THE INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

MEMBERS

ASSOCIATE MEMBERS

Britain and Ireland Argentina and Brazil Canada Australia Czech Republic China Germany Egypt Japan France New Zealand Greece Russia Italy 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

Kyoto, Japan 27th August – 1st September 2017

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 Kyoto, Japan 27th August – 1st September 2017

Plenary Session. Monday, 28th August 2017. 9:00am

The President of IAPWS, Professor Hans-Joachim Kretzschmar, welcomed the Executive Committee (EC) and other IAPWS members to Tokyo for the Executive Committee and Working Group (WG) Meetings of IAPWS. He first asked the Chair of the Japan National Committee, Professor Masaru Nakahara, to welcome the EC to Kyoto. The President then officially opened the 2017 EC Meetings by introducing the National Delegates. All of the Member countries of IAPWS were in attendance as well as Associate Members with the exception of Argentina/Brazil, France, Greece and Switzerland. In total there were 65 people assembled for the EC meeting.

1. <u>Adoption of Agenda</u>

Provisional agendas had been posted on the IAPWS Website for all IAPWS members by the Executive Secretary in May 2017. There were a few additions and the final agenda was then approved by the Heads of all National Delegations, and forms Attachment 1 of these minutes.

2. IAPWS Business and Appointment of Committees

2.1 IAPWS Business Since Last EC Meeting in Dresden, September 2016

The Executive Secretary first indicated that two documents had been circulated to the National Committees during the year since the Dresden meeting for final approval. The Executive Secretary reminded the EC of these documents:

- Revised Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use. Dresden EC Minute 7.2 indicated that the Revised Release could be finalized after the Dresden meeing. The minor changes and the editorial work were completed and the document was circulated for a Postal Ballot on 1st October 2016. No objections were received by 30th December 2016 so the Revised Release became an official IAPWS document.
- IAPWS AN6-16. Relationship between Various IAPWS Documents and the International Thermodynamic Equation of Seawater – 2010 (TEOS-10). The Dresden EC Minute 9.3 noted that TPWS and SCSW would develop a new Advisory Note 6, on clarifying the IAPWS documents which contribute to TEOS-10. The Executive Committee (EC) authorized a Postal Ballot following review by the Editorial Committee. This review was completed after Dresden and the document was circulated to National Committees for the Postal Ballot on

6th October 2016. No objections were received by 6th January 2017 so AN6-16 became an official IAPWS document.

- Italy became an Associate Member after a postal ballot on 11th November 2016
- China became an Associate Member after a postal ballot on 24th March 2017.
- The Czech Republic National Committee nominated Dr. Jan Hruby to be the next IAPWS Vice President.

2.2 <u>Press Release</u>.

The President asked Cook to chair the development of the Highlights/Press Release on the IAPWS proceedings during the week. It was also suggested that Nakahara assist in this development. The Clerks of Minutes from each WG were asked to provide input. The Press Release is discussed in Minute 17.1 and is Attachment 10.

2.3 <u>Evaluation Committee on International Collaboration</u>.

The President indicated that no proposals had been received by the Executive Secretary prior to the meeting, and that any 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 any proposals received would consist of the WG Chairmen, with the President and Executive Secretary as ex. officio members. A chairman would be chosen by the Committee. (See Minute 15.1 for further discussion on International Collaborations).

2.4 <u>IAPWS Awards Committees</u>

2.4.1 <u>Helmholtz Award Committee</u>

The President indicated that there was a Helmholtz Awardee this year, Dr. Pavel Gotovtsev, from the Kurchatov Institute in Moscow. Unfortunately, he was not able to attend the meetings in Kyoto.

The Executive Secretary then reminded the EC that the Helmholtz Committee for the 2018 award would consist of a member from SIAPWS, USA, BIAPWS, Canada and Czech Republic. SIAPWS will provide the committee chairman. The President asked SIAPWS delegate, Thomsen, to organize the committee and to report back to the EC on Friday with the names of the members of this committee (see Minute 16.1).

2.4.2 <u>Honorary Fellow Award Committee</u>

The President indicated that there had been no nominations for an IAPWS Honorary Fellow in 2017. He then requested that Friend (Chairman) and Nakahara form the Committee for 2018. The President would be ex. Officio.

2.4.3 Gibbs Award

The President indicated that there were two nominations for the IAPWS prestigious award which would be presented at the 17th ICPWS in Prague. He reminded the EC that the Gibbs Award is awarded every five years at each ICPWS. The selection committee was formed at the 2016 EC Meetings in Dresden, Germany but because of changes in Working Groups and absences for the 2017 EC Meetings, the President indicated that the committee would consist of Friend (TPWS)(Chair), Okita (IRS), Pawlowicz (SCSW), Nakahara (PCAS) and Rziha (PCC). The results of this committee's review is included in Minute16.3.

2.5 Promoting IAPWS

The President requested each Working Group to discuss options for promoting IAPWS worldwide, and for the Chairs to report back to the EC with suggestions.

2.6 <u>17th ICPWS. Activities of International Program Committee (IPC)</u>

The President requested the Chair of the Organizing Committee for the 17th ICPWS, Hruby, to introduce this topic. Hruby first reminded the EC of the 2nd - 7th September 2018 dates for the ICPWS to be held at the Marrott Hotel in Prague, Czech Republic. He then briefed the EC on the location, the formation of the local organizing committee and the sponsors. The International Program Committee (IPC) had met during the Dresden IAPWS EC Week and will meet again during the Kyoto EC week. A further report on the 17th ICPWS is found in Minute 14.2.

2.7 OPAL Website for IAPWS Documents and Presentations

The President reminded the EC of the Opal Website for storage of IAPWS Working Group files and presentations. This is a password protected site for use by the IAPWS Working Groups.

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

3.1 <u>Releases, Guidelines and Certified Research Needs</u>.

The Executive Secretary indicated that three ICRNs needed attention during the week: #22 on steam chemistry in the phase transition zone (PTZ), #29 on uncertainties in coolant sampling for low concentration metals, and #27 on thermodynamic properties of humid gases and CO₂ - rich mixtures needs a closing statement

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 Working Group (WG) Chairmen of the Week's Activities

President Kretzschmar 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 8).

Following this item, the President closed the opening session of the EC at 9:50 am.

Activities During the Week in Kyoto

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, 30th August 2017 and the Symposium Program is shown in Attachment 3.

Executive Committee Meeting. Friday, 1st September 2017

President Kretzschmar opened the continuation of the EC Meeting at 9:00 am. Each of the Member countries of IAPWS except Germany was in attendance as well as Associate Members with the exception of Argentina/Brazil, France, Greece and Switzerland. In total there were 25 people assembled for the EC meeting. Kretzschmar first asked the EC if there were any additional items that should be added to the Agenda. None were suggested.

5. Acceptance of Minutes of Previous Meeting

President Kretzschmar asked for comments and changes to the minutes of the EC meeting held in Dresden, Germany in 2016. No changes were noted, thus the 2016 Minutes were accepted.

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

President Kretzschmar provided a short report. He was most enthused about the new IAPWS Membership of New Zealand and the Associate memberships of China, Italy and Egypt. He encouraged the IRS working group that they should continue advising IAPWS of the industrial requirements. He noted that the Technical Guidance Documents (TGD) of PCC are penetrating into the power plant chemistry and creating worldwide interest. These are putting IAPWS in a leadership position. The President thought the new IAPWS Release on Heavy Water will be very important. IAPWS needs to find new areas of activity and some possibilities are: renewables, solar power, refrigeration, air-conditioning, supply and disposal technology, and geothermal technology. He recognized that members with longterm experience in IAPWS are very important to help find the right future directions and decisions. Finally, he indicated that the working groups and national committees should try to make IAPWS better recognized around the world.

7. <u>Report and Recommendations of the Thermophysical Properties of Water and Steam (TPWS)</u> <u>Working Group</u>

TPWS Chairman Harvey opened this item by indicating that he would report on the activities relating to TPWS although a number of joint meetings with IRS and SCSW had taken place during the week. Full Minutes and the Agenda for TPWS can be found in Attachment 4.

7.1 The Working Group (WG) considered a new Release on the IAPWS Formulation 2017 for the Thermodynamic Properties of Heavy Water Substance. The WG voted to approve the draft Release, with the condition that members be given until the end of October 2017 to bring up additional issues. The WG Chair and Chair of the Evaluation TG were authorized to resolve any such issues that are raised. The WG requests the EC to authorize a Postal Ballot to be conducted after this additional period has passed and after the Editorial Committee has approved the draft.

The EC approved this Request Unanimously.

- 7.2 Harvey next provided the EC with seven informational items:
 - A Task Group of Harvey and Wagner with input from Feistel will work on refinements to the uncertainty statements in IAPWS-95 for the properties of vapors at low pressures, with the intention to have a revision ready in time for the 2018 meeting.
 - A Task Group was appointed to assess aspects of the IAPWS-95 formulation where there may be room for improvement. Members are Harvey, Hrubý, Okita, Span and Orlov.
 - Kalová replaces Vinš as the Chair of the Task Group working toward revising the IAPWS formulation for the surface tension of pure water.
 - A Task Group (Holten, Harvey and Feistel) was appointed to work on a formulation for the vapor pressure of supercooled liquid water, to be added to the IAPWS Guideline on Thermodynamic Properties of Supercooled Water. The goal is for the Revised Guideline to be ready for IAPWS adoption in 2018.
 - A joint Task Group between TPWS and PCAS (Yoshida, Harvey and Meier) was appointed to work on an IAPWS Guideline on the Diffusivity of Water and Heavy Water.
 - A joint Task Group between TPWS and IRS was formed to prepare a new ICRN on the dew point for acid gases. Members are Okita (chair), Span, and Orlov.
 - The Task Group on Interfacial Properties of Supercooled Water is no longer active and was officially dissolved.

7.3 <u>ICRNs</u>.

Harvey reported that ICRN-27 (properties of humid gases and CO2-rich mixtures) was closed in 2014. Span and Harvey will prepare closing statement before the 2018 meetings in Prague.

7.4 <u>TPWS Membership</u>.

Chairman Harvey requested EC approval for three new TPWS WG members who had been approved by the WG:

- Kishor Nayar (MIT, USA),
- Vito Fernicola (INRIM, Italy),
- Raffaella Romeo (INRIM, Italy).

Harvey also requested EC approval for Meier (Helmut Schmidt University, Hamburg) to be elected as an additional Vice Chair of TPWS.

The EC approved these Membership Changes Unanimously.

7.5 <u>Promoting IAPWS</u>.

Chairman Harvey informed the EC that the TPWS/IRS/SCSW combined working group had discussed the following items that could be used to promote IAPWS around the world:

- Inviting top level people of other international organizations to ICPWS (and try to get our people similarly invited to their meetings).
- Translations of TGDs into other languages.
- Online communities, etc.
- Encourage people publishing IAPWS work to mention IAPWS in prominent place (like Abstract or Title).
- Wikipedia pages.
- IAPWS-related software can be a point of contact. Or some sort of table of values for key properties available on web.
- Mention of IAPWS in organization of related conferences.

8. <u>Report and Recommendations of the Industrial Requirements and Solutions (IRS) Working</u> <u>Group</u>

IRS Chairman Okita indicated that many of the activities of IRS during the week had been reported in the TPWS report. Minutes for IRS and the Agenda can be found in Attachment 5. In response to Dresden Minute 8.5 which questioned the future of the IRS Working Group with the EC, Chairman Okita indicated that IRS will continue as an active IAPWS Working Group. He then reported on the following informational items for future activities.

8.1 Wet Steam Properties Calculation for Industrial Use.

A new Task Group (Nový, Hrubý, Orlov, Span and Meier) was formed on how to correctly calculate or estimate thermophysical and transport properties of wet steam which are not part of the IAPWS-IF97 standard.

8.2 <u>Scientific Formulation</u>

A new Task Group (Hrubý, Harvey, Okita, Orlov and Span) has been set up to revise and upgrade the existing IAPWS-95.

8.3 <u>Wet Steam Data from Operating Turbines</u>

A new Task Group (Okita, Nový, Senoo, Weber, Singh, and Hiegemann) has been set up to gather steam turbine measured wet steam data and share it among the members.

8.4 IRS Membership.

Chairman Okita requested EC approval for two new IRS WG members who had been approved by the WG:

- Olaf Lemp (GE, Germany),
- Shigeki Senoo (Mitsubishi Hitachi Power Systems, Japan),

Okita indicated that Lemp was replacing Daur, who had retired and should be removed as a member of IRS.

The EC approved these Membership Changes Unanimously.

9. <u>Report and Recommendations of the Sub-Committee on Seawater (SCSW)</u>

SCSW Chairman Pawlowicz reported on the following items. Minutes for SCSW and the Agenda can be found in Attachment 6.

9.1 Information for EC.

The Chairman first provided four informational items:

- The Task Group on extending the range of formulation for thermodynamic properties of seawater was ordered to continue their work, including evaluation of new compressibility data.
- Reports on Joint Committee on the Properties of Seawater (JCS) and IAPWS/BIPM Cooperation. Two of the four Metrologia papers published in 2017 received a "Highlight of 2016" award from the journal.
- Successful trip by IAPWS representative (Feistel) to BIPM-CCT meeting in May 2017. Next step in cooperation focussed on traceably defining relative humidity and moving it into the SI is to invite key BIPM representative(s) to planned seawater property workshops at ICPWS.
- Task group for the Surface Tension of Seawater has been formed (Nayar, Hruby, Harvey) with an Evaluation Task Group (Feistel).

9.2 <u>Membership</u>.

Pawlowicz proposed four new members who had been approved by SCSW:

- Yohei Kayukawa (AIST, Japan),
- Kishor Nayar (MIT, USA),
- Aina Wu (NCOSM, China),
- Jeremy Lovell-Smith (IRL, New Zealand) (already a member of TPWS).

The EC approved these Membership Changes Unanimously.

10. <u>Report and Recommendations of Physical Chemistry of Aqueous Systems</u> <u>Working Group (PCAS)</u>

Chairman Anderko couldn't attend the Kyoto meetings so Nakahara acted as chairman. He provided the PCAS Report to the EC. Full Minutes can be found in Attachment 7. He indicated that the PCAS working group had a number of presentations and joint sessions which are delineated in the PCAS Minutes. He also informed the EC that the PCAS working group expects more applications of computational approaches in the future.

10.1 <u>Membership</u>

Acting Chairman Nakahara proposed two membership additons for PCAS:

- James Bellows (James Bellows & Associates, USA) (already a member of other working groups)
- Shigeki Senoo (Mitsubishi Hitachi Power Systems, Ltd., Japan)

The EC approved these Membership Changes Unanimously.

11. <u>Report and Recommendations of Power Cycle Chemistry Working Group (PCC)</u>

Chairman Rziha who had chaired the PCC all week had to leave Kyoto for business activities on Friday and did not attend the EC meeting. Executive Secretary, Dooley, provided the PCC Report to the EC. Full Minutes can be found in Attachment 8. The following items were covered:

11.1 <u>Technical Guidance Documents (TGD)</u>.

The PCC working group had discussed extensively the TGD developments. The TGD Task Group (Chair: Dooley) activities can be summarized as follows.

- *Monitoring Corrosion Products in Flexible (cycling and two-shifting) Plants.* The Task Group (Addison and Thomsen (Joint Chairs), Cook, McCann, and Dooley) will finalize a White Paper for the 2018 Meeting. Extensive plant sampling and detailed evaluation is on-going. An IAPWS Map on corrosion product decay will be formulated
- Ensuring the Integrity and Reliability of Demineralised Makeup Water Supply to the Unit Cycle. The Task Group (Joy, Chair) plan to develop the final TGD by the 2018 Meeting

- Application of Film Forming Products (FFP) in Nuclear Plants. The Task Group (Cook, Chair) will develop a White Paper by the 2018 Meeting.
- Application of Film Forming Products (FFP) in Industrial Plants. The Task Group (Dooley, Hater and Lendi (Joint Chairs), Rziha, and Carvalho) plan to develop the final TGD by the 2018 Meeting. The development will involve the same team that developed the TGD on FFP in Fossil and Combined Cycle Plants (TGD8-16) plus a number of new contributors from industrial plants.
- *Air In-Leakage in Steam Water Cycles.* The Task Group (Carvalho (Chair), Dooley, Rziha and Thomsen) plan to develop the final TGD by the 2018 Meeting.
- Aspects of Geothermal Steam Chemistry. The Task Group (Addison, Chair, plus representatives from Geothermal Countries) will develop a White Paper for the 2018 Meeting. This will be used to determine if a TGD can be developed.
- *Condensate Polishing*. Discussion took place on developing a new TGD. Because the overall subject was considered enormous, a Task Group (Khalifa (Chair), Addison, Buecher, Thomsen, Leidich and Joy) was formed to explore developing a White Paper for the 2018 meeting with a concentration on application of condensate polishing for combined cycle/HRSG plants. This will not be a design document, but will provide guidance on justifying polishing for these plants.

11.2 IAPWS Certified Research Needs (ICRN).

The PCC Working Group had discussed the ICRNs and the following information was provided to the EC for approval.

- ICRN 22 on *Steam Chemistry in the Phase Transition Zone (PTZ)*. This document has been finalized and will have a new expiry date of September 2019. The document will receive a light review by the Editorial Committee and then be sent for Postal Ballot.
- ICRN 29 on *Uncertainties in Coolant Sampling for Low Concentration Metals* (Fe, Cu, Co, etc). This document has been finalized and will have a new expiry date of September 2021. The document will receive a light review by the Editorial Committee and then be sent for Postal Ballot.

The EC approved these ICRN Actions Unanimously.

11.3 PCC Membership.

The PCC Working Group requested that the following new members be approved:

- Adam Caswell (EdF Energy, UK)
- Steve McGee (COG, Canada)
- Tian Li (TPRI, China)

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 documents delineated in Minute 2.1. The Committee had also inserted new document identifiers on all title pages and the IAPWS Logo on some title pages (including TGDs). They had also updated Advisory Note 2 (role of different IAPWS documents for pure water thermodynamic properties).

Harvey then indicated that a large number of documents will need editorial review over the next year and requested early notification.

13. <u>Membership and Associates</u>

13.1 Member Dues.

The Executive Secretary indicated that all IAPWS Members had paid their 2017 dues.

13.2 <u>Reports on Current Associate Members</u>

Status Report on IAPWS Associate Member, Australia. Chairman Joy provided a short presentation. The Australian National Committee (AUSAPWS) has continued to focus on the Power Cycle Chemistry area but is also developing a wider focus in seawater, carbon sequestration and thermodynamics. AUSAPWS currently has over 70 members from the power generation industry, universities, service companies and consultants, including the Australian Power Institute (API). It has good involvement with the API Chemistry Conference and the IAPWS supported Australasian HRSG Users Group (AHUG). Joy indicated that AUSAPWS has developed By-Laws and is finalizing funding arrangements with API, other companies and sponsorships to complete AUSAPWS funding. Joy indicated that AUSAPWS is planning to apply for full IAPWS Membership in 2018 maybe before the Prague meetings.

<u>Status Report on IAPWS Associate Member, China.</u> Delegate Tian Li provided a short report and indicated that the Associate Membership had been approved by the Chemical Standardization Technical Committee of Power Plants within the China Electric Power Enterprise Federation in May 2017. This Chemical Standardization Technical Committee is an academic group composed of nearly 40 experts from various research institutes in China, and mainly carries out the formulation and revision of China's standards in Power plant chemistry, and organizes some academic activities in power plant chemistry. For example, they have just completed review of the criteria: 1) inspection procedures for on-line chemical instrument of power plant, 2) quality criteria of water and steam for power plant and steam-generating equipment, and 3) guideline for the acceptance of biological aerated filter in fossil fuel power plants. Another IAPWS interest in China is the Marine Information Technology Research Institute with two delegates attending the Kyoto meeting, mainly to participate in the discussions of the Subcommittee on Seawater.

<u>Status Report on IAPWS Associate Member, Egypt.</u> Chairman Khalifa provided a short report based on the Country Report in Attachment 14. Khalifa indicated that four seminars had been organized during the last year to introduce IAPWS to the Egyptian industry and to review the IAPWS TGD. They plan to continue the promotions through 2018 and conduct the necessary administrative tasks.

<u>Status Report on IAPWS Associate Member, Italy.</u> Delegate Vito Fernicola provided a short report and indicated that they are trying to revamp the national committee with ENEL, Universities and manufacturers in Italy.

<u>Status Report on IAPWS Associate Member, Switzerland.</u> The Secretary of the Swiss National Committee (SCPWS) provided a country report in Attachment 20. This report indicates that no team of sponsors has yet been assembled to commit on a mid- or long-term basis to supporting a regular Swiss membership fee. The SCPWS has been very active and hosted the First International Conference on Film Forming Amines and Products in April 2017 in Lucerne, Switzerland. The conference was very successful and found wide international acceptance, but the goal of finding new participating institutions was not achieved.

<u>Activities of other Associate Members of IAPWS</u>. The Executive Secretary provided short updates on Argentina/Brazil, France and Greece, and indicated that there was little activity in any of these Associate Members. After some discussion and referral to the IAPWS Statutes and By-Laws, the EC agreed unanimously at this time to keep these Associate Members and to initiate further discussion during the 17th ICPWS in Prague in 2018.

14. Executive Secretary's Report

14.1 IAPWS Bank Accounts, Financial, Auditors and IAPWS Dues

The Executive Secretary reported that IAPWS is on a sound financial footing with currently about £58,000GBP in total in the UK and US bank accounts. The status as at 4^{th} August 2017 in the bank accounts had been provided to each National Delegate prior to the EC meeting.

The Executive Secretary next reported that the 2016 financial statements had been forwarded to the IAPWS Auditors in January 2017. Professor Savarik in Czech Republic and Dr. Hencke in Germany had reviewed and approved the financial statements. These approvals had also been provided to the Heads of all the National Delegates present prior to the EC meeting.

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 2018. He also mentioned that IAPWS By-Law #1 provided the basis of the dues structure, and that this would be used to assess the dues for Australia if they apply for membership in 2018.

The EC Unanimously Agreed to this Proposal.

The Executive Secretary had also provided a rough estimate of the income and known planned expenditures for 2017 / 2018.

14.2 Time and Place of the 2018, 2019 and 2020 Meetings

<u>2018 IAPWS Meetings and the 17th ICPWS.</u> The Head of the Czech Republic NC, Hruby, continued his report as a continuation from Monday (Minute 2.6). He indicated that the International Program Committee (IPC) had met during the Kyoto week and had developed a list of suggested symposia topics representative of all the IAPWS working groups. The third IPC meeting will take place in Prague on 22nd and 23rd March 2018 after abstracts have been received.

<u>2019 IAPWS Meetings</u>. The Executive Secretary informed the EC that Canada had been requested to consider hosting the 2019 IAPWS meetings. Canadian NC Chair, Cook indicated that the meetings will be in Banff, Alberta in mid- to late- September 2019.

15. <u>Guidelines, Releases, Certified Research Needs, and International Collaborations</u>

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 Project.

The President requested the Chairman of the 2017 International Collaboration Committee (WG and SC Chairs) to report on the findings of that committee during the week. Chairman Harvey reported that one collaborative project had been proposed. The following is an overview of the proposed project. The details are provided in Attachment 9:

• Corrosion Product Sampling, Analysis and Assessment.

The IAPWS sponsors are Thomsen (SIAPWS), Addison (New Zealand) and McCann (BIAPWS). The young scientist is thought to be a student in the Chemical Department of Aarhus University in Denmark who is currently taking a semester on water chemistry at Stavanger University in Norway. It is proposed that IAPWS funding of £20,000GBP would cover subsistence and travel for visits to power plants in UK, Ireland, and New Zealand. The location may be exchanged dependent on availability of local staff. The student will also spend time at a laboratory in SIAPWS to analyze the data and to ensure quality control.

Harvey indicated that the Evaluation Committee supported the proposal, but had raised concern about whether the time proposed for each visit would be sufficient. and that the technical content was of interest to IAPWS. He indicated that the proposal was directly

in line with amending the current TGD on corrosion product sampling and analysis so that IAPWS could take a leadership position for flexible plants. The Chairman then proposed to the EC that the project is approved for up to £20,000GBP, and if further funds are required to complete the work then the PCC Chairman should come back to the EC. The President indicated that the IAPWS finances were in good condition and conducted a vote by the EC.

The EC Approved the Motion to Fund this Collaborative Project Unanimously.

16. IAPWS Awards

16.1 IAPWS Helmholtz Award

The President asked the SIAPWS Delegate, Thomsen, for the names of the 2018 Helmholtz Award Committee. The 2018 Helmholtz Committee will consist of: Chairman Jensen (SIAPWS), Friend (USA), Cooper (BIAPWS), Cook (Canada) and Vins (Czech Republic).

Action: Nominations will be due to the Executive Secretary by 31st January 2018.

16.2 IAPWS Honorary Fellowships

The President reminded the EC of the Awards Committee for 2018 with Friend (USA) as Chairman and Nakahara (Japan) as member with the IAPWS President as ex.-officio member.

Action: Nominations are due to the Executive Secretary by 31st January 2018.

16.3 IAPWS Gibbs Award

The President requested the Chair of the Selection Committee to provide an update to the EC. Chairman Friend told the EC that the committee had met twice during the Kyoto week and that deliberations were still on-going. He expects that a decision will be made by mid-October 2017 to select one of the nominations or request a further solicitation.

17. <u>New Business</u>

17.1 Press Release

The President mentioned that Cook had been asked at the EC meeting on Monday to develop a Press Release. This was developed with input provided by each WG and SC. Cook indicated that a document had been prepared. The final version is Attachment 10. The President indicated that this release will be sent to all NCs and WGs of IAPWS and it should be distributed as widely as possible and sent to any journals and publications.

17.2 Japan National Committee Feedback on the Kyoto Meetings.

The Conference Chair, Nakahara, thought the IAPWS meetings had been a great success with 80 full time participants. He was very happy with the feedback and thanked everybody for attending. The EC applauded in thanking the Japan NC team for the great organization of the meetings, symposium and IAPWS Dinner.

17.3 Other New Business

President Kretzschmar asked the EC if there was any further business.

No other business was raised.

17.4 <u>Reports from National Committees</u>.

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
Egypt	Attachment 14
Germany	Attachment 15
Japan	Attachment 16
New Zealand	Attachment 17
Russia	Attachment 18
SIAPWS	Attachment 19
Switzerland	Attachment 20
USA	Attachment 21

17.5 Participants

Attachment 22 provides a list of participants at the IAPWS EC and WG Meetings in Kyoto, Japan in August/September 2017.

17.6 List of Members

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

18. <u>Closing Remarks and Adjournment</u>

The President thanked everybody for participating at this EC meeting. Then he formally closed the 2017 EC meeting at 12:08 pm.

AGENDA for the EXECUTIVE COMMITTEE of IAPWS

Kyoto, Japan. 28th August – 1st September 2017

Monday, 28th August 2017. Opening Plenary Session (9:00 – 10:15 am)

Opening Remarks, Welcome and Introductions by IAPWS President H-J. Kretzschmar Adoption of Agenda

- 2. IAPWS Business and Appointment of Committees
 - 2.1 IAPWS Business since Last EC Meeting in Dresden, September 2016
 - 2.2 IAPWS Highlights / Press Release
 - 2.3 Evaluation Committee on International Collaboration
 - 2.4 IAPWS Awards for 2018 (Honorary Fellow, Gibbs, Helmholtz)
 - 2.5 Promoting IAPWS including Cover Pages of IAPWS Documents
 - 2.6 17th ICPWS. Activities of International Program Committee (IPC)
 - 2.7 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, 1st September 2017. Executive Committee Meeting. (9:00am – 1:00 pm)

- 5. Acceptance of Minutes of Previous Meeting
- 6. President's Report

1.

- 7. Report and Recommendations of Joint TPWS, IRS and the Sub-Committee on Seawater
- 8. Report and Recommendations of Separate IRS Meetings
- 9. Report and Recommendations of Separate Sub-committee on Seawater Meetings
- 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 of Current Associate Members
- 14. Executive Secretary's Report
 - 14.1 IAPWS Bank Accounts, Financials, Auditors and Dues
 - 14.2 Time and Place of 2019 and 2020 Meetings.
 - Includes Czech Republic on the 17th ICPWS in 2018
- 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 Gibbs Award
- 17. New Business
 - 17.1 Press Release
 - 17.2 Japan Committee feedback on 2017 Meetings and Symposium
 - 17.3 Other items raised during the IAPWS week
- 18. Adjournment

Schedule of IAPWS Meetings						
	Kvoto, Jar	oan. 27 th August – 1 st September 2017				
(All technical meetings will be in the Kyoto Research Park (KRP))						
Sunday 27 Aug.	7:00 pm	Informal Get-together and Registration Science Center Club, Kyoto Research Park				
Monday 28 Aug.	9:00am	Executive Committee - Opening Plenary Session				
	10:15am	Coffee / Tea Break				
	10:30am	TPWS/IRS/SCSW Joint Meeting				
(To set agendas	for the week and to c	conduct IAPWS Business, thus allowing remainder of week for technical matters)				
	10:30am	PCAS and PCC Separate Meetings				
	(To conduct IAPWS	Business, thus allowing remainder of week for technical matters)				
	12:00pm	LUIICII TDWS/IDS/SCSW/ Loint Masting				
	1:30pm.	PWS/IKS/SCSW Joint Meeting				
	1:30pm.	PCC and PCAS Separate wG Meetings				
Tuesday 29 Aug.	9:00am	PCAS Workshop (other WG Members will be welcome)				
	9:00am	PCC Workshop (other WG Members will be welcome)				
	9:00am	TPWS/IRS/SCSW Joint Working Group Meeting				
	10:30am	TPWS/IRS/SCSW Joint or Separate Meetings				
	10:30am	PCC and PCAS Separate Meetings				
	12:00pm	Lunch				
	1:30pm	TPWS/IRS/SCSW Joint Meeting.				
	1:30pm	PCC/PCAS/IRS Joint WG Meeting and Workshop				
	3:30pm	PCC and PCAS Separate Meetings				
Wadnas 30 Aug	0.000m 1.00	IADWS Symposium				
wealles. 50 Aug.	9.00am – 4.00 (Water and Steam	• Fnergy Efficiency and Environmental Sustainability)				
	(Water and Steam	. Energy Enterency and Environmental Sustainability)				
Thursday 31 Aug	9:00am	IRS, SCSW and PCC Separate WG Meetings				
	9:00am	TPWS/PCAS Joint WG Meeting				
	12:00pm	Lunch				
	1:30pm	Separate meetings of Working Groups				
	4.20	(If needed to prepare for Executive meeting)				
	4:30pm	Excursion (Piwaka amiga MICHICAN)				
	6:30nm	IAPWS Dinner/Ranquet				
	0.50pm.	(Biwako Hotel)				
Friday 1 Sept.	9:00am	Executive Meeting (9:00am - 1: 00pm) (Will include at least one member from each National Delegation)				

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 29th August 2017

IAPWS Symposium 2017

Wednesday, 30 August

9:00-9:10

Opening remarks, Symposium information

Helmholtz Awarding and Lecture

9:10-9:40

Dr. Pavel Gotovtsev (National Research Centre "Kurchatov Institute", Russia)

"Application of Machine Learning for Water Technologies? from Power Cycle Chemistry to Green Cities"

Symposium Lectures

"Water and Steam: Energy Efficiency and Environmental Sustainability"

9:40-10:30 Session 1

Chair: Prof. Kenji Yasuoka (Keio University)

Prof. Nobuyuki Matubayasi (Osaka University)

"Polymer as Energy-Saving Medium for Water Absorption: All-Atom Analysis toward Rational Design"

Dr. Ken Yoshida (Tokushima University)

"Self-Diffusion Coefficients of Sub- and Supercritical Water: Available Data, Reliable Fitting Functions, and Effects of Temperature and Density"

10:30-10:50 Coffee break

10:50-11:40 Session 2

Chair: Prof. Nobuyuki Matubayasi (Osaka University)

Dr. Hiroshi Uchida (Japan Agency for Marine-Earth Science and Technology)

"Long-Term Change in the Deep Ocean Resulting from Global Warming"

Prof. Kenji Yasuoka (Keio University)

"Molecular Simulation for Clathrate Hydrate"

11:40-13:20 Lunch

13:20-14:35 Session 3

Chair: Dr. Hideo Hirano (Former CRIEPI)

Prof. Shozo Kaneko (University of Tokyo)

"Development of High Efficiency Air-blown IGCC"

Mr. Masaki Iijima (Mitsubishi Heavy Industries, Ltd.)

"Commercialize Flue Gas CO2 Capture from Power Plant"

Dr. Ayumu Morita (Hitachi, Ltd.)

"Technical Issues of Future Power Network with a Large Amount of Renewable Energy Sources"

14:35–14:55 Coffee break

14:55-16:35 Session 4

Chair: Prof. Koichi Watanabe (Keio University)

Mr. Nobuo Okita (Toshiba)

"Steam Turbine Cycles for Renewable Energies - Geothermal, Solar Thermal and Binary Generation -"

Dr. Hideo Hirano (Former CRIEPI)

"Current Status of Combined Cycle/HRSG Power Plant and Ultra-Supercritical Steam Power Plant, and

Development of Advanced Ultra-Supercritical Steam Power Plant"

Dr. Shigeki Senoo (Mitsubishi Hitachi Power Systems, Ltd.)

"Nonequilibrium Condensation Model and Numerical Analysis for Wet Steam Turbines"

Prof. Tadashi Tanuma (Teikyo University)

"Aerodynamic Blade Designs Including Wet Steam Turbine Stages"

16:35-16:40

Closing remarks

Polymer as Energy-Saving Medium for Water Absorption: All-Atom Analysis toward Rational Design

Nobuyuki Matubayasi

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Polymer emerges as a material for selective absorption of small molecules. It plays key roles in such processes as desalination and gas separation, and the energy consumption at separation often reduces with polymer membrane compared to conventional distillation. Separation with polymer is distinct from distillation in that while the latter relies upon macroscopic phase diagrams, a rational design of the former requires insights into intermolecular interaction at atomic resolution. Atomistic analysis is thus necessary for the polymer medium, and molecular dynamics (MD) simulation is a method for meeting this necessity. In the present work, we develop a free-energy method for assessing the extent of water absorption into polymer [1]. We treat the polymer as a solvent and water as a solute, and employ a theory of solutions to accurately and efficiently compute the free energy of water dissolution [2]. It is demonstrated that all-atom treatment is predictive for the free energy irrespective of the hydrophobicity and hydrophilicity of the polymer, and the computed free energy of dissolution is discussed in connection to the structures of the polymers and their interactions with water.

References

[1] T. Kawakami et al., J. Chem. Phys., 137, 234903 (2012).

[2] S. Sakuraba et al., J. Comput. Chem., 35, 1592 (2014).

Self-Diffusion Coefficients of Sub- and Supercritical Water: Available Data, Reliable Fitting

Functions, and Effects of Temperature and Density

Ken Yoshida

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The dynamic insights into water and steam at high temperatures are of great importance to develop the highperformance power generation that is associated with efficient transformation of the kinetic energy into the mechanical. To the end the self-diffusion coefficient data is required because it represents water mass transport phenomenon. We have proposed a useful and reliable scaling law for the self-diffusion coefficients of water, that can be applied over a wide range of thermodynamic states from ambient to the supercritical [1]. The scaled expression can be used for the correlation and evaluation of the available literature data. It can be applied also for the inter- and extrapolation to the practically inaccessible extreme conditions using molecular dynamics (MD) simulation as a key guide. It has been clarified that the self-diffusion is characterized by the large temperature effect and relatively small density effect due to the attractive and directional hydrogen bonding of water [2].

References

K. Yoshida, N. Matubayasi, Y. Uosaki and M. Nakahara, J. Chem. Eng. Data, 55, 2815 (2010).
K. Yoshida, N. Matubayasi, Y. Uosaki and M. Nakahara, J. Chem. Phys., 137, 194506 (2012); Id. J. Chem. Phys., 138, 134508 (2013); Id. J. Solution Chem., 43, 1499 (2014).

Long-term Change in the Deep Ocean Resulting from Global Warming

Hiroshi Uchida

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The Earth's climate system is driven by energy from the sun. Ocean and atmosphere circulations transfer this energy from the Earth's surface at low latitudes to higher latitudes. The ocean's central role in the climate system results from its great capacity to store and transport heat and freshwater to exchange these with the atmosphere. The surface water cooled around the Antarctica sinks to the bottom and forms the bottom water by spreading to all over the world ocean. To obtain an accurate picture of ocean circulation, land-to-land and surface-to-bottom global hydrographic data were gathered in the World Ocean Circulation Experiment (WOCE) in the 1990s. In the 2000s, reoccupations of the WOCE hydrographic sections have been carried out to document decadal changes of the ocean circulation. In this study, long-term changes of water properties (temperature, salinity and dissolved oxygen) and volume transport of the bottom water in the North Pacific were examined based on those high-quality hydrographic data repeatedly obtained along zonal WOCE sections at 47°N, 30°N and 25°N. For depths below 4000 m, significant trends were detected for temperature (1.5 ± 0.09 mK per decade) and dissolved oxygen (-0.99±0.12 µmol/kg per decade), although salinity trend was not significant. Half of the decrease in oxygen might be casued by remineralization due to increasing residence time probably caused by slowing the deep meridional overturning circulation resulting from Global Warming.

Molecular Simulation for Clathrate Hydrate

Kenji Yasuoka

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Clathrate hydrates of natural gas are suitable for industrial use such as transportation and storage. Clathrate hydrates are crystalline compounds composed of guest substances and hydrogen-bonded host water molecules. Molecular simulation is useful for studying clathrate hydrates. To clarify the thermodynamic stability of clathrate hydrate molecular dynamics simulations were applied and the free energy of clathrate hydrates were estimated [1]. Molecular vibrations of guest molecules in hydrate cages were calculated by *ab initio* molecular dynamics simulations [2]. Cage occupancy of guest molecules were also simulated by Gibbs ensemble Monte Carlo simulations [3]. Nucleation phenomena of clathrate hydrates were studied [4]. Phase equilibrium conditions were estimated by a statistical thermodynamics model [5].

References

- Y. Okano and K. Yasuoka, J. Chem. Phys. **124**, 024510(2006).; T. Miyoshi et al., J. Chem. Phys., **126**, 234506(2007).; T. Miyoshi et al., J. Phys. Chem. C, **111**, 3799(2007).; T. Miyoshi et al., Molecular Simulation, **33**, 65(2007).
- [2] M. Hiratsuka et al., J. Chem. Phys., 136, 044508(2012).; J. Chem. Phys. 137, 144306 (2012).; Molec. Simul., 41, 813 (2015).; Phys. Chem. Chem. Phys., 17, 12639 (2015).
- [3] P. E. Brumby et al., Fluid Phase Equilibria, 413, 242 (2016).
- [4] D. Yuhara et al., Faraday Discussions, **179**, 463 (2015).
- [5] E. Sato et al., Jpn. J. Appl. Phys., 46, 5944-5950(2007).; F. Takeuchi et al., Int. J. Thermophys., 30, 1838(2009).

Development of High Efficiency Air-blown IGCC

(IGCC: Integrated coal Gasification Combined Cycle)

Shozo Kaneko

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Japan imports 96% of its fossil fuels from abroad. From the standpoint of energy security, Japanese Government decided the Guideline for Energy Mix 2030 aiming at 27% by natural gas and 26% by coal on power generation(kWh) basis. On the other hand Japan declared ambitious 26% reduction of CO₂ from 2013 result. Raising efficiency of coal fired power plant is of the first priority technical requirement. Japan has undergone development of air-blown IGCC(Integrated coal gasification Combined Cycle) technology for more than 30 years, starting from small 2 tons/day PDU(Process Development Unit) in 1982, then 200 tons/day Pilot Plant and finally 250MW IGCC Demonstration Project. The 250MW Demonstration Plant started operation in 2008 and completed successfully in 2013 after fulfilling all the targets [1]. Two commercial scale IGCCs of 540MW each are decided to be constructed as the Fukushima Restoration projects, one in Nakoso in Iwaki City, the other in Hirono, Hirono-cho both in Fukushima Prefecture. Hirono IGCC site is only 20 km away from Fukushima-Daiichi Nuclear Power Station of Tokyo Electric Power Company. Construction work already started for Nakoso IGCC Plant which will start commercial operation in mid-2020, supplying eelectricity to Tokyo Metropolitan Area serving the Tokyo Olympic Games in 2020.

[1] S. Kaneko, J.of Energy Engineering E4015018(2015), American Society of Civil Engineers.

Commercialize Flue Gas CO₂ Capture from Power Plant

Masaki Iijima

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Mitsubishi Heavy Industries, LTD.(MHI) started R&D since 1990 together with The Kansai Electric Power Company (KEPCO) targeting power plant flue gas CO₂ capture for the purpose of global warming prevention.

MHI has delivered various commercial flue gas CO₂ capture plants for chemicals and general use such as urea, methanol and beverages since 1999.

Power plant flue gas CO₂ capture is the final target for Enhanced Oil Recovery (EOR) and CO₂ Capture and Storage (CCS) purposes, and recently MHI delivered largest (4,776 Ton/D) coal fired power plant flue gas CO₂ capture plant in the world for EOR purposes in Texas USA.

How MHI carried out the R&D and increased the experiences based on commercial plants and demonstration plant are presented.

References

[1] Takashi Kamijo et.al. KM CDR process project update and new novel solvent development, International Conference on Greenhouse Gas Control Technologies 13 2016.

[2] Takashi Kamijo et.al. Development of the World's Largest Post-Combustion Carbon Capture Plant for Coal-fired Power Plant MHI Technical Reports 2015.

Technical Issues of Future Power Network with a Large Amount of Renewable Energy Sources

Ayumu Morita

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Renewable energy penetration is soaring worldwide. For instance, the added capacity in 2016 is 138.6GW, or approximately the total capacity of Canada. In Japan, in accordance to the Basic Energy Plan of the government, generation through renewable energy sources will be increased from 8.5% to 22-24% between 2015 to 2030 in order to comply with the of CO_2 emission reduction in COP21. As a contributer to this effort, Hitachi has provided many mega-solar systems and wind turbines, and will continue to develop advanced models. One key technology for this effort is our unique down-wind type turbine. This is a wind turbine that efficiently captures wind with the weatherclock effect by placing the turbine on the downwind side of the tower.

When installing a large amount of photovoltaics (PV) and wind turbines (WT), Japan expects to face various network issues. Generating 20% of electricity through renewable energy sources would propose two major issues. First is a shortage of tranmission capacity. Deployment of PV and WT is concentrated in areas with good weather, northern Japan, while demand would be concentrated towards the center—such as Tokyo. This would require us to enhance transmission system to increase capacity. Another issue is network instability.

Since PV and WT are unstable energy sources with power conditioning system, voltage and frequency fluctuations would occur in steady-state operation and influence of contingencies would be much greater due to lack of synchronous inertia. To solve these issues, we propose an integrated control concept, where generators, networks and consumers work together. In this presentation, system integrity protection scheme (SIPS) for a wide-area network and virtual power plant (VPP) for a local area are introduced as elements to the integrated control concept.

Steam Turbine Cycles for Renewable Energies: Geothermal, Solar thermal and Binary Generation

Nobuo Okita

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Renewable energy systems (RES) focused on reduction of carbon dioxide have been recently considered as practical alternatives to fossil fuel power plant. In such RES, steam turbine cycles are adopted to produce stable and reliable electricity. Geothermal energy system is known as one of the most stable RES, however its resources area is limited to volcanic area or hot spring fields. Toshiba and other Japanese suppliers of turbines for geothermal systems have wide experience in various kinds of geothermal cycle over the world. We have faced issues such as erosion/corrosion by the wet steam mixed with non-condensable gases and impurities and measuring method of wetness. Some items are resolved but some still partly remain.

Another renewable steam cycle is a solar thermal system well known as CSP. It is also limited to sunny places and it supplies unstable power with low temperature and moist exhaust steam. Nevertheless, the solar system combined with biomass boiler and binary generation can supply more stable power even at lower heat area like in Japan. Binary turbine and its combination with flash steam turbine would also contribute to use geothermal resources effectively and widely to lower temperature and more gas mixture in the steam.

We would be able to plan and offer practical RES with more efficient and economical steam turbine cycles based on our experiences and by the expectation to IAPWS of solving issues on water, steam and aqueous solutions as working fluid and heat transfer fluid.

Current Status of Combined Cycle/HRSG Power Plant and Ultra-Supercritical Steam Power Plant, and

Development of Advanced Ultra-Supercritical Steam Power Plant

Hideo Hirano

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As for the combined cycle/HRSG power plant, Higashi-Niigata thermal power plant began commercial operation as the first Japanese combined cycle power plant in December, 1984. For about 33 years after 1984, the 23 combined cycle/HRSG power plants including 130 units have been installed until July 31, 2017. All combined cycle/HRSG power plants use the LNG for fuel. On the other hand, as for the Ultra-Super Critical (USC) power plant, Kawagoe thermal power plant started commercial operation as the first Japanese USC power plant in June, 1989. For about 28 years after 1989, the 17 USC power plants including 27 units have been installed until July 31, 2017. All combined cycle/IRSG power plants use the coal for fuel.

Although some problems are left behind on both the combined cycle/HRSG power plant and USC power plant, the thermal efficiency of combined cycle/HRSG power plants were improved from 48.6% LHV to 61% LHV, and the thermal efficiency of USC power plants were improved from 43% LHV to 45% LHV, respectively. The combined cycle/HRSG power plant and USC power plant have been positioned as the main source of power generation in Japan. In recent years, from a viewpoint of CO₂ reduction of global warming prevention, improvement in the further efficiency is required, and the development and utilization of the 1700°C class combined cycle/HRSG power plant and Advanced-USC power plant are progressing.

References : [1] S. Nakamura et. al. Technical Development and Future Prospect of A-USC, MHI Technical Report Vol.48, No.3, 2011. (In Japanese)

Nonequilibrium condensation model and numerical analysis for wet steam turbines

Shigeki Senoo

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In most conventional power plants the steam turbines are supplied with superheated steam but, during the course of its expansion, the condition of the steam enters the two-phase region and the last few low-pressure stages operate in the wet regime. The main practical consequences of operating in the wet regime are blade erosion and corrosion damage, and deterioration in thermal efficiency due to a variety of two-phase effects collectively known as wetness losses. The adverse impact of condensation on efficiency has been appreciated from the very early days of steam turbines and considerable progress has been made in many aspects of condensing-flow research. Three dimensional, nonequilibrium calculations are now possible for multistage turbines, even fundamental uncertainties remain regarding nucleation and droplet growth models, and numerical methods are still unable to predict the broad droplet size distributions observed in real turbines. The derivation of theories for nucleation and droplet growth to model droplet size spectra in nonequilibrium condensating steam flow will be presented together with both numerical and experimantal results in the latest international collaboration project [1].

References

[1] Senoo, S., and White, A.J., Chap.9: Analysis and Design of Wet Steam Stages, Advances in Steam Turbines for Modern Power Plants, Elsevier, pp.165-218, (2016)

Aerodynamic Blade Designs Including Wet Steam Turbine Stages

Tadashi Tanuma

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The power-generation percentage by steam turbines in all power stations including renewable energy power stations was 60% in 2012, and estimated to become 47% in 2040 [1]. Almost all turbine stages in nuclear, geothermal and concentrated solar power stations operate in wet steam conditions. Even in steam turbines for modern ultra-supercritical thermal power stations, last a few low-pressure turbine stages operate in wet steam conditions. These data show that understanding of accurate properties of wet steam flows and condensation water flows should be critical for design of blades in steam turbine stages [2]. Velocities of steam flows in steam turbine stages become high when the steam goes through throats of the flow paths and the velocities sometimes go over the sonic speed in last a few low-pressure long blade flow paths. In these conditions, non-equilibrium condensations can take place in blade flow paths and these phenomena lead to changes of pressures, velocities and flow angles of inlet and outlet of stationary and rotating blades. Aerodynamic blade designs including these wet steam turbine stages with these non-equilibrium wetness effects will be presented.

References

[1] T. Tanuma, Chapter 1: Introduction to steam turbines for power plants, Advances in Steam Turbines for Modern Power Plants, Elsevier, pp.3-9, (2016)

[2] T. Tanuma, Chapter 6: Design and analysis for aerodynamic efficiency enhancement of steam turbines, Advances in Steam Turbines for Modern Power Plants, Elsevier, pp.109-126, (2016)

IAPWS Thermophysical Properties of Water and Steam WG Kyoto, Japan, 28–31 August 2017

NOTE: These Minutes include many items that were held jointly with the IRS Working Group and/or the Subcommittee on Seawater (SCSW). 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, August 28, 2017 by the TPWS Chair, Allan Harvey. The agenda (Attachment A) was adopted after some additions. The Chair noted that the 2016 Minutes had been circulated and approved by email shortly after the 2016 meeting. J. Hrubý was appointed Clerk of Minutes for TPWS.

3. No new Collaborative Project was suggested at TPWS.

4. Possible topics for 17th ICPWS in Prague 2018 have been discussed. Suggested were sessions on uncertainties of thermophysical property formulations, thermophysical properties of aqueous systems, molecular modeling, metastable states. (Other may be included at the IPC meeting.). R. Span stressed that ICPWS should have strong focal points in order to remain a significant meeting. The form of publication of presented research has been discussed. D. Friend suggested that International Journal of Thermophysics may be interested in publishing a special issue dedicated to ICPWS. R. Span suggested that extended abstracts could be published in Energy Procedia.

<u>NOTE</u>: Item 5 except for point 5.5 is reported on in the IRS minutes.

5. Industrial Requirements and Solutions for Steam Property Calculations, joint with WG IRS

5.1 Report of the Task Group "Categories of industrial requirements" (N. Okita, A. Nový, I. Weber)

5.2 Report of the Task Group "Industrial Advisory Note" (M. Hiegemann, B. Rukes, A. Singh, A. Harvey)

5.3 Report of the Task Group "Wet steam properties survey" (I. Weber, H. J. Kretzschmar, N. Okita, A. Nový)

5.4 Acid dew point under low sulfur contents (N. Okita)

5.5 As a result of the discussion on the need of a new industrial formulation initiated by J. Bellows) it has been suggested that the process should start with an updated scientific formulation. A task group for reconsideration of the IAPWS scientific formulation has been established (A. Harvey as chair, members N. Okita, D. Friend, R. Span, K. Orlov, J. Hrubý). The mission of the TG is to explore possible deficiencies of the present scientific formulation, consider new requirements such as modeling mixtures and phase interfaces, and stimulate new research when needed.

6. Heavy Water Properties (joint with WG IRS)

6.1 Stefan Herrig (co-authors R. Span, A. Harvey) reported on the results of the Task Group on Heavy Water Thermodynamic Properties. Collaboration between NIST and RUB in the development of a new formulation started in 2013. The new equation has the form of reduced Helmholtz energy as function of dimensionless temperature and density. It has 24 terms, is valid up to 825 K and 1200 MPa. New ideal gas part is based on recent data by Simkó et al. (2017) and it is accurate to within 0.02%. Many pieces of data such as gas density data by Kell, data for liquid at very high pressures are fitted significantly better than with the present IAPWS formulation. New second virial coefficient data was used for (quantum computations down to 200 K), speed of sound (RUB and PTB), supercooled density data (IT Prague). Draft release submitted, publication is being prepared.

6.2 H.-J. Kretzschmar presented the Report of Evaluation Task Group for Heavy Water Formulation (other members M. Duška, V. Holten, T. Beuthe). After a few amendments the formal aspects fulfill all requirements. correctness: derivatives clearly described, speed of sound equations had to be corrected. Supercooled heavy water with experimental data. High level of experimental data. Minor changes needed. Document appears as complete. Three reviewers implemented independently. Test values were corrected. Computing time is similar to the previous equation. The new equation has smaller number of terms but contains fitted exponents. The evaluation task group recommends to accept the Draft as an IAPWS Release. In discussion: K. Orlov said that he implemented the equation and wants it to be very clear that the molecular weight given in the Release should be used to convert to mass-based properties unless there is special knowledge of a different isotopic composition for the specific system.

6.3 Discussion of procedure toward adoption of Release for Heavy Water Thermodynamics. Because the document was circulated only recently, it was decided that people (especially those not in Kyoto) should be given more time to examine it, although the members present felt it was ready for adoption. The WG voted to approve the draft Release, with the condition that members be given until the end of October to bring up additional issues. The WG Chair and Chair of the Evaluation TG were authorized to resolve any such issues that are raised. The WG requests the EC to authorize a Postal Ballot to be conducted after this additional period has passed and after the Editorial Committee has approved the draft.

6.4 Report of TG for Heavy Water Transport Properties (J. Sengers, M. Assael, M. Huber, R. Perkins) A. Harvey reported on behalf of the Task Group that it had collected data but otherwise was just beginning its work.

6.5 R. Romeo (co-authors P. A. Giuliano Albo, S. Lago, L. Rosso) informed about preliminary measurements of density of heavy water through an isochoric method up to 170 MPa. The mass was determined gravimetrically. Coefficients of thermal expansion and pressure expansion for the cell have been determined by comparing the measured data with IAPWS-95 formulation. Estimated standard uncertainty in terms of density is 0.02%. In the discussion, some experimental aspects have been opened, such as the fact that the pressure transducer, containing some volume of the sample, was not immersed in the bath.

7. Possible Improvements of IAPWS-95 Release

7.1 A. Harvey (in collaboration with W. Wagner) reported on possible refinement of uncertainty estimates in the IAPWS-95 Release. Uncertainty estimates for thermodynamic properties in the gas phase may be reduced as the ideal gas limit is approached. In particular, heat capacity, speed of sound and density have been considered. It has been proposed that sentences will be added to the captions of the uncertainty diagrams informing that the uncertainties became smaller at low pressure. The proposal (**TG consisting of Harvey and Wagner**) should be circulated in order that it can be adopted at the 2018 meeting. R. Feistel suggested that more quantitative statements should be possible; he and Harvey will investigate the possibilities.

8. J. Kalová and J. Hrubý reported on behalf of the Task Group on Surface Tension of Ordinary Water (joint with WG IRS and SC SW, members V. Vinš, A. Harvey, O. Hellmuth, V. Holten, J. Hrubý, J. Kalová, R. Mareš, J. Pátek, F. Caupin). R. Mareš performed capillary rise measurements in thin capillary (I.D. 0.097 mm) down to -32 °C. V. Vinš and co-authors measured surface tension of supercooled water using the horizontal capillary method. Both measurements support previous conclusion that the surface tension of supercooled water is close to the extrapolated IAPWS standard. Further, J. Kalová presented results of a literature review. F. Caupin in a message required that the equation should have the proper critical exponent (1.260 is the currently adopted value; neither the present IAPWS equation nor new equation by Pátek et al. use this value). In the following discussion it has been mentioned that new surface tension data should be generated in the high-temperature region, where only old Soviet data is available. J. Kalová was appointed as the new chair of the TG. The TG will work towards a new IAPWS equation for the surface tension, but no deadlines were set as it is felt that this is not an urgent task.

9. Humid Air Fugacity and Enhancement Factor, joint with SC SW

9.1 A. Harvey reported on his investigation of explicit approximations to the Poynting factor. The enhancement factor is the ratio between the actual partial pressure of (water) vapor in a mixture equilibrium condition to its saturation pressure in the pure state. The Poynting is a part of the enhancement factor which represents the effect of pressure on the fugacity of a pure liquid or solid phase. Approximations for pressure-independent molar volume ("first order") and considering pressure-independent compressibility ("second order") have been considered. Approximations have been compared with the Poynting factor computed directly from IAPWS-95 or the IAPWS ice formulation up to 20 MPa at temperatures 473 K down to 173 K for ice and down to 235 K for supercooled water. For the second-order correction, the difference to the accurate values was below 0.1 ppm for pressures up to 1 MPa.

10. Metastable Water (joint with SC SW)

10.1 J. Hrubý reported about the progress of measurements of the density of supercooled ordinary and heavy water performed by M. Duška and coworkers. Because M. Duška was in the past year at a research stay in the USA (next item), only evaluation of the 2016 data was performed in this period. The reproducibility of the heavy water measurements was within 0.005%, the standard uncertainty of the "relative density" (the ratio of density at given pressure and temperature to the density at the same pressure and reference temperature of 25 °C) is

roughly 0.01%. The data were provided to the developers of the developers of the new IAPWS formulation of thermodynamic properties of heavy water.

10.2 J. Hrubý (main author M. Duška, co-author M. Anisimov) presented a preliminary report on modeling thermodynamic properties of supercooled heavy water. This work has been performed in frame of the Young Scientist IAPWS Fellowship Project "Towards an IAPWS Guideline for the Thermodynamic Properties of Supercooled Heavy Water". A new model based on the two-state concept has been developed. The properties of liquid water are expressed in the form of a Gibbs energy of a mixture, including parts for "pure components", representing the various molecular structures, ideal mixing part and an excess part. In contrast to the model by V. Holten and co-authors which used a high-order empirical polynomial for component A (denser structure), the new model uses a simple expansion around spinodal suggested originally by Speedy (outside the two-state concept). The work is ongoing and final results of the project will be presented at 17th ICPWS in 2018.

10.3 V. Fernicola (coauthors (L. Rosso, G. Beltramino, S. Tabandeh, P. A. Giuliano Albo) informed about vapor pressure measurements over subcooled water down to 255 K. Measurements have been performed with a new setup. The sample cell was formed by a fused silica capillary (I.D. 0.500 mm) forming a U-tube. The sample was outgassed repeated freeze quenching, degassing in vacuum, and thawing under low pressure. The cell is connected to a capacitance pressure transducer, which is at higher temperature. Pressure transducer calibrated at the triple point of water using the IAPWS-adopted value. Combined standard uncertainties range from 0.03% at 273 K to 0.08% at 255 K.

10.4 J. Hrubý reported on behalf of a Task Group on Superheated liquid water (second member R. Feistel, joint with WG IRS and SCSW). The results of comparison of IAPWS-95 computations with experimental data in the superheated liquid region have been presented in Dresden. The main result was that IAPWS-95 can be safely extrapolated to the superheated liquid region. Existing old data on the density and speed of sound for superheated water have large uncertainties and their importance is rather qualitative. R. Feistel informed that the study is not anymore needed for the purpose of the definition of relative humidity, for which it had been required.

10.5 Report on Task Group on ICRN for Interfacial Properties of Supercooled Water (O. Hellmuth, J. Hrubý, J. Sengers) The TG was closed because it had no output.

10.6 A. Harvey (co-author V. Holten) reported on the saturation pressure of supercooled water. Various correlations are used for the saturation pressure of supercooled water. Most of them are extrapolations based on data above the triple point. The saturation pressure can be determined using thermodynamics by starting at the triple point and integrating the Clapeyron equation, or, alternatively, by developing a thermodynamic potential and finding the saturation conditions. The second option has been used and the saturation pressure was computed using the equation in the 2015 Guideline for properties of supercooled water for the liquid phase and IAPWS-95 for the gas phase. Differences with respect to the often used correlation by Murphy and Koop is primarily due to different data for the heat capacity of supercooled water used for the computations. **A Task Group (A. Harvey, V. Holten, R. Feistel) was appointed to develop this into a new section to be inserted into the supercooled water Guideline.** The Chair was

authorized to appoint an Evaluation Task Group at the appropriate time; J. Lovell-Smith volunteered for that Task Group.

10.7 A. Harvey reported for the Task Group on possible revision of IAPWS formulations for melting curves (other members V. Holten, H.-J. Kretzschmar) The main point was that V. Holten was working on thermodynamic potentials for various ices which might lead to new melting curves, which would also take advantage of better knowledge of the Ih-III-L triple point. However, there was no progress during the year.

<u>NOTE</u>: Items 11-15 are reported in the SCSW Minutes.

11. Report of Task Group on Extension of Range of Formulation for Thermodynamic Properties of Sea Water (joint with WGs IRS and SC SW) (R. Feistel) (Tuesday)

12. Cooperation with other international bodies (joint with SC SW) (Tuesday)

13. Reports on seawater-related topics (joint with SCSW) (Tuesday)

(see attached agenda for individual titles)

14. Proposed new IAPWS seawater-related documents (joint with SCSW) (Tuesday)

14.1 Report on Guideline for Electrical Conductivity of Seawater (R. Pawlowicz)

14.2 Report of Task Group on Supplementary Release for a simplified density equation for oceanographic use (R. Pawlowicz, T. McDougall, P. Barker)

14.3 Report of Task Group on Advisory Note on IAPWS documents contributing to TEOS-10 (R. Feistel, A. Harvey, R. Pawlowicz)

15. Reports on miscellaneous TPWS scientific topics (joint with WG IRS and SC SW)

15.1 Report of Task Group on Covariance in IAPWS work (R. Feistel, J. Hruby, S. Seitz, J. Lovell-Smith, D. Friend)

15.2 Unleashing empirical equations with "Nonlinear Fitting" and "GUM Tree Calculator" (J. Lovell-Smith, P. Saunders, R. Feistel)

15.3 GLS Uncertainty Propagation of Systematic Error (R. Feistel, J. Lovell-Smith)

16. Joint session with WG PCAS [Thursday morning]

16.1 S. Senoo reported on a nonequilibrium condensation model and numerical analysis for wet steam turbines (joint topic with IRS, also presented at IAPWS Symposium on Wednesday). The basic physical principles are nucleation and droplet growth. Homogeneous nucleation is considered, although some effect of heterogeneous nucleation is admitted. Classical nucleation theory with a non-isothermal correction by Kantrowitz was used to predict the nucleation rate. In subsequent discussion it has been said that the processes in wet steam flows are of interest to IAPWS and that relevant ICRNs exist (ICRN

22, Steam Chemistry in the Turbine Phase-Transition Zone and ICRN 28, Thermophysical Properties of Metastable Steam).

16.2 J. Hrubý reported on the progress toward improved ideal-gas properties of ordinary and heavy water performed by a group of authors primarily based in spectroscopy led by Prof. A. Csaszar. Final results for $H_2^{16}O$ (the main isotopologue in ordinary water) have been published. Further, final results for deuterated isotopologues $D_2^{16}O$, $D_2^{17}O$, and $D_2^{18}O$, and heavy water (their mixture) were published in 2017 (and used in the new IAPWS formulation for heavy water). The ideal gas properties are computed using a partition function based on a large database of experimental and quantum-mechanically computed energy levels. The developers were encouraged to provide data for the remaining water isotopologues so that the ideal-gas heat capacity for ordinary water could eventually be replaced.

16.3 A. Harvey reported on first-principles calculations of second and third virial coefficients for H₂O and D₂O. Experimentally, the second virial coefficient is known from 350 to773 K, little data exist down to 323 K and up to 1173 K. The third virial coefficient is known from 400 to 773 K. The computations consider quantum effects, flexibility of molecules, and isotopic differences (including D₂O). Significant differences of the new computations with respect to the 2004 formulation by Harvey and Lemmon are only at low temperatures. The quantum correction is needed below about 800 K, semiclassical approach is good down to about 400 K. Preliminary results were shown for the third virial coefficient. Third virial coefficient by IAPWS-95 seems to underpredict the experimental data at low temperatures. The computations with rigid molecules seems to confirm the IAPWS-95 curve, but this is not definitive since flexibility may be significant as it is for the second virial.

16.4 K. Yoshida presented a proposal for IAPWS Guideline on self-diffusion coefficient of water (also presented at IAPWS Symposium on Wednesday). The formulation is based on article J. Chem. Eng. Data 55 (2010) 2815-2823. It has been agreed that an IAPWS document on self-diffusion coefficient is needed. **Task group has been established, including K. Yoshida, K. Maier, and A. Harvey.**

17. IAPWS Certified Research Needs (ICRNs)

17.1 ICRN 27: Thermophysical Properties of Humid Gases and CO2-Rich Mixtures: Closing statement will be prepared by R. Span.

17.2 N. Okita discused a possible ICRN for acid gas dew points. In particular, interest is in dew point under low sulfur contents (SO3 below 1 ppm). Problems occur in combustion of NG containing sulfur. Sulfuric acid and nitric acid are formed causing stress corrosion cracking. Existing empirical formulation predicts dew points more than 25 K lower than a theoretical model. Siemens point of view: apply water dew point when the predicted dew point is below the water dew point. R. Span mentioned that reasonably good correlations can be found for SO2 and SO3. A difficulty is providing the distribution between SO2 and SO3 which depends on complex catalytic effects. A TG has been established including N. Okita (chair), K. Orlov, and R. Span.

18. Reports on other TPWS activities

18.1 A. Harvey reported that there are no changes needing an update of the Guideline on Fundamental Constants.

18.2 A. Harvey reported that no amendment is needed to Advisory Note 2.

19. Other Business

19.1 Report on International Collaborative Projects. No new International Collaborative Projects have been proposed.

19.2 Further discussion of ICPWS topics. J. Hrubý acknowledged an update of ICPWS topics based on the contributions of IPC members. He asked the IRS members to reconsider the structure of their topics.

19.3 Ideas for promoting IAPWS has been discussed: Inviting top-level people to other international organizations to ICPWS, translations of TGDs into other languages, online communities, encourage people publishing IAPWS work to mention IAPWS in a prominent place, Wikipedia pages, IAPWS-related software can be a point of contact, mentioning IAPWS when organizing related conferences.

20. Membership and Vice-Chair election: K. Nayor, R. Romeo and V. Fernicola have been unanimously elected as TPWS members. Prof. Karsten Meier has been unanimously elected as a second TPWS vice chair.

21. Contribution to Press Release

The Chair and the Clerk of Minutes were assigned to prepare the contribution to the Press Release.

22. 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.

23. Adjournment

The meeting was adjourned at 14:15 on Thursday, August 31.

Preliminary Agenda for the IAPWS Working Group

Thermophysical Properties of Water and Steam (TPWS)

Kyoto, Japan, August 28-31, 2017

- 1. Opening Remarks; Adoption of Agenda
- 2. Appointment of Clerk of Minutes
- 3. Potential International Collaborative Projects [Monday]
- 4. Discussion of topics for 2018 ICPWS in Prague
- 5. Industrial Requirements and Solutions for Steam Property Calculations, joint with WG IRS
 - 5.1 Report of the Task Group "Categories of industrial requirements" (N. Okita, A. Nový, I. Weber)
 - 5.2 Report of the Task Group "Industrial Advisory Note" (<u>M. Hiegemann</u>, B. Rukes, A. Singh, A. Harvey)
 - 5.3 Report of the Task Group "Wet steam properties survey" (I. Weber, H. J. Kretzschmar, N. Okita, A. Nový)
 - 5.4 Acid dew point under low sulfur contents (N. Okita)
 - 5.5 Is it time for a new industrial formulation? (J. Bellows)
- 6. Heavy Water Properties (joint with WG IRS)
 - 6.1 Report of Task Group on Heavy Water Thermodynamic Properties (R. Span, A. Harvey, <u>S. Herrig</u>)
 - 6.2 Report of Evaluation Task Group for Heavy Water Formulation (H.-J. Kretzschmar)
 - 6.3 Discussion of procedure toward adoption of Release for Heavy Water Thermodynamics
 - 6.4 Report of TG for Heavy Water Transport Properties (J. Sengers, M. Assael, M. Huber, R. Perkins)
 - 6.5 Heavy water density through an isochoric method: preliminary results (<u>R. Romeo</u>, P. A. Giuliano Albo, S. Lago, L. Rosso)
- 7. Possible Improvements of IAPWS-95 Release
 - 7.1 Report on Uncertainty Estimates of IAPWS-95 for vapors at low pressures (W. Wagner, <u>A. Harvey</u>)
- Report of Task Group on Surface Tension of Ordinary Water (joint with WG IRS and SC SW) (V. Vinš, A. Harvey, O. Hellmuth, V. Holten, <u>J. Hrubý</u>, <u>J. Kalová</u>, R. Mareš, J. Pátek, F. Caupin)
- 9. Humid Air Fugacity and Enhancement Factor, joint with SC SW
 - 9.1 Report on Investigation of explicit approximations to the Poynting factor (A. Harvey)

- 10. Metastable Water (joint with SC SW)
 - 10.1 Measurements of the density of supercooled ordinary and heavy water (M. Duška, J. Hrubý)
 - 10.2 Report on modeling thermodynamic properties of supercooled heavy water (M. Duška, J. Hrubý)
 - 10.3 Some difficult, but challenging, vapour pressure measurements over subcooled water down to 253 K (L. Rosso, G. Beltramino, S. Tabandeh, <u>V. Fernicola</u>, P. A. Giuliano Albo)
 - 10.4 Report of Task Group on Superheated liquid water, joint with WG IRS and SCSW (J. Hrubý, R. Feistel)
 - 10.5 Report on Task Group on ICRN for Interfacial Properties of Supercooled Water (O. Hellmuth, J. Hrubý, J. Sengers)
 - 10.6 Report on the vapor pressure of supercooled water (V. Holten, <u>A. Harvey</u>)
 - 10.7 Report of Task Group on possible revision of IAPWS formulations for melting curves (V. Holten, <u>A. Harvey</u>, H.-J. Kretzschmar)
- 11. Report of Task Group on Extension of Range of Formulation for Thermodynamic Properties of Sea Water (joint with WGs IRS and SC SW) (R. Feistel) (<u>Tuesday</u>)
- 12. Cooperation with other international bodies (joint with SC SW) (Tuesday)
 - 12.1 IAPWS/IAPSO/SCOR Joint Committee on Seawater, including updates to TEOS-10 (R. Pawlowicz)
 - 12.2 BIPM/IAPWS cooperation (R. Feistel)
- 13. Reports on seawater-related topics (joint with SCSW) (Tuesday)
 - 13.1 Absolute Salinity measurements by a vibrating tube densimeter and a refractive index salinometer (H. Uchida)
 - 13.1a Current situation of the absolute density measurements of seawater (<u>Y. Kayukawa</u>, H. Uchida)
 - 13.2 Surface Tension of seawater (K.G. Nayar)
 - 13.3 Isothermal compressibility of seawater and predicting seawater properties for desalination applications (K.G. Nayar)
 - 13.4 Progress on pH-related topics (S. Seitz)
 - 13.5 Improving the metrological traceability of seawater pH measurements (A. Dickson presented by R. Pawlowicz)
- 14. Proposed new IAPWS seawater-related documents (joint with SCSW) (Tuesday)
 - 14.1 Report on Guideline for Electrical Conductivity of Seawater (R. Pawlowicz)
 - 14.2 Report of Task Group on Supplementary Release for a simplified density equation for oceanographic use (<u>R. Pawlowicz</u>, T. McDougall, P. Barker)
 - 14.3 Report of Task Group on Advisory Note on IAPWS documents contributing to TEOS-10 (R. Feistel, A. Harvey, R. Pawlowicz)
- 15. Reports on miscellaneous TPWS scientific topics (joint with WG IRS and SC SW)
 - 15.1 Report of Task Group on Covariance in IAPWS work (<u>R. Feistel</u>, J. Hruby, S. Seitz, J. Lovell-Smith, D. Friend)

- 15.2 Unleashing empirical equations with "Nonlinear Fitting" and "GUM Tree Calculator" (J. Lovell-Smith, P. Saunders, R. Feistel)
- 15.3 GLS Uncertainty Propagation of Systematic Error (R. Feistel, J. Lovell-Smith)
- 16. Joint session with WG PCAS [Thursday morning]
 - 16.1 Nonequilibrium condensation model and numerical analysis for wet steam turbines (S. Senoo) [joint topic with IRS]
 - Progress toward improved ideal-gas properties of ordinary and heavy water (J. Hrubý)
 - 16.3 First-principles calculation of second and third virial coefficients for H₂O and D₂O (A. Harvey)
 - 16.4 Possible IAPWS Guideline for self-diffusion coefficient of water (K. Yoshida)
- 17. IAPWS Certified Research Needs (ICRNs)
 - 17.1 ICRN 27: Thermophysical Properties of Humid Gases and CO₂-Rich Mixtures (closing statement needed) (R. Span, A. Harvey)
 - 17.2 Discussion of possible ICRN for acid gas dew points (N. Okita)
- 18. Reports on other TPWS activities
 - 18.1 Guideline on Fundamental Constants (A. Harvey)
 - 18.2 Advisory Note 2 (J. Cooper, A. Harvey)
- 19. Other Business
 - 19.1 Report on International Collaborative Projects
 - 19.2 Further BRIEF discussion of ICPWS topics (J. Hruby)
 - 19.3 Ideas for promoting IAPWS
- 20. Membership and Vice-Chair election
- 21. Contribution to Press Release
- 22. Preparation of the Formal Motion to the EC
- 23. Adjournment

August 28, 2017

A.H. Harvey (Chair), J. Hrubý (Vice-Chair)
Minutes of the IAPWS working group IRS, Kyoto, 28. – 31. August 2017

(Numbering of topics follows TPWS agenda, except where denoted "...-IRS")

1. Nobuo Okita opened the session for IRS at about 10:30 am, 28. August 2017. The agenda was adopted without changes.

- 2. Adam Nový was appointed clerk of minutes.
- 3. Covered in TPWS minutes.
- 4. Covered in TPWS minutes.
- 5. Industrial Requirements and Solutions for Steam Property Calculations [joint with TPWS]

5.1 Report of the Task Group "Categories of industrial requirements" (N. Okita, A. Nový, I.

<u>Weber)</u>

N. Okita explained the purpose of the T.G. and presented the gathered and sorted topics of the potential areas of interest of IRS group. The items were sorted from different point of views and supported by examples. There was discussion following the presentation. D. Friend asked about the form to be circulated within IAPWS members, what will be the final form, set of ICRNs or document available on the webpages? N. Okita answered that the final form is not known yet as it is the initial kickoff and is about to be considered.

TODO:

1) Categorize items in terms of expected IAPWS output (ICRNs, Guidelines, Standards, etc.) and discuss the distance to IAPWS business.

2) Make the categories available in comprehensive to all IAPWS members to comment.

5.2 Report of the Task Group "Industrial Advisory Note" (M. Hiegemann, B. Rukes, A. Singh, A. Harvey)

M. Hiegeman was not present and no progress is known on this project. A. Harvey reminded the original purpose of the TG, to prepare a guideline for industrial application, which clarifies what IAPWS document should be used for in the industrial applications. The discussion concluded that it would be good to keep the task open

TODO:

1) Check the status from M. Hiegeman, and ask him, whether he will continue himself, otherwise find a new chair of the TG.

5.3 Report of the Task Group "Wet steam properties survey" (I. Weber, H. J. Kretzschmar, N. Okita, A. Nový)

There was presented survey by A. Nový summarizing the wet steam properties calculation used in some of Doosan Škoda in house IF-97 libraries and steam turbine calculation software. It was pointed out, that no standard and/or guideline exist for some of wet steam property calculation (speed of sound, viscosity, etc.). There was long discussion following, leading to setting up new T.G.: "Advisory Note on Wet Steam Properties Calculation" (<u>A. Nový</u>, J. Hrubý, K. Orlov, R. Span, K. Meier). The purpose will be to put together advisory note for industrial use, how to correctly calculate or estimate thermo-physical and transport properties of wet steam which are not part of the IAPWS-IF97 standard.

TODO:

- 1) Prepare list of the wet steam properties to be addressed.
- 2) Look up possible existing solutions (literature, models, measurements, etc.).

5.4 Acid dew point under low sulfur contents (N. Okita)

N. Okita presented the background, issues and status in Japan regarding the problems connected with dew point under low sulfur content related to HRSG for GTCC. It was pointed out, that the current knowledge does not include low Sulphur concentration areas and is solved in different ways within different companies. Suggestion to IAPWS is to unify method or data for predicting dew point under low sulfur contents and post/revise ICRN 23. Discussion will be followed by the "point of view" of Alstom and Siemens at the Thursday meeting for new ICRN. TODO:

1) Decide next step, unify the methodic leading to guideline and/or revise the ICRN 23. Discussed on item 17.2 (Covered in TPWS minutes)

5.5 Is it time for a new industrial formulation? (J. Bellows)

J. Bellows presented excellent overview of the IAPWS formulations prepared through the history and pointed out some important facts. There was every 30 years new formulation and bringing new formulation takes about 5 to 10 years. He also reminded the requirements for accuracy and speed and also so called long term stability. The main idea was, that it is "Time to start thinking". The discussion was then started. After discussing the strong and weak parts of both existing formulations IAPWS-95 and IAPWS-IF97 (considering range, regions, calculation speed, applicability, TTSE, SBTL, etc.), it was concluded, that the best approach would be to revise the existing scientific formulation IAPWS-95 and the eventual "new industrial formulation" to be derived from the "new scientific formulation". For this purpose the new T.G.: "New Scientific Formulation" has been set up (<u>A. Harvey</u>, J. Hrubý, N. Okita, K. Orlov, R. Span). TODO:

- 1) Revise existing IAPWS-95 its weaknesses and potential upgrades, for example in range, data background, two-phase region etc. and also consider "mixture compatibility", as advised by R. Span.
- 6 15. Covered in TPWS / SCSW minutes.

16-IRS. Discussion on the future of IRS

16.1 Nonequilibrium condensation model and numerical analysis for wet steam turbines (S.

<u>Senoo</u> [joint session with WG TPWS and PCAS] Covered in TPWS minutes

<u>16.2-IRS. Discussion on wet steam properties</u> [IRS separate meeting with S. Senoo]

S. Senoo presented the details of specific requirements towards IAPWS regarding the wet steam in steam turbines modeling. 1) two-phase flow problem, especially focused on water film breakup model and droplets deposition model on the turbine blades. 2) Wetness measurement equipment and techniques. 3) Lack of measured wet steam data from operating power plants. The points 1) and 2) may be in future be addressed by formulating ICRNs or creating Guidelines or Technical guidance documents. For the point 3) new T.G. "Wet steam Data from Operating Turbines" has been set up (<u>N. Okita</u>, A. Nový, S. Senoo?, I. Weber?, A. Singh?, M. Hiegemann?). The task group should gather the steam turbine measured wet steam data and share it within the T.G. members. TODO:

1) Ask I. Weber?, A. Singh?, M. Hiegeman? Whether they want to participate.

2) Prepare form of gathering and sharing.

3) Ask ASME for possible assistance.

16.3-IRS. Evaluation of distance to IAPWS business and stakes holders [IRS separate meeting] Discussing the list of possible topics of IRS busines as presented in point 5.1. The discussion led to conclusion, that within IRS we are unable to judge the items distance to IAPWS so the other W.G. will be asked for help. The T.G. "Categories of industrial requirements" about to be expanded with at least one representative of each IAPWS W.G., to properly judge the items distance to IAPWS business. TODO:

1) Ask chairs of W.G.s for candidates to expand the T.G. "Categories of industrial requirements"

16.4-IRS Features and problems of the geothermal steam turbine cycle [IRS separate meeting with N. Yamaguchi]

N. Yamaguchi presented the details of specific requirements towards IAPWS regarding the geothermal power plants. There were five main areas of interest mentioned.

1) Steam – gas mixture thermo-physical properties

2) Wetness measurement

3) Steam scrubbing

4) Silica content measurement and affecting of silica scaling

5) Modeling two-phase flow for binary type power plant heat exchanger

The discussion concluded that topics 3) and 4) to be moved to PCC W.G. topic 5) to be treated

individually outside IAPWS at this moment. The topic 1) is to be covered by future ICRN. Topic 2) was not addressed with specific solution and was left for future decision.

TODO:

Prepare draft of ICRN regarding point1) Steam – gas mixture in geothermal power plant turbine thermophysical properties within the Japanese committee possibly with support by New Zealand and reviewed by the geothermal session of ICPWS 2018 for common requirements.

17. IAPWS Certified Research Needs (ICRNs)

Covered in TPWS minutes.

- 18. Covered in TPWS / SCSW minutes.
- 19. Other business: No report for IRS
- 20. Membership
 - 1) Michael Daur has retired. Replacing M. Daur, Olaf E. Lemp (Germany) was proposed as new IRS member.
 - 2) Shigeki Senoo (Japan) was proposed as new IRS member by H. J. Kretszchmar and seconded by N. Okita

IRS unanimously accepted both new members.

Other changes:

There were noticed changes in e-mail addresses of F. Blangetti, M. Heigemann and P. Murphy.

- 21. Contribution to Press release will be done by the WG chair
- 22. Formal motion to the EC will be prepared by the WG chair
- 23. The IRS meeting was adjourned 31. August 2017, about 12:10 pm.

Minutes of Joint Meeting with TPSW/SCSW

Chair: R. Feistel Clerk of Minutes: R. Pawlowicz, Kyoto, Aug 2017.

Agenda approved.

These minutes include agenda items in the joint TPWS/SCSW/IRS agenda that are specifically oriented to SCSW. For other agenda items consult the minutes of the other WG.

.1. Opening remarks, adoption of Agenda. The session was opened by Allan Harvey. Agenda was corrected with the addition of 12.2 (BIPM/IAPWS collaboration) which somehow got deleted. Also the addition of 13.1b, due to a mixup with the 13.1 speaker.

11. Report of Task Group on Extension of Range of Formulation for Thermodynamic Properties of Sea Water: Feistel is still hoping for a Gibbs function over a wider range for industrial purposes. New soundspeed data now available. Density measurements (perhaps) also will be available. but there may be some inconsistency with the new and old data. Numbers were promised for last Christmas but a paper still in preparation...so wait until next year.

12.1 SCOR/IAPWS/IAPSO Joint Committee on the Properties of Seawater (JCS) including updates to TEOS-10. Pawlowicz reports Web site accesses and software downloads have reached a steady state. Relative humidity work has now proceeded so that cooperation from other societies is required, details in the next talk. Some questions about TEOS-10 software and how best to organize it.

12.2 Report on BIPM/IAPWS collaboration – Feistel reports on recent progress, including his attendance at a recent BIPM meeting. has been coopted as member of BIPM/CCT WG-RH. An update was provided on downloads of the Metrologia papers, two parts of which received a "Highlight of 2016" award, with an extension of open-access. A brief outline was provided of the proposed RH definition based on fugacity ratio rather than partial pressure ratio. A proposal was put forward to BIPM/CCT WG-RH and was received with mostly positive comments. Suzanne Picard is appointed to by official point of contact with IAPWS at ICPWS workshops., which can now officially say they are "officially endorsed by BIPM".

There are some options to get BIPM to take up RH (and "change the SI") – but it will be difficult (although not impossible). 2 companion papers planned. Robert Wielgosz has been informed about efforts and has passed this on to CCQM and EAWG but cooperation not so advanced there as for RH matters.

Questions – does BIPM have anything like RH? (dimensionless variable). Yes, angle and dB (also under discussion). Is fugacity too advanced a concept for teaching people? Yes, but...so was Gibbs functions. Should it be called something like "relative fugacity" instead of "relative humidity"? The question is still open. Would RH depend on IAPWS formulations? Not as a definition, but it would be important as (for example) a mise en pratique. A note – it will be important to get the meteorological community on board, and right now they aren't.

13.1 Absolute Salinity measurements by a vibrating tube densimeter and a refractive index salinometer. Uchida has a refractive index salinometer for the lab (in a constant T bath). In theory the setup has a resolution about 1 order of magnitude smaller than is needed for the "salinity/density problem", but (as always) and equation for the refractive index of seawater is needed. Also tested – the linearity of Anton Paar density meters. First, SSW test of 8 density meters showed offset of 4 to 11 ppm. Low-salinity seawater was tested with a different offset. So diluted SSW was used – negative offset at all salinities except very close to zero. Theory is that isotopic composition of water used for dilutions was to blame!

Discussion – some skepticism about whether there is a real effect from a single source, or just the sum of many tiny effects.

13.1b Current situation of the absolute density measurements of sea water: Kayukawa described his hydrostatic weighing machine for density. Uses an Si sinker with a thermal oxidation layer to prevent dissolution. Updates for this year – has calibrated sinker, made some other modifications. New measurements give good results for ultrapure water (and MilliQ), but seawater measurements are also a little low. Perhaps because of evaporation?

Q: Hruby wonders about the effects of surface tension on the wire. Issue is not resolved.

13.2 Surface tension of seawater: Nayar provides overview of the topics of the Lienhard research group of which he is a part (practical desalination interests, software for seawater properties). He explained that surface tension is important for membrane systems, esp. at high temps and high salinities. He ran tests on pure water, artificial seawater, some kind of standard seawater. Proposes to work towards a new IAPWS release on surface tension (as per the ICRN 16).

Discussion on dependence on IAPWS pure water surface tension.

Since paper published – needs a task group and an evaluation task group.

Task group for the Surface Tension of Seawater: Nayar, Hruby, Harvey. Wait until December in case of new measurements at low temperature by Hruby. Eval task group Rainer Feistel.

13.3 Isothermal compressibility of seawater. Nayar explains that there is a lack of high salinity/high pressure data – but this is the range needed for desalination. An extrapolation was developed to get SOMETHING in this range. Proposes to use this to improve the industrial formulation.

Q: Various questions about usefulness of high S/P measurements?

This is a topic for the new task group to prepare result for the existing task group on extended Industrial Formulation for seawater. This is best done by adding Nayar and Lovell-Smith to the existing task group.

13.4 – Progress on pH-related topics Seitz explains that there are pH measurements in seawater at S<5 and S>25, but there is a gap between them! Explanation of Harned cell measurements. Some preliminary results are shown, but there are differences with previous measurements that MAY be explained by composition differences with the artificial seawaters used (different workers use different recipes for the artificial seawater)

13.5. Improving the metrological traceability of seawater pH measurements Pawlowicz presented some slides from Dickson describing the upcoming Harned cell measurements and Pitzer model development in SCOR WG 145 which will help towards improving the pH problem identified by JCS.

14.1 Report on Guideline for Electrical Conductivity of Seawater Pawlowicz reports that there have been some setbacks in progress, but a plan has been made to work around them.

14.2 Report of Task Group on Supplementary Release for a simplified density equation for oceanographic use Task group is closed due to lack of interest in converting an existing publication to an IAPWS document.

14.3 Report of Task Group on Advisory Note on IAPWS documents contributing to TEOS-10 Advisory note written – task group closed.

15.1 Report of Task Group on Covariance in IAPWS work – two papers published, to be described in 15.2 and 15.3

15.2 Unleashing empirical equations with "Nonlinear Fitting" and "GUM Tree Calculator" Lovell describes the history of uncertainty models developed for measurements of relative humidity using a two-pressure humidity generator. The error depends somewhat on the correlation of errors at different temperatures. Uncertainty tends to drop once correlation taken into account. Also described 'GUM TREE' – a software package to simplify the application of GUM.

15.3 GLS Uncertainty Propagation of Systematic Error. Systematic error has been added to covariance matrix as applied to IAPWS95, but uncertainties are still somewhat smaller than seem believable. A hypothesis is that "GUM uncertainty" is a measuring a different thing than "IAPWS uncertainty:.

Vigorous discussion about what this means. Great controversy! Standard IAPWS uncertainties are (roughly) held to explain the degree of scatter about the fit (the "model"). The GUM propagation approach (roughly) shows the uncertainty of the fit. The two disagree. The clerk's theory is that a disagreement between a priori and a posteriori statistics suggests that the model is in error and should be improved. However, there remains the question of what to do when the "model" is taken as fixed.

20. Membership

Proposed members for SCSW: Yohei Kayukawa, Kishor Nayar, and Aina Wu, and Jeremy Lovell (already member of TPWS). Unanimously approved.

PCAS WG Minutes Kyoto, Japan, 27 August - 1 September, 2017

Present:	
Masaru Nakahara (Chair, on behalf of Andre Anderko)	nakahara@scl.kyoto-u.ac.jp
James C. Bellows	jcbellows2@aol.com
Milan Sedlar	m.sedlar@sigma.cz
Masakatsu Ueno	mueno@kvd.biglobe.ne.jp
Shigeki Senoo	shigeki1_senoo@mhps.com
Ken Yoshida	yoshida.ken@tokushima-u.ac.jp

Masaru Nakahara opened the meeting on behalf of the chair Andre Anderko, who was not able to attend the Meeting in Kyoto. The agenda was approved without any additions. Ken Yoshida was appointed as the clerk of minutes.

Minutes of the 2016 meeting were approved.

The possibility of issuing international collaboration was discussed and no proposals were made.

The possibility of issuing ICRNs was discussed and no proposals were made.

PCAS Workshop (Monday)

The following presentations were made in the PCAS workshop:

Dr. K. Yoshida gave a brief summary of his talk in IAPWS Symposium on Wednesday about the formulation of the self-diffusion coefficient and the analysis of the temperature and density effects in combination with MD simulation. It was indicated that a guideline in preparation on this topic is to be proposed in TPWS/PCAS Joint session on Thursday and EC on Friday, and the attendees adopted this proposal unanimously.

Dr. M. Sedlar summarized and discussed the topics related his talk in PCC/PCAS/IRS Joint WG Meeting on Tuesday in the afternoon, titled "Cavitation phenomena in balancing drums of high-performance feed pumps".

Dr. S. Senoo summarized and discussed the topics related his talk in IAPWS Symposium on Wednesday, titled "Nonequilibrium Condensation Model and Numerical Analysis for Wet Steam Turbines".

PCAS Workshop (Tuesday morning)

The following presentation was made in the PCAS workshop:

Prof. N. Matubayasi gave a talk about the free energy calculation of water in various polymers and its application to the rational design of polymers to improve the energy efficiency of separation processes. He showed his strategies to treat the polymers as the "solvent" for water for the analysis of adsorption and permeation of water in polymers, and shed light on the discussion about the segment size of the polymer chains that can be treated as a unit size of a "solvent molecule".

PCC/PCAS Joint Workshop (Tuesday afternoon)

The following presentations were made:

Cavitation phenomena in balancing drums of high-performance feed pumps (M. Sedlar) Presentation has shown the possibilities to predict numerically cavitation phenomena inside the balancing drum of a feed pump. Calculations include full bubble dynamics and real properties of water (nuclei number density distribution). Also a new grand project has been introduced, aiming to capture the influence of acoustic phenomena inside the drum.

Features and problems of the geothermal steam turbine cycle (N. Yamaguchi)

Novel technology for silica scaling control in geothermal power plant (Y. Kawahara)

PCAS Workshop (Tuesday afternoon)

The draft of the paragraph for the Press Release was composed and accepted.

The proposal of international collaboration of SIAPWS was considered. It is decided that PCAS WG is going to suggest the improvement of the proposal; especially it was suggested that the goals of the project need to be more clearly specified. The PCAS WG's position in the Evaluation Committee is entrusted to Prof. Nakahara.

TPWS/PCAS Joint Workshop (Thursday)

The following presentations were made:

Non-equilibrium condensation model and numerical analysis for wet steam turbines (S. Senoo) Progress toward improved ideal-gas properties of ordinary and heavy water (J. Hrubý) First-principles calculation of second and third virial coefficients for H₂O and D₂O (A. Harvey) Possible guideline on the self-diffusion coefficient of light and heavy water over wide ranges (K. Yoshida)

K. Yoshida proposed to move forward the evaluation processes of the guideline of the selfdiffusion coefficient. The proposal was approved.

Membership

It was decided that Dr. James C. Bellows (James Bellows and Associates, USA) and Dr. Shigeki Senoo (Mitsubishi Hitachi Power Systems, Ltd., Japan) will be recommended to EC Friday Meeting as the new PCAS WG members.

Miscellaneous

Masaru Nakahara attended as the PCAS representative for the Gibbs Award Committee on behalf of Andre Anderko.

IAPWS 2017 Kyoto Minutes of PCC meeting 10:30AM Monday, Aug 28th 2017

- Agenda from past meeting was adopted; minutes from Dresden meeting are available on IAPWS website, no objections were noted, minutes adopted
- From 2016 minutes re: TGDs' action items: one action on the ICRN26 (aluminum alloys use in cooling towers) action was to provide overview at Kyoto meeting; no input noted to be carried over to next meeting in Prague
- On the topic of international collaboration......K. Thomsen presented on TGD of "Monitoring of corrosion products on flexible plants"....concluded that much further work is required before confident to convert it into a TGD; AUS/NZ and SIAPWS. PCC decided it is necessary to work for 6+ months to develop database to develop such confidence....joint proposal will be made to the EC; Rziha notes that such work is critically important in CCPP worldwide. Critical to gain more knowledge on how these waves of oxides by pressure variation, loads, chemistry; also with layup strategies. Path forward is to circulate printed version of TGD, add a contract student (Aarhus Univ.); particle size distribution evaluations to be included
- B. Dooley provided background to PCC newcomers on TGDs; PCC Group has been working on TGDs since 2008, have become international standards around the world for conventional fossil and CCP plants, and also biomass (at request of SIAPWS); has expanded access by plants to this invaluable information worldwide; there are currently 8 TGDs (TGD-01-08, TGD2-09/2015, TGG3-10; TGD4-11/2015, TGD5-13, TGD6-13/2014.....TGD7-16, TGD8-16); reminds all that before a TGD can be introduced, a lot of data has to be evaluated (a rigorous process); discusses HRSG HP Evaporator Tube selection for both HGP and VGP-type HRSGs; there is an IAPWS "deposition map" available giving deposit loading vs Pressure.....useful to determine chemical cleaning, encompassing a 150-plant database ; described base case vs. Customization of each TGD
- B. Dooley further expanded on rigorous process for TGD, its truly international character, both in perspective and direction; it follows a process of draft/circulation/many revisions/editorial committee/then to 24 national committees /EC approval....ultimately leads to an International Standard
- TGDs planned for next 12 months: Demin water Impact in Steam Water Cycle, Air In-leakage Impact on Steam Water Cycle, FFP for Industrial plants, FFP Nuclear Secondary, plus 2 white papers; white papers can transition into TGD in 1-3 years.
- Refreshment of published TGDs need to reflect "state-of-the-art expertise"
- M. Rziha asks for suggestions for new TGDs; B. Dooley explains timeline for current set of TGDs-in-waiting
- Kirk Buecher is there a set date for implementing TGDs? within IAPWS, B. Dooley states No, only ICRNs have set deadlines
- K. Thomsen 1st presentation: Update on TGD CP sampling & analysis (Results of field testing) "Monitoring Corrosion Products in Flexible (cycling and two-shifting) Plants"

 M. Nielsen presented "Corrosion Product Monitoring By Online Turbidity, Total iron & Filtration Samples"; followed by K. Thomsen 2nd Presentation – Update on TGD CP sampling & analysis (focusing on statistical distribution aspects" - "Distribution of Particles and CP concentrations"

• M. Rziha asked if there were objections to the submitted international collaboration project; None were noted, M. Rziha proposes submitting a formal application to IAPWS Executive Committee (EC)

• Presentation given by J. P. Jensen "Permit for discharge of excess water to recipient - Flue gas condensation"

• Presentation given by Zhang Xiaoni on High-salinity Water Reuse in Coal-fired Power Plants

• Presentation by Xuxiang Jia (Wuhan University) on "Hydrodynamics/Kinetics Study on Flow Rate and Expansion of Ion-exchange Resins"

• Presentation by G. Joy on progress of TGD on Demin Water (fossil & nuclear) - "Ensuring the Integrity and Reliability of Demineralized Makeup Water Supply to the Unit Cycle"; pledge made to accelerate progress of this TGD and publish at EC meeting in Prague, 2018.

• Presentation by L. Carvalho on progress of TGD on Air In-leakage In Steam Water Cycles; Carvalho presented skeleton of TGD and current 13-page TGD draft; AIL subcommittee (Carvalho-Chair; Dooley/Rziha/Thomsen) will meet the following day in break-out session to finalize TGD writing assignments. Monika Nielsen asks to be excused from further subcommittee work due to work load; Carvalho asks if there are more volunteers to join, none noted at the meeting.

Day #2 Tuesday, August 29th 2017

- Presentation "Fundamental Investigation on powder scale occurring in OT plants"
- W. Cook gave an update on Canada/NZ International collaboration project; Electrochemical Corrosion Study, based on two ICRN (ICRN 25 & ICRN 20); matrix needed to try to match various Action Level guidelines around the world (Dooley). Work done @17MPa/sat. T 332C; W. Hater asked if organic acids will be tested on this rig? Cook: YES, and possibly filming amines effects but this is not a priority right now;
- W. Cook made a 2nd presentation Concept of HEPro Measurement....
- W. Hater presented on Film Forming Amine Products (FFPAs); "Introduction to the TGD for FFP in Industrial Plants"; discussion followed on potential additional TGD on FFP for closed loop cooling and heating systems justification based on a different philosophy than boilers, lower temperature system; B. Dooley stated that there is now the issue of the use of FFPs that are not "amine-based"; the subcommittee members present in Kyoto (Hater, Rziha, Dooley, Carvalho, Dosan of Kurita) will meet in a separate meeting on Wednesday 10AM) to discuss issue of "non-amines" in TGD
- W. Cook gave an update on Film Forming Amines and FFPs for use in the Second loop of Nuclear (PCC Nuclear Subcommittee FFP task group); discussion stressed differences around steam generator integrity in nuclear field and "nuclear qualification" around chemical impurities, etc.; also that a white paper is a better approach (rather than TGD), this should be done for the 2018 Prague meeting to decide direction; issue ICRNs for key parameters; B. Dooley suggested getting Anderko & P. Tremaine (from PCAS) to look at chemical properties aspect; Cook states that only nuclear secondary loop is included; Dooley states IAPWS can take a leadership position in developing a white paper on this topic; there is an AREVA program using ODA; there is an EPRI study by K. Fruzzetti; IAPWS white paper should go ahead

- M. Sedlar gave a presentation on "Cavitation Phenomena In Balancing Drums of Highperformance Feed Pumps"
- Naoko Yamaguchi presentated on "Features & Problems of Geothermal Steam Turbine Cycle"
- Yoshitaka Kawahara presented on "Novel Technology for Silica Scaling Control in Geothermal Plant"; B. Dooley formally invited Naoko Kawahara to join TGDs on Geothermal and IAPWS; also that there is a need for an ICRN;
- PCC breaks up into sessions in the afternoon for TGD working groups

DAY 3 - Wednesday, Aug 30th 2017 - no PCC activities due to main IAPWS symposium program

DAY 4 – Thursday Aug 31st 2017

• **PRESENTATIONS:**

- "Review of Different Demineralization Technologies for Low Salinty Water in the Power Industry" - Moataz Khalifa
- "Proposal for new TGD for Condensate Polishing" Moataz Khalifa. Discussion:
 - White Paper under preparation target Q2 2018.
 - TGD skeleton prepared for Prague meeting.
 - Considered too large a scope for proposed TGD as presented.
 - Agreed content:
 - 1. Do one generation system type CCGT including conventional or an Air Cooled Condenser or a Heller tower.
 - 2. Not a detailed design manual
 - 3. Cover essential elements to consider in deciding whether to include a polisher (CPP) in a plant, and key features on operating CPP
 - 4. Include decision considerations in installing or retro-fitting a CPP
 - Task Group members:
 - Moataz Khalifa Chair
 - David Addison
 - Kirk Buecher
 - Karsten Thomsen
 - Frank Udo Leidich
 - Gary Joy
- "Update on Corrosion product TGD" Karsten Thomson. Covered modification of previous presentation based on comments made at the meeting – to include a peak level assessment for the various start up steps.

• 17th ICPWS:

Reviewed and assigned promoters for the nominated ICPWS PCC sessions:

- 1. IAPWS Technical Guidance Documents (TGD's) (Dooley, Rziha)
- 2. Re-use of Water and Water Savings (Rziha, Karsten Thomsen, Joergen Peter Jensen)
- 3. Chemistry in Geothermal Plants (Addison, Kawahara, Yamaguchi, Tomarov, Rziha)
- 4. Chemistry in Nuclear Plants (Cook, Adam Caswell, Ishihara, Rziha)
- Chemistry in Combined Cycle and Fossil Fired Plants (Rziha; Dooley, Leidich, McCann; Hirano; Tian Li)
- 6. Film Forming Amines and Film Forming Products (Hater, Lendi, Dooley, Keith Fruzetti, Rziha)

• ICRN REVIEW

o ICRN 22 – Steam Chemistry in PTZ

Date Extension Statement to be sent to Editorial Committee – to extend to September 2018.

- ICRN 29 Corrosion Product Transport. Work finalized by Derek Lister. Date Extension Statement to be sent to Editorial Committee extend date to 2021.
- No new ICRNs proposed.

• DISCUSSION OF FUTURE PCC ACTIVITIES

- PCC / PCAS INTERACTION:
 - Previous discussion with PCAS to look at Film Forming Amines and Products, and for Andre Anderko (PCAS) to discuss with Peter Tremaine about work proposals.
 - Proposal for the 2018 and 2019 Meetings:
 - Continue with Joint workshops
 - But include a discussion time slot to discuss key PCC issues for PCAS
- OTHER ITEMS:
 - Proposal for an ICRN on FFA and Products
 - Proposal for TGDs to show the review process. Noted that all current TGDs have been revised except – TGD1 Boiler Carryover.
 - Discussion on whether White papers could be available on IAPWS website. At present White Papers considered as Working Documents and could be available on OPAL. Could consider publishing a White Paper if a TGD is not prepared. To be considered on a case by case basis.

• PCC PUBLIC RELATIONS:

- Encouragement for PCC members to promote IAPWS and PCC.
- Propose to publish PPChem document on PCC meeting.
- o PCC already supports international conferences on HRSGs and FFP

• CHANGES IN PCC ELECTED OFFICERS:

• No changes to PCC elected Officers

• **PROPOSED NEW PCC MEMBERS:**

- Adam Caswell EdF, UK
- Steve McGee Candu Owners Group (COG), Canada
- o Tian Li TPRI, China

Application for International Collaboration Corrosion Product Sampling, Analysis and Assessment

Background

The IAPWS TGD on corrosion product sampling and analysis has already taken a leadership position for fossil and combined cycle plants worldwide. Not only does this TGD provide details on how and where to take samples and to analyze them properly to determine total iron and copper levels, but it also provides limits for iron and copper, which illustrate optimized cycle chemistry according the IAPWS treatment TGD for AVT, OT, PT and CT. These levels have become standards worldwide. However, it is recognized that for heavily flexibly operating plant (fast start, cycling and two-shifting) these limits may not provide a rugged assessment of the cycle chemistry or whether FAC is under control. Therefore, this Corrosion Product Sampling and Analysis TGD needs revision with new assessment methodology being developed. This first requires cooperation with a range of power plants applying a variety of chemistry conditions that already conduct or are willing to conduct the corrosion product monitoring campaigns with parallel measurements of both classical analysis (as defined by the IAPWS TGD) and on-line methods during flexible load conditions and start-ups. A number of organisations have already taken part, but they often lack resources and the right setup of monitors to cover the demands fully. IAPWS in NZ/AU, UK/Ireland, and Scandinavia have formulated an approach, which will use a young scientist supported by an IAPWS International Collaborative Project. The Young Scientist will work under the direction of three IAPWS Members (Karsten Thomsen, SIAPWS, David Addison, New Zealand, and Paul McCann, BIAPWS) and cooperate with host plants that will conduct the field tests. It is planned that the Young Scientist will spend two weeks at three host sites. This will involve organizing monitoring campaigns, securing proper sampling conditions, applying and testing on-line instrumentation, and overseeing that the data acquired and submitted have the best possible quality. Most the equipment to conduct the tests and the analyses will be provided by the host site. All the analysis will be conducted or quality assured by the young scientist under the direction of the IAPWS monitor in SIAPWS, which will involve spending at least two weeks at a SIAPWS laboratory.

Technical Aspects and Goals

This planned activity will keep IAPWS in the leadership position with regards to corrosion products monitoring and assessment. The ultimate goal of the activity is to develop an IAPWS Map for the Decay of Corrosion Product Levels for flexible plant. The field tests conducted to date have demonstrated that on-line measurements such as turbidity and particle number/distribution may be used to follow particle levels and transport during start-up and flexible operation. The close relation between particle size distribution (PSD) and corrosion product (CP) distribution has been demonstrated both from basic principles and experimentally. Both PSD and CP distribution follow the log-normal distribution, and this new insight leads to a change in data processing of CP data and the use of new characteristic parameters to describe the level and variability of the CPs. These findings need to be confirmed for a number of cases representing the different chemistry typically applied in different plants. The ultimate goal is to establish a TGD covering sampling, analysis, and assessment of CPs for plants operating in flexible mode. This includes establishing an IAPWS Map for guiding values for levels, transport, and decay after startup. Of course, such values must be based on reliable and comparable data. Getting those within a reasonable period is the focus of this project. There is a great demand for such guidance worldwide, because power plant operating in flexible mode are numerous and the guidance so far has focused on plants in base load. The IAPWS Map will allow plants to determine whether both the operating and shutdown chemistry is optimized. For combined cycle plants, it will also link very closely with the IAPWS Map for HRSG HP Evaporator deposits (IAPWS TGD). The scientific content of the project will lead to a handful of

publications describing the connection between the fundamental PSD and the levels and distribution of CPs actually measured, the application of on-line methods as valuable tools to optimize the layup and shutdown chemistry, and the new data model leading to a change in routine data processing of CP data. In many senses, new territory is discovered in this study.

Young Scientist

SIAPWS has contact to a student at the Chemistry Department of Aarhus University who is interested in this project. He will be able to conduct the project for the master thesis. He is a very promising person who has A grades in almost every course so far. He is currently taking a semester at Stavanger University in Norway, focused on water chemistry courses, showing that he able to adapt and cooperate under foreign conditions.

Budget

Expenses to be covered:

- 1. Travel Scandinavia to UK, EI, FI x 1 each
- 2. Travel to NZ/AU x 1
- 3. Travel to IAPWS meeting x 1
- 4. Living expenses during stays

Additional analyses – the purpose is to supplement the analyses performed by/at the plants, such that all relevant measures are available for the evaluation in relation to the TGD development work. Quality of the data will be a focus point, and only laboratories that are able to document appropriate quality assurance at least at the level of the current TGD will be used.

Total budget is estimated at 20.000 GBP. The budget will be further refined, once the precise extent of the field trials is known.

On behalf of IAPWS organizations in Australia, New Zealand, United Kingdom and Ireland, and Scandinavia

Karsten Thomsen

SIAPWS Chair, member of PCC and the TGD task group

PRESS RELEASE

INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

2017 ANNUAL MEETING, KYOTO, JAPAN

Continuing a series of conferences that began in 1929 in London, 102 scientists, engineers and accompanying persons from 13 countries attended the annual meeting of the International Association for the Properties of Water and Steam (IAPWS). The Japanese National Committee of IAPWS hosted the meeting between the 27th August and the 1st September 2017 at the Kyoto Research Park in Kyoto, Japan. The highlights of the IAPWS working group sessions and other proceedings of the executive committee are summarized in this release.

The primary purpose of the annual IAPWS meeting is to connect researchers and scientists with the engineers who use their information. This information exchange provides the researchers with guidance on topical problems within industry and provides the engineers with the latest research results. Areas of application include power cycle chemistry, high temperature aqueous technologies applicable to steam cycles and fuel cells, the use of high temperature water and supercritical steam in chemical and metallurgical processes, supercritical synthesis of new materials and destruction of toxic wastes, hydrothermal geochemistry, hydrometallurgy, oceanography and global climate modelling, power cycles with CO₂ capture and storage systems and combined heat and power systems including district heating.

IAPWS produces releases and guidelines on the recommended scientific formulations for physical and chemical properties of water in its various forms as well as technical guidance documents that are the concerted opinion of IAPWS members on the best operating practices for power plant chemistry. IAPWS also documents certified research needs that represent the opinion of experts in their respective fields that a research topic is greatly needed to fill a current gap in knowledge. All this information is freely available and can be found on the IAPWS website at www.iapws.org.

In the Working Group on Thermophysical Properties of Water and Steam (TPWS), preliminary approval was given to a new formulation for the thermodynamic properties of heavy water (D₂O). The new formulation makes use of new, high quality data from several research groups and uses state-of-the-art molecular calculations to constrain its gas phase properties. Replacing the previous standard that was developed over 35 years ago will allow more reliable and accurate analysis for certain types of nuclear plant and will provide more accurate properties for scientific studies. Also discussed were new experimental and modelling results for supercooled water and heavy water. These results assist in understanding aspects of the fundamental physics of liquid water that give rise to unusual (and in some cases biologically important) behavior of water at low temperatures.

The Industrial Requirements and Solutions (IRS) working group discussed matters around droplet nucleation and wet steam to increase efficiency and to protect from erosion of turbine

blades. This resulted in a task group to assess and develop the requirements for an industrial solution for discussion during the 17th ICPWS in 2018 and a targeted release in collaboration with ASME.

The Working Group on Physical Chemistry of Aqueous Systems (PCAS) discussed cavitation in pumps and condensation in steam turbines. Another topic was computational approaches such as free energy calculation of water adsorption in various polymers and its application to the rational design of polymers to improve the energy efficiency of separation processes. A new IAPWS Guideline has been proposed concerning the formulation of the self-diffusion coefficient over a wide range of temperature and density, which is expected to be completed in 2018.

The Subcommittee on Seawater continued working towards the traceability of marine measurements. Software and documents on the web site (http://www.teos-10.org/) continue to be heavily downloaded. Also, a recent set of review papers on this topic has been very well received in the scientific community. Significant progress has been made in talks with the International Bureau of Weights and Measures (BIPM) towards standardizing a traceable definition of relative humidity and getting this widely accepted. Several talks were also given on density measurements of different real seawaters. A series of open workshops are planned for next year's International Conference on the Properties of Water and Steam.

The Power Cycle Chemistry (PCC) working group worked intensively on the development of several new technical guidance documents (TGDs) involving demineralized water requirements, the effects of air in-leakage into steam-water cycles and the use of film forming amines and products in industrial plants and nuclear plants. Considerable progress was made and presented on a white paper for corrosion product sampling for plants on flexible operation. Steam requirements for geothermal plants was highlighted as an area of future interest for PCC.

IAPWS produces Certified Research Needs (ICRNs) as guidance for funding agencies and as an aid to people doing research in defining important research. To date, these have covered a variety of areas related to the properties of water and steam, seawater and the chemistry of power plants. A list of currently active ICRNs and closing statements on the progress made for those that have expired can be found on the IAPWS website.

А symposium entitled "Water and Steam: Energy Efficiency and Environmental Sustainability" was held on 29th Wednesday August 2017. The symposium included discussions on deep ocean temperatures, molecular simulation. modelling and design for



wet steam turbine stages. Several presentations were given focused on integrating advanced thermal power plants into the renewable energy infrastructure through coal gasification, CO₂ capture and ultra-supercritical power cycles. The IAPWS Helmholtz award lecture is

traditionally the cornerstone of the IAPWS Symposium. This year's award winner was Dr. Pavel Gotovtsev from the National Research Centre "Kurchatov Institute" in Russia. Dr. Gotovtsev was to present a talk entitled "Application of Machine Learning for Water Technologies - From Power Cycle Chemistry to Green Cities"; however, he was unable to attend the meeting. The IAPWS Helmholtz award is given annually to developing or early career scientists and engineers who are working in a field of interest to IAPWS. It includes an opportunity to attend the annual IAPWS meeting and to present the Helmholtz Award lecture.

The Executive Committee of IAPWS welcomed last year's new members New Zealand (Full Member), Egypt and China (Associate Members) and was pleased to have renewed participation from Italy (Associate Member). 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 17th International Conference on the Properties of Water and Steam (ICPWS), September 2nd through 7th, 2018 in Prague, Czech Republic (www.icpws2018.com). Further information on the conference and working group meetings can be found on the conference webpage or at the IAPWS website (www.iapws.org) respectively.

People interested in IAPWS documents and activities should contact the Chairs of their IAPWS National Committee (see the IAPWS website for contact details) or contact the IAPWS Executive Secretary, Dr. Barry Dooley, bdooley@IAPWS.org. People do not need to be citizens or residents of member countries to participate in IAPWS activities.



Group photo of the participants of the 2017 IAPWS meeting, Kyoto, Japan.

Chair:Mr. M. Sparrey, ABB Ltd., Oldends Lane, Stonehouse, Gloucestershire, UKVice-Chair:vacantSecretary:Dr M. Robson, RWE npower, Laboratory Building, TSG Ferrybridge, Knottingley, UKTreasurer:Mr H.W. Lloyd, UK

BIAPWS ANNUAL REPORT 2017

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 period from August 2016 to July 2017. A list of publications by BIAPWS members during this period is included in Appendix A. If you would like to know more about BIAPWS, please feel free to visit our web site www.biapws.org or e-mail BIAPWS at contact.us@biapws.co.uk.

2 BIAPWS MEMBERSHIP AND MEETINGS

BIAPWS membership remains strong, with current support provided by twenty-three industrial sponsors, six honorary members, five ordinary members and eleven corresponding members.

BIAPWS committee meetings are held three times a year and attendance at these continues to be good, typically with around thirty people present. A recent change has been to expand the technical sessions at BIAPWS committee meetings to add value to meeting attendance.

Industrial member's representatives are able to bring a colleague to the meetings to benefit from and contribute to the discussions.

3 BIAPWS POWER PLANT CHEMISTRY SYMPOSIUM

Each year, BIAPWS organises an annual symposia on power plant chemistry and water treatment. The 18^{th} in this series of symposia was held at the University of Warwick, Coventry, on 14 - 15 June 2017. The symposium consists of introductory sessions on the fundamentals of power plant chemistry and water treatment, followed by more detailed technical presentations. The event remains well supported, with around 100 delegates and 13 exhibition spaces taken up in 2017.

A copy of the symposium programme is included in Appendix B. A paper summarising the proceedings of the 2017 event has been published in Power Plant Chemistry journal.

4 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. At the 2017 IAPWS annual meeting in Kyoto, Japan, BIAPWS will be represented by M. Sparrey and Adam Caswell of EDF. In addition, BIAPWS is represented on the executive committee of IAPWS.

5 **BIAPWS AWARDS**

BIAPWS offers selected sponsorship opportunities for student placements and schools events that aim to raise the awareness and generate new interest amongst students in the areas of science and technology relevant to the properties of water and steam, including power plant chemistry. This initiative has in the past proven highly successful, with many previous winners of the BIAPWS Student Award going on to full time employment in power generation.

Over the last 12 months, BIAPWS received no opportunities for sponsorship in 2017.

6 BIAPWS WEBSITE

The public facing pages aim to promote a better understanding of what BIAPWS and IAPWS are and what our activities include. The member's area now includes a library of technical information for our members from BIAPWS meetings and symposia. Further developments are planned to include training resources.

7 BSI REPRESENTATION

BIAPWS is currently represented on the three British Standards and Euro Norm Committees listed below of relevance to power plant chemistry and water treatment. However, there have not been any significant developments in recent years.

- PVE/2: Water Tube and Shell Boilers. The UK standards committee has 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".
- CII/62: Treatment of water for boilers. The UK standards committee also has responsibility for BS 2486:1997: "Recommendations for Treatment of Water for Steam Boilers and Water Heaters".
- EH/3/6: Water quality sampling. The UK standards committee is responsible for BS 6068-6.7:1994 (ISO 5667-7:1993): "Guidance on Sampling of Water and Steam in Boiler Plants".

8 INTERACTION WITH PROFESSIONAL ORGANISATIONS

BIAPWS maintains correspondence with a number of professional bodies with the aim of sharing information and closer working.

- BIAPWS is represented on the Energy Sector Interest Group of the Royal Society of Chemistry by John Greene;
- BIAPWS is also represented on the Water Science Forum of the Royal Society of Chemistry by Eric Huff;
- Richard Hill, who is a committee member of the Institution of Chemical Engineers (IChemE) Water Subject Group, is also a Corresponding Member of BIAPWS.

Mike Sparrey Chair, British & Irish Association for the Properties of Water and Steam September 2017

APPENDIX A:

LIST OF UK AND IRELAND ORIGINATED REFERENCE PAPERS IN AREAS OF INTEREST. NO UPDATES CURRENTLY SUPPLIED IN 2017.

APPENDIX B:

WARWICK CONFERENCES The University of Warwick, Coventry, CV4 7AL UK http://www.warwickconferences.com/

Early bird registration fees are available until 31 March 2017

PROGRAMME

WEDNESDAY 14TH JUNE 2017, 12:00 - 17:00

INTRODUCTIONS TO POWER PLANT CHEMISTRY

- 12:00 Registration and Lunch
- 13:20 Welcome and introduction Mike Sparrey, Chair, BIAPWS
- 13:30 Session 1: New Nuclear Update
- Presenters: Ruth Oakley (EDF Energy Generation)

Presenter to be confirmed (Horizon Nuclear Power)

- Chair: Andy Rudge (EDF Energy Generation)
- 15:00 Break
- 15:30 Session 2: Amine Chemistry
- Presenters: Properties and Chemistry of Amines Alan Pomfret (GE Water)

Film-Forming Amines using the IAPWS Guidelines - Andre deBache (Kurita Europe)

- Chair: Andy Rudge (EDF Energy Generation)
- 17:00 Close
- 19:30 Evening meal and entertainment, Warwick Conferences

BIAPWS Symposium 2017 Final

BRITISH AND IRISH ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

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



THURSDAY 15TH JUNE 2017, 09:00 - 16:00

POWER PLANT CHEMISTRY AND CORROSION

08:30	Registration and Coffee	
09:00	Welcome and introduction	Mike Sparrey, Chair, BIAPWS
09:05	Exhibitor introductions	Mike Sparrey, Chair, BIAPWS
	Session 1	Chair: John Greene, Consultant
09:20	The Real Story on Steam Turbine Phase Transition Zone Damage	Barry Dooley, Structural Integrity Associates
09:50	CCGT Plant Preservation	Paul McCann, Uniper Technologies Ltd
10:20	Break	
10:50	Cation Conductivity Measurement by Electrodeionisation	Julie Gath, SWAN
11:20	Cooling Water pH Discharge Monitoring	Mark Robson, RWE Generation UK PLC
11:50	Open Discussion Session	
12:00	Lunch	
	Session 2	Chair: Eric Huff, BIAPWS
13:00	Session 2 A Recent History of the Advanced Gas Reactor (AGR) Pod Boilers	Chair: Eric Huff, BIAPWS Ellie Laney, EDF Energy Generation
13:00 13:30	Session 2 A Recent History of the Advanced Gas Reactor (AGR) Pod Boilers Off-Load Corrosion in AGR Reheaters – Summary of Investigative Work	Chair: Eric Huff, BIAPWS Ellie Laney, EDF Energy Generation Adam Caswell, EDF Energy Generation
13:00 13:30 14:00	Session 2 A Recent History of the Advanced Gas Reactor (AGR) Pod Boilers Off-Load Corrosion in AGR Reheaters – Summary of Investigative Work Break	Chair: Eric Huff, BIAPWS Ellie Laney, EDF Energy Generation Adam Caswell, EDF Energy Generation
13:00 13:30 14:00 14:30	Session 2 A Recent History of the Advanced Gas Reactor (AGR) Pod Boilers Off-Load Corrosion in AGR Reheaters – Summary of Investigative Work Break Four Years' Experience of Film-Forming Amine Treatment on a CCGT - The Analytical Chemistry Challenges and Achievements	Chair: Eric Huff, BIAPWS Ellie Laney, EDF Energy Generation Adam Caswell, EDF Energy Generation Bill Smith, Uniper, and John Greene, Consultant
13:00 13:30 14:00 14:30 15:00	Session 2 A Recent History of the Advanced Gas Reactor (AGR) Pod Boilers Off-Load Corrosion in AGR Reheaters – Summary of Investigative Work Break Four Years' Experience of Film-Forming Amine Treatment on a CCGT - The Analytical Chemistry Challenges and Achievements A Modern Approach to Monitoring and Controlling Boiler Chemistry	Chair: Eric Huff, BIAPWS Ellie Laney, EDF Energy Generation Adam Caswell, EDF Energy Generation Bill Smith, Uniper, and John Greene, Consultant Andrew Mosley and Mark Robson, RWE Generation UK PLC
13:00 13:30 14:00 14:30 15:00 15:30	Session 2 A Recent History of the Advanced Gas Reactor (AGR) Pod Boilers Off-Load Corrosion in AGR Reheaters – Summary of Investigative Work Break Four Years' Experience of Film-Forming Amine Treatment on a CCGT - The Analytical Chemistry Challenges and Achievements A Modern Approach to Monitoring and Controlling Boiler Chemistry Open Discussion Session	Chair: Eric Huff, BIAPWS Ellie Laney, EDF Energy Generation Adam Caswell, EDF Energy Generation Bill Smith, Uniper, and John Greene, Consultant Andrew Mosley and Mark Robson, RWE Generation UK PLC
13:00 13:30 14:00 14:30 15:00 15:30 15:55	Session 2 A Recent History of the Advanced Gas Reactor (AGR) Pod Boilers Off-Load Corrosion in AGR Reheaters – Summary of Investigative Work Break Four Years' Experience of Film-Forming Amine Treatment on a CCGT - The Analytical Chemistry Challenges and Achievements A Modern Approach to Monitoring and Controlling Boiler Chemistry Open Discussion Session Closing Remarks	Chair: Eric Huff, BIAPWS Ellie Laney, EDF Energy Generation Adam Caswell, EDF Energy Generation Bill Smith, Uniper, and John Greene, Consultant Andrew Mosley and Mark Robson, RWE Generation UK PLC Mike Sparrey, Chair, BIAPWS

BIAPWS 2017 Programme & Registration

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IAPWS Canadian National Committee

Annual Report 2017

Submitted to IAPWS EC, Kyoto, Japan, September 1, 2017

CNC Executive: William Cook (Chair); Derek Lister; Peter Tremaine; Melonie Myszczyszyn; Rich Pawlowicz; Steve McGee (CANDU Owners Group Representative, Treasurer), Craig Stuart.

1. Canadian National Committee: Dues for the Canadian National Committee (CNC) of IAPWS are supported by the National Research Council of Canada (NRC). 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 an initial five-year term, including travel support for the academic members of the CNC. In December 2012, COG agreed to another five-year term as the CNC's industrial sponsor (2013-2017). We are currently in the second year of an agreement with COG and the NRC for a third five-year term. Thanks to Steve McGee for ensuring the renewal proceeded smoothly.

The CNC recruited Dr. Craig Stuart, Senior Scientist – CNL, as Dr. Dave Guzonas' replacement so that CNL and the Canadian nuclear industry's interests continue to be well represented within IAPWS.

2. CNC Member Activities

2.1 Activities at the University of New Brunswick (UNB) <u>Derek Lister</u>

Heat exchanger fouling; the recirculating water loop built for studying deposit formation on heat-exchange surfaces has been refurbished with a new test section (including a simulated heat exchanger tube with a high heat-flux heater) and control system. A scoping study to assess the operation of the loop in sub-cooled boiling in the test section and the effect on magnetite particle deposition ended with heater burn-out; at the same time, the study using atomic-force microscopy to evaluate the forces between magnetite particles and bubble surfaces in water ended when the AFM became no longer available. Emphasis has switched to bench studies of adsorption of film-forming amines on magnetite with experiments on magnetite powder and sintered magnetite pellets.

Flow-accelerated corrosion (FAC); experiments on the effects of FFA on FAC are proceeding in two recirculating water loops. Under feedwater conditions at 140°C, a commercial product is being investigated for its efficiency in mitigating FAC with no pH additive in flows of different Reynolds numbers. The effect of the FFA on FAC in steam-water mixtures has been determined.

Modelling reactor primary circuit contamination; inserting FAC mechanisms and in-core effects into models for material transport has led to predictions of the transport of radioactive corrosion products in a CANDU primary coolant system. To translate the results to predictions of radiation field build-up, experiments are in progress to simulate and then verify by measurement the radiation field from radioactivated bundles of tubes in heat-exchanger configurations.

Developing a robust probe for measuring FAC in-situ in operating plant; three probes have been successively installed downstream of the boiler feed pump in a coal-fired power station. After analysis of the results from the first probe, refinements were made to the system before the second probe was installed. The third probe has been installed and removed while analysis of the results from the second has proved inconclusive because of the intermittent power production of the plant.

Verifying the effects of dissolved iron on FAC; experiments injecting iron into a coolant stream by promoting FAC upstream of an in-situ FAC probe are complete. The measured effects have been successfully described in terms of UNB's mechanistic model, indicating that the FAC rate is not directly proportional to the concentration of dissolved iron.

Measuring the effusion rate of hydrogen through steel; in a collaborative project with UNB's Centre for Nuclear Energy Research, the development of an in-situ probe (HEPro) for monitoring FAC by measuring the rate of effusion of corrosion hydrogen through pipe walls is being supported by investigating the details of hydrogen diffusion around the probe structure. Using a commercial CFD code, the pathways of diffusion into the probe have been visualised and the effect of the wall thickness of the probe evaluated. In collaboration with CNER, a project measuring the ingress of hydrogen into a steel undergoing FAC has already demonstrated that the phenomenon is different under reactor primary coolant conditions and feedwater conditions.

Electrochemical influences in FAC; an in-situ FAC probe in a high-temperature water loop is made the working electrode of a three-electrode system and the corrosion characteristics are separately investigated by electrochemical techniques. The project is currently investigating the phenomena in bent tubes.

Willy Cook

W. Cook has been Director of the Centre for Nuclear Energy Research (CNER), a research institute on UNB's campus, for the past two years. CNER has over two-decades of research / collaboration with the nuclear industry and has developed and patented online sensors for monitoring corrosion of plant piping insitu, HEPro. Additional field trials to show the utility of the sensors for nuclear power plants are currently in preparation. CNER continues to grow its consulting expertise and provides services to Canada's nuclear industry including active engagement with local nuclear power generating stations and Canadian Nuclear Laboratories.

Experience with the use of CNER's HEPro has demonstrated that it is very sensitive and can measure changes in FAC rate of carbon steel with subtle changes in system chemistry conditions. A program is currently underway to investigate the effects of IX resin replacement on iron concentration in the CANDU heat transport system and what affect this may have on FAC of the carbon steel outlet feeder pipes.

Hydrogen control in CANDU cooling systems is a project initiated in 2014 in conjunction with industrial collaborators. Current CANDUs have several nuclear auxiliary light water systems that are exposed to intense radiation fields. Suppression of water radiolysis and mitigation of hydrogen production in these systems using alternate oxygen scavenging chemicals to hydrazine is a primary goal. The experimental program is now complete and results demonstrate that corrosion processes on carbon steel can significantly affect the reaction kinetics and production from water radiolysis.

W. Cook and David Addison (Thermal Chemistry Inc. – New Zealand) were awarded an IAPWS International Collaboration project 2015. The focus of the project was to establish capabilities at UNB / CNER's laboratories to measure, electrochemically, the effects of mixed contaminants on boiler materials. D. Addison again visited UNB / CNER in May 2017 and the test rig was redesigned, relocated and recommissioned.

3.2. Activities at the University of Guelph (Peter Tremaine)

In 2016, Peter Tremaine was appointed to a newly created NSERC/UNENE Senior Industrial Research Chair in High Temperature Aqueous Chemistry. The objective is to expand mission-oriented basic research and modelling expertise at Guelph in areas related to primary coolant chemistry, moderator chemistry, steam generator chemistry and nuclear waste management. Recruitment of a tenure-track junior faculty member to address succession planning issues is in the final stages. In addition to UNENE, the industrial partners are the CANDU Owners Group, the Nuclear Waste Management Organization and the Electric Power Research Institute.

Other current and recent projects include (i) Solvation and Equilibria of Ions and Organic Solutes in Water up to Near-Critical Conditions (ii) CANDU Nuclear Reactor Chemistry: D₂O Isotope Effects on Acidbase Ionization and Metal Hydrolysis (UNENE/NSREC CRD Grant), (iii) Generation IV Nuclear Reactor Chemistry: Ion Pairs and Complexes in Sub-critical and Supercritical Water (NRCan/AECL/ NSERC CRD Grants), (iv) Carbon Capture and Sequestration by Novel Phase-Separating Solvents (NSERC International Strategic Grant with University Blaise Pascal, France)

3.3. Activities at the University of British Columbia (Rich Pawlowicz)

IAPWS-related activities continue to concentrate on investigations into the effect of chemical composition changes in seawater on its physical properties, and coordination of international activities in supporting and extending the seawater standard TEOS-10 through chairmanship of the Joint SCOR/IAPWS/IAPSO Committee on the Properties of Seawater (JCS).

Field measurements of "density anomaly": (1) Continued measurements of river anomalies were made in the Canadian Arctic Archipelago as part of a Canadian GEOTRACES rivers project (with H. Uchida and K. Brown)

3.4. CANDU Owner's Group (COG) Activities (Steve McGee)

COG is a not-for-profit corporation with voluntary funding from international CANDU-owning utilities and Canadian National Laboratories. The COG mission is to improve the performance of CANDU stations worldwide through member collaboration. COG Canadian R&D program members include Ontario Power Generation, Bruce Power Limited Partnership, New Brunswick Power and Canadian Nuclear Laboratories.

CANDU Industry-IAPWS Engagement

In September 2016, the COG Research and Development (R&D) Chemistry, Materials and Components Technical Committee members toured the laboratories of CNER and UNB which are instrumental in performing IAPWS research. Willy Cook and Peter Tremaine have participated in COG Chemistry Working Group meetings and COG workshops and have also provided input to the annual COG R&D planning process. W. Cook keeps the Working Group members informed of the Canadian IAPWS activities.

4. Activities Planned

The CNC activities over the next few years will continue the work that is currently ongoing, as described above.

An IAPWS CNC workshop for Canadian industry and academic stakeholders is in the planning stages for December 2017. The goal would be to raise the profile of the Canadian National Committee and IAPWS activities with researchers in Canada doing complementary research within the fossil and HRSG community. Topics included FFA/FFP use and modelling and simulation of aqueous energy production and extraction.

The CNC has started the planning process to host the 2019 IAPWS meetings. Preliminary scouting of locations has led to Banff, Alberta and we are now finalizing the dates, venue and arrangements.

Each of the CNC members and IAPWS-involved researchers in Canada are involved in industry-sponsored research with organizations such as EPRI and the CANDU Owners Group pertinent to topics of interest to IAPWS.

5. Select List of Publications

- 1. Pawlowicz, R., **Ocean Salinity**, Encyclopedia of Sustainable Technologies, Elsevier, 11pp, (accepted Dec/2016, in press).
- H. Arcis, J. Ferguson, G. Zimmerman, L. Applegarth, C. Pye, S. Sasidharanpillai, J. Cox, D. Hussey, D. Wells and P. Tremaine, Speciation and Thermodynamic Stability of Boric Acid, Borate and Polyborates under PWR Primary Coolant Conditions by AC Conductivity and Raman Spectroscopy, Nuclear Plant Chemistry NPC 2016, Brighton, UK, Oct. 2 to 7 (2-16).
- 3. H. Arcis, J.P. Ferguson, G.H. Zimmerman, and P.R. Tremaine, The Limiting Conductivity of the Borate Ion and its Ion-Pair Formation Constants with Sodium and Potassium under hydrothermal Conditions. *Phys. Chem. Chem. Phys.* **18**, 24081-24094 (2016).
- 4. H. Arcis, J.P. Ferguson, L.M.S.G.A. Applegarth, G. H. Zimmerman, and P. R. Tremaine, Ionization of Boric Acid in Water from 298 K to 623 K by AC Conductivity and Raman Spectroscopy. *J. Chem. Thermodyn.* **106** 187–198 (2017).
- 5. D.E. Nieto Roca, C.M. Romero and P.R. Tremaine, Ionization constants of DL-2-aminobutyric acid and DL-norvaline under hydrothermal conditions by UV-visible spectroscopy, *J. Solution Chem.* **46**, 388-423 (2017).
- J.P. Ferguson, H. Arcis, G.H. Zimmerman, and P.R. Tremaine Ion-Pair Formation Constants of Lithium Borate and Lithium Hydroxide under Pressurized Water Nuclear Reactor Coolant Conditions, *Ind. Eng. Chem. Research.* 56,8121-8132 (2017).
- C. McGregor, O. Fandino, J.S. Cox, K. Ballerat-Busserolles and P.R. Tremaine Standard Partial Molar Heat Capacities and Volumes of Aqueous N-Methylpiperidine and N-Methylpiperidinium Chloride from 283 K to 393 K. J. Chem. Thermodynamics 113, 377-387 (2017).
- 8. A.R. Lowe, J.S. Cox, P.R. Tremaine. Thermodynamics of Aqueous Adenine: Standard Partial Molar Volumes and Heat Capacities of Adenine, Adeninium Chloride, and Sodium Adeninate from T = 278.15 to 363.15 K. *J. Chem. Thermodynamics* **112**, 129-145 (2017).
- L. Applegarth, C. Pye, J.S. Cox, P.R. Tremaine. A Raman Spectroscopic and Ab Initio Investigation of Aqueous Boric Acid, Borate and Polyborate Speciation from 25 to 80 °C. *Ind. Eng. Chem. Research.* (Submitted).
- P. Tremaine, H. Arcis, L. Applegarth, J. Cox, J. Ferguson, C. Pye, S. Sasidharanpillai, G. Zimmerman; EPRI Project Managers D. Wells D. Hussey. Thermodynamic Properties and Structure of Boric Acid Species under PWR Coolant Conditions -Speciation of Aqueous Borate and Polyborates by AC Conductivity and Raman Spectroscopy up to 350°C *EPRI Technical Report* 3002008159 (2016)
- 11. Swift, R. and Cook, W.G., C. Bradley, R.C. Newman, *Validation of Constant Load C-ring Apex Stresses for SCC Testing in Supercritical Water*, Journal of Nuclear Engineering and Radiation Science, vol.3, no.2, pp. 021004-021004-7, March 2017.

- 12. Steeves, G. and Cook, W.G., *Development of Kinetic Models for the Long-term Corrosion Behaviour of Candidate Alloys for the Canadian SCWR*, Journal of Nuclear Engineering and Radiation Science, vol.3, no.3, pp. 031001-031000-7, July 2017.
- Lyons, J., Cook, W., Stuart, C. and Gardner, E., Synergistic Effects Between Radiation Chemistry and Carbon Steel Corrosion in the Calandria Vault and End Shield Cooling System of a CANDU Reactor, Proceedings of the 2017 Canadian Nuclear Society Annual Student Conference, Niagara Falls, June 2017.
- 14. Cook, W., Brown, G., Smith, B. and Thompson, P., *Status Update: Evolution of Radiation Fields in the Point Lepreau CANDU Reactor Following Refurbishment*, Proceedings of the 2017 Canadian Nuclear Society Annual Conference, Niagara Falls, June 2017.
- 15. Cook, W., Brown, G., Smith, B. and Stuart, C., *Evolution of Radiation Fields in the Point Lepreau CANDU Reactor Following Refurbishment*, Nuclear Plant Chemistry Conference (NPC 2016), Brighton, UK, October 2016.
- 16. Stuart, C., Lee, J., Gardner, E. and Cook, W., *Steam Cycle Contamination and Remediation following the Refurbishment Outage at the Point Lepreau Generating Station*, Nuclear Plant Chemistry Conference (NPC 2016), Brighton, UK, October 2016.
- 17. Lyons, J., Cook, W., Stuart, C. and Gardner, E., *Synergistic Effects Between Radiation Chemistry and Carbon Steel Corrosion in the Calandria Vault and End Shield Cooling System of a CANDU Reactor*, Nuclear Plant Chemistry Conference (NPC 2016), Brighton, UK, October 2016.
- S. Mahboubi, Y, Jiao, W. Cook, W. Zheng, D. Guzonas, G. Botton, J. Kish, Stability of Chromia (Cr2O3)-Based Scales Formed During Corrosion of Austenitic Fe-Cr-Ni Alloys in Flowing Oxygenated Supercritical Water, Corrosion, v 72, n 9, p 1170-1180, September 2016.
- Uchida, S., Naitoh, M., Okada, H., Hanawa, S. and Lister, D.H. (2016). "Effects of Oxide Film on ECP and Corrosion of Steel." Proc. EUROCORR2016, Annual Congress European Federation of Corrosion, Montpellier, France, (September 11-15).
- Lister, D.H. (2016). "Studies on Two-phase FAC; Modelling and Effects of Amine Breakdown Products". Power Cycle Chemistry Working Group, IAPWS 2016 Annual Meeting, Dresden, Germany, (Sept. 11-16).
- Mohajery, K., Liu, L., Lister, D.H. and Uchida, S. (2016). "Flow-Accelerated Corrosion in Two-phase Steam-Water Flows: Experiments and Modelling". Proc. 20th International Conference on Water Chemistry of Nuclear Reactor Systems, Brighton, UK. Nucl. Inst. (October 2-7).
- Palazhchenko, O.Y. and Lister, D.H. (2016) "The Impact of Crud Behaviour on the Predictions of Activity Transport in CANDU-6 Reactors", Proc. 20th International Conference on Water Chemistry of Nuclear Reactor Systems, Brighton, UK. Nucl. Inst. (October 2-7).

REPORT on IAPWS-related activities: May 2016 – May 2017

submitted by the

Czech National Committee for the Properties of Water and Steam (CZ NC PWS) to the Executive Committee Meeting of 2017 IAPWS Meeting, Kyoto, Japan, September 2017

National Committee | Contact

CZ NC PWS Institute of Thermomechanics of the CAS, v. v. i. Dolejškova 1402/5, 182 00 Praha Czech Republic Fax: +420 286 584 695 E-mail: secr.czncpws@it.cas.cz Committee Chairman: Dr. Tomáš Němec (nemec@it.cas.cz)

Participating institutions

The following Czech Institutions participated in the research of thermophysical properties and chemical processes between May 2016 and May 2017:

Institute of Thermomechanics of the CAS, v. v. i., ("IT CAS"), 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"), Department of Power Engineering ("ICT-DPE") and Department of Physical Chemistry ("ICT-DPC"), 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

DOOSAN ŠKODA POWER, Plzeň, Inc., Tylova 57, CZ-316 00 Plzeň

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

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

University of South Bohemia ("USB"), Faculty of Science, Branišovská 31A, CZ-370 05 České Budějovice

The founder of CZ NC PWS is the Czech Academy of Sciences.

The activities described below were sponsored by the Czech Science Foundation (GAČR), DOOSAN 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 2014-2017:

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

List of IAPWS-Related Activities

The international collaboration between CZ NC PWS and IAPWS was funded from the project of IT CAS and TUL sponsored by MŠMT since 2016 (project no. LG15040). The project support will end on 31/12/2017.

Dr. Hrubý and Dr. Vinš (IT CAS) and their collaborators from IT CAS, UWB, USB and abroad continued their experimental investigation of surface tension of supercooled water [1,2].

Dr. Hrubý (IT CAS) has completed a multi-year collaborative project with a group of molecular spectroscopists and quantum chemists focused on calculation of properties of water molecules composed of ¹H [3] and deuterium ²H [4] and three isotopes of oxygen, ¹⁶O, ¹⁷O, and ¹⁸O. The resulting thermodynamic data replaces previous data that were several decades old. The uncertainty of the new data in the technically most relevant temperature range up to 1,000°C is much smaller than the uncertainty of any thinkable thermodynamic measurement. The new data has already been used for the development of the new IAPWS equation of state for heavy water.

Assoc. Prof. Kolovratník (CTU) and Dr. Bartoš (CTU/IT CAS) carried out pneumatic and optical measurements of a wet steam flow upstream of the last stage of a nuclear-power-station steam turbine [5-9]. On September 12-14, 2016, the Wet Steam Conference 2016 was held at the Faculty of Mechanical Engineering of Czech Technical University.

Prof. Šafařík (CTU) had a Keynote Lecture on the speed of sound in steam [10] and published a book on thermodynamics of moist air [11].

Dr. Sedlář (SIGMA) and his collaborators studied cavitation erosion in water pumps and the problem of cavitation instabilities under hydrodynamic conditions [12, 13].

The team of Prof. Šedlbauer (TUL) published a paper [14] on chemical and biological process engineering and Prof. Majer (TUL) studied solubility data on correlation of solubility [15-16].

The team of Assoc. Prof. Hnědkovský (ICT-IPC) studied thermodynamic properties of aqueous solutes in water [17-24].

References

- Vinš V., Hošek J., Hykl J., Hrubý J.: Experimental Data for the Surface Tension of Supercooled Water Measured with a Horizontal Capillary Tube, Asian Thermophysical Properties Conference (ATPC) 2016, Yokohama (Japan), October 2-4, 2016.
- [2] Vinš V., Harvey A., Hellmuth O., Holten V., Hrubý J., Kalová J., Mareš R., Pátek J.: Report of Task Group on Surface Tension of Ordinary Water – 2016, Annual IAPWS Meeting, Dresden (Germany), September 12, 2016.
- [3] Furtenbacher T., Szidarovszky T., Hrubý J., Kyuberis A.A., Zobov N.F., Polyansky O.L., Tennyson J., Czsászár A.G.: Definitive Ideal-Gas Thermochemical Functions of the (H2O)-O-16 Molecule. Journal of Physical Chemical Reference Data 45, 2016, 043104
- [4] Simko I., Furtenbacher T., Hrubý J., Zobov N.F., Polyansky O.L., Tennyson J., Gamache R.R., Szidarovszky T., Dénes N., Czászár A.G.: Recommended Ideal-Gas Thermochemical Functions for Heavy Water and its Substituent Isotopologues. Journal of Physical Chemical Reference Data 46, 2017 023104
- [5] Hoznedl M., Kolovratník M.,Sedlák K., Bednář L., Kalista R., Bartoš O., Mrózek L.: Flow Conditions at the Last Stage and in the Exhaust Hood of the Turbine 1090 MW for Saturated Steam. In : Proceedings of the Wet Steam Conference in Prague, 2016, pp.102-116
- [6] Kolovratník M.: Evolution of Steam in Steam Turbines, Conference on Turbomachines, Pilsen, 2016 (in Czech)
- [7] Kolovratník M., Yun K., Bartoš O.: Control of the Probe Influence on the Flow Field in LP Steam Turbine. In Proceedings of the International Conference Experimental Fluid Mechanics 2016. Liberec, 2016, pp. 344-348
- [8] Hrubý J., Duška M., Němec T., Kolovratník M.: Consistency of Empirical Corrections of the Classical Nucleation Theory for Nucleation in Steam with Nucleation Experiments and Molecular Simulations. In : Proceedings of the Wet Steam Conference in Prague, 2016, pp. 182-200
- [9] Bartoš O., Hrubý J., Kolovratník M.: Experimental Research of Heterogeneous Nuclei in Expansion Chamber. In : Proceedings of the Wet Steam Conference in Prague, 2016, pp.240-245
- [10] Šafařík P.: On Speed of Sound in Steam, Conference ANSYS 2017, Svratka, 2017 (in Czech)
- [11] Šafařík P., Vestfálová M.: Thermodynamics of Moist Air, CTU Publishing House, 2017 (in Czech)
- [12] Sedlář, M., Ji, B., Krátký, T., Rebok, T., Huzlík, R.: Numerical and Experimental Investigation of Three-Dimensional Cavitating Flow around a Straight NACA2412 Hydrofoil. Ocean Engineering, 123, 2016, pp. 357-382.
- [13] Volkov, A.V., Parygin, A.G., Naumov, A.V., Vikhlyantsev, A.A., Šoukal, J., Sedlář, M., Komárek, M.: Influence of Hydrophobization of Impellers of Centrifugal Pumps on Their Operating Characteristics. Thermal Engineering, Vol. 63, 2016, pp. 841-847.
- [14] Janos P., Agapovova E., Fikarova J., Sedlbauer J., Janos P.(Jr.): Biosorption of Sulfonic Azodyes on Spruce Wood Shavings: Kinetics and Sorption Mechanisms. Environmental Engineering and Management Journal, 15, 2016, pp.2671-2680.
- [15] Majer V.: Solubility data of H₂S in H₂O and NaCl(aq) over a wide range of temperature and pressure; experimental data and correlation scheme, Annual IAPWS Meeting, Dresden (Germany), September 12, 2016.

- [16] Akinfiev N.N., Majer V., Shvarov, Ju.V.: Thermodynamic description of H₂S-H₂O-NaCl solutions at temperatures to 573 K and pressures to 40 MPa,, Chemical Geology, 2016, 424, pp.1-11.
- [17] Hu, B., Hnedkovsky, L., Hefter, G.: Densities and Apparent Molar Volumes of Aqueous Solutions of Li2SO4 and LiCF3SO3 at Temperatures from 293 to 343 K, Journal of Chemical and Engineering Data, 61 (10), 2016, pp. 3618-3626.
- [18] Hu, B., Hnědkovský, L., Hefter, G.: Heat Capacities of Aqueous Solutions of Lithium Sulfate, Lithium Perchlorate, and Lithium Trifluoromethanesulfonate at 298.15 K, Journal of Chemical and Engineering Data, 61 (6), 2016, pp. 2149-2154.
- [19] Hu, B., Hnedkovsky, L., Li, W., Hefter, G.: Densities and Molar Volumes of Aqueous Solutions of LiClO4 at Temperatures from 293 K to 343 K, Journal of Chemical and Engineering Data, 61 (4), 2016, pp. 1388-1394.
- [20] Cibulka, I.: Partial Molar Volumes of Organic Solutes in Water. XXVII. Two Aliphatic Polyethers (Triglyme, Tetraglyme) at Temperatures T = 298-573 K and Pressures up to 30 MPa, Journal of Chemical Thermodynamics, 101, 2016, pp. 78-83.
- [21] Cibulka, I.: Partial Molar Volumes and Partial Molar Isentropic Compressions of Four Poly (Ethylene Glycols) at Infinite Dilution in Water at Temperatures T = (278 to 343) K and Atmospheric Pressure, Journal of Chemical and Engineering Data, 61 (2), 2016, pp. 748-759.
- [22] Slavíček, P., Kryzhevoi, N.V., Aziz, E.F., Winter, B.: Relaxation Processes in Aqueous Systems upon X-ray Ionization: Entanglement of Electronic and Nuclear Dynamics, Journal of Physical Chemistry Letters, 7 (2), 2016, pp. 234-243.
- [23] Kolafa, J.: Solubility of NaCl in Water and Its Melting Point by Molecular Dynamics in the Slab Geometry and a New BK3-Compatible Force Field, Journal of Chemical Physics, 145 (20), Art. No. 204509, 2016.
- [24] Ondo, D.: Calorimetric Study on the Interaction of Didecyldimethylammonium and Decyltrimethylammonium Cations with Native Cyclodextrins in Water, Journal of Chemical Thermodynamics, 97, 2016, pp. 235-243.

Report On Egyptian National Committee Status and Activities Q4-2016 / Q3-2017

1. Purpose of the report

The purpose of this report is to present the status and activities of Egypt's national committee during 2017 as well as plans for 2018.

2. Importance of National Committee to Egypt

With the current expansion in power generating facilities in Egypt, building national capacity in the field of properties of water and steam specially the power cycle chemistry becomes mandatory in order to maintain and improve performance of this plants and to form a national forum for discussion and research. Egypt by 2020 will reach about 80,000 MW generating capacity, also there is a plan for coal fired complex and Nuclear power complex. We believe that the Egyptian NC will become the window for international collaboration in these fields.

3. Activities during 2017

After Dresden meeting we start to prepare a plan for promoting to our initiative of joining IAPWS and establishing our national committee. Communication started within electricity sector and a lot of correspondence and calls made to arrange for meeting and seminars.

It was decided to focus with Electricity sector to accelerate the start of NC and later will continue our initial plan for communicating other universities and research institutes. Many seminars arranged to promote to NC and illustrate the initiative as well as provide technical sessions about selected IAPWS's TGDs. The following is a list of activities made during 2017:

a. PGESCo seminar

- Location : Cairo
- Date : 8th of May 2017
- Attendance: 39 of Sector heads and plants mangers



b. <u>UEEPC Seminar</u>

- Location : Kuriemat
- Date: 11th of July 2017
- Attendance: 29 of Plant's managers, chemists and operators within UEEPC




c. <u>WDEPC seminar</u>

- Location : Alexandria
- Date : 18th of July 2017
- Attendance : + 17 of Plant's managers, chemists and operators
- Attendees from power generation research department





d. CEPC seminar

- Location : Cairo North Power Station
- Date 25th July 2017
- Attendance : +29
- Plant's managers, chemists and operators



During all of the four seminars the following presentation is made:

- Introduction about IAPWS
- Initiative Of Obtaining IAPWS Membership For Building National Capability
- Egypt's IAPWS committee
- Technical discussion on TGD3-10(2015)
- Technical discussion on TGD4-11(2015)
- Technical discussion on TGD5-13

-

4. Plans for 2018

In 2018 we will continue our promoting effort and already arranged another two seminars to MDEPC and EDEPC.

Also we planned to list of activities in order to finalize establishment of NC in 2018 and to run it activities. The following list of planned activities:

- Conduct more seminars and travel to everyone has an interest of NC
- Prepare more technical session on IAPWS's TGDs
- Finalize an application form of national committee
- Finalize legal issues
- Maintain bank account
- Set a communication channel with members
- Arrange for the 1st meeting and announce of NC establishment

German National Committee to IAPWS Executive Committee

Research Activities on the Thermodynamic Properties of Water and Steam of the German National Committee in the Period 2016/2017

www.iapws.de

Chair: Ingo Weber, Siemens Power and Gas, Erlangen

Vice Chair: Prof. Dr. Hans-Joachim Kretzschmar, Zittau/Goerlitz University of Applied Sciences, Zittau

Annual Meeting of the German National Committee

The 2017 Annual Meeting of the German National Committee took place at the Helmut Schmidt University in Hamburg on 17th March 2017. 25 Colleagues attended this meeting. Six papers were presented in the scientific session.

In the following, activities of certain members of the German National committee are summarized.

Baltic Sea Research Institute, Warnemuende Dr. Rainer Feistel

Projects

- 1. Development of a draft Advisory Note No. 6: "Relationship between Various IAPWS Documents and the International Thermodynamic Equation of Seawater 2010 (TEOS-10)".
- 2. Preparation of a paper about Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air to be submitted to an international journal.
- 3. Preparation of a paper about unleashing empirical equations using nonlinear fitting & GUM tree calculator (published in Int. J. Thermophys.).
- 4. Preparation of a paper toward a fundamental definition on relative humidity (published in Metrologia).

Recent Publications

 Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.: Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air.

N.N. (2017), in preparation.

- Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.: Digital Supplement to "Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air". N.N. (2017), in preparation.
- Lovell-Smith, J. W.; Saunders, P.; Feistel, R.: Unleashing Empirical Equations with "Nonlinear Fitting" and "GUM Tree Calculator". Int. J. Thermophys. 38 (2017), 148. DOI 10.1007/s10765-017-2282-y

- Feistel, R.; Lovell-Smith, J. W.: Defining relative humidity in terms of water activity. Part 1: definition. Metrologia 54 (2017) 566-576. https://doi.org/10.1088/1681-7575/aa7083
- o Feistel, R .:

Salzgehalt des Meeres und relative Feuchte der Luft: Rolle im Klima-system und Probleme ihrer Definition. Vortrag in der Klasse für Naturwissenschaften und Technikwissenschaften am 10. 11. 2016.

Zeitschrift der Leibniz-Sozietät e. V. Leibniz Online 25 (2017). https://leibnizsozietaet.de/wp-content/uploads/2017/01/Feistel.pdf

• Feistel, R.; Lovell-Smith, J. W.:

Uncertainty propagation using dispersion matrices accounting for systematic error in least-squares regression.

Metrologia 54 (2017), submitted.

• IAPWS:

Relationship between Various IAPWS Documents and the International Thermodynamic Equation of Seawater – 2010 (TEOS-10).

The International Association for the Properties of Water and Steam (2016). Available at http://www.iapws.org.

Highlight 2016 in the journal "Metrologia":

 Feistel, R.; Wielgosz, R.; Bell, S. A.; Camões, M. F.; Cooper, J. R.; Dexter, P.; Dickson, A. G.; Fisicaro, P.; Harvey, A. H.; Heinonen, M.; Hellmuth, O.; Kretzschmar, H.-J.; Lovell-Smith, J. W.; McDougall, T. J.; Pawlowicz, R.; Ridout, P.; Seitz, S.; Spitzer, P.; Stoica, D.; Wolf, H.: Metrological challenges for measurements of key climatological observables: Oceanic salinity and pH, and atmospheric humidity. Part 1: Overview. Metrologia 53 (2016), R1-R11, doi: 10.1088/0026-1394/53/1/R1.

Lovell-Smith, J. W.; Feistel, R.; Harvey, A. H.; Hellmuth, O.; Bell, S. A.; Heinonen, M.; Cooper, J. R.:

Metrological challenges for measurements of key climatological observables. Part 4: Atmospheric relative humidity.

Metrologia 53 (2016), R40-R59, doi: 10.1088/0026-1394/53/1/R40.

German Aerospace Center (DLR), Cologne Institute of Propulsion Technology Prof. Dr. Francesca di Mare

Project

- 1. Implementation of the Fast Steam Property Algorithms Based on Spline Interpolation into the CFD Code TRACE.
 - The "IAPWS Guideline on the Fast Calculation of Steam and Water Properties in Computational Fluid Dynamics Using the Spline-Based Table Look-Up Method (SBTL)" has been implemented into the CFD code TRACE.
 - On this basis the implementation has been further improved, especially regarding the software architecture, solution algorithm and boundary treatment.

• The capability of the SBTL-method has been tested on Laval-nozzle and Cascade test cases. The calculation of a real steam engine configuration is targeted next.

Recent Publications

Kunick, M.; Kretzschmar, H.-J.; Gampe, U.; di Mare, F.; Hrubý, J.; Duška, M.; Vinš, V.; Singh, A.; Miyagawa, K.; Weber, I.; Pawellek, R.; Novi, A.; Blangetti, F.; Wagner, W.; Friend, D. G.; Harvey, A. H.:
Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL),
J. Eng. Gas Turbines Power, in preparation.

Helmholtz Centre for Environmental Research – UFZ, Magdeburg PD Dr. Bertram Boehrer

Project

1. Properties of limnic waters and effect on circulation of lakes.

Recent Publications

 Moreira, S., Schultze, M., Rahn, K., Boehrer, B.: A practical approach to lake water density from electrical conductivity and temperature. Hydrol. Earth Syst. Sci. 20 (2016), 2975-2986. doi: 10.5194/hess-20-2975-2016

Leibniz Institute for Tropospheric Research, Leipzig Dr. Olaf Hellmuth

Projects

- 1. Investigation on Virial Approximation for Humid Air
- 2. Preparation of a Paper about Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air
- 3. Preparation of Three Further Volumes on New Particle Formation in the Earth Atmosphere

Recent Publications

 Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.: Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air.

N.N. (2017), in preparation.

 Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.: Digital Supplement to "Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air". N.N. (2017), in preparation.

Physikalisch-Technische Bundesanstalt Braunschweig und Berlin, Braunschweig Dr. Henning Wolf

Highlight 2016 in the journal "Metrologia":

 Feistel, R.; Wielgosz, R.; Bell, S. A.; Camões, M. F.; Cooper, J. R.; Dexter, P.; Dickson, A. G.; Fisicaro, P.; Harvey, A. H.; Heinonen, M.; Hellmuth, O.; Kretzschmar, H.-J.; Lovell-Smith, J. W.; McDougall, T. J.; Pawlowicz, R.; Ridout, P.; Seitz, S.; Spitzer, P.; Stoica, D.; Wolf, H.: Metrological challenges for measurements of key climatological observables: Oceanic salinity and pH, and atmospheric humidity. Part 1: Overview. Metrologia 53 (2016), R1-R11, doi: 10.1088/0026-1394/53/1/R1.R

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

Projects:

- 1. Improvement of accurate models available for CCS-relevant mixtures. Within this project humid mixtures are of particular interest, since existing models from the GERG-2008 package for natural gases are not designed for higher concentrations of water. A first version of this new-mixture model was published in Journal of Chemical Thermodynamics (Gernert and Span, 2016). Software enabling the application of the latest version of our property models has been made available and is by now used by more than 80 groups worldwide (both in academia and in industry). Current work addresses an improved description of less well measured minor mixtures. In conjunction with the Norsk Research Center on CCS (NCCS) a project has been granted, which will provide funding for continued work on this subject.
- 2. The work on models describing hydrate formation has been continued in cooperation with Dr. V. Vinš and Dr. J. Hruby. S. Hielscher continues the work at RUB as Ph.D. candidate. Andreas Jäger has changed to TU Dresden, where he involves the institute of Technical Thermodynamics headed by Prof. Cornelia Breitkopf into the work on hydrates. Three journal articles describing the latest status of the hydrate model in detail were published (Vinš *et al.*, 2016, 2017; Jäger *et al.*, 2016).
- 3. Development of a new reference equation of state for heavy water. This work is linked to an IAPWS grant awarded in 2012 and to a close cooperation with Dr. A. H. Harvey and Dr. E. W. Lemmon at NIST in Boulder, CO. The work on the new equation of state has largely been finished. A draft release will be submitted to the evaluation task group and will be presented at the 2017 IAPWS meeting in Kyoto.

Recent Publications

o Gernert, J.; Span, R.:

EOS-CG: A Helmholtz energy mixture model for humid gases and CCS mixtures. J. Chem. Thermodyn. 93 (2016), 274-293.

 Vinš, V.; Jäger, A.; Span, R.; Hrubý, J.: Model for gas hydrates applied to CCS systems part I. Parameter study of the van der Waals and Platteeuw model. Fluid Phase Equilib. 427 (2016), 268-281.

- Vinš, V.; Jäger, A.; Hrubý, J.; Span, R.: Model for gas hydrates applied to CCS systems part II. Fitting of parameters for models of hydrates of pure gases. Fluid Phase Equilib. 435 (2017), 104-117.
- Jäger, A.; Vinš, V.; Span, R.; Hrubý, J.: Model for gas hydrates applied to CCS systems part III. Results and implementation in TREND 2.0. Fluid Phase Equilib. 429 (2016), 55-66.

Ruhr University Bochum Faculty of Mechanical Engineering, Chair of Thermodynamics Prof. em. Dr. Dr. e. h. Wolfgang Wagner

Project

1. Preparation of the 3rd edition of the book "International Steam Tables".

Recent Publications

Kunick, M.; Kretzschmar, H.-J.; Gampe, U.; di Mare, F.; Hrubý, J.; Duška, M.; Vinš, V.; Singh, A.; Miyagawa, K.; Weber, I.; Pawellek, R.; Novi, A.; Blangetti, F.; Wagner, W.; Friend, D. G.; Harvey, A. H.:

Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL),

J. Eng. Gas Turbines Power, in preparation.

Siemens Energy Solutions, Erlangen Michael Rziha

Projects

- 1. Development of new Technical Guidance Documents:
 - Application of Film Forming Amines in Fossil, Combined Cycle, and Biomass Power Plants Released 2016 in Dresden
 - HRSG High Pressure Evaporator Sampling for Internal Deposit Identification and Determining the Need to Chemical Clean – Released 2016 in Dresden
- 2. Developing of drafts for a new technical guidance documents
 - Monitoring Corrosion Products in Flexible (cycling and two-shifting) Plants. White paper is developed for presentation at the 2017 Meeting. TGD will be further developed based on this input.
 - Ensuring the Integrity and Reliability of Demineralized Makeup Water Supply to the Unit Cycle. Skeleton and list of contents is finalized. Further progress will be discussed during 2017 meeting.
 - Air In-Leakage in Steam Water Cycles. White paper in preparation.
 - Film Forming Products. Following the release of the IAPWS TGD on FFP for Fossil and Combined Cycle Plants and the IAPWS International Conference on FFP in Lucerne, IAPWS will be developing two new TGD on FFP:
 - a) Application of Film Forming Products in Nuclear Plants. The Task Group will have a working session during the Kyoto week.

- b) Application of Film Forming Products in Industrial Plants.
- Aspects of Geothermal Steam Chemistry. A White Paper for the 2017 Meeting is in preparation. This will be used to determine if a TGD can be developed.

Siemens Energy Solutions, Erlangen Ingo Weber, Stefan Bennoit, Julien Bonifay

Projects

- 1. Implementation of the fast steam property spline-interpolation algorithms into the heat cycle simulation code KRAWAL
 - The "IAPWS Guideline on the Fast Calculation of Steam and Water Properties in Computational Fluid Dynamics Using the Spline-Based Table Look-Up Method (SBTL)" has been implemented into the heat cycle code KRAWAL which is used worldwide by Siemens.
 - The computing time consumption of KRAWAL has been significantly reduced.
- 2. Implementation of the fast steam property spline-interpolation algorithms into the non-stationary power-plant simulation code DYNAPLANT
 - The "IAPWS Guideline on the Fast Calculation of Steam and Water Properties in Computational Fluid Dynamics Using the Spline-Based Table Look-Up Method (SBTL)" has been implemented into the non-stationary power-plant simulation code DYNAPLANT.
 - The computing time consumption of DYNAPLANT has been significantly reduced.

Recent Publications

Kunick, M.; Kretzschmar, H.-J.; Gampe, U.; di Mare, F.; Hrubý, J.; Duška, M.; Vinš, V.; Singh, A.; Miyagawa, K.; Weber, I.; Pawellek, R.; Novi, A.; Blangetti, F.; Wagner, W.; Friend, D. G.; Harvey, A. H.:

Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL),

J. Eng. Gas Turbines Power, in preparation.

STEAG Energy Services, Zwingenberg Dr. Reiner Pawellek, Dr. Tobias Löw

Project

- 1. Implementation of the fast steam property spline-interpolation algorithms into the heat cycle simulation code EBSILON
 - The "IAPWS Guideline on the Fast Calculation of Steam and Water Properties in Computational Fluid Dynamics Using the Spline-Based Table Look-Up Method (SBTL)" has been implemented into the heat cycle code EBSILON which is used worldwide by the power industry.
 - The computing time consumption of EBSILON has been significantly reduced.

Recent Publications

Kunick, M.; Kretzschmar, H.-J.; Gampe, U.; di Mare, F.; Hrubý, J.; Duška, M.; Vinš, V.; Singh, A.; Miyagawa, K.; Weber, I.; Pawellek, R.; Novi, A.; Blangetti, F.; Wagner, W.; Friend, D. G.; Harvey, A. H.:

Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL),

J. Eng. Gas Turbines Power, in preparation.

Zittau/Görlitz University of Applied Sciences Department of Technical Thermodynamics Prof. Dr. Hans-Joachim Kretzschmar, Dr. Sebastian Herrmann, Matthias Kunick

Projects

- 1. Development of fast property calculation algorithms based on spline interpolation
 - The Spline-Based Table Look-Up Method (SBTL) is being applied to the mixture humid air.
- 2. Application of the developed SBTL method for calculating thermodynamic properties

The developed spline-based property libraries have been implemented into the following process simulation codes:

- Non-stationary thermo-hydraulic codes SubChanFlow and TwoPorFlow of the Karlsruhe Institute of Technology KIT
- o Non-stationary thermo-hydraulic code RELAP-7 of the Idaho National Laboratory INL
- o Heat-cycle simulation program EBSILON of STEAG Energy Services
- o Heat-cycle simulation program KRAWAL of Siemens Energy Solutions
- o Non-stationary heat-cycle simulation program DYNAPLANT of Siemens Energy Solutions.
- 3. Development of algorithms for the transport properties of moist air, ASHRAE Research Project 1767.
- 4. Preparation of a new ASHRAE standard for calculating moist air properties, ASHRAE Project SPC 213P.
- 5. Reworking on the 3rd edition of the book "International Steam Tables".

Recent Publications

- Kunick, M.; Berry, R. A.; Martineau, R. C.; Kretzschmar, H.-J.; Gampe, U.: Application of the new IAPWS Guideline on the fast and accurate calculation of steam and water properties with the Spline-Based Table Look-Up Method (SBTL) in RELAP-7. Kerntechnik 82/3 (2017), 264-279.
- Herrmann, S.; Kretzschmar, H.-J.; Gatley, D. P.: In: 2017 ASHRAE HANDBOOK FUNDAMENTALS, SI and I-P Editions, Chapter 1 PSYCHROMETRICS, Table 2 Thermodynamic Properties of Moist Air at Standard Atmospheric Pressure. Table 3 Thermodynamic Properties of Water at Saturation. American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., Atlanta, GA (2017), ISBN 978-1-939200-58-0. www.ashrae.org
- Kunick, M.; Kretzschmar, H.-J.; Gampe, U.; di Mare, F.; Hrubý, J.; Duška, M.; Vinš, V.; Singh, A.; Miyagawa, K.; Weber, I.; Pawellek, R.; Novi, A.; Blangetti, F.; Wagner, W.; Friend, D. G.; Harvey, A. H.:
 Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL).

J. Eng. Gas Turbines Power, in preparation.

o Kunick, M.:

Fast Calculation of Thermophysical Properties in Extensive Process Simulations with the Spline-Based Table Look-Up Method (SBTL).

Fortschritt-Berichte VDI, in preparation.

- Vogel, E., Herrmann, S.: New Formulation for the Viscosity of Propane. J. Phys. Chem. Ref. Data 45 (2016), 043103.
- Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.: Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air.

N.N. (2017), in preparation.

 Hellmuth, O.; Feistel, R.; Lovell-Smith, J. W.; Kalová, J.; Kretzschmar, H.-J.; Herrmann, S.: Digital Supplement to "Virial Approximation of the TEOS-10 Equation for the Enhancement Factor of Water in Humid Air". N.N. (2017), in preparation.

Current Status of Research Activities in Japan Submitted to the Executive Committee Meeting, IAPWS, Kyoto, Japan, August 2017

Japanese National Committee, Chaired by Professor Masaru Nakahara International Association for the Properties of Water and Steam c/o The 139th Committee on Steam Properties Japan Society for the Promotion of Science (JSPS) 5-3-1, Kojimachi, Chiyoda-ku Tokyo 102-0083, Japan

I. Overview:

The Japan National Committee, supported by JSPS, of IAPWS continues to endeavor to make closer and innovative interactions between engineering and academic groups with respect to the international and domestic energy-related issues. The key points are cleaner, greener, and more sustainable energy as well as high efficiency and safety. We are discussing about the science and engineering of fuels, boilers, turbines, and water-treatment. Now we take it into account the power generation from geothermal and biomass energies. Our activities in the publication are shown below.

II. Recent Publications:

Nakahara, Masaru

Professor Emeritus of Kyoto University, Institute for Chemical Research email: nakahara@scl.kyoto-u.ac.jp

- Nakahara, M.; Yoshida K.; "Chronological Scientific Tables 2017", pp.502-509, 514-517, Maruzen Publishing Co., Ltd., Tokyo, ISBN 978-4-621-30096-1 (2016).
- [2] Yoshida, K.; Matubayasi, N.; Nakahara, M.; Uosaki, Y.; "Effect of Rotation on Vibrational Spectrum of Supercritical Water: Analysis of Dependencies on Density and Hydrogen Isotopes", *The Review of High Pressure Science and Technology*, 26, 323-332 (2016).
- [3] Nakahara, M.; Yoshida K.; "Handbook of Scientific Tables", Maruzen Publishing Co., Ltd., Tokyo and World Scientific Publishing Co, Singapore, in press.

Hirano, Hideo

Retired Senior Research Scientist, Central Research Institute of Electric Power Industry e-mail: hhirano0879@jcom.home.ne.jp

- [1] Hirano, H.; Shimokado, T; Kamisasa, M; "Trend of The Water Conditioning for Boiler Water : Application of New Volatile Treatments AVT(LO) and AVT(O)", Boiler Yearbook, 2016 year editions, Japan Boiler Association, pp. 44-54 (2016). (In Japanese)
- [2] Hirotaka, K.; Hirano, H.; Katsumura, Y; et al., "BWR Water Chemistry Guidelines and PWR Primary Water Chemistry Guidelines in Japan – Purpose and Technical Background", *Nuclear Engineering* and Design, 309, 161-174 (2016).

Yasuoka, Kenji

Professor, Department of Mechanical Engineering, Keio University email: yasuoka@mech.keio.ac.jp

URL: http://www.yasuoka.mech.keio.ac.jp

- [1] Doi, H.; Okuwaki, K.; Mochizuki, Y.; Ozawa, T.; Yasuoka, K.; "Dissipative Particle Dynamics (DPD) Simulations With Fragment Molecular Orbital (FMO) Based Effective Parameters for 1-Parmitoyl-2-Oleoyl Phosphatidyl Choline (POPC) Membrane", *Chem. Phys. Lett.*, 684, 427-432 (2017). DOI : 10.1016/j.cplett.2017.07.032
- [2] Winarto; Yamamoto, E.; Yasuoka, K.; "Water Molecules in a Carbon Nanotube Under an Applied Electric Field at Various Temperatures and Pressures", *Water*, 9, 473 (2017). (14 pages) DOI : 10.3390/w9070473
- [3] Doi, H.; Yasuoka, K.; "Replica Exchange Molecular Simulation of Lennard-Jones Particles in a Two-Dimensional Confined System", *AIP Advances*, 7, 055018 (2017). (9 pages) DOI: 10.1063/1.4984815
- [4] Tomobe, K.; Yamamoto, E.; Yasui, M.; Yasuoka, K.; "Effects of Temperature, Concentration, and Isomer on The Hydration Structure in Monosaccharide Solutions", *Phys. Chem. Chem. Phys.*, 19, 15239-15246 (2017). DOI : 10.1039/C7CP02392H
- [5] Shibuya, T.; Yasuoka, K.; Mirbt, S.; Sanyal, B.; "Subsurface Polaron Concentration as a Factor in The Chemistry of Reduced TiO2 (110) Surfaces", J. Phys. Chem. C, 121, 11325-11334 (2017). DOI : 10.1021/acs.jpcc.7b00935
- [6] Tomobe, K.; Yamamoto, E.; Kholmurodov, K.; Yasuoka, K.; "Water Permeation Through the Internal Water Pathway in Activated GPCR Rhodopsin", *PLOS ONE*, **12**, e0176876 (2017). DOI : 10.1371/journal.pone.0176876
- [7] Nomura, K.; Kaneko, T.; Bai, J.; Francisco, J. S.; Yasuoka, K.; Zeng, X. C.; "Evidence of Low-Density and High-Density Liquid Phases and Isochore End Point for Water Confined to Carbon Nanotube", *PNAS*, **114**, 4066-4071 (2017). DOI : 10.1073/pnas.1701609
- [8] Yamamoto, E.; Akimoto, T.; Kalli, A. C.; Yasuoka, K.; Sansom, M. S. P.; "Dynamic Interactions Between a Membrane Binding Protein and Lipids Induce Fluctuating Diffusivity", *Science Advances*, 3, e1601871 (2017). (6 pages) DOI: 10.1126/sciadv.1601871
- [9] Takahashi, K. Z.; Nishimura, R.; Yasuoka, K.; Masubuchi, Y.; "Molecular Dynamics Simulations for Resolving Scaling Laws of Polythylene Melts", *Polymers*, 9, 24 (2017). (12 pages) DOI : 10.3390/polym9010024

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- [1] Miyamoto, H.; Shoji, Y.; Akasaka, R.; Lemmon, E. W.; "The Precise Measurement of Vapor-Liquid Equilibrium Properties of The CO₂/Isopentane Binary Mixture, and Fitted Parameters for a Helmholtz Energy Mixture Model", *Int. J. Thermophys.*, accepted manuscript, (2017).
- [2] Yoneda, Y.; Sato, S.; Matsumoto, T.; Miyamoto, H.; "Density of Methylcyclohexane at Temperatures up to 600 K and Pressures up to 200 MPa", *Int J Thermophys.*, **38**, 106 (2017).
- [3] Kimura, T.; Kayukawa, Y.; Miyamoto, H.; Saito, K.; "Critical Parameters and Critical-Region (p,ρ,T) Data of trans-1,1,1,3-Tetrafluorobut-2-ene [HFO-1354mzy(E)]", *Int J Thermophys.*, **38**, 122 (2017).
- [4] Matsumoto T.; Miyamoto, H.; " $P\rho T$ and Saturation Properties of Isopentane at 280 to 440 K and up to 200 MPa", *J. Chem. Thermodyn.* **101**, 150-156 (2016).

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- URL: http://pub2.db.tokushima-u.ac.jp/ERD/person/189117/work-en.html
- [1] Nakahara, M.; Yoshida K.; "Chronological Scientific Tables 2017", pp.502-509, 514-517, Maruzen Publishing Co., Ltd., Tokyo, ISBN 978-4-621-30096-1 (2016).
- [2] Yoshida, K.; Matubayasi, N.; Nakahara, M.; Uosaki, Y.; "Effect of Rotation on Vibrational Spectrum of Supercritical Water: Analysis of Dependencies on Density and Hydrogen Isotopes", *The Review of High Pressure Science and Technology*, **26**, 323-332 (2016).
- [3] Nakahara, M.; Yoshida K.; "Handbook of Scientific Tables", Maruzen Publishing Co., Ltd., Tokyo and World Scientific Publishing Co, Singapore, in press.

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- Kawada, S.; Komori, M.; Fujimoto, K.; Yoshii, N.; Okazaki, S.; "Molecular Dynamics Study of the Formation Mechanisms of Ionic SDS and Nonionic C12E8 Micelles and n-Dodecane Droplets", *Chem. Phys. Lett.*, **646**, 36-40 (2016).
 DOI: 10.1016/j.cplett.2015.12.062
- [2] Wang, L.; Fujimoto, K.; Yoshii, N.; Okazaki, S.; "A Molecular Dynamics Study of the Breathing and Deforming Modes of the Spherical Ionic SDS and Nonionic C12E8 Micelles", J. Chem. Phys., 144, 034903 (2016). DOI: 10.1063/1.4940031
- [3] Hamasaka, S.; Muto, T.; Andoh, Y.; Fujimoto, K.; Kato, K.; Takata, S.; Okazaki, S.; Uozumi, Y;
 "Detailed Structural Analysis of a Self-Assembled Vesicular Amphiphilic NCN-Pincer Palladium Complex by Using Wide-Angle X-Ray Scattering and Molecular Dynamics Calculations", *Chem. Eur. J.*, 23(6), 1209 (2016).

DOI:10.1002/chem.201605213

- [4] Kuo, A.; Shinoda, W.; Okazaki, S; "Molecular Dynamics Study of the Morphology of Hydrated Perfluorosulfonic Acid Polymer Membranes", J. Phys. Chem. C, 120(45), 25832-25842 (2016). DOI: 10.1021/acs.jpcc.6b08015
- [5] Kitabata, M.; Fujimoto, K.; Yoshii, N.; Okazaki, S; "A Molecular Dynamics Study of Local Pressures and Interfacial Tensions of SDS Micelles and Dodecane Droplets in Water Micelles and Dodecane Droplets in Water", J. Chem. Phys., 144(22), 224701 (2016). DOI: 10.1063/1.4953405
- [6] Andoh, Y.; Yamada, A.; Yoshii, N.; Okazaki, S; "Evaluation of Atomic Pressure in the Multiple Time-step Integration Algorithm", J. Comput. Chem., 38(10), 704-713 (2017). DOI: 10.1002/jcc.24731

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 Uchida, S.; Hanawa, S.; Naitoh, M.; Okada, H.; Lister, D. H.; "Effects of Oxide Film on ECP and of Steel", *EUROCORR2016*, Sep 12-15, 2016, Montpellier, France, European Federation of Corrosion (2016) (CD).

- [2] Katsumura, Y.; Uchida, S.; "Latest Activities of the Water Chemistry Group in Japan", Int. Conf.On Water Chemistry of Nuclear power Systems, NPC2016, Oct. 2-7, 2016 Brighton, UK, Nuclear Institute (2016) (CD).
- [3] Uchida, S.; Itoh, A.; Naitoh, M.; Okada, H.; Pellegrini, M.; Nagai, H.; "Evaluation of Fission Product Behavior in Fukushima Daiichi NPP Under Svere Accident– Understanding Their Behavior Based on Coupling of the Forward and Backward Evaluation Procedures", *Int. Conf. On Water Chemistry* of Nuclear power Systems, NPC2016, Oct. 2-7, 2016 Brighton, UK, Nuclear Institute (2016) (CD).
- [4] Mohajery, K.; Lister, D. H.; Uchida, S.; "Flow-Accelerated Corrosion in Two-Phase Steam-Water Flows: Experiments and Modelling", *Int. Conf.On Water Chemistry of Nuclear power Systems*, *NPC2016*, Oct. 2-7, 2016 Brighton, UK, Nuclear Institute (2016) (CD).
- [5] Hanawa, S.; Uchida, S.; Hata, K.; Chimi, Y.; Kasahara, S.; Nishiyama, Y.; "Study of Irradiation Effects on ECP Using In-pile in the JMTR", *Int. Conf.On Water Chemistry of Nuclear power Systems, NPC2016*, Oct. 2-7, 2016 Brighton, UK, Nuclear Institute (2016) (CD).
- [6] Hanawa, S.; Uchida, S.; Hata, K.; Chimi, Y.; Kasahara, S.; Nishiyama, Y.; "Evaluation of ECP Measured in the In-pile Environment", *Int. Conf.On Water Chemistry of Nuclear power Systems*, NPC2016, Oct. 2-7, 2016 Brighton, UK, Nuclear Institute (2016) (CD).
- [7] Kawamura, H.; Hirano, H.; Katsumura, Y.; Uchida, S.; Mizuno, T.; Kitajima, H.; Tsuzuki, Y.; Terachi, T.; Nagase, M.; Usui, N.; Takagi, J.; Urata, H.; Shoda, Y.; Nishimura, T.; "BWR Water Chemistry Guidelines and PWR Primary Water Chemistry Guidelines in Japan - Purpose and Technical Background", *Nucl. Eng. Design*, 309, 161-174 (2016).
- [8] Uchida, S.; Okada, H.; Naitoh, M.; Kojima, F.; Koshizuka, S.; Lister, D. H.; "Improving Plant Reliability Based on Inspection and Maintenance of Local Wall Thinning due to Flow-Accelerated Corrosion", *Power Plant Chemistry*, 18 (6), 288-300 (2016).

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- Watanabe, N.; Kikuchi, T.; Ishibashi, T.; Tsuchiya, N.; "v-X-type Relative Permeability Curves for Steam-Water Two-Phase Flows in Fractured Geothermal Reservoirs", *Geothermics*, 65, 269-279 (2017).
- [2] Watanabe, N.; Numakura, T.; Sakaguchi, K.; Saishu, H.; Okamoto, A.; Ingebritsen, S. E.; Tsuchiya, N.; "Potentially Exploitable Supercritical Geothermal Resources in the Ductile Crust", *Nature Geoscience*, **10** (2), 140-144 (2017).
- [3] Tsubokawa, Y.; Ishikawa, M.; Kawakami, T.; Hokada, T.; Satish-Kumar, M.; Tsuchiya, N.; Grantham, G. H.; "Pressure–Temperature–Time Path of a Metapelite from Mefjell, Sør Rondane Mountains, East Antarctica", *Journal of Mineralogical and Petrological Sciences*, **112** (2), 77-87 (2017).
- [4] Watanabe, N.; Egawa, M.; Sakaguchi, K.; Ishibashi, T.; Tsuchiya, N.; "Hydraulic Fracturing and Permeability Enhancement in Granite from Subcritical/Brittle to Supercritical/Ductile Conditions", *Geophysical Research Letters*, **44**, 5468-5475 (2017).
- [5] Tsuchiya, N.; Ishikawa, H.; Saito, R.; Hiran, N.; "Development of Portable Thermoluminescence Measurement Equipment for Geothermal Exploration" *J. Geotherm. Res. Soc. Japan*, **38**(4) 127-131 (2016).
- [6] Tsuchiya, N.; Yamada, R.; Uno, M.; "Supercritical Geothermal Reservoir Revealed by a Granite– Porphyry System", *Geothermics*, **63**, 182-194 (2016).

- [7] Ishibashi, T.; Watanabe, N.; Asanuma, H.; Tsuchiya, N.; "Linking Microearthquakes to Fracture Permeability Change: The Role of Surface Roughness", *Geophysical Research Letters*, **43** (14), 7486-7493 (2016).
- [8] Burenjargal, U.; Okamoto, A.; Tsuchiya, N.; Uno, M.; Horie, K.; Hokada, T.; "Contrasting Geochemical Signatures of Devonian and Permian Granitoids from the Tseel Terrane, SW Mongolia", *Journal of Geosciences*, **61** (1), 51-66 (2016).
- [9] Yamasaki, S.-I.; Takeda, A.; Kimura, K.; Tsuchiya, N.; "Underestimation of Chromium And Zirconium in Soils by Hydrofluoric Acid Digestion and Inductively Coupled Plasma-Mass Spectrometry", *Soil Science and Plant Nutrition*, **62** (2), 121-126 (2016).

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- Hwang, E. T.; Orchard, K.; Hojo, D.; Beton, J.; Lockwood, C. W.; Adschiri, T.; Butt, J. N.; Reisner, E.; Jeuken, L.; "Exploring Step by Step Assembly of Nanoparticle: Cytochrome Biohybrid Photoanodes", *ChemElectroChem*, 4, 1959–1968 (2017). DOI: 10. 1002 /celc. 201700030
- Fujii, T.; Kawasaki, S.; Adschiri, T.; "Kinetic Study of Octanoic Acid Enhanced Crystal Growth of Boehmite Under Sub- and Supercritical Hydrothermal Conditions", *Journal of Supercritical Fluids*, 118, 148-152 (2016). DOI: 10.1016/j.supflu.2016.08.005
- [3] Fujii, T.; Kawasaki, S.; Suzuki, A.; Adschiri, T.; "High-Speed Morphology Control of Boehmite Nanoparticles by Supercritical Hydrothermal Treatment with Carboxylic Acids", *Crystal Growth & Design*, **16**, 1996-2001 (2016). DOI:10.1021/acs.cgd.5b01584
- [4] Aoki, N.; Sato, A.; Sasaki, H.; Litwinowicz, A. A.; Seong, G. M.; Aida, T.; Hojo, D.; Takami, S.; Adschiri, T.; "Kinetics Study to Identify Reaction-Controlled Conditions for Supercritical Hydrothermal Nanoparticle Synthesis with Flow-Type Reactors", *Journal of Supercritical Fluids*, 110, 161-166 (2016). DOI: 10.1016/j.supflu.2015.11.015
- [5] Sugioka, K.; Ozawa, K.; Kubo, M.; Tsukada, T.; Takami, S.; Adschiri, T.; Sugimoto, K.; Takenaka, N.; Saito, Y.; "Relationship Between Size Distribution of Synthesized Nanoparticles and Flow and Thermal Fields in a Flow-Type Reactor for Supercritical Hydrothermal Synthesis", *Journal of Supercritical Fluids*, **109**, 43-50 (2016). DOI: 10.1016/j.supflu. 2015.11.008

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- URL: http://www.cheng.es.osaka-u.ac.jp/matubayasi/english/index.html
- [1] Shimizu, S.; Matubayasi, N.; "The origin of cooperative solubilisation by hydrotropes", *Phys. Chem. Chem. Phys.*, **18**, 25621-25628 (2016). DOI: 10.1039/c6cp04823d
- [2] Harris, R. C.; Deng, N.; Levy, R. M.; Ishizuka, R.; Matubayasi, N.; "Computing Conformational Free Energy Differences in Explicit Solvent: An Efficient Thermodynamic Cycle Using an Auxiliary Potential and a Free Energy Functional Constructed from the End Points", *J. Comput. Chem.*, 38, 1198-1208 (2017). DOI: 10.1002/jcc.24668
- [3] Takahashi, H.; Umino, S.; Miki, Y.; Ishizuka, R.; Maeda, S.; Morita, A.; Suzuki, M.; Matubayasi, N.; "Drastic Compensation of Electronic and Solvation Effects on ATP Hydrolysis Revealed through Large-Scale QM/MM Simulations Combined with a Theory of Solutions", *J. Phys. Chem. B*, 121, 2279-2287 (2017). DOI: 10.1021/acs.jpcb.7b00637
- [4] Shimizu, S.; Stenner, R.; Matubayasi, N.; "Gastrophysics: Statistical Thermodynamics of Biomolecular Denaturation and Gelation from the Kirkwood-Buff Theory Towards the

Understanding of Tofu", *Food Hydrocolloids*, **62**, 128-139 (2017). DOI: 10.1016/j.foodhyd.2016.07.022

- [5] Matubayasi, N.; "Free-Energy Analysis of Protein Solvation with All-Atom Molecular Dynamics Simulation Combined with a Theory of Solutions", *Current Opinion in Structural Biology*, **43**, 45-54 (2017). DOI: 10.1016/j.sbi.2016.10.005
- [6] Levy, R. M.; Cui, D.; Zhang, B. W.; Matubayasi, N.; "Relationship Between Solvation Thermodynamics from IST and DFT Perspectives", J. Phys. Chem. B, 121, 3825-3841 (2017). DOI: 10.1021/acs.jpcb.6b12889
- [7] Kobayashi, S.; Fujii, S.; Koga, A.; Wakai, S.; Matubayasi, N.; Sambongi, Y.; "Pseudomonas aeruginosa Cytochrome c₅₅₁ Denaturation by Five Systematic Urea Derivatives that Differ in the Alkyl Chain Length", Bioscience, Biotechnology, and Biochemistry, 81, 1274-1278 (2017). DOI: 10.1080/09168451.2017.1303361
- [8] Yamamori, Y.; Matubayasi, N.; "Interaction-Component Analysis of the Effects of Urea and its Alkylated Derivatives on the Structure of T4-Lysozyme", J. Chem. Phys., 146, 225103 (13 pages) (2017). DOI: 10.1063/1.4985222
- [9] Maneffa, A. J.; Stenner, R.; Matharu, A. S.; Clark, J. H.; Matubayasi, N.; Shimizu, S.; "Water Activity in Liquid Food Systems: A Molecular Scale Interpretation", *Food Chemistry*, 237, 1133-1138 (2017). DOI: 10.1016/j.foodchem.2017.06.046
- [10] Sayou, M.; Ishizuka, R.; Matubayasi, N.; "Energetic Analysis of Adsorption and Absorption of Small Molecule to Nanodroplet of Water", J. Phys. Chem. B, 121, 5995-6001 (2017). DOI: 10.1021/acs.jpcb.7b01554
- [11] Shimizu, S.; Matubayasi, N.; "Osmolyte Depletion Viewed in Terms of the Dividing Membrane and its Work of Expansion Against Osmotic Pressure", *Biophysical Chemistry*, in press (2017). DOI: 10.1016/j.bpc.2017.02.003
- [12] Matubayasi, N.; "Energy Representation Approach", Reference Module in Chemistry, Molecular
Sciences and Chemical Engineering, in press (2017).
DOI: 10.1016/B978-0-12-409547-2.11485-4
- [13] Shimizu, S.; Matubayasi, N.; "Unifying Hydrotropy Under Gibbs Phase Rule", *Phys. Chem. Chem. Phys.*, **19**, in press (2017). DOI: 10.1039/c7cp02132a
- [14] Ishizuka, R.; Matubayasi, N.; "Effective Charges of Ionic Liquid Determined Self-Consistently Through Combination of Molecular Dynamics Simulation and Density-Functional Theory", J. Comput. Chem., 38, in press (2017). DOI: 10.1002/jcc.24880
- [15] Mori, H.; Matubayasi, N.; "MD Simulation Analysis of Resin Filling into Nano-Sized Pore Formed on Metal Surface", Appl. Surf. Sci., in press (2017). DOI: 10.1016/j.apsusc.2017.08.123

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- [1] Matsuno, T.; Tabuchi, Y.; Hosomi, R.; Hasegawa, T.; Kometani, N.; Tsuji, K.; "Sample Preparation for TXRF Analysis of Metal Particles in Used Machine Oils and Preliminary Research for Application of Principal Component Analysis", *Advances in X-ray Analysis*, **59**, 112-119 (2016).
- [2] Takimoto, Y.; Yamanashi, M.; Kato, S.; Shoji, T.; Kometani, N.; Tsuji, K.; "WD-XRF Imaging With Polycapillary Optics Under Glancing Incidence Geometry", *Advances in X-ray Analysis*, **59**, 120-124 (2016).
- [3] Kometani, N.; Hirata, S.; Chikada, M.; "Photocatalytic Reduction of CO₂ by Pt-Loaded TiO₂ in the Mixture of Sub- and Supercritical Water and CO₂", *J. Supercritical Fluids*, **120**, 443-447 (2017). DOI: 10.1016/j.supflu.2016.05.031

[4] Nishiyama, T.; Matsuura, K.; Sato, E.; Kometani, N.; Horibe, H.; "Degradation of Hydrophilic Polymers in Aqueous Solution by Using Ozone Microbubble", J. Photopolym. Sci. Technol., 30, 285-289 (2017). DOI: 10.2494/photopolymer.30.285

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- [1] Kimura, T.; Kayukawa, Y.; Miyamoto, H.; Saito, K.; "Critical Parameters and Critical-Region (p, ρ, T) Data of trans-1,1,1,3-Tetrafluorobut-2-ene [HFO-1354mzy(E)]", *Int. J. Thermophys.*, 38, (2017). DOI: 10.1007/s10765-017-2256-0
- [2] Kimura, T.; Kayukawa,; Saito, K.; "Pressure–Volume–Temperature Property Measurements for trans-1,1,1,3-Tetrafluoro-2-butene [HFO-1354mzy(E)]", J. Chem. Eng. Data, 62, 1422–1426 (2017). DOI: 10.1021/acs.jced.6b00980

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[1] Smith, B.; McCann, P.; Uchida, K.; Mori, S.; Jasper, J.; Hater, W.; "Determination of Oleyl Propylenediamine, a Commonly Used Film Forming Amine, on the Surfaces of Water-Steam Cycles", *Power Plant Chemistry*, **19** (3), 129-140 (2017).

New Zealand Association for the Properties of Water and Steam (NZAPWS) Annual Report

Date: 28 August 2017

Key Achievements:

- 1. NZAPWS is now a full member country of IAPWS¹
- 2. NZAPWS is now fully funded via a industry sponsorship model with contrubutions from generating utilities, industrial steam users and water/steam related chemical vendors providing sufficient funding to:
 - a. Pay our annual IAPWS full country membership fees (Paid 22 June 2017)
 - Provide travel funding assistance to NZAPWS members to attend IAPWS meetings/conferences – for 2017 – Jeremy Lovell-Smith to represent New Zealand
 - c. Provide funding to undertake an annual NZAPWS meeting/conference in NZ
 - d. Provide a source of funds for future related research.
- 3. NZAPWS has an active membership covering the following areas:
 - a. Fossil power generation
 - b. Industrial steam production and use for dairy product production
 - c. Geothermal power generation (subsurface and surface operations)
 - d. Humidity research and services
 - e. Water/steam analytical services
 - f. Water/steam chemical treatment and services

Key Activities:

- 1. A very successful technical seminar was held in May 2017 in Rotorua, NZ with 45 attendees and a wide ranging program of technical presentations covering;
 - a. Geothermal steam chemistry
 - b. Industrial steam chemistry
 - c. Humidity
 - d. Water and steam chemical analysis
 - e. Cooling water systems
 - f. Steam heat transfer
 - g. IAPWS related research and Technical Guidance Documents
- 2. Formation of a new NZAPWS committee taking NZAPWS forward
- 3. David Addison has had ongoing involvement in the PCC Corrosion Product Sampling working group

¹ Once again showing our superiority to Australia by achieving full IAPWS membership status first.

- 4. David Addison has had ongoing involvement in a PCC IAPWS International Collaboration project with the University of New Brunswick (DR Willy Cook) working on high temperature electrochemical corrosion monitoring
- 5. David Addison and Ian Richardson have continued working on geothermal related aspects for a IAPWS white paper
- 6. Jeremy Lovell-Smith has contributed to (a) TPWS through continuing investigation into the use of Generalised Least Squares (GLS) to propagate input data covariance into the IAPWS equation parameters and to (b) JCS through work on the definition of relative humidity.

Publications:

- 1. E. Buscarlet, I. Richardson, S. Addison, H. Moon, J. Quinao; *Geochemical Modelling of Plant and Reservoir Processes at the Ngatamariki Geothermal Field* New Zealand Geothermal Workshop, 2016
- I.M. Richardson, D.R. Addison, S.J. Addison, T.J. Gresham and R.J. Lawson; *Online Steam Purity Analysis for Geothermal Power Generation;* New Zealand Geothermal Workshop, 2016
- R. Lawson, T. Gresham, I. Richardson, F. Siega, S. Addison, Long Run Polymerization Experiments at the Kawerau Geothermal Limited Power Plant; New Zealand Geothermal Workshop, 2016
- 4. J. Weir, D. Addison; *Ion Exchange Challenges in a Dairy Product Processing Factory Cogeneration Plant;* PPChem, 2017, 19(3)
- Lovell-Smith, J. W., Saunders, P., & Feistel, R. (2017). Unleashing Empirical Equations with "Nonlinear Fitting" and "GUM Tree Calculator". International Journal of Thermophysics, 38(10), 148.
- 6. Feistel, R., & Lovell-Smith, J. W. (2017). Defining relative humidity in terms of water activity. Part 1: definition. Metrologia, 54, 566.
- 7. C. Morris, E Mroczek, *Geothermal Turbine Scaling*, PPChem 2016 (18(3)

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International Association for the Properties of Water and Steam Russian National Committee (RNC)

Report Second Half-Year of 2016 – First Half-Year of 2017

Russian National Committee of IAPWS and National Research University "MPEI" held International Conference «Using Film Forming Amines in Power Industry» 9-10 November 2016, Moscow, MPEI. Registered participants: 188, active participants: 146.



Titles of presentations:

- 1. IAPWS TGDs for water chemistry in power industry;
- 2. IAPWS TGD for the water chemistry with film-forming amines;
- 3. The use of ODA in the Russian power industry;
- 4. Summarizing the experience of protection against atmospheric corrosion of power equipment of TPP and NPP by at ODACON conservation technology;
- 5. Perspective directions of use of film-forming amines in the power industry;
- 6. Experience of water chemistry with the use of complex reagents on the example of Vologda CCPP with 100 MW capacity;
- 7. FFAP treatment during abnormal operations;
- 8. Experience of polyamines in power plants;
- 9. Experience in the application of FFA for pre-cleaning and preservation of HGST in CCPP;
- 10. A review of studies on the use of film-forming amines for correctional water treatment;
- 11. The influence of complex reagents on the basis of PA sensors on automatic analysers in the system of chemical control at TPP;
- 12. The results of operation of power units of Zhambyl GRES with a water-based complex reagents with POA;
- 13. The use of reagents based on FFA for water chemistry at "Sitienergo" power plant;

- 14. The use of reagents based on FFA for water chemistry at Kaliningradskaya TPP-2 with 450 MW capacity;
- 15. Experience with the use of reagents on the basis of FFA at the Ivanovo CCPP.

List of other activities

- RNC active participation in organization of next seminars for engineers and technology specialist from Russian power engineering companies:
- 16. Cycle chemistry at power plants;
- 17. Today technologies for cycle chemistry monitoring systems;
- 18. Today experience of water treatment systems operation;
- 19. Water treatment and cycle chemistry for combine cycle power plants.
 - Two meetings of RNC have been held.

Publications list

Books

- 1. Ochkov V., Orlov K., Voloshchuk V. Thermal Engineering Studies with Excel, Mathcad and Internet. Springer, ISBN 978-3-319-26673-2 (in English).
- 2. Alexandrov A.A., Orlov K.A., Ochkov V.F. Thermo-physical properties of power industry working fluids: reference book. 2nd edition, 2017. -226 [8] pp (in Russian).

Articles

- 3. Yudovskaya, M.A., Distler, V.V., Prokofiev, V.Y., Akinfiev, N.N. Gold mineralisation and orogenic metamorphism in the Lena province of Siberia as assessed from Chertovo Koryto and Sukhoi Log deposits. Geoscience Frontiers Volume 7, Issue 3, May 2016, Pages 453-481
- Kokh, M.A., Akinfiev, N.N., Pokrovski, G.S., Salvi, S., Guillaume, D. The role of carbon dioxide in the transport and fractionation of metals by geological fluids Geochimica et Cosmochimica Acta Volume 197, 15 January 2017, Pages 433-466
- Tyapkov, V.F., Petrova, T.I., Dyachenko, F.V., Borodastov, A.K. Use of amines for adjusting the second-loop chemical regime in NPPs with VVER October 2016, Volume 120, Issue 6, pp 412– 417
- 6. Petrova, T.I., Orlov, K.A., Dooley, R.B. International water and steam quality standards on thermal power plants at all-volatile treatment December 2016, Volume 63, Issue 12, pp 896–902
- 7. Petrova, T.I., Orlov, K.A., Dooley, R.B. International water and steam quality standards for thermal power station drum-type and waste heat recovery boilers with the treatment of boiler water with phosphates and NaOH January 2017, Volume 64, Issue 1, pp 61–67
- 8. Ustyuzhanin, E.E., Ochkov, V.F., Shishakov, V.V., Rykov, S.V. Internet calculations of thermodynamic properties of substances: Some problems and results. Journal of Physics: Conference Series, Volume 774, Number 1

- Ochkov V., Nikulcev E., Gurke S. Displaying formulas as embedded calculations in scientific literature, textbooks and educational web apps. Computer modelling and new technologies. 2017 V 21, №1, P. 7-12
- P.M. Gotovtsev, Ya.E. Sergeeva, A.V. Komova, I.A. Konova, K.V. Gorin, G.U. Badranova, V.M. Pojidaev and R.G. Vasilov. Mathematical Modeling of Intracellular Processes. Chapter at book Advances in Mathematics Research. Ed. Albert R. Baswell Volume 21. Nova Publishing. 2017. P.1 30. ISBN: 978-1-53610-470-7
- A. N. Reshetilov, J. V. Plekhanova, S. E. Tarasov, A. G. Bykov, M. A. Gutorov, S. V. Alferov, T. K. Tenchurin, S. N. Chvalun, A. S. Orekhov, A. D. Shepelevd, P. M. Gotovtsev, and R. G. Vasilov. Evaluation Properties of Bioelectrodes Based on Carbon Superfine Materials Containing Model Microorganisms *Gluconobacter*. Nanotechnologies in Russia, 2017, Vol. 12, Nos. 1–2, pp. 107–115.
- Ya. E. Sergeeva, E. B. Mostova, K. V. Goria, A. V. Komova, I. A. Konova, V. M. Pojidaev, P. M. Gotovtsev, R. G. Vasilov, and S. P. Sineoky. Calculation of Biodiesel Fuel Characteristics Based on the Fatty Acid Composition of the Lipids of Some Biotechnologically Important Microorganisms. Applied Biochemistry and Microbiology, 2017, Vol. 53, No. 8, pp. 27–33.
- A.N. Reshetilov, Yu.V. Plekhanova, S.E. Tarasov, V.A. Arlyapov, V.V. Kolesov, M.A. Gutorov, P.M. Gotovtsev, and R.G. Vasilov. Effect of Some Carbon Nanomaterials on Ethanol Oxidation by *Gluconobacter oxydans* Bacterial Cells. Applied Biochemistry and Microbiology, 2017, Vol. 53, No. 1, pp. 122–128.
- 14. P.M. Gotovtsev, Ya.E. Sergeeva, A.V. Komova, I.A. Konova, K.V. Gorin, G.U. Badranova, V.M. Pojidaev and R.G. Vasilov. Mathematical Modeling of Intracellular Processes. International Journal of Mathematics, Game Theory, and Algebra. 2016 V.25 № 2
- 15. A.V. Borgolov, K.V. Gorin, V.M. Pozhidaev, Y.E. Sergeeva, P.M. Gotovtsev, R.G. Vasilov. Mathematical Modeling of Triglyceride Transesterification through Enzymatic Catalysis in a Continuous Flow Bioreactor. Indian Journal of Science and Technology. Vol.9 Issue 47 December 2016
- P.M. Gotovtsev, A.V. Dyakov. Biotechnology and Internet of Things for Green Smart City Application. IEEE World Forum of Internet of Things. Proceedings. Reston USA 12 – 14 December 2016. PP – 542-546
- Voronov, V.N., Yegoshina, O.V., Bolshakova, N.A., Yarovoi, V.O., Latt, A.M. Effect of water chemistry upsets on the dynamics of corrective reagent dosing systems at thermal power stations. December 2016, Volume 63, Issue 12, pp 903–907
- 18. V.M. Pojidaev, K.V. Gorin, Ya.E. Sergeeva, P.M. Gotovtsev, R.G. Vasilov. Conversion of phototrophic microorganism biomass to biooil by electrosynthesis. Ovchinnikov bulletin of biotechnology and physical and chemical biology 2016 (12) №4, 29-35 (*Russian*)
- 19. A. N. Reshetilov, A. E. Kitova, M. V. Machulin, S. E. Tarasov, M. A. Gutorov, S. V. Alferov, V.V. Kolesov, P.M. Gotovtsev, R.G. Vasilov. Biosensor based on *Gluconobacter* cells and thermally expanded graphite. Sensors systems. 2016 V30 № 4, c. 351–354 (*Russian*)
- O.V. Egoshina, V.O. Yarovoy, M.M. Sazanova. Investigation of methods polyamins concentration measurements in thermal power plants. New in Russian power engineering. 2016 №10, 25 32 (*Russian*)
- 21. Ochkov, V.F., Bodryakov A.V., Hor'kov S.N. Hybrid computations using PC. Cloud of Science. 2016 V4 №2 P.168-189 (*Russian*)
- 22. Ochkov, V.F., Orlov K.A., Voloshuk V.V., Dudolin A.A., Oleynikova E.N., Aung tu ra Tun. Thermophysical properties of substances for computation of energy efficiency. Energy saving and water treatment. 2016 V3 (101), P. 43-57 (*Russian*).

SIAPWS annual report for 2016

The annual meeting 2016 was successful with 16 participants at the event that was hosted by Nordjyllandsværket in Denmark. The workshop was interesting with good presentations and discussion afterwards, and the meeting ended with a visit to the ultrasupercritical plant NJV3 and the laboratory, which is specialised in tribology and water chemistry. The discussion at the meeting lead to a decision that the Executive Committee (EC) should focus on improving the exchange of information and experiences across SIAPWS in the coming year, especially with attention on transfer of knowledge to the younger members.

The EC took the task up and discussed several ideas that came together in SIAPWS Water Chemistry Network, a Facebook and web-based network intended for fast transfer of experience, registration and organisation of lasting information, and course activities covering the main aspects of the SIAPWS work field. The main idea is that you should be able to participate from your desk and pc and only occasionally travel to meet your colleagues physically.

The Matarvattenkonferensen in November was the setting for the first presentation of the network and invitation of our colleagues to take part. The first months of the network has seen a slow start, but the EC hopes that colleagues will join as they learn more about the network. The demand that only members of SIAPWS (company or personal) have the full access to the information may be an obstacle. This is necessary of several reasons – access to both IAPWS/PCC and SIAPWS website demands login, and the IAPWS materials is restricted to members only.

The annual IAPWS meeting took place in Dresden this year. As usual, it was an intensive week with workshops, presentations, and discussions. The work in the Power Cycle Chemistry (PCC) group during the year led to release of two new Technical Guidance Documents (TGDs) on criteria for chemical cleaning of Heat Recovery Steam Generators (HRSGs) and application of film forming amines for feed water conditioning. The last one is the first international guide describing the basic chemicals and application of these compounds in the water-steam circuit – *pro et contra*.

The upcoming revision of the TGD on Corrosion Product Sampling and Analysis was another hot topic. The driver for the revision is the wish of many users for guidance regarding plants that operate in flexible mode with frequent load changes and start/stops. This work is well under way, and currently a number of field trials are performed to cover missing knowledge with respect to corrosion product formation and transport under start-up and flexible conditions.

The work on a new TGD on air in-leakage in water-steam circuits has been initiated. This is a common disturbance, the source is often not easy to reveal, and it is costly since the plant efficiency decreases. The intention of the TGD is give systematic guidance on how to test for air in-leakage and methods to locate the source/leak.

SIAPWS takes part in both of the task groups working with the TGD's mentioned here, and several members contribute to the field trials.

Executive Committee

Chair	Karsten Thomsen	Cashier	Kaj Thomsen
Vice-chair, secretary	Jørgen Peter Jensen	Coordinator	Roger Lundberg

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

Report on IAPWS related activities – September 2016 / August 2017

Submitted to the EC Meeting of IAPWS, Kyoto, Japan – August 2017.

National Committee Contacts: President: Marco Lendi, E-mail: marco.lendi@swan.ch Secretary: Tapio Werder, E-mail: tapio.werder@waesseri.com

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

Prof. Dr. Horst-Michael Prasser, Institute of Energy Technology, Swiss Federal Institute of Technology, Zürich, E-Mail: prasser@lke.mavt.ethz.ch Dr. Michael Hiegemann, General Electric (Switzerland) GmbH, Baden, Switzerland, E-Mail: michael.hiegemann@ge.com

Dr. Robert Svoboda, Svoboda Consulting, Wettingen, E-Mail: r.svoboda@swissonline.ch

Marco Lendi, Swan Analytical Instruments, Hinwil, E-Mail: marco.lendi@swan.ch Tapio Werder, PowerPlant Chemistry Journal, Hinwil, E-Mail: tapio.werder@waesseri.com

Research activities in the reporting period: No new projects were reported

Contributions to current IAPWS activities: Vice-chairman of Subcommittee on Sea-Water: M. Hiegemann Vice-chairman of PCC Sub-Task Group on Film Forming Amines (FFA): Marco Lendi

Status of Associate Membership to IAPWS:

Up to now, no team of sponsors to commit on mid- or long-term to a regular Swiss membership fee has yet been assembled. Activities were therefore limited to few individuals. SCPWS hosted the First International Conference on Film Forming Amines and Products in April 2017 in Lucerne, Switzerland. The organization of this conference was the main activity of the board of SCWPS in the past year. The conference in Lucerne was intended to serve to promote SCPWS within Switzerland and to find new participating institutions. Although the conference found wide international acceptance, in regard to finding new participating institutions, the goal was not achieved. The board of SCPWS is currently planning a smaller event in Spring 2018 to find new participating institutions in Switzerland.

- It is therefore requested to extend the Associate Membership for another term.

M. Lendi, August 2017

U.S. National Committee to IAPWS 2017 Report on Activities of Potential Interest to IAPWS

Communicated from the Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, CO:

- In a collaboration with the Ruhr University of Bochum (Germany), we completed a new reference equation of state for the thermodynamic properties of heavy water. This EOS is now undergoing testing by an IAPWS Evaluation Task Group, and a paper is being drafted.
- Work is beginning on a related IAPWS project to develop new transport property correlations for heavy water.
- In collaboration with researchers at Fondazione Bruno Kessler (Italy), Nicolaus Copernicus University (Poland), and the University of Delaware (USA), two state-of-the-art flexible models for the water pair potential have been used to calculate second virial coefficients B(T) for both H₂O and D₂O. The calculations use the path-integral Monte Carlo method, which fully accounts for both intermolecular and intramolecular quantum effects. The results agree with experimental data, but cover a wider range of temperatures. The effect of molecular flexibility is found to be significant in comparison to the uncertainty of the calculations and of the experimental data, implying that the rigid models often used for water are insufficient if the best quantitative accuracy for virial coefficients is desired. The results for D₂O served as input for the new IAPWS EOS for heavy water.
- Calculations are in progress for the third virial coefficient C(T) for both H₂O and D₂O, which requires state-of-the-art 3-body potentials. We have discovered that the only high-quality flexible 3-body model has too many "holes" to be useful in virial calculations, so we are using a better-behaved rigid potential for the 3-body contribution.

Communicated from the University of Maryland, College Park

In 2017 we have published four papers relevant to IAPWS activities, including the last two supported by the Young Scientist IAPWS Fellowship Project *Towards an IAPWS Guideline for the Thermodynamic Properties of Supercooled Heavy Water*.

- John W. Biddle, Rakesh S. Singh, Evan M. Sparano, Francesco Ricci, Miguel A. González, Chantal Valeriani, José L. F. Abascal, Pablo G. Debenedetti, Mikhail A. Anisimov, and Frédéric Caupin, *Two-structure thermodynamics for the TIP4P/2005 model of water covering supercooled and deeply stretched regions*, J. Chem. Phys. **146**, 034502 (2017).
- Andrei A. Novikov, Anton P. Semenov, Viviana Monje-Galvan, Vladimir N. Kuryakov, Jeffery B. Klauda, and Mikhail A., *Action of Hydrotropes at the Water/Oil Interface*, J. Phys. Chem. C (2017) DOI:10.1021/acs.jpcc.7b05156
- Mikhail A. Anisimov, Michal Duška, Frédéric Caupin, Lauren E. Amrhein, Amanda Rosenbaum, Richard J. Sadus, *Thermodynamics of Fluid Polyamorphism*, arXiv:1708.03573 [cond-mat.stat-mech]
- Michal Duška, Jan Hrubý, Frédéric Caupin, Mikhail A. Anisimov *Communication: Two-structure thermodynamics unifying all scenarios for water anomalies* arXiv:1708.04054 [cond-mat.stat-mech]

Communicated from the ASME Research & Technology Committee on Water and Steam in Thermal Systems

The Water Technology Subcommittee has published the *Consensus on Pre-Commissioning Stages for Cogeneration and Combined Cycle Power Plants* (ASME, 2017 ISBN: 9780791861264). Work continues on an update to the document: *Consensus on Operating Practices for the Control of Feedwater and Boiler Water Chemistry in Modern Industrial Boilers*. We have also started working on a new project – the steam/water cycle equipment inspection guidelines series. The project will consist of a series of guideline pamphlets each focused on a specific piece of equipment in the steam/water cycle and will provide the user with information on how to plan for, conduct, and interpret the results of inspections. The guidelines are aimed at power plant and industrial boiler house staff and aiding those persons in planning for inspections, working with the certified inspector, and understanding the results of the inspection reports. Work has started on the first 3 guidelines: deaerators, fire tube boilers, and drum style water tube boilers.

Communicated from OLI Systems

• Aqueous solution chemistry of actinides

OLI has finalized a comprehensive model for predicting the properties of actinide species in aqueous solutions. The model is based on the previously developed Mixed-Solvent Electrolyte (MSE) thermodynamic framework. It provides a detailed treatment of speciation and solubility of U(IV, VI), Np(IV, V, VI), Pu(III, IV, V, VI), Am(III), and Cm(III) in various environments including salt, acid and base solutions in wide ranges of temperatures. The model has been designed for applications in nuclear waste management, environmental studies of radionuclide behavior and nuclear fuel processing. The work has been published in:

P. Wang, A. Anderko, J.J. Kosinski, R.D. Springer, and M.M. Lencka, "Modeling Speciation and Solubility in Aqueous Systems Containing U(IV, VI), Np(IV, V, VI), Pu(III, IV, V, VI), Am(III), and Cm(III) in Wide Concentration Ranges," J. Solution Chem., 46 (2017) 521-588

• Aqueous solution chemistry of rare-earth elements

OLI Systems participates in the Department of Energy's Critical Materials Institute as a provider of simulation tools for solution chemistry and thermodynamic properties. Recently, the work has been focused on the properties of aqueous systems and solid phases containing chlorides, sulfates, and carbonates of rare earth elements. The recently completed work has been published in the following papers:

R. Shivaramaiah, W. Lee, A. Navrotsky, D. Yu, P. Kim, H. Wu, Z. Hu, R. Riman, and A Anderko, "Location and Stability of Europium in Calcium Sulfate and its Relevance to Rare Earth Recovery from Phosphogypsum Waste," American Mineralogist, 101 (2016) 1854-1861

S.G. Srinivasan, R. Shivaramaiah, P.R.C. Kent, A.G. Stack+, R. Riman, A. Anderko, A. Navrotsky, V.S. Bryantsev, "A Comparative Study of Surface Energies and Water Adsorption on Ce-Bastnästite, La-Bastnästite, and Calcite via Density Functional Theory and Water Adsorption Calorimetry," Physical Chemistry Chemical Physics, 19 (2017) 7820-7832.

• Corrosion chemistry

A major effort has been devoted to investigating the effect of solution chemistry on corrosion phenomena. The MSE model has been applied to model the behavior of corrosion products in environments containing carbon dioxide, hydrogen sulfide and salts. Preliminary results of this work have been published in: S. Smith, A. Anderko, and P. Wang, "Effects of Non-Ideal Chemistry on Corrosion Testing," Materials Performance, 56 (2017) 44-47

• Other topics

As continuation of our work on modeling natural aqueous environments, we focused on the behavior of systems containing hydrocarbons, carbon dioxide and hydrogen sulfide. A small part of this work has been published in:

J. Loring, D. Bacon, R. Springer, A. Anderko, S. Gopinath, C. Yonkofski, C. Thompson, B. McGrail, K. Rosso, and H. Schaef, "Water Solubility at Saturation for CO2-CH4 Mixtures at 50 °C and 90 bar," J. Chem. Eng. Data, 62 (2017) 1608-1614

Also, we have completed a project on simulating the behavior of calcium, magnesium, and zinc silicates in aqueous systems. This project has been designed to address the need to predict phenomena associated with SAGD (steam-assisted gravity drainage) processes.

Name	Middle name	Vorname	Country
Ryo		Akasaka	Japan
Yoshifumi		Asahi	Japan
James	С	Bellows	USA
Kirk		Buecher	USA
Luis		Carvalho	Canada
Adam		Caswell	UK
Dorthe		Christensen	Denmark
Willy		Cook	Canada
Barry		Dooley	UK
Rainer	Erich	Feistel	Germany
Sabine		Feistel	Germany
Vito	Claudio	FERNICOLA	Italy
Daniel	G.	Friend	USA
hitoshi		fukushima	Japan
Qiulin		Gong	China
Satoshi		Hanawa	Japan
Allan		Harvey	USA
Wolfgang		Hater	Germany
Stefan		Herrig	Germany
Hideo		Hirano	Japan
Jan		Hruby	Czech
Taro		Ichihara	Japan
Masaki		lijima	Japan
Kenichi		Imai	Japan
Nobuo		Ishihara	Japan
Jorgen	Peter	Jensen	Denmark
Lidde	Bagge	Jensen	Denmark
Xuxiang		Jia	China
Gary	Arthur	Joy	Australia
Теа		Joy	Australia
Jana		Kalová	Czech
Masato		Kanedome	Japan
Shozo		Kaneko	Japan
sachi		katsura	Japan
Toru		Kawaeda	Japan
Yoshitaka		Kawahara	Japan
Hirotaka		Kawamura	Japan
Yohei		Kayukawa	Japan

List of Participants in IAPWS2017 (in Kyoto)

Moataz		Khalifa	Egypt
Haruka		Kido	Japan
Hans-Joachim		Kretzschmar	Germany
Monika		Kretzschmar	Germany
Petra		Kusova	Czech
tian		li	China
HaiYan		Li	China
DEREK		LISTER	Canada
Jeremy		Lovell-Smith	New Zealand
Nobuyuki		Matubayasi	Japan
Steven	Pullman	McGee	Canada
Nancy		McGee	Canada
David		McGee	Canada
Elizabeth		McGee	Canada
Karsten		Meier	Germany
Kiyoshi		Miyagawa	Japan
Hiroyuki		Miyamoto	Japan
Shintaro		Mori	Japan
AYUMU		MORITA	Japan
Ichiro		Myougan	Japan
MASARU		NAKAHARA	Japan
MAYUMI		NAKAHARA	Japan
Kishor	Govind	Nayar	USA
zhang	xiao	ni	China
Monika		Nielsen	Denmark
Anders		Nielsen	Denmark
Tomoki		Nishiyama	Japan
Adam		Novy	Czech
nobuo		okita	Japan
Hirohito		Okuhara	Japan
Konstantin		Orlov	Russia
Darunee		Paenkaew	USA
Reiner		Pawellek	Germany
Rich		Pawlowicz	Canada
Zhouhai		Qian	China
Raffaella		Romeo	Italy
Dagmar		Rosenberg	Germany
Michael		Rziha	Germany
Satoshi		Saito	Japan
Tetsuya		Sawatsubashi	Japan
Milan		Sedlar	Czech

Steffen		Seitz	Germany
Shigeki		Senoo	Japan
Sho		Shinotsuka	Japan
Roland		Span	Germany
Michael	Amos	Sparrey	υκ
Toshio	Tahara	Tahara	Japan
Tadashi		Tanuma	Japan
Karsten	Normann	Thomsen	Denmark
Hiroshi		Uchida	Japan
Masakatsu		Ueno	Japan
Sayako		Ueno	Japan
Yoichi		Wada	Japan
Koichi		WATANABE	Japan
Fujiko		WATANABE	Japan
Aina		Wu	China
Naoko		Yamaguchi	Japan
Kenji		Yasuoka	Japan
Ken		Yoshida	Japan
Chuan		Zhang	China
Mincong		Zheng	China