THE INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

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

Rotorua, New Zealand
28th November and 2nd December 2022

Prepared by Barry Dooley

IAPWS

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of the
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28th November and 2nd December 2022

Plenary Session. Monday, 28th November 2022. 9:00am

At 9:00 the President of IAPWS, Professor Masaru Nakahara welcomed the Executive Committee (EC) and other IAPWS members to the Executive Committee (EC) Meeting. He first asked the Chair of the New Zealand National Committee, Mr. David Addison, to welcome the EC to Rotorua, New Zealand. Addison thanked the sponsors of this IAPWS meeting. The President then officially opened the 2022 EC Meetings by introducing the National Delegates. All of the IAPWS Members except BIAPWS were in attendance, and only Italy of the Associate Member countries was in attendance. In total there were 32 people assembled for the EC meeting.

1. Adoption of Agenda

Provisional agendas had been e-mailed to all IAPWS members by the Executive Secretary in July 2022. There were no additions and the final agenda forms Attachment 1 of these minutes.

2. IAPWS Business and Appointment of Committees

2.1 IAPWS Business Since Last EC Meeting, Virtual 17th September 2021

During the year since the last IAPWS EC Meeting activity took place on the following documents with regards to IAPWS activities:

- *Release on the IAPWS Formulation 2021 for the Thermal Conductivity of Heavy Water 2020.* IAPWS 2021 Minute 6.1 indicated that the WG had approved the release and requested the EC to authorize a Postal Ballot following review by the Editorial Committee. The document was circulated for a Postal Ballot on 29th September 2021. No objections were received by 29th December 2021, so the Release became an official IAPWS document (IAPWS R18-21).
- On 19th June 2022 a postal ballot was conducted based on the recommendation of a Task Group formed by the IAPWS President which indicated that the Russian National Committee should be suspended from the IAPWS Executive Committee, with such suspension being indicated on the IAPWS website with the accompanying note: *The IAPWS Executive Committee has suspended the membership of the Russian National Committee because of Russia's war of aggression against Ukraine*. The postal ballot was completed on 18th July 2022 and the motion was approved. The Task Group and activity will be reviewed at the next IAPWS EC meeting in New Zealand (see Minute 2.6).
- On 15th June 2022 a special postal ballot was conducted at the request of the PCC Chair to undertake an additional task/project on the Corrosion Product Sampling, Analysis and Assessment Project. This International Collaboration Project (ICP) was initially approved by the Working Group Chairs and the EC in Banff at the 2019 IAPWS meetings. This additional activity will involve the collection and production of standardized Quality Control samples for corrosion products. This will ensure high quality data, minimise errors and help to produce a future world class IAPWS Technical Guidance Document (TGD). The full proposal is Attachment 2 to these minutes. No objections were received by 15th September 2022, so the additional ICP was approved.

2.2 IAPWS Highlights and Press Release

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 a person from NZAPWS assist in this development and in this regard Addison agreed to assist Cook. The Clerks of Minutes from each WG were asked to provide input. The Press Release is discussed in Minute 18.1 and is Attachment 13.

2.3 Evaluation Committee on International Collaboration.

The President indicated that two proposal had been received by the Executive Secretary prior to the meeting, and that any other 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 IAPWS Awards Committees for 2023

2.4.1 Honorary Fellow Award Committee

A committee of Harvey (Chairman) and Kretzschmar were selected for the 2023 Honorary Fellow award with the President and Executive Secretary as ex. Officio members.

Action: Nominations are due to the Executive Secretary by 31st January 2023.

2.4.2 Helmholtz Award Committee

The Executive Secretary reminded the EC that the Helmholtz Award selection committee for the 2023 award would consist of a member from Australia (Chair) (McAllister), BIAPWS (Morris), Canada (Palazhchenko), Czech Republic (Hruby) and Germany/Switzerland (Hellmann).

Action: Nominations are due to the Executive Secretary by 31st January 2023.

2.4.3 Gibbs Award Committee

The President reminded the EC that the Gibbs Award is awarded about every five years at each ICPWS. He then requested that the heads of National Committees, Working Groups and Sub-committees provide a nomination for the 2024 Gibbs Award by 1st May 2023 to the Executive Secretary. A Gibbs Award selection committee also needed to be formed early and the President requested that one person from each Working Group be nominated at the Friday EC meeting and the award committee will then be chosen with no duplication of country.

2.5 Update Report on 18th ICPWS

The President requested the Head of the US National Committee (Friend) to report the status details on hosting the 18th ICPWS in 2024. Friend indicated the following points:

- The U.S. National Committee will Host the ICPWS between 23rd and 28th June 2024 in Boulder, Colorado in conjunction with the triennial Symposium on Thermophysical Properties (STP)

- The logistics and activities will be integrated with ICPWS and STP being differentiated as feasible/appropriate
- Harvey and Friend will be Co-Chairs
- U.S. National Committee for IAPWS will serve as host with the organization having a Local Organizing Committee (LOC) and an International Program Committee (IPC). The IPC will include WG chairs and the Executive Secretary.
- The IAPWS IPC will provide two organizers for ICPWS sessions and one for Joint Sessions and will select and organize ICPWS papers. The joint conference will be located on the Colorado University campus at Boulder.

Friend indicated that because of the joint nature of the conference that the US National Committee will probably not need any seed money up front. But he proposed that the usual ICPWS Donation of £25,000.00GBP be approved by the EC just in case.

The EC approved this proposal unanimously.

Friend also suggested that the IPC members should meet during the week to review the draft announcement and prepare topic areas.

2.6 Situation in Ukraine

As delineated in Minute 2.1 the IAPWS EC had by postal ballot approved (18th July 2022) suspending membership of the Russian National Committee. The President requested the Chair of the Committee (Friend) to review the situation and lead a discussion of any possible IAPWS future activities. Friend indicated that there had not been any changes to the aggression and suggested to the EC that there were no reasons to change the suspended membership. Action would be initiated when there was a change in the conflict.

2.7 Other Business Requiring Extensive Discussions

No other business was raised by the EC.

3. EC Mandate to Working Groups and Membership

The following mandates were given to the WG Chairmen for action during the week.

3.1 Releases, Guidelines and Certified Research Needs.

The Executive Secretary indicated that the following ICRNs needed attention during the week: #16 Thermophysical Properties of Seawater, #22 Steam Chemistry in the Phase Transition Zone (PTZ), #25 Corrosion Mechanisms, #26 Behaviour of Aluminium in Water/Steam, #29 Uncertainties in Coolant Sampling for Low Concentration Metals, and #30 Thermophysical Properties of Supercooled Water.

3.2 Working Group Directions.

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

4. Preview of the IAPWS Week's Activities

President Nakahara indicated that there would be the IAPWS Symposium and a NZAPWS Workshop on Wednesday and Thursday, 30th November and 1st December 2022 respectively. The details are included in Attachments 3 and 4. He then asked each WG Chair to provide an outline of activities during the week

Following this item, the President closed the opening session of the EC at 10:02am.

Activities During the Week
The first day activities of the Executive Committee were followed by Working Group meetings, the IAPWS Symposium and NZAPWS Workshop (the programme for the week is included in Attachment 5).

Executive Committee Meeting. Friday, 2nd December 2022
President Nakahara opened the continuation of the EC Meeting at 9:04 am. All of the IAPWS Members except BIAPWS were in attendance, and only Italy of the Associate Member countries was in attendance. In total there were 18 people assembled for the EC meeting.

Nakahara asked the EC if there were any additional items that should be added to the EC Agenda. None were suggested.

5. Acceptance of Minutes of Previous Meeting

President Nakahara asked for comments and changes to the minutes of the Virtual EC meeting held on 17th September 2021. No changes were noted; thus the 2021 Minutes were accepted.

6. President's Report

President Nakahara had provided his report at the opening of the IAPWS Symposium. This is provided in these minutes as Attachment 6.

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

Minutes of the TPWS WG conducted during the week are in Attachment 7. TPWS Chairman Meier discussed the following items with the EC:

7.1 Replacement of the IAPWS-95 Formulation.

Planning is beginning on what will be a large project to replace IAPWS-95. The first step will be organization and evaluation of available experimental data. The WG recommended a proposed International Collaboration project to accomplish this step (see Minute15.1).

7.2 Trace Water Measurements in Ultra Pure Gases

The PROMETH2O project (www.prometh2o.eu) is developing the European metrological infrastructure and the measurement technologies to provide a robust traceability for water measurements in ultra high purity gases, filling the gap and meeting the needs of improved trace water measurement methods and standards for the amount fraction range between 5 ppm and 5 ppb (or, equivalently, between -65°C and -105°C frost point temperature).

7.3 Second Cross Virial Coefficients of Aqueous Gas Mixtures

A Guideline for a Virial Equation of State for Aqueous Gas Mixtures will be developed based on theoretically calculated virial coefficients using ab initio potentials. This may also include enhancement factors coordinated with the PROMETH2O project. A Task Group for the development of the Guideline was appointed consisting of Fernicola, Harvey, Hellmann, and Meier.

7.4 ICRN -16. Thermophysical Properties of Seawater.

This ICRN was originally adopted in 2007, revised in 2010 and 2014, and expired 2019. In the absence of members of the SCSW, TPWS appointed Hrubý and Pawlowicz as a Task Group to bring a recommendation to the 2023 IAPWS meeting.

7.5 ICRN-30. Thermophysical Properties of Supercooled Water.

This ICRN was originally adopted in 2015 and expired in 2020. This area is important enough that a new ICRN should be produced. A Task Group for the Thermophysical Properties of Supercooled Water was appointed in 2021 (Hellmuth (chair), Caupin and Lago). The Task Group was asked to prepare a closing statement for ICRN-30 and draft a new ICRN for 2022. Hellmuth resigned as Chair of the Task Group so Meier was requested to contact Caupin to check if he could lead the Task Group. If this is not possible, it will be discussed at the 2023 Meeting how to proceed.

7.6 Future of the Subcommittee on Seawater

The TPWS Chair reported that there were no attendees from SCSW at 2022 meeting, but messages had been received from Pawlowicz and Feistel during the meeting. The JCS (Joint Committee on Seawater) was active during the Covid-19 pandemic and Pawlowicz is still the Chair of JCS. Feistel resigned as Vice Chair of JCS, and no successor has yet been found. Seitz replaced McDougall as 2nd Vice Chair of JCS. Meier reported that TPWS wants SCSW to continue and that Pawlowicz, Feistel and Seitz will be asked to chair the subcommittee and plan for continuation at 2023 meeting.

7.7 TPWS Membership and Officers

The TPWS Chair proposed one new WG member:

Dr. Michal Duška (Czech Republic), Institute of Thermomechanics, Czech Academy of Science.

The EC approved the new WG member unanimously.

The TPWS Chair also informed the EC that Harvey will step down as Vice-Chair after the IAPWS 2022 Meeting.

The EC approved this new TPWS officer arrangement unanimously.

8. Industrial Requirements and Solutions (IRS) Working Group

Minutes of the IRS WG conducted during the week are in Attachment 8.

8.1 Task Group Updates

The IRS Chairman Okita provided the EC with updates on five Task Groups. None needed EC approval.

- Task Group on Categories of industrial requirements. Will continue with extended new topics such as hydrogen combustion, clouds micro and macrophysics related to aviation. It will be discussed to cooperate with ASME.
- Task Group on Wet steam properties calculation. Will continue and will interface with the International Wet Steam Modeling Project.
- Task Group on Wet steam data from operating turbines. Will continue with the key being to understand the film forming on stator blade and forming droplets from the water film.

- Task Group on ICRN for acid gas dew points. Will continue. The ICRN is withdrawn and a possible TGD to maintain reliability is considered. A white paper for the TGD will be prepared for the next annual meeting.
- Report of the joint Task Group on White paper on geothermal plant issues. Will continue. A JPAPWS 2nd draft is expected by January 2023 and possible approval of final document at the meeting in 2023 in Italy.

8.2 IRS Officers

The IRS Chair proposed di Mare as the new chair and Harwood as the new vice-chair:

Dr. Francesca di Mare, Ruhr-Universität, Bochum, Germany
Mr. Richard Harwood, Siemens Energy, Inc. USA

The EC approved this new IRS officer arrangement unanimously.

The EC thanked Okita for his excellent leadership of the IRS WG.

9. Sub-Committee on Seawater (SCSW)

Unfortunately, the SCSW Chair, Pawlowicz, could not be present for the EC meeting.

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

Minutes of the PCAS WG conducted during the week are in Attachment 9.

IRS Chairman Yoshida discussed the following items with the EC:

10.1 New Task Group on Ionization of Water

A new PCAS Task Group was proposed by Arcis and Tremaine on developing a revised formulation for the water ionization constant (Kw). A joint PCAS/TPWS Evaluation Task Group is also proposed to first review the revised formulations derived to represent the limiting conductivity of ionized water, and second to evaluate the upcoming revised correlation for Kw. The following members were suggested: Harvey, Palmer, Corti and Wang.

10.2 PCAS Membership

The PCAS Chair proposed one new WG member:

Dr. Amish Patel, University of Pennsylvania, USA, who was the 2022 Helmholtz awardee.

The PCAS Chair also informed the EC that Dr. Frantisek Marsik, Czech Academy of Science, Czech Republic, had requested to be removed from the WG.

The EC approved these WG member changes unanimously.

10.3 On-going and Continuing Task Groups

The PCAS Chair informed the EC of the following activities:

- Guideline on self-diffusion coefficient. Led by Yoshida, in collaboration with TPWS. Development is underway and will be continued.

- Guideline on ionization constant of light water. Led by Arcis and Tremaine, in collaboration with TPWS. Development is underway and will be continued.
- Geothermal White Paper. Collaboration with PCC and IRS. Development is underway and will be continued.
- Possibility of organizing a new group on radiation chemistry. Efforts to reach out to interested researchers in the field are ongoing. There has already been discussion about a joint effort with PCC.

11. Power Cycle Chemistry Working Group (PCC)

Minutes of the PCC WG conducted during the week are in Attachment 10.

PCC Chairman Addison first indicated that ~25 people from New Zealand, Asia, Europe, UK and USA participated in the PCC meetings. He then discussed the following items with the EC:

11.1 Technical Guidance Documents (TGD)

The PCC Chair provided the EC with the following updates on the TGD that were either in preparation or being considered at the 2022 EC meeting:

1. Chemistry in Geothermal plants (White Paper)
2. Corrosion Product Sampling, Monitoring for Flexible and Fast Starting Plants (White Paper and update of TGD)
3. Water Treatment of Flue Gas Condensate White Paper – Draft TGD
4. Chemistry for Electrode Boilers (White Paper)
5. FFS application in Nuclear Plants (White paper and TGD)
6. Demin Water Integrity – retired
7. Condensate Polishing Plants for HRSG plants - retired
8. Informed Alarm Systems – retired.

There is also a joint IRS/PCAS/PCC TGD proposed on Acid Dew Points. A Task Group has been established.

At the 2023 PCC meeting it is intended to review all current TGDs and develop an update/revision program (if required).

11.2 International Collaboration Projects (ICP)

The PCC Chair informed the EC that no new collaborations had been proposed but indicated that the following two current ICP were active:

- Boiler Corrosion – Canada/NZ – work continuing with expanded project but no visits due to COVID.
- Corrosion Products – SIAPWS/BIAPWS/NZAPWS – fully in progress

11.3 PCC Membership and Officers

The PCC Chair proposed the following new WG members:

1. Benjamin Loder, University of New Brunswick, Canada
2. Mads Skovbjerg, VTT Technical Research Centre of Finland, Finland
3. Duncan McAllister, Loy Yang B Power Station, Australia
4. David Rodman, Nalco Water, Australia
5. Pam Yakabuskie, Canadian Nuclear Laboratories, Canada
6. Harold Stansfield, Waltron Bull and Roberts, United States

The EC approved these new WG member changes unanimously.

The PCC Chair next indicated that Rziha will step down as PCC Vice Chair as per 2021 IAPWS meeting. Buecher (USA) was nominated by the PCC WG as PCC Vice Chair.

The EC approved these new PCC officer arrangements unanimously.

12. Editorial Committee Report

Editorial Committee Chairman Harvey reported that in the preceding year, the Editorial Committee (Harvey, Cook and Cooper) had not reviewed any IAPWS Documents prior to publication.

13. Membership and Associates

13.1 Report on Membership

First, the Executive Secretary reported that only Germany had not paid the 2022 dues by the end of October 2022.

The Head of the German National Committee proposed to the EC that a new joint IAPWS national committee be formed from the German National Committee of IAPWS and the Swiss Associate Member committee. The name of this joint committee will be German – Swiss Association for the Properties of Water and Steam (GSAPWS). It is proposed that the following people are the initial officers:

First Chairman: Kretzschmar
Second Chairman: Rziha
Deputy Chairman: Meier
Deputy Chairman: Werder

This proposal led to much discussion on joint membership, dues for joint members, and the current IAPWS dues structure. This discussion resulted in the following four motions to the EC:

- The new joint GSAPWS committee should be approved
- An invoice for the 2022 IAPWS Dues will be prepared and forwarded to GSAPWS for payment in 2022
- The invoice for the 2023 IAPWS Dues will be prepared and forwarded to GSAPWS for payment in 2023
- A Task Group (Friend and Addison) will review the IAPWS Dues structure and report back to the EC at the 2023 meetings in Turin.

The EC approved these motions unanimously.

13.2 Reports on Current Associate Members

The Executive Secretary reported on contacts with Associate Members on their IAPWS status.

Status Report on IAPWS Associate Member, Italy. The delegate of the Italian National Committee, Albo, who was present reported that the Italian National Committee is

planning to become a full member of IAPWS in early 2023 as ITAPWS. The internal approval processes are complete and INRIM have been contacting potential participants.

Status Report on IAPWS Associate Member, Greece. Mr. Antony Thanos, Chair of HIAPWS, indicated that from September 2021 an effort had been carried out to expand the list of people in Greece with an interest in IAPWS activities. Academic and research institutions in Greece were contacted, as well as Greek EPC companies with worldwide activities, Greek power plant operators and people in Cyprus. Fifteen additional people responded positively from all the above sectors, and they were added to the mailing list of HIAPWS, which now includes sixty-five members, who are regularly informed on IAPWS activities. They organized a web symposium for the members of HIAPWS in order to further communicate IAPWS activities and update the HIAPWS status.

Status Report on IAPWS Associate Member, Israel. The Head of ISRAPWS, (Nussbaum) reported that they have built a local community of Operators, Managers, Chemists, and others involved in the operation, maintenance, and design of power plants and process factories. They maintain an annual symposium for the members with information sharing and raise problems through direct personal contacts and presentations sessions.

Status Report on IAPWS Associate Member, China. The new head of the China National committee (Long) reported that the China electric power plant chemical standardization technical committee became an Associate member of IAPWS in May 2017. This group is composed of nearly 40 experts from various research institutes in China. It mainly carries out the formulation and revision of China's standards in Power plant chemistry and organizes some academic activities of power plant chemistry.

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 £125,000.00GBP in total in the UK and US bank accounts. The status as at 31st October 2022 in the bank accounts had been provided to the Head of each IAPWS Member country prior to the EC meeting.

The Executive Secretary next reported that the 2021 financial statements had been forwarded to the IAPWS Auditors in January 2021. Professor Savarik in Czech Republic and Dr. Delfs of VDI in Germany had reviewed and approved the financial statements. These approvals had also been provided to the Heads of each IAPWS Member National Committee prior to the EC meeting.

The Executive Secretary proposed that these organizations be re-appointed to act as auditors The Delegate of the Czech Republic National Committee, Novy, responded that he will have to check with the Czech National Committee and will respond then. The German Delegate, Kretzschmar, indicated positively.

The EC Approved these Actions Unanimously.

The Executive Secretary proposed to the EC that the dues structure for member countries remains unchanged for 2023.

The EC Unanimously Agreed to this Proposal in association with Minute 13.1.

14.2 Time and Place of the 2023, 2024 and 2025 IAPWS Meetings

2023 IAPWS Meetings. The Delegate of the Italian National Committee, Albo, indicated that the Italian NC confirms that the 2023 meetings are planned to be held in Turin on 3 – 8 September 2023. Full details will be provided on the website http://iapws2023.inrim.it/.

2024 IAPWS Meetings. The annual meetings will be held in conjunction with the 18th ICPWS which was discussed in Minute 2.5.

2025 IAPWS Meetings. The IAPWS President and Executive Secretary had reviewed past meeting locations and had asked the Head of SIAPWS, Nielsen, to review with her committee the possibility of holding the 2025 meetings. At the EC meeting she indicated that SIAPWS will be pleased to host the meetings which will be held in Helsinki between 22 – 27 June 2025.

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

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

15.1 International Collaboration Projects.

The President requested the Chairman of the 2022 International Collaboration Committee (WG Chairs) to report on the findings of that committee during the week. Chairman Meier reported that the following two collaboration project had been proposed:

1. *Impact of Metal Ion Complexation on the Radiation Chemistry of Acetohydroxamic Acid in Aqueous Solutions.*
   IAPWS Sponsors: Dr. Jacy K. Conrad, Idaho National Laboratory, USA and Dr. Hugues Arcis, National Nuclear Laboratory, UK.
   Proposed young Scientist: Ms. Elen Clayton, Dalton Nuclear Institute, The University of Manchester, UK.
   Budget: £20,000 GBP (three research stays at INL and BNL)
2. *Towards a Replacement for the IAPWS Formulation 1995: Detailed Analysis of Available Data.*
   IAPWS Sponsors: Dr. Allan Harvey, NIST, USA, Dr. Roland Span, Ruhr-Universität Bochum, Germany and Dr. Jan Hrubý, Czech Academy of Sciences, Czech Republic.
   Proposed young Scientist: Dr. Aleš Blahut, Czech Academy of Sciences, Czech Republic.
   Budget: £9,300 GBP (one stay at NIST, four visits at RUB)

The full proposals are Attachments 11 and 12. Chairman Meier indicated that the committee considered both proposals technically sound for IAPWS and recommended funding both. This led to discussion by the EC of available funds and eventually a decision to vote on each individually. EC members with an interest in either proposal were asked to leave the room.

The EC Unanimously Approved both Proposals for International Collaboration Projects.

16. IAPWS Awards

16.1 Helmholtz Award.

It was noted that the 2022 Helmholtz Awardee (Dr. Patel) provided the Helmholtz lecture at the IAPWS Symposium on Wednesday 30th November 2022. The lecture was preceded by the IAPWS President presenting the Award and reading the citation.

The Helmholtz Award Committee for 2022 had been formulated in Minute 2.4.2.

16.2 Honorary Fellow Award.

The IAPWS President also indicated that there had been two Awardees for 2022: Professor Rich Pawlowicz of Canada and Dr. Frank Udo-Leidich of GSAPWS. As neither of the awardees were present at the EC the awards were given to the heads of the respective national committees for presentation at a later suitable time.

16.3 Gibbs Award.

The President reminded the EC that the process for the Gibbs Award had been formulated at the Monday EC meeting (Minute 2.4.3). Each of the Working Group Chairs in their reports had provided the proposed member of the selection committee:

- TPWS: Meier (Germany)
- IRS: Okita (Japan)
- PCAS: Anderko (USA)
- PCC: Addison (New Zealand)

17. Election of IAPWS Officers for 2023 and 2024

The Executive Secretary indicated that according to IAPWS By-Law 8, the election of the next Vice President should be made at the end of the EC meeting in even years. The Executive Secretary indicated that together with the IAPWS President the recent history had been checked which suggested that the SIAPWS Committee should be asked to nominate one of their committee members for the position. The SIAPWS Chair, Nielsen, had been contacted and was asked to provide her committee's decision. She indicated that SIAPWS had selected her for the position.

The EC Unanimously Approved this Process and Selection.

The current President, Nakahara will step down on 31st December 2022. The current Vice President, Friend, will become the President on 1st January 2023 and Nielsen will become the IAPWS Vice President at the same time.

The EC thanked Nakahara for his leadership over the last two years which had been a tremendously difficult period for IAPWS during the pandemic with no live meetings. The EC applauded.

18. New Business

18.1 Press Release

The President mentioned that Cook (Chair) and Addison had been asked at the EC meeting on Monday to develop a Press Release. This was developed with input provided by each WG. Cook indicated that a document had been prepared. The final version is Attachment 13. 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.

18.2 Reports from National Committees.

Written reports on progress in member countries provided during and after the EC meeting are attached to these minutes as follows:

Czech Republic	Attachment 14
USA	Attachment 15
Japan	Attachment 16

18.3 New Zealand National Committee Feedback on the 2022 EC and WG Meetings.

The Head of the New Zealand National Committee, Addison, thought the IAPWS meetings had been a great success. There had been 60 people attending for the symposium and 113 for the Workshop.

The IAPWS President thanked Addison for organizing the IAPWS week in Rotorua. Applause from EC in appreciation.

18.4 Participants

Attachment 17 provides a list of participants at the IAPWS Meetings in Rotorua, New Zealand in November/December 2022.

18.5 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 EC Meeting. This will be forwarded electronically to the Head of each National Committee and the Working Group Chairs.

19. Closing Remarks and Adjournment

No further business was raised by the EC. The President thanked everybody for participating at this EC meeting. The 2022 EC meeting was closed at 11:50 am.

AGENDA for the EXECUTIVE COMMITTEE of IAPWS
Rotorua, New Zealand. 27th November – 2nd December 2022

Monday, 28th November 2022. Opening Plenary Session (9:00 – 10:15 am)

Opening Remarks, Welcome and Introductions by IAPWS President M. Nakahara
1. Adoption of Agenda
2. IAPWS Business and Appointment of Committees
   - 2.1 IAPWS Business since Last Virtual EC Meeting September 2021
   - 2.2 IAPWS Highlights / Press Release
   - 2.3 Evaluation Committee on International Collaboration
   - 2.4 IAPWS Awards for 2023 (Honorary Fellow, Helmholtz, Gibbs)
   - 2.5 Update Report on 18th ICPWS (ICPWS Chairman Friend)
   - 2.6 Situation in Ukraine (Task Group Chair: Friend)
   - 2.8 Other business requiring special/extensive discussions
3. EC Mandate to Working Groups and Membership
   - 3.1 Releases, Guidelines and ICRNs
4. Preview of Week's WG Activities by WG Chairmen

Friday, 2nd December 2022. Executive Committee Meeting. (9:00am – 1:00 pm)

5. Acceptance of Minutes of Previous Meeting
6. President's Report
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 application of German/Swiss Committee and Members Defaulting on Dues.
    - 13.2 Reports of Current Associate Members (China, Egypt, Greece, India, Italy and Israel)
14. Executive Secretary's Report
    - 14.1 IAPWS Bank Accounts, Financials, Auditors and Dues
    - 14.2 Time and Place of 2023 (Italy) and 2024 (USA) Meetings.
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
17. Election of IAPWS Officers for 2023 and 2024
18. New Business
    - 18.1 Press Release
    - 18.2 New Zealand National Committee feedback on 2022 Annual Meeting
    - 18.3 Other items raised during the IAPWS week
19. Adjournment

IAPWS

Barry Dooley
13th October 2022

Scandinavian IAPWS Committee
c/o IDA, Kalvebod Brygge 31-33
1780 København V

21 December 2022

SIAPWS
ALL ABOUT WATER

Application for International Collaboration
Grant for an International Round Robin
in relation to the 2019 project
Corrosion Product Sampling, Analysis and Assessment

Background

At the 2019 IAPWS meeting in Banff, Canada, the funding for an International Collaboration Project was granted by the EC. The purpose of the project was to make the final investigations and put the plant experience together to finalise a new TGD for corrosion product sampling and analysis for flexible plants, i.e., plant operating in a very variable mode with frequent start/stops and continuously varying load. One key result of this collaboration project is to calibrate and fine-tune the IAPWS Decay Map which was developed as part of the initial IAPWS collaboration. The initial plan was to run the project in 2020, but this was halted by the outbreak of Covid-19 worldwide. Since the beginning of 2022, work has been going on to start the project, a host site (VTT in Finland) has been found, and the project opportunity has been advertised to students in the Nordic countries. The project is expected to run from August 2022 and 6-12 months forward. Collection of plant experience, i.e., data from start-ups tracked by the proposed quantitative method developed in the first international project, is a major focus point this time. To make sure that the data sets from many plants are comparable and not hampered by analysis errors, an international round robin is proposed as an additional task of the original collaborative project, but which was not included in the submittal to the IAPWS EC in Canada. Participation in this will ensure that the methods used for later data collection for the international project are verified at the laboratories taking part and the results compared with those of a group of competent laboratories.
This application applies for an additional grant to be able to realise the round robin that is seen as a critical step to achieve the best possible data quality for calibration of the IAPWS Decay Map. The extra grant will cover the work hours and the costs of preparation and shipping of the many sample sets (around 30) to the participants worldwide, data processing, and reporting of the results.

Technical Aspects and Goals (from the original application in Banff, October 2019)

This planned activity will keep IAPWS in the leadership position with regards to corrosion products monitoring and assessment. The final goal of the activity is to develop the IAPWS Corrosion Product Decay Map that will represent the first standardized method for quantification and comparison of the effects of operational and shutdown chemistry regimes. The field tests conducted to date have demonstrated that, provided correct sampling and subsequent sample handling, on-line measurements such as turbidity and particle number/distribution are useful and reliable means 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 further confirmed to cover all the different chemistries typically applied in various all-ferrous and mixed-metallurgy plants. The outcome of the project will be a master thesis and key reference for the final product: The extension to the present TGD covering sampling, analysis, and assessment of CPs for plants operating in flexible mode. This will allow further minimization of CP transport and the negative consequences during operation, but the most important guidance will be the systematic method to quantify CP transport during start-up

and the IAPWS Decay Map defining the relevant guiding values. Of course, such values must be based on reliable and comparable data. Getting those within the next 1-1½ year 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 Decay 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 measured, the application of on-line methods as valuable tools to optimise 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.

Planning of the Round Robin for 2022

The round robin is planned in detail, and an invitation to participate both in the round robin and the subsequent data collection has been set up at the SIAPWS web-site: IAPWS Round Robin and Collaborative Project for Corrosion Products. This page is not yet public, but it is ready for use introducing both purposes.
Vattenfall in Sweden has volunteered their plant in Uppsala as site for preparation of the authentic grab and filter samples to be distributed. The plant consists of several municipal waste boilers in operation around the year, so adequate sampling points and levels of iron are present.
The subtasks to produce the set of equal samples to be distributed to the participants are outlined here:
Task 1

- Initiation of Ferrozine method at lab, calibration, test on QC-samples, test on grab samples
- Data handling - set up of Excel forms for data registration

Task 2

- Initial test of sample points taking both grab and filter samples
- Sampling at a several possible sample point to select those with suitable iron levels

Task 3

- Purchase of sample bottles needed for the round robin (and chemicals for analysis)

Task 4

- Test run on selected sample points
- Sampling grab and filter samples over 1-2 hours from selected sampling point
- Analysis of samples to document suitable iron levels, stability, and equal levels between grab and filter samples

Task 5

- Sampling from selected sample points and analysis to ensure levels consistent with earlier results
- Sampling for test items, i.e., grab and filter samples for participant and test of homogeneity
- Filtration of filter samples, drying of filter in protected place

Task 6

- Selection of samples for homogeneity test
- Analysis of samples for homogeneity test
- Evaluation of samples: OK for round robin or not?

Task 7

- Preparation of QC-samples to be distributed

- Packing of grab samples, filters, and QC-samples for the participants
- Shipping of sample sets to participants

Task 8

- Registration of submitted data into Excel forms
- Data processing according to the standard ISO 13528:2015
- Preparation of graphical display of results

Task 9

- Writing of common report
- QA of report
- Distribution of report
- Informing individual participant on their lab-ID

Budget for the Round Robin

Expenses to be covered:

Task	**Description of task**	**Budget (GBP)**
1	Preparing and testing of samples	4,100
2	Lab equipment (chemical for analysis, ultrapure membrane filters, ultrapure sample bottles)	2,600
3	Boxes and wrapping for sample bottles and filters including shipping of samples to participants worldwide	2,300
4	Registration of and communication with participants including initial registration and processing of the data submitted.	3,000
	Total	**12,000**

Total budget is estimated to 12,000 GBP.

On behalf of IAPWS organisation in the Nordic countries (Sweden, Norway, Denmark, Finland), Britain and Ireland and New Zealand.
Monika Nielsen, SIAPWS Chair, member of PCC and the International Collaboration Project Steering Group.
Ryan Morris, BIAPWS Chair.
David Addison, NZAPWS Chair, PPC Chair.

THE 2022 IAPWS Symposium Program

9:00 – 9:10 **Introductory Remarks**
Prof. Masaru Nakahara - IAPWS President, Kyoto University, Japan

9:10 – 9:55 **Helmholtz Lecture and Award Presentation**
How do Surfaces with Nanoscale Heterogeneity Perturb Water Structure?
Dr Amish Patel Associate Professor in Chemical and Biomolecular Engineering at the University of Pennsylvania, US

9:55 – 10:05 **Welcome to IAPWS and the IAPWS and NZAPWS Supercritical Geothermal Symposium**
David Addison Chairperson NZAPWS, IAPWS PCC Chairperson,
Principal Consultant, Thermal Chemistry Limited, NZ

10:05 – 10:50 **KEYNOTE:**
New Zealand's Energy and Geothermal Future. Opportunities and Challenges
Vince Hawksworth Chief Executive, Mercury NZ Limited

10:50 – 11:20 ***MORNING TEA***

11:20 – 11:35 **Geothermal the Next Generation Research Programme Introduction** –
Including thoughts on Using the Fluids at the surface and drilling to access the super critical resources
Brian Carey Geothermal Resource Management Specialist - GNS Science

11:35 – 12:35 **Volcanism in the Taupo Zone and Geophysics**
OVERVIEW: • Magnetotellurics • Seismic Attenuation Studies - identifying rock mush • Magnetics • Depth to 560o C conditions derived for Curie Point Modelling
Pre-recorded Video Presentations
Dr Geoff Kilgour, Dr Craig Miller, Dr Ted Bertrand, Dr Stephen Banister -GNS Science

12:35 – 13:20 ***LUNCH***

13:20 – 14:00 **Overview of conditions and issues**
GNS Experimental capability • Silica and anhydrite solution studies at super critical conditions
Dr Bruce Mountain, Dr Peter Rendel

14:00 – 14:20 **Geothermal steam sampling and online analysis of trace sodium and silica and interference removal via gas transfer membranes and sulfide to sulphate converters**
David Addison Principal Consultant, Thermal Chemistry Limited, NZ

14:20 – 14:50 ***AFTERNOON TEA***

14:50 – 15:50 **MODELLING** • Methodology for national inventory of supercritical resources Modelling to assess project potential • Deep sub critical models and the supercritical to sub critical transition with the challenges crossing the critical point in modelling • Modelling well outputs producing from 6 km deep supercritical wells
Chris Bromley Dr Warwick Kissling Dr John Burnell Julius Riveria GNS Science

15:50 – 16:10 **Geothermal Supercritical Fluid Steam Transformer Design Concepts**
Peter Rop (presented by David Addison) NEM Energy, Netherlands

16:10 – 16:40 **Reducing Greenhouse Gas Emissions from Geothermal Power Generation**
Ian Richardson Capability Lead - Operations Generation & Development, Contact Energy, NZ

16:40 – 16:50 **Clean Energy European Metrology Network**
Dr P. Alberto Giuliano Albo Researcher, Istituto Nazionale di Ricerca Metrologica, Italy

16:50 – 17:00 **OPEN DISCUSSION: Geothermal supercritical**

17:00 – 17:15 **Closing Remarks**
David Addison Chairperson NZAPWS,
IAPWS PCC Chairperson, Principal Consultant, Thermal Chemistry Ltd

The 2022 IAPWS Workshop Program

8:30 – 8:45 **Welcome to NZAPWS Future of Steam Workshop**
David Addison, NZAPWS Chairperson

8:45 – 9:05 **Update on IAPWS TGDs**
Barry Dooley, IAPWS Executive Secretary

9:05 – 9:15 **Introduction to electrode boilers in NZ, projects, issues and solutions**
David Addison, Principal Consultant, Thermal Chemistry Limited

9:15 – 9:35 **Orsted 's (Denmark) Experience and Issues with Electrode Boilers**
Monika Nielsen SIAPWS Chairperson / Lead Chemistry Specialist, Orsted, Denmark

9:35 – 9:55 **Synlait Electrode Boiler Project**
Alan Beuzenberg, Energy and Utilities Manager, Synlait

9:55 – 10:15 **Mataura Valley Milk Electrode Boiler Project**
Robert Barrack, Technical Director, Process Systems, Aurecon¬†

10:15 – 10:40 ***MORNING TEA***

10:40 – 11:00 **Electrode Boilers verses Resistive Element Boilers. The Pros and Cons of each**
Brendon Stephenson, General Manager, Energy Plant Solutions

11:00 – 11:20 **WoolWorks Electrode Boiler Project**
Anita Zunker, Engineering Manager, PEI Group Limited

11:20 – 11:35 **Decarbonising steam generation by electrifying your existent fossil fuel boiler – technology and case studies**
Fabiano Gatto, General Manager - Spirax Sarco New Zealand

11:35 – 11:55 **OPEN DISCUSSION: Electrode boilers in NZ and water/steam related issues**
Electrode Boiler Discussion Panel Electrode Boiler Presenters

11:55 – 12:15 **Geothermal Industrial Steam Opportunities at the Kawerau Steam Field**
Robbie Watt, General Manager - Geothermal, Ngati Tuwharetoa Geothermal Assets Ltd

12:15 – 13:00 ***LUNCH***

13:00 – 13:20 **Computational fluid dynamics (CFD) and non-linear finite element analysis (FEA) modelling for Industrial Boilers**
Paul Bosauder, Principal Engineer and Director, Sequence

13:20 – 13:40 **Fonterra's Future for Steam**
Tony Oosten, Energy and Climate Manager, Fonterra

13:40 – 14:00 **Fonterra Stirlling Biomass Boiler Project**
Ian Hall Senior Engineering Project Manager, Fonterra

14:00 – 14:20 **Coal Boiler to Biomass Conversion Considerations**
Ian Brownlie Project Engineering Team Leader, Windsor Energy

14:20 – 14:25 **AUSAPWS Update**
Justin West AUSAPWS

14:25 – 14:35 **Application of IAPWS TGDs to solve industrial steam plant problems – Dissolved Oxygen Case Study**
Justin West Industrial Water Services - Australia

14:35 – 15:00 ***AFTERNOON TEA***
15:00 – 15:20 **OPEN DISCUSSION: Future of Steam in NZ All Presenters**
15:20 – 15:40 **Industrial boilers analyser considerations**
Mar Nogales Swan Analytical Switzerland

15:40 – 16:00 **Considerations for Future Utility Systems Combining Biomass and Electrode Boilers** Dr Marty Atkins Senior Lecturer, School of Engineering - The University of Waikato
16:00 – 16:20 **Water as a Working Fluid in Industrial Heat Pumps**
Dr Tim Walmsley Senior Lecturer, School of Engineering - The University of Waikato

16:20 – 16:40 **Formation Mechanism and Microscopic Structure of Corrosion Protective Coating for Steam Piping by Film-Forming Amine**
Dr Ken Yoshida Associate Professor - Tokushima University

16:40 – 17:00 **New Generation Film Forming Substances for Industrial Applications**
Bill Snodgrass Product Application Engineer, Veolia Water Technologies and Solutions

17:00 – 17:20 **Industrial applications for FFS in NZ**
Marty Templeton Managing Director, Visentia

17:20 – 17:30 **Closing Remarks**
David Addison NZAPWS Chairperson

Schedule of IAPWS Meetings
Rotorua, New Zealand. 27th November – 2nd December 2022
(All technical meetings will be at the Novotel Rotorua Lakeside)

Sunday 27 Nov.	6:00 – 7:30 pm	Welcome Reception and Registration **Rotorua Novotel**
Monday 28 Nov.	9:00 am	**Executive Committee - Opening Plenary Session**
	10:15 am	Coffee / Tea Break
	10:30 am	TPWS/IRS Joint Meeting (To set agendas for the week and to conduct IAPWS Business, thus allowing remainder of week for technical matters)
	10:30 am	PCAS and PCC Separate Meetings (To conduct IAPWS Business, thus allowing remainder of week for technical matters)
	12:00 pm	Lunch
	1:30 pm.	TPWS/IRS Joint Meeting
	1:30–3:30 pm	PCC and PCAS Joint Meeting
	3:30 pm	PCC and PCAS Separate Meetings
Tuesday 29 Nov.	9:00 am	PCAS and TPWS Joint Meeting
	9:00 am–Noon	PCC WG Meeting
	9:00am	TPWS/IRS Joint or Separate Meetings
	10:30 am	TPWS/IRS Joint or Separate Meetings
	10:30 am	PCAS Separate Meeting
	12:00 pm	Lunch
	1:30 pm	TPWS/IRS/PCAS/PCC Joint Meeting.
	1:30 pm	PCAS and IRS Joint Meeting
	3:30 pm	PCC and PCAS Separate Meetings

Wednes. 30 Nov.	9:00 am–5:00 pm	**IAPWS Symposium Supercritical and Subcritical Geothermal Steam Chemistry**
	6:30 pm.	**IAPWS Dinner/Banquet**. (Te Puia, Rotorua. https://www.tepuia.com)
Thurs. 1 Dec.	9:00 am–5:00 pm	**NZAPWS Workshop** **The Future of Industrial Steam in New Zealand**
	9:00 am	TPWS/IRS Separate or joint WG Meetings or Part of Workshop
	9:00 am	PCAS Separate WG Meeting or Part of Workshop
	12:00 pm	Lunch
	1:30 pm	Separate meetings of Working Groups (if needed)
Friday 2 Dec.	9:00 am	**Executive Meeting (9:00am - 1:00pm)** (Will include at least one member from each National Member Delegation)
	1:30 pm	**IAPWS Technical Visits** (Geothermal Power Station/Facility – Mercury Kawerau or Geothermal. Tuwharetoa Travel arranged to leave at 1:30pm)

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

23rd November 2022

IAPWS President's Report

Welcome to the delegates and everybody else to the IAPWS Meeting 2022 here in Rotorua, New Zealand. This time we have the traditional face-to-face type of annual meeting following the one in Banff (2019). We have been suffering from the pandemic COVID-19 and the CIVILIZATION DESTRUCTION in Ukraine by Russia. We hope that this aggression will stop as soon as possible. I thank the Chair of NZAPWS, Mr. David Addison, for great efforts in assembling this meeting. I am happy to have a chance of expressing my thoughts about the present situation and future perspectives of our organization, IAPWS,

Many thanks to the hard-working chairs, Karsten Meier, Nobuo Okita, Ken Yoshida, and David Addison, respectively, of the IAPWS Working Groups; TPWS, (Thermophysical Properties of Water and Steam), IRS (Industrial Requirements), PCAS (Physical Chemistry of Aqueous Systems), and PCC (Power Cycle Chemistry). All the chairs have worked elaborately to make creative contributions to IAPWS. Many participants have joined us to stimulate and deepen our discussions in the IAPWS 2022 meetings in New Zealand. Consider how best to utilize such IAPWS products as Releases, Guidelines, Technical Guidance Documents (TGD), and IAPWS Certified Research Needs (ICRN). All of these are characteristic of the IAPWS business. The useful IAPWS products are now popular all over the world. You can make access to the IAPWS website when you have any interest or question about water/steam (WS). I am sure you can learn about the treatment, handling, and monitoring of WS as well as the scientific formulation and meaning. Here are so many good engineers and scientists.

Where are we going now with Water and Steam in IAPWS? Any kind of technology is unavoidably subjected to changes after some level of saturation. In the ancient age, humans discovered how fire could be combined with hot water and steam to generate power required for cooking. In the longterm human dreams are variable and unsaturated. Hundreds of years after the Renaissance, James Watt succeeded in dramatically improving the steam engine that employs Water and Steam by a boiler. Many ideas employed at that time have been transferred to the technology used in power/electricity generation. Now we meet input and output energy problems as fuels are burned to transform the chemical bond energy to heat. For example, steam engines have been taken over by electric motors on a large scale. We should recognize electricity is required for our life; even EVs (Electric Vehicles) that can reduce carbon emissions and cool down Earth to some extent. EVs can't run without electricity. It is said: The cheaper the better. The cheaper the more poisonous. Don't forget about possible dangers around us. Nothing is perfect; Water and Steam are not exceptional.

It is highly expected that Earth can be cooled down by decarbonation or CCS. At present nobody knows to what extent we can reduce the global warming rate by sustainable energies. I hope something more will be done by the geothermal energy inherent in Earth. As mentioned in the last year's president statement, most of the energies, originate from the Sun as in the form of light and heat with the broad range of electromagnetic wavelength. The Sun is continuously producing huge amounts of atomic energy by nuclear fusion reaction of hydrogen. Geothermal energy is being born in the Earth's core that has nuclear fission reactions at the high temperature and high pressure. The nuclear high energy generated in the core is transformed into thermal energy through the deep and thick magma, hot melted rock below the Earth surface. Strong radiation is mostly confined in the core and screened and diluted before reaching the very thin Earth crust. Moreover, the use of geothermal energy can reduce the possibility of dangerous explosions of volcanoes by releasing the excess atomic energy in the Earth core and help us cool down Earth as well as the sustainable ones. Through geothermal power we can use inexhaustible WS as the heat energy carrier. WS are friendly to Earth while such light-element heat carriers as Li and He are very expensive. I mean WS power will continue under the influence of a variety of technological developments.

We tend to fear the radioactivity produced by nuclear reactions. When we feel a fear danger it is important to recognize the permissibility range of danger, the concentration, the degree of dilution or the strength. Of course, the time scale difference is to be understood between the two cases mentioned. Some of the nuclear reaction products have a long lifetime, say, a few ten thousand years that are much shorter than the time spent by human beings from the birth. We are not killed by viruses if the concentration is lower than the limit. The dilution and the decay timer of radioactive species are of great importance. Nuclear energies can't be neglected until sustainable energies have been sufficiently developed. We should be patient. Humans are tough. We are always thinking about devising a new way to overcome such rough water as a deluge and the strong electricity from lightning. We should be careful and sensitive enough to the possible negative factors brought to us by the demerits of technical developments and democracy. We love peace at any time and are to be responsible for the future.

The behavior of Water and Steam is controlled by the free energy changes. The hydration/solvation free energy is key to understanding metal/water interfaces. The stability changes in the interfacial binding among water, organics, and metals are not singly dependent on the products but also on the initial states. In the case of IAPWS businesses the hydration states sensitively vary according to the density and temperature of supercritical water. Recently novel developments have been made for a better understanding of interfacial structure, interactions, and reactions through molecular-level theoretical calculations. They can be used for complicated engineering and biochemical interfacial phenomena, where no analytical solution formulae are available yet. Machine learning using computers is changing the way of molecular simulations based on ab-initio force fields and dramatically expanding the size

and time scales. For the future of IAPWS we should work together to expand engineering by inventing new techniques/methods necessary for the safety and efficiency. Energy-security co-operation contributes to worldwide peace. We should not miss the good chance at this time. Thank you for your exciting attention. Finally, thanks Barry for your beautiful arrangement of the EC meetings.

IAPWS Thermophysical Properties of Water and Steam WG
Rotorua, New Zealand, 28-29 November 2022

NOTE: These Minutes include some items that were held jointly with the IRS and/or PCAS Working Groups. 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, November 28, 2022, at approximately 10:30 by the TPWS Chair, Karsten Meier. A modified Agenda was adopted (Attachment A). The 2021 Minutes had been circulated and approved by email shortly after the 2021 virtual meeting. Allan Harvey was appointed Clerk of Minutes for TPWS.

3. Tributes for deceased colleagues.

A. Harvey presented brief tributes to three IAPWS contributors who had died in recent years: Bob Spencer (IAPWS Honorary Fellow), Bill Parry, and Christopher Wormald. H.-J. Kretzschmar read a tribute to Francisco (Pancho) Blangetti that had been prepared by Michael Hiegemann and Bobby Swoboda. The Chair led the Working Groups in a moment of silence.

4. Potential International Collaborative Projects

The Working Group discussed a proposed project (involving the Czech Republic, Germany, and the U.S.) titled "Towards a replacement for the IAPWS Formulation 1995: Detailed analysis of available data". **The WG unanimously endorsed the proposal**.

5. State of Development of a New Formulation for the Thermodynamic Properties of Ordinary Water (Replacement of IAPWS-95). (A. Harvey, D. Friend, J. Hrubý, N. Okita, K. Orlov, R. Span)

A. Harvey reported on the various reasons for replacing IAPWS-95 in the coming years (including small flaws in the equation of state, new data including many good sound-speed measurements, advances in technology for developing reference equations of state). There are still some data needs as expressed in IAPWS ICRN 31, but it seems unlikely that many of these needs will be met in the timeframe envisioned for the effort. A question was raised about when a new EOS might be ready, but it is too early to say. It was discussed that the new EOS should behave accurately for the metastable vapor and liquid below the triple point, and that more rigorous uncertainty information would be desirable.

6. Metrology for trace water in ultra-pure process gases (P. Alberto Giuliano Albo)

P.A. Giuliano Albo reported on the PROMET-H2O project led by his colleague Vito Fernicola. The purpose is to develop metrology for measurement of trace amounts of water in ultra-pure process gases in applications including energy systems and semiconductor processing. Pressures will be up to 1 MPa, with dew-point temperatures ranging from −105 °C to −65 °C corresponding to roughly 5 ppb to 5 ppm H_2O in the gas. Several different experimental approaches are being explored, and there will be some component of developing recommended enhancement factors for ice in common gases. It was discussed that those recommendations might be made into an IAPWS Guideline (see item 11.2).

7. IAPWS Certified Research Needs (ICRNs)

Two expired ICRNs were discussed, although in neither case were the key people present. For ICRN-16 (Properties of Seawater), **J. Hruby and R. Pawlowicz (if the latter is willing) were appointed as a Task Group to evaluate the situation and bring a recommendation to the 2023 meeting**. For ICRN-30 (Properties of Supercooled Water), some new data have become available but a new leader of the IAPWS efforts in that area is needed as O. Hellmuth is not able to continue. **The WG Chair will contact F. Caupin about taking the lead in revising the ICRN**. If that is not possible, we will discuss in 2023 how to proceed, perhaps by making a Closing Statement.

NOTE: Item 8 is reported on in the IRS minutes.

8.1 Report of the Task Group "Categories of industrial requirements" (N. Okita, chairs or representatives of other WG)

8.2 Report of the Task Group "Wet steam properties calculation" (A. Nový, J. Hrubý, K. Orlov, R. Span, K. Meier, Francesca di Mare, S. Senoo, M. Kunick)

9. Heavy Water Properties

9.1 Progress on a formulation for the static dielectric constant of heavy water (J. Cox, J. Young, A. Harvey, and P. Tremaine)

A. Harvey reported on behalf of the Task Group, which has been slowed by the departure of J. Young from NIST. Work is expected to resume in early 2023. The plan is to make one formulation that would be a simple modification or correction to the IAPWS H_2O formulation, limited to the liquid up to perhaps 300 °C, and then a second, comprehensive formulation covering the whole fluid range that would not have the flaws of the H_2O formulation. The time frame is still unclear due to limited availability of personnel. It was recalled that in 2021 we authorized the WG Chair to appoint an Evaluation Task Group during the year if it was warranted.

10. Report of Task Group on surface tension of ordinary water (joint with WG IRS and SC SW) (J. Kalová, V. Vinš, A. Harvey, O. Hellmuth, V. Holten, J. Hrubý, R. Mareš, F. Caupin)

J. Hrubý reported that a new correlation had been published in the past year by Kalová and Mareš. In the discussion, the consensus was that, in the absence of new data (particularly at high temperatures), there was no clear reason to produce a new formulation for IAPWS. However, at some temperatures the uncertainty estimates in the IAPWS formulation are too large, so a revision of those estimates could be worthwhile.

11. Joint session with WG PCAS

11.1 Crystal growth of urea and its modulation by additives as analyzed by all-atom MD simulation and free-energy calculation (N. Matubayasi)

This was a technical presentation about insights gained by molecular simulation on the relative growth rates of different crystal planes in urea.

11.2 Cross second virial coefficients for binary mixtures of water vapor with carbon monoxide, sulfur dioxide, hydrogen sulfide, and hydrogen from ab initio intermolecular potentials (R. Hellmann, K. Meier)

K. Meier reported on the project of calculating high-quality second virial coefficients for water-gas systems based on state-of-the-art ab initio pair potentials. Future calculations will involve water with argon and the light alkanes. These can contribute to calculation of enhancement factors in various contexts.

In subsequent discussion, it was noted that this has overlap with the enhancement factor needs of the PROMET-H2O project discussed in item 6. An IAPWS Guideline on values of $B_{12}(T)$ and/or on the enhancement factor of water and ice in common gases would be useful for a variety of purposes. **A Task Group was appointed consisting of K. Meier, R. Hellmann, A. Harvey, and V. Fernicola (if he is willing to join), with the mission to decide what makes the most sense for a Guideline and to work toward preparing recommended values in convenient form.**

11.3 (This item was cancelled).

11.4 Challenges in modeling the ammonia/water system (I. Bell, A. Harvey)

A. Harvey, on behalf of his colleague Ian Bell, presented some of the problems with the present IAPWS model for the thermodynamics of ammonia/water, along with the data situation for sound speed where the sets of data seem to not be mutually consistent. Some high-quality liquid sound speeds, even if only near atmospheric pressure, would be very helpful in sorting out the proper behaviour. Several factors making this mixture difficult to study were discussed.

12. Reports on seawater-related topics

12.1 New accurate data for the density of cold and supercooled seawater at practical salinity 35 and pressures up to 110 MPa (A. Blahut, J. Hrubý, V. Vinš)

J. Hrubý presented his group's measurements of seawater density extending to 100 MPa and about 10 K of supercooling below the freezing curve. Compared to the IAPWS seawater formulation, there are some significant differences in thermal expansivity in the supercooled region and to some extent along the melting curve.

12.2 A new approach to a comprehensive formulation of thermodynamic properties of seawater (J. Hrubý, A. Blahut)

J. Hrubý reported a new approach to seawater thermodynamics his group has taken involving scaling the pure-water equation and adding an extended Debye-Hückel term. The maximum density points are used in the scaling from the IAPWS supercooled water guideline. Initial results seem promising.

12.3 Discussion on future of Subcommittee on Seawater

The absence of our seawater contingent from this meeting, and from IAPWS in the past 2 years or so, was noted. An email had been received from SCSW Chair Rich Pawlowicz about his difficulty in participating and wondering if the Subcommittee

should be folded back into the TPWS Working Group. The Joint Committee on Seawater is still somewhat active with Pawlowicz as Chair and Steffen Seitz of PTB as a Vice-Chair, but its current work is less IAPWS-related. **It was recommended that the SCSW remain as it is in IAPWS for now, with the following steps to be taken to attempt to revive it: K. Meier contact Pawlowicz, Feistel, and Seitz to get their input on a way forward. P.A. Giuliano Albo contact people he knows in physical oceanography in Italy and France to invite them to the 2023 IAPWS meeting.**

13. TPWS/IRS/PCAS/PCC joint session

This item is reported in the PCC Minutes.

15. Membership

Michal Duška (Czech Republic) was unanimously elected as a new TPWS member.

16. Election of Vice-Chair

A. Harvey will step down as Vice-Chair after the conclusion of this meeting. K. Meier remains as Chair and J. Hrubý remains as Vice-Chair.

17. Contribution to Press Release

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

18. 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.

19. Adjournment

The meeting was adjourned at approximately 17:00 on Tuesday, November 29.

Agenda for the IAPWS Working Group

Thermophysical Properties of Water and Steam (TPWS)
Rotorua, New Zealand, Nov. 27 – Dec. 2, 2022

1. Opening Remarks; Adoption of Agenda [Monday morning]
2. Appointment of Clerk of Minutes
3. Minute's Silence for Deceased Members and Colleagues (A. Harvey, H.-J. Kretzschmar)
4. Potential International Collaborative Projects
5. State of Development of a New Formulation for the Thermodynamic Properties of Ordinary Water (Replacement of IAPWS-95)
   - 5.1 Report of Task Group (A. Harvey, D. Friend, J. Hrubý, N. Okita, K. Orlov, R. Span)
6. Reports on miscellaneous TPWS scientific topics
   - 6.1 Metrology for trace water in ultra-pure process gasses (P. Alberto Giuliano Albo)
7. IAPWS Certified Research Needs (ICRNs)
   - 7.1 ICRN 16: Thermophysical Properties of Seawater (R. Pawlowicz)
   - 7.2 ICRN 30: Thermophysical Properties of Supercooled Water (O. Hellmuth)
8. Industrial Requirements and Solutions for Property Calculations (joint with WG IRS) [Monday afternoon]
   - 8.1 Report of the Task Group "Categories of industrial requirements" (N. Okita, chairs or representatives of other WG)
   - 8.2 Report of the Task Group "Wet steam properties calculation" (A. Nový, J. Hrubý, K. Orlov, R. Span, K. Meier, Francesca di Mare, S. Senoo, M. Kunick)
9. Heavy Water Properties (joint with WG IRS)
   - 9.1 Progress on a formulation for the static dielectric constant of heavy water (J. Cox, J. Young, A. Harvey, and P. Tremaine)
   - 9.2 Appointment of a Task Group for the evaluation of the formulation of the static dielectric constant of heavy water
10. Report of Task Group on surface tension of ordinary water (joint with WG IRS and SC SW) (J. Kalová, V. Vinš, A. Harvey, O. Hellmuth, V. Holten, J. Hrubý, R. Mareš, F. Caupin)
11. Joint session with WG PCAS [Tuesday morning]
    - 11.1 Crystal growth of urea and its modulation by additives as analyzed by all-atom MD simulation and free-energy calculation (N. Matubayasi)
    - 11.2 Cross second virial coefficients for binary mixtures of water vapor with carbon monoxide, sulfur dioxide, hydrogen sulfide, and hydrogen from *ab initio* intermolecular potentials (R. Hellmann, K. Meier)
    - 11.3 Speed of sound measurements in mixtures of ammonia and water (M. Brown, A. Harvey)

11.4 Challenges in modeling the ammonia/water system (I. Bell, A. Harvey)

12. Reports on seawater-related topics (joint with WG PCAS and SC SW)
    12.1 New accurate data for the density of cold and supercooled seawater at practical salinity 35 and pressures up to 110 MPa (A. Blahut, J. Hrubý, V. Vinš)
    12.2 A new approach to a comprehensive formulation of thermodynamic properties of seawater (J. Hrubý, A. Blahut)
    12.3 Discussion on the future of the Subcommittee on Sea Water
13. TPWS/IRS/PCAS/PCC joint session [Tuesday afternoon]
    13.1 Electrode boiler chemistry issues update and possible TGD discussions (D. Addison, M. Nielson)
    13.2 ICRN 32 Conductivity of Electrolytes in Aqueous Solutions presentation and discussion
    13.3 Strategies to improve criteria on steam for steam turbine (geothermal) (S. Terada)
    13.4 Report of the joint Task Group "White paper on geothermal plant issues" (N. Okita, F. di Mare, D. Addison, S. Terada)
    13.5 Report of the Task Group "Wet steam data from operating turbines" (S. Senoo, N. Okita, A. Anderko)
    13.6 Report of the joint Task Group on ICRN for acid gas dew points (N. Okita, S. Senoo, T. Němec)

Tuesday afternoon session splits into separate WG sessions

14. Other Business
    14.1 Report on International Collaborative Projects
15. Membership
16. Election of Vice-Chair
17. Contribution to Press Release
18. Preparation of the Formal Motion to the EC

November 27, 2022

K. Meier (Chair), A.H. Harvey, J. Hrubý (Vice-Chairs)

Minutes of the IAPWS working group IRS,
Rotorua, New Zealand, Nov. 27 - Dec. 2, 2022
(Numbering of topics follows TPWS agenda, except where denoted "…-IRS")

1. The Chair, Nobuo Okita, opened the IRS (joint with TPWS) at 10:30 am, 28. November 2022. Agenda was adopted without changes.
2. Appointed Adam Nový as a clerk of minutes for IRS

3. Potential International Collaborative Project

Young scientist project has been proposed by A. Harvey, R. Span and J. Hrubý. The project is for 2023-2024 for young scientist Aleš Blahut from Czech Institute of Thermomechanics – Czech Academy Of Sciences. The work should be a preliminary preparation for IAPWS-95 replacement and will be focused on review of available data, identifying possible problems and preparing the structure for equations. IAPWS funding of 9.300 GBP will be used for foreign stay.

The following discussion:

D. Friend recommended to openly communicating the proposal to all national committees to avoid collisions with other proposals. The proposal was unanimously agreed to pass to EC.

TODO:

Move proposal to EC

4. State of Development of a New Formulation for the Thermodynamic Properties of Ordinary Water (Replacement of IAPWS-95)

4.1 Report of Task Group (A. Harvey, D. Friend, J. Hrubý, N. Okita, K. Orlov, R. Span)

A. Harvey summarized known problems to be reviewed like EOS deficiencies, unphysical behavior, oscillating and extrapolation problems. Also considered availability of new data and in parallel identifying regions where data are needed. Summary of collected information and considering possible preliminary EOS.

The following discussion:

K. Mayer considerations about time frame about 2 years and then decide how to move on. Other discussed super cooled water region, low temperatures (high Mach) below triple point (H_2 combustion). D. Friend mentioned uncertainties, but it was concluded, to be determined later.

5. IAPWS Certified Research Needs (ICRNs)

5.1 ICRN 16: Thermophysical Properties of Seawater (R. Pawlowicz)

R. Pawlowicz not present and no other member of SCSW, ICRN expired

5.2 ICRN 30: Thermophysical Properties of Supercooled Water (O. Hellmuth)

O. Hellmuth also not present and no other member of SCSW, ICRN expired

Both ICRNs are expired and both are related to SCSW, which is now not active because of personal reasons of the members.

The following discussion to both ICRNs:

D. Friend suggested that there is no problem leave it as is until next year. After broader discussion, the TPWS and IRS members agreed to take no action and wait until the next

meeting whether there will be any activity and possible personal changes in SCSW. The JCS is active, but now the link to IAPWS is missing.

TODO:

The TPWS and IRS members concluded to contact Chair and Vice-chair of SCSW and/or S. Seitz, who might be interested.

6. Industrial Requirements and Solutions for Property Calculations, joint with WG TPWS [Monday afternoon]

6.1 Report of the Task Group "Categories of industrial requirements" (N. Okita, chairs or representatives of other WG)

N. Okita presented the status of gathered categories and highlighted new items. N. Okita accented the most relevant categories like condensation, corrosion and geothermal steam. The grouping of categories into A, B, C groups according to the IAPWS distance. Then the modified part were overviewed. There were new categories added namely, hydrogen combustion, clouds micro and macrophysics related to aviation, ammonia and water-ammonia mixtures, which were brought to discussion. Short-term topics 1y Industrial calculation needs (CFD), Wet steam data/simulation, ASME cooperation. Long-term 3y mixtures H_2O plus some substance, CO_2 cycles. New possible mission including PCAS, wet steam, non-condensable gases and scrubbing/moisture removal.

The following discussion:

A. Harvey asked, what is expected from ASME and the answer was to attract industry people to IAPWS to bring new challenges relevant to IAPWS. J. Hruby suggested to avoid clouds physics as it is the topic covered by other groups within ocean, weather and climate modeling. K. Meier suggested $N+H_2O$ mixtures and also pure helium used in primary thermometers. Later K. Meier also suggested sharing the categories list within all IAPWS members because it is a very complete and complex work. A. Harvey mentioned, that hydrogen combustion can be understand in two ways, hydrogen clean or included for example in LNG combustion. D. Friend mentioned possible activity for ICPWS 2024. Consider whitepaper on wet steam properties and also on mixtures in the farther future.

Continuing discussion separately in IRS (as item 9-IRS). H. J. Kretzschmar noted that power industry in Germany is moving away from the coal and nuclear. H. J. Kretzschmar also commented the ammonia and ammonia-water mixtures used for Kalina cycle, desalination and in heat pumps. Regarding the hydrogen combustion, there was also mentioned that within ASME there exist combustion committee. It was concluded, that wet steam is still the most important topic followed by the geothermal steam. Next can be the hydrogen combustion and clouds micro-macrophysics related to aviation industry. The lowest relevance has the ammonia and ammonia-water mixtures (Kalina, desalination heat pumps), The idea of contact with ASME has been accepted. Panel discussion in ASME conference is also useful if it can be held. After the program of ASME Turbo Expo 2023 (June 26-30) is submitted, we can survey which items are attracted. Same for other ASME conferences.

TODO:

Get involved in ASME Turbo Expo 2023 in Boston to observe the industry needs.

6.2 Report of the Task Group "Wet steam properties Calculation" (A. Nový, J. Hrubý, K. Orlov, R. Span, K. Meier, Francesca di Mare, S. Senoo, M. Kunick)

A. Novy reported no progress on the theoretical models and calculations. Presented new measurement nozzle for wet steam measurements, which will be operational in next year within Doosan Skoda company's R&D.

The following discussion:
Possible forms of funding for providing experiments and possible forms of support from IAPWS (ICRNs, International Collaborative Projects). Possible connection with International Wet Steam Modeling Project
TODO:
Get in touch with the International Wet Steam Modeling Project possible contact should be Markus Schatz.

7. Heavy Water Properties (joint with WG TPWS)

7.1 Progress on a Formulation for the Static Dielectric Constant of Heavy Water (J. Cox, J. Young, A. Harvey, and P. Tremaine)

A. Harvey gave the summary of work done, two formulations suggested first for solution chemist with limited region and second completely new and flawless. The work will resume in 2023

The following discussion:

D. Friend asked for the result for if it should be one or two equations. A. Harvey concluded that it will be determined, when finished. Refer to the TPWS minutes more in detail.

7.2 Appointment of a Task Group for the Evaluation of the Formulation of the Static Dielectric Constant of Heavy Water

Refer to the TPWS minutes.

8. Report of Task Group on Surface Tension of Ordinary Water (joint with WG TPWS and SC SW) (J. Kalová, V. Vinš, A. Harvey, O. Hellmuth, V. Holten, J. Hrubý, R. Mareš, F. Caupin)

J. Hrubý presented on behalf of J. Kalova, who is not active due personal reasons, basic information. Refer to the TPWS minutes more in detail.

9-IRS -New item for considering IRS task group (Francesca di Mare, N. Okita)

Refer to the item 6-1 (included in the latter half of item 6-1)

13. TPWS/IRS/PCAS/PCC joint session

13.1 Electrode Boiler Chemistry Issues Update and Possible TGD Discussions (D. Addison, Monika Nielson)

D. Addison gave overview of real operation problems in e-boiler regarding corrosion of electrodes and their surroundings. D. Addison accented limited technical knowledge, no scientific literature and no industry published data regarding this kind of problems. Finally, the problems were treated by adjusting the design and operation modus. H2 levels are monitored and kept at normal levels. For the hydrogen, levels there are also no knowledge about the levels. Refer to the PCC minutes more in detail.

13.2 ICRN 32 Conductivity of Electrolytes in Aqueous Solutions Presentation and Discussion

Refer to the TPWS/PCC minutes.

13.3 Strategies to improve criteria on steam for steam turbine (geothermal) (S. Terada)

S Terada gave overview in focus of balancing purity vs operating costs. Limits for steam purity needs to be revised to avoid corrosive substances, scale and possible erosion and/or corrosion.

13.4 Report of the joint Task Group "White paper on geothermal plant issues" (N. Okita, Francesca di Mare, D. Addison, S. Terada)

D. Addison summarized the status of the prepared Whitepaper on Geothermal Steam Purity and Recent Data Collection Update. Overview of scaling, corrosion, erosion and steam purity problems. There were auxiliary devices described (separators, scrubber, condensing traps). There was also servicing and revision scheme of geothermal turbines discussed. The purity limits are being discussed and adjusted between NZAPWS and JPAPWS 2nd draft is expected by January 2023 and possible approval of final document in 2023 Italy.

13.5 Report of the joint Task Group "Wet Steam Data from Operating Turbines" (S. Senoo, N. Okita, A. Anderko)

S. Senoo gave overview of problematic of coarse droplets causing erosion of the last stages in steam turbines. There were measurements of droplets spectrum presented. The key is to understand the film forming on stator blade and forming droplets from the water film. The film was measured and visualized. The measurements were done on Mitsubishi experimental turbine.

The following discussion:

B. Dooly noted, that erosion can be also related to electrostatic discharge and that works on this topic are published. J. Hruby added that on the similar topic there is another group of people working at the Czech Technical University in Prague (O. Bartoš)

13.6 Report of the joint Task Group on ICRN for acid gas dew points (N. Okita, S. Senoo, T. Němec) [Joint with PCAS]

N. Okita presented an update on the topic, the theoretical model for dew point ASPEN Model-3 was found to be sufficient, as there were not big differences between model and application at existing plants condition. Consider simulation of wider range of SO3 concentration to lower SO3 contents than 0.08ppm. However, ICRN is now not necessary as the exhaust temperature is decided by other factors such as draft forth of exhaust gas in case of lower than 0.01ppm SO3. Possible TGD on reliability against corrosion and on high efficiency case by case in operation and types. Discussed with PCC chair D. Addison.

TODO:

White paper for the TGD to be prepared until the next annual meeting.

10-IRS. Other Business

10.1 Report on New Item for considering IRS Task Group

IRS continue to investigate "wet steam" including geothermal steam.
Then, IRS would extend the mission such as hydrogen combustion and clouds micro-macrophysics related to aviation industry, and ammonia and ammonia-water mixtures.
IRS agree to contact with ASME members to collaborate for new topics.

10.2 Nomination for Gibbs Award committee

N. Okita has been nominated by the IRS WG

11-IRS. Membership

11.1. Election of new chair and new vice chair of IRS

It was unanimously confirmed to propose Francesca di Mare as new chair and Richard Harwood as new vice-chair to EC.

12-IRS. Preparation of the Formal Motion to the EC

Propose Francesca di Mare as new chair and Richard Harwood as new vice-chair to EC

15-IRS. Contribution to Press release will be done by the WG chair.

15-IRS. Adjournment

Adjourned at about 17:00 November 29, 2022

PCAS WG Minutes

Rotorua, New Zealand, November 27 – December 2, 2022

Present:

Ken Yoshida (chair)	yoshida.ken@tokushima-u.ac.jp
Masaru Nakahara	nakahara@scl.kyoto-u.ac.jp
Jane Ferguson	jane.ferguson@unb.ca
Amish Patel	pamish@seas.upenn.edu
Nobyuki Matubayasi	nobuyuki@cheng.es.osaka-u.ac.jp

PCAS separate meeting, 11/28 morning

(1) Agenda approved

(2) J. Ferguson appointed as the clerk of minutes

(3) Minutes of the 2021 meeting approved

(4) PCAS members in attendance each gave introduction and overview of their PCAS related research activities

(5) Possibility of ICRNs
IRS/PCAS joint task group is no longer considering ICRN for acid gas dew points, to be discussed in greater detail in the PCAS/IRS joint session

(6) International collaboration
K. Yoshida presented ICRN proposal from J. Conrad (INL, USA) and H. Arcis (NNL, UK) on the impact of metal ion complexation on the radiation chemistry of acetohydroxamic acid in aqueous solutions
PCAS reviewed document, discussed interest in increasing the expertise on radiolysis in PCAS
All members strongly support official recommendation of this proposal to the EC
K. Yoshida volunteered as PCAS representative on the Evaluation Committee of International Collaboration Projects

(7) Discussion of future activities of PCAS
K. Yoshida presented slide from H. Arcis on the proposal of a new TG for an updated formulation for the ionization constant of light water
Members all in agreement to support this to EC

(8) K. Yoshida volunteered as PCAS representative on the Gibbs Award Selection Committee and ICP Selection Committee

(9) Discussion of the possibility of releases and guidelines
K. Yoshida reported that development of guidelines for the self-diffusion of water is ongoing, not at a stage yet to circulate guidelines, but making progress, and will continue to update in coming years
K. Yoshida reported on behalf of P. Tremaine and A. Harvey that development of guidelines for the dielectric constant of heavy water is ongoing, no updates
K. Yoshida reported on behalf of H. Arcis that the formation of a radiolysis group is in progress, H. Arcis has contacted researchers in that field but not ready yet for proposal to the EC.

PCC/PCAS joint session, 11/28 afternoon.

The following presentations were given:

O. Palazhchenko – Iron oxide precipitation and lithium adsorption on spent ion exchange resin at alkaline conditions typical to NPPs

N. Matubayasi – MD-DFT approach to the electrical conductivity of ionic liquids

D. Addison & B. Dooley – Film forming substances unknowns/knowledge gaps for ICRN

Expressed need for ICRN, joint PCC with PCAS to address FFS knowledge gaps

David Addison (PCC), Barry Dooley (PCC), Duncan McAllister (PCC), Dave Robin (PCC), Ken Yoshida (PCAS) will form the team to put together this ICRN

B. Loder – Boiler electrochemical corrosion studies test rig results – IAPWS Canada/NZ international collaboration project

TPWS/PCAS joint session, 11/29 morning

The following presentations were given:

N. Matubayasi - Crystal growth of urea and its modulation by additives as analyzed by all-atom MD simulation and free-energy calculation

K. Meier - Cross second virial coefficients for binary mixtures of water vapor with carbon monoxide, sulfur dioxide, hydrogen sulfide, and hydrogen from ab initio intermolecular potentials

A. Harvey - Challenges in modeling the ammonia/water system

J. Hrubý - New accurate data for the density of cold and supercooled seawater at practical salinity 35 and pressures up to 110 MPa

J. Hrubý - A new approach to a comprehensive formulation of thermodynamic properties of seawater

TPWS/IRS/PCAS/PCC joint session, 11/29 afternoon

The following presentations were given:

N. Matubayasi - Crystal growth of urea and its modulation by additives as analyzed by all-atom MD simulation and free-energy calculation

D. Addison - Electrode boiler chemistry issues update and possible TGD discussions

S. Terada – Strategies to improve criteria on steam of steam turbine (geothermal)

D. Addison – Report of the joint Task Group “White paper on geothermal plant issues”

S. Senoo – Report of the Task Group “Wet steam data from operating turbines”

N. Okita – Report of task group on ICRN for acid gas dew points

PCAS separate session, 11/29 afternoon

PCAS Membership

New member Amish Patel (University of Pennsylvania, USA)

Removal of member Frantisek Marsik (Czech Republic), self-requested

Unanimously approved

Planning activities for 2022/2023

Guidelines for self-diffusivity of water

New SC or WG for radiation chemistry ongoing

Discussion of possibility for a joint effort between PCAS and PCC

Discussion among PCAS attendees of the possibility of initiating TG instead of proceeding directly to SC or WG

Preparation of report for Executive meeting

Discussion of whether it is premature to present this to EC as a possible SC or WG. Confirmed that wording on EC slide is appropriate, "Possibility of organizing a new group of radiation chemistry. Efforts to reach out to interested researchers in the field are ongoing"
Discussion of PCAS/PCC joint ICRN on FFS – still in planning stages, next step is drafting ICRN. K. Yoshida will communicate with D. Addison and B. Dooley to confirm PCAS is willing to participate.

Comments on ICPWS announcement

List of Other Symposium Sessions of Interest to ICPWS – Recommend removing "Exhibits" and "Posters" from this list with technical topics and be grouped separately

Members approved wording of draft press release of PCAS activities

Power Cycle Chemistry Working Group (PCC WG)
Rotorua, New Zealand, November 27 – December 1st

1. Adoption of Agenda and Minutes Approval

IAPWS 2022 PCC WG members were welcomed by David Addison.
Willy Cook requested an addition to the agenda – discussion of radiolysis task group to be formed, possibly by PCC.
The agenda was adopted. The agenda is attached as PCC Attachment A.
Minutes from PCC Virtual/online 2021 were approved with no changes.

2. Appointment of PCC WG Clerk of Minutes

Olga Palazhchenko (Canada) was appointed as clerk.

3. Review of Actions from last PCC WG Meeting

No significant updates to report on.

4. IAPWS TGDs Updates

Session chaired by Executive Secretary Barry Dooley.
Dooley provided background information that 11 TGDs have previously been developed. Dooley emphasized that importance of the TGDs should be shared with the NZ geothermal community, highlighting that TGDs are unique in that they contain a base case and customization aspects for every plant worldwide. Dooley requested that the separate TGD WGs arrange to meet during the ICPWS week to progress activities.

Progress on Draft TGDs or Whitepapers:

Whitepaper: Application of Film Forming Substances (FFS) in Nuclear Power Plants (NPPs)
Slides from Jorg Fandrich to support this TGD were provided – Dooley gave highlights of slides to PCC

- New reactors under construction and new designs built, highlights importance of FFS for ongoing materials protection
- Highlighted differences of NPPs to fossil units
- Progress has been made overall

Discussion by PCC members on importance of FPPs in nuclear plants due to large number of stations (particularly in North America) undergoing mid-life refurbishment within next 5-10 years.

TGD: Monitoring of Corrosion Products in Flexible and Two-Shifting Plants
Additional presentation delivered by Mads Skovbjerg to provide update on round robin process

- IAPWS Round Robin (RR)
    - 10-month endeavour is underway, where Mads has visited 5 plants
    - RR proved necessary QA before IAPWS Collection Campaign
    - Labs that followed protocol for iron analysis performed well, while those that did not saw significant outliers

- Mads will circulate results of round robin to labs with suggestions for improvement

- IAPWS Collection Campaign summary provided by Mads:
  - Measurements of CPs during start-ups
  - Online measurements (preferred) and grab samples
  - Analysis by laboratories at which data were collected
  - Mads will do data analysis of data provided by laboratories in Spring 2023

Whitepaper: Flue Gas Condensation

Monika Nielsen delivered presentation to provide update on first draft of whitepaper and discussion by PCC followed. First draft has been complete.

- Question raised on if materials of construction and corrosion are covered in white paper. They are not currently, but Monika will take this feedback to SIAPWS.
- **ACTION**: **David Addison will send whitepaper to PCC. One month will be given to PCC to provide feedback.**
  - PCC comments will be sent back to Monika.

Retirement of TGDs/Whitepapers:

TGD: Ensuring Integrity and Reliability of Demin Makeup Water Supply to the Unit Cycle

- Retired – no further comments from PCC.

Whitepaper: Condensate Polishing for Combined Cycle/HRSG Plants (not a TGD)

- Retired – no further comments from PCC.

Addition of smart alarms to Instrumentation TGD

- Retired. This was already noted in the 2021 virtual meeting minutes.

Refreshment of TGDs:

David Addison asked for discussion on review of TGDs, importance of refreshing/reviewing previous documents

- E.g., Instrumentation TGD should be refreshed to include geothermal and electrode boilers
- More guidance for more industrial plants – firmer tables would facilitate their use, perhaps in an appendix
- Importance of Instrumentation TGD highlighted – don't want to lose the clear messages or add a lot of extra work for PCC members
- Perhaps formal process that every 3 years refresh is needed for TGDs to make sure current, even if no changes are made.
- Should distinguish if this process is to be formal, updating of technology an issue
- Review process would start the same process as creating a new TGD, locking it into a long process, noting that verification of new technology is required before inclusion
- Most of current documents would need to be reviewed if a frequency of ~3 years was selected. TGDs should be "owned" by someone
- Questionnaire to go to PCC should be generated. After survey results come back, a priority list, review period, etc. will be established. Overall TGD task group will review.

- **ACTION: David Addison will send out a survey to PCC to provide comments on refreshing and updates needed for each current TGD, then go forward from there: what improvements, advancements, etc. are needed.**

ICRN Updates:

David Addison/Barry Dooley - Film Forming Substances Unknowns/Knowledge gaps for ICRN

- Still many unknowns and misapplications in the FFS space
- When done correctly, FFS work extremely well; need to do to understand mechanisms
- ICRN is needed – input from PCAS necessary
- ICRN team formed: David Addison (New Zealand), Barry Dooley (UK), Ken Yoshida (Japan), Duncan McAllister (Australia), and David Rodman (Australia)

ICRN 32: Conductivity of Electrolytes in Aqueous Solutions
ACTION: David Addison will circulate ICRN to national committees post IAPWS2022 to prepare for a postal ballot

5. Joint PCAS and PCC WG Meeting

Ben Loder – Boiler Electrochemical Corrosion Studies Test Rig Results– IAPWS Canada/NZ International Collaboration Project

- This is an update on an international collaboration between Canada (Willy Cook) and New Zealand (David Addison)
- Progress has been made and a lively discussion between Cook, Dooley, Loder, and Addison followed.

Willy Cook – Laboratory study of the impact of ODA on ion exchange resins

- Good discussion on ODA fouling tests on IX resin completed at UNB, with questions by many PCC members on further plans for testing with commercial filming products and details of procedure to regenerate resin, e.g., brine cleaning. Willy indicated that these are important follow-up tests for future work.

6. PCC Presentations

Taro Ichihara Hydrogen Damage in Power Boiler - A Study of Damage Selectivity and Conditions

- Good discussion with PCC members on poor welding and re-welding to fix this on previously damaged tubes exacerbating the hydrogen damage and subsequent failure. Suggestions were made to Taro on additions to his work

Mar Nogales – Operational Experience with EDI technology for CACE Measurement

- Suggestion of backwash of middle component/cartridge as additional R&D direction.

7. TPWS/IRS/PCAS/PCC Joint Session

David Addison – Electrode Boiler Hydrogen Generation from Arcing Events

- Steam hydrogen monitoring should be installed in electrode boilers
- Expressed need for TGD in this area
- Discussion on ratios of oxygen and hydrogen, and suspicious non-stoichiometric ratios
- Either additional oxygen production source or quenching of hydrogen

David Addison - Geothermal Steam Purity White Paper and Recent Data Collection Update and Discussion

- Progress on whitepaper being made
- A technical paper has been put together
- Some proposed steam chemistry limits for second draft of whitepaper
- Proposed timeline:
    - Draft #2 of whitepaper underway for Jan 2023
    - To circulate to wider IAPWS
    - Draft of TGD for May/June
    - Goal to present TGD at IAPWS Italy 2023

Report of the joint PCAS/IRC Task Group Wet Steam Data from Operating Turbines:

- Goal of erosion reduction in steam turbine due to coarse water droplets
- 2 remaining issues:
    - Measurement technologies of droplets in steam turbines
    - Modelling – using CFD techniques
- Looking for collaborators to help task group with these issues
    - Barry Dooley indicated that 10-15 years ago an international conference already featured a lot of measurements of droplets – will provide information to task group

Report of the joint PCAS/IRC Task Group on ICRN for Acid Gas Dew Points:

- Needs are for natural gas GTCCs
- Task group has decided that ICRN is now necessary
- Possible TGD needed to maintain reliability against corrosion for existing plants for newly developed natural gas GTCC
- PCC Chair comment: doesn't currently fit scope of any of the current areas, perhaps additional resources and manpower needed to support this whitepaper/TGD.
- Task group will be formed and revealed to PCC at later date.

ICRN for Acid Dew Points
ACTION: David Addison to work with PCAS on draft future TGD

8. PCC WG Business

a. Gibbs Award 2024 Committee PCC

The Executive Secretary reminded PCC that this is IAPWS' most prestigious award for early career individuals.
ACTION: Nominations to the Executive Secretary are due by January 2023.

b. Progress Reports 2021/2022 and Future PCC Activities

- No new TGDs underway
- Geothermal whitepaper – progress being made
- Revision to flexible/two shifting plants TGD underway
- Face to face meeting in 2023 Turin for updates on international collaborations
- Task group for electrode boilers: Monika Nielsen (Denmark), Willy Cook (Canada), and David Addison (New Zealand) will begin work on this
- Pathway for updating TGDs discussed, and survey will be provided to PCC
- IAPWS Radiolysis Database collaboration
    - Pam Yakabuskie expressed need for centralized and updated location for kinetic rate constants necessary to model radiolysis processes
    - This used to be managed by University of Notre Dame, later moving to NIST, but is difficult to access and has not been updated since 1995. Either NIST radiolysis kinetics information needs updating or a new platform is required
    - Barry Dooley indicated that PCAS and TPWS already have an existing proposal in this area, or something adjacent. This work doesn't fit PCC's mandate, but PCC will support and is in general agreement of importance of this work
    - **ACTION: Pam Yakabuskie to interface with PCAS on existing radiation chemistry activities and will propose a collaboration specific to radiolysis.**
    - **ACTION: on request by Willy Cook, David Addison or Barry Dooley will circulate existing PCAS proposal submission to PCC**

c. Future Direction of PCC Discussion

- Management/actions for remote chemistry support, particularly when station event/accident takes place - likely not technical enough for TGD, but important topic to consider
- More PCC focus at ICPWS
    - PCC Chair noted that structure of ICPWS makes it difficult to get regular PCC business done – may need to commit 1 afternoon during the week just for PCC WG work.
- More paper submissions to PPCHEM are needed – PCC to keep this in mind
- PCC webinars will be delivered
    - **ACTION: David Addison to organize two webinars (quarter 1 of 2023 and quarter 3 of 2023)**
    - Efficacy of webinars will be reported on and assessed in Turin 2023.
- Suggestions provided by Kirk Buecher on new directions for IAPWS, e.g., biomass and hydrogen generation
    - PCC Chair expressed some concerns that PCC does not currently have sufficient expertise nor is the direction of the technology mature enough (scope is too broad) for concrete actions to be taken on this by PCC/IAPWS

  - **ACTION: Kirk Buecher to assess scope and cross-over of hydrogen generation space with PCC and other WGs' mandates. To present his findings (perhaps reaching out to his contacts) in Turin 2023.**
- PCC will continue to think about other web-based activities, e.g., LinkedIn activity.
- **ACTION: David Addison will update IAPWS website with more details and a refresh on the mandate of PCC**

d. International Collaboration

- No international collaborations put forward this year.
- **ACTION: PCC members to submit plans or paperwork for desired upcoming collaborations before Italy ICPWS 2023.**
  - Potential new collaboration for electrode boilers

e. ICRNs – Review and Possible New Additions

- ICRNS to be sent out for review:
  - ICRN 32 Conductivity of Electrolytes in Aqueous Solutions to be sent out by David Addison
- Needed Future ICRNS:
  - ICRN for electrode boilers needed, will be put together by Monika Nielsen (Denmark), Willy Cook (Canada), and David Addison (New Zealand)
  - ICRN for FFS needed Barry Dooley (UK) and David Addison (New Zealand)

- Closing of ICRNS:
  - ICRN 19: Improved Coolant Sampling and Analysis of Low Concentration Metals (Fe, Cu, Co, etc.). Issued September 2006. Expired September 2009. Derek Lister

    Possibly a misnomer as ICRN 29 in IAPWS records. No progress has been made on this in a while.
    ACTION: David Addison will follow up with Derek Lister on details about this ICRN.

  - ICRN 22: Steam Chemistry in the Turbine Phase-Transition Zone. Issued July 2010. Expires September 2015. M. Stastny
    ACTION: Barry Dooley will write a closing statement for this ICRN and provide to PCC Chair before EC on Friday.

  - ICRN 26: Behavior of Aluminum in the Steam Water Cycle of Power Plants. Issued September 2011. Renewed June 2014. Expires June 2019. Bobby Svoboda
    ACTION: David Addison to ask Bobby Svoboda for closing statement.

- Renewal of ICRNS:
    - ICRN 25: Corrosion mechanisms related to the presence of contaminants in steam/water circuits, particularly in boiler water. Issued June 2014. Expires June 2019. Willy Cook
    - **ACTION: David Addison to extend ICRN 25 until September 2025**

f. PCC Public Relations

ACTION: Willy Cook and David Addison will put together press release for 2022 NZ Meeting.

g. Changes in PCC Membership and Election of Officers

The Executive Secretary emphasized that being a member of PCC requires active participation and that membership should be taken as a meaningful responsibility
This was seconded by the PCC Chair, highlighting that only attending IAPWS events is not "active" participation, and contribution via partaking in task groups, working on documents (whitepapers or TGDs), etc. is also very important.
The following WG members were nominated to join PCC:

1. Benjamin Loder, University of New Brunswick, Canada
2. Mads Skovbjerg, VTT Technical Research Centre of Finland, Finland
3. Duncan McAllister, Loy Yang B Power Station, Australia
4. David Rodman, Nalco Water, Australia
5. Pam Yakabuskie, Canadian Nuclear Laboratories, Canada
6. Harold Stansfield, Waltron Bull and Roberts, United States

New members should provide the PCC Chair or the Executive Secretary with their contact information before the EC meeting on Friday.
Previous meeting (2021) established that the vice chair position would expire in one year. Two vice chair positions need to be filled to replace Michael Rziha and Paul McCann.

- Barry Dooley nominated Kirk Buecher (USA) and Willy Cook seconded the nomination.
- PCC accepted Kirk as new vice chair unanimously.
- **ACTION: PCC Chair David Addison will make recommendation to EC on Friday to introduce one new vice chair**

- Barry Dooley nominated Taro Ichihara (Japan) as the second vice chair.
- Taro Ichihara requested a letter for his employer outlining the responsibilities of this position before he can accept the nomination
- **ACTION: PCC Chair David Addison will provide Taro with requested information for his manager.**

h. Adjournment

Meeting adjourned 5:03 PM November 29th, 2022.

Summary of Actions from PCC 2022

#	PCC Area	Action	Whom By	Due Date
1	Flue Gas Condensation	Flue Gas Condensation whitepaper to be sent to PCC	David Addison	PCC will need 1 month to provide comments, send ASAP
2	Updates to TGDs	Send survey to PCC to provide comments on updates needed for each current TGD	David Addison	Before Turin 2023
3	ICRN 32: Conductivity of Electrolytes in Aqueous Solutions	Circulate ICRN to national committees during the week so decision can be made by EC at end of week	David Addison	Before Dec. 2nd 2022
4	Future PCC directions	Organize two webinars	David Addison	Webinar 1: Q1 of 2023 and Webinar 2: Q3 of 2023
5	Future PCC directions	Assess scope and cross-over of hydrogen generation space with PCC and other WGs' mandates. To present his findings in Turin	Kirk Buecher	Turin 2023
6	International collaborations	Submit plans or paperwork for desired upcoming international collaborations	PCC Members	Before Turin 2023
7	PCC description on IAPWS website	Update IAPWS website with more details and a refresh on the mandate of PCC	David Addison	Before Turin 2023
8	Status of ICRN 19: Improved Coolant Sampling and Analysis of Low Concentration Metals	Follow up with Derek Lister on details about ICRN 19 (potential misnomer as ICRN 29 in PCC records)	David Addison	
9	Status of ICRN 22: Steam Chemistry in the Turbine Phase-Transition Zone	Write closing statement for ICRN 22, and provide to PCC Chair	Barry Dooley	December 2nd, 2022 EC meeting
10	Status of ICRN 26: Behavior of Aluminum in the Steam Water Cycle of Power Plants	Obtain closing statement from Bobby Svoboda	David Addison	

11	Status of ICRN 25: Corrosion mechanisms related to the presence of contaminants in steam/water circuits	Extension of ICRN 25 until Sept. 2025	David Addison	
12	Press Release	Put together press release for 2022 NZ Meeting	Willy Cook David Addison	December 2nd, 2022 EC meeting
13	Vice chair replacement	Recommendation to EC on to introduce one new vice chair: Kirk Buecher	David Addison	December 2nd, 2022 EC meeting
14	Vice chair replacement	Provide Taro Ichihara with requested information for his manager on duties of vice chair position	David Addison	
15	Future PCC directions: radiation chemistry and radiolysis collaboration	Interface with PCAS on existing radiation chemistry activities and will propose a collaboration specific to radiolysis.	Pam Yakabuskie	Prior to Turin 2023 meeting
16	Future PCC directions: radiation chemistry and radiolysis collaboration	Circulate existing PCAS proposal submission on radiation chemistry task group to PCC	David Addison or Barry Dooley	

Impact of Metal Ion Complexation on the Radiation Chemistry of Acetohydroxamic Acid in Aqueous Solutions

IAPWS Sponsors

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Background

As the world population continues to grow, increasing global energy demands necessitate high power density and low carbon emission solutions such as nuclear power. Reprocessing used nuclear fuel (UNF)—for the recovery and re-use of uranium in new fuel—is key to achieving a sustainable and secure nuclear fuel cycle that could meet the base load for these energy demands. Currently, a major reprocessing research focus is on the development of next generation solvent extraction technologies that promote the efficient recovery of high purity uranium product streams from UNF.

Acetohydroxamic acid (AHA) has been proposed as a safer and more effective substitute for hydrazine-stabilized reductants for the selective separation of plutonium and neptunium from co-extracted uranium [1]. Under typical UNF reprocessing conditions, AHA would be dissolved in concentrated aqueous nitric acid (HNO_3) and exposed to the intense multicomponent ionizing radiation fields resulting from the radioactive constituents of the dissolved UNF. These conditions ultimately promote hydrolytic and radiolytic degradation processes that limit the effectiveness and longevity of AHA. The hydrolytic behavior of AHA has been well documented [2-,3,4,5,6], and our knowledge of its radiation chemistry is maturing [7-8,9,10,11,12,13].

The radiolysis of water and aqueous HNO_3:

$H2O \rightsquigarrow e_{aq}^-, H^\bullet, {}^\bullet OH, H_2O_2, H_2, H_{aq}^+,$ (**1**)

$HNO3 \rightsquigarrow e_{aq}^-, {}^\bullet NO_3, HNO_2, O^\bullet, H_{aq}^+,$ (**2**)

lead to the formation of reactive radical (eaq–, $H^\bullet$, $^\bullet OH$, and $NO_3^\bullet$) and molecular (H_2O_2 and HNO_2) species that exhibit chemistry with AHA that ultimately leads to its conversion into acetic acid, hydroxylamine, and nitrous oxide gas [11,12]. This foundational radiation chemistry can now be modeled and predicted in the presence and absence of hydrolytic contributions [11,12].

However, this current understanding of AHA radiation chemistry is limited to aqueous solutions in the absence of metal ions, whereas, under envisioned UNF reprocessing conditions, AHA will be present as a mixture of the "free" ligand and its neptunium/plutonium ion complexes, the radiation chemistries of which can be significantly different [14-, 15,16,17,18,19,20,21,22,23,24]. For example, the complexation of trivalent iron ions, Fe(III), by ethylenediaminetetraacetic acid (EDTA), has been shown to enhance the steady-state rate of EDTA radiolysis [15-,16,17,18]. This has been explained by the Fe(III) ion center providing additional reaction pathways for the products of water radiolysis (**Equation 1**) [17,19]. Similar behavior is expected for the metal ion complexes of AHA, and thus this knowledge is essential for the accurate assessment and prediction of the effectiveness and longevity of AHA under envisioned UNF reprocessing conditions.

Research Scope

The proposed research aims to use a combination of steady-state gamma and time-resolved electron pulse irradiation techniques, coupled with multiscale computer modeling calculations, to determine the impact of metal loading on the radiation chemistry of AHA in aqueous solutions (water, nitrate, and perchloric and nitric acids). For this work, Fe(III) is the metal ion chosen for evaluating the impact of complexation on the rate of AHA radiolysis, and the subsequent distribution of AHA degradation products, as compared to previously reported metal-free AHA systems [11,12]. Iron has been chosen for this project because it is typically found as a solute from the corrosion of steel-based alloy systems, it is readily complexed by AHA [5], non-radioactive, and its impact on AHA hydrolysis has been well studied [5]. To achieve this research goal, the Visiting Young Scientist will execute three parallel research objectives over the course of 9 months, beginning in October 2023:

1. ***Steady-State Gamma Irradiations***. The *Idaho National Laboratory* (INL) *Center for Radiation Chemistry Research* (CR2) cobalt-60 gamma irradiators and wet chemistry laboratories will be used for the preparation, irradiation, and subsequent analysis of 0.5 M AHA samples. Gamma irradiated samples will be interrogated by a series of previously benchmarked analytical techniques and methods [11-,12,13], including UV-visible-nIR absorption spectroscopy, and ion and gas chromatography, all of which the Visiting Young Scientist will be trained in. The steady-state irradiation results will provide the necessary data to begin multiscale model expansion and evaluation.
2. ***Time-Resolved Electron Pulse Irradiations***. The reaction kinetics of metal ion complexes of AHA and its degradation products are currently unknown, and yet needed to construct an accurate reaction set for multiscale model development. Therefore, chemical kinetics will be measured using the *Brookhaven National Laboratory* (BNL) *Laser Electron Accelerator Facility* (LEAF)—of which both Conrad and Horne hold visiting scientist status—for the reaction of Fe(III) AHA complexes (and where possible Fe(III) complexes of AHA degradation products) with the transient radical products from water and aqueous nitrate radiolysis, specifically e_{aq}^-, $H^\bullet$, $^\bullet OH$, and $NO_3^\bullet$. Isolation of these radicals is trivial, the

methods for which have been previously reported [**Error! Bookmark not defined.**,**Error! Bookmark not defined.**]. The resulting second-order rate coefficients from these kinetic data will be used to expand the current AHA multiscale model reaction sets for the impact of metal ion complexation.

3. ***Multiscale Model Development***. The data acquired by the two previous experimental research objectives will be used to expand and evaluate current multiscale models for AHA radiolysis in aqueous solutions [**Error! Bookmark not defined.**,**Error! Bookmark not defined.**]. The multiscale modeling approach uses a combination of stochastic [25,26] and deterministic modeling methods, which leverage the INL *High Performance Computing Center* resources and desktop kinetic modeling software (MCPA *FACSIMLE* [27]), respectively.

Visiting Young Scientist

Ms. Elen Clayton (*Dalton Nuclear Institute, The University of Manchester, Manchester, M1 7HF, UK*) is a graduate student in the second year of her Ph.D. on the "*Development of a New UK Radiolysis Flow Loop for Determination of Radiolytic Solvent Stability*," which entails the construction and evaluation of a recirculation loop with capability to investigate the irradiation of biphasic mixtures—as seen in processes for the recovery of uranium from UNF. Elen is uniquely qualified to carry out this work because she has excellent knowledge of the radiation chemistry of water, AHA, and other components of next generation UNF reprocessing technologies due to her previous work towards her Master's degree dissertation: "*Development of a Kinetic Model for the Hydrolytic and Radiolytic Degradation of Acetohydroxamic Acid.*" Elen's master's project focused on the computer simulation of AHA decomposition *via* hydrolytic and radiolytic pathways in a UNF recycling process. The research proposed here would provide Elen with the opportunity to be involved in the experimental study of the radiation chemistry of AHA. This presents an opportunity for Elen to network internationally and learn from specialists in the field of radiation chemistry, and to develop and hone laboratory skills; both of which are essential for a future career in radiation chemistry research. Overall, this project will contribute to the mentorship and comprehensive radiation chemistry training of Ms. Elen Clayton, essential to the completion of her Ph.D. thesis.

Deliverable

At the end of this 9-month project, the proposed research will lead to the expansion of current predictive modeling of AHA radiolysis capabilities to include metal-loaded systems. This project aligns well with the goals of the IAPWS Physical Chemistry of Aqueous Systems Working Group. A report of completed research activities will be delivered to the IAPWS and could directly contribute to the publication of IAPWS documents, such as Guidelines on the anticipated lifetime of AHA in the extreme environments found in UNF reprocessing flowsheets. Further, results will be disseminated through publication of a peer-reviewed journal manuscript (at a minimum *Radiation Physics and Chemistry*, Impact Factor = 2.858 as of 2022) and presentation of our findings at the 2024 *Actinide Separations Conference* and the *18th International Conference on the Properties of Water and Steam.*

Budget (£20,000.00)

- Student Travel Support (return flights from the UK to Idaho Falls, USA): £3,000.00
- Student Travel Support (research trip to BNL): £800.00
- Student Housing/Accommodation Support (£200 per week): £7,200.00
- Student Living Expenses (£250 per week): £9,000.00

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(27) MCPA Software FACSIMILE Kinetic Modeling Software Package

Proposal for IAPWS International Collaborative Project

Towards a replacement for the IAPWS Formulation 1995: Detailed analysis of available data

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November 18, 2022

Abstract

Support is requested for an IAPWS Fellowship for a young scientist to pursue research "Towards a replacement for the IAPWS Formulation 1995: Detailed analysis of available data".

Introduction

For more than two decades, the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use [1,2] (IAPWS-95) served to a broad public as a reference equation for computing thermodynamic properties of ordinary water. For a variety of reasons, notably the availability of new experimental data and recognition of some shortcomings in the IAPWS-95 functional form, such as poor extrapolation into metastable regions and problematic performance in mixture models, IAPWS intends to replace IAPWS-95 in the coming decade. One of the reasons is that new experimental data are available for various thermodynamic properties in different regions. Also, new accurate statistical mechanical computations are available for the gas phase and molecular simulations have been performed providing the approximate course of thermodynamic properties in metastable regions and at extreme conditions. Beyond this, there have been efforts to arrive at realistic uncertainty statements for the computed properties complying with the present best practice of uncertainty assessment. The multitude of available thermodynamic data makes water prominent among other fluids. However, the fact that the data exist in the form of partially overlapping clouds of measurements for various thermodynamic properties makes the question of the most likely location of the thermodynamic surface highly non-trivial. In order to properly asses the value of individual datasets and to judge their mutual consistency, one needs to study the original experimental reports and, preferably based on the assessor's experimental background, identify the decisive sources and magnitudes of uncertainties, and to transform gained information into a form suitable for data correlation.

The Lehrstuhl für Thermodynamik at Ruhr-Universität Bochum (RUB) and the Applied Chemicals and Materials Division of the National Institute of Standards and Technology (NIST), Boulder, are world-wide leaders in the area of development of reference multi-parameter equations of state and in reference thermodynamic measurements. The Institute of Thermomechanics of the Czech Academy of Sciences (IT CAS) possesses experimental and data-handling expertise based on the running program of accurate experimental determination of density of cold and supercooled aqueous systems.

Young investigator

Young scientist Aleš Blahut graduated from the University of Chemistry and Technology in Prague, has working experience from the Czech Metrology Institute, and currently performs research of thermodynamic properties of supercooled water and aqueous systems at the Institute of Thermomechanics. He is uniquely qualified to pursue this research. A Curriculum Vitae of Aleš Blahut is presented in Attachment I.

Implementation of project

The project is to be done during 2023 and 2024. During this period, the young scientist will be employed at the Institute of Thermomechanics in Prague and he will collaborate with colleagues at the

National Institute of Standards and Technology (NIST) in Boulder and at Ruhr-Universität Bochum (RUB). IAPWS support is requested for several short research stays of the young scientist abroad. We plan 4 one-week stays at RUB (two in 2023, two in 2024) and one two-week stay at NIST. A final Report will be provided at the 2025 IAPWS Meeting.

The specific goals of the Young Scientist Project will be:

- For a selected range of parameters, tentatively the whole liquid and supercritical region, including metastable regions of supercooled, superheated, and stretched water, develop a complete database of relevant experimental or simulated data (i.e., data with significant information content) with a brief characterization of each dataset in terms of the experimental methods, sources of uncertainty, and uncertainty estimates, in particular concerting various systematic effects.
- Participate in the development of a preliminary thermodynamic formulation aiming at a replacement of IAPWS-95. The developed model will provide intimate know how and required partial derivatives for the data analysis and it will be useful as an intermediate step helping to identify ways of improvement of IAPWS-95 shortcomings.

By completing this project, the young scientist will learn modern methods of development of reference equation of state. For IAPWS, the results should bring significant progress towards a new and advanced “flagship” formulation of thermodynamic properties of ordinary water.

Budget (in GBP)

Support for a one-week stay at RUB: 1,200 GBP. Support for a two-week stay at NIST: 4,500 GBP. The project includes 4 stays at RUB and one stay at NIST.
Total Young Scientist Grant: 9,300 GBP.

References

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Attachment: Curriculum Vitae of Aleš Blahut

INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER & STEAM

ROTORUA, NEW ZEALAND
27TH NOVEMBER - 2ND DECEMBER
ANNUAL MEETING 2022

Press Release

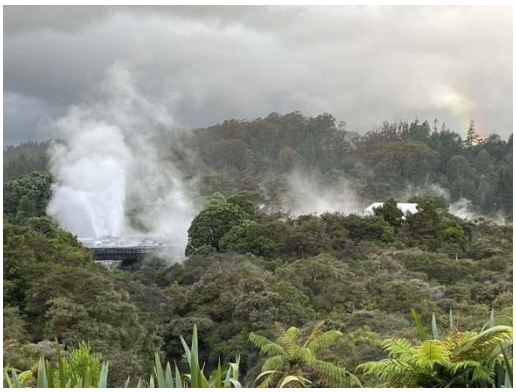
International Association for the Properties of Water and Steam (IAPWS)
2022 Executive Committee and Working Group Meetings

Rotorua, New Zealand, November 27th – December 2nd, 2022

Following two years of online meetings, the IAPWS Executive Committee and Working Groups resumed their Annual meeting in-person and descended on the Novotel Lakeside Hotel in Rotorua, New Zealand. The main meetings included, 33 scientists, engineers and guests representing 13 countries and continues a series of meetings that began in 1929 in London, UK with the purpose to connect researchers and scientists with the engineers who use their work providing the researchers with guidance on topical problems within industry and providing the engineers with the latest research results. Areas of application include power cycle chemistry, high temperature aqueous technologies applicable to steam cycles, geothermal steam, electrode boilers, the use of high temperature water and supercritical steam in chemical and metallurgical processes, hydrothermal geochemistry, oceanography and global climate modelling, power cycles with CO_2 capture and storage systems and combined heat and power systems.

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**.

The 2022 IAPWS Symposium was a joint event with Geothermal, The Next Generation and the New Zealand Geological and Nuclear Sciences (GNS) Crown Research Institute and was focused on the developing area of supercritical steam chemistry and potential applications and brought together geothermal researchers and IAPWS members to discuss and expand on this interesting area of science. The Symposium - "Supercritical and Subcritical Geothermal Steam Chemistry" - was held on Wednesday November 30th and included 65 delegates. The IAPWS Helmholtz award is presented to a developing



or early career scientist or engineer who is working in a field of interest to IAPWS. It includes an opportunity to attend the IAPWS meeting to present the Helmholtz Award lecture during the IAPWS Symposium. This year, the Helmholtz award was presented to Dr. Amish Patel, Associate Professor in Chemical and Biomolecular Engineering at the University of Pennsylvania, USA "For seminal theoretical and computational contributions to fundamental understanding of hydrophobicity, protein hydration and solvation of complex surfaces, and their application to the design of biologically derived materials." Dr. Patel delivered an enlightening lecture about molecular dynamics modelling of superhydrophobic surfaces entitled "How do Surfaces with nanoscale Heterogeneity Perturb Water Structure". Following the symposium, the IAPWS banquet was held at the Te Puia Geothermal Park and Maori Art and Crafts Institute. Delegates were treated to stunning visuals and were able to witness the power of water and steam in action with New Zealand's largest geyser performing for all.

On Thursday December 1st, the IAPWS delegates participated in the NZAPWS Workshop entitled "Future of Industrial Steam in New Zealand" that welcomed over 110 participants from around New Zealand including steam users, equipment suppliers, engineers and chemists. Presentations focused on new electrode boiler systems, integration and upgrading biomass boiler systems and understanding mechanisms through which film forming substances mitigate corrosion.

IAPWS, through the various working groups, produces releases and guidelines, technical guidance documents (TGD) and IAPWS certified research needs (ICRN). These can all be found for free download on the IAPWS website at www.iapws.org. Throughout the week, the working groups progressed their activities, as reported below.

The Working Group on Thermophysical Properties of Water and Steam is beginning a project to replace the existing standard for the thermodynamic properties of water and steam, known as IAPWS-95. The new formulation will take advantage of new data from experiment and from molecular theory, and also of the advances since 1995 in technology for developing equations of state. As a first step, a project is being initiated to organize and evaluate the available data. The PROMETH2O project (www.prometh2o.eu) is developing the European metrological infrastructure and the measurement technologies to provide a robust traceability to trace water measurements in ultra high purity gases, filling the gap and meeting the needs of improved trace water measurement methods and standards for the amount fraction range between 5 ppm and 5 ppb (or, equivalently, between -65 °C and -105 °C frost point temperature).

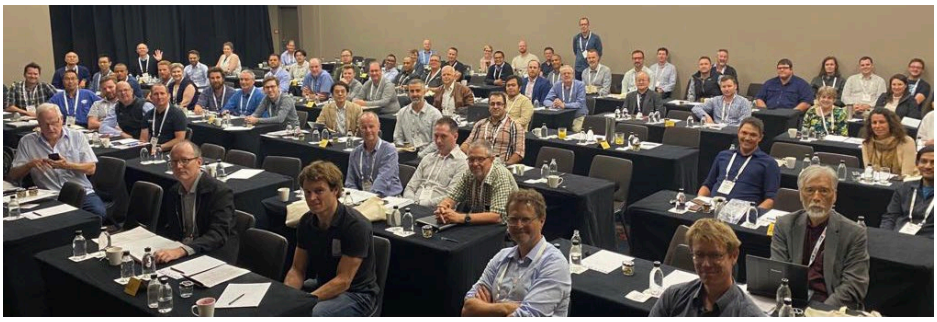
The main topics discussed within the Industrial Requirements Working Group were the engineering requirements for wet steam calculations, new models for estimating low sulfur dewpoint in GTCC and new topics to extend the existing IRS scope. IRS are discussing these with other working groups and will be documented in white papers (dew point, new items, geothermal wet steam) and/or other forms. New topics such as hydrogen combustion, clouds micro- and macro-physics related to aviation are also considered to cooperate with ASME for evaluating attractive fields.

The Physical Chemistry of Aqueous Systems (PCAS) working group discussed MD-DFT approaches for electrical conductivity, all-atom MD analysis of crystal growth processes, structures and film-formation mechanisms of film-forming amines, and the ionization constant of water. The development of an IAPWS guideline for water self-diffusion is underway and will be continued.

The Power Cycle Chemistry (PCC) working group had an extremely productive meeting with a focus on re-establishing face-to-face contact between PCC members and restarting various projects that have been delayed over the past two years. Specific attention was on the area of film forming substances (FFS) with joint discussions between PCC and PCAS and a focus on identifying areas with a lack of information related to FFS and where future research/investigations are needed. An ICRN is currently in development. Progress updates on active International Collaboration projects related to corrosion product sampling and boiler corrosion were made and a draft TGD was presented on Flue Gas Condensate recovery which will be circulated for review and for approval in 2023. Updates on the joint PCC/IRS geothermal steam purity white paper were presented by both JAPWS and NZAPWS with progress intended to continue towards the completion of a draft TGD and possible approval in 2023.

The Executive Committee reviewed and approved all the above-mentioned working group activities, new chairs for working groups and also acknowledged two new IAPWS Fellows –Rich Pawlowicz (Canada) "For excellent leadership of the IAPWS Subcommittee on Seawater and the IAPSO/SCOR/IAPWS Joint Committee on the Properties of Seawater, including facilitating their cooperation with the BIPM" and Frank-Udo Leidich (Germany) "For longterm leadership in the Power Cycle Chemistry Working Group including service as Vice Chair and participation in the development of important Technical Guidance Documents, as well as for promotion of the use of these documents in industry."

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 in Turin, Italy from the 3rd – 8th September 2023. Further information on meetings can be found at the IAPWS website (www.iapws.org) as it becomes available. People interested in IAPWS documents and activities should contact the chairman of their IAPWS National Committee (see website) or the IAPWS Executive Secretary, Dr. R. Barry Dooley, bdooley@iapws.org. People do not need to be citizens or residents of member countries to participate.



IAPWS and NZAPWS Workshop, December 1, 2022
Rotorua, New Zealand

Czech Society for the Properties of Water and Steam
Annual Report 2022

Submitted to IAPWS Executive Committee, November 2022

Steering board of CZPWS
Chair: Tomáš Němec (Institute of Thermomechanics of the Czech Academy of Sciences - IT CAS, nemec@it.cas.cz), Vice-Chair: Josef Šedlbauer (Technical University of Liberec), Secretary: Jan Hrubý (IT CAS), Member: Radim Mareš (University of West Bohemia), Member: Milan Sedlář (SIGMA Research and Development Institute).

CZPWS Meetings
Annual meeting of the CZPWS was held on June 15, 2022. The form of the meeting was hybrid. CZPWS members were informed about the activities of CZPWS Chair and approved CZPWS Financial Statements. Until 2021, payment of CZPWS Member Due to IAPWS was provided from a national grant led by T. Němec. This grant ended. CZPWS became a member of the Council of Scientific Societies of the Czech Republic (CSSCR). Member fee for 2022 and future CZPWS Member Dues to IAPWS will be paid based on the CZPWS membership in CSSCR. New steering board of CZPWS was elected for period 2023-2027: Jan Hrubý (chair), Milan Sedlář (vice-chair), Ondřej Bartoš (scientific secretary), Vladimír Majer (member), Adam Nový (member).

RESEARCH ACTIVITES
Calibration of vibrating tube densimeters using the IAPWS standards
Experimentalists from IT CAS in Prague continued in measurement of density of various fluids using accurate vibrating tube densimeteres (VTD). A calibration technique for highly sensitive commercial instrument Anton Paar DMA 5000 M operated at 0.1 MPa was developed based on the comparison with the IAPWS-95 equation of state for water and the IAPWS G8-10 guideline for humid air [1]. The uncertainty of the liquid density was thoroughly analyzed together with other aspects influencing the quality of obtained data such as the relation between fluid viscosity and damping, the isotopic composition of the calibration water, the measurement procedure covering VTD cleaning and filling, and the effect of water contained in samples. The high-pressure VTD Anton Paar DMA HP is currently being brought into operation [7]. Both densimeters are intended for accurate measurement of density of aqueous solutions.

Surface tension and vapor pressure of supercooled water
Recent work on surface tension of supercooled water at University of West Bohemia in Pilsen was reported by R. Mareš and J. Kalová [5]. J. Kalová also published a study of the vapor pressure of supercooled water [6].

Cavitation

The problems studied in the SIGMA Research and Development Institute and the Centre of Hydraulic Research in the period of June 2021 – June 2022 have been related mainly to the model-ling of cavitation erosion during the hydrodynamic cavitation and models of cavitation

instabilities. In cooperation with the Institute of Physics of the Czech Academy of Sciences, a new cavitation erosion stand has been used to test cavitation resistance of steel samples treated with LSP. In cooperation with the Moscow Power Engineering Institute, the Technical University of Liberec and the Wuhan University, the experimental and numerical modelling of unsteady cavitation phenomena in water has continued in the framework of internal grant projects. The experiments and numerical simulations have concentrated on the thermal effects of cavitation and on the in-fluence of surface hydrophobicity on cavitation phenomena [2]. The Centre of Hydraulic Research in cooperation with the Palacky University in Olomouc finished a new hot-water stand for testing high-performance pumps at the temperatures up to 190 °C, maximum pressure up to 40 bar and power input up to 11 MW. In cooperation with the Institute of Thermomechanics of the Czech Academy of Sciences and the Czech Technical University in Prague, experimental and numerical modelling of unsteady multiphase flow has continued, taking into account the interface of water and air [3], [4].

Publications

1. Prokopová O., Blahut A., Čenský M., Součková M., Vinš V.: Comments on temperature calibration and uncertainty estimate of the vibrating tube densimeter operated at atmospheric pressure, J. Chem. Thermodynamics 173 (2022) 106855.
2. Sedlář M., Komárek M., Šoukal J., Volkov A.V., Ryzhenkov A.V., Druzhinin A.A., Grigoriev S.V., Kachalin G.V, Kalakutskaya O.V.: Experimental and Numerical Studies into the Cavitation Impact of the Hydrofoil Surface with Different Treatments. Thermal Engineering, 69 (2022), 418-428. doi: 10.1134/S0040601522060064
3. Furst J., Halada T., Sedlář M., Krátký T., Procházka P., Komárek M.: Numerical analysis of flow phenomena in discharge object with siphon using lattice-Boltzmann method and CFD. Mathematics, 9 (2021), 1734. doi: 10.3390/math9151734
4. Uruba V., Procházka P., Sedlář M., Komárek M., Duda D.: Experimental and Numerical Study on Vortical Structures and their Dynamics in a Pump Sump. Water 2022, 14(13), 2039; doi.org/10.3390/w14132039
5. Kalová J., Mareš R., Temperature Dependence of the Surface Tension of Water, Including the Supercooled Region, Int. J. Thermophysics, 43, 10 (2022), doi.org/10.1007/s10765-022-03077-
6. Kalová J, Vapor Pressure of Supercooled Water, Int. J. Thermophysics, s (2022) 43: 165, doi.org/10.1007/s10765-022-03095-w

Conference Proceedings

7. Olga Prokopová, Miroslav Čenský, Aleš Blahut, Václav Vinš: *Design and testing of the supporting setup for the high-pressure vibrating tube densimeter*, EPJ Web of Conferences 264 (2022) 01033.

U.S. National Committee to IAPWS
2022 Report on Activities of Potential Interest to IAPWS
21 November 2022

Communicated from the Applied Chemicals and Materials Division, National Institute of Standards and Technology, Boulder, CO (Allan Harvey)**:**

In an IAPWS project, in collaboration with Marc Assael (Aristotle University, Greece) and Jan Sengers (University of Maryland and NIST), a new thermal conductivity formulation for heavy water was developed and approved as an IAPWS Release (IAPWS R18-21). The archival paper was published: M.L. Huber, R.A. Perkins, M.J. Assael, S.A. Monogenidou, R. Hellmann, and J.V. Sengers, "New International Formulation for the Thermal Conductivity of Heavy Water," *Journal of Physical and Chemical Reference Data* **51**, 013102 (2022).

A collaboration between NIST and the group of Prof. Tremaine at the University of Guelph has the objective of developing a standard formulation for the static dielectric constant of heavy water. Thus far, we have gathered the available data and made preliminary comparisons based on the existing H_2O correlation in order to see where there are gaps in the data that might need to be filled in based on H_2O behavior. It is hoped that a new formulation will be ready before the 2023 IAPWS meeting.

In December 2021, the History and Heritage Committee of ASME (American Society of Mechanical Engineers) designated "Standardized Steam Property Tables" as Historic Mechanical Engineering Landmark #276. This reflects the centennial of the ASME's efforts on standardized steam tables, which began in 1921. The accompanying brochure and other information are on the ASME website: https://www.asme.org/about-asme/engineering-history/landmarks/276-standardized-steam-property-tables.

Also in conjunction with the 100th anniversary of ASME steam tables efforts, a historical perspective article was published: A.H. Harvey and J.C. Bellows, "A Century of ASME Steam Tables," *Mechanical Engineering* **144**(1), 44 (2021/2022).

A review article has been prepared on the thermophysical properties of water, with an emphasis on IAPWS formulations: A.H. Harvey, J. Hrubý, and K. Meier, "Improved and Always Improving: Reference Formulations for Thermophysical Properties of Water," *Journal of Physical and Chemical Reference Data*, submitted (2022).

Communicated from the ASME Research and Technology Committee on Water and Steam in Thermal Systems (Bob Bartholomew)

The Water Technology Subcommittee has completed work on a new guideline, *Deaerator Performance Monitoring and Inspection Guideline*. This document is now available from ASME as an e-book for a nominal fee at https://asmedigitalcollection.asme.org/ebooks/book/291/Deaerator-Performance-Monitoring-and-Inspection.

Communicated from the Idaho National Laboratory *Center for Radiation Chemistry*, Idaho Falls, ID (Jacy Conrad)

Advancements in the Radiation Chemistry of Aqueous Systems

The *Idaho National Laboratory* (INL) Center for *Radiation Chemistry Research* (CR2) has provided significant fundamental insight into the radiation-induced behavior of various aqueous chemical systems relevant to the nuclear fuel cycle.

Elucidating the radiation-induced behavior of actinides in aqueous media
New insights were gained on the behavior of rare actinide ions in aqueous solutions of interest for the manipulation of actinide and nuclear fuel cycle materials. By employing novel electron pulse radiolysis techniques—utilizing the *Brookhaven National Laboratory* (BNL) *Laser Electron Accelerator Facility* (LEAF)—the INL CR2 measured the first-ever transient di- and tetra-valent californium and berkelium ion spectra and lifetimes, in addition to the associated kinetics arising from the reaction of the corresponding trivalent states with transient aqueous radiolysis products, specifically the hydrated electron (e_{aq}^-), hydrogen atom ($H^\bullet$), and hydroxyl radical ($^\bullet OH$) from water radiolysis. The lifetimes of these non-traditional late actinide oxidation states are of the order of microseconds, which is more than sufficient to influence the chemistry of their immediate (coordination sphere) and surrounding (bulk aqueous solution) environments. This work was funded by the U.S. Department of Energy (DOE) Office of Science, Office of Basic Energy Sciences, under Award DESC0021372, and published in the following paper:

- G.P. Horne, B.M. Rotermund, T.S. Grimes, J.M. Sperling, D.S. Meeker, P.R. Zalupski, N. Beck, D. Gomez Martinez, A. Beshay, D.R. Peterman, B.H. Layne, J. Johnson, A.R. Cook, T.E. Albrecht-Schönzart, and S.P. Mezyk, Transient Radiation-Induced Berkelium(III) and Californium(III) Redox Chemistry in Aqueous Solution. Inorganic Chemistry, **2022**, 61 (28), 10822, DOI: https://doi.org/10.1021/acs.inorgchem.2c01106.

Kinetics measured for the radiation-induced reduction of aqueous hexavalent chromium ions to 325 °C
Highly toxic hexavalent chromium [Cr(VI)] is found in industrial wastewaters, including those from nuclear power plants, as a leachate from stainless steels. Electron pulse radiolysis using the *Notre Dame Radiation Laboratory* (NDRL) *Linear Accelerator* (LINAC) was employed to measure chemical kinetics and Arrhenius parameters for the reactions of Cr(VI) with water radiolysis products to 325 °C. It was determined that Cr(VI) is reduced to Cr(III) under irradiation, however, the oxidation between Cr(V) and the $^\bullet OH$ radical needs to be suppressed for complete reduction to occur. These new findings can be incorporated into models of chromium speciation under the extreme conditions present in operating nuclear reactors. The results of this work, funded by the INL Laboratory Research & Development (LDRD) Program under the U.S. Department of Energy (DOE) Idaho Operations Office Contract DE-AC07-05ID14517 have been published in the following paper:

- J.K Conrad, A. Lisouskaya, D.M. Bartels, Pulse Radiolysis and Transient Absorption of Aqueous Cr(VI) Solutions up to 325 °C. ACS Omega, **2022**, 7(43), 39071-39077, DOI: https://doi.org/10.1021/acsomega.2c04807.

Predictive multiscale model for the degradation pathways of acetohydroxamic acid in aqueous solutions under irradiation
Acetohydroxamic acid (AHA) has been proposed for use in used nuclear fuel reprocessing flowsheets for the reduction and complexation of plutonium and neptunium ions. New reaction

kinetics were measured for the reactions of AHA with the primary radiolysis products of water and nitric acid solutions, including the e_{aq}^-, H• atom, •OH and nitrate (NO_3•) radicals, using electron pulse radiolysis at the BNL LEAF and the NDRL LINAC. Using these measured kinetic rate coefficients, a predictive multiscale computer model has been developed for the radical-induced behavior of AHA in acidic aqueous solutions. This model has been rigorously evaluated against steady-state irradiations performed using the INL CR2 cobalt-60 gamma irradiator. These findings give a complete picture of the degradation pathways of AHA under proposed used nuclear fuel reprocessing conditions. This work, funded by the U.S. Department of Energy Assistant Secretary for Nuclear Energy, Material Recovery and Waste Form Development Campaign yielded the recent publication:

- J.K Conrad, C.D. Pilgrim, S.M. Pimblott, S.P. Mezyk, G.P. and Horne, Multiscale Modelling of the Radical-Induced Chemistry of Acetohydroxamic Acid in Aqueous Solution. RSC Advances, **2022**, 12(46), 29757-29766. DOI: https://doi.org/10.1039/D2RA03392E.

Communicated from the University of Maryland, College Park (Jan Sengers)

The IAPWS project on the development of new formulations for the viscosity and thermal conductivity of H2O and D2O has now been completed with the publication of

"New international formulation for the thermal conductivity of heavy water", M.L. Huber, R.A. Perkins, M.J. Assael, S.A. Monogenidou, R. Hellmann, and J.V. Sengers, J. Phys. Chem. Ref. Data 51, 013102 (2022), 19pp. https://doi.org/10.1063/5.0084222.

Communicated from EPRI, Palo Alto, CA (Chuck Marks, Dominion Engineering)

Aqueous chemistry of boric acid and alkali borates at elevated temperature
In recent years EPRI has led a collaborative effort of participants from multiple countries in obtaining new data on speciation and volatility of boric acid at elevated temperatures, developing new models for the activity coefficients of boric acid species, and developing expressions for the equilibrium coefficients for relevant reactions at infinite dilution. The results of this work are being incorporated into EPRI's ChemWorks Tools / MULTEQ and BOA software for modeling of nuclear reactor coolant chemistry.

Re-evaluation of the water dissociation equilibrium at high temperatures
As part of the boric acid work discussed above, a comparison of calculations with ChemWorks Tools and OLI's software indicated that differences in the treatment of the dissociation of water contributed significantly more to uncertainty in high temperature chemistry calculations than uncertainty in the speciation of boric acid. Comparisons of the IAWPS formulation with legacy formulations (e.g., that of Marshall and Franck) had previously indicated comparable uncertainty, but few experimental data were available to reduce the uncertainty. EPRI has begun an evaluation of the new data developed by Arcis, et al. with the objective of developing a new expression for the ionization of water at elevated temperatures.

Current Status of Research Activities in Japan
Submitted to the Executive Committee Meeting, IAPWS,
December, 2022

Japanese National Committee, Chaired by Professor Kenji Yasuoka
International Association for the Properties of Water and Steam
c/o The Japan Association for the Properties of Water and Steam
Chaired by Professor Kenji Yasuoka
3-14-1 Hiyoshi, Kohoku-ku,
Yokohama 223-8522, Japan

I. Overview:

The Japan National Committee 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 of our attention are cleaner, greener, and more sustainable energy as well as high efficiency and safety. We are discussing 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:

Yasuoka, Kenji
Professor, Department of Mechanical Engineering, Keio University
email: yasuoka@mech.keio.ac.jp
URL: https://k-ris.keio.ac.jp/html/100011311_en.html

Correlation between ordering and shear thinning in confined OMCTS liquids
Y. Kobayashi, N. Arai, K. Yasuoka
J. Chem. Phys., 157, 114506 (10 pages), 2022

Impact of free energy of polymers on polymorphism of polymer-grafted nanoparticles
M. Ishiyama, K. Yasuoka, M. Asai
Soft Matter, 18, 6318-6325, 2022

Optimal Replica-Exchange Molecular Simulations in Combination with Evolution Strategies
A. Kowaguchi, K. Endo, P. E. Brumby, K. Nomura, K. Yasuoka
J. Chem. Inf. Model., DOI: 10.1021/acs.jcim.2c00608

Differences in ligand-induced protein dynamics extracted from an unsupervised deep learning approach correlate with protein–ligand binding affinities
I. Yasuda, K. Endo, E. Yamamoto, Y. Hirano, K. Yasuoka
Commun. Biol., 5, 481 (9 pages), 2022

A stochastic Hamiltonian formulation applied to dissipative particle dynamics
L. Peng, N. Arai, K. Yasuoka
Appl. Math. Compu., 426, 127126 (13 pages), 2022

Efficient Monte Carlo Sampling for Molecular Systems Using Continuous Normalizing Flow
K. Endo, D. Yuhara, K. Yasuoka
J. Chem. Theory Comput., 18, 1395-1405, 2022

Natural quantum reservoir computing for temporal information processing
Y. Suzuki, Q Gao, K. C. Pradel, K. Yasuoka, N. Yamamoto
Sci. Rep., 12, 1353 (15 pages), 2022

An Efficient Random Number Generation Method for Molecular Simulation
K. Okada, P. E. Brumby, K. Yasuoka
J. Chem. Inf. Model., 62, 71-78, 2022

Water molecules in CNT–Si3N4 membrane: Properties and the separation effect for water–alcohol solution
Winarto, E. Yamamoto, K. Yasuoka
J. Chem. Phys., 155, 104701 (11 pages), 2021

On effective radii of dodecahedral cages in semiclathrate hydrates for van der Waals and Platteeuw model
S. Muromachi, S. Takeya, D. Yuhara, K. Yasuoka
Fluid Phase Equil., 527, 112846 (6 pages), 2021

The influence of random number generation in dissipative particle dynamics simulations using a cryptographic hash function
K. Okada, P.E. Brumby, K. Yasuoka
PLoS ONE, 16, e0250593 (8 pages), 2021

Phase Transitions and Hysteresis for a Simple Model Liquid Crystal by Replica-Exchange Monte Carlo Simulations
A. Kowaguchi, P. E. Brumby, K. Yasuoka
Molecules, 26, 1421 (14 pages), 2021

Matubayasi, Nobuyuki
Professor, Graduate School of Engineering Science, Osaka University
email: nobuyuki@cheng.es.osaka-u.ac.jp
URL: http://www.cheng.es.osaka-u.ac.jp/matubayasi/english/index.html

Molecular dynamics study of the interactions between a hydrophilic polymer brush on graphene and amino acid side chain analogues in water
T. Yagasaki, N. Matubayasi
Phys. Chem. Chem. Phys., 24, 22877-22888, 2022

Constructing a Memory Kernel of the Returning Probability to Efficiently Describe Molecular Binding Processes
K. Kasahara, R. Masayama, Y. Matsubara, N. Matubayasi
Chem. Lett., 51, 823-827, 2022

Crystal Growth of Urea and Its Modulation by Additives as Analyzed by All-Atom MD Simulation and Solution Theory
S. Tanaka, N. Yamamoto, K. Kasahara, Y. Ishii, N. Matubayasi
J. Phys. Chem. B, 126, 5274-5290, 2022

Surface Area Estimation: Replacing the Brunauer-Emmett-Teller Model with the Statistical Thermodynamic Fluctuation Theory
S. Shimizu, N. Matubayasi
Langmuir, 38, 7989-8002, 2022

Nonpolarizable Force Fields through the Self-Consistent Modeling Scheme with MD and DFT Methods: From Ionic Liquids to Self-Assembled Ionic Liquid Crystals
Y. Ishii, N. Matubayasi, H. Washizu
J. Phys. Chem. B, 126, 4611-4622, 2022

Adsorption Energetics of Amino Acid Analogs on Polymer/Water Interfaces Studied by All-Atom Molecular Dynamics Simulation and a Theory of Solutions
N. Yasoshima, T. Ishiyama, N. Matubayasi
J. Phys. Chem. B, 126, 4389-4400, 2022

All-atom molecular simulation study of cellulose acetate: amorphous structure and the dissolution of small molecule
R. Matsuba, H. Kubota, N. Matubayasi
Cellulose, 29, 5463-5478, 2022

Explaining reaction coordinates of alanine dipeptide isomerization obtained from deep neural networks using Explainable Artificial Intelligence (XAI)
T. Kikutsuji, Y. Mori, K. Okazaki, T. Mori, K. Kim, N. Matubayasi
J. Chem. Phys., 156, 154108 (8 pages), 2022

Anion-cation contrast of small molecule solvation in salt solutions
S. Hervø-Hansen, J. Heyda, M. Lund, N. Matubayasi
Phys. Chem. Chem. Phys., 24, 3238-3249, 2022

Simulating the nematic-isotropic phase transition of liquid crystal model via generalized replica-exchange method
K. Takemoto, Y. Ishii, H. Washizu, K. Kim, N. Matubayasi
J. Chem. Phys., 156, 014901 (8 pages), 2022

Ensemble transformation in the fluctuation theory
S. Shimizu, N. Matubayasi
Physica A, 585, 126430 (14 pages), 2022; Physica A, 605, 127987 (1 pages), 2022

Molecular Structure and Vibrational Spectra of Water Molecules Sorbed in Poly(2-methoxyethylacrylate) Revealed by Molecular Dynamics Simulation
N. Yasoshima, T. Ishiyama, M. Gemmei-Ide, N. Matubayasi
J. Chem. Phys B, 125, 12095-12103, 2021

Atomistic description of molecular binding processes based on returning probability theory
K. Kasahara, R. Masayama, K. Okita, N. Matubayasi
J. Chem. Phys., 155, 204503 (15 pages) 2021

Effects of chain length on Rouse modes and non-Gaussianity in linear and ring polymer melts
S. Goto, K. Kim, N. Matubayasi
J. Chem. Phys., 155, 124901 (10 pages), 2021

Crystallization of Polyethylene Brushes and Its Effect on Interactions with Water
T. Yagasaki, N. Matubayasi
Macromolecules, 54, 8303-8313, 2021

Temperature Dependence of Sorption
S. Shimizu, N. Matubayasi
Langmuir, 37, 11008-11017, 2021

Breakdown of the Stokes-Einstein relation in supercooled liquids: a cage-jump perspective
R. Pastore, T. Kikutsuji, F. Rusciano, N. Matubayasi, K. Kim, F. Greco
J. Chem. Phys., 155, 114503 (7 pages), 2021

Cooperative Sorption on Porous Materials
S. Shimizu, N. Matubayasi
Langmuir, 37, 10279-10290, 2021

Water Dissolved in a Variety of Polymers Studied by Molecular Dynamics Simulation and a Theory of Solutions
H. Kojima, K. Handa, K. Yamada, N. Matubayasi
J. Phys. Chem. B, 125, 9357-9371, 2021

Molecular insights on confined water in the nanochannels of self-assembled ionic liquid crystal
Y. Ishii, N. Matubayasi, G. Watanabe, T. Kato, H. Washizu
Sci. Adv., 7, eabf0669 (14 pages), 2021

Construction of isostructural hydrogen-bonded organic frameworks: limitations and possibilities of pore expansion
Y. Suzuki, M. Gutiérrez, S. Tanaka, E. Gomez, N. Tohnai, N. Yasuda, N. Matubayasi, A. Douhal, I. Hisaki
Chem. Sci., 12, 9607-9618, 2021

Adsorbate-adsorbate interactions on microporous materials
S. Shimizu, N. Matubayasi
Micropor. Mesopor. Mater., 323, 111254 (8 pages), 2021

Sorption: A Statistical Thermodynamic Fluctuation Theory
S. Shimizu, N. Matubayasi
Langmuir, 37, 7380-7391, 2021
Transition pathway of hydrogen bond switching in supercooled water analyzed by the Markov state model
T. Kikutsuji, K. Kim, N. Matubayasi
J. Chem. Phys., 154, 234501 (7 pages), 2021

Understanding the scaling of boson peak through insensitivity of elastic heterogeneity to bending rigidity in polymer glasses
N. Tomoshige, S. Goto, H. Mizuno, T. Mori, K. Kim, N. Matubayasi
J. Phys.: Condens. Matter, 33, 274002 (7 pages), 2021

Cooperativity in micellar solubilization
S. Shimizu, N. Matubayasi
Phys. Chem. Chem. Phys., 23, 8705-8716, 2021

Spatial-Decomposition Analysis of Electrical Conductivity in Mixtures of Ionic Liquid and Sodium Salt for Sodium-Ion Battery Electrolytes
L. Hakim, Y. Ishii, N. Matubayasi
J. Phys. Chem. B, 125, 3374-3385, 2021

Implicit function theorem and Jacobians in solvation and adsorption
S. Shimizu, N. Matubayasi
Physica A, 570, 125801 (11 pages), 2021

Phase stability condition and liquid-liquid phase separation under mesoscale confinement
S. Shimizu, N. Matubayasi.
Physica A, 563, 125385 (13 pages), 2021

Solvation energetics of protein and its aggregates analyzed by all-atom molecular dynamics simulation and the energy-representation theory of solvation
N. Matubayasi
Chem. Comm., 57, 9968-9978, 2021

All-Atom Analysis of Partitioning Functions of Molecular Aggregates through Development of a Statistical-Mechanical Theory of Solutions
N. Matubayasi
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