

## PCAS WG Minutes

Boulder, US, June 23 – 28, 2024

Present:

Ken Yoshida (chair)

Hugues Arcis (vice-chair)

Andre Anderko

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### PCAS separate meeting, June, 23 morning

- (1) Agenda approved
- (2) H. Arcis appointed as the clerk of minutes
- (3) Minutes of the 2023 meeting approved
- (4) PCAS members in attendance each gave introduction and overview of their PCAS related research activities
- (5) Possibility of ICRNs  
Creation of an ICRN on FFS led by PCC WG is one of possible ICRNs to which PCAS can contribute.
- (6) International collaboration  
Two International Collaboration Projects (ICP) have been submitted (Iodine radiolysis by Arcis and Stuart, and FFA characterization by Yoshida and Cook). Both proposals were endorsed by PCAS, and Andre Anderko was appointed as the PCAS representative for the evaluation IAPWS Committee.
- (7) Discussion of future activities of PCAS  
One of PCAS's main challenges is expanding its active membership. To address this, we decided to invite participants at this year's ICPWS who showed interest in PCAS activities to join PCAS. We made these announcements at the start of each session. This approach proved successful, resulting in productive conversations with interested participants and recommendations for new members.
- (8) Discussion of the possibility of releases and guidelines  
Major revision to release on formulation for the ionization constant of light water (complete)  
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  
A joint PCAS-PCC Task Group to work on radiation chemistry and water radiolysis concepts of critical interest for irradiated aqueous systems such as those in nuclear reactors, has been proposed by Dr. Pam Yakabuskie (CNL, Canada), Dr. Hugues Arcis (NNL, UK) Dr. Jacy Conrad (INL, USA) and Dr. Martin Bachet (EdF, France). It has been identified that there is a need to re-establish access to, and continue the building of the worldwide database for reactions of water radiolysis products with impurities, and particularly to expand the database to include reaction rate constants at higher temperatures. This data forms the basis for fundamental development of radiolysis models for primary circuit chemistry and waste management streams. Radiation chemistry is an important concept for many aspects of the nuclear fuel cycle, with implications for reactor operation and chemistry control, severe accident modelling and development of mitigation plans, and waste management activities

**TPWS/PCAS joint session, June, 23 afternoon.**

The following presentations were given:

- Categories of Industrial Requirements and sulfuric acid dew points (N. Okita).
- Proposal for the development of a new industrial formulation for the properties of water and steam (M. Kunick) (joint with WG IRS, PCAS and SCSW) [afternoon]
- Progress on a formulation for the static dielectric constant of heavy water (J. Cox, A. Harvey, and P. Tremaine) – no progress due to staff moving to new positions; possible progress expected in 2024.
- IAPWS representative for Consultative Committee for Thermometry / Working Group on humidity (CCT-WG-Hu) – A. Harvey has volunteered pending there are virtual arrangements for the meetings in Paris (France).

**ICPWS plenary session, June 24**

IAPWS Gibbs Award Lecture: Thermodynamics of Water in the “Steam Engine” Climate – Rainer Feistel

**ICPWS/PCAS session, June 24*****Physical Chemistry of Aqueous Systems 1: Thermodynamics and Transport Properties – Chair K. Yoshida***

A Revised Formulation for the Ionization Constant of Water over a Wide Range of Temperatures and Densities, Including Near-Critical Conditions – Hugues Arcis

Improvements in Internal Consistency of Inorganic Thermodynamic Data at 298.15 K – Darrell Nordstrom

The Observation of Molecular Symmetry Evolutions in Extremely Supersaturated Aqueous Solution – Yong Chan Cho

Equilibria of Aqueous Solutions of Disodium Terephthalate, Terephthalic Acid, and Compressed Carbon Dioxide for Separations – Trevisan Melfi

Protein Diffusion in Aqueous Solution for Revealing Spectrally Silent Conformation Change – Masahide Terazima

***Physical Chemistry of Aqueous Systems 2: High Temperatures-High Pressures, Electrochemistry, and Corrosion – Chair A. Anderko***

High Pressure, High Temperature Rotating Cylinder Electrode for Electrochemical Corrosion Studies in Flowing Systems – Andrei Yermalayeu

Electrochemical and Fluid Properties of Electrolyte Solutions in All-Vanadium Redox Flow Batteries – Jana Heiß

Microscopic Investigations Towards the Practical Implementation of Film Forming Amines as Corrosion Inhibitors in High-Temperature Aqueous Systems – Ken Yoshida

Gibbs Energy Local Basis Function Representations for Aqueous NaCl and Ammonia-Water Solutions to 10 GPa and 2000 K – J. Michael Brown

***Physical Chemistry of Aqueous Systems 3: Thermodynamic Modeling – Chair H. Arcis***

A Novel Standard Gibbs Energy of Formation Model for High-Enthalpy Water Systems – Derek Hall

Modeling Speciation and Phase Equilibria of Aqueous Boric Acid and Metal Borates from Ambient to Hydrothermal Conditions – Andre Anderko

A Thermodynamically Sound and Numerically Robust Modelling Framework for Mixed Aqueous Electrolyte Solutions and for Redefining pH – Eric May

Quantifying Ion-Ion Association in Mixed Electrolyte Systems Using Bulk Thermodynamic Experimental Data – Elizabeth Ploetz

### **ICPWS/PCAS session, June 25, morning**

#### ***Physical Chemistry of Aqueous Systems 4: Aqueous Solution Chemistry – Chair K. Yoshida***

MB-pol Data-Driven Many-Body Potential: Realistic Simulations of Water Across All Phases – Francesco Paesani

Structure and Dynamics of Water-in-Salt LiTFSI Electrolytes from First-Principles Molecular Dynamics Simulations – Ilja Siepmann

Ion Dehydration Under Operating Conditions for Brine Treatment – Nathanael Schwindt

Optimization of the Route to Produce Magnetic Nanofluids – Matthias Buschmann

### **PCC/PCAS joint session, June, 25 afternoon.**

The following presentations were given:

- Future of PCC Workshop – Paul McCann
- Electrode Boiler update – David Addison
- EPRI Nuclear Activities – Ian Duncanson
- Possibilities of Future PCC/PCAS Collaboration – David Addison
  - K. Yoshida pointed out that the work on updating the TGDs on FFS could serve as a model for collaborative efforts between PCC and PCAS.

### **ICPWS evening session, June, 25.**

- ICPWS/STP - IAPWS Helmholtz Award Lecture & General Meetings of IAPWS

### **ICPWS/PCAS session, June 26, afternoon**

#### ***Nuclear Reactor and Fuel Cycle Chemistry – Chairs J. Conrad & H. Arcis***

Impact of KOH Primary Coolant Chemistry on Pressurized Water Reactor's Operating with Fuel Crud – Hugues Arcis

Phase Behavior and Thermodynamic Solubility Constants for Novel Nickel Sulfate Phases Formed Under Secondary Coolant Hideout Conditions – Maryanne Stones

A Re-evaluation of the Boric Acid Thermodynamics for PWR Systems – Hugues Arcis

A Simple Model for Salting In or Out in Reactor Conditions – Martin Bachet

In-situ High Temperature Radiation-Induced Metal Cation Redox Chemistry – Jacy K. Conrad

### **PCAS separate session, June 27 morning**

PCAS New Membership proposed at the Friday EC meeting:

- Dr. Elizabeth Ploetz (Kansas State University, USA)
- Prof. Francesco Paesani (University of California San Diego, USA)
- Dr. Martin Bachet (EdF, France)
- Prof. Greg Zimmerman (Commonwealth University of Pennsylvania, USA)