PCAS WG Minutes

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

Present: Ken Yoshida (chair) Masaru Nakahara Jane Ferguson Amish Patel Nobyuki Matubayasi

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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