PCAS WG Minutes

Torino, Italy, September 4 – September 7, 2023

Present:

Ken Yoshida (chair)	yoshida.ken@tokushima-u.ac.jp
Hugues Arcis (vice-chair)	hugues.arcis@uknnl.com
Masaru Nakahara	nakahara@scl.kyoto-u.ac.jp
Milan Sedlár	m.sedlar@sigma.cz

PCAS separate meeting, 9/4 morning

(1) Agenda approved
(2) H. Arcis appointed as the clerk of minutes
(3) Minutes of the 2022 meeting approved
(4) PCAS members in attendance each gave introduction and overview of their PCAS related research activities
(5) Possibility of ICRNs
None planned at the moment.

(6) International collaboration
No updates to date on International Collaboration Projects (ICP) [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]

(7) Discussion of future activities of PCAS

PCC/PCAS joint session, 9/4 afternoon.

The following presentations were given:

Nobuo Okita, Toshiba, Dew Point of Low Sulphur Exhaust Gas

Ken Yoshida, Tokushima University, Reaction pathways and mechanisms of alkylamines in supercritical water as studied by NMR spectroscopy

It was recognized this is one of the only labs that can support the development of basic knowledge understanding for FFS kinetics – Recommendation for IAPWS Japan/NZ international collaboration project

David Addison (PCC), Ken Yoshida (PCAS) to prepare proposal for international collaboration project

Hal Stansfield, Waltron, FFA fouling of analytical instruments and mitigations

David Addison/Barry Dooley –Outline of FFS unknowns draft ICRN

Folmer Fogh, Ørsted Bioenergy & Thermal Power-Flue Gas Condensation White Paper/Draft TGD

B. Dooley, Technical guidance documents – status at September 2023

TPWS/PCAS joint session, 9/4 afternoon

The following presentations were given:

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.

Multimodal CO_2-transport - Current developments, the relevance of thermodynamic properties and open questions regarding the formation of corrosive phases (R. Span)

TPWS/PCAS joint session, 9/5 morning

The following presentations were given:

Cross second and third virial coefficients and dilute-gas transport properties of the water–argon system from first-principles calculations (R. Hellmann)

A new model for thermodynamic properties of mixtures based on Helmholtz energy formulations of the components yielding a proper composition dependence of virial coefficients. Preliminary results for water-gas systems. (J. Hrubý)

A Calibration facility for investigating trace water sensors in moist hydrogen in a wide range of gas pressure and water concentration (R. Nobakht, R. Cuccaro, R. Salerno, V. Fernicola)

Measurements of the surface tension of the binary mixtures water + ethylene glycol and water + methanol at temperatures down to -25 °C (V. Vinš, M. Součková, M. Čenský, O. Prokopová, A. Blahut and J. Hrubý)

PCAS separate session, 9/5 morning

(8) Discussion of the possibility of releases and guidelines
Potential new release on formulation for the ionization constant of light water

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

H. Arcis reported 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.

TPWS/PCAS joint session, 9/5 afternoon

The following presentation was given:

Revaluation of the database and formulation for the water ionization constant (K_w) (H. Arcis)

IAPWS Symposium, 9/6

PCAS separate session, 9/7 morning

The following presentation was given:

Comparison of experimental and calculated ionization constants for subcritical/supercritical water (M. Nakahara, K. Yoshida)

Thermal effects of cavitation in water (M. Sedlář)

(9) PCAS New Membership

None. Limited member attendance has been raised as a challenge. Efforts are being continued to recruit new members.

(10) Planning activities for 2023/2024

Possible new release on the ionization constant of water. Comments of evaluation task group (A. Harvey, A. Anderko) expected to be received before 2024 meeting.

PCAS expects to attract new members with the upcoming symposium session "Nuclear Reactor and Fuel Cycle Chemistry" at the 2024 meeting and accelerate the efforts towards the possibility of organizing a new group of radiation chemistry. Efforts to reach out to interested researchers in the field are still ongoing.

PCAS will coordinate with PCC to understand how they could support FFA/FFS and which academics could be invited to join PCAS.

Preparation of report for Executive meeting

It was decided to report to the EC that member Don Palmer of the Evaluation Task Group on K_w of water would be replaced by member Andre Anderko.

The wording of the EC slides was confirmed as appropriate, and some minor changes were made.

Members approved wording of draft press release of PCAS activities.