

## **Minutes, PCAS Working group meeting**

*IAPWS Annual Conference, NIST, Gaithersburg, September 10-14, 2001*

*Members present:* A. Anderko, H. Corti, R. Fernandez-Prini, J.P. Jensen, S. Lvov, V. Majer, W. Marshall, D. Palmer, G. Perboni, A. Plyasunov, M. Ueno, R. Wood

### **Monday morning, September 10; Separate PCAS WG meeting**

1. The chairman (V. Majer) opened the session; the agenda for the PCAS WG sessions during the Conference was approved; S. Lvov was appointed as the clerk of minutes. The minutes of the 2000 (Prague) PCAS WG meetings were approved. V. Majer addressed the issue of the main areas of interest of PCAS WG (1. pH of water HT/Hp, 2. group contribution scheme for predicting standard thermodynamic properties of aqueous organic solutes HT/Hp, 3. ion association in aqueous alkali metal electrolytes at high temperatures to supercritical conditions) and proposed to focus on these areas as was decided in Prague. The corresponding guidelines should be prepared during the next 3 years from 2002 to 2004. R. Fernandez-Prini asked if co-ordinators should be designated for the three domains of the WG's interest. S. Lvov supported R. Fernandez-Prini's request. V. Majer proposed to think about it further and to discuss this issue on Thursday.

2. R. Fernandez-Prini presented his thoughts on possible communications and collaborations between IAPWS and IUPAC after the General Assembly in Brisbane, Australia where he participated. It was concluded that these international organizations can compliment each other and the WG members could use some advantages of the possible collaborations. An IUPAC document on "Guidelines for IUPAC Projects" was presented, discussed, and distributed for initiating possible proposals under the auspices of both organizations (an IUPAC document was distributed to the WG members). V. Majer shared his experience working with IUPAC and mentioned that IUPAC was recently reorganized and the procedure of presenting proposals was modified. V. Majer expressed his opinion that perhaps a joint IAPWS/IUPAC workshop could be jointly supported by the two organisations. D. Palmer addressed a possible mechanism of submitting the proposals saying that IAPWS should probably approve it before any formal action in the direction of IUPAC.

3. D. Palmer presented a proposal for an international collaboration between ORNL and the Moscow Power Engineering Technical University on "Investigation of Lithium and Boric Acid Hideout in Pressure Water Reactors under Axial Offset Anomalous Conditions" (document distributed to group members). The young investigator is Yulia V. Zhgenti (resume made available to WG members). It is planed that Mrs. Zhgenti will be visiting ORNL for a period of 4 months. The proposal and the support requested from IAPWS (\$9,400) were approved by PCAS WG.

## **Attachment 8**

4. V. Mayer addressed the issue of IAPWS membership. After a short discussion it was proposed that recommendation of PCAS WG should be as follows. If a member of the WG did not participate in the PCAS WG meetings for 5 years, the WG Chairmen should request an appropriate national representative to ask this member if he/she wishes to continue an affiliation with IAPWS. It was decided to continue this discussion and finally formulate the statement on Thursday.

5. ICRNS were discussed in which PCAS WG was involved.

### **Monday afternoon, September 11; Joint meeting of PCC and TPWS WGs for a workshop**

K. Daucik welcomed the participants and announced the program of the workshop on "Copper in Water/Steam Cycles", for the list of presentations, see Minutes of PCC WG. The two presentations of S. Lvov were of particular interest for PCAS WG.

1. S. Lvov presented preliminary results on Development of high temperature Pourbaix diagrams for Cu-Ni-Zn-Alloys in water-ammonia power plant environments. The data bases of available thermodynamic values and correlations have been created for Cu, Ni, and Zn oxides, hydroxides, metal alloys, and aqueous species. A deficit in thermodynamic properties of aqueous species was found and additional experimental studies were recommended to be carried out especially for  $\text{Cu}^+$  amine and hydroxide complexes at temperatures up to 300°C. D. Palmer informed the participants that high temperature amine/hydroxide complexation studies are in progress at ORNL.

2. S. Lvov gave a second presentation on high temperature zeta potential measurements at metal oxide/water interface. It was reported that a high temperature micro-electrophoresis instrument for measuring zeta potentials at oxide/water interfaces was designed and constructed. The first studies of  $\text{ZrO}_2$ /water and  $\text{TiO}_2$ /water zeta potentials showed the capability of the developed system.  $\text{TiO}_2$ /water zeta potential measurements are currently being carried out at Penn State University.

### **Tuesday morning, September 11; Separate PCAS WG meeting**

On Tuesday morning there was a half-hour PCAS WG meeting before a separate PCAS workshop started.

1. V. Mayer started a discussion on ICRNS # 10, 11, and 12. After a short discussion, it was decided that ICRN # 10 should be renewed for an additional period of 3 years up to May 2002. The ICRNS # 11 and 12 should be closed (Palmer and Lvov will prepare closing statements).

2. D. Palmer proposed to organize a separate meeting on Atlas and to continue a discussion on this topic at the Thursday WG meeting.

PCAS workshop: the following short contributions on priority activities (ion pairing, group contributions for organic solutes, pH measurements) were scheduled:

R.H. WOOD: Recent conductance studies

M. UENO: Density and temperature dependencies of the electrolyte conductance in the sub- and supercritical water: A test of the Hubbard-Onsager continuum dielectric friction theory

A. PLYASUNOV: Second cross virial coefficients for interactions involving water: data compilation and some correlations.

A. PLYASUNOV: Group contribution method for aqueous solutes at elevated T and P: Why to start with the thermodynamic functions of hydration at 298.15 K?"

V. MAJER: Progress on the development of group contribution method for hydration properties of organic aqueous solutes

S. LVOV: High temperature pH measurements for industrial applications

The workshop was interrupted at 10:05 A.M. after presentation of Dr. Ueno due to tragic events on the East Coast. The program was continued on Thursday morning, see below, without contribution of S. Lvov who had to return to Penn State.

**Wednesday, September 12; Joint PCAS and TPWS WGs workshop "Molecular simulation of water and aqueous solutions" (improvised at the hotel)**

I Svishchev, Trent University, chair of the Task group on molecular simulation, was chairing the workshop, which started at 8:30 AM. Igor made a short introduction explaining objectives of the task group.

The scheduled presentations:

I.SVISHCHEV: The standard formulations for computer simulated water: linking research and industrial applications

R.MOUNTAIN: Water potentials

F.STARR: Supercooled states: How unusual is water?

S.OKAZAKI: Molecular dynamics study of sub- and supercritical water based upon polarizable potential model - PVT, dielectric constant, and clusters

A.CHIALVO: Ion pair formation in supercritical electrolyte solutions of NaCl, HCl, and CuCl

R.H. WOOD: "Free energies and structure of high level ab initio models from simulations

of Lennard-Jones plus charge models; free energy of hydration of Na<sup>+</sup> and Cl<sup>-</sup>

K.YASUOKA: Molecular Dynamics Simulation of Vapor-Liquid nucleation

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The presentation of Prof. Wood's had to be cancelled since he had to return to Delaware on Tuesday evening.

The WG members continued after the workshop the joint session with TPWS (see the TPWS WG minutes) The PCAS WG member A. Anderko presented a contribution on phase equilibria and pH in the water-ammonia- carbon dioxide.

### **Wednesday afternoon, September 12; Discussion regarding improvement of collaborations between PCC and PCAS WGs workshop**

1. J. Bellows opened the session and expressed a feeling regarding failing communication between the two WGs. In his view PCAS WG should be better informed about the needs of PCC and should address them in their activities.
2. V. Majer responded in the name of PCAS WG. It is difficult to expect some targeted research without additional funding available. Since IAPWS does not have vocation of a funding agency the support for specific actions of interest to PCC should be provided by companies to which the PCC members are affiliated. The PCAS WG members are funded in their home institutions mainly for fundamental research, they are ready to address topics proposed by PCC but can not do it without additional support. It can be also expected that more researchers active in the field of high temperature aqueous systems will be attending the IAPWS annual meeting provided it will be a platform for initiating applied research contracts.
3. After a short discussion it was decided to organise during annual meetings round table discussion where PCC WG members will expose their problems and PCAS WG will provide possibly "state of art" information on topics of interest

### **Thursday morning, September 13; Separate PCAS WG meeting**

1. The PCAS internal talks that were interrupted on Tuesday morning were continued. Andrey Plyasunov (Washington University) presented the first talk on the "Second Cross Virial Coefficients for Interactions involving Water: Data compilations and some co-relations". He also presented a second talk on "Group additivity co-relations of thermodynamic properties for aqueous organic compounds". Dr.Vladimir Majer gave the final talk on the current status of research on co-relation models for hydration properties of non-electrolyte organic solutes (mainly dealing with Henry's law constants) in his research group.

## Attachment 8

2. Co-ordinators of the three tasks for the future consideration of PCAS were chosen: S. Lvov to lead pH project; R. Wood for non-electrolyte group contribution methods and D. Palmer for ion association;. These three tasks will be reported on in 2002, 2003 and 2004, respectively, and may lead to guidelines being proposed on each task.
3. New members proposed for approval by EC: Dr. Masakatsu Ueno (Japan) and Dr Andrey Plyasunov (USA) and Ariel Chialvo (USA).
4. The PCAS WG expressed their concerns regarding the future of IAPWS. In several countries the participation in IAPWS National Committees is limited and financial contributions are difficult to obtain. It would be useful to gain new member countries and reinforce the existing memberships. The functioning of IAPWS should become more flexible and less bureaucratic. IAPWS should also consider opening up towards other fields where high temperature aqueous systems are of high interest (geologic fluids, reservoir chemistry, hydrothermal oxidation and reactions). The ratio between technical (annual) meetings and IAPWS scientific conferences (4:1) is not favourable. People from academia do not have money and time to attend technical meetings every year, this is the reason why attendance in the PCAS WG meetings is relatively low and IAPWS is not well known among physical and solution chemists.