### THE INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

### **MEMBERS**

Argentina and Brazil Britain and Ireland Canada Czech Republic Denmark France Germany Italy Japan Russia United States of America

#### ASSOCIATE MEMBERS Greece

### 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

Kyoto, Japan 29 August – 3 September, 2004

### **Prepared by: Barry Dooley**



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### Minutes of the Meetings of the Executive Committee of the International Association for the Properties of Water and Steam held in Kyoto, Japan 29 August – 3 September, 2004

### Plenary Session. Sunday, 29 August 2004. 9:00am

The President of IAPWS, Professor Koichi Watanabe, welcomed the EC and other IAPWS members to Kyoto for the EC and WG Meetings of IAPWS as well as for 14<sup>th</sup> ICPWS. He indicated that over 220 people had pre-registered for the ICPWS from about 20 countries with about 70 coming from overseas.

The President then officially opened the 2004 EC Meetings by introducing the National Delegates. Each of the member countries of IAPWS was in attendance with the exception of Canada, France and Italy. There were about 40 people in attendance.

### 1. <u>Adoption of Agenda</u>

A provisional agenda had been posted on the IAPWS Website for all IAPWS members by the Executive Secretary in June 2004. There were no suggestions for additional items. The agenda was then approved by the Heads of all National Delegations and forms Attachment 1 of these minutes.

### 2. <u>Preparation for IAPWS General Assembly</u>

The President indicated that the EC would defer discussion on this until later in the day.

At 4:30pm the EC reassembled. The Executive Secretary indicated that the next ICPWS would be in 2008 and that no member had offered to host the conference. He indicated that BIAPWS was next in line to host the ICPWS followed by Germany. He proposed to the EC that the BIAPWS Delegate (Cooper) officially request the BIAPWS Joint Committee to inform the Executive Secretary by the end of 2004 if they could host the 15<sup>th</sup> ICPWS. In the event that the BIAPWS committee could not, then Germany would be the backup location.

### The EC approved this suggested approach unanimously.

- 3. <u>IAPWS Business and Appointment of Committees</u>
  - 3.1 Press Release.

The President asked Bellows and Oguchi to serve on this Committee. The Press Release is discussed in Minute 18.2 and Attachment 18.

3.2 Evaluation Committee on International Collaboration.

The President indicated that no proposals had been received by the Executive Secretary prior to the meeting. The President reminded the EC that the Committee to review any proposals received by the end of the day would consist of the WG Chairmen, with the President and Executive Secretary as ex. officio members. A chairman would be chosen if any suggestions are received. The discussion of this Committee is reported in Minute 15.3 and Attachment 10.

3.3 IAPWS Awards Committees

### 3.3.1 Helmholtz Award Committee

The President indicated that no suggestions had been made for the 2004 Award which was very disappointing for IAPWS. He then reminded the EC that the Helmholtz Committee for the 2005 award would consist of a member from Argentina/Brazil, BIAPWS, Canada, Czech Republic and France. The President asked the Argentina/Brazil delegate (Corti) to organize the committee and to report back to the EC on Friday with the names of the members of this committee (Minute 16.2). The procedures to be followed are delineated in the 1999 EC Canada Minutes.

### 3.3.2 Honorary Fellow Award Committee

The President asked the Executive Secretary to review the procedures and status of the Committee. He then asked Daucik to join Fernandez-Prini on the Committee for 2004. Fernandez-Prini will be the Chairman.

3.4 IAPWS Restructuring

The President requested an update from each of the chairpersons of the four Committees and five Task Groups within the restructuring activities discussed at the Denmark EC Meetings (Committees and Task Forces. Vejle Minutes, Attachment 2).

Committees:

- Nuclear Power. Chairman Uchida outlined the work accomplished during the last year
- Fuel Cells and Hydrogen Technology. Chairman Lvov was not present at the EC meeting.

- Effectiveness of ICRNS. Chairman Bellows indicated that there had been insufficient time for any activity.
- Awards. Chairman Cooper outlined his review of the IAPWS Awards and made a number of suggestions for achieving better IAPWS recognition.

Task Forces:

- Properties and Formulations for High Temperature Aqueous Systems. Chairman Mayer was not present at the EC meeting.
- Electrochemical Processes in High Temperature Aqueous Systems. Chairman Lvov was not present at the EC meeting.
- Education and Outreach. Chairman Corti outlined the input from Greece and BIAPWS.
- Environmental Issues. Chairman Okita presented an initial report.
- Metastability, Nucleation, Early Condensate, Droplet Sprays, Cavitation. Chairman Marsik provided an initial list of names of people who should be interested in joining this Task Force.

After each chairperson had presented the initial information, the President requested that work should continue during the week with a final presentation to the EC on Friday. See Minute 18.1 and Attachments 11-17.

3.5 IAPWS Statutes and By-Laws

The President requested the Chairman of the Task Group (Harvey) to report on the activities of the Committee (Assael, Cooper and Miyagawa). Attachment 2 provides the information on the changes suggested. The BIAPWS Delegate (Cooper) then suggested that these changes only constitute an "Amendment" of the Statutes and By-Laws, rather than a "Revision". He also suggested that the flavour of Section 14 of the Statutes ("Taking Effect of these Statutes") should not be changed from the September 1994 version, and that the Statutes and By-Laws should be submitted to the General Meeting for adoption. The President suggested that these items needed to be considered by the EC later in the day.

At 4:30pm, the EC reassembled and the President re-proposed the items suggested by Cooper.

# The EC unanimously approved the suggestions by the BIAPWS Delegate, and that the Statutes and By-Laws will be submitted to the General Meeting for adoption.

3.6 Other Business Considered to Require Special/Extensive Discussions

There were no other items suggested by the EC

### 4. EC Mandate to Working Groups and Membership

4.1 Releases, Guidelines and Certified Research Needs.

The President asked the Executive Secretary to review the status of various Releases, Guidelines and Advisory Notes that would need action by the WGs and the EC during the week. The Executive Secretary indicated that the following four documents had been forwarded to the Heads of National Committees during the year:

- Revised Supplementary Release on Backward Equations for the Functions T(p,h), v(p,h) and T(p,s), v(p,s) for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam.
- Supplementary Release on Backward Equations p(h,s) for Region 3, Equations as a Function of h and s for the Region Boundaries, and an Equation  $T_{sat}$  (h,s) for Region 4 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam.
- Guideline on the Henry's Constant and Vapor-Liquid Distribution Constant for Gases in H<sub>2</sub>O and D<sub>2</sub>O at High Temperatures.
- Advisory Note No. 2. Roles of Various IAPWS Documents Concerning the Thermodynamic Properties of Ordinary Water Substance.

The Executive Secretary reminded the EC that comments on any of these documents were due by the end of the day and that the EC would then be asked to approve these IAWPS documents at the EC meeting on Friday (Minutes 8.1, 8.2 and 15.1). The Executive Secretary then noted that ICRNs 1, 5, 10, and 13 would need action by the respective WGs during the week (Minute 15.2).

### 5. <u>Preview by WG Chairmen of Weeks Activities</u>

President Watanabe indicated that in the interest of time the EC would forego these previews this year. The details of these WG meetings are covered in detail in Minutes 8, 9, 10, and 11.

### Activities During the Week

The first day activities of the WGs and Executive Committee were followed by WG meetings on Sunday 29 August 2004. The 14<sup>th</sup> ICPWS was held from Monday, 30 August 2004 to Thursday, 2 September 2004.

The full IAPWS program for the week is shown in Attachment 3.

### Executive Committee Meeting. Friday, 3 September 2004

President Watanabe opened the continuation of the EC Meeting at 9:05am. All members of IAPWS were present except Italy. He first asked if there were any additional items that should be added to the Agenda. None were suggested.

### 6. <u>Acceptance of Minutes of Previous Meeting</u>

President Watanabe asked for comments and changes to the minutes of the EC meeting held in Vejle, Denmark in August 2003. The Executive Secretary indicated that an errata sheet had been developed for the 2003 Minutes and posted on the IPAWS Website. No further changes were noted, thus the 2003 Minutes were accepted.

### 7. <u>President's Report</u>

President Watanabe provided the following comments:

- He had provided his main report for the General Meeting (General Meeting Minutes).
- He wished again to to indicate that the ICPWS was a nice assembly of people and illustrated the collaboration within the IAPWS community, which he hoped would continue.
- IAPWS is currently restructuring, but is basically on track.
- He will be forwarding a signed copy of the just published IAPWS "Atlas" to Professor Ulrich Franck.

### 8. <u>Report and Recommendations of Thermophysical Properties of Water and Steam</u> <u>Working Group (TPWS)</u>

Chairman Friend highlighted only those activities from the TPWS working sessions during the week, which needed action by the EC. He indicated that most of the WG activities had been conducted with IRS. Full minutes can be found in Attachment 4.

8.1 The TPWS and IRS WGs had voted to recommend the adoption of the Supplementary Release "Supplementary Release on Backward Equations p(h,s) for Region 3, Equations as a Function of h and s for the Region Boundaries, and an Equation  $T_{sat}(h,s)$  for Region 4 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" after some minor revisions had been addressed in conjunction with the Editorial Committee. The Chairman proposed that this supplementary release be approved by the EC

### The EC approved this supplementary release unanimously

8.2 The WGs had voted to recommend the adoption of the revised Supplementary Release "Revised Supplementary Release on Backward Equations for the Functions T(p,h), v(p,h), and T(p,s), v(p,s) for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam". Chairman Friend then proposed to the EC that this release be approved.

### The EC approved the release unanimously.

8.3 Chairman Friend noted that the *Journal of Engineering for Gas Turbines and Power* was imposing excess page charges (\$200 for each page above nine) for the publication of the comprehensive article reporting the first Supplementary release with additional backward equations, adopted in 2001. This might amount to approximately \$2000. The WG felt that this was a necessary expense for the dissemination of IAPWS standards. Friend requested approval from the EC that these page charges could be paid from IAPWS funds.

# After much discussion, the EC approved this payment with one objection from Canada.

- 8.4 Chairman Friend noted that a WG member was frequently asked about the status of IAPWS recommendations as an engineering standard, and the relationship with ISO. He wanted to inform the EC that it had been decided to draft a FAQ on this issue for the IAPWS Website and that Harvey and Span will work on this.
- 8.5 Chairman Friend next raised the issue of WG membership. He indicated that last year some WG members were asked to attempt to contact members who had not been active to see if they wished to continue. As a result of this, he proposed to the EC that Dr. Agayev (Azerbaijan) and Dr. Mayinger (Germany) should be withdrawn from TPWS membership.

### The EC approved these membership changes unanimously.

8.6 Chairman Friend indicated that the WG now realized that Advisory Note #2 should be updated to reflect the new Supplementary Releases (Approved in Minutes 8.1 and 8.2). He indicated that Cooper will draft the updated language. This Advisory Note will then be forwarded to the Executive Secretary for circulation to the National Committees.

### The EC approved this process unanimously.

8.7 Chairman Friend noted that in regard to the issue raised about attracting people (especially young people) to annual meetings, the TPWS WG wished to recommend to the EC that the Executive Secretary should send invitations for the Annual Meetings directly to each WG member (either

by postal mail or e-mail) rather than relying solely on the Website. This raised much discussion. The President finally indicated that the consensus was for the Heads of National Committees and WG Heads to forward the information supplied by the Executive Secretary to them and to the IAWPS Website to any special invitees. Then an individual invitation could be formulated.

### 9. <u>Report and Recommendations of Industrial Requirements and Solutions Working</u> <u>Group (IRS)</u>

Chairman Miyagawa provided the IRS Report to the EC. Full minutes can be found in Attachment 5. The Chairman indicated that all the technical items had been covered by Friend in the TPWS report. He only had two items that needed action by the EC.

9.1 With regards to membership of IRS, Chairman Miyagawa requested that three people be removed from the membership: Perstrup, Meyer-Pittroff and Perera. He then proposed one new member, Daur from Alstom Power in Germany.

### The EC approved these membership changes unanimously.

9.2 Chairman Miyagawa expressed his wish to step down as the WG chairman at the end of 2004 and proposed to the EC that Parry becomes the chairman with Weber as the vice chairman.

### The EC approved these IRS leadership changes unanimously.

# 10. <u>Report and Recommendations of Physical Chemistry of Aqueous Solutions</u> <u>Working Group (PCAS)</u>

Chairman Mayer provided the PCAS Report to the EC. Full minutes can be found in Attachment 6.

10.1 The Chairman indicated that he will be stepping down as of January 2005. He proposed to the EC that Lvov becomes the new chairman and that Corti becomes vice chairman.

### The EC approved these leadership changes unanimously.

10.2 Chairman Mayer next informed the EC about the PCAS Priority Areas: a) pH of water at high temperatures, b) prediction of standard state properties of non-electrolytes, and c) ion pairing in 1-1 electrolytes. The PCAS WG will be discontinuing work in the last area.

10.3 Chairman Mayer next proposed Sedlář of Sigma Research and Development Institute as a new WG member.

### The EC approved this membership addition unanimously.

10.4 Chairman Mayer next introduced a proposal for a new project to the EC on "Establishing Recommended Data on Thermodynamic Properties of Hydration for Selected Organic Solutes". He indicated that the proposal and an appendix had been provided to each National Committee during the week. These are Attachment 7. The Chairman requested that the EC approve the requested funding of 12K euros (with 5K in 2005, 5K in 2006 and 2K in 2007). Some discussion ensued about the ownership of the common data base between IUPAC and IAPWS, the likelihood of funding from IUPAC, and how the data base will be updated. The President delayed the EC vote on this item until after the EC had been informed about the IAPWS finances (Minute 14.1). At that time the EC was asked to approve the full funding over the period 2005 – 2007.

### The EC approved the funding for this project unanimously.

10.5 Chairman Mayer next introduced another proposal for a new project to the EC on "Hydrothermal Experimental Data: Phase Equilibria and Solution Properties in Binary and Ternary Systems". He again indicated that the proposal and an appendix had been provided to each National Committee during the week. These are Attachment 8. The Chairman indicated that no financial support was being requested from IAPWS. Some discussion ensued about whether the timetable was realistic, and that the EC wanted to ensure that IAPWS received full credit by having the IAPWS logo prominently displayed on the front of the book. The President asked the EC to approve the project

### The EC approved the project unanimously.

11. <u>Report and Recommendations of Plant Cycle Chemistry Working Group (PCC)</u>

Chairman Zeijseink highlighted those activities that needed action/approval by the EC. A full written report of the PCC WG activities forms Attachment 9.

- 11.1. The Chairman indicated that the new procedure for Guidelines/ICRN had not yet been fully developed, but that the WG intended to test it out on a new priority item involving mechanical carryover. Attachment A to the PCC WG minutes is a first draft.
- 11.2. The Chairman indicated that PCC had developed a proposed International Collaborative proposal on flow-accelerated corrosion.

11.3 The Chairman proposed Therkildsen from Energi E2 in Denmark as a new member of the WG.

### The EC approved this membership addition unanimously

### 12. Editorial Committee Report

Chairman Harvey reported that the Editorial Committee had reviewed and approved four IAPWS documents during the last year: the Supplementary Release on Backwards Equations, the revised Supplementary Release on Backwards Equations, the Guideline on Henry's Constant, and the Advisory Note #2.

### 13. <u>Membership and Associates</u>

13.1 Membership.

The Executive Secretary requested the Greece Delegate, Assael, to provide an update on the membership of Greece in IAPWS. Assael indicated that he now had agreement that the IAPWS Membership dues would be paid for 2005 and that Greece was now ready to apply for full membership in 2005.

### The EC approved this new full IAPWS member unanimously

13.2 Members Defaulting on Dues.

The Executive Secretary indicated that according to the latest Swiss bank account statement (31 July 2004), the following countries had not paid the 2004 IAPWS dues: Canada, France, Japan, USA, and Russia. In 2003 France had not paid the dues. In 2002 France paid a partial payment. In response: a) the Canada delegate indicated that the Canadian NRC was in the process of paying, b) the Japan delegate indicated that the invoice had been sent to the payment authority, c) the US ensured the EC that the dues would be paid, d) the Russia delegate indicated that Russia will fully pay the dues but cannot do this each year, and e) the France delegate once again reminded the EC of the revitalization of the French national committee. The Executive Secretary indicated that there had been no change in the Italian national committee situation and there was still no active committee in Italy.

### 14. <u>Executive Secretary's Report</u>

14.1 Financial, Auditors and Dues

The Executive Secretary reported that IAPWS remained on a sound financial footing with currently over SFrs 85,000 in the Swiss bank

account and over \$17,500 in the US account for a total of \$86,037 combined. The status as at 16 August 2004 in the bank accounts had been provided to each National Delegate present at the EC meeting.

The Executive Secretary next reported that the 2003 financial statements had been forwarded to the Auditors in January 2004. Mr. Miyagawa in Japan had reviewed and approved them. VDI in Germany had not to date replied. The financial statements for 2003 and the Auditors reports had also been provided to all the National Delegates present.

The Executive Secretary proposed that these organizations continue to act as auditors.

### The EC approved this unanimously.

The Executive Secretary proposed to the EC that the dues structure for member countries remain unchanged for 2005, and that the dues for the new Greece National Committee would be set at 1,600 SFrs for 2005.

### The EC unanimously agreed to this proposal.

The Executive Secretary also provided a rough estimate of the income and known planned expenditures for 2004. This lead to some discussion about the overall planned IAPWS expenditures. The BIAPWS delegate specifically wished to know whether there would be the same level of support for the BIAPWS committee if they decided to hold the 15<sup>th</sup> ICPWS in the UK or Ireland in 2008. Instead of suggesting a specific amount, the following proposal was formulated for the EC: "The EC would agree to support the BIAPWS (or Germany if BIAPWS cannot hold the next conference) committee for the next ICPWS, to about the same level as was provided to Japan for the 14<sup>th</sup> ICPWS, upon receiving an official request".

### The EC approved of this proposal unanimously

### 14.2 Time and Place of the 2005 and 2006 Meetings

The 2005 EC Meetings will be held in Greece. The Executive Secretary asked the delegate from Greece to provide the details. Assael indicated that the next EC and WG meetings would be held at the Santorini Palace Hotel at Fira on the Island of Santorini from Sunday, 3 July to Friday, 8 July, 2004. He planned to very quickly establish a website, and requested early registration and booking.

The Executive Secretary indicated the location of the 2006 EC Meetings was dependent on the response from BIAPWS (and maybe Germany)

about hosting the 2008 ICPWS. The countries next in line to host the EC Meetings are Russia, France, Germany and Britain/Ireland. Discussions with the Russia delegate had indicated that it was financially not possible for Russia to host the meetings, but that France was prepared to consider holding the 2006 or 2007 meetings depending on the revitalization of the national committee. The EC was asked to approve delaying the decision of a location for 2006 until the 2005 EC meetings.

### The EC approved this delay unanimously.

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

15.1 Guidelines and Releases

Four documents had been forwarded to National Committee for postal ballot during the year. The overall status of these documents follows:

- Revised Supplementary Release on Backward Equations for the Functions T(p,h), v(p,h) and T(p,s), v(p,s) for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam. This was approved by the EC during the TPWS WG presentation (Minute 8.2).
- Supplementary Release on Backward Equations p(h,s) for Region 3, Equations as a Function of *h* and *s* for the Region Boundaries, and an Equation  $T_{\text{sat}}(h,s)$  for Region 4 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam. This was approved by the EC during the TPWS WG presentation (Minute 8.1).
- Guideline on the Henry's Constant and Vapor-Liquid Distribution Constant for Gases in H<sub>2</sub>O and D<sub>2</sub>O at High Temperatures. One small change had been raised by the Japanese National Committee, which had been dealt with during the TPWS WG meeting and approved by the Editorial Committee.

### The EC approved this Guideline unanimously

- Advisory Note No. 2. Roles of Various IAPWS Documents Concerning the Thermodynamic Properties of Ordinary Water Substance. The EC had already approved of the process to finalize this Advisory Note during the TPWS WG presentation (Minute 8.6)
- 15.2 IAPWS Certified Research Needs (ICRNS)

The President indicated that discussion on ICRNs should have been dealt with during the WG meetings as requested during the Plenary EC Meeting on Sunday, 29 August 2004. The following actions were developed:

- ICRN 1. This will be "Closed August 2004". The PCC Chairman will provide a closing statement to the Executive Secretary within two months.
- ICRN 5. This will be "Closed August 2004". The PCC Chairman will provide a closing statement to the Executive Secretary within two months.
- ICRN 10. This needs new life. It will be extended to, and then revised in, July 2005. The new PCAS Chairman, Lvov, has the responsibility.
- ICRN 13. This needs new life. It will be extended to, and then revised in, July 2005. The PCC Chairman, Zeijseink, has the responsibility to contact one of the original authors, Gabrielli.

### The EC approved all these actions on ICRNs unanimously

15.3 International Collaborative Projects.

The President asked the Chair of the Committee (Friend) to report on the discussions during the week. The Chairman indicated that only one proposal had been received. The details of this proposal are provided in Attachment 10. The Chairman summarized the proposal for the EC. The IAPWS Sponsors are Uchida (Japan) and Tremaine (Canada). A young Japanese investigator will travel to UNB in the Canada to investigate the experimental techniques being used there to assess flow-accelerated corrosion. The period of performance will be four months at a proposed budget cost of \$5,000 for travel expenses and costs.

After some discussion by the EC, the President asked the Japanese and Canadian delegates to leave the room and then asked the EC for approval

### The EC approved the project unanimously.

### 16. <u>IAPWS Awards</u>

### 16.1 IAPWS Honorary Fellowships

The President reported that Tremaine (Canada) and Miyagawa (Japan) had been elected Honorary IAPWS Fellows, following the established procedure and after unanimous approval through the postal ballot conducted by the Executive Secretary. The Fellowship Awards had been presented at the IAPWS Dinner on Thursday evening.

The President reminded the EC of the Awards Committee for 2005 with Fernandez-Prini as Chairman and Daucik as member. The IAPWS President in 2005 (Marsik) will be an ex.-officio member.

### 16.2 IAPWS Helmholtz Award

The President asked the Argentina-Brazil Delegate for the names of the Helmholtz Award Committee for 2005. Corti (Chairman) indicated that the members would be Harries (BIAPWS), Svishchev (Canada), Mares (Czech Republic) and Mayer (France). Nominations are due to the Executive Secretary by January 31, 2005.

### 17. Election of Officers for 2005 and 2006

The President indicated that he would step down at the end of 2004 and that Vice President Marsik will assume the position of IAPWS President on January 1, 2005. According to the Statutes, the election of the next Vice President should be made at the end of the EC meeting in even years. The President and Executive Secretary had checked the recent history and proposed that the BIAPWS Joint Committee should be asked to nominate one of their committee members for the position. The President asked the EC if there were any other suggestions. None were suggested, so he then requested the EC approves this selection.

### The EC unanimously approved this selection.

Action: The BIAPWS Joint Committee should inform the Executive Secretary of their nomination for Vice President after the next meeting of their committee, and before the end of 2004.

### 18. <u>New Business</u>

### 18.1 IAPWS Restructuring

The President reminded the EC that some initial discussions had taken place at the Plenary meeting of the EC on Sunday, 29 August 2004 (Minute 3.4), and that he had requested each of the Committee and Task Group Chairmen to return at the Friday EC meeting with a final report. He then requested each chairman to provide the status.

### Committees:

- Nuclear Power. Chairman Uchida indicated that there were no significant changes from his presentation on Sunday and provided Attachment 11 as a final report of his committee.
- Fuel Cells and Hydrogen Technology. Chairman Lvov presented his committee report. (Attachment 12)
- Effectiveness of ICRNS. Chairman Bellows was not present at the EC meeting.
- Awards. Chairman Cooper indicated that there were no further activities. He provided his committee report (Attachment 13) and

indicated that this committee should now be closed. However, the suggested actions should be addressed in Greece.

Task Forces:

- Properties and Formulations for High Temperature Aqueous Systems. Chairman Mayer indicated that this Task Group had been discussed in the PCAS WG and that his report is included within the PCAS Minutes (Attachment 6).
- Electrochemical Processes in High Temperature Aqueous Systems. Chairman Lvov presented his report. (Attachment 14).
- Education and Outreach. Chairman Corti indicated no significant changes and provided his report (Attachment 15).
- Environmental Issues. Chairman Okita indicated no significant changes and provided his report (Attachment 16).
- Metastability, Nucleation, Early Condensate, Droplet Sprays, Cavitation. Chairman Marsik indicated no significant changes and provided his report (Attachment 17).
- 18.2 Press Release

The President requested that the Press Release be projected for review by the EC. The final version is contained in Attachment 18.

### The EC approved this unanimously.

18.3 14th ICPWS, Kyoto, Japan. August 29 – September 3, 2004

The President reported that the final count at the 14<sup>th</sup> ICPWS was 235 people, and that 195 papers had been presented.

18.4 Review of Progress of Research in Member Countries

Written reports on progress in member countries were not reported to the EC but were distributed to other members and the Executive Secretary during the ICPWS/IAPWS week. They are attached to these minutes as follows:

Britain and Ireland	Attachment 19
Czech Republic	Attachment 20
Denmark	Attachment 21
Germany	Attachment 22
Greece	Attachment 23
Japan	Attachment 24
Russia	Attachment 25
USA	Attachment 26

### 18.5 Participants

Attachment 27 provides a list of participants at the ICPWS and IAPWS EC and WG Meetings in Kyoto, Japan in August 2004.

### 18.6 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 Kyoto Meetings. This will be forwarded electronically to the Head of each National Committee.

### 19. <u>Closing Remarks and Adjournment</u>

The President thanked everybody for their patience during this EC meeting. He indicated that he had enjoyed his second IAPWS Presidency, and then formally closed the 2004 EC meetings at 12:30pm.

# AGENDA for the EXECUTIVE COMMITTEE IAPWS

# KYOTO, JAPAN. 29 AUGUST – 3 SEPTEMBER, 2004

### Sunday, 29 August 2004. Opening Session (9:00 - 10:30am)

Opening Remarks and Welcome

- 1. Adoption of Agenda
- 2 Preparation for IAPWS General Assembly
  - 2.1 Host Country for 15<sup>th</sup> ICPWS
- 3. IAPWS Business and Appointment of Committees
  - 3.1 Press Release
  - 3.2 Evaluation Committee on International Collaboration
  - 3.3 IAPWS Awards Committees (Honorary Fellow and Helmholtz)
  - 3.4 IAPWS Restructuring (Committees and Task Forces. Vejle Minutes, Attachment 2)
  - 3.5 IAPWS Statutes and By-Laws
  - 3.6 Other business requiring special/extensive discussions
- 4. EC Mandate to Working Groups and Membership
  - 4.1 Releases, Guidelines and Certified Research Needs (New and Expiring)
  - 4.2 WG Directions
- 5. Preview by WG Chairpersons of Week's Activities

### Friday, 3 September 2004. Executive Meeting. (9:00am - 12:00noon)

- 6. Acceptance of Minutes of Previous Meeting
- 7. President's Report
- 8. Report and Recommendations of TPWS
- 9. Report and Recommendations of IRS
- 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 Members Defaulting on Dues)
- 14. Executive Secretary's Report
  - 14.1 Financial, Auditors and Dues
  - 14.2 Time and Place of 2005/2006 Meetings
  - Guidelines, Releases, Certified Research Needs and International Collaborations
- 16. IAPWS Awards (Helmholtz and Honorary Fellowship)
- 17. Election of Officers for 2005/2006
- 18. New Business
  - 17.1 IAPWS Restructuring
  - 17.2 Press Release
  - 17.3 14<sup>th</sup> ICPWS Report

19. Adjournment



15.

# STATUTES & BY-LAWS

- Task Group: Harvey (Chair), Assael, Cooper, Miyagawa
- Mandate from 2003 meeting (Minute 12.3): "Look primarily at the areas of documents and awards within the Statutes and By-Laws."
- <u>Reasons</u>: Duplication in existing Statutes and By-Laws, some documents not mentioned, most awards (Gibbs, Helmholtz) not mentioned, some procedures did not reflect current practice or were ambiguous.
- <u>General Philosophy</u>: Make Statutes simpler since they are harder to change. Put details in By-Laws.

# CHANGES TO STATUTES

- Remove details about Releases & Guidelines (now in By-Laws), keep statement authorizing documents (Section 2.2).
- Add sentence authorizing awards (Section 5.3.3)

# CHANGES TO BY-LAWS

- Define existing types of documents (Release, Guideline, Supplementary Release, Advisory Note), EC may issue others (Section 3).
- Procedures for adopting documents adjusted to reflect current practice, possibility of electronic distribution (Sections 3, 6).
- <u>Awards</u>: Addition of Gibbs and Helmholtz, further explanation of IAPWS Fellow procedure. All reflect current ways of doing things. (Section 7).

# STATUTES AND BY-LAWS: FURTHER COMMENTS

- Task Group restricted itself to narrow mandate (documents, awards).
- There may be other changes to Statutes and By-Laws that should be considered for the next ICPWS. Any Task Group for a comprehensive review of Statutes and By-Laws should be formed at least <u>two</u> years in advance.
- Possible areas for change:
  - 1) Move details of ICRNs to By-Laws?

2) Do we need the General Meeting to set policy, or should it just be informational?

- 3) Something in By-Laws about Website?
- 4) Update postal ballot procedures?

# Schedule IAPWS Meetings and ICPWS Kyoto, Japan. 29 August – 3 September 2004

(Kyoto International Conference Hall)

Sunday 29 Aug. 9:00am EC Initial Meeting 10:30am TPWS/IRS Joint Meeting 10:30am PCAS Separate Meeting 10:30amPCC Separate Meeting 1:30pm Meeting of all WGs

Registration for ICPWS will be from 3:00-7:00pm

5-7:00pm IAPWS Informal Reception (Swan Banquet Hall)

Monday 30 Aug. 9:00am. Opening Plenary Session – ICPWS 2:00pm Poster Session - ICPWS 3:30pm. ICPWS Symposia - Afternoon

Tuesday 31 Aug. 9:00am. ICPWS Symposia All Day 3:40pm Poster Session - ICPWS

5:10-6:00pm General Meeting of IAPWS

Wednesday 1 Sept. 9:00am ICPWS Symposia – Morning

1:30pm Excursion

Thursday 2 Sept. 9:00am. ICPWS Symposia All Day

7:00pm. IAPWS Banquet (Sakura Banquet Hall)

Friday 3 Sept. 9:00am. Executive Meeting (9:00 - 12:00noon) (To include one member from each National Delegation)

TPWS - Thermophysical Properties of Water and Steam WG

- PCAS Physical Chemistry of Aqueous Solutions WG
- PCC Power Cycle Chemistry WG
- IRS Industrial Requirements and Solutions WG

Barry Dooley 16 August 2004



Minutes

### IAPWS Thermophysical Properties of Water and Steam WG

KYOTO, JAPAN 28 AUGUST TO 3 SEPTEMBER 2004

NOTE: Items are listed according to their order on the agenda, which is attached as Attachment A. **Bold print** denotes significant actions. These minutes include some items (4-6) that were done jointly with the WG IRS.

1-3. The meeting was opened at 11 AM on Sunday, August 29 by the Chair, Dan Friend. The agenda (Attachment A) was adopted. Allan Harvey was appointed Clerk of Minutes. The minutes of the 2003 IAPWS TPWS WG meeting in Denmark were approved.

4. The draft Supplementary Release "Supplementary Release on Backward Equations p(h,s) for Region 3, Equations as a Function of h and s for the Region Boundaries, and an Equation  $T_{sat}(h,s)$  for Region 4 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" was distributed along with the favorable report of the evaluation task group. Concern was raised that the draft did not sufficiently deal with the issue of a short extrapolation into the metastable region below the triple point. It was decided that Prof. Kretzschmar, in conjunction with the Editorial Committee, should add a few words to address this issue. The WGs voted to recommend the adoption of the Supplementary Release "Supplementary Release on Backward Equations p(h,s) for Region 3, Equations as a Function of h and s for the Region Boundaries, and an Equation  $T_{sat}(h,s)$  for Region 4 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" after this minor revision.

5. The draft revised Supplementary Release "Revised Supplementary Release on Backward Equations for the Functions T(p,h), v(p,h), and T(p,s), v(p,s) for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" was distributed along with the favorable report of the evaluation task group. The WGs voted to recommend the adoption of the revised Supplementary Release "Revised Supplementary Release on Backward Equations for the Functions T(p,h), v(p,h), and T(p,s), v(p,s) for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam". Thanks was expressed to both the developers and the evaluation task group for all their hard work on both of these Supplementary Releases.

6. A report was given by Prof. Kretzschmar about the work of the Task Group on backward equations. A new Supplementary Release was proposed for the function v(p,T) for Region 3. The proposal divided Region 3 into 20 subregions (or 26 if it was desired to cover all of Region 3, allowing larger deviations very near the critical point); there was some discussion as to whether this was desirable. It was decided to go ahead, but with a version that covered all of Region 3, sacrificing the consistency requirements very close to the critical point. The WGs voted to appoint the same evaluation task group (chaired by Mr. Miyagawa) as for item #4 above,

# and to adopt a similar schedule of work (with the evaluation completed by the end of January) with the goal of adoption at the 2005 meeting in Greece.

6a. It was brought up that the *Journal of Engineering for Gas Turbines and Power* was imposing excess page charges (\$200 for each page above nine) for the publication of the comprehensive article reporting the first Supplementary release with additional backward equations, adopted in 2001. This might amount to approximately \$2000. It was felt that this was a necessary expense for the dissemination of IAPWS standards. **The WGs voted to ask the EC to pay these page charges from IAPWS funds.** 

7a. Dr. Harvey recommended that no changes be made for the Fundamental Constants Guideline this year.

7b. Dr. Harvey had nothing to report on the Website, but solicited the WGs for more Frequently Asked Questions. Prof. Span mentioned that he was frequently asked about the status of IAPWS recommendations as an engineering standard, relationship with ISO, etc. It was decided to draft a FAQ on this issue; Dr. Harvey and Prof. Span will work on this.

7c. Dr. Friend summarized the current status of the project to revise the standard for the viscosity of ordinary water. Progress has been made, and a finished version should be available by the end of 2004 to send to the evaluation task group. The next project will the the thermal conductivity of ordinary water.

7d. There was nothing to report regarding the liason with the IEC.

7e. Mr. Cooper reported no progress on the project for updating the  $D_2O$  thermodynamic property release for the ITS-90 temperature scale. He hopes to have a draft of the proposed release and the accompanying report by the end of 2004.

7f. Prof. Span reported the status of the project in the EU on humid air properties for combustion gases and humid air turbines. There are still major needs, particularly for experimental work, for both thermodynamic and transport properties. A task group of Span, Kretzschmar, Harvey and Cooper was appointed to explore how TPWS might help in this work and how it might turn into an output of some kind for TPWS.

7g. Dr. Yasuoka, the Interim Chair of the Simulation Task Group, reported on the previous work of the task group and on some existing resources. A meeting of the Task Group and invited researchers was held and decided to hold annual symposia before focusing on a specific IAPWS output.

8. With regard to membership, last year some WG members were asked to attempt to contact members who had not been active to see if they wished to continue. As a result of this, **Dr. Agayev (Azerbaijan) and Dr. Mayinger (Germany) are withdrawn from TPWS membership** Dr. Friend expressed his intention to step down as Chair of the TPWS WG following next year's meeting in Greece; no replacement has been designated at this time.

9. Prof. Wagner brought to the attention of the WG his work with Prof. Feistel on a fundamental equation for the thermodynamic properties of ice. The WG decided that it would be desirable to have an IAPWS document for the thermodynamic properties of ice. Prof. Wagner

was authorized to proceed in this direction, with the goal of having a draft document for next year's meeting in Greece, at which time an evaluation task group will be appointed.

Mr. Cooper pointed out that Advisory Note #2 should be updated to reflect the new Supplementary Releases (items 4 and 5 above) if they are adopted by the EC. He will draft the updated language.

# The WG voted to recommend such an update to the EC if the proposed Supplementary Releases are adopted.

With regard to the issue raised in the EC meeting about attracting people (especially young people) to meetings, the TPWS WG recommends to the EC that the Executive Secretary should send invitations to the Annual Meetings directly to each WG member (either by postal mail or e-mail) rather than relying solely on the Website.

Dr. Harvey reported on conversations in Kyoto with Drs. Fujii and Tanaka of the National Metrology Institute of Japan, who are involved in the CCM (Consultative Committee for Mass and Related Quantities) and CIPM (International Committee on Weight and Measures). The CCM has adopted a standard for metrology for the density of ordinary water at near-ambient pressures between 0 °C and 40 °C, and questions arise about the relationship of this recommendation to the IAPWS standard. Drs. Fujii and Tanaka are interested in publishing a short note in *Metrologia* to clarify these issues. **Dr. Harvey and Prof. Span were appointed as liasons to deal with the CCM on this issue.** 

10. The Chair and Clerk of Minutes were appointed to prepare the formal motion of the TPWS WG to the EC.

11. The meeting was adjourned at 6:20 PM on Tuesday, August 31.

### **TPWS Attachment A**

### Agenda

### IAPWS Thermophysical Properties of Water and Steam WG

KYOTO, JAPAN 28 AUGUST TO 3 SEPTEMBER 2004

- 1. Opening Remarks; Adoption of Agenda
- 2. Appointment of Clerk of Minutes
- 3. Approval of Minutes of TPWS WG in Vejle, Denmark, August 2003
- \*Supplementary Release on Backward Equations for Region 3, Equations as a Function of h and s for the Region Boundaries, and an Equation for Wet Steam of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam

   4a) Report of the Evaluation Task Group
   4b) Acceptance of the Supplementary Release
- 5. \*Revised Supplementary Release on Backward Equations for the Functions T(p,h), v(p,h), and T(p,s), v(p,s) for Region 3 of the IAPWS Industrial Formulation 1997 for
- v(p,h), and T(p,s), v(p,s) for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam
  - 5a) Report of the Evaluation Task Group
  - 5b) Acceptance of the Supplementary Release
- 6. \*Progress Report of the Task Group for the Development of IAPWS-IF97 Backward Equations in Region 3 (Proposal: supplementary release on v(p,T) equation)
- 7. Reports on Various TPWS Activities
  - (a) Fundamental Constants
  - (b) Website Issues
  - (c) Transport Properties
  - (d) Liaison with IEC
  - (e)  $D_2O$  Properties
  - (f) Humid Air
  - (g) <sup>+</sup>Simulation Task Group
- 8. Membership; Officers
- 9. Other Business
- 10. Preparation of the Formal Motion to the EC
- 11. Adjournment

\* Joint with WG IRS + Joint with WG PCAS

Minutes of the Industrial Requirements & Solutions Working Group

### Kyoto, Japan, August 29 – September 3, 2004

**Note:** Most meetings were held as joint sessions with the TPWS working group. All agenda items of the joint sessions (IRS items 4 to 7) can be found in the TPWS minutes.

Sunday, August 29, 2004, 10:30am

### 1. Opening Remarks, Adoption of Agenda

Chairman Kyoshi Miyagawa welcomed the IRS members to the Kyoto meeting. The previously circulated agenda has been revised – item 7 of the final agenda was added. The agenda was adopted with this amendment. It is provided as IRS attachment A.

### 2. Appointment of Clerk of Minutes

Ingo Weber was appointed clerk of minutes.

#### **3.** Approval of Minutes of Vejle Meeting, August 2003 The minutes of the Vejle meeting was approved without objection.

Tuesday, August 31, 2004, 5:45pm

### 8. Membership

The working group suggests the following changes to the membership roster

Removals: Claus Perstrup Prof. Roland Meyer-Pittroff

George Perrera

Additions:

Dipl.-Ing. Michael Daur Alstom Power GmbH Department GB-ET Augsberger Str. 712 70329 Stuttgart Germany email: michael.daur@power.alstom.com phone: +49 711 9171569

### 9. Other Business

Chairman Kiyoshi Miyagawa expressed his wish to step down from the WG chairman position. The working group members expressed their sincere thanks for his very fruitful and efficient chairmanship. According to traditional procedure the current vice chairman follows in this position. Consequently the WG suggests to nominate Bill Parry for chairman. Bill Parry expressed his confidence in continuous attendance of the WG meetings. As successor for the vice-chairman position the WG suggests Ingo Weber.

### 10. Preparation of Report to Executive Committee

This item will be undertaken by the Chairman and the Clerk of Minutes.

### 11. Adjournment

Chairman Miyagawa thanked all participants for their attention and adjourned the meeting at 6:00pm.

### **IRS** Attachment A

### Agenda

### of

### Industrial Requirement and Solutions Working Group Kyoto, Japan. 28 August to 3 September 2004

- 1. Opening Remarks, Adoption of Agenda
- 2. Appointment of Clerk of Minutes
- 3. Approval of Minutes of Vejle Meeting, August 2003
- 4. Supplementary Release on Backward Equations for Region 3, Equations as a Function of h and s for the Region Boundaries, and an Equation for Wet Steam of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam
  - 4a) Report of the Evaluation Task Group
  - 4b) Acceptance of the Supplementary Release
- Revised Supplementary Release on Backward Equations for the Functions T(p,h), v(p,h), and T(p,s), v(p,s) for Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam
  - 5a) Report of the Evaluation Task Group
  - 5b) Acceptance of the Supplementary Release
- Progress Report of the Task Group for the Development of IAPWS-IF97 Backward Equations in Region 3
  - (Proposal: supplementary release on v(p,T) equation)
- Article on p1(h,s) and p2(h,s) Backward Equations IAPWS support for the excess page charge of ASME Journal of Engineering for Gas Turbines and Power.
- 8. Membership
- 9. Other Business
- 10. Preparation of Report to Executive Committee
- 11. Adjournment

Note: The items 4 to 7 will be discussed at the joint session with WG TPWS.

### Minutes of PCAS WG, 2004 Meeting held August 29, 2004, 14:00 – 17:00 Kyoto, Japan

**Participating members:** Vladimir Majer (chair), Serguei Lvov (vice chair), Horacio Corti, Donald Palmer, Masaru Nakahara, Roberto Fernandez-Prini, Robert Wood, Andre Anderko, František Maršik, Josef Hruby, Josef Sedlbauer, Vladimir Valyashko

### PRELIMINARIES

V. Majer called the meeting to order. Minutes of the previous meeting in Vejle, Denmark were accepted without comment. Andre Anderko was appointed as clerk of minutes.

### Committee Leadership

V. Majer is stepping down as chairman as of January 2005. S. Lvov is ready to take over chairmanship. H. Corti is scheduled to become vice chairman, he expressed, however, some concern regarding his commitment to vice-chairmanship of the IAPWS Committee on educational outreach.

### **Priority Areas**

*pH of water at high temperatures*. D. Palmer reported on the progress in this area. A questionnaire was sent out to experts in this field (Kunio Arai, Horacio Corti, Arthur Covington, Kang Ding, Glenn Hefter, Kevin Knauss, Serguei Lvov, Digby Macdonald, Eric Maughan, Donald Palmer, Peter Tremaine, Shinsuke Uchida, David Wesolowski, Thomas Wolery, Scott Wood, Andre Zeijseink). The topics are: definition of pH at high temperature and methods of measurement. So far, five people have responded. The goal is to prepare a publication with recommendations and submit it to a journal. PCAS WG approved this action unanimously.

**Prediction of standard-state properties of nonelectrolytes.** V. Majer, in collaboration with R. Fernandez-Prini and J. Sedlbauer, prepared a plan of the project and distributed it to the attendees. The objective is to prepare a technical report as an IAPWS guideline, an article to be published in Journal of Physical and Chemical Reference Data and a freely accessible database. Databases that are already in place at Arizona State and University of Liberec will be included in the project. Approximately 200 organic substances will be targeted to cover the largest number of structures rather than the largest number of individual species. Funding from IAPWS has been requested (12 k€ for 2.5 years) to facilitate the mobility of young researchers (under 40 years of age, not members of our group). The mobility support is intended mainly for visits to other labs rather than meeting participation. The possible young researchers include P. Vrbka (Institute of Chemical Technology, Prague), L. Mendez de Leo, H. Bianchi (Atomic Energy Commission, Buenos Aires), V. Diky (NIST – Boulder), K. Ballerat (Blaise Pascal University), N.V.

Plyasunova (Arizona State) and M. Slavik (U. of Liberec). V. Majer has sent the proposal to national delegates and the Executive Secretary; PCAS approved this action unanimously.

*Ion pairing in 1-1 electrolytes*. Donald Palmer reported no progress in this area. Robert Wood indicated the availability of results for 1-2 electrolytes from conductance measurements and predicted values from ab initio methods. Donald Palmer has results on complexation in ZnCl<sub>2</sub> and NiCl<sub>2</sub>. However, these results are not directly relevant to this project. The PCAS WG does not want pursue activity in this area.

### "Atlas" Monograph

D. Palmer reported that the monograph "Aqueous Systems at Elevated Temperatures and Pressure: Physical Chemistry in Water, Steam and Hydrothermal Solutions" was published by Elsevier in July 2004. IAPWS invested 10000 \$ in technical preparation of the manuscript, royalties from sales will go to IAPWS. A copy will be sent to E.U. Franck in recognition of his early initiative to write this book. R. Fernandez-Prini indicated that the publishers expect to sell 1000-2000 copies. V. Majer thanked the Editors (D. Palmer, R. Fernandez-Prini and A. Harvey) for their work and dedication.

# Book on thermodynamic data and measurement methods at high temperatures

V. Majer reported that an initiative to develop a compilation of high-temperature data (under coordination of V. Valyashko) was presented at Vejle 2003. Some criticism was raised in Vejle because of the lack of critical evaluation of the data and the arbitrary nature of the proposed lower temperature limit (200 °C), which would results in possible splitting of data sets. An Advisory board (Vladimir Valyashko, Vladimir Majer and Marc Assael) was nominated by EC to prepare a more detailed proposal of procedure so that the project can be considered for IAPWS sponsorship. A broad discussion on these aspects and timing of the project has taken place during winter and spring 2004.

In a later part of the meeting, Vladimir Valyashko gave a brief presentation on the proposed book. The objective is to give the user information on experimental methods, experimental data and their treatment. The originally proposed chapters were (1) phase equilibria (V. Valyashko, (2) PVT properties (H. Corti, V. Majer), (3) calorimetric data (V. Majer), (4) isopiestic data (Miroslaw Gruszkiewicz), (5) electrochemical data (D. Palmer, S. Lvov), (6) electrical conductivity (H.), (7) thermal conductivity (I. Abdulagatov, M. Assael) and (8) viscosity (I. Abdulagatov, M. Assael).

D. Palmer, M. Gruszkiewicz and S. Lvov expressed their difficulties to contribute to this project because of other heavy commitments. V. Majer attempted to enlist Christopher Wormald to collaborate, but it is unclear whether this will materialize. On the other hand, H. Corti has already written his chapter; also, most data are already in the computer.

Discussion on this topic continued during the week and a sound consensus was reached. Finally a proposal was formulated by the Advisory board for EC on September 2. The chapter on isopiestic data will be cancelled; V. Majer will take as a coauthor his research associate (K. Ballerat), S. Lvov will lead the chapter on electrochemical properties and will be helped by D. Palmer regarding the ORNL data.

### Reports regarding new Task groups and Committees

*Metastability, Nucleation, Early Condensate, Droplet Sprays and Condensation*. This group should provide a forum for researchers and practitioners to engage in debate on contemporary issues regarding the nonequilibrium thermodynamics of water and aqueous systems.

V. Marsik (Chair) listed persons (mainly out of IAPWS) working in this field and presented areas of interest to IAPWS: phase transitions and phase diagrams of aqueous systems, saturation line - bubble points and dew points, metastable water and metastable aqueous systems, nucleation – cavitation - boiling – condensation, bubble and droplet formation - two-phase flow, measuring techniques for transient quantities.

Recommendation to IAPWS: establish a task group within IAPWS.

### Electrochemical Processes in High-Temperature Aqueous Systems

Serguei Lvov (Chair) gave a list of researchers involved in this task group (D. Macdonald, E. Maughan, M. Nakahara, T. Petrova, and S. Uchida) and listed main areas of interest to IAPWS: potentiometry, pH Measurements, electrochemical monitoring of solution chemistry, electrochemical kinetics measurements, corrosion metals and alloys, electrokinetic measurements, electrochemical production of substances (for example, hydrogen production), electrochemical production of electrical energy (for example, fuel cells), electrochemical conductance measurements.

Recommendations of PCAS WG: (*i*) continue the Task Group activities in 2004/2005, (*ii*) add D. Palmer to the members list, (*iii*) communicate with PCC WG to formulate details of the listed above areas of research.

### Fuel Cell and H<sub>2</sub> Technologies

S. Lvov (Chair) reported on an initiative to establish a Committee with J. Pierre (invited consultant from Siemens Westinghouse, Pittsburg, PA). Several other PCAS WG members expressed interest.

The main areas that are important to IAPWS were suggested as follows: electrolysis of water, electrochemical oxidation of fuels, electrochemical reduction of oxygen, conductivity of water containing proton conducting membranes, electrochemical and chemical production of hydrogen using hydrothermal processes, development of fuel cell–turbine hybrid systems.

Recommendations of PCAS WG: create a task group on fuel cell and H<sub>2</sub> technologies: S. Lvov (chairman), H. Corti, M. Nakahara, and F. Marsik.

### Properties and formulations for high temperature aqueous systems

V. Majer consulted on this topic A. Harvey, R. Fernandez-Prini, F. Marsik and J. Sedlbauer. The problem can be divided in two parts: (i) dilute solutions with interactions solute – solvent prevailing: these issues are addressed in a proposal of a project on hydration properties,

(ii) concentrated solutions with interactions solute – solute playing also important role: this issue should be addressed in the next stage.

Recommendation to PCAS WG: support the hydration project, persons participating in this project will form the task group.

### New members

V. Marsik proposed M. Sedlář of Sigma Research and Development Institute as WG member. Approved.

# THE INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

http://www.iapws.org

### Working group "Physical chemistry of aqueous solutions" (PCAS)

Chair: Vladimir Majer, <u>vladimir.majer@univ-bpclermont.fr</u>, Blaise Pascal University / CNRS, Clermont-Ferrand, France Vice-Chair: Serguei Lvov, <u>lvov@psu.edu</u>, Pennsylvania State University, University Park, PA, USA

# Establishing recommended data on thermodynamic properties of hydration for selected organic solutes

proposal for a project to be conducted under auspices of IAPWS and IUPAC (2005-2007)

### Task group chairman: Vladimir MAJER

### Task group members:

V. DOHNAL, P. Vrbka, Ustav fysikalni chemie, Vysoka skola chemicko-technologicka – Praha, 16628 Prague 6, CZECH REPUBLIC, *vladimir.dohnal@vscht.cz* 

R. FERNANDEZ-PRINI, J. ALVAREZ, H. Bianchi, L. Mendez de Leo, U.A. Quimica, Comision Nacional Energia Atomica, 1429 Buenos Aires, ARGENTINA, <u>*rfprini@cnea.gov.ar*</u>

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E.L. SHOCK, A.V. PLYASUNOV, N.V. Plyasunova, Department of Geological Sciences and Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287, USA, *Everett.Shock@asu.edu* 

### **Objective:**

The objective of the project is to establish a database of thermodynamic properties of hydration for approximately 200 selected organic solutes at reference condition of 298.15 K and 0.1 MPa and as a function of temperature and pressure up to the near-critical region of water. The values of hydration properties for solutes covering different molecular structures will be calculated from the reliable experimental data for aqueous and pure solutes. The established database will be used as a standard for testing and establishment of new physico-chemical models and methods of molecular simulation as well as for developing semi-theoretical prediction schemes of interest for chemical engineering ,power cycle chemistry, environmental chemistry and geochemistry.

### **Description:**

Thermodynamic properties of hydration (TPH) covered in the project are: the Gibbs energy of hydration  $\Delta_{hvd}G_2^{\circ}$ , and its temperature and pressure derivatives (the enthalpy of hydration  $\Delta_{\rm hyd} H_2^{\circ}$ , the heat capacity of hydration  $\Delta_{\rm hyd} C_{p,2}^{\circ}$  and the partial molar volume at infinite dilution  $V_2^{\circ}$ ), other TPH result from their combinations; for exact definitions and interrelationship see Appendix 1. TPH express the difference between the property of a solute in the standard state of infinite dilution at a given temperature and pressure and that of an ideal gas at the same temperature and reference pressure of 0.1 MPa. Thus they characterise the transfer of a solute from a state where molecules are not interacting to the state where the solute molecules interact solely with the water solvent. Due to this definition they can be used conveniently in testing and conception of theoretical models and simulation approaches for dilute aqueous solutions developed by physical chemists. At the same time, TPH allow an easy calculation of partition coefficients (such as the Henry's law constant, air-water partition coefficient, relative volatility, etc.) and of the thermodynamic reaction constants for aqueous systems. Therefore they also have a practical value of interest for engineers and environmental chemists. In addition, the high temperature / high pressure TPH are particularly useful for characterization of phase and chemical equilibria in hydrothermal and power cycle systems.

TPH cannot be directly measured but are calculated from the experimental data characterising aqueous and pure solutes, which result from phase equilibrium, calorimetric and volumetric measurements. Appendix 1 summarises equations used to calculate TPH and lists types of experimental data that can be exploited.

The task group will select from the primary literature the best available experimental results for establishing a database of reliable values of TPH for 100 - 200 organic solutes and several common gases. In selecting the solutes, three main criteria will be observed: *i*) coverage

of the widest range of molecular structures, indispensable for the development of theoretical models and group contribution prediction schemes *ii*) availability of reliable experimental data, particularly with regard to the HT/HP region, *iii*) technological and environmental importance of individual solutes. The database will comprise values at the reference condition  $T_r = 298.15$  K and  $p_r = 0.1$  MPa for about 200 solutes and at elevated temperatures (T < 673 K) and pressures (p < 40 MPa) for about 100 solutes. For several solutes the recommended TPH will be given up to the critical region of water where they undergo remarkable changes. A tentative list of the classes of solutes covered and their respective numbers are given in Appendix 2. Every effort will be made to supply a database that will not be biased by use of any particular correlation model for interpolating or extrapolating the data.

This project requires collaboration of researchers having complementary knowledge in data evaluation and in different experimental techniques used for obtaining data for aqueous and pure solutes. Participation of investigators from at least six institutions in four countries is expected. The Buenos Aires, NIST Boulder and Prague groups have particular expertise regarding experimental data on the Gibbs energy level for aqueous solutions while the Aubière (Clermont-Ferrand) group will focus mainly on derivative properties. They will all collaborate with the Tempe and Liberec groups where extensive databases for aqueous solutes are already available. TRC of NIST Boulder will supply all the recommended experimental data for pure organic compounds (under coordination of <u>M. Frenkel</u>). A particular feature of this project will be the participation of younger researchers, some of them in early stages of their careers, beside confirmed experts (listed in capitals) who collaborated already in the past and are members of international scientific bodies (IAPWS, IUPAC, IACT).

### **Outcome:**

*i)* technical report to be presented as an IAPWS guideline, *ii)* a comprehensive article to be published in Journal of Physical and Chemical Reference Data, *iii)* a database (list of values, no software) freely accessible through the IAPWS and IUPAC web pages.

Time frame: Planned start date January 2005, duration of project 30 months

### Milestones:

- October 2005 system selection closed, main experimental data sets selected

- <u>March 2006</u> determination of recommended data for TPH at  $T_r = 298.15$  K and  $p_r=0.1$ MPa completed

- <u>August 2006</u> recommended TPH at HT/HP calculated for most systems, workshop organized during the International Conference on Chemical Thermodynamics in Boulder, CO

- January 2007 consistency verification and refinements completed

- <u>June 2007</u> review paper submitted to JPCRD, the proposed IAPWS guide line circulated for evaluation, data base prepared to be available through the IAPWS web page after approval of the guideline at the IAPWS annual meeting

### Anticipated impact:

The data on TPH are of interest for:

- *physical chemists* (model developers and simulators)

- *chemical engineers* (schemes for calculating phase and chemical equilibria in industrial aqueous systems including <u>power cycles</u>)

- *environmental chemists* (partitioning of solutes between air and water, cleanup of aqueous effluents)

- *theoretical geochemists* (development of prediction schemes for thermodynamic equilibrium constants

of hydrothermal reactions)

### Budget requested from IAPWS:

Total: <u>12k€</u> (5 k€ in 2005, 5 k€ in 2006, 2 k€ in 2007)

This budget will be used for *i*) facilitating mobility of young researchers (who are not members of IAPWS working groups) when working on project tasks (8 k $\in$ ), *ii*) data compilation, evaluation and transfer, establishment of a database (4 k $\in$ ).

### Budget requested from other sources:

- IUPAC: <u>14 k€</u>

- Participating laboratories: contribution to the project estimated to <u>48 k€</u>

*Note:* This proposal was prepared by Vladimir Majer and consulted with Roberto Fernandez-Prini (PCAS WG) and Allan Harvey (TPWS WG) before its submission to IAPWS EC for discussion and vote during the 14<sup>th</sup> ICPWS in Kyoto (August 29 – September 3, 2004).

#### **Appendix 1 to Attachment 7**

#### Establishing recommended data on hydration properties for selected organic solutes

#### APPENDIX 1

#### Thermodynamic background and main classes of experimental data needed

Thermodynamic property (function) of hydration (TPH) – difference between a property in the standard state of infinite dilution (temperature and pressure of the system) and in the state of an ideal gas (temperature of the system and standard pressure of 0.1 MPa)

$$\Delta_{\text{hyd}} X_2^{\circ} = X_2^{\circ} [T, p] - X_2^{\text{1g}} [T, p_{\circ}] \qquad p_{\circ} = 0.1 \text{ MPa}$$

Gibbs energy of hydration  $\Delta_{hvd}G_2^\circ$  :

Relationship with the Henry's law constant:  $\Delta_{\text{hyd}}G_2^\circ = G_2^\circ - G_2^{\text{ig}} = RT \ln(k_{\text{H},2} / p_\circ)$ Relationship with the Gibbs energy associated with dissolution of a liquid or solid solute

$$\Delta_{\text{hyd}}G_2^\circ = \Delta_{\text{sol}}G_2^\circ + RT\ln(f_2^\bullet/p_\circ) = \Delta_{\text{sol}}G_2^\circ + RT\ln(\phi_2^\bullet p_2^{\text{sat}}/p_\circ) + \int_{p_2^{\text{sat}}}^p V_2^\bullet dp$$

Relationship of  $\Delta_{sol}G_2^{\circ}$  to the symmetric limiting activity coefficient (liquid solutes)  $\Delta_{sol}G_2^{\circ} = G_2^{\circ} - G_2^{\bullet l} = RT \ln \gamma_2^{R^{\infty}}$ 

Relationship of  $\Delta_{sol}G_2^{\circ}$  to the solubility (sparingly soluble liquid or solid solutes)  $\Delta_{sol}G^{\circ} = G_2^{\circ} - G_2^{\bullet} = -RT \ln x_2^{sol} \gamma_2^{H} \cong -RT \ln x_2^{sol}$ 

#### Experimental data needed:

(*aq*) - Henry's law constants (gases), limiting activity coefficients (hydrophilic and moderately hydrophobic liquid solutes), solubilities (hydrophobic liquid and solid solutes) (*pure*) - vapour pressures, gas nonideality corrections, densities of pure solutes

#### Enthalpy of hydration $\Delta_{hyd}H_2^\circ$ :

Relationship with the enthalpy associated with dissolution

$$\Delta_{\text{hyd}}H_2^\circ = \Delta_{\text{sol}}H_2^\circ + \int_0^p (V_2^\bullet - T(\partial V_2^\bullet / \partial T)_p) dp \quad T > T_c$$

#### **Appendix 1 to Attachment 7**

$$\Delta_{\text{hyd}}H_2^\circ = \Delta_{\text{sol}}H_2^\circ - \Delta_{\text{vap}}H_2^\bullet + \int_0^{p_2^{\text{sat}}} (V_2^\bullet - T(\partial V_2^\bullet/\partial T)_p) dp \cong \Delta_{\text{sol}}H_2^\circ - \Delta_{\text{vap}}H_2^\bullet T < T_c$$

Relationship of  $\Delta_{sol}H_2^{\circ}$  to the data resulting from calorimetric experiments

$$\Delta_{\text{sol}} H_2^{\circ} = (H_2^{\circ} - H_2^{\bullet}) = \lim_{n_2 \to 0} (\Delta_{\text{sol}} H / n_2)$$

Experimental data needed:

(*aq*) - enthalpies of solution (dilute aqueous solutions)

(*pure*) - residual enthalpies (enthalpic departure function resulting from pVT data) for gases and supercritical fluids, enthalpies of vaporization (liquids) / sublimation (solids)

Heat capacity of hydration  $\Delta_{hyd} C_{p,2}^{\circ}$ :

$$\Delta_{\text{hyd}} C_{p,2}^{\circ} = C_{p,2}^{\circ} - C_{p,2}^{\text{ig}}$$

Relationship of  $\Delta_{\text{hyd}} C_{p,2}^{\circ}$  to the data resulting from calorimetric experiments

$$C_{p,2}^{\circ} = c_{p,1} \cdot M_2 + \lim_{m_2 \to 0} \left( \frac{c_p - c_{p,1}}{m_2} \right)$$

Experimental data needed:

(aq)- specific heat capacities (heat capacity differences) of dilute aqueous solutions (pure)- ideal gas heat capacities of solute

#### Partial molar volume at infinite dilution $V_2^{\circ}$ :

$$V_2^{\circ} = \frac{M_2}{\rho_1} - \frac{1}{\rho_1^2} \lim_{m_2 \to 0} \left(\frac{\rho - \rho_1}{m_2}\right)$$

Experimental data needed:

(aq)- densities (density differences) of dilute aqueous solutions

#### **Appendix 1 to Attachment 7**

#### **Relationship between individual TPH:**

$$\Delta_{\text{hyd}} G_2^\circ = \Delta_{\text{hyd}} G_2^\circ [T_r, p_r] - (T - T_r) \Delta_{\text{hyd}} S_2^\circ [T_r, p_r] + + \int_{T_r}^T \left( \Delta_{\text{hyd}} C_{p,2}^\circ \right)_{p_r} dT - T \int_{T_r}^T \left( \Delta_{\text{hyd}} C_{p,2}^\circ \right)_{p_r} d\ln T + \int_{p_r}^p \left( V_2^\circ \right)_T dp$$

where

$$\Delta_{\text{hyd}}S_2^{\circ}[T_r, p_r] = (\Delta_{\text{hyd}}H_2^{\circ}[T_r, p_r] - \Delta_{\text{hyd}}G_2^{\circ}[T_r, p_r])/T_r$$

 $T_r = 298.15 \text{ K}, \quad p_r = p_o = 0.1 \text{ MPa}$ 

*Symbols* : 2 solute, 1 solvent ; superscript • - pure solute property, superscript  $^{\circ}$ - standard state of infinite dilution, superscript ig – ideal gas

*Note:* thermodynamic properties of water are obtained from the equation of state for ordinary water substance (IAPWS-95 formulation)

## Appendix 2 to Attachment 7

### APPENDIX 2

## Classes of compounds covered and tentative numbers of solutes included

Compounds of carbons and hydrogen (C-H) Alkanes Cycloalkanes Unsaturated aliphatic hydrocarbons Aromatic and unsaturated monocyclic hydrocarbons Polycyclic hydrocarbons	55
Compounds of carbon, hydrogen and halogen (C-Hal, C-H-Hal) Fluoroderivatives Chloroderivatives Bromoderivatives Iododerivatives Mixed halogen derivatives	20
Compounds of carbon, hydrogen and nitrogen (C-H-N) Amines Nitriles Heterocyclic nitrogen compounds Miscellaneous nitrogen compounds	30
Compounds of carbon, hydrogen and oxygen (C-H-O) Ethers Alcohols and phenols Carbonyl compounds Acids Esters Heterocyclic oxygen compounds Miscellaneous oxygen compounds	60
Compounds of carbon, hydrogen and sulphur (C-H-S) Sulphides Thiols Heterocyclic sulphur compounds	15

## Appendix 2 to Attachment 7

Other organic compounds	10
Compounds of carbon, hydrogen, halogen and oxygen (C-H-Hal-O)	
Compounds of carbon, hydrogen, nitrogen and oxygen (C-H-N-O)	
Compounds of carbon, hydrogen, oxygen and sulphur (C-H-O-S)	
Miscellaneous compounds	

Inorganic gases (H $_2$  O $_2$ , N $_2$ , CO $_2$ , NH $_3$ , H $_2$ S, ...)

10

## THE INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

http://www.iapws.org

#### Working group "Physical chemistry of aqueous solutions" (PCAS)

Chair: Vladimir Majer, <u>vladimir.majer@univ-bpclermont.fr</u>, Blaise Pascal University / CNRS, Clermont-Ferrand, France Vice-Chair: Serguei Lvov, <u>lvov@psu.edu</u>, Pennsylvania State University, University Park, PA, USA

## Hydrothermal Experimental Data; Phase Equilibria and Solution Properties in Binary and Ternary Systems

Outline of the book to be published under auspices of IAPWS and proposal of a procedure (2004-2005)

Following the presentation of the proposal for a book on hydrothermal data at the IAPWS annual meeting in Vejle (2003), the Advisory Board (M. Assael, V. Majer and V. Valyashko), nominated by the EC, has undertaken a broad consultation with authors and a consensus was reached in Kyoto (August 2004). The following proposal was developed:

**1.** The main goal of the project is to prepare a monograph "Hydrothermal Experimental Data; Phase Equilibria and Solution Properties in Binary and Ternary Systems" dealing with

- high temperature measurement techniques,
- experimental data review and assessment,
- presentation of experimental values in tabular forms.

The database of experimental values on hydrothermal systems reaching to temperatures above 200°C was established by V.M.Valyashko and N.S.Ivanova (Kurnakov Institute RAS, Moscow, Russia) between 1998-2003. This database will provide a solid basis for the preparation of the book. A preliminary agreement was reached at the end of 2003 with the Publisher (John Wiley Ltd., London, UK).

**2.** The monograph will be organized into 7 chapters, each chapter dealing with a property of hydrothermal systems. The Editor of the book will be *V.M. Valyashko, Russia. J.M.H. Levelt Sengers* and *D.A. Palmer* have agreed to act as the English Editors after the chapters are available in the final form. The list of properties and responsible authors is as follows:

Chapter I (Phase Equilibrium data – V.M. Valyashko, Russia) Chapter II (pVTX data – H. Corti, Argentina, V. Majer, France) Chapter III (Calorimetric data – V. Majer, K. Ballerat, France) Chapter IV (Electrochemical data – S.N. Lvov, D.A. Palmer, USA) Chapter V (Electrical conductivity data – H. Corti, Argentina) Chapter VI (Thermal conductivity data – I. Abdulagatov, Russia/USA, M.J. Assael Greece)

*Chapter VII (Viscosity data - I. Abdulagatov, Russia/USA, M.J. Assael Greece)* The collective of authors is free to invite possibly other scientists to participate in the preparation of the book.

Each Chapter will consist of two parts: *text part* (thermodynamic background and the review of techniques, experimental data and treatment procedures) and *summary table* overviewing the data. This table will show for each property the following information: nonaqueous component(s) of system (chemical formula and name), range of parameters (concentration, temperature, pressure), type of data in the literature source, indication of data quality, code for the experimental technique used, literature reference, code for connection to the CD database and possibly other additional information. An <u>Appendix</u> on a CD will be produced presenting the direct experimental data (one table per system and reference). Brief specific information regarding the data presented, and information on the accuracy claimed by the author (if available), will precede each table.

**3.** Additionally to the aforementioned points, the members of the PCAS WG have come to the following agreement:

**3.a.** The collection will focus mainly on the data reaching above 200°C. This data limit will not be, however, considered as restrictive. For certain properties the chapter authors may consider the data below this limit if it makes sense and a better explanation of the nature of the data is so achieved.

**3.b.** The chapters will have no temperature limitation in a description of experimental techniques, property behavior or the methods of experimental data treatment. Moreover, the summary table will indicate the temperature ranges as reported by the original authors. The tables in the CD Appendix will contain mainly the data above 200°C; in some cases this temperature limit can be lowered provided the chapter authors add the data to the database.

**3.c.** Values of T, p, and x in the Summary Tables will be presented in uniform units (temperature - K. pressure - MPa, concentration range - molality or mole per cent as convenient). Experimental data in the CD Appendix will be presented as reported by authors. However, in a limited number of cases where a conversion is desirable (obsolete units etc.), all information necessary will be provided.

**3.d.** Copies of original papers presenting experimental data will be available to authors from V. Valyashko when necessary.

#### 4. <u>Timetable:</u>

October 1, 2004Final list of authors and chapter outlines submitted to the Editor. Every<br/>author should submit an official confirmation of his participation in the book preparation.February 1, 2005Authors decide on the final list of data sources to be included and if<br/>necessary complete the database accordingly. Papers published in the open literature, including<br/>theses, until the end of 2004 will be considered.July 1, 2005Drafts of chapters sent to the Editor.December 15, 2005Final manuscript ready for the submission to the Publisher.

**5.** The preliminary agreement with John Wiley Ltd. regarding the book is as follows. The book will contain about 500 printed pages. The Publisher will pay \$ 10 per printed page. The payment for the CD material will be the total sum of \$ 3500.

Since **no financial support from IAPWS is requested for this project** the payment from the Publisher will go to the authors and for compensating the expenses with the manuscript and data base preparation.

Submitted to EC by the Advisory board members. M. Assael, V. Majer, V. Valyashko Kyoto, September 1, 2004

#### **Appendix to Attachment 8**

#### Appendix (book outline)

### Hydrothermal Experimental Data; Phase Equilibria and Solution Properties in Binary and Ternary Systems

#### V.M. VALYASHKO, Editor Kurnakov Institute RAS, Moscow, Russia

## *CHAPTER I* "Phase Equilibria in Binary and Ternary Hydrothermal Systems" (V.M. VALYASHKO, Kurnakov Institute RAS, Moscow, Russia)

Introduction

Binary Systems (Fluid and complete phase diagrams; Theoretical derivation and systematic classification of binary phase diagrams).

Ternary Systems (Graphical representation; Theoretical derivation and systematic classification of ternary phase diagrams)

Estimation of Thermodynamic Functions and Equilibrium Constants from Experimental Data on Phase Equilibria.

Methods and Equipment for Studying Hydrothermal Phase Equilibria

Some Regularities of Hydrothermal Phase Behavior in Experimentally Studied Systems.

## *CHAPTER II* "PVTX Properties of Hydrothermal Solutions" (H.R. CORTI, Comision Nacional de Energia Atomica, Buenos Aires, Argentina; Vladimir MAJER, Blaise Pascal University, Clermont-Ferrand, France))

Basic Principles and Definitions

Experimental Methods

Theoretical Treatment of PVTX-data for Ionic and Nonionic Solutes (*Standard partial molar volume; Partial molar volumes near critical conditions; Excess volume; Ion association effects on excess volumes*) General Trends in Temperature, Pressure and Composition Dependencies of Standard Partial Molar Volume and Excess Volume for Ionic and Nonionic Solutes.

Recommendations for the Calculation of Standard and Excess Properties from Experimental Data.

## *CHAPTER III* "Calorimetric Properties of Dilute Hydrothermal solutions" (V. MAJER, K. BALLERAT, Blaise Pascal University / CNRS, Clermont-Ferrand, France )

Thermodynamic Background: Heat Of Solutions, Heat Of Dilution, and Heat Capacity

Experimental methods

Theoretical Treatment of Calorimetric Data for Ionic and Molecular Solutes (*Standard and Excess Properties, Near Critical Behaviour, Ion Association Effects*)

General Trends in Temperature, Pressure and Composition; Depenencies of Standard and Excess Properties ror Ionic And Molecular Solutes

Recommendations for the Calculation of Standard and Excess Properties from Experimental Data.

#### **Appendix to Attachment 8**

# *CHAPTER IV* "High-Temperature Electrochemical Measurements of Aqueous Solutions" (S.N. LVOV, Pennsylvania State University, University Park, USA, D.A. PALMER, ORNL, Oak Ridge, USA)

Introduction Conventional High Temperature Electrochemical Cells Hydrogen-Electrode Concentration Cell Hydrothermal Electrochemical Measurements

## CHAPTER V "Electrical Conductivity in Hydrothermal Binary and Ternary solutions" (H.R. CORTI, Comision Nacional de Energia Atomica, Buenos Aires, Argentina)

**Basic Principles and Definitions** 

Experimental Methods

Data Treatment (*Dissociated and associated electrolytes*; *Getting information from electrical conductivity data*)

General Trends (Specific conductivity as a function of temperature, concentration and density. The limiting molar conductivity; Molar conductivity as a function of concentration, temperature and density; Association constants)

Conductivity in Ternary Systems

## *Chapter VI* "Thermal Conductivity of Hydrothermal Solutions" (I.M. ABDULAGATOV, NIST, Boulder, USA; M.J. ASSAEL, Aristotle University, Thessaloniki, Greece)

Introduction

Experimental Methods (Parallel Plate, Coaxial Cylinders and Transient Hot – Wire Apparatus, Theoretical Bases and Uncertainties of the Measurements)

Experimental Thermal Conductivity Data for Hydrothermal Solutions (*Temperature, pressure and concentration dependencies of the thermal conductivity of aqueous solutions*)

## *Chapter VII* "Viscosity of Hydrothermal Solutions" (I.M. ABDULAGATOV, NIST, Boulder, USA; M.J. ASSAEL, Aristotle University, Thessaloniki, Greece) Introduction

Experimental Methods of the Viscosity Measurements at High Temperatures and High Pressures (*Capillary flow and oscillating disk apparatus; Theoretical bases and uncertainties of the measurements*) Experimental Viscosity Data for Aqueous Solutions at High Temperatures and High Pressures (*Temperature, pressure and concentration dependencies of the viscosity of aqueous solutions*)

#### Minutes of PCC meeting, August 28, 2004.

Agenda approved as modified. (Modified agenda attached as PCC Attachment B.)

James Bellows volunteered as clerk of minutes.

Minutes of previous meeting approved.

International collaborations:

- Procedure reviewed
- Possibilities in Nuclear task force
- Possibilities in Environmental task force
- Possibilities in Metastable task force
- Michael Rziha and Shunsuke Uchida will generate a proposal for an international collaboration on FAC

#### Priority list

Problems suggested:

- 1. Formation and Exfoliation Mechanism of Scale (oxide films) of Steam lines Important new topic
- 2. Mechanism and Influence of Cu Deposition This is essenstially a solved problem from a scientific viewpoint
- 3. Behavior of TOC (total organic carbon) in Steam Lines of USC Plants
- 4. Mechanism of Decomposition of Ion-exchange Resin Operating conditions, quality control of resin; leak rates are slow, but sulfate is one of the products
- 5. Development of High Temperature Sensors
- 6. Improved analysis of low concentration of Fe ion Is the ionic iron the problem
- 7. Corrosion mechanisms that are relatied to the presence of contaminants in steam/water circuits
- 8. The relationships between the chemistry of the contaminants and their concentration at point of measurement
- 9. The quantification of risk
- 10. The appreciation of the fate of corrosion products
- 11. Economically viable solution for improved steam/water separation in HRSGs Is this a monitoring issue? Is a standard the real need? Is the accurate measurement the real issue? Michael Rziha and Bobby Svoboda with Jim Bellows—See PCC 2004 ATTACHMENT A
- 12. Improvement of heat transfer in condensers—dropwise vs filmwise condensation
- 13. Corrosion interaction between materials and supercritical water/steam—influence of supercritical parameters—effect on protective layers—also effect of radiation
- 14. Deposition of contaminants and corrosion products in steam and water circuits—involves supersaturation, mass transfer, adsorption, crystal nucleation, deposit re-dissolution, scouring and exfoliation
- 15. Otakar's list (Bellows talk to Dan Friend for list)

Bold item in suggestions taken for action as a trial of the new procedure

Review of environmental effects task force (Ask Mr. Okita for electronic copy. Not available as of September 2, 2004.)

Additional issues for PCC

- 1. Steam cooling
- 2. Steam injection
- 3. SCWO
- 4. SCR, SNCR?
- 5. Erosion and corrosion

Review of nuclear task force

(See accompanying copy of power point slides)

[JCB personal notes: One PWR has injected noble metals into the primary to reduce corrosion. In BWRs, hydrogen peroxide is important, but is lost by conversion to oxygen in sample line, leading to difficulties in knowledge. Need theoretical model of water radiolysis for controlling hydrogen injection; hydrogen promotes cracking. Often use Ti sample lines since Co is critical analysis and stainless steel leaches Co at similar concentrations.]

Additional issues for PCC

4. Relationship between species at beginning of hot sample line and the species at the cooled end.

Agreement: Andre Zeijsinck and Jim Bellows will get all the lists together and make a unified list to be distributed.

Topics for next year Nuclear chemistry

- Nuclear chemistry
- Sampling
- Differences and common ground
- Amine chemistry

Combined cycle chemistry

- Cycling
- Common problems

IRCNs

- Evaluation of Binary Nucleation Models—close with a statement that the sponsor is no longer active in IAPWS and the matter is closed.
- Origin and fate of organics—Andre Zeijseink will close this
- Surface tension of aqueous solutions—Fabio and Gabrielli, who is sponsor—Andre will check minutes for other actions with respect to it—possibly close with "no longer active" statements

See *PowerPlant Chemistry* July 2004 for EN12952-12:2003 "Recommendations for Treatment of water for steam boiler."

#### PCC Attachment A

## IAPWS MEETING KYOTO, 2004 / PCC

### Proposal for new Task group within PCC:

## GUIDELINE FOR DETECTION AND DETERMINATION OF MECHANICAL CARRY OVER

Mechanical carry over in drum boilers has a significant impact on steam purity, as well as on the lifetime of SH-tubes.

Recent experiences reported to PCC demonstrates that mechanical carryover is often detected too late. Reasons for this are, among others,

- Lack of monitoring device and possibilities (design of sampling system)
- Lack of up to date procedures
- Rarely included in plant chemistry control procedures

Therefore it is proposed to settle a task group which elaborates a guideline for detection and determination of mechanical carry over.

- Routine checks for mechanical carry over are required, since efficiency of demisters may degrade by time (e. g. by mechanical defects, wear).
   A minimum frequency for check on mechanical carryover shall be recommended.
- Chemistry of boiler water may also influence the mechanical carryover.
   Adequate information in this respect shall be given.
- Maintenance work may effect the performance of demisters desired or accidentally (e. g. unwanted damages during maintenance work in boiler drums).
   ⇒ Recommendation shall be given to re-check on mechanical carryover when works had been performed in boiler drums.
- Method description for performing the check on mechanical carryover shall be prepared and shall include recommendations such as
  - Minimum requirements for sampling systems (sampling location, on line monitoring device, sampling probes, etc.).
  - Analytical methods and suggestions for possible tracer selection (e. g. Na<sub>3</sub>PO<sub>4</sub>, NaOH, LiOH, <sup>24</sup>Na, Li<sub>2</sub>CO<sub>3</sub>, etc.).
  - Evaluation of gained values.

### PCC Attachment A

- Recommendations for quick cross check / diagnosis shall be given, such as using cation conductivity, Na-monitoring, temperatures.
- ➤ Target levels for mechanical carryover shall be described (→ boiler specification, ABMA, etc.).

PCC Attachment B



August 29, 2004

#### The International Association for the Properties of Water and Steam http://www.iapws.org

#### Working group 'Power Cycle Chemistry (PCC)

IAPWS PCC WG Meetings in Kyoto, Japan August 29, 2004

#### Starting time 10:30 16:30, including lunch 12:00-13:30

- 1. Amendments/Adoption of Agenda
- 2. Election of Clerk of Minutes
- 3. Approval of Minutes of 2003 Meeting in Veijle, Denmark, action points
- 4. International Collaborations, the process
- Priority List Review, progress on ICRN's, selection of an ICRN and drafting of an x year research plan, responses BIAPWS and Japanese comittees
   5a (BCC response to Nuclear committee and 14:30 Environmental committee)
  - 5a (PCC-response to Nuclear committee and 14:30 Environmental committee)
- 6. IAPWS Certified Research Needs, Closing statements
- 7. European Standard STANDARD EN12952-12:2003 " Recommendations for Treatment of water for steam boiler
- 8. Development of a PCC- corrosion-risk assessment guide (UK proposal)
- 9. Improvement of Fe-analysis in low ppb level (Japanese proposal)
- 10. Guidelines from EBA, discussion of draft guideline for boiler water (Daucik, Svoboda)
- 11. Membership
- 12. Next year's topics
- 13. Election of Officers
- 14. Preparation of the Report to EC
- 15. Miscellaneous and Adjournment

#### For more information:

#### PCC Chairman

André Zeijseink, andre.zeijseink@kema.com, KEMA, Arnhem, The Netherlands

#### Vice-Chairmen

Michael Rziha, <u>michael.rziha@erlll.siemens.de</u>, Siemens, Erlangen, Germany Robert Svoboda, <u>robert.svoboda@power.alstom.com</u>, Alstom, Baden, Switzerland



August 29, 2004

## The International Association for the Properties of Water and Steam <u>http://www.iapws.org</u>

#### Working group 'Power Cycle Chemistry (PCC)

Chair: André Zeijseink, <u>andre.zeijseink@kema.com</u> Vice-Chair: Michael Rziha, michael.rziha@siemens.com, Siemens, Erlangen, Germany Robert Svoboda, <u>robert.svoboda@power.alstom.com</u>, Alstom, Baden, Switzerland

#### Flow-Accelerated Corrosion of Carbon Steel in PWR Secondary Cooling Water Conditions

Proposal for An International Collaboration on Flow Assisted Corrosion between Japan and Canada (2004-2005)

#### Proposed by

Prof. Shunsuke Uchida, Tohoku University, Japan, shunsuke.uchida@qse.tohoku.ac.jp Prof. Peter R. Tremaine, University of Guelph, tremaine@uoguelph.ca

Supported by "Nuclear Committee" of IAPWS

#### **Objectives:**

Latest accident of ruptures of the feed water piping in Mihama-3 plant realized us importance of flow assisted corrosions (FAC) of carbon steel under reducing aqueous conditions. Latest research results on FAC showed that too low electrochemical corrosion potential (ECP) also enhanced FAC. The safety zone of ECP for avoid sereous FAC should be reevaluated based on the latest data. An "International Collaboration" in proposed for developing abilities of young researchers, Tomonori Satoh\*, on understanding of FAC and setting future subjects in the fields of engineering.

#### **Description:**

1. Date survey:

Tremendous amounts of data are avilable on FAC. The latest ones shows the effects of ECP on FAC. Too low ECP often enhanced FAC. In order to point out the threshold ECP to avoid FAC, the data should be compiled. The data on the effects of temperature, materials, geometry and flow velocity on FAC should be also compiled. [TU,UNB, VGB, Framatom-ANP]

200\$

2. Understanding the gaps between the experimental conditions and operational conditions in the plants

ECP measurement in the operating plants is still difficult technology. Oxygen concentrations, conductivity and pH are usual data to identify corrosive conditions. To bridge the gaps between

ECP and measured elemental data ([O<sub>2</sub>], conductivity, pH, temperature, materials, geometory and flow velocity), suitable model based on the experimantal data are to be proposed.

[TU, UNB, VGB, Framatom-ANP]

- Learning sufficient skill to promote the experiments on FAC By joining the FAC test loop experiments in UNB, sufficient skill to promote the experiments on FAC is to be obtained. [TU, UNB]
- 4. Propose future subjects on FAC experiments

It is very difficult to understand total phenomena of FAC in the operating plants. Furthur studies should be concluded. Future subjects on FAC and some bridging techniques are proposed.

[TU,UNB, VGB, Framatom-ANP] The details should be discussed with Prof. D. H. Lister of UNB and others in the related institutes.

#### **Deliverables:**

Brief reports corresponding to the descriptions mentioned above will be submitted to the PCC working group and also to the Executive Committee of the IAPWS.

#### Time frame:

Planned start date: October 1, 2004

#### **Milestones:**

litestonest	
- December 30	Date survey, To select the experimental subject to be carried out at University of
	New Branswick
- Feburary 10	Preparation for the experiments and travelling
- March 25	Experimental works
- April 30	Compiling the report
The details shoul	d be discussed with Prof. D. H. Lister of UNB and others in the related institutes.

#### Anticipated impact:

The data obtained during the international collaboration can be appreciated by the Nuclear Committee.

The educated young researcher should become key persons in near future in the field of researches in interactions between materials and water at elevated temperature.

#### Budget requested from IAPWS for the period of October 1, 2004 through May 30, 2005

Total: 5,000\$ (travelling: 2,000\$, living: 3,000\$)

Details; Tickets for Round Trip INarita- New York - Montreal - Frederikton, Canada]

2,000\$

Tickets for Local Round Trip [Sendai - Narita] Travelling cut to 2,000\$ Hotels (50\$/day x 40days) 2,000\$ Local Transportation (Rent Car 1000\$/month x 1.5 months) 1,500\$ Living cut to 3,000\$

#### **Budget requested from other sources:**

Total: 5,000\$ (experiment supplies: 5,000\$)

The amounts will be supported by Tohoku University.

The details should be discussed with Prof. D. H. Lister of UNB and others in the related institutes.

#### Abbreviations

- TU: Tohoku University
- UNB: University of New Branswick
- VGB: VGB PowerTech e.V

* Tomonori Sat	oh	
Name:	Tomon	ori Satoh
Student:	PhD Co	burse, Quantum Science and Energy Enineering, Graduate School of Engineering,
		I University
Birth date:		, 1975 (29 years old)
Birthplace:	Aomor	
Education:		antum Science and Energy Enineering, Tohoku University (Mar, 2000)
		antum Science and Energy Enineering, Tohoku University (Mar, 2002)
		uantum Science and Energy Enineering, Tohoku University
		(Promised on Mar, 2005)
Awards:	2002	Okamoto Award [Financial support to attend Int. Water Chemistry Conf. of
		Nuclear Power Systems, Avignon, France, Apr. 2002]
	2003	Okamoto Award [Financial support to attend 11th Int. Sym. Environmental
		Degradation of Materials of muclear power paints, Stevenson,
		WA, USA, Aug. 2003]
	2003	Inoue Award, Aoba Industrial Forum, Sendai
		"Determination of Corrosive Conditions of BWR primary cooling Systems"
	2004	36th Award for Emerging Technology, Atomic Energy Society of Japan
		"Development of a method to determine water chemistry in a crack tip under
		irradiation for evaluating irradiation assisted stress corrosion cracking
		(IASCC)"
Major Publicatio	ons:	
5		wa, K. Iinuma, Y. Satoh and S. Uchida, "Water Chemistry in a Crack Tip

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#### Final report on "Nuclear Committee" of IAPWS

September 2, 2004

Nuclear Committee Members Dr. Clifford Davis

USA

Idaho National Engineering & Environmental Laboratory,

Prof. Derek H. Lister Prof. Takayuki Mizuno Dr. A. Rudge Dr. Ulrich Staudt Prof. Hiroshi Takaku Dr. Hideki Takiguchi Prof. Shunsuke Uchida, Dr. Milan Zmitko

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### ABSTRACT

In order to submit research subjects related to water chemistry of nuclear power cycles to IAPWS, a committee, "Nuclear Committee" has been organized and discussed about water chemistry and materials in power plants for a year. Precise and reliable evaluations of water chemistry data are required to improve plant reliability and safety. For this, quality assurance of the water chemistry data acquisition system is needed. At the same time, theoretical models are being applied to bridge the gaps between measured water chemistry data and the information desired to understand the interaction of materials and cooling water in plants. Major models which have already been applied for plant evaluation are:

(1) water radiolysis models for BWRs and PWRs;

(2) crevice radiolysis model for SCC in BWRs; and

(3) crevice pH model for SG tubing in PWRs.

High temperature water chemistry sensors and automatic plant diagnostic systems based on water chemistry data have been applied in only restricted areas. ECP sensors are gaining popularity as tools to determine the effects of hydrogen injection in BWR systems.

#### 1. Introduction

The IAPWS used to be supported mainly by scientists and engineers related to thermal power plants. Recently, few members came from nuclear power fields. These members have been expected to submit some new research subjects related to nuclear power plants. At the 2003 annual meeting of ICPWS in Vejle, Denmark (August 2003) a new committee "Nuclear Committee" was established to discuss chemical phenomena shown in nuclear power plants, to summarize them from the scientific viewpoints and then to submit the suitable research subjects.

Scientists would like to understand phenomena in plants, while plant operators and supervisors would like to have economical and comfortable plant operations. The gaps between both should be bridged based on phenomenological approaches. Unfortunately, only few subjects will be proposed by plant chemists. Scientists should join to plant chemists to pick up the subjects in plants. Collaboration tasks are desirable

to understand effectively phenomena related to plant chemistry and material behaviors in plants. Major phenomena and subjects are listed as a result of discussion among scientists, which should be reviewed by plant chemists for submitting to the IAPWS members.

One of the benefits of nuclear power plants circuit chemistry is existence of radioactive species. As a result of radioactive analysis, behavior of low concentration species can be often measurable, their histories in the circuits, e.g., generation, transfer and final accumulation, are traceable and then fundamental phenomena are understandable. High radiation level around nuclear reactor systems often prevents easier accessibility to the plants to acquire water chemistry data thought. Comparative studies of PWR and BWR circuit chemistry are often beneficial to understand phenomena at elevated temperature, though their chemical conditions are much different each other. Comparative studies of nuclear and thermal power circuits are also useful to understand phenomena, though both temperature ranges are much different.

#### 2. Water Chemistry Data Acquisition Systems

Cooling systems, major components and water chemistry differ in BWR and PWR plants. Procedures to measure water chemistry are also different in both reactor systems. At the same, common points in both reactor systems should also be discussed from the viewpoints of water chemistry data acquisition systems.

It is easy how to take data from the in-line monitors into the computer systems; water chemistry data from the sampled2 water used to be inputted into the computer system by plant chemists through keyboard entry. Large improvements have been reported in the latest plants on automatic analysis of chemical and radioactive nuclide data. Chemical species and radioactive nuclides collected on membrane filters are analyzed by X-ray fluorescence analyzer and gamma ray spectrometer, respectively, and then the measured data are transferred from the analyzers to the computer system directly [1]. Accumulated data are stored in a host computer (data server) allowing easy observation of plant water chemistry. The data numbers are also reduced to be compiled for daily, weekly and monthly documents (reports). Plant chemists, operators and supervisors through the computer network share the original data and also the reduced data. On-line ion chromatographs have been applied in plants for fully automatic data acquisition for the concentrations of anion and cation species, where the data are transferred to the laboratory data server through floppy disks or in the direct connection through the computer network [1]. The water chemistry data server is the center of the water chemistry data net work system, connecting with the operation and control computer systems to take plant operational data and to give water chemistry conditions to plant operators.

Trend and transient analyses are important evaluation procedures. General patterns of the data are compared with those of other plant data. Fuel integrity checking is one of the most important procedures for plant chemists and an important concern for plant operators and supervisors.

There are some gaps between the measured water chemistry data and information to understand plant conditions and interactions between materials and cooling water, which are shown in Table 1.

Table 1 Gaps between	desired information and me	easured data (Beyond water chemistry data)		
Desired information	Measured WC data Major measures to bridge the gaps			
to understand in-plant	in plants			
phenomena				
Corrosive conditions	• Measured [O <sub>2</sub> , H <sub>2</sub> ]	<ul> <li>Theoretical models for water radiolysis</li> </ul>		
[H <sub>2</sub> O <sub>2</sub> , O <sub>2</sub> , H <sub>2</sub> ]		• HT O <sub>2</sub> sensors		
		• ECP sensors		
Crevice water chemistry	<ul> <li>Bulk water chemistry</li> </ul>	<ul> <li>Theoretical crevice radiolysis models</li> </ul>		
		<ul> <li>Theoretical &amp; empirical models for</li> </ul>		
		impurity concentration in crack tip		
Crack propagation rate	<ul> <li>Crack growth rate</li> </ul>	• HT crack growth rate sensors		
	in simulated condition	<ul> <li>Theoretical &amp; empirical models for</li> </ul>		
		crack propagation rate		
Soluble and insoluble	<ul> <li>Saturated concentrations</li> </ul>	<ul> <li>Solubility analysis &amp; deposition/release</li> </ul>		
metallic species	along sampling lime	analysis along sampling lime		
		<ul> <li>High temperature conductivity sensors</li> </ul>		
High temperature pH	• pH at cooled water	Theoretical evaluation		
		• HT pH sensors		
Properties of oxide film	Characterization	Theoretical oxidation models		
on sampled specimens	of oxide film	• HT impedance sensors		
		UT: high tomporature		

	Table 1	Gaps between	desired informat	tion and measur	ed data (Beyo	nd water chemistry data	ι)
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To evaluate plant condition by using water chemistry data, two points should be carefully considered. The first point is quality assurance of water chemistry data and the other is bridging the gaps between desired information and measured data.

#### 3. Major subjects to be proposed to PCAS group

Newly proposed subjects from the viewpoints of nuclear plant chemistry (Table 2) are discussed as follows.

1) Water chemistry general Quality assurance of Water Chemistry Da				
2) Water chemistry control	Chemical dosage			
3) Sampling and analytical technology	Suitable sampling procedures			
	Automatic analytical procedures			
4) Development and application of water chemistry sensors	High temperature water chemistry sensors			
5) Understanding materials-water interactions*	Corrosive conditions			
	ECP, radiolytic species, $H_2O_2$			
	Water radiolysis models for BWRs and PWRs			
	Crevice radiolysis model for SCC in BWRs			
	Crevice pH model for SG tubing in PWRs			
	Oxidation and reduction of metals			
	Cupper behavior			
	Solubility of metallic ions in steam			
	Nucleation and condensation of impurities in steam			
	Condensation and deposition of metallic			
	Oxide film morphology at elevated temperature			
	Flow assisted corrosion (FAC)			

Table 2 Proposed major subjects for discussion

\* Major gaps between the desired information to understand the phenomena and measured data

#### 3.1 Water chemistry general

(1) Quality Assurance of Water Chemistry Data

Evaluation should be based on reliable data. For this, quality assurance of water chemistry data is essential. Standardization of data acquisition procedures is required to obtain qualified data, where sampling location & periods, sampling procedures and analytical instruments to determine chemical and radioactive components, calibration procedures for the instrument and their frequencies, training of plant chemists and documentation guides are clearly defined.

At the same time traceability of water chemistry data is required. For this, standard procedures for document management should be established. Quality assurance of water chemistry data in thermal power plants have been established and the details are published as one of the Japan Industrial Standards [5].

Enthusiastic promotion of quality assurance of water chemistry data in nuclear power plants based on light water reactors and establishing the standard for water chemistry data acquisition and processing are being carried on as one of the most important activities of the Research Committee on "Water Chemistry Standard" of Atomic Energy Society of Japan.

#### 3.2 Water chemistry control

Corrosive conditions are control by chemical dosage, e.g., hydrogen injection for reducing  $[O_2]$ , pH control for reducing corrosion rate, Zn injection for reducing activation deposition. For this, water radiolysis should be clearly understood in nuclear plant circuits. Theoretical models have been developed but more precise data base obtained at elevated temperature should be obtained to support the water radiolysis model and to keep sufficient accuracy.

#### 3.3 Sampling and analytical technology

Changes in mass and chemical forms of targets species during cooling down process along the sampling line should be clearly understood. Kinetic evaluation of chemical form change and deposition and release of species on tubing wall are carefully analyzed. Each of phenomena should be discussed in oxidation and reduction of metallic species.

#### 3.4 Development and application of water chemistry sensors

(1) High temperature water chemistry sensors

Water chemistry at elevated temperature are extrapolated by applying suitable model to evaluate interaction between water and materials in plant circuits. In order to confirm justification of the extrapolation, direct measurements of water chemistry parameters with high temperature water chemistry sensors are desirable. High temperature sensors for oxygen, hydrogen, hydrogen peroxide, pH and conductivity and in-situ measurement devices for oxide surface observation, morphology, electrochemical corrosion potential and crack propagation are requested. These sensors are applied in laboratories first and then applied in plants if they have sufficient reliability.

Some of high temperature sensors applied at operating plants [1], [5]. Most of them are sensors for structural material integrity test. High temperature reference electrodes for electrochemical corrosion potential measurements and contact tension specimens for crack propagation measurements are applied for task force of hydrogen water chemistry.

In order to obtain a reductive environment and thus mitigate secondary side corrosion of steam generator tubing, the optimum hydrazine content in the secondary system of PWR should be discussed based on ECP measurement. However, ECP would be carried out only in a very few units. Once the optimum hydrazine condition is defined, the plant staff will only routinely monitor hydrazine and ECP measurements can be terminated. In stead of direct ECP measurement, a combination approach of concentration measurement of anions and cations with ion chromatograph and empirical calculation based on crevice concentration factors and pH evaluation has been successfully applied to determine the corrosive conditions at the tubing and the crevice between the tubing and the supporting plate.

#### 3.5 Understanding materials-water interaction

(1) Corrosive conditions

ECP (electrochemical corrosion potential) can be measured in several locations in the primary coolant at elevated temperature and extrapolated to the location of interest to evaluate corrosive conditions of the target structures. Conductivities and pH are measured at room temperature and their effects on the materials should be considered by extrapolating them to values at elevated temperature. One of the most important radiolytic species,  $H_2O_2$ , which cannot be measured in the sampled water, should be determined by the theoretical rater radiolysis model along with  $O_2$  and  $H_2$  at the location of interest [6].

- (i) water radiolysis models for evaluating corrosive conditions in BWRs and PWRs [7], [8];
- (ii) crevice radiolysis model for estimating crack growth rate of SCC in BWRs [9]; and
- (iii) crevice pH model for evaluating corrosive conditions in crevices between SG tubing and tube support plate in PWRs [10].

Major gaps between the desired information to understand the phenomena and measured data are shown in Table 5 with measures to bridge these gaps.

(2) Oxidation and reduction of metals

Most fundamental phenomena of water and metal interaction at elevated temperature are oxidation and reduction of metals. The phenomena are affected by parameters determined by the results of interaction as well as by combined parameters of materials and water. Oxidation and reduction themselves are a kind of synthetic science consisting of electrochemistry, metallurgy, physics and chemistry. Corrosion, erosion, dissolution, precipitation, adsorption and deposition

and fouling are related to oxidation and reduction of metals. It is wondered if scientific fields desire much breakdown of oxidation and reduction. The items are breakdown into several elemental items, which are as follows.

(i) Cupper behavior

Cupper behavior should be understood with considering oxidation and reduction on metal. Cupper ion affects oxidation of other metallic ions and at the same time be affected by coexisted ionic species and particles. Catalytic effects of cupper on oxidation and reduction of co-existed impurities are important to be determine, though it is difficult to measure them

- Solubility of metallic ions in steam
   Solubility of metallic ions in steam is also considered as a part of oxidation and reduction of metals in steam. It will be difficult to avoid the contribution of co-existed mists to solubility in steam.
- (iii) Nucleation and condensation of impurities in steam

Condensation of impurities on heated surfaces is one of the important subjects. Their concentrations are d determined by balance of deposition and release, which might be affected by co-existed impurities. Compatibility of deposits with surfaces will be one of the key parameters to determine condensation and particle growth.

- (iv) Condensation and deposition of metallic impurities in aqueous solution and steam Compatibility of deposits with surfaces will be one of the key parameters to determine condensation and particle growth.
- (v) Oxide film morphology at elevated temperature

Oxide film morphology at elevated temperature will be changed during cooling down periods. Exact examinations of the films give us important information but sometimes they are not correct. Direct measurements of oxide film properties are desired.

It is important to discussed the border between the contributions of basic research and plant application. Perfect understanding the phenomena and their application are orthodox approaches but the goals are so far. Plant chemists should be submit some speculation or their candidates, while scientists screening them based on scientific consideration.

(3) Flow induce corrosion

Erosion-corrosion is one of key issues of car4bone steel corrosion for both BWRs and PWRs.

#### 4. Conclusions

Major subjects to be proposedFor PCAS are summarized in Table 2.

In order to improve plant reliability and safety, precise and reliable evaluations of water chemistry data have been required. For this, quality assurance of the water chemistry data acquisition system is required. The quality assurance should be supported by standard procedures for water chemistry data acquisition; these are going to be established by a committee designated by the Atomic Energy Society of Japan. Measured water chemistry data often give us only restricted information to understand materials water interaction in the plants. Theoretical models are being applied to bridge the gaps between measured water chemistry data and information desired to understand the interactions of materials and cooling water in plants. Major models already in use are:

- (1) water radiolysis models for evaluating corrosive conditions in BWRs and PWRs;
- (2) crevice radiolysis model for estimating crack growth rate of SCC in BWRs; and
- (3) crevice pH model for evaluating corrosive conditions in crevices between SG tubing and tube support plate in PWRs.

High temperature water chemistry sensors and automatic plant diagnostic systems have been applied in only restricted areas, but they will be applied in plants after more experience is obtained with off line Attachment 11.

diagnostic systems. ECP sensors are growing in popularity as devices to determine the effects of hydrogen injection in BWR systems.

As a result of discussion on the results of Nuclear Committee during IAPWS 2004, an international collaboration program on flow assisted corrosion has been proposed.

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Abbreviations ABWR · advanced BWR AC: autoclave ATR: advanced thermal reactor BD: bottom drain line BWR: boiling water reactor CT: compact tension ECP: electrochemical corrosion potential FP: radioactive fission IAPWS: International Association of Properties of Water and Steam ICPWS: International Conference on Properties of Water and Steam IGSCC: intergranular stress corrosion JIS : Japanese Industrial Standards KK: Kashiwazaki Kariha LPRM: local power range monitor housing PCAS: Physical Chemistry of Aqueous Solutions PCC: Power cycle chemistry PWR: pressurized water reactor

PWSCC: primary water stress corrosion cracking

SSRT: slow strain rate test

#### REPORT

#### IAPWS Committee: Fuel Cell and H<sub>2</sub> Technologies

<u>Mandate:</u> update IAPWS on ongoing research, advice on problems IAPWS could work on, and on whether a task group should be formed. The committee will work for a year, and report at Kyoto, after which it is disbanded.

<u>Recommended members:</u> S. Lvov (chairman) and L. Shockling (Siemens Westinghouse Power Corporation).

Mr. Shockling was contacted by e-mail but never replied on the request to participate in the Committee. Dr. J. Pierre from Siemens Westinghouse, Pittsburg, PA was asked served as a consultant on the Committee.

<u>Committee Members (2003/04):</u> S. Lvov (chairman), J. Pierre (invited consultant from Siemens Westinghouse, Pittsburg, PA)

The main areas of R&D in Fuel Cell and H<sub>2</sub> Technologies those are important to IAPWS:

- (1) Electrolysis of Water
- (2) Electrochemical Oxidation of Fuels
- (3) Electrochemical Reduction of Oxygen
- (4) Properties of Proton Conducting Membranes
- (5) Electrochemical and Chemical Production of Hydrogen using Hydrothermal Cycles
- (6) Development of Fuel Cell–Turbine Hybrid Systems

All the areas of R&D mention above have "high priority" status in the roadmap plans of DOE, DOD, ARO, etc. and substantially funded or likely to be funded by these agencies during next 5-10 years.

The Committee activities in 2003/04 were discussed at PCAS WG meeting on Sunday, August 29<sup>th</sup>, and the WG recommendations are as follows:

(1) create an IAPWS Task Group on Fuel Cell and H<sub>2</sub> Technologies
(2) recommend the following task group members: S. Lvov (chairman), H. Corti, M. Nakahara, and F. Marsik.

### Structure of IAPWS, Awards

Following the consideration of a survey on the operation and structure of IAPWS at Vejle 2003 groups were established to consider matters of importance to IAPWS. One of these groups, Bellows, Bignold, Olavessen, Rukes and Cooper(chair) was to consider awards and was given the following mandates:

A. Advise EC on

- (1) Forms of IAPWS recognition of companies' support of IAPWS activities.
- (2) Desirability of formal written appointment by IAPWS President of WG chairs
- (3) Letter of appreciation at termination.
- (4) Desirability of new IAPWS Award for excellent leadership of WG.

B. Work with Editorial Committee on proper definition and conditions of IAPWS Awards in Bylaws, in time for vote at Kyoto meeting.

#### **Current Awards**

The details of the three current IAPWS Awards given below are useful when considering A. (4) and B. above.

[A] Gibbs Award This Award should be given to a distinguished scientist or engineer who has made a substantial contribution to the development of knowledge on the properties of water, steam and aqueous solutions at high temperatures and pressures, as well as to other areas of underlying science and technology of interest to IAPWS. The Award will not be monetary, but will consist of a plaque and or certificate and or medal that carries a considerable prestige.

The Award will be presented to the recipient on the occasion of ICPWS, and the recipient shall be invited as one of the keynote speakers at the plenary session of the Conference.

The Gibbs Award was established in 1997.

[B] Helmholtz Award This Award will be given to promising mid-career scientists and engineers (not more than one each year), who are making significant contributions to improve the existing knowledge of the properties of water, steam and aqueous solutions, or other areas within the scope of IAPWS activities interests. The candidate will normally be under the age of forty at the time of nomination.

The Helmholtz Award aims to encourage mid-career experts who may not yet be active in the IAPWS community, and to provide an opportunity for presenting their achievements at the Symposium associated with the annual IAPWS meeting. The Award will consist of a plaque and/or certificate and is intended to be a prestigious Incentive to the career of the recipient. This Award will also provide financial support from the IAPWS for nominal travel expenses required to attend the annual meeting.

The Helmholtz Award was established in 1997.

[C] Honorary Fellowships made to IAPWS members who have made outstanding contributions to the Association, first awarded in 1981.

#### Comments on and recommendations for mandate A

A. (1) Forms of IAPWS recognition of companies' support of IAPWS

Companies support IAPWS in the following ways.

(i) Payment of subscriptions to the members (National Committees), who then pay the annual dues to IAPWS and also the expenses of the deputy representing the member at the annual IAPWS EC meeting.

(ii) Pay the expenses of their employees, who are members of IAPWS Working Groups, to attend the annual IAPWS meeting.

(iii) Financial support for an ICPWS, normally from companies in the country of the member hosting the particular ICPWS.

Recognition of (i) appears to lie with the National Committee and can take various forms such as

(a) declaration of sponsorship of the National Committee on its web site and elsewhere.(b) Provide complementary copies of IAPWS publications such as the Atlas or the proceedings of the ICPWS.

(c) invitations of other company employees to any symposia or other events of interest to the company that the National Committee have organised.

(Recommend (a), (b) and (c) to National Committees)

Recognition of (ii) If the employee is a member of the National Committee then actions under (i) cover this situation. In the case of a WG member who is employed by an organisation that does not sponsor a National Committee then it may be the case that letters of invitation to IAPWS WG meetings, letters of welcome to WG membership and letters of thanks for involvement in IAPWS tasks, may be of value. (the use of web registration IAPWS meetings looses one of these).

(Recommend to EC)

Recognition of (iii) is made in appropriate acknowledgement in ICPWS documents including the proceedings.

(Recommend to ICPWS Organising Committee)

The use of plaques for (i) or (ii) seems to have difficulties in ascertaining that all companies who have supported IAPWS though National Committees treated equally.

A. (2) Desirability of formal written appointment by IAPWS President of WG chairs. It is important to establish the formal letter of appointment.

(Recommend to EC)

A. (3) Letter of appreciation at termination. It is highly desirable that the retiring WG chair should receive a letter of appreciation. (*Recommend to EC*)

A. (4) Desirability of new IAPWS Award for excellent leadership of WG. Any retiring WG chair, who has made a significant contribution to the business of IAPWS will be a strong candidate for Honorary Fellowship. It should not be necessary to create another award.

#### REPORT

#### IAPWS Task Group: Electrochemical Processes in High-Temperature Aqueous Systems

<u>Mandate:</u> The task group should be formulated and start their work as soon as possible. It should be operational, and report by the time of the Kyoto meeting. The chair should have the discretion to select further members and co-opted experts.

<u>Members:</u> S. Lvov (chairman), D. Macdonald, E. Maughan, M. Nakahara, T. Petrova, and S. Uchida

The Task Group has extensively communicated in 2003/04 by e-mail and formulated the following areas of R&D that are important to IAPWS:

- (1) Potentiometry
- (2) pH Measurements
- (3) Electrochemical Monitoring of Solution Chemistry
- (4) Electrochemical Kinetics Measurements
- (5) Corrosion Metals and Alloys
- (6) Electrokinetic Measurements
- (7) Electrochemical Production of Substances (for example, hydrogen production)
- (8) Electrochemical Production of Electrical Energy (for example, fuel cells)
- (9) Electrochemical Conductance Measurements.

The Task Group activities in 2003/04 were discussed at PCAS WG meeting on Sunday, August 29<sup>th</sup>, and the WG recommendations are as follows:

(1) continue the Task Group activities in 2004/2005,

- (2) add D. Palmer to the members list
- (3) communicate to PCC to formulate details of the listed above areas of research

## EDUCATION AND OUTREACH TASK GROUP

According to the Minutes of the Vejle meeting (pp. 19-20) the tasks of this TG are:

- Define educational and outreach projects.
- Work with national committees active in this area.
- Attract volunteers.
- Explore possibilities of obtaining funding.

#### • Proposed projects.

After discussions with members of different National Committees the proposed activities in the near future should aim to three targets: young researchers, university students and high school students. They are the following (in decreasing order of priority)

1- Promote the participation of PhD students and young researchers in Annual IAPWS meetings

This activity could start at the next IAPWS meeting at Greece, with the participation of local and foreign students. The best option seems to be organize one or two special sessions in the framework of WG joint meetings.

Funds for encouraging the participation of students in IAPWS activities would come from IAPWS (directly or through funds required for international collaborations). Local agencies could eventually contribute.

2- Develop an educational web page and expand the FAQ section of the IAPWS web site. FAQ items could be added, such as those related to new technology (fuel cells for instance), environmental issues, etc.

Additionally, an independent web page could be created, linked to the IAPWS site, which aims to a different people target: university students and high school students and teachers. The content of this web page has to be defined in connection with point (3) during the next year.

3- Educational Booklet.

It aims to develope educational material for university and high school students related with the use of water and steam in the power industry. Its content will be defined during the next year and it will be complementary with other electronic educational tools (CD, web page). It is a long term project (2-3 years).

#### Task Group Members

Confirmed members of this Task Group are: H.Corti (ABBC, chair), M.Assael (Greece), R.Harris (BIAPWS), L.Trevani (Canada), L.Olavessen (USA), A.Harvey (USA, consultant). One of the task for the next year is try to attract volunteers of other National Committees representing different WGs.

### Funding

#### The first activity will require IAPWS support.

The preparation of electronic and printed material will require funds from local or international agencies.

#### New Task Group – Environmental issues

*Rev.1 Sep.1<sup>st</sup>, 2004* August 29<sup>th</sup>, 2004 Nobuo Okita

- 1. Main task and object for the new task group Investigate current status and future directions, and research the subjects to which IAPWS can contribute as for environmental issues.
- 2. Task member First-level subcommittee members: Okita, Parry, Weber, Zeijseink Additional, full committee: Nakahara, Assael, Olavessen, Span, Regazzoni(Argentina)
- 3. Key technologies to be considered Three stages QFD (quality function deployment) is carried out as below in order to collect and select the key technologies for solutions to environmental issues.

Solutions Issues	High efficiency	Recycle	Treatment	Zero emission	Maintain efficiency
CO2 emissions	++		+	+++	+
Mercury ( heavy metal ) emissions	+	+	++	+++	+
NOx & SOx emissions	+	+	++	+++	+
Effluent		++	+++	+	
Waste		+++	++	+	
Sea or river water temperature rise	+++				++

#### OFD-1: Concept of solutions

Notes) +: weak correlation ++: moderate correlation +++: strong correlation

QID 2. Itelinology	neius ioi solutioi					
Fields Solutions	High temp. Low NOx CC	USC plant	Nuclear energy	Renewable energy	Other new cycles & systems	Energy Storage
High efficiency	+++	++	+		+++	+
Recycle	+	+	++	+++	++	++
Water treatment	++	++	+++	+	+	
Flue gas treatment	+++	+++	++	+	+	
Fuel treatment			++	++	+++	++
Zero emission	+		++	++	+++	
Maintain efficiency	++	+	+	+	+	+++

#### OFD-2: Technology fields for solutions

Technologies Fields & Solutions		Steam cooling	Steam-Water injection	SCWO	SCR SNCR	OT	Chemical reactions	Anti-erosion corrosion
Fields	High temp. & Low NOx CC	+++	++	++	++	++		
	USC plant	++		++	+++	++		+++
	Nuclear energy			+++		+++	+	++
	Geothermal system		++	++			+	+++
	Fuel cell			+			+++	
	Biomass energy			++	++	++	++	++
	PFBC, A-PFBC		++		+++	+	++	++
	IGCC,IGFC	+	++	+	++	+	+++	++
	HAT (SAT) cycle		+++		+	+	++	+
	New H2 system	++	++			+	+++	++
	Energy Storage						+++	
Solutions	High efficiency	+++	++				+	+
	Recycle			++			+	
	Water treatment			+++		+++	++	
	Flue gas treatment			+++	+++		++	
	Fuel treatment		+++	++	++		+	
	Zero emission			++			+++	
	Maintain efficiency	++	++			++		+++

QFD-3: Key Technologies for solutions relating to water and steam ( to be discussed)

4. Experts and related committees (to be discussed)

Japan: Dr. Nakahara & Dr. Matsubayashi, Kyoto University (SCWO)

Dr. Hamamatsu & Ikemoto, CRIEPI (Environment Issues)

Dr. Takaku, Shinshu University (Water treatment)

Dr. Yamazaki & Dr. Uchida, Tohoku University (Chemical reactions& Nuclear energy)

National Institute of Advanced Industrial Science and Technologies (General issues) Supercritical Fluid Research Center (SCWO)

National Institute for Environmental Studies (Environment Issues)

Toyohashi University of Technology (SCWO)

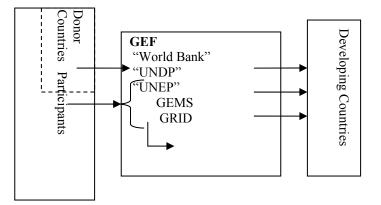
Germany: International Journal for Electricity and Heat Generation (General issues) Department of Business and Labor of the German government (General Issues)

USA: U.S. Environmental Protection Agency (Environment Issues, SCR) :www.epa.gov Energy and Environmental Research Center (Environment Issues, SCR)

www.undeerc.org

Institute of Clean Air Companies (SCR, SNCR) : www.icac.com EPRI (General Issues) : www.epri.com

Reference: International Organizations for environmental issues



GEF: Global Environmental Facility UNDP:United Nations Development Programme UNEP: United Nations Environment Programme GEMS: Global Environment Monitoring System GRID: Global Resource Information Database

#### 5. Current status and future direction in Japan and USA

(2) High Temperature & Low NOx Combined Cycle

1450degC Gas turbine combined cycle using steam cooling for combustion is operating in Tohoku Electric Power Co.

1500degC Gas turbine combined cycle using steam cooling for  $1^{st} \& 2^{nd}$  blades is under construction in Tokyo Electric Power Co. More than 58%(LHV) of plant efficiency can be realized.

Steam purification for the cooling is strictly controlled in order to maintain reliability.

NOx is guaranteed below 5ppm at the stuck by using dry low NOx combustor and SCR with ammonia.

Future direction will be more than 59% of plant efficiency and below 3ppm of NOx emission.

In USA, in order to avoid "yellow plume" form exhaust gas at low load, quick start of gas turbine is important.

(2) USC plant

The highest temperature is 600/610deg C and the highest pressure is 31MPa in operating plants. Technologies for the 630/630deg C has been developed and completed, however, Japanese domestic demand for electricity is not so high now. Then it will take more time in Japan to realize USC plant with such high temperature.

Future direction will be more than 700deg C USC plant which is considered to be a national R & D project in future.

In USA, the highest applied steam condition is 1050 F with subcritical pressure, because utilities prioritize reliability.

(3) Nuclear energy

ABWR is operated applying OT in Tokyo Electric Power Co. APWR is under construction. Plu-Thermal plan for recycle of used fuel is under consideration. Economical comparison has been discussed recently.

Future direction will be discussed further, however, it is necessary as base load in Japan.

In USA, new nuclear plants are constructed only for upgrade to exist plants, because new site can not be permitted for construction.

(4) Geothermal system

Geothermal plants are operated in Tohoku Electric Power Co. and Kyushu Electric Power Co. Binary plant is also operated as a test plant.

Water injection system is applied for cleaning steam and preventing from scale adherence to the 1<sup>st</sup> nozzles and blades. *One of the most important issue is anti-corrosion technology.* 

New technology for preventing from scale adherence to the return well is also investigated. Future direction will be to investigate how to recover or maintain the energy of steam from the well.

(5) Fuel cell

Several kinds of fuel cell are developed and operated as follows,

"Molten Carbonate Fuel Cell (MCFC)"

"Solid Oxide Fuel Cell (SOFC)"

"Phosphoric Acid Fuel Cell (PAFC)"

"Proton Exchange Membrane Fuel Cell (PEFC)"

High temperature fuel cell (MCFC & SOFC) will have great potential for future use as an alternative source of generating electricity.

(6) Biomass energy

Recently in Japan, biomass energy is focused and introduced as an economical energy by industrial users. Utilities are investigating it. Biomass fuel can be cheaply obtained rather than the conventional oil fuel.

Future direction will be to maintain reliability by boiler tube selection and flue gas treatment.

(7) PFBC and A-PFBC

Three units of PFBC with 850deg C class gas turbine are operated in commercial use and one unit is under construction.

A-PFBC with 1350deg C class gas turbine is investigated for future application

(8) IGCC and IGFC

An IGCC plant is operated as a test plant at Nakoso power station.

Future application will be IGFC system with fuel cell for higher efficiency.

(9) HAT cycle

HAT cycle or SAT cycle is under investigation as low NOx and high efficiency cycle.

SAT (Steam and Air Turbine) cycle with chemical reaction for the flue gas will reach higher efficiency.

(10) New H2 system

Hydrogen turbine system had been developed in the national R&D programme. However, it has been stopped because of the difficulty in obtaining and treating economically the hydrogen fuel. Material development or selection is half done.

Chemically recuperated gas turbine system is under investigation.

Future issue to be resolved will be economical treating system for hydrogen fuel with other use such as fuel cell.

- (6) Current status and future direction in other countries
  - (1) Germany
    - Coal Fired Steam Power Plants:

Current efficiency level 47% (anthracite) and 43% (lignite). Through progress in thermodynamic and flow design, materials and coal drying techniques increase of efficiency estimated to about 51% until 2010. Fields of interests are:

- Material development for highest process parameters (700/720 C, 375 bar)
- Highly efficient steam turbines (700 to 800 C, 350 to 400 bar)
- Low NOX through optimized combustion
- Optimization of coal drying process for lignite
- Improved modeling of combustion and fouling
- Improved numerical design tools

Combined Cycle Power Plants (CCPP):

Current efficiency level 58%. Through progress in thermodynamic and flow design and materials increase of efficiency estimated to about 65% until 2010. Fields of interests are:

- Optimized design for turbine components
- Reduction of cooling air consumption in gas turbines
- Improved combustors
- Improved design and modeling tools

Integrated Gasification Combined Cycle (IGCC):

Currently several demonstration plants in Europe existing. Further demonstration project intended for 2010 - 2015. Main focus is profitability improvement and incorporation of progress in CCPP design.

Future concepts of interest (not before 2020): CCPP with pressurized pulverized coal combustion CCPP with pressurized fluidized bed combustion and partial gasification Externally fired Combined Cycle (EFCC) Hybrid power plants (CCPP with fuel cells, IGCC with fuel cells) Humid Air Turbine cycle (HAT)

#### Fuel Cells:

Pressurized high temperature fuel cells (solid oxide (SOFC), molten carbonate (MCFC))

(Source: COORETEC report on R&D concepts on low emission fossil fired power plants, Issued by the Department of Business and Labor of the German government, 12/2003)

(2) Argentina

There is interest in the academic sector and also in the government to promote the use of hydrogen, particularly that obtained from eolic and solar renewable sources to generate energy in fuel cells.

(7) The subject to which IAPWS can contribute

The previous QFDs suggest that the selected key technologies are the candidates of the subject to which IAPWS can contribute.

Each technology will be able to be discussed in the following WG's.

"Steam cooling" : TPWS, IRS, *PCAC and PCC* "Steam injection" : TPWS, IRS, *PCAS and PCC* 

"SCWO" : PCAS and PCC "SCR, SNCR" : PCAS "OT" : PCC "Chemical Reactions" : PCAS and IRS "Anti-erosion & corrosion" : PCC and IRS

 Task object, directions in future and functions for the selected subjects To be discussed in Kyoto referring the held symposium . Firstly collect each country's current status and future directions as described in item #5, then draft the summary of the results and discuss further.

#### 9. Schedule

During Kyoto meeting: Extending the survey I did for Japan to the other member countries should be an urgent task for the respective national committees. Most importantly, review the item 7 in which I have outlined areas IAPWS could contribute to.

### Task group

# Metastability, Nucleation, Early condensate, Droplet Sprays and Cavitation

# Main subjects:

The group will provide a forum for leading researchers and practitioners to engage in debate on contemporary issues governing the state-of-the-art in nonequilibrium and metastable of water and aqueous systems. In particular:

- Phase transitions and phase diagrams of aqueous systems Saturation line, bubble points and dew points
- Metastable water and metastable aqueous systems Nucleation, cavitation, boiling and condensation
- Bubble and droplet formation and two-phase flow
- Measuring techniques for transient quantities.

More details about the task group problems see the lectures in the Symposium 4 *Nonequilibrium,Metastable and Critical States* 

Some researchers out of IAPWS active

# in this TASK GROUP activities

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# Press Release 14<sup>th</sup> International Conference on the Properties of Water and Steam and International Association for the Properties of Water and Steam 2004 Meeting

Continuing the series of conferences started in 1929, 235 scientists and engineers from 19 countries met in Kyoto, Japan at the 14<sup>th</sup> International Conference on the Properties of Water and Steam. Over 180 papers were given on thermodynamic and transport properties of pure water and steam, on critical phenomena, on chemistry in subcritical and supercritical water, on chemical processes occurring in power plant equipment, and on power cycle chemistry. The conference connects academic researchers with engineers who use their information. It provides the researcher with guidance on useful problems and provides the engineers with the latest research.

The International Conference on the Properties of Water and Steam (ICPWS) is sponsored every 4 years by the International Association for the Properties of Water and Steam (IAPWS). The General Meeting of IAPWS met at the conference and reviewed the progress since the 13<sup>th</sup> ICPWS in 1999. Major progress was demonstrated in the scientific understanding of copper transport in power plants, formulation of the thermodynamic properties of the ammonia-water system over the range of interest in power generation and in fast calculation of accurate steam properties. Work continues on properties of metastable steam. IAPWS also produces guidelines, and certified research needs. Information may be found at the IAPWS website: www.iapws.org.

IAPWS has recently completed *Aqueous Systems at Elevated Pressures*, a compendium of thermodynamic and thermochemical properties, techniques for measurement, techniques for representation of data for pure water and steam and for aqueous solutions, including the partition between water and steam. The work stresses applications to the power industry, geochemistry and other hydrothermal industries. This book includes both theory and data and is intended to be used by a graduate chemist or engineer. The book is available from Elsevier.

IAPWS Power Cycle Chemistry Working group maintains a priority list of research concerns for power cycle chemistry. Heading this list is a scientific understanding of the processes that promote transport and deposition of copper and its oxides in steam turbines. Second on the list is an understanding of the sources, formation and decomposition rates, and corrosion consequences of organic chemicals, particularly but not exclusively, carboxylic acids.

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 Greece in July, 2005. The 15<sup>th</sup> ICPWS will be held in 2008. Further information on both meetings can be found at the IAPWS website, www.iapws.org, as it becomes available.

To: Professor K Watanabe, Chairman of IAPWSFrom: Dr. R R Harries, Chairman of BIAPWSCc: Dr. B Dooley, International Secretary, IAPWS

28 July 2004

# A REVIEW OF THE CURRENT STATUS OF BIAPWS IN 2004

## Overview

BIAPWS is a joint association within the United Kingdom and the Republic of Ireland.

BIAPWS is in healthy position, both financially and with respect to active membership. It has nine corporate sponsors, three members with academic links and four associate members who are in consultancy or are retired from the power generation industry.

BIAPWS has an active role in promoting research and disseminating information within appropriate industries and academic areas. This is achieved through organisation of symposia and workshops and through the BIAPWS Award for final year undergraduate students.

## Membership

The nine corporate sponsors are full members of BIAPWS and represent the power generation industry (7 members), power plant manufacturer (1), technical support and consultancy (1) and power plant chemical instrumentation manufacturer (1). BIAPWS continues to encourage membership from other power plant generators and related industries as well as academia.

The academic support has reduced in the last few years, but three universities are currently associate members, with two actively engaged with the committee.

There are currently four individual associate members, all of whom have now retired from the power generation industry and have been active within BIAPWS for a number of years. These individual members retain their technical knowledge through part time consultancy and are a key factor in the operation of the BIAPWS committee.

It is inevitable, that with all of the sponsors and a high percentage of the membership being drawn from the power generation industry, topics relevant to that industry have a higher priority than academic research. It has proved difficult to establish the level of academic research into topics of interest to BIAPWS / IAPWS, but there is a general feeling that little research of specific interest is currently being conducted within the UK.

All corporate sponsors are required to pay an annual membership fee as a condition of continued membership. These fees allow BIAPWS to pay its IAPWS dues, to fund a delegate to the annual IAPWS international meeting, to organise symposia and workshops within the UK and, more recently, to sponsor the BIAPWS award.

## Education and Outreach

BIAPWS sees one of its primary functions to act as a central point of communication and information for matters of steam and water chemistry between the power generation industry, manufacturers of power plant equipment, academia and other interested parties.

This is achieved by regular committee meetings at which representatives from the major UK and Irish power generation companies can meet and exchange views in a neutral environment. At these meetings they also interact with equipment suppliers and with academic institutions.

The second area of education and outreach is the regular organisation of technical symposia. Seven symposia have been held since 1995, initially annually, but latterly at 18 month intervals. The major topic is linked to power plant steam and water chemistry, and BIAPWS provides the only UK and Irish national forum for a regular symposia on power plant chemistry. As such it achieves a very important function and has regularly attracted attendances of 80 people, including speakers and attendees from other European countries. These symposia are a very effective way of raising awareness of BIAPWS within the UK and Ireland.

At the last symposium, in May 2003, a new initiative was started, whereby BIAPWS organised half-day workshop sessions on the days before and after the symposium, with two power plant related topics in each workshop. The first workshop was reasonably successful, the second was less well attended. This was believed, partly, to be due to the poor economic state of the UK power generation industry. For the 2004 symposium, planned for autumn 2004, it is proposed to have only one half-day workshop session with three or four topics, some of which will be linked to papers presented in the main symposium. The symposium itself will be targeted at power plant operators. It is hoped this "added value" will attract attendees to both the workshop and symposium. The third initiative has been the BIAPWS Award, started in 2002 and first awarded in 2003. Its aim is to raise the awareness of undergraduates about research and careers in areas and industries associated with the properties of water and steam. It offers a prize of £1000 (\$1800US) for a dissertation based on a final year undergraduate project with suitable association to the aims, ideals and topic areas of IAPWS. In 2003 the winning dissertation was on the topic of "Third Phase formation in the Purex Process". It was awarded to Ms Lindsay Plant of Manchester University.

Currently two members of the BIAPWS committee are active on a committee set up by the European Power Plant Suppliers Association in determining a common set of boiler chemistry and steam purity guidelines for new power plants supplied by these European companies. BIAPWS is currently co-ordinating responses from members on the recently issued European Standard EN 12952 – 12: 2003 "Water Tube Boilers and Auxiliary Installations – Part 12: Requirements for Boiler Feedwater and Boiler Water Quality".

## The future

BIAPWS will aim to continue to expand its membership with appropriate companies and institutions.

BIAPWS will seek to find further ways of bringing awareness of the topics of steam and water, its scientific properties and its technical applications and challenges to a wider audience, particularly through developing an interest by undergraduates and pre-university students in science and engineering associated with water and steam.

**Richard Harries, Chairman BIAPWS** 

# The Czech National Committee

International Association for the Properties of Water and Steam

## **REPORT on IAPWS related activities – July 2003 / August 2004**

Submitted to the EC Meeting of IAPWS, Kyoto - August 2004.

### National Committee Contacts:

CZ NC PWS - Institute of Thermomechasnics, Dolejskova 5, 182 00 Prague 8, Czech Republic Fax: + 420 2 858 4695, E-mails: secr.czncpws@it.cas.cz Prof. R.Mareš, Fax: + 420 19 7429986, E-mail: maresr@kke.zcu.cz

- Following Institutions participated in the research into the thermophysical properties and chemical processes:
- Institute of Thermomechanics (IT) AS CR, Department of Thermodynamics, Dolejskova 5, CZ-182 00 Prague 8
- **Czech Technical University in Prague** (CTU), Faculty of Mechanical Engineering, Department of Fluid Mechanics and Power Engineering, Technická 4, CZ-166 07 Prague 6
- **Technical University Brno** (TU), Faculty of Mechanical Engineering, Department of Thermomechanics and Nuclear Energetics, Technická 2, CZ-616 69 Brno
- **Institute of Chemical Technology Prague** (ICT), Power Engineering Department (ICT-IE) and Department of Physical Chemistry (ICT-IPC), Technická 5, CZ-166 28 Prague 6
- **University of West Bohemia in Pilsen** (UWB), Faculty of Mechanical Engineering, Department of Power System Engineering, Univerzitní 8, CZ-306 14 Plzen
- SKODA ENERGO, Turbines, Plzeň, Inc., Tylova 57, CZ-316 00 Plzen
- Nuclear Research Institute plc. (NRI), Rez, CZ-250 68 Rez

Technical University of Liberec (TUL), Department of Chemistry, CZ-461 19 Liberec.

Activities were sponsored by the Grant Agency of the Academy of Sciences and Grant Agency of the Czech Republic, SKODA ENERGO-Turbines, Plzen Inc., Ministry of Education, Youth and Physical Training of the Czech Republic, and Ministry of Industry and Trade of the Czech Republic.

- Dr. Sifner (IT) prepared information about history and results of the research into thermophysical properties of water and steam in Czechoslovakia and Czech Republic. /for use by CZ NC/ [1,2,3].
- Prof. Mares (UWB) prepared an information about Aleksandrov's equation for viscosity of ordinary water and with collaborators investigated wet steam flow [4,5,6].
- Prof. Marsik (IT) with co-authors finished and sent to press the manuscript of the Chapter 7: "Binary Homogeneous Nucleation in Selected Aqueous Solutions", in the frame of the ATLAS Project [7].
- Prof. Marsik (IT) with his research team carried out investigations into metastable state of water and steam, condensation, evaporation, and cavitation [8 to 14].
- Prof. Sedlbauer (TUL) with Profs. Majer and Wood finished and sent to press the manuscript of Chapter 4: "Calculation of Standard Thermodynamic Properties of Aqueous Electrolytes and Nonelectrolytes", in the frame of the ATLAS Project [15].

- Prof. Sedlbauer (TUL) with Prof. Wood developed a new model for simultaneous description of thermodynamic properties of aqueous ions at extreme conditions. The model is based on the Sedlbauer-O'Connell-Wood equation for standard part of the chemical potential and Mean Spherical Approximation for the excess part of the property [16 to 20].
- Dr. Hruby (IT) performed experimental and theoretical investigation of homogeneous nucleation of dropplets of pure water and water solutions from superheated steam/vapor mixtures and studied properties of subcooled water [21, 22].
- Research activities at the CTU have continued during the period 8/2003 8/2004 in further improving our knowledge on the droplet nucleation process occurring in LP steam turbines by means of analysis of realized diagnostics of wet steam in 1000 MW and 210 MW steam turbine of nuclear and fossil power station, respectively.

The diagnostics of wet steam at the exit of L-0 turbine stage (from the root to the blade tip) consisted in prediction of droplet size spectra, moisture level, and electrostatic charge of the droplet population.

Combined extinction and charge probe developed at the CTU was found to be suitable equipment for measurement of separate contributions of the fine and coarse droplets in the wet steam charge density. The data obtained in the mentioned turbine tests have been used in improving computational model of the droplet nucleation in LP steam turbines [23].

- Dr. Jiricek (ICT-IE) with collaborators evaluated deposits from steam turbine buckets on the basis of elemental analysis and spectroscopic examination. Compounds responsible for underlying steel corrosion brought by steam carry-over were identified [24].
- Dr. Jiricek (ICT-IE) studied corrosion inhibition in runway deicers based on potassium acetate. In the new formulation, toxic triazoles are avoided and optimized additives gave the fluid with low impact on aircraft materials measured by standard tests for aircraft maintenance chemicals [25, 26].
- Dr. Hnedkovsky (ICT-IPC) with collaborators investigated properties of organic solutes in water. Published articles are in [27 to 43].
- Prof. Stastny (SKODA ENERGO) with co-workers studied effects of deposits on the blades of MP parts of steam turbine in fossil power station, measured degradation of steam turbine blade surfaces by deposits of chemicals and compared numerical models of the water steam flow with hetero-homogeneous condensation in nozzles with experiments [44, 45].
- Dr. Zmitko (NRI) collaborated with nuclear power plants mainly in the fields of water chemistry, corrosion problems and radiation control. Following activities were carried out :
  - monitoring and evaluation of primary water chemistry and radiation situation at units 1 and 2 of the Temelín Nuclear Power Station.
  - data processing technologies and system for diagnostics for water chemistry and corrosion control in Nuclear Power Plants (DAWAC). [46 to 48].

### Young Scientists IAPWS Fellowships:

Mr. T. Nemec finished the IAPWS Young Scientists Project (CZ-US) "Thermodynamics of Binary Homogeneous Nucleation in Superheated Steam " under supervising Prof. Maršík, Dr.Hrubý, Dr. Palmer, and Dr. Simonson. The project was focused on three areas of interest in the binary homogeneous nucleation research:

- preparation of a database of nucleation-relevant thermodynamic properties for several water-admixture binaries relevant to power cycles,
- to employ this database in a nucleation simulation program,
- solving the kinetic equations of nucleation.

His Final Report for the IAPWS Young Scientists Fellowship is in Appendix 1.

The new publications of the fellowship holder are in [8, 9, 49].

#### IAPWS Certified Research Needs

Ad item 1.11 from the Minutes of EC IAPWS, Veile, DK, 2003

- a) Members of the CZ NC PWS interested in PCC problems, looked through the proposal of the new procedure for development of ICNRs (PCC Attachment A, pg.44 in Minutes) and agree with the proposal.
- b) They reviewed the priority list ICRNs accepted on September 25, 2003 in Veile and recommend to continue namely in solving
  - Copper Depositions
  - Nucleation and Condensation in Steam Turbines
  - Physical and Chemical Processes of Concentration and Deposition in the Power Cycle

and recommend for discussion and inclusion of three new tasks:

- A) Improving of the Heat Transfer of the Condenser Tubes in Power Plants. (Improving the Thermic Efficiency of Clausius-Rankine Cycle)
- B) Properties of Supercritical Water (SCW), Solubility of Salts, Corrosion Products and Oxide Protection Layers.
- C) Protection of alloys by coatings, hot corrosion in molten salts.

The deputy of the CZ PCC group (Dr.Zmitko) is prepared to give explanation for the proposed tasks under points A through C).

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### THERMODYNAMICS OF BINARY HOMOGENEOUS NUCLEATION IN SUPERHEATED STEAM – YOUNG SCIENTISTS IAPWS PROJECT – FINAL REPORT

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#### BACKGROUND

Nucleation, a physical phenomenon which is closely connected to the nature of the world around us, is the area of interest of this project. Even though we focus on its special case only, the vapor – liquid nucleation, we can follow more than a century of scientific investigations of this problem. The broad area of application makes the nucleation very important nowadays; the two following cases are discussed mainly. The formation of aerosols in the atmosphere is very important in the study of various atmospheric processes. And the condensate creation in power cycles gives some restrictions on the power cycle design and efficiency.

Let me mention the most important milestones in the nucleation theory development. The early works of Gibbs [1] are usually referenced as the first attempt to describe the nucleation process. The nucleation theory development was started by Becker and Döring [2]. Their unary nucleation theory was fine-tuned later by Zeldovich [3]. The next big step into the field of binary nucleation was done by Reiss [4]. Then Stauffer [5] derived a proper expression for the binary nucleation rate and Trinkaus [6] generalized the theory to multicomponent mixtures. This approach to the nucleation problem is usually called the Classical Nucleation Theory (CNT).

Of course, the development of the nucleation theory was pushed forward by the enhancements and improvements of experimental nucleation techniques. Unfortunately, the results of these nucleation experiments (nucleation rate, size and composition of the critical cluster) showed significant deviations from the values predicted by the CNT. Many scientists tried to remove the discrepancies by introducing various revisions or consistency enhancements of the CNT, but these modifications were applicable to a specific small set of mixtures only, never reaching a general validity.

Our mission is to review the framework of the CNT. Evaluating the nucleation properties based on the CNT for a wide set of mixtures, and comparing them with available experimental results can help us to pinpoint the weaknesses of the CNT.

#### RESULTS

There is an obvious choice for the systems suitable for our purpose – aqueous binary systems. The nucleation of water with various admixtures has been investigated experimentally in many studies, especially in connection with the atmospheric aerosol formation and the power cycle condensation. Moreover, the properties of aqueous systems necessary for accurate evaluation of the nucleation properties using the CNT have been measured in most cases already. The only bottleneck in nucleation calculations remains the availability of thermodynamic properties of the investigated mixtures. Luckily, the aqueous chemistry group at ORNL, where I spent almost 5 months (March – July 2003) under the supervision of Don A. Palmer during this project, turned out to be the most suitable place for finding the necessary thermodynamic data and getting help with their representation.

We have studied several types of aqueous mixtures, introducing different thermodynamic models. Water with alcohols (methanol, ethanol, propanol) served for comparison with experiments. Other dissociative admixtures were implemented  $(H_2SO_4, HNO_3, HCl, NaOH, NaCl)$  with a slightly different approach. Ammonia which can be described either by a non-dissociative model or by a dissociative one was very useful for calibrating our two nucleation models. As a result, I have developed an easy-to-use windows-based program called Conan. It calculates all the nucleation properties of the above mentioned systems at given temperature, pressure and composition. Moreover, it evaluates the sensitivity of the results to the errors in thermodynamic properties used throughout the calculations. The Conan software is available upon request.

The comparison of the Conan results and available experimental nucleation rates (e.g. Mirabel [7], Flageollet [8], or Wyslouzil [9]) shows a systematic deviation mentioned earlier. But we can follow the nature of these differences for a wide set of distinct aqueous systems. This gives us some ideas how to solve this problem; the CNT enhancement based on these results will be the next step in our research. Later, we will focus on multicomponent systems.

A short summary of this project was presented at the annual IAPWS Meeting in Vejle, Denmark, 24 - 30 August 2003.

#### COLLABORATIVE PROJECTS

Some of the results of this research will appear in the chapter "Binary Homogeneous Nucleation in Selected Aqueous Vapor Mixtures" of the upcoming ATLAS book edited by Don A. Palmer.

#### BUDGET

Living expenses (\$9000) in Oak Ridge were covered by the IAPWS Fellowship. Air tickets and health insurance (\$1000) were covered by the grant no. 60251 of the Grant Agency of the Academy of Sciences of the Czech Republic.

#### ACKNOWLEDGEMENTS

I would like to acknowledge the indispensable help of both my supervisors D. A. Palmer and F. Maršík, and important comments from M. Gruszkiewitz, A. Chialvo, and J. M. Simonson (ORNL), and A. H. Harvey (NIST). Finally, I would like to thank IAPWS for making this fruitful research possible.

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## **Danish National IAPWS Committee - DIAPWS**

c/o IDA, Kalvebod Brygge 31 - 33, 1780 Copenhagen V

18 February 2003

# IAPWS REPORT 2003

The research activities in 2003 in Denmark in the field of properties of water and steam were mainly concentrated on continuation of activities started in the 2002. Due to the difficult economic situation new research has not been initiated.

Measurement of the solubility of sodium sulphate in steam in the vicinity of the critical point was made as a collaborative project supported by the EU.

Mathematical modelling of thermodynamic properties of ammonia / water mixtures is in progress at the Technical University of Denmark, Copenhagen. The model takes the chemical interaction between ammonia and water into account improving its fit to the experimental data.

Measurements and modelling of density and viscosity of multicomponent aqueous electrolyte solutions are in progress at the Technical University of Denmark, Copenhagen. The aim is to the predict the scaling in hydrogeological systems.

Modelling of multicomponent aqueous electrolyte systems and application of models to the recycling process for fertilizer from ash residues is in progress at the Technical University of Denmark, Copenhagen.

Modelling of ion exchange processes has started at the Technical University of Denmark, Copenhagen.

Publications in 2003:

Søren Gregers Christensen and Kaj Thomsen, "Modeling of Vapor-Liquid-Solid Equilibria in Acidic Aqueous Solutions", Ind. & Eng. Chem. Res. 42(2003)4260-4268, issue 18

Svend-Erik Therkildsen, "Water Chemistry Control and Monitoring Concept for Avoiding Chemistry-Related Failures in Small Combined Heat and Power Plants", Power Plant Chemistry, Vol. 5 (2003) No.9, p. 553-560.

### German National Committee to IAPWS

# Research Activities on the Thermodynamic Properties of Water and Steam Report "Research in Progress 2004"

- 1. Supplementary backward equations p(h,s) for regions 1 and 2 of IAPWS-IF97
  - The comprehensive article on the backward equations p(h,s) in regions 1 and 2 was finished and finally accepted by the "Journal of Engineering for Gas Turbines and Power".
- 2. Supplementary backward equations *T*(*p*,*h*), *v*(*p*,*h*), and *T*(*p*,*s*), *v*(*p*,*s*) for region 3 of IAPWS-IF97
  - In addition to the backward equations T(p,h), v(p,h), and T(p,s), v(p,s), equations  $p_{sat}(h)$  and  $p_{sat}(s)$  for the region boundary between region 3 and wet-steam region 4 were developed.
  - The Draft of "Revised Supplementary Release on Backward Equations for the Functions T(p,h), v(p,h), and T(p,s), v(p,s) for region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" was prepared.
  - The evaluation of the revised release was supported.
  - The comprehensive article on the backward and boundary equations was prepared.
- 3. Supplementary backward and boundary equations p(h,s) for region 3 of IAPWS-IF97
  - The evaluation of the "Supplementary Release on Backward Equations p(h,s) for Region 3, Equations as a Function of *h* and *s* for the Region Boundaries, and an Equation  $T_{sat}(h,s)$  for Wet Steam of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" was supported.
- 4. Supplementary backward equations v(p,T) for region 3 of IAPWS-IF97
  - The development of backward equations v(p,T) in region 3 was completed.
  - The Draft of "Supplementary Release on Backward Equations for Specific Volume as a Function of Pressure and Temperature v(p,T) for region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" was prepared.

- Investigations on thermodynamic properties of humid air part of the project "Advanced Adiabatic Compressed Air Energy Storage" (AA-CAES) of the European Union
  - The property data base for humid air was completed.
  - Comparison calculations of different models for calculating thermodynamic properties of humid air were performed.
- 6. Property libraries for water and steam, combustion Gas mixtures, and humid air
  - The program libraries FluidEXL for Excel<sup>®</sup> FluidMAT for Mathcad<sup>®</sup>

were extended .

- 7. Implementation of the industrial formulation IAPWS-IF97 on pocket calculators
  - The program FluidTl for the model TI 83 of Texas Instruments was prepared.

Zittau, August 25, 2004

H.-J. Kretzschmar

## The Hellenic National Committee International Association for the Properties of Water and Steam

### **REPORT on IAPWS related activities**

Submitted to the EC Meeting of IAPWS, Kyoto - August 2004

### National Committee Contact: Prof. Marc J. Assael, Chemical Engineering Department, Aristotle University 54124 Thessaloniki, Greece

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#### SCIENTIFIC WORK

The work concentrated in the area of transport properties. More specifically:

#### 1) Maintenance of the Water & Heavy Water Viscosity & Thermal Conductivity Data Bank

As part of a joint project between the International Association for the Properties of Water and Steam and the International Association for Transport Properties (formerly known as Subcommittee on Transport Properties of the International Union of Pure and Applied Chemistry Commission I.2 on Thermodynamics), all available and reliable experimental data on the viscosity and thermal conductivity of ordinary water and steam, as well as heavy water, have been collected and converted to the current temperature scale (ITS-90) and a common set of units. The data are grouped according to state into four regions: liquid phase (excluding data at 0.101 325 MPa), steam (vapor) phase, supercritical phase ( $T > T_c$  for any pressure), and liquid at ambient pressure (0.101 325 MPa) between the triple point temperature and the normal boiling point temperature. Moreover, in the case of water, for each point with measured temperature and pressure (or at specified saturation conditions) a density has been computed with the current scientific standard thermodynamic formulation (IAPWS95), and each experimental datum has been compared with the viscosity or thermal conductivity calculated from the current standard formulations for these properties.

Fluid	Property	No of Points	Temperature range (K)	Maximum Pressure (MPa)
Water	Viscosity	4181	254 - 1316	346
	Thermal Conductivity	5111	255 - 1072	785
Heavy Water	Viscosity	1244	277 - 779	468
	Thermal Conductivity	2380	277 - 1043	250

The data bank is kept updated.

#### 2) New Formulation for the Viscosity of Water

Work in this area is presently progressing fast with the cooperation of Dr D. Friend and Prof. J. Sengers (USA), Prof. E. Vogel (Germany), and A. Nagashima (Japan). It was hoped that a new improved formulation for the viscosity of water would have been ready to be proposed at the

ICPWS Meeting in Kyoto. However, this was slightly delayed, due to the measurement of new data by Prof. E. Vogel, which had to be added.

The new formulation for the viscosity,  $\eta$ , will have a better theoretical form, which is described by the following equation

 $\eta = (\eta_0 + \eta_1 + \eta_{ex})\eta_{cr}$ 

where,  $\eta_0$ , is the viscosity at the dilute gas limit,  $\eta_1$ , the initial density dependence,  $\eta_{ex}$ , the excess viscosity, and  $\eta_c$ , the viscosity in the critical region.

- a) Viscosity at the Dilute Gas Limit
  Following the 4-month stay of Ms Metaxa in NIST in 2003, the work on the viscosity of water
  vapor at the dilute gas limit, has successfully been concluded with the cooperation of Dr Dan
  Friend at NIST (USA), and Prof. E. Vogel (Germany). Thus, a modified form of the IAPWS
  1997 formulation is proposed for the viscosity of water vapor at the dilute gas limit.
  In order to derive this form, more data than the existing correlations, were employed. The
  data were evaluated using an extension of the international recommended procedure for Key
  Comparison Reference Values with the cooperation of the Statistics Division at NIST. The
  resulting proposed equation has a 1.6% uncertainty at the 95% confidence limit.
- b) Initial density dependence contribution Work is now completed by Ms Metaxa in cooperation with Prof. E. Vogel (Germany). The resulting correlation was sent to Dr Dan Friend (NIST) who will carry out the formulation of the excess viscosity and critical contribution in cooperation with Prof. S.V Sengers (USA)
- *c) Excess Viscosity and Critical Contribution* Work in these final areas of the formulation, is near each end.

#### 3) New Formulation for the Viscosity of Heavy Water

Following the above procedure for the viscosity of water, a new formulation for the viscosity at the Dilute-Gas Limit was developed.

#### NON-SCIENTIFIC WORK

Work is still (Oh yes indeed!!) under progress in forming a full National Committee (This is going to be the longest-time-taken-to-be-formed National Committee in the history of IAPWS!). Although some industries and institutions have responded positively, no National Committee has as yet been appointed. The Hellenic Association of Chemical Engineers, which is the body representing Greece, is still thinking about it. Nevertheless, it has been agreed that in December 2004 the full fees will be paid and Greece will become a full member.

### Current Status of Research Activities in Japan Submitted to the ExecutiveCommittee Meeting, IAPWS, Kyoto, Japan, August 2004

by

Japanese National Committee International Association for the Properties of Water and Steam c/o The 139<sup>th</sup> Committee on Steam Properties Japan Society for the Promotion of Science (JSPS) 6, Ichiban-cho, Chiyoda-ku Tokyo 102-8471, Japan

The Japanese National Committee to the IAPWS is playing an active function as the 139th Committee on Steam Properties chaired by Professor Koichi Watanabe, Keio University, at the Japan Society for the Promotion of Science (JSPS), Tokyo. The Committee is extensively concentrating every effort to organize the 14th ICPWS to be held in Kyoto, from August 29 through September 3, 2004. We are expecting more than 230 participants from 20 countries worldwide and 195 papers to be presented at the 14th ICPWS.

The following research projects on the thermophysical and physical-chemical properties of water substances including various aqueous systems of technological importance are currently in progress at several universities and institutions in Japan.

At the Division of Chemistry, Graduate School of Science, Hokkaido University, Sapporo, Prof. S. Ikawa and coworkers are engaged in spectroscopic measurements of water-hydrocarbon mixtures at high temperatures and pressures. Near-infrared absorption spectra of water and water-benzene mixtures were measured at temperatures and pressures in the ranges of 373-673 K and 20-400 bar, respectively. Enthalpy for dimerization of water molecules in the gas and gaslike phase has been estimated to be 15 . . kJ/mol from a pressure-temperature dependence of the molar absorption intensity [*J. Chem. Phys.*, 119 (23), 12432 (2003)]. Anomalously large volume expansion on the mixing of water and benzene has been found in the region enclosed by an extended line of the three-phase equilibrium curve and the one-phase critical curve of the mixtures, and the gas-liquid equilibrium curve of water. It becomes as large as 7 times expansion at 573 K and 100 bar and at molar fraction of benzene of 0.18 [*J. Chem. Phys.*, 121 (6), 2694 (2004)]. [contact: Prof. S. Ikawa; E-mail: sikawa@sci.hokudai.ac.jp].

At the Department of Quantum Science and Energy Engineering, Graduate School of Engineering, Tohoku University, Sendai, Prof. S. Uchida is promoting a second phase of the project on water chemistry of BWR. The effects of hydrogen peroxide on corrosion and IGSCC of stainless steel in high temperature pure water have

been examined by using the high temperature high pressure hydrogen peroxide water loops with controlled hydrogen peroxide concentrations and lower possible oxygen concentrations. By changing concentrations of H<sub>2</sub>O<sub>2</sub> and O<sub>2</sub>, in situ measurements of electrochemical corrosion potential (ECP) and frequency dependent complex impedance (FDCI) of test specimens were carried out and then characteristics of oxide film on the specimens were determined by multilateral surface analyses, i. e., X-ray diffraction (XRD), laser Raman spectroscopy (LRS), Rutherford back scattering spectroscopy (RBS), secondary ion mass spectroscopy (SIMS), and X-ray photoelectron spectroscopy (XPS). The ECP and FDCI data of the specimens exposed to 100 ppb H<sub>2</sub>O<sub>2</sub> were not affected by co-existing O<sub>2</sub> with the same level oxidant concentration and they were also not affected by pre-exposure to 200 ppb O<sub>2</sub>. From the viewpoint of ECP, this meant that corrosive conditions of hydrogen water chemistry were the same as those of normal water chemistry. Smaller oxide dissolution resistance and larger electric resistance of the oxide film were obtained for the specimens exposed to 100 ppb  $H_2O_2$ .  $H_2O_2$  exposure led to thicker oxide layers than  $O_2$  exposure and Cr depletion did. The hematite ratio in the oxide films of the specimens exposed to H<sub>2</sub>O<sub>2</sub> was expressed as a linear function of  $[H_2O_2]$ . The hematite ratio was measurable for 8 ppm  $O_2$ , but negligibly small for 200 ppb O<sub>2</sub>. As a result of theoretical approaches to understand crack tip water chemistry under gamma and neutron irradiations, Mr. Tomonori Satoh (a doctor course student) got a 2003 Award for Emerging Technology of the Atomic Energy Society of Japan. [Latest publication: (1) S. Uchida, et al., Proc 11th Int. Conf. on Environmental Degradation on Materials in Nuclear Power Systems; Water Reactors, Aug. 10-14, 2003, Stevenson, Washington, American Nuclear Society (2003) (CD). (2) T. Satoh, et al., ibid. (3) H. Takiguchi, et al., J. Nucl. Sci. Technol., 41, 214 (2004). (4) S. Uchida, et al., Proc. the 14th Pacific Basin Nuclear Conference (2004) (CD). (5) T. Satoh, et al., J. Nucl. Sci. Technol., 41, 610 (2004). (6) H. Takiguchi, et al., J. Nucl. Sci. Technol., 41, 601 (2004)] [contact: Prof. S. Uchida; E-mail: shunsuke.uchida@gse.tohoku.ac.jp].

At the Graduate School of Environmental Studies, Tohoku University, Sendai, Profs. N. Yamasaki, H. Enomoto, K. Tohji, N. Tsuchiya, and their group are covering wide field related to hydrothermal material science and geofluid science. Material research group developed several kinds of advanced and functional materials [Yamasaki et al., J. Ceram. Soc. Jpn., 111,221-225(2003)], such as synthetic diamond, stratified materials on carbon nano-tube using hydrothermal process, and the liquefaction and gasification of heavy oil, the SCWO of rice husk for production of sodium acetate, the separation and extraction of useful materials from bio-mass using superheated steam, and the formation of organic materials by the hydrothermal reduction of carbon dioxide( ex. [Liu et al., Energy Conversion and Management, 44, 1399-1410 (2003)]). Geofluid science research group is conducting water-rock interaction under sub- and supercritical condition [Tsuchiya et al., Geothermal Resources Council Trans., 27, 111-114 (2003)], including multi-phase and multi-component solutions. We organized 1<sup>st</sup> international workshop on WATER DYNAMICS (17-19th March 2004, Sendai), which focused on the role of water in Earth processes, Life science and Material design. The workshop was unique objectives covering very wide range of water and steam properties and utilization.

We are planning 2<sup>nd</sup> workshop of WATER DYNAMICS in 11-12th November 2004 in Sendai International Center.

[contact: Prof. N. Tsuchiya; tsuchiya@mail.kankyo.tohoku.ac.jp

At the Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Prof. T. ADSCHIRI and his group are developing a new process of supercritical hydrothermal synthesis of nano particles. Specific features of this method have been found: (i) nano particle formation, (ii) single crystal formation, (iii) ability to control particle morphology to some extent with pressure and temperature, and (iv) ability to provide homogeneous reducing or oxidizing atmospheres by introducing gases or additional components (O2, H2). The method can be used for various applications, including magnetic material (BaO6Fe2O3), phosphor (Tb:YAG), metallic Ni nanoparticles, Li ion battery material (LiCoO2, LiMn2O4). For the rational design of this process, they developed a simulation method of supercritical hydrothermal synthesis, based on the fluid dynamics at supercritical conditions, kinetics, solubility estimation, nucleation, particle growth, and particle coagulation. Recently, they demonstrated that by using the supercritical hydrothermal synthesis, organic-inorganic hybrid nanoparticles could be synthesized due to homogeneous phase formation under the conditions. Hydrophilic or hydrophobic nature of the nanoparticles can be controlled by the organic modification on the surface of the particles, which paves a way to various applications of nanoparticles. [contact: Prof. T. Adschiri; e-mail: ajiri@tagen.tohoku.ac.jp]

At the Material Properties and Metrological Statistics Division, National Metrology Institute of Japan (NMIJ, formerly NRLM), National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, a section lead by Dr. K. FUJII is working on the density and viscosity standards. Absolute density measurements of silicon crystals with a relative standard uncertainty of better than  $1 \times 107$  and a determination of the Avogadro constant by the X-ray crystal density (XRCD) method are conducted for replacing the present definition of the kilogram [K. Fujii, A. Waseda, N. Kuramoto, S. Mizushima, M. Tanaka, S. Valkiers, P. Taylor, R. Kessel, and P. De Bièvre, "Evaluation of the molar volume of silicon crystals for a determination of the Avogadro constant," IEEE Trans. Instrum. Meas., 2003, 52, 646-651], resulting in the Avogadro constant of 6.022  $1375(12) \times 10^{23}$  mol<sup>1</sup>. The data from the NMIJ were used for finding the best set of the fundamental physical constants most recently recommended by the CODATA Task Group on Fundamental Constants. Using the silicon density standard, densities of standard liquids are calibrated by a magnetic suspension density meter developed at the NMIJ [N. Kuramoto, K. Fujii, and A. Waseda, "Accurate density measurements of reference liquids by a magnetic suspension balance," Metrologia, 2004, 41, S84-S94]. A relative standard uncertainty of  $4 \times 10^6$  has been achieved in the density measurement of organic liquids used for calibrating the vibrating-tube densimeters. In his group a new absolute viscosity measurement by the falling ball method is in progress. Nano-technologies for measuring the falling distance and diameters of small silicon spheres are developed for providing reference data of transport properties of liquid water

with a relative standard uncertainty of 0.01 %. Dr. K. FUJII is working as a chairman of the WG-Density, CCM (Consultative Committee for Mass and Related Quantities) to organize the research activities on the density standards at the National Metrology Institutes. A new density-of-water table that has a specified isotopic abundance was recommended by the WG-Density and approved by the CCM [M. Tanaka, G. Gerard, R. Davis, A. Peuto, and N. Bignel, "Recommended table for the density of water between 0 °C and 40 °C based on recent experimental reports," Metrologia, 2001, 38, 301-309]. This new table is recommended as a metrological standard for the density of SMOW [contact: Dr. K. Fujii, Chief, Fluid Properties Section, NMIJ; E-mail: fujii.kenichi@aist.go.jp].

At the Division of Environmental Materials & Energy, Department of Environmental Science & Technology, Faculty of Engineering, Shinshu University, Nagano City, Prof. Hiroshi Takaku works since Feb.1, 2000. Previously, he worked approximately for 31 years at Central Research Institute of Electric Power Industry in Japan (CRIEPI) where he engaged in the study of the field of the corrosion, material properties and water chemistry both in nuclear and fossil power plants. In the simulated geothermal waters containing the mixed corrosive chemicals such as chloride, sulfide, carbon dioxide, hydrogen sulfide and others, he and his coworkers are studying the corrosion of the steam turbine materials for the geothermal power plants, and Ti-Ni base shape memory alloys for the heat engine actuator. They are also studying the corrosion of boiler materials and other equipments materials. [Latest publications: (1) N. kawai, H. Takaku, et al, Zairyo-to-Kankyo (J. of Corrosion Engineering in Japan), 49 (2000) 612-618, (2) T. Sakuma, H. Takaku, et al. Transactions of Materials Research Society of Japan, 26 (2001), 167-170, (3) H. Takaku, et al, Materials Transactions, 43 (2002), 840-845, (4) H. Sakai, H. Takaku, et al, Proc. International Conference on Power Engineering (ICOPE-03, ASME-JSME-CSPE), Vol.3 (2003), 297-302, (5) Y. Horiuchi, H. Takaku, et al, Transactions of Materials Research Society of Japan, 29 (2003)] [contact: Prof. H. Takaku; E-mail: takakuh@gipwc.shinshu-u.ac.jp]

Mr. K. MIYAGAWA is developing Tubular Taylor Series Expansion Method (TTSE) for rapid calculation of thermophysical properties of water substance and other fluid. In the IAPWS meeting in Vejle, Denmark in 2003, the IAPWS guideline "Guideline on the Tabular Taylor Series Expansion (TTSE) Method for Calculation of Thermodynamic Properties of Water and Steam Applied to IAPWS-95 as an Example" was adopted. Mr. Miyagawa is developing a new version of TTSE programs that calculates transport properties with high speed and high accuracies. It will be useful to analyze transient phenomena in heat transfer and fluid mechanics. He will present it at the 14th ICPWS in Kyoto, Japan in August 2004. [contact: Mr. K. Miyagawa; E-mail: miyagawa.kiyoshi@nifty.com]

At the Department of Mechanical Sciences and Engineering, Tokyo Institute of Technology, Tokyo, Prof. A. SAITO, Assoc. Prof. S. OKAWA, and their group are

studying the effect of the shape of fallen particles on heterogeneous nucleation of water using Molecular Dynamics Simulaiton, and finding that the small projection on the surface influences the freezing. [Trans. JSRAE, 20, 2, 135-142, (2003) in Japaneses] They are also studying the effect of the difference in lattice constant of particle on freezing [Trans. JARAE, 20, 2, 155-162, (2003) in Japanese], and the effect of various kinds of external forces on freezing of supercooled water [6th ASME-JSME Thermal Engineering Joint Conference, (in CD-ROM), (2003)] [contact: Dr. S. Okawa; E-mail: sokawa@ mech.titech.ac.jp].

At Materials Science Research Laboratory, Central Research Institute of Electric Power Industry (CRIEPI), Yokosuka, Kanagawa, Dr. M. Domae and his coworkers constructed a Raman spectroscopic system for solid sample in high temperature water up to 400 °C, as a part of a national research project, "Fundamental R&D on Water Chemistry of Supercritical Pressure Water under Radiation Environment". They measured Raman spectra of several metal oxides in high temperature water, finding that alumina is stable in air-saturated water of 250 °C. [contact: Dr. M. Domae; E-mail: domae@criepi.denken.or.jp]

At the Center for Mechanical Engineering and Applied Mechanics, Keio University, Yokohama, Prof. M. UEMATSU and his group have constructed PVT apparatus for aqueous ammonia mixtures in the range of temperatures to 800 K and pressures to 20 MPa. Isobaric specific heat capacities for water + methanol mixtures are being measured by new calorimeter for temperatures from 250 K to 400 K at pressures to 20 MPa. [contact: Prof. M Uematsu; E-mail: uematsu@mech.keio.ac.jp].

At the Department of Mechanical Engineering, Keio University, Yokohama, Dr. K. YASUOKA and his group are studying the molecular dynamics (MD) simulation to clarify the mechanism for the dissociation and formation of clathrate hydrate. They adopt the MD simulation for the adosorption and desorption of ethanol molecules to liquid-vapor water surface. They have got the results, nucleation rate etc., for the bubble nucleation process. They started to evaluate the water model contained in HIV-1 Protease. These four topics are presented in 14th ICPWS. [contact: Dr. K. Yasuoka; E-mail: yasuoka@mech.keio.ac.jp].

At the Department of Mechanical Engineering, Kanagawa Institute of Technology, Atsugi, Prof. K. OGUCHI and his group are measuring the *PVTx* properties of ammonia + water mixtures. They have measured the *PVTx* properties of aqueous dilute solutions of ammonia in the range of temperatures from 265 K to 305 K, pressures up to 16 MPa, densities from 975 kg·m<sup>-3</sup> to 989 kg·m<sup>-3</sup>, and compositions up to 0.10 mole fraction of ammonia including pure water, focusing their attentions on the maximum density phenomena, and also in the range of temperatures from 298 K to 309 K, pressures up to 15.6 MPa, densities from 810 kg·m<sup>-3</sup> to 823 kg·m<sup>-3</sup>, and compositions up to 0.5133

mole fraction and 0.5357 mole fraction of ammonia. Some of their results were presented at the 14<sup>th</sup> ICPWS. [contact: Prof. K. Oguchi; E-mail: oguchi@me.kanagawa-it.ac.jp].

At the Department of Computational Molecular Science, Institute for Molecular Science, Prof. S. Okazaki and his group analyzed dissipation mechanism of excess vibrational energy of the solute molecules in ambient and supercritical water based upon mixed quantum-classical molecular dynamics calculation. Dynamics of coherence between vibrational states has also been investigated starting from a certain coherent initial state based upon path integral influence functional theory. [M. Sato and S. Okazaki, J. Mol. Liq. in press, M. Sato and S. Okazaki, Mol. Simul. in press, and T. Mikami and S. Okazaki, J. Chem. Phys. in press]. [contact: Prof. S. Okazaki; E-mail: okazaki@ims.ac.jp].

At the Department of Applied Chemistry, Ritsumeikan University, Shiga, Prof. S. SAWAMURA studies the hydrophobic hydration under high pressure up to 400 MPa in the stand point of the partial molar volume and the visicosity of H2O and D2O in the high-pressure and low-temperature region [see: H. Matsuo, Fluid Phase Equilibria **20** (2002), 227-238. Sawamura, S., Rev. High Press. Sci. Tech. 13, (2003) 157-164]. At the same department, Prof. Y. TANIGUCHI and Prof. M. KATO are measuring the infrared, Raman, and NMR spectra for biological compounds at high pressures [see: W. Dzwolak, et al, Biochim. Biophys. Acta **1595** (2002), 131-144; K. Fumino, et al. J. Mol. Liq. **100** (2002), 119-128; R. Kitahara, et al., Protein Science, 12. 207-217 (2003); Y. Shiratori, et al., Bull. Chem. Soc. Jpn, **76** (2003), 501-507.] [contact: Prof. Sawamura, S.; sawamura@se.ritsumei.ac.jp].

At the Institute for Chemical Research, Kyoto University, Uji, Kyoto, Prof. M. NAKAHARA, Prof. N. MATUBAYASI, Dr. C. WAKAI, and their coworkers study the structure, dynamics, and reactions in super- and subcritical water by means of multinuclear NMR (nuclear magnetic resonance) spectroscopy, computer simulation, and Raman spectroscopy. Their current focus are (1) the thermodynamics, structure, and dynamics of aqueous solutions over a wide range of thermodynamic conditions ["NMR Study on the Reorientational Relaxation in Supercritical Alcohol", T. Yamaguchi, N. MATUBAYASI, and M. NAKAHARA, J. Phys. Chem. A 108, 1319-1324 (2004)] and (2) the molecular mechanism of noncatalytic reactions in hydrothermal conditions. ["Hot Water Induces an Acid-Catalyzed Reaction in Its Undissociated Form", Y. Nagai, N. Matubayasi, and M. Nakahara, Bull. Chem. Soc. Japan 77, 691-697 (2004)]. [contact: Prof. M. Nakahara; E-mail: nakahara@scl.kyoto-u.ac.jp]

At the Department of Molecular Science and Technology, Doshisha University, Kyotanabe, Kyoto, Prof. M. UENO, Prof. IBUKI and their group have studied the electric conductivities of NaCl, KCl, and CsCl in liquid methanol along the liquid-vapor

coexistence curve up to the critical temperature to examine the validity of the Hubbard-Onsager dielectric friction theory, and compared the results with those in water [T. Hoshina, N.Tsuchihashi, K. Ibuki, and M. Ueno, J. Chem. Phys., **120**, 4355-4365 (2004)]. They have also measured the NMR spin-lattice relaxation times of <sup>2</sup>H and <sup>1</sup>N nuclei in acetonitrile-water mixtures at 30°C under high pressure up to 300 MPa together with density and viscosity measurements to investigate the rotational motion of water and acetonitrile molecules in the mixtures [in press, M. Ueno, S. Ueyama, S. Hashimoto, N. Tsuchihashi, and K. Ibuki, J. Solution Chem., **33**, 823-842 (2004)]. Computer simulations have been carried out to test a new theory of the dynamics of diffusion-controlled reactions based on the Fokker-Planck-Kramers equation [K. Ibuki and M. Ueno, J. Chem. Phys., **119**, 7054-7064 (2003)]. [contact: Prof. M. Ueno; E-mail: mueno@mail.doshisha.ac.jp]

At the Department of Mechanical Enginnering Science, Kyushu University, Fukuoka, Prof. Emeritus T. Ito and Prof. Y. Takata have released the 12.1 version of the Computer Program Package for Thermophysical Properties, PROPATH. Its new version is now under development. This software consists of 5 subsets. The water substances with different formulations are available. By using E-PROPATH, one of the 5 subsets, one can calculate properties as functions of MS-EXCEL software. [contact: Prof. Y. Takata; E-mail: takata@mech.kyushu-u.ac.jp or http://gibbs.mech.kyushu-u.ac.jp/propath/index.html]

At Toshiba Corporation, Keihin Product Operations, Dr. T. Tanuma and his coworkers are studying the application of the nonequilibrium wet steam CFD analysis for steam turbine blade design as a collaborative program with Professor S. Yamamoto, Department of Mechanical Engineering, Tohoku University, Japan and Professor X. Yuan, Department of Thermal Engineering, Tsinghua University, China. The research results indicate that the CFD method for compressible viscous wet steam flows in steam turbines is useful for optimization of blade designs (profile geometry, surface pressure distributions, blade exit angles, blade throat, etc.) in nonequilibrium wet steam conditions including rotor blade flow paths which are affected with passing stator blade wakes in real turbine stages. In a recent paper, the application results of nonequilibrium wet steam flow through steam turbine stages have been reported [The Proceedings of the 13th Pacific Basin Nuclear Conference October 21-25, 2002,

Shenzhen, China], [contact: Dr. T. Tanuma, tadashi.tanuma@toshiba.co.jp].

# International Association for the Properties of Water and Steam Russian National Committee

#### Report of Russian National Committee (2003 – 2004) List of Publications

- 1. Bogachev A.F., Ul'yanov V.V., Yurkov V.A., Prutskova A.V. Diagnostics of the Period Between Washings in the Operation of High-Pressure Drum Boilers on the Basis of Temperature Inserts and Indicators of the Quality of Water Chemistry Conditions. Thermal engineering. 2004, Vol. 51, № 7, p. 511.
- 2. Grishin A.A., Larin B.M., Malakhov I.A., Fedoseev B.S. An Investigation of the Sorbtion–Desorbtion of Organic Impurities of Natural Waters on Anionite Filters. Thermal engineering. 2004, Vol. 51, № 7, p. 517.
- 3. Man'kina N.N., Karkarin A.P., Kirilina A.V., Zagretdinov I.Sh., Kir'yanov I.I., LyspakA.I. The Results of the Introduction of Oxygenated Steam–Water Cleaning, Passivation, and Preservation of the Flow Path of the Type PK-38 Boiler st. no. 6 of the Krasnoyarsk GRES-2 District Power Station. Thermal engineering. 2004, Vol. 51, № 7, p. 522.
- Petrova T.I., Vidoikovich S., Zonov A.A., Petrov A.Yu. Effect of Acetic Acid on the Contamination of Saturated Steam by Sulfates and Fluorides. Thermal engineering. 2004, Vol. 51, № 7, p. 526.
- 5. Malakhov I.A., Askerniya A.A., Borovkova I.I., Malakhov G.I. Technological Aspects of Choosing Optimal Feedwater-Demineralization Schemes for Steam Generators of Thermal Power Stations and Industrial Enterprises. Thermal engineering. 2004, Vol. 51, № 7, p. 530.
- 6. Dubrovskii I.Ya., Eskin N.B., Tugov A.N., Anikeev A.V. Experimental Investigations of the Behavior of Octadecyl Amine in Superheated Steam and on Metals Coming into Contact with It. Thermal engineering. 2004, Vol. 51, № 7, p. 544
- Petrova T.I., Ryzhenkov V.A., Kurshakov A.V., Zroichikov N.A., Chernov V.F., Galas I.V. Using Film-Forming Amine for Conservation of Process Equipmentat the Mosenergo Cogeneration Station TETs-23. Thermal engineering. 2003, Vol. 50, № 9, p. 760.
- 8. Petrova T.I., Furunzhiyeva A.V. Use of chelamine at fossil power plants with drum boilers. Energosberezheniye i vodopodgotovka, 2004, №1, pp. 3 8.
- 9. Zaripov Z.I., Burtsev S.A., Bulaev S.A., Mukhamedzyanov G.Kh. Heat capacity and temperature conductivity of aqueous solutions of alkali metals in wide range of pressures. J.Phys. Chem. (Rus), 2004. Vol. 78. No. 5. P. 814 -818.

- 10. Grigoriev E.B. Thermal conductivity of triple aqueous solutions of lantanium salts Teploenergetika. 2003. No. 6. P. 64 66.
- Bazaev A.R, Bazaev E.A. P,ρ,T,x -relation of gas mixtures water -hydrocarbon in wide range of parameters of state. Thermophys.of High Temperatures. 2004. Vol. 42. No. 1. P. 48 -57.
- Podmurnaya O.A., Gudkov O.I., Dubovikov A.A. Equilibrium concentration of mixtures of nitrogen with water at the pressures up to 10 MPa. J. Phys. Chem. (Rus). 2004. Vol. 78. No. 2. P. 373 -375.
- 13. Alexandrov A.A. The equations for thermophysical properties of aqueous solution of sodium hydroxide. Submitted to 14 ICPWS.

# U.S. National Committee to IAPWS 2004 Report on Activities of Potential Interest to IAPWS

#### Communicated from Arizona State University, Tempe, AZ:

- Correlations and estimations for the second cross virial coefficients for interactions involving water. (Plyasunov A. V., Shock E. L. (2003) Second cross virial coefficients for interactions involving water. Critical data compilation; J. Chem. Eng. Data, 48, 808-821; Plyasunov A. V., Shock E. L., Wood R. H. (2003) Second cross virial coefficients for interactions involving water. Correlations and group contributions values. J. Chem. Eng. Data, 48, 1463-1470.)
- Correlations and estimations for the Krichevskii parameter for volatile nonelectrolytes in water. (Plyasunov A.V., Shock E.L. (2004) *Prediction of the Krichevskii parameter for volatile nonelectrolytes in water* Fluid Phase Equil., in press.)
- Correlations and estimations for the vapor-liquid distribution constants for volatile nonelectrolytes in water. (Plyasunov A.V., Shock E.L. (2003) *Prediction of the vapor-liquid distribution constants for volatile nonelectrolytes in water up to its critical temperature* Geochim. Cosmochim. Acta, 67, 4981-5009.)
- Additional work on high pressure equation of state for water. (Mark R. Frank, Yingwei Fei, Jingzhu Hu. (2004) Constraining the equation of state of fluid H2O to 80 GPa using the melting curve, bulk modulus, and thermal expansivity of Ice VII Geochim. Cosmochim. Acta, 68, 2781-2790; Evan H. Abramson, J. Michael Brown (2004) Equation of state of water based on speeds of sound measured in the diamond-anvil cell Geochim. Cosmochim. Acta, 68, 1827-1835)

#### **Communicated from the University of Maryland, College Park, MD:**

- A new study of criticality in aqueous solutions was completed. It was concluded that the asymptotic critical behavior of aqueous electrolyte solutions is the same as in non-electrolyte solutions, but that the non-asymptotic crossover critical behavior is non-monotonic. An anomalous critical behavior in aqueous solutions of 3-methylpyridine and sodium bromide previously observed that was attributed to the formation of a micro-heterogeneous phase turned out to be caused by long-living non-equilibrium states. Further experimental studies showed the ubiquitous presence of mesoscopic non-equilibrium aggregates in electrolyte aqueous solutions. The physical and chemical variables that govern the appearance of long-living non-equilibrium structures are not yet understood. (A.F. Kostko, M.A. Anisimov, and J.V. Sengers, *On the nature of criticality in aqueous solutions of 3-methylpyridine and sodium bromide*, Phys. Rev. E, in press.)
- J.V. Sengers continued his collaboration with the Physical and Chemical Properties at the National Institute of Standards and Technology, Boulder, CO towards the development of a new formulation for the viscosity of water and steam.

#### Communicated from Jonas, Inc., Wilmington, DE:

- Low Temperature Corrosion Problems in Fossil Power Plants State of Knowledge: (Jonas, Inc. EPRI project with contributions by others) The objective of the project was to provide a basic understanding of common, low temperature (up to 150°C) corrosion problems in fossil fueled power plants, to present solutions currently applied to those problems, case histories, and available pertinent references. "Missing Knowledge" for each component. Emphasis was placed on those areas identified as severe problems by the participants of an informal survey. (*Low Temperature Corrosion Problems in Fossil Power Plants State of Knowledge*. EPRI, Palo Alto, CA: December 2003. 1004924).
- ChemExpert: Further development (network) and applications of the EPRI water chemistry control expert system. (O. Jonas, L. Machemer, and B. Dooley. "EPRI ChemExpert: Cycle Chemistry Advisor for Fossil Power Plants." *EPRI 6th International Conference on Cycle Chemistry in Fossil Plants*. June 27-29, 2000, Columbus, Ohio.)

- Experimental Investigation of Local Environments in a PWR LP Turbine; ETA + Boric Acid Water Treatment: Includes new instrument to collect early condensate, Converging-Diverging Nozzle, Deposit Collector/Simulator, and a Drying Probe. Joint EPRI - utility - Jonas, Inc. project. (Report pending)
- Stress Corrosion Cracking in PWR and BWR Component Cooling Water Systems: The purpose of this project was to identify the root cause(s) of the stress corrosion cracking which is occurring near carbon steel welds in the component cooling water systems of several nuclear pressurized water reactor (PWR) units and one boiling water reactor (BWR) unit. (Report Pending)
- Condition Monitoring for Damage Assessment: Two German PWRs, each instrumented at over 1000 points. Data used to evaluate fatigue, FAC, SCC, and other damage.
- Water Cooling of High Voltage Electrical Cables: Effort to replace oil cooling with water cooling; selection of water chemistry and corrosion testing.

#### Communicated from The Pennsylvania State University, University Park, PA:

- High Temperature Thermodynamics of Aqueous Solutions (Bandura A. V., and Lvov S.N. *The Ionization Constant of Water over Wide Ranges of Temperature and Density, J. Phys. Chem. Ref. Data*, 2004, in press)
- High Temperature Aqueous Electrochemistry (Lvov S.N. and Palmer D.A. *Electrochemical Studies of High-Temperature Aqueous Systems*, Chapter 12, in "The Physical and Chemical Properties of Aqueous Systems at Elevated Temperatures and Pressures: Water, Steam and Hydrothermal Solutions," D.A. Palmer, R. Fernandez-Prini and A.H. Harvey, Eds., 2004, Wiley; Lvov S.N. *Electrochemistry of High Temperature Subcritical and Supercritical Aqueous Systems*, Volume 5, D.D. Macdonald, Vol. Ed., in "Encyclopedia of Electrochemistry," M. Stratmann and A. Bard, Eds., 2004, Wiley-VCH, in press).
- Elevated Temperature Proton Exchange Membrane Fuel Cells (Zhou X.Y., Weston J., Chakova E., Lvov S. N., Hofmann M., Ambler C. M., and Allcock H. R. *High Temperature Transport Properties of Polyphosphazene Membranes for Direct Methanol Fuel Cells, Electrochimica Acta,* 48, 2003, 2173-2180)
- High Temperature Solid Oxide Fuel Cells (Zhou Z.F., Gallo C., Pague M.B., Schobert H., and Lvov S.N., *Direct Oxidation of Jet Fuels and Pennsylvania Crude Oil in a Solid Oxide Fuel Cell, Journal of Power Sources*, 133, 2004, 181-187)
- High Temperature Potentiometery and pH measurements (Seneviratne D.S., Papangelakis V. G., Zhou X.Y., and Lvov S.N. Potentiometric pH Measurements in Acidic Sulfate Solutions at 250°C Relevant to Pressure Leaching, *Hydrometallurgy*, 68, 2003, 131-139; Lvov S. N., Zhou X. Y., Ulmer G. C., Barnes H. L., Macdonald D. D., Ulyanov S.M., Benning L. G, Grandstaff D. E., Manna M., and Vicenzi E. *Progress on the Yttria-Stabilized Zirconia Sensors for Hydrothermal pH Measurements*, Chemical Geology, 198, 2003, 141-162:Zhou X.Y., Lvov S.N., and Ulyanov S.M. "Yttria-Stabilized Zirconia Membrane Electrode", United States Patent # 6,517,694, February 11, 2003.)
- High Temperature Electrokinetic Studies of Solid Oxide/Water Interface: (Zhou X.Y., Wei X.J., M.V. Fedkin, Strass K.H., and Lvov S.N. A Zetameter for Microelectrophoresis Studies of the Oxide/Water Interface at Temperatures up to 200 °C. Rev. Sci. Instrum., 74, 2003, 2501-2506; Fedkin M.V., Zhou X.Y., Kubicki J.D., Bandura A.V., Lvov S.N., Machesky M.L., and Wesolowski D.J. High Temperature Microelectrophoresis Studies of the Rutile/Aqueous Solution Interface, Langmuir, 19, 2003, 3797-3804; Zhang Z., Fenter P., Cheng L., Sturchio N. C., Bedzyk M. J., Predota M., Bandura A., Kubicki J. D., Lvov S.N., Cummings P.T., Chialvo A.A., Ridley M.K., Benezeth, P., Anovitz L, Palmer D.A., Machesky M.L., and Wesolowski D.J. Ion Adsorption at the Rutile-Water Interface: Linking Molecular and Macroscopic Properties, Langmuir, 20, 2004, 4954-4969).

#### Communicated from the National Institute of Standards and Technology, Boulder, CO:

- Magomed Aliev from the Dagestan Scientific Center (Russian Academy of Sciences) will visit NIST (Boulder) in October, 2004 to work with Drs. Joseph Magee and Ilmutdin Abdulagatov on the project *An Experimental Study of PVTx Properties for the System Ammonia* + *Water at High Temperatures and Pressures* under IAPWS support.
- Collaborations between the Dagestan Scientific Center and NIST continue with a manuscript on experimental *PVTx* studies of light water + heavy water and a series of manuscripts on *PVTx* and *Cv* for the methanol + water system.
- Collaborations with the Japan National Defense Academy and Keio University continue with manuscripts on heat capacity measurements on alkanol (methanol, ethanol and 1-propanol) + water systems.
- Manuscripts have been completed on experimental enthalpies of dilution of salts in water, including the first such reported measurement for a room-temperature molten salt (C. S. Oakes, J. A. Rard and D. G. Archer, *Enthalpies of Dilution of NdCl<sub>3</sub>(aq) at Temperatures from 297.89 K to 372.09 K and an Extended Pitzer Ion-interaction Model for the NdCl<sub>3</sub> + H<sub>2</sub>O System, J. Chem. Eng. Data 49, 313-325, 2004; D. G. Archer, <i>Enth alpy of Solution of Potassium Tetrafluoroborate in Water and Aqueous Sodium Fluoride. Thermodynamic Properties of the Aqueous Tetrafluoroborate Anion and Potassium Tetrafluoroborate*, in review).
- Collaboration continues with theoretical chemists in England on development of intermolecular pair potentials for aqueous systems and calculation of second virial coefficients that have smaller uncertainties than those obtained by experiment. We expect this work to find application for humidity standards and for calculating thermodynamic properties of combustion gases. (Water/hydrogen M.P. Hodges et al., J. Chem. Phys. **120**, 710, 2004; water/nitrogen system is nearly complete)
- Work is continuing on the joint IAPWS and IUPAC efforts to update the formulations for the transport properties of water and steam; preliminary correlating surface for viscosity has been completed.
- In collaboration with experimentalists at NIST/Gaithersburg, we have characterized the refractive index of liquid water in the far ultraviolet (193 nm) for a technology called immersion lithography, which is being developed for manufacturing computer chips. The project combined experimental work with modeling efforts to describe the variation of the index with temperature, pressure, and dissolved air.

List of Participants			
Name	Affiliation	Country	
Prof. Tadafumi Adschiri	Tohoku University	Japan	
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Mr. Yoshimichi Andoh	Keio University	Japan	
Prof. Mikhail A. Anisimov	University of Maryland, College Park	United States	
Ms. Elena V. Jouravleva		United States	Α
Mr. Takeshi Aramaki	Keio University	Japan	
Mr. Haruhiko Asano	Chubu Electric Power Co., Inc	Japan	
Mr. Denis J. Aspden	ESKOM	South Africa	
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Ms. Theodora I. Kyriafini		Greece	Α
Mr. Kazunori Bada	Tohoku University	Japan	
Dr. James C. Bellows	Siemens Westinghouse Power	United States	
	Corporation		
Mr. Toshifumi Bito	Kawasaki Heavy Industries Ltd.	Japan	
Dr. Li Bo	AIST	Japan	
Dr. Nanno Bolt	KEMA	Netherlands	
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		Kingdom	
Prof. Alina Ciach	Institute of Physical Chemistry, Polish Academy od Sciences	Poland	
Mr. Patrick J. Colman	Electricity Supply Board	Ireland	
Ms. Judith M. Colman		Ireland	Α
Ms. Lesley P. Colman		Ireland	А
		United	
Dr. Jeff R. Cooper	Queen Mary University of London	Kingdom	
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