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

Dr. Barry Dooley EPRI 3412 Hillview Ave, Palo Alto, California, 94304, USA. Phone: 650-855-2458 Fax: 650-855-1026 e-mail: bdooley@epri.com

Minutes of the Meetings

of the

Executive Committee

of the

International Association for the Properties of

Water and Steam

Vejle, Denmark August 24 – 30, 2003

Prepared by: Barry Dooley



CONTENTS

		<u>Page</u>
IAP	WS Minutes	1
<u>ATT</u>	ACHMENTS	
1	Agenda for EC	17
2	Committee Report on the Structure of IAPWS	18
3	IAPWS Symposium Program	21
4	IAPWS Schedule for the week	22
5	TPWS Minutes	23
6	IRS Minutes and Attachments	27
7	PCAS Minutes	32
8	PCC Minutes and Attachment	36
9	IAPWS Releases, Guidelines, Advisory Notes and ICRNs	45
10	IAPWS Collaborative Grant Proposal	49
11	Press Release	54
12	Britain and Ireland Report of Current Research and Attachment	55
13	Czech Report of Current Research	57
14	Denmark Report of Current Research	62
15	Germany Report of Current Research	63
16	Hellenic Report of Current Research	65
17	Japan Report of Current Research	68
18	Russia Report of Current Research	73
19	USA Report of Current Research	76
20	List of Participants at the 2002 EC and WG Meetings in Buenos Aires	79

Minutes of the Meetings of the Executive Committee of the International Association for the Properties of Water and Steam held in Vejle, Denmark August 24 – 30, 2003

Plenary Session. Monday, 25 August 2003

The new President of IAPWS, Professor Koichi Watanabe, welcomed the EC and other IAPWS members to Vejle for the EC and WG Meetings of IAPWS. He then introduced the Chairman of the Danish National Committee, Karol Daucik, who welcomed IAPWS to Denmark. Mr. Daucik indicated that all the EC and WG meetings would take place in Hotel Australia.

The President then officially opened the 2003 EC Meetings by introducing the National Delegates. Each of the member countries of IAPWS was in attendance with the exception of Argentina/Brazil, Canada, and Italy. He particularly mentioned and welcomed the new IAPWS Vice President, Professor Marsik from the Czech Republic. There were 42 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 February 2003. The President and Executive Secretary indicated three additions/changes to this agenda, and then requested any other additions and changes to the agenda. There were no further suggestions for additional items. The agenda was then approved by the Heads of all National Delegations and forms Attachment 1 of these minutes.

2. IAPWS Business and Appointment of Committees

2.1 Press Release.

The President asked Bellows, Daucik and Bignold to serve on this Committee. The Press Release is discussed in Minute 17.4 and Attachment 11.

2.2 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. He requested that Zeijseink be the Chairman of the Committee if any proposals were received. The discussion of this Committee is reported in Minute 15.1 and Attachment 10.

2.3 Helmholtz Award Committee

The President indicated that the 2003 Award would be presented at the IAPWS Symposium. He then reminded the EC that the Helmholtz Committee for the 2004 award would consist of the Delegates from Russia, USA, Argentina/Brazil, BIAPWS, and Canada. The President asked the Russian Delegate (Petrova) 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.

2.4 Gibbs Award

The President indicated that only one Nomination had been received by the Executive Secretary prior to the meeting. Any other nominations were due by the end of the day. The President then reminded the EC that the Evaluation Committee had been determined at the 2002 EC Meeting, but a number of these people were missing from this year's EC Meeting. He then modified the committee to consist of Harvey (TPWS), Miyagawa (IRS), Palmer (PCAS), and Daucik (PCC), with Cooper as Chairman. The President asked the Committee to meet during the week and report back to the EC on Friday. See Minute 16.3.

2.5 IAPWS Atlas

The President requested an update from one of the Editors of the Atlas (Palmer). Palmer indicated that the Atlas was almost finished. The deadline for submission to the Publisher is the end of September. The total number of chapters will be 18, however 2 are not yet ready. An estimate of the cost to prepare the chapters for publication is currently about \$5,000 compared to the original estimate of about \$40,000.

2.6 IAPWS on the Internet (IAPWS Website <u>www.IAPWS.org</u>)

The President indicated that this informational item would be delayed until Friday as Harvey was delayed in arriving in Denmark. (See Minute 17.2).

2.7 Publishing Addresses and E-mail Addresses on IAPWS Website

The President indicated that this item had been raised during the last year by BIAPWS, and asked the BIAWPS Delegate (Bignold) to make a few comments. Bignold indicated that BIAWPS was very satisfied with the action taken by the past President and the Executive Secretary in removing all e-mail addresses associated with Participation Lists for annual meetings on the IAPWS Website.

2.8 IAPWS Structure

The President asked the Chairperson (Levelt Sengers) of the IAPWS Structure Committee to review the status of the Survey that has been conducted over the last year. The Committee consisted of IAPWS past Presidents (Levelt Sengers as Chair, Watanabe, Fernandez-Prini and Cooper). A survey was sent to all NCs, responses were received and collated. Levelt Sengers provided a brief overview of the main conclusions and recommendations from the report. The President indicated that there wasn't sufficient time during the plenary session to discuss in detail, and suggested that a new committee be formed as a number of the original members were not present this week. Members of the new committee were Levelt Sengers (Chair), Marsik, Cooper and a PCC Representative (established later as Svoboda). This item is discussed further in Minutes 5.1 and 17.3.

2.9 IAPWS Products

The President asked Cooper as the only member of Editorial Committee present to address the aspect of the definition of Products in the IAPWS Statutes and By-Laws. Cooper suggested to delay this report until Friday's EC Meeting as Harvey was delayed in arriving in Denmark. This item is discussed in Minute 12.

2.10 Other Business Considered to Require Special/Extensive Discussions

The Executive Secretary informed the EC that he had received a letter from Tremaine concerning the situation of the Canadian NC in re-aligning industrial sponsorship. Tremaine wished to assure the EC that the Canadian NC was very active in trying to rebuild the NC. At this stage the French NC Delegate, Mayer, also informed the EC of a similar situation in France with regards to funding and support. He requested assistance from members of the PCC WG to provide names in France that should be interested in IAPWS activities, and could be contacted to assist in developing a one-day symposium on Cycle Chemistry.

- 3. EC Mandate to Working Groups and Membership
 - 3.1 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. Discussion and Approval of these are included later in the WG Minutes. The Executive Secretary also indicated that ICRNs 1, 5, 10, and 13 would need action by the respective WGs during the week

3.2 14th ICPWS

The President, as Chairman of the ICPWS Conference Organizing Committee, provided an overview of the organization of the Conference todate, which included outlines of the proposed Plenary lectures, invited lectures, finances, and logistics. He then requested the WGs to review the proposed program symposia and to help in fine-tuning. Abstracts will be required by December 15, 2003. A website has already been created (14icpws.iapws.jp/). The ICPWS is discussed further in Minutes 5.2 and 17.1.

3.3 WG Directions.

The President suggested that the presentation on IAPWS Structure in Minute 2.8 leads to a clear redirection of the WGs, particularly for PCC and PCAS. He thus requested the WGs to thoroughly review their operating regimes, their leadership and succession planning. He also requested that each WG takes a very close look at their membership list in terms of dormant members.

3.4 Reports to EC

The President again used the IAPWS Structure discussion (Minute 2.8) to remind the WG Chairmen that their reports to the EC on Friday should only include those items that needed action or approval by the EC.

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

President Watanabe requested each WG chairman to provide an overview of their respective planned meetings and activities throughout the week. The details of these WG meetings are covered in detail in Minutes 8, 9, 10, and 11. The

President concluded the morning by inviting the WGs to convene a joint session of WGs on Thursday between 1:30-3pm.

5. <u>Special Joint Meeting of all Working Groups</u>

President Watanabe called all members of the WGs together at about 1:40pm on Thursday, 28 August 2003. This meeting dealt with the following two items:

5.1 Structure of IAPWS

The President referred to the item of the same name of last Monday (Minute 2.8) and asked the Chairperson (Levelt Sengers) of the IAPWS Structure Committee to provide an update. Levelt Sengers reminded the assembly of the 37-page report and the set of recommendations contained within, and her new Committee (Cooper, Marsik, and Svoboda). She indicated that she would only cover the recommendations on Task Groups and Committees. She provided information, which is contained in Attachment 2. She then outlined the 4 Committees and 5 Task Groups, which had since Monday been populated by the IAPWS WGs with a chairperson and a number of suggested working members.

The President next asked each WG Chairman for some overall Responses on the Complete Restructuring Document. The TPWS Chairman responded: a) there was no need to change the TPWS or IRS WG names, b) there is now a shortened amount of time for WG activities at annual meetings and that there should be more time allowed in 2005, and c) TPWS /IRS had no objection to a four year cycle for ICPWS, but that there was no overwhelming desire to change from the current five year cycle. The PCAS Chairman responded: a) there was no need to change the WG name, b) there must be more PCAS-PCC interaction, and c) the WG recommends to change to a four year cycle for ICPWS, and that the papers should be published in Journals instead of an ICPWS Proceedings Book. The PCC Chairman responded: a) there is somewhat of a dilemma in that the WG needs to have technical content in meetings to attract people to the WG and the annual meetings, but that the PCC WG is regarded within IAPWS as the driver for ideas, b) there needs to be a compromise with a focus on certain items and also the development of reference documents for the other groups, and c) the output of PCC will not drastically change and for example at next years meeting there will be a focus on ultrasupercritical plants.

The President then requested that Chairperson Levelt Sengers make any necessary changes based on this feedback, and then report back to the EC again on Friday (Minute 17.3).

5.2 14^{th} ICPWS

The President next reviewed the proposed symposia with each of the WGs to try to finalize the organizer of each and the invited speaker.

Activities During the Week

The first day activities of the WGs and Executive Committee were followed by WG meetings from Monday–Thursday. The IAPWS Symposium "Aqueous Thermodynamics in Power Generation" was held on Wednesday, 27 August 2003. The Symposium program is given in Attachment 3.

The full IAPWS program for the week is shown in Attachment 4.

Executive Committee Meeting. Friday, 29 August 2003

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

6. Acceptance of Minutes of Previous Meeting

President Watanabe asked for comments and changes to the minutes of the EC meeting held in Buenos Aires, in July 2002. None were provided, thus the 2002 Minutes were accepted.

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

President Watanabe provided the following comments:

- On behalf of IAPWS he wanted to thank the Danish National Committee for organizing an excellent week and the Symposium.
- The important task of looking at the structure of IAPWS had blossomed out into a comprehensive report, which had been outlined on Monday (Minute 2.8).
- In conjunction with the restructuring task, he was very pleased to report that the new direction for PCC seemed improved and that this will lead to a nice collaboration with PCAS at future meetings. He looked forward to this being very productive.
- The 14th ICPWS would be held in Kyoto, Japan in 2004. The two program committee meetings had now produced a set of clear objectives and ideas for the final planning process. The second circular will be issued in mid-September. The deadline for Abstracts will be 15 December 2003.
- The President wants to enhance the presence of IAPWS outside the organization and proposed: a) a liaison with IEC or other organizations as

cosponsors, and b) agreement with other organizations for international collaboration (such as IUPAC).

• The President also wanted to develop a guideline/criteria on how to involve new people in IAWPS

Some discussion ensued with respect to the last two items, and the President developed the following action for the NCs:

Action for each National Committee: Each delegate should discuss these items with their National Committee and be prepared to make suggestions at next year's meeting.

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. Full minutes can be found in Attachment 5.

- 8.1 Most meetings were held jointly with WG IRS, but many items will be reported separately
- 8.2 Advisory Note #2 on "The Roles of Various IAPWS Documents Concerning the Thermodynamic Properties of Ordinary Water Substance". The document, as revised, was approved by the TPWS and IRS WGs. The WGs recommend that it is now ready for postal ballot. The WGs also recommend that a brief discussion of obsolete IAPWS documents should be included on the IAWPS web site.

The EC approved these two recommendations unanimously.

Action: Advisory Note #2 will be sent to the Executive secretary for Postal Ballot.

8.3 The Guideline on the "Henry's Constant and Vapor-Liquid Distribution Constants for Gases in H_2O and D_2O at High Temperatures". The document was approved by the WGs after a significant change. The WGs now recommend a postal ballot.

Action: The Guideline will be sent to the Executive secretary for Postal Ballot.

8.4 Transport properties. The international collaborative project was completed and the final report distributed. Work by the WG on the "Revised Release on the IAPS Formulation 1985 for the Viscosity of Ordinary Water Substance" noted some minor errors, which were

corrected. TheWG endorsed the Release and now recommends that the EC approves the document

The EC approved the Release unanimously

- 8.5 Status of simulation task group. The Chair of the joint TG was unable to attend the meeting. Professor Yasuoka was selected as an interim chairman until ICPWS in 2004.
- 8.6 Membership. The WG recommends that Yasuoka (Japan) and Mares (Czech Republic) and Span (Germany) should be added to WG membership. Several inactive members will be contacted.

The EC approved these WG membership changes unanimously.

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 6. The Chairman indicated that there were three recommendations to put to the EC.

9.1 "Supplementary Release on Backward Equations for the Functions T(p,h), v(p,h), and T(p,s), and v(p,s) for the Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam". The WGs TPWS and IRS recommend to the EC that the draft distributed to National Committees for preview be accepted by IAPWS as a supplementary release. The WGs TPWS and IRS further recommend that the proposed code be treated as part of the IAPWS-IF97 authorized code.

The EC approved the Release and the code proposal unanimously.

9.2 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". This guideline had been distributed to National Committees for Postal Ballot. No objections had been received by the Executive Secretary. The WG made a few changes to the front page (changing the authorized date, place, and related terms from those of 2002 to 2003 IAPWS annual meeting). The guideline referenced downloadable software is now available from the Japanese National Committee website.

The WGs IRS and TPWS now recommend to the EC that this guideline be approved.

The EC approved the Guideline unanimously.

9.3. Advisory Note No. 1 "Uncertainties in Enthalpy for IAPWS-95 and IAPWS-IF97". The WGs TPWS and IRS recommend that the draft distributed to National Committees previously for preview be accepted by IAPWS as an IAPWS product. It is also recommended that the Release "IAPWS Skeleton Tables 1985 for the Thermodynamic Properties of Ordinary Water Substance" be withdrawn from the IAPWS Listing of Releases and Guidelines, as approved by the EC at the 2002 annual meeting. It is also recommended that the EC allow creation of a document list on the IAPWS website, which would record for historical purposes, all outdated IAPWS releases, guidelines, and ICRNs.

The EC approved these three recommendations unanimously

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

Chairman Mayer provided the PCAS Report to the EC. Full minutes can be found in Attachment 7. Chairman Mayer mentioned that there were numerous Joint Sessions and Workshops with other WGs during the week.

10.1 The Chairman indicated that the WG had discussed the leadership of the WG and indicated that for the period starting after the next ICPWS, the Chair Designate would be Lvov, with Corti as the Vice Chair designate.

The EC approved these leadership changes unanimously.

- 10.2 International Collaborative Projects. The Chairman reported that the PCAS WG would like to simplify and standardize the final report format. After some discussion and suggestions by the EC, the President requested that the PCAS Chairman together with Palmer draft out a suggested format and forward it to the Editorial Committee in readiness for the EC Meetings in 2004.
- 10.3. The Chairmen indicated that he wished to report on three proposed IAPWS Products:
 - 10.3.1. Preparation of a document on pH Measurements at High Temperatures. This had been discussed at a joint PCAS/PCC Meeting and it had been agreed that members from both WGs would work to assemble the document.
 - 10.3.2 Preparation of a monograph on experimental techniques for high temperature measurements and collection of direct experimental data (T>200°C). The Chairman outlined the proposed members

of the team that would assemble the document and an initial table of contents with eight chapters. Valyashko was proposed as the leader of the project as he has already performed lots of work in this area. After the President called a coffee break to allow National Committees to confer, he indicated that there appeared to be concensus that the project was worthwhile. The President then developed the following action.

- Action: An editoral/advisory board consisting of Mayer, Assael and Valyashko should develop a Proposal of Procedure, which would include an outline of each chapter, the proposed author(s), the philosophy of the book and any necessary background. This Proposal should be forwarded to the Executive Secretary for a Postal Ballot.
- Establishing recommended data on hydration properties for 10.3.3. selected organic solutes. This proposal for the generation of an international data base under the auspices of IAPWS and IUPAC, has an objective of establishing recommended values for hydration properties of selected organic solutes on the basis of the best available experimental data. The Chairman suggested a number of WG Members who would work on the project, and indicated that the project would need funding from IAPWS (\$12,000) and IUPAC (\$12,000) for technical support. This lead to much discussion about spending IAPWS funds. Finally the President developed a proposal to establish a small committee of Mayer and Fernandez-Prini to develop a comprehensive statement to include the definition, philosophy, selected data, systems and a budget. The President mentioned that this statement should include consideration of who will update the data base. The statement should be sent within six months (end of February 2004) to the Executive Secretary for a Postal Ballot.

The EC approved this proposal unanimously.

10.4. WG Membership. The Chairman indicated that there were no new proposals for membership, but that the WG had reviewed the current membership and recommended that Haymet, Brunner, Longhi and Servida be removed.

The EC approved these membership changes with one abstention.

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 8.

11.1. The Chairman indicated that the WG had decided not to produce an amended Priority List, but had spent some time on developing a new procedure for developing ICRNs on high priority items. The Chairman also indicated that the WG would like to propose that each National Committee provide an indication of the priority items in their country. The Chairman next indicated that he will via email make clear to PCC members what is required to produce a proposal, and frequently remind members to actively pursue the objective of making a proposal for International Collaboration. The President asked for any comments and then developed the following action:

Action: Each National Committee should discuss the priorities within their country and bring a listing to the next EC Meeting in Japan. Each National Committee should also provide feedback on the proposed procedure for developing ICRNs on high priority items. This is included as PCC Attachment A to the PCC Minutes in Attachment 8.

11.2. The Chairman indicated that the PCC had no new proposals for membership, but indicated that he would contact members who had been inactive for three years or more to determine if they still wished to be a member.

At this stage in the EC, the President thanked the PCC Chairman for the outstanding work he had done during the week in bringing together ideas so that IAPWS overall could move forward. He indicated that the principle objectives of the IAPWS Annual Meetings include: a) to prepare and disseminate IAPWS Documents, such as Releases and Guidelines being the international standards, Advisory Notes and ICRNs for the better understanding of various properties on behaviour pertinent to water, steam and aqueous systems, b) to update the property standards disseminated worldwide in the past, and c) to discuss several business items on how IAPWS can enhance the international collaboration not only within IAPWS, but also by co-opting with other relevant organizations such as IUPAC.

The President then indicated that it is certainly true that the annual IAPWS meetings are a wonderful opportunity for all IAPWS members to exchange views on updated knowledge for science and technology within the framework of IAPWS activities. However, one of the important issues is that IAPWS is not a gathering merely for the purpose of having a forum, but for all WGs to collaborate together to pursue the common goals of IAPWS just mentioned. In other words, it is essential that all WGs must challenge, along the same road map, to aim the scientific and technical achievements throughout the discussion at each WG's annual meetings.

12. Editorial Committee Report

Chairman Harvey reported on the Editorial Committee activities since the last EC Meetings in 2002.

- 12.1 The Editorial Committee has reviewed five IAPWS documents during the last year: the Guideline on TTSE, the Supplementary Release on Backwards Equations, the Guideline on Henry's Constant, Advisory Note #1, and the Revised Release on Viscosity
- 12.2 The Editorial Committee was asked in Buenos Aires to "review the names of products within the IAPWS Statutes and By-Laws". The Chairman indicated that essentially any new product can be issued by the EC within the existing Statutes and By-Laws even though not explicitly defined.
- 12.3 As an extension to Minute 12.2, the Chairman then wished to inform the EC that: a) there was a number of areas where the Statutes and By-Laws were inconsistent with the current way in which some IAPWS business was conducted, and b) there was some redundancy within the Statutes and the By-Laws. Some discussion on this matter ensued. The President finally developed the proposal that a Task force should be assigned by the EC (Harvey, Miyagawa, Assael and Cooper) to look primarily at the areas of documents and awards within the Statutes and By-Laws. Any changes should be made and a Revised Version of the Statutes and By-Laws should be sent to the Executive Secretary for Postal Ballot so that it can be approved by the General Assembly in Japan.

The EC approved this proposal unanimously.

- 13. <u>Membership and Associates</u>
 - 13.1 Members Defaulting on Dues.

The Executive Secretary indicated that according to the latest Swiss bank account statement (31 July 2003), the following countries had not paid the 2003 IAPWS dues: Argentina/Brazil, France, Italy, and Russia. In 2002 France (partial), Germany, Italy and Russia had also not paid their dues. Since the July 2003 Bank statement, the Executive Secretary had received a note from the Russian NC indicating that the 2002 and 2003 Dues had been paid into the Swiss Bank. The Delegate from Argentina/Brazil was absent from the EC meeting. The Delegate from France had reported about the situation in France in the opening EC session (Minute 2.10). The situation with Italy had been reported at the 2002 EC meeting.

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 137,000 in the Swiss bank account and over \$6,500 in the US account for a total of \$108,538 combined. The status as at 31 July 2003 in the bank accounts had been provided to each National Delegate present at the EC meeting.

The Executive Secretary next reported that the 2002 financial statements had been forwarded to the Auditors in January 2003. Both VDI in Germany and Mr. Miyagawa in Japan had reviewed and approved them. The financial statements for 2002 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 2004.

The EC unanimously agreed to this proposal.

The Executive Secretary also provided a rough estimate of the income and known planned expenditures for 2003.

14.2 Time and Place of the 2003 and 2004 Meetings

The ICPWS will be held in Kyoto, Japan in August 2004. The Executive Secretary asked the delegate from Greece to provide a few details of initial ideas and plans for the 2005 meetings. The President thanked Assael and asked him to provide further details at the EC Meeting in Japan.

15. <u>Guidelines, Releases, Certified Research Needs, International Collaborations</u>

President Watanabe indicated that discussion on Guidelines, Releases and ICRNs had been dealt with during the WG presentations. A listing of all IAPWS Releases, Guidelines, Advisory Notes and ICRNs is provided as Attachment 9.

15.1 International Collaborative Projects.

The President asked the Chair of the Committee (Zeijseink) 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 Attachments 10. The Chairman summarized the proposal for the EC. The IAPWS Sponsors are Harvey (US) and Alexandrov (Russia). A young investigator from the Dagestan Scientific Center will travel to NIST in the USA to address PVT Properties for the Ammonia/Water system. The period of performance will be one year at a proposed budget cost of \$10,000 for travel expenses and costs.

After some discussion by the EC, the President 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 Karol Daucik (Denmark) had been elected Honorary IAPWS Fellow, following the established procedure and after unanimous approval through the postal ballot conducted by the Executive Secretary. The Fellowship Award had been presented to Daucik at the IAPWS Dinner on Thursday evening.

The President next discussed the Awards Committee, and requested that Cooper become the chair of the committee for the 2004 Award. He also suggested that Fernandez-Prini should become the second member of the committee.

16.2 IAPWS Helmholtz Award

The President asked the Russian Delegate for the names of the Helmholtz Award Committee for 2004. Petrova indicated that Alexandrov from Russia would be the Chairman, and that the following would be members: Argentina/Brazil (Japas), BIAPWS (Bignold), Canada (Svishchev), and USA (Harvey). Nominations are due to the Executive Secretary by January 31, 2004.

16.3 IAPWS Gibbs Award

The President requested the appointed Chairman of the Gibbs Award Committee to provide a report of the discussions during the week. Cooper indicated that three people had been nominated. The committee had reviewed proposals for three people in detail. The Chairman then recommended to the EC that Professor R. Wood of the University of Delaware should become the 2004 IAPWS Gibbs Awardee.

The EC approved this nomination unanimously.

17. <u>New Business</u>

17.1 14th ICPWS, Kyoto, Japan. August 29 – September 3, 2004

The Chairman of the Japanese Organizing Committee, Watanabe, provided details of the activities during the week. The Organizing and Program Committees had met twice. There is now a complete set of proposed Symposia together with an organizer and an invited speaker. The topics for the Plenary Lectures have been decided. The Second Conference Brochure will be available by September 15, 2003, and the closing date for abstracts will be 15 December 2003. The EC will meet on Sunday 29 August 2003.

17.2. IAPWS Website (http://www.iapws.org)

The President requested Harvey to provide an update of activities on the IAPWS Website.

Harvey first indicated that the website now contained: a) all IAPWS Releases, Guidelines and ICRNs, b) details for all annual meetings including this Denmark meeting, c) the IAPWS Minutes from EC meetings, and d) a new section on IAPWS News. He then indicated that there had not been any new Frequently Asked Questions developed. He thought that maybe there should be some better descriptions of the WGs, and suggested that the IAPWS Atlas should be mentioned in a promotional fashion.

17.3. IAPWS Restructuring

The President requested the Chair of the Committee (Levelt Sengers) to provide a final status report on any outstanding items, which were not covered in the Thursday Special Session (Minute 5). The Chair reminded the EC of the Committees and Task Groups that had been set up. Attachment 2 provides the final makeup. She then raised the issues of changes to the WGs and the cycle frequency of ICPWS. After some discussion, the President indicated that it appeared that the consensus was that changes to the WG structure were not required. He then developed a proposal for the EC to move the ICPWS to a four-year cycle.

The EC approved the proposal by majority with 4 abstentions.

The President next asked the EC to approve the formation of the Committees and Task Groups.

The EC approved these unanimously.

The President then thanked the Chair, her committee, the WG Chairmen, and National Committees for the tremendous work they had conducted to thoroughly review so many aspects of IAPWS operation. He then requested the EC to dissolve the IAPWS Restructuring Committee.

The EC approved this unanimously.

17.4 Press Release

The President requested Bellows to present the News Release to the EC. This is contained in Attachment 11.

The EC approved this unanimously.

17.5 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 IAPWS week. They are attached to these minutes as follows:

Britain and Ireland	Attachment 12
Czech Republic	Attachment 13
Denmark	Attachment 14
Germany	Attachment 15
Greece	Attachment 16
Japan	Attachment 17
Russia	Attachment 18
USA	Attachment 19

17.6 Participants

Attachment 20 provides a list of participants at the EC and WG Meetings in Vejle in August 2003.

17.7 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 Denmark Meetings. This will be forwarded electronically to the Head of each National Committee.

18. Closing Remarks and Adjournment

The President thanked the Danish National Committee for their hospitality during the week. He then formally closed the 2003 EC meetings at 2:45pm.

AGENDA for the EXECUTIVE COMMITTEE IAPWS

DENMARK. 24-30 AUGUST 2003

Monday, 25 August 2003. Opening Session (8:30-10:00am)

Opening Remarks and Welcome

1. Adoption of Agenda

- 2. IAPWS Business and Appointment of Committees
 - 2.1 Press Release
 - 2.2 Evaluation Committee on International Collaboration
 - 2.3 IAPWS Helmholtz Award Committee
 - 2.4 IAPWS Gibbs Award (2002 Minutes. Minute 15.3)
 - 2.5 IAPWS Atlas (Update by Palmer)
 - 2.6 IAPWS on the Internet.
 - 2.7 IAPWS Members and e-mail addresses
 - 2.8 IAPWS Structure (2002 Minutes. Minute 17.4)
 - 2.9 IAPWS Products (2002 Minutes. Minute 17.5)
 - 2.10 Other business requiring special/extensive discussions
- 3. EC Mandate to Working Groups and Membership
 - 3.1 Releases, Guidelines and Certified Research Needs (New and Expiring)
 - 3.2 14th ICPWS in Kyoto, Japan
 - 3.3 WG Directions
 - 3.4 Reports to EC
- 4. Preview by WG Chairpersons of Week's Activities

Thursday, 28 August 2003. Special Joint WG Session (1:30-3:00pm)

- 5. Special Joint WG Session
 - 5.1 Structure of IAPWS
 - 5.2 14th ICPWS

Friday, 29 August 2003. Executive Meeting. (9:00am - 4:00pm)

- 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)

- Executive Secretary's Report
 - 14.1 Financial, Auditors and Dues
 - 14.2 Time and Place of 2005 Meeting
- 15. Guidelines, Releases, Certified Research Needs and International Collaborations
- 16. IAPWS Awards (Gibbs, Helmholtz, and Honorary Fellowship)
- 17. New Business

14.

- 17.1 Planning Details of 14th ICPWS
- 17.2 IAPWS Website
- 17.3 IAPWS Restructuring
- 17.4 Press Release
- 18. Adjournment

Committee on the Structure of IAPWS Levelt Sengers, chair, Cooper, Marsik, Svoboda Denmark, Aug. 28, 2003 Report to Plenary Session/EC

The Committee for the Structure of IAPWS proposes the formation of four committees and five task groups. The committees will work for a year, and report at Kyoto, after which they are disbanded. They require an EC vote. The task groups will report at Kyoto, and may continue as seen fit. Names marked by * indicate individuals who have been contacted and have agreed to serve or act.

COMMITTEES

NUCLEAR POWER SYSTEMS

Mandate: update IAPWS on developments in various countries, and delineate tasks for IAPWS.

Proposed Chair: Uchida*

Members: Svoboda*, Palmer*. Mayer* will try to find contact at CEA/Framatom Levelt Sengers* will find names of co-opted experts at EPRI, NEEL Idaho and Canada Svoboda* will find contacts in Argentina/Brazil and EDF. Cooper* will ask Andy Rudge (BIAPWS) as co-opted expert. PCC* will provide contact names.

FUEL CELLS AND HYDROGEN TECHNOLOGY

Mandate: update IAPWS on ongoing research, advise on problems IAPWS could work on, and on whether a task group should be formed.

Proposed chair: Serguei Lvov* Members: Rukes, co-opted experts from Siemens-Westinghouse/Pittsburgh, DOE, Weber* will recommend contact at Siemens-Westinghouse, Parry* will recommend contact at GE. Wagner will contact Rukes.

EFFECTIVENESS OF ICRNs

Mandate: assemble the statistics and analyze the fate of past ICRNs: their success rate in generating proposals, obtaining funding, and solving the problem at hand.

Proposed chair: Jim Bellows*
Members: Zeijseink*, Daucik*, Wagner*, Palmer*, Parry*, Friend*
Awards
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.

Proposed chair: Jeff Cooper* Members: Bellows*, Bignold, Olavessen*, Rukes Wagner will contact Rukes Cooper will contact Bignold.

TASK GROUPS

The task groups should be formed and start their work as soon as possible. They should be operational, and report, by the time of the Kyoto meeting. Again, the chairs should have the discretion to select further members and co-opted experts.

PROPERTIES AND FORMULATIONS FOR HIGH-TEMPERATURE AQUEOUS SYSTEMS

Task: expand the existing PCAS task group by formulating a comprehensive program encompassing PCAS, TPWS and PCC expertise in this field.

Proposed chair: Vladimir Mayer* Members: Harvey*, Jensen* Mayer* will contact Fernandez-Prini, Plyasunov, Anderko. Marsik* will contact Sedlbauer.

ELECTROCHEMICAL PROCESSES IN HIGH-TEMPERATURE AQUEOUS SYSTEMS

Task: Formulate a research program for IAPWS. Augment existing expertise by attracting co-opted experts and new members

Proposed Chair: Serguei Lvov* Members: Petrova*, Eric Maughan*, Nakahara*, Uchida*, and a research associate of Digby Macdonald, Lvov* will ask Macdonald for the associate.

Education and Outreach

Task: Define educational and outreach projects IAPWS should engage in. Work with national committees active in this area. Attract volunteers. Explore possibilities of obtaining funding.

Proposed chair: Corti Members: Assael*, Harris*, Nagashima, Olavessen, a member from Canada Natl. Committee. Consultant: Harvey* Levelt Sengers* contacts Corti. Backup: Assael*. Levelt Sengers contacts Canadian national committee.

ENVIRONMENTAL ISSUES

Task: Deal with environmental consequences of electric power generation, including use of new fuels, and methods proposed for their mitigation, including SCWO. Define areas to which IAPWS can contribute, and pinpoint sources of funding.

Proposed chair: Ochita* First-level subcommittee members: Ochita*, Parry*, Weber*, Zeijseink* Additional, full committee: Nakahara*, Assael*, Olavessen* (with company support) Kretschmar* will ask Spann; Levelt Sengers* will solicit Argentina/Brazil rep.

METASTABILITY, NUCLEATION, EARLY CONDENSATE, DROPLET SPRAYS, CAVITATION

Task: Define and attract expertise needed, define problems to work on.

Proposed chair: Marsik* Members: Bellows*, Stastny* Levelt Sengers* contacts Anisimov Marsik* contacts young engineer at hydropumps company, Guenter Schnerr, Karlsruhe, Rini van Dongen, Eindhoven, Christopher Brenner, Cal. Tech. Zeijeink will contact Cees van Geld, Eindhoven.

Symposium, Wednesday 27 August 2003 Aqueous Thermodynamics in Power Generation

Morning Session Helmholtz Award and Danish Research and Development Chairperson: Karol Daucik, Elsam, Denmark				
09:00	Presentation of the Helmholtz Award by the president of IAPWS			
09:05	E. Luijten New Techniques for the Determination of Phase Properties of Aqueous Systems via Computer Simulations			
09:50	S.Hansen Process Design and Optimisation of the Avedøre2 Multi Fuel Power Plant			
10:20	Coffee break			
10:50	R. Blum Development of 700° Ultrasupercritical Fossil Power Plant			
11:20	A. García Scaling in Geothermal Units			
11:50	K. Thomsen Utilization of Bio-ash			
12:30	Lunch			

Afternoon session

The Physical and Chemical Properties of Aqueous Systems at Elevated Temperatures and Pressures: Water, Steam and Hydrothermal Solutions

Chairperson: Dr. Jørgen Peter Jensen, Energi E2, Denmark

14:00	J.M.H. Levelt Sengers Near-Critical Behaviour of Aqueous Systems
14:30	A.H. Harvey Aqueous Solubility of Volatile Nonelectrolytes
15:00	Coffee break
15:30	F. Marsik Binary Homogeneous Nucleation in Selected Aqueous Solutions
16:00	D.A. Palmer Partitioning of Electrolytes to Steam and Their Solubility in Superheated Steam
16:30	V. Valyashko Phase Equilibria in Binary and Ternary Water-salt Systems

under Sub- and Supercritical Conditions

Schedule

IAPWS Meetings

Vejle, Denmark. 24-30 August 2003 (All meetings will be at Hotel Australia, Vejle, Denmark)

Sunday 24 August.	3:00-5:0 6:00pm	3:00-5:00pm International Program Committee for the 14 th ICPWS 6:00pm Informal Get-together and Registration			
		(Hosted by Danish National Committee)			
Monday 25 August.	8:30am. 10:00am	Opening Plenary Session - Executive Committee TPWS/IRS Joint Meeting			
(To set agendas for the w	week and to cor	duct IAPWS Business, thus allowing remainder of week	k for technical matters)		
	10:00am	. PCAS and PCC Separate Meetings			
	(To cond	act IAPWS Business, thus allowing remainder of week f	for technical matters)		
	1:30pm.	TPWS and IRS Joint or Separate Meetings			
	1:30pm.	PCC/PCAS Joint WG Meeting and Workshop			
Join	it WG Work	shops: pH Measurements at Different Tempera	atures, and		
		Ultra-Supercritical Plants			
Tuesday 26 August.	8:30am.	PCAS/PCC Joint Workshop			
	Chemist	ry in Ultra Supercritical Plants			
	8:30am.	TPWS and IRS Joint or Separate Working Groups	s Meetings.		
	1:30pm	All WG Meeting	-		
	2:30pm	IRS and PCC Separate WG Meetings			
	2:30pm	TPWS/PCAS Joint Meeting			
		Topics of Interest to Both WGs			
Wednes. 27 August.	9:00-5:00	IAPWS Symposium			
C	"Aqueo	us Thermodynamics in Power Generation"			
Thursday 28 August	8.30am	TPWS/IRS/PCAS/PCC Separate or Joint WG Me	etings		
Thursday 20 August.	1.30nm	Special Session of all Working Groups	etings		
	1.5 opin.	7:00 pm IAPWS Dinner			
	(Hosted	by Danish National Committee)			
Friday 20 August	0:00am	Executive Meeting (0:00em 4:00nm)			
Filday 29 August.	(Will incl	ude at least one member from each National Delegation)		
Saturday 30 August.	9:00am.	Technical Visit to Skaerbaekvaerket Plant			
	1.5				
TPWS - Thermophysi	cal Properties	of Water and Steam WG			
PCC - Power Cycl	e Chemistry VI Aque	VG	Barry Dooley		
IRS - Industrial R	equirements	and Solutions WG	August 2003		
in a substantial in	- 1 an entrentes		. Iugust 2005		

Minutes of IAPWS Thermophysical Properties of Water and Steam WG

Vejle, Denmark 25–28 August 2003

NOTE: Items are listed according to their order on the revised agenda. **Bold print** denotes significant actions taken. For some of the agenda items discussed jointly with the IRS working group, reference is made to those minutes.

1-3. A few additions were made to the preliminary agenda, after which it was adopted. Allan Harvey was appointed Clerk of Minutes. The minutes from the 2002 TPWS WG meeting in Buenos Aires were approved without objection.

4. Dr. Friend reviewed the status of IAPWS documents and highlighted those that would be discussed during the week.

5 The preliminary report on the future of IAPWS was discussed. With regard to specific items affecting TPWS, the following conclusions were reached. There is no need to change the TPWS name. With regard to suggestions about reducing the length of the IAPWS week, the WG had concerns about any plan that would reduce the amount of time available for the Working Groups, especially for the meeting following the ICPWS where more time might be needed. The WG had no objection to holding the ICPWS at 4-year intervals, provided willing host countries were available.

Some people were proposed for some of the new committees being formed. Allan Harvey agreed to serve on *Properties and Formulations for High-Temperature Aqueous Systems.* Bill Parry (GE) and Ingo Weber (Siemens) agreed to check within their companies for possible interest in the *Fuel Cells* Task Group. Bill Parry agreed to serve on *Effectiveness of ICRNs.* Marc Assael agreed to serve on the *Educational* Task Group, and Prof. Watanabe will contact a member of the Japanese delegation who might be interested. Dr. Okita agreed to serve on the *Environmental Issues* Task Group.

6. Suggestions were made for organizing sessions at the upcoming ICPWS, and were transmitted to the organizing committee.

7-11. For these items, all of which are joint with the IRS Working Group related to different IAPWS products, see the IRS minutes.

12. Mr. Cooper gave a report on the proposed Advisory Note 2 on the role of various IAPWS documents relating to thermodynamic properties of ordinary water. After some

discussion, it was decided that Surface Tension should be added to the document. With some additional editorial changes, the WG was satisfied with the document. The joint Working Groups TPWS and IRS recommend this document to the EC, and suggest that it be sent for approval by postal ballot in the coming year.

The issue of obsolete IAPWS documents came up in this discussion (and also for agenda item 11). It was decided that the Website should have a brief section about obsolete IAPWS documents, which Allan Harvey and Jeff Cooper will prepare.

13. Jeff Cooper gave a presentation on his study of the effect on the existing formulation for D2O thermodynamic properties of changing the reducing temperatures to the current ITS-90 scale. The WG felt a need to have more time to look at the proposed changes, and at the documentation of their effects. The following schedule was adopted. By the end of 2003, Jeff Cooper will produce a draft of a revised release, and supporting documentation. The WG Chair will circulate this to the D2O Task Group, and then to the WG members by Feb. 15. WG members will have until March 31 to comment. Mr. Cooper will produce a revised version by April 30, which will be reviewed by the Editorial Committee by May 31. Then the WG Chair will send it to the Executive Secretary to be distributed to National Delegates, in anticipation of a vote for approval at the 2004 EC meeting.

14. Jeff Cooper reported that the IEC steam turbine committee was currently dormant due to lack of a chair. He will continue as a liaison.

15. Allan Harvey, chair of the Task Group on this issue, reported that there was **no need to revise the Fundamental Constants guideline this year**.

16-24. A Joint Session was held with PCAS on Tuesday afternoon. The contributions are listed on the Agenda. Item 18 required some action, as approval of a new Guideline on Henry's constants and vapor-liquid distribution constants (replacing two existing Guidelines) was requested. It was decided that some information about uncertainties should be added to the Guideline. The WGs TPWS and PCAS endorsed the proposed Guideline subject to this revision, and desires that it be sent for postal ballot for EC approval once the revision is made.

25. Prof. Yasuoka gave a presentation on his molecular dynamics simulations of the ethanol/water interface.

26. Dr. Friend described the progress of the Transport Properties Task Group, which was greatly enhanced by the IAPWS Project that allowed Ifigenia Metaxa to visit NIST in Boulder.

Allan Harvey described the minor discontinuity that had been discovered in the existing release for the viscosity of ordinary water, and its suggested resolution, which had already been endorsed by the Transport Properties TG. **TPWS approved this minor revision to the viscosity Release and requests the EC to approve the revision at this meeting.**

Marc Assael reported on the work done by I. Metaxa on the IAPWS Collaborative Project on the low-density limit of the viscosity of water. He also described future plans to work toward a new formulation for the viscosity; it is hoped that a preliminary version will be finished by next year's meeting in Kyoto.

P. Kones and R. Mares reported on their evaluation of the equation published by Alexandrov for the viscosity of water and steam. It was the decision of the Transport Properties Task Group that, though the Alexandrov formulation has some good points, it will not be adopted as a new standard, and a new formulation will be adopted instead.

A question was raised about the thermal conductivity, and it was stated that the Task Group would start working on that more seriously as the viscosity project drew nearer to a close.

27. There was no further discussion of EC mandates to the WG in addition to that reported in items 5 and 6 above.

28. Several items left over from Tuesday's joint symposium with PCAS were discussed.

With regard to the project underway in the EU on properties of humid air (item 16), the WG chair will write a letter to the Chair of this part of the project ("Working Package 4") expressing the interest of TPWS in this area to see if any mutually beneficial interactions can be developed.

With regard to the proposal by V. Mayer for development of recommended data values of hydration properties of organic solutes (item 21), Allan Harvey was appointed to represent TPWS in discussions of this project.

With regard to the proposed compilation by V. Valyashko on high-temperature experimental data for aqueous mixtures, the WG had concerns about IAPWS involvement at this late stage in the project and about the lack of data evaluation. Marc Assael and Anneke Levelt Sengers were appointed to discuss these issues with Prof. Valyashko before deciding on any further steps.

29. The Chair reminded the WG of the usefulness of collaborative projects and invited them to think of ideas for next year.

30. Under this item, there was discussion of the Simulation Task Group, which does not appear to have accomplished much toward its goals. In the absence of the TG chair, it was suggested that Prof. Yasuoka lead the effort for the next year (looking toward the ICPWS in Kyoto) toward finding fruitful directions for simulation for IAPWS. The WG Chair will write a letter to the previous TG Chair expressing thanks for his service and inviting him to contribute in the future. Since this TG is joint with PCAS, Dr. Friend will consult the PCAS Chair to be sure this course of action is acceptable to that WG.

31. Dr. Kenji Yasuoka (Japan) and Dr. Radim Mares (Czech Republic) were proposed to become members of TPWS, and were unanimously approved. It was also noted that Prof. Roland Span (Germany) had been added to the WG last year, but that this was not reflected in the IAPWS membership roster. In response to the request of the IAPWS President to examine the status of inactive members, 4 members were identified to be contacted to see if they wish to continue. Prof. Wagner will contact Schiebener (Germany) and Mayinger (Germany). The British and Irish Commmittee will contact Watson (BIAPWS). Dr. Friend will contact Agayev (Azerbaijan).

- **32.** There was no further new business.
- **33-34.** The Chair and Clerk of Minutes were authorized to prepare the motion to the EC and the report to the meeting of all Working Groups, and the meeting was adjourned.

MINUTES OF INDUSTRIAL REQUIREMENT AND SOLUTIONS WORKING GROUP

VEJLE, DENMARK – AUGUST 25 - 30, 2003

Note: Most meetings were held in joint session with TPWS. TPWS agenda items 7 through 11 are documented within these minutes. All others will be found in Minutes of TPWS Working Group.

Agenda Item 1 – Opening Remarks; Adoption of Agenda

After chairman Dr. Friend had conducted the initial TPWS business, IRS chairman Mr. Kiyoshi Miyagawa conducted opening business for the Industrial Requirement and Solutions working group. He expressed appreciation to Mr. Ingo Weber for acting as chairman for the working group last year held in Buenos Aires. The agenda was modified to add items 4 and 5; otherwise it was the same as originally distributed prior to meeting. It is provided as IRS Attachment A.

Agenda Item 2 – Appointment of Clerk

Dr. Bill Parry was appointed clerk of the minutes.

Agenda Item 3 – Approval of Minutes

Minutes from the 2002 annual meeting held in Buenos Aires were approved without objection.

<u>Agenda Item 4 (TPWS Agenda Item 5) – Discussion of future of IAPWS as related</u> <u>to Working Groups.</u>

See TPWS minutes for this item.

Agenda Item 5 (TPWS Agenda Item 6) – 14th ICPWS to be held next year in Kyoto, Japan

See TPWS minutes for this item.

<u>Agenda Item 6 (TPWS Item 7) – Supplementary Release on Backward Equations</u> <u>for the functions T(p,h), v(p,h), and T(p,s), and v(p,s) for the Critical and</u> Supercritical Regions to IAPWS-IF97.

At the September 2002, Buenos Aires Meeting, a draft of the supplementary release was proposed and an evaluation task group was established. In March 2003, the evaluation report and revised draft were sent to IRS and TPWS members. In May, technical discussion closed and the revised draft was sent to IRS and TPWS Working Group members. Tests were performed by Evaluation Task Group, including reproducibility and accuracy requirements of IAPWS-97 and consistency at boundary between sub regions. The computing speed was verified by independently derived software.

It was the recommendation of the task group to have the draft be accepted by IAPWS as a supplementary release. The Task Group further recommends that the proposed code be treated as part of the IAPWS-IF97 authorized code. Dr. Friend made a motion to present the supplementary release of these equations to the executive committee for adoption as recommended by the task group. Dr. Allan Harvey seconded this motion. The motion was accepted without dissention.

<u>Agenda Item 7 (TPWS Item 8) – Progress Report on Development of IAPWS-IF97</u> <u>Backward Equations in Region 3</u>

Prof. Hans-Joachim Kretzschmar gave an overview on the progress for development of supplementary backward equations. Ms. K. Knobloch then gave a detailed talk describing the work in developing backward functions in region 3 of IAPWS-IF97 for the functions $p_3(h,s)$, $T_3(h,s)$, and $v_3(h,s)$. The resultant backward equations reduce the need for time consuming twodimensional iterations. They meet the accuracy requirements of IAPWS-IF97, and result in 11 times faster result than the iteration process. Backward equations for determining the region boundaries as a function of h,s were presented which showed a 14 times resultant speed advantage over IAPWS-IF97. Finally, a backward calculation for $T_{sat}(h,s)$ was presented. This routine was 11 times faster than IAPWS-IF97. Several questions were asked including reference to a survey which indicated that 2/3 of those questioned did not see a need for a backwards set of equations in region 3. It was pointed out that there was currently renewed interest in supercritical and ultracritical cycles which will require more calculations in region 3 for both turbine and boiler manufacturers.

Mr. Miyagawa started discussion for Proposal for new Region 3 Supplementary Release. Ingo Weber suggested an establishment of Evaluation Task Group. Mr. Miyagawa proposed using same task group, Miyagawa (chairman), Okita, Gallagher, and Weber who were members of the prior task group. Testing task group will develop their own testing software, and independently access the accuracy of the proposed group. Based on his past experience, Mr. Miyagawa proposed the evaluation report to WG by January 2004, Draft Release to WG and Editorial Committee by February 2004, and Final Release to executive secretary for distribution to the National Committees by April, 2004.

<u>Agenda Item 8 (TPWS Item 9) – Progress Report of the Guideline on Tabular</u> <u>Taylor Series Expansion (TTSE)</u>

Chairman Miyagawa reported that the guideline had been approved by Editorial Committee, the approved draft had been sent to the executive secretary, and the guideline had been distributed to National Representatives for Postal Ballot. The EC has approved the Guideline in its current form, and the guideline referenced downloadable software is now available from the Japanese National Committee website. A demonstration by Dr. Kenji Yasuoka in real time showed how the method can be accessed from the Japanese National Website. The Website can be accessed at "http://www.iapws.jp."

As a result of the software availability and normal acceptance procedures being complete, the joint IRS and TPWS will recommend to the EC that this guideline be approved.

<u>Agenda Item 9 (TPWS Item 10) – Topics on the TTSE method, expansion of TTSE</u> *p-h* version for transport properties

Mr. Kiyoshi Miyagawa made a presentation on the TTSE Method for Transport Properties. He pointed out the calculation of μ (dynamic viscosity) is a time consuming process with either IAPWS-95 or IAPWS-IF97 due to the contained exponential function. Similarly, λ (thermal conductivity) can be calculated with either IAPWS-95 or IAPWS-IF97 (with some loss in accuracy near critical region), but this is even a more time consuming process due to three contained exponential functions, an exponentiation by a non-integer value, and two call of derivatives of thermodynamic properties. He then showed that TTSE can be used for μ in the *p*-*h* plane where the behavior is smooth. The resulting calculations with TTSE have less than a 0.1%deviation from the original IAPWS-95 except at high pressure and very low enthalpy where the IAPWS equation is not applicable. Unfortunately, the behavior of λ on the *p*-*h* plane is not as well defined, and shows a steep peek at the critical point. The TTSE results show deviations of less than 0.1% except near the critical point. It is recommended to use the original formulation near the critical region to obtain accurate results. Isobaric specific heat (c_p) is similar to thermal conductivity in that deviations occur near the critical point; therefore, the same approach is used as with thermal conductivity. The Prandtl Number $(Pr) = c_P \mu / \lambda$ was evaluated by the two methods; as expected, the TTSE method is significantly faster.

Dr. Dan Friend urged continuation of TTSE method but felt that a release of this methodology should be delayed until the expected release of the new Transport Properties which should take place within two years. He also pointed out that the current recommendation of transport properties is to use either IAPWS-95 or IF97; the resulting difference between the two is less than the expected deviation in actual transport properties. Dr. Dan Friend asked whether computational speed is as important for transport properties. Mr. Ingo Weber, Dr. Bill Parry, and Mr. Jeff Cooper responded that speed was important, especially in CFD work.

Agenda Item 10 (TPWS item 11) – Uncertainties in the enthalpies of IAPWS-95 and IAPWS-IF97; status of skeleton tables

Prof. Wolfgang Wagner presented a method to determine the uncertainties in enthalpy in IAPWS-95. Prof. Wagner showed uncertainty results for enthalpy for the prior IAPS-84; this was in the form of Pressure plotted on the ordinate versus Temperature on the abscissa showing the percentage uncertainty for different regions. These were calculated based on differences between experimental c_p data and c_p derived from IAPS-84. However, there is no experimental data of enthalpies related to the zero point. Therefore, Prof. Wagner decided to consider primarily the differences in enthalpy among the best equations of state represented by IAPWS-95, Hill (1990). and Saul and Wagner (1989). Additionally, he considered the older formulations IAPS-84, Pollak (1974), and International Skeleton Tables IST-85. He created a plot of Pressure versus temperature with regions of uncertainty in enthalpy expressed in kJ/kg. These range from +/- 0.1 kJ/kg up to a small area of +/-15 kJ/kg at very high pressure and temperature. He then considered uncertainties in percent change in enthalpy based on an isobaric change in temperature; a plot of Pressure versus Temperature shows the vast majority of results with +/-0.2% or less. Near the critical point, there is a small area of +/-2%. He also considered two different types of adiabatic paths, adiabatic reversible (constant entropy), and adiabatic irreversible (simulating normal turbine expansions). The resulting uncertainty regions on a P vs. T plot show that the most of the region are $\pm - 0.4\%$ or below, with the small areas near the critical point being \pm 5%. There was no substantial difference in the results whether reversible or irreversible

He also compared IAPWS-IF97 to IAPWS-95. The plot of *P* vs. *T* shows that most of the regions are with +/- 1 kJ/kg. Near the critical point the uncertainty is +/- 15 kJ/kg. He also investigated the uncertainty of IAPWS-IF97 versus IAPWS-95 using the isobaric methodology. The *P* vs. *T* plot has most of its area at or below +/- 0.3%, with a small area near the critical point being +/- 2%.

A series of questions followed the presentation. Prof. Wagner was asked to publish the method and results in a technical paper which he said he would consider.

Dr. Friend then started discussion on acceptance of Advisory Note No. 1 which details the results of the enthalpy uncertainty. Mr. Jeff Cooper felt that a procedure for acceptance had not yet been established. Consensus was reached to recommend to EC that this Advisory Note be approved. The need for a skeleton table is no longer necessary with the adoption of the Advisory Note, and therefore, consensus was reached to recommend to the EC that the skeleton document be withdrawn. Much discussion ensued about whether to list or not list the skeleton table. There was strong opinion that a section be created on the IAPWS website listing outdated IAPWS releases (IST85, IFC67, etc.). Dr. Friend asked Dr. Harvey to draft such a document for inclusion on the website for outdated documents.

<u>Agenda Item 11 (TPWS Agenda Item 12) – Progress on document concerning</u> <u>differences among IAPWS products for calculating water properties</u>

See TPWS Minutes for this item.

Agenda Item 12 – Membership

There are no changes to current membership. However, the chairman will write to each National Committee for those IRS members who have not attended the last three IAPWS meeting so ascertain whether that member is still interested in serving on the committee.

Agenda Item 13 – Other Business

There was no Other Business.

Agenda Item 14 – Preparation of Report to Executive Committee

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

<u>Agenda Item 15 – Adjournment</u>

The chairman thanked all participants for their attention and involvement and adjourned the meeting.

IRS Attachment A

Agenda of Industrial Requirement and Solutions Working Group Vejle, Denmark August 24 through 30, 2003

- 1. Opening Remarks, Adoption of Agenda
- 2. Appointment of Clerk of Minutes
- 3. Approval of Minutes of Buenos Aires Meeting, July 2002
- 4. Discussion of future of IAPWS as related to Working Group
- 5. Discussion of ICPWS-14
- 6. Supplementary Release on Backward Equations for the Functions T(p,h), v(p,h) and T(p,s), v(p,s) for the Critical and Supercritical Regions of IAPWS-IF97
 - 4a) Report of the Evaluation Task Group
 - 4b) 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 *p*(*h*,*s*) equations)
- 8. Progress of the Guideline on Tabular Taylor Series Expansion (TTSE) Method
- 9. Topics on the TTSE method, expansion of TTSE *p*-*h* version for transport properties
- 10. Uncertainties in the enthalpies of IAPWS-95 and IAPWS-IF97; status of skeleton tables
- 11. Progress on document concerning differences among IAPWS products for calculating water properties
- 12. Membership
- 13. Other Business
- 14. Preparation of Report to Executive Committee
- 15. Adjournment

Minutes of PCAS, 2003

Monday Morning (25 August 2003)

DP adopted as clerk of minutes

Minutes of previous IAPWS meeting in Argentina accepted without comment.

Participating members: Sergeui N. Lvov, Vladimir Mayer, Masaru Nakahara, Tomas Nemec, Donald A. Palmer, Masakatsu Ueno, Vladimir M. Valyashko,

ALS - IAPWS questionnaire

Crucial to the establishment of a better relationship with PCC and for the future of IAPWS is the increasing importance of aqueous chemistry rather than refinement of the properties of water and steam. We need to identify specific products from IAPWS WG's, particularly for industrial attendees. We need for PCC to prioritize a problem and with support from PCAS frame this problem (or more than one problem) during the course of this meeting. We need task groups that go beyond the membership of IAPWS to deal with common needs and future goals. There should be a slew of committees set up this week to treat a range of issues. For example, the first issue would be fuel cells with the aim of showing how IAPWS will play a role. This committee could be made up of SL, FM and Horacio Corti, and others. Electrochemistry at high temperatures is another topic (SL, DP, Digby Macdonald, and others). A subtask group would be to establish guidelines for pH measurements at high temperatures. The formation of this subtask group was mentioned at the PCAS WG meeting in Argentina and members were initially suggested (DP, SL, Peter Tremaine, MN, HC). SL asked if it is possible to attract chemists from the nuclear power industry. The answer is that nuclear is on the rise, and that IAPWS has had members in the past from the nuclear power industry so that we should be able to attract members in the future. ALS urges PCAS members to get involved in these task groups. Education is another issue that PCAS should consider having members on this committee. There are many good ideas in this area in the report that ALS described at the EC meeting on Monday morning. The subject was raised about our attempts to have PCAS and TPWS becoming interested in computer simulation modeling, but as no members with this expertise are currently in attendance, this subject will languish this year. How do we involve more "simulators" in IAPWS on a regular basis? Perhaps next year at the ICPWS the symposium on simulations will provide a basis for this area within IAPWS. DP suggested that we need to have more than one person responsible for new areas to avoid losing these initiatives.

VM asked if there were any applications for the collaborative young scientist program. However, there were none from PCAS this year.

VM raised the question of the symposia for the 2004 ICPWS. The list of symposia in the first circular was found to be no longer valid as it was revised on Sunday. SL proposed a rewording and recombination of two symposia into "Electrochemistry for Power Generation and other Technologies". This title would fit the currently proposed last topic on the current list from Sunday. It was decided to delay further discussion until Thursday.

Monday afternoon - joint PCC/PCAS workshop

1. Andre Zeijseink On the Importance of pH Measurements in Power Plant Cycles

Question: SL Why not add NaCl to the pure water samples to measure pH directly? AZ This has been tried sparingly, but not over a long period of time due to cost of probes. TP You give a value of 5.5 for the neutral pH of pure water at 350C. Was this an experimental or calculated value. The consensus of opinion was that this value was calculated based on fitting a large body of experimental data. 2. Jim Bellows Calculation of pH from Specific and Cation Conductivity (no handout was available)

Question: MB Did you try the calculation of pH with NaCl added? Yes. EM confirmed that you can only calculate the pH in alkaline solutions as stated in the VGB guidelines.

3. Eric Maughan Practical Aspects of pH Measurement

Question: SL Have you considered diffusion potentials in your low temperature glass electrode measurements? By using KCl in the reference compartment, and dilute buffers and very dilute test solutions, the diffusion potential can be ignored. DP Do you recommend the use of Ross combination glass electrodes? Yes, and Equilthal electrodes are also very reliable.

4. Don Palmer Report on the pH of High Temperature Water

Question: SL Are there plans at ORNL to make a flow concentration cell for supercritical conditions? Yes, by replacing Teflon with ceramics a prototype as been made to go initially to 400C. VM How reliable are pH measurements at high temperature using spectrophotometric indicators? We could not find any complete estimate of experimental errors in the papers by Johnston and coworkers, but we estimate that these errors may be +/- 0.1 pH units. However, these researchers are no longer active in this area.

5. Serguei Lvov Can We Measure pH of High Temperature Water?

6. Yulia Zhgenti An Experimental Investigation of Borate/Lithium Adsorption from Solution onto Zirconium Dioxide in the Water-Steam Cycle of Power Plants

Question: SL Is knowledge of the zeta potential important to your study? Yes, because adsorption of ions changes the zeta potential. MB Do lithium cations adsorb because borate is adsorbed on the ZrO_2 surface? No, lithium cations adsorb independently on the negative ZrO_2 surface, and borate may be either adsorbed directly on the surface in place of hydroxide ions or are incorporated in the electric double layer.

7. Erik Maughan Theoretical and Practical Aspects for the Verification of Carbon Dioxide in the Water-Steam Cycle of Power Plants

Question: Is the instrument that you have described available commercially? Yes. 8. Shunsuke Uchida Development of High Temperature Water Chemistry Sensors

Question: SL You mentioned that ECP instrumentation has been installed in BWR's in Japan, what reference electrode was used and how do they allow concentrated solutions in the reference electrode to be used in the BWR environment? We use either an Ag/AgCl or Fe/Fe₃O₄ reference electrode in a line where the water then goes to the drain and not back into the reactor.

9. Erik Maughan Automatic on-line Calibration Method for pH of Ammoniacal Water Circuits.10. Geoff Bignold A Spreadsheet for Calculation of Speciation, pH and Conductivity from Measured Concentrations of a Range of Anions and Cations.

Question: MB A comment that spreadsheets will at least predict which are the important species in water at various conditions. DP A further comment that the reliability of these predictions depends on the reliability of the database on which they are based. For example, $Mg(OH)^+$ is now believed not to be an important hydrolysis product of Mg^{2+} which rather hydrolyses directly to $Mg(OH)_2$.

Monday afternoon final PCC/PCAS Discussion

At the request of AZ for a combined action by PCC and PCAS, DP suggested that interested participants from both groups and invited specialists from outside IAPWS prepare a document for eventual publication on the subject of pH with particular emphasis on high temperature applications, comparison of techniques. equipment, calibration schemes and standards with consistent consideration of experimental uncertainties. MB noted that for power plant applications there was no need for uncertainty analyses as the expected reliability is only +/- 0.3 pH units at present. EM commented that although there is a critical need for reliable pH measurements in power plants, the task group must also consider the use of conductivity to predict pH. So a two-way approach should be adopted, conductivity and direct pH measurement. AZ commented that in Holland there was an attempt to use pH meters in power plants, but these were not successful (reliable) and therefore this approach was abandoned. SL claimed that chemists possess the technology to measure pH at high temperatures and this technology could be implemented now in a bypass mode to within a precision of 0.1 pH units. However, the equipment is bulky and expensive (ca. \$50,000). BD responded that this effort has been funded for over ten years and is still far too unreliable to be installed in working plants. Therefore power plants continue to use relatively inexpensive conductance monitors for fossil and BWR plants. He further stated that in terms of new instrumentation only ORP monitors have been adopted successfully through initial education by EPRI of the plant chemists and engineers. Forty percent of fossil plants with copper in their cycles now employ ORP monitors. Education of the power

industry following the publication of a comprehensive paper on pH measurements would be a logical next step. JB commented that information retrieved from power cycle monitors is now considered by plant operators in terms of the cost of shut down versus continued power generation and the resulting estimated cost of plant damage. BD said that corrosion fatigue is the most common and expensive problem facing the industry, but we should concentrate first on the question of pH as we have the expertise necessary within the two working groups. BS suggested that we also consider creating a task group to expand the spreadsheet presented by GB to extend the range to 120C and perhaps produce commercial software based on this model. However, BD quickly responded that there are too many legal barriers for IAPWS to go into such a venture.

It was concluded that an outline for the report by the pH/conductivity task group be prepared by two members of PCC and two from PCAS. Andre Zeijseink and Shunsuke Uchida (PCC), and Serguei Lvov and Donald Palmer (PCAS) volunteered to prepare this outline shortly after the Danish meeting. Others to be involved in this project are: Erik Maughan, Geoff Bignold and Horacio Corti with external help by Arthur Covington and Digby Macdonald, if they agree to participate. It is planned to have a draft of this report available by the next ICPWS meeting in Kyoto.

Thursday Morning (28 August 2003)

The first item dealt with the recommendations for the restructuring of IAPWS (the following numbers refer to the recommendation numbers in the report).

- 1. No change
- 2. IAPWS name change: we should retain the general title, even though it does not reflect the exact nature of the organization, but we vote to insert "systems" instead of "mixtures" in the subtitle.
- 3. No change
- 4. PCAS would like to have more interaction with PCC, but we leave the recommendations for PCC to PCC.
- 5. We recommend a wording change to the recommendation "jointly and separately".
- 6. Agree
- 7. Agree
- 8. Agree
- 9. We recommend a four year cycle for ICPWS. We do not wish to suggest changes to the forthcoming ICPWS meeting in Kyoto. We recommend publication of papers in special issues of journals in addition to or instead of the publication of the traditional ICPWS book/CD.

Committees:

Nuclear – we support the establishment of the nuclear power task group (Palmer) Fuel cell – accept

ICRN's – PCAS members present report that they have had no direct or indirect benefit or use of ICRN's. We feel further that the creation of task groups which are proactive substitute for ICRN's in a positive way. For example, the task group on pH has been created, but we are about to close our ICRN on pH, because it has run its course and the same questions still remain.

Awards – agree (nomination of awards committee, PCAS recommends Mr. Okita) Task groups

Properties and formulation for high temperature aqueous solutions – we need a co-chair from TPWS to serve with Vladimir Majer

Electrochemical processes in high-temperature aqueous systems – we recommend Masaru Nakahara and Shunsuke Uchida as additional members.

Education and Outreach – The Monograph is an educational tool and the Japanese national committee has a plan to include students in the forthcoming ICPWS.

Environmental Issues – PCAS nominates Masaru Nakahara and Vladimir Majer.

Metastability, nucleation, early condensate, droplet sprays and cavitation – PCAS has no further members to add.
Suggested symposium topics for the 2004 ICPWS meeting in Kyoto that involve PCAS directly

Thermophysical properties and phase equilibria in aqueous solutions: experiment and modeling (Harvey, Majer) - conditionally invited lecturer to be Dan Friend

Structure, dynamics and molecular simulation in aqueous systems (Ikawa and Okazaki, Mountain) - conditionally invited lecturer to be Guillot

Processes and chemical reactions in hydrothermal systems (Yamasaki, Palmer) – conditionally invited lecturer to be Yoshimura

Apparatus, materials and monitoring instrumentation for applications at high temperatures and pressures (Ueno, Sawamura, Maughan) - conditionally invited lecturer to be ?

Nonequilibrium, metastable and critical states (Marsik, Sengers) - conditionally invited lecturer to be Michael Anisimov

Fuel systems and electrochemistry of aqueous systems (Lvov, Japanese) - conditionally invited lecturer to be Robert Savenil

New task groups / committees

PCAS accepts participation in the project on the Data Book "Hydrothermal Experimental Data. Phase Equilibria and Solution Properties in Binary and Ternary Systems" edited by Vladimir Valyashko that contains eight chapters. The participating IAPWS members are H. Corti, S.N. Lvov, V. Majer, D. Friend and D.A. Palmer.

The Hydration Properties project, which is carried over from the previous year, continues with additional participation from Andre Plyasonov, Shedelbauer, Fernandez-Prini and Harvey.

Minutes of the PCC Working Group Meeting 25 - 28 August 2003

Monday 25 August 2003

1. Amendments / Adoption of Agenda

The agenda was modified to include additional items with the required input target times as requested by the Executive committee at the plenary session.

2. Election of Clerk of Minutes

Mr K McGrath was appointed.

3. Approval of minutes of 2002 Meeting in Buenos Aires, Argentina

The minutes were approved.

4. International Collaboration

K Daucik explained the process for producing a proposal for International Collaboration, which would seek IAPWS support for a Young Scientist to work in a member country. A Zeijseink suggested that we could not make a proposal by the Friday deadline at this meeting. Instead PCC members should actively consider making suggestions for a proposal for next year. A Zeijseink will via email make clear to PCC members what is required to produce a proposal and frequently remind members to actively pursue the objective of making a proposal. Action A Zeijseink.

5. Priority List

The view of the members, after considerable discussion, was that the current list was in need of updating. A Zeijseink said that more action was needed to clear the existing ICRNs – many of which were felt to have generated work had already been reported on. Speaking for US National Committee J Bellows, suggested that PCC should take one issue from the list and work on it to produce a research plan that could be passed to PCAS Working Group. While many members felt this was a positive suggestion that would produce tangible results B Dooley suggested that PCC members should go further than this and that it is important to have a new list of topics. B Dooley's view was that PCC should provide information on the topic, which would assist PCAS and also provide

information on PCC's identified requirements to outsiders as a guidance document. A Zeijseink had not received any inputs on identified topics from any of the National Committees. G. Bignold said that BIAPWS had discussed the current list in committee and there were disparate views on plant type and respective needs given by the BIAPWS sponsors. A Zeijseink said that with a well-developed research proposal it should be possible to obtain funding. Some PCC members said it was important not to raise false hopes in PCAS that funding would be obtainable. To conclude the discussion A Zeijseink said that PCC needed to appoint a task force to work this week and develop the process for producing a proposal. J Bellows, L Olavessen and E Maughan were to be the task force members and report back to PCC on Thursday, 28 August. This group should also especially consider the types of output the PCC could provide for its own use and for interested colleagues, within and outside of IAPWS. As an example the provision of a CD-ROM with the presentation would be valuable. In summary, A Zeijseink said it would not be possible this week to have a new list since no National Committee had responded formally. He further advised that from within the PCC membership there are already ideas for a new list but these would have to be validated and formally submitted by the National Committees for next year's meeting. Action A Zeijseink to contact National Committee Chairmen to progress input for a new list.

6. Report on Future of IAPWS

A Zeijseink advised the PCC that the Executive Committee had requested input of PCC on the recommendations in the Report on the Future of IAPWS. R Svoboda was appointed as PCC representative on the Committee, which will be finalising the recommendations to the Executive Committee. Action R Svoboda to represent PCC. In discussion it was agreed PCC should try to invite members with nuclear interests / expertise to join PCC. It was recognised there was a need to offer interesting material and involvement to encourage new people to support PCC and IAPWS. Action PCC membership to make suggestions to A Zeijseink. It was agreed appropriate that the minutes would include a list of the presentations made at this year's PCC sessions. A Sengers said that PCC should take one of the presentation items and explain to PCAS members in such a way that they understand the issues and could then be better equipped to work out a solution. This would help collaboration between the two groups.

7. Suggestion for Gibbs Award Nominee

In view of short time scale required by Executive Committee, A Zeijseink will ask permission to make an input by Thursday. Action A Zeijseink.

8. Joint workshop PCAS/PCC WGs Part 1 "pH Measurements at Different

Temperatures"

The following papers were presented. Copies of the papers and further information can be obtained from the authors.

A. ZEIJSEINK J. BELLOWS E. MAUGHAN D. PALMER, S. LVOV S. LVOV Y.V. ZHGENTI, D. PALMER, P. BENEZETH, D. WESELOWSKI, L. ANOVITZ	On the importance of pH measurements in Power Plant cycles. Calculation of pH from specific and cation conductivity. Practical aspects of pH measurement. Report on the pH of high temperature water. Can we measure pH of high temperature water outside a lab? An experimental investigation of borate/lithium adsorption from solution onto zirconium dioxide fuel-cladding surfaces: model of AOA phenomenon.
G. BIGNOLD	A spreadsheet for calculation of speciation, pH and conductivity
H.D. PFLUG, E. MAUGHAN	Theoretical and practical aspects for the verification of carbon dioxide in the water-steam cycle of power plants.
S. UCHIDA	Development of high temperature water chemistry sensors.
H.D. PFLUG, E. MAUGHAN	Automatic on-line calibration method for pH of ammoniacal water circuits.

8.1 Following the presentations on pH issues, a discussion took place between PCC and PCAS members on the need for future work. The question was raised 'Do power plants need to have the facility to measure pH at high temperature?'. A Zeijseink noted that a lot of work had been carried out in the laboratory to develop a high temperature pH sensor. At the present time, in most instances power plants had chosen to measure pH at low temperature and not to adopt measurement at high pH. Some plants did not have instrumentation to measure pH but calculated a value from conductivity measurements. The only possible support for adoption of pH measurement at high temperature was from BWR plants and support unlikely from fossil plants. It was felt that power plant chemists accept the existing systems and use their readings. The question was raised 'If there are inherent inaccuracies should there be an aim to improve measurement capability?'. Answering this question was considered to be important for some nuclear plant chemists. S Lvov said that the Zirconia pH measuring equipment was not as simple as a conventional pH cell. It was expensive (USD50K), bulky and required to be fitted on a bypass system with a pump incorporated. Using such equipment would allow measurement of pH at

350C at better than +/- 0.1 pH units. He asked is there any need to proceed with development to meet power plant need? There was general agreement that an outline of a guidance paper on the needs for pH measurement in power plants should be prepared. The objective would be to produce the paper within oneyear. For the outline two representatives from industry would be Nuclear Plant - S Uchido and Fossil Plant - E Maughan together with three research representatives – D Palmer, S Lvov and D MacDonald. To produce the paper researchers and users would be involved in a Task Group. For the group the following names were suggested: - D Palmer, S Lvov, D MacDonald, A Zeijseink, G Bignold, H Corti, J Bellows and A Covington. Action A Zeijseink to initiate the contact with the proposed nominees and progress the task to meet the one-year target for the guidance paper.

Tuesday 26 August 2003

Joint Workshop PCAS/PCC WGs Part 2 "Chemistry in Ultra Supercritical Plant (USC) and Other Issues"

The following papers were presented. Copies of the papers and further information can be obtained from the authors.

A. ZEIJSEINK, K. DAUCIK	Issues and requirements for chemistry in USC plant from a European perspective.		
B.D. DOOLEY	EPRI's materials program for USC.		
T. KOBAYASHI	Practical experiences with USC Kawagoe Power Plant in Japan		
J.P. JENSEN, L.S. PEDERSEN	Water Treatment at Avedøre 2 - a USC boiler.		
K. DAUCIK	Chemistry of Water/Steam Cycle in Elsam's USC		
	Units - Intentions and real experience.		
A. ZEIJSEINK	Development of water chemistry guidelines for the		
	European AD-700 USC plant		
S. LVOV	Development of hydrothermal coating technology for corrosion mitigation in high temperature aqueous		
	systems.		
T. NEMEC, F. MARSIK, D. PALMER	Binary nucleation of selected power cycle and environmentally relevant water mixtures.		

8.2 Following the presentations on Ultra Supercritical Power Plant issues, a discussion took place between PCC and PCAS members present on the need to develop an ICRN on USC water-technology. In opening the discussion, V Majer commented that at temperatures >500C physical chemistry experiments become more complicated and molecular simulation techniques could be a necessary solution. Working on aspects of importance for USC could be the future topic for the PCC / PCAS collaboration. S Lvov said that collaborative work had been started with Perboni to model behaviour at high temperature and low pressure. S Lvov offered (and PCC agreed) to give a short talk to PCC members on Molecular Modelling on Thursday 28 August. (Due to time restrictions this did

not restrictions this did not take place.) In some of the presentations on USC, materials testing rig work was described. Results from such work would influence and direct research needs. PCC members agreed that work for a PCC Task Group to define the USC issues, as a Guidance Document to issue to PCAS, is more long term than defining needs for pH measurements. A. Zeijseink said he would seek out opportunities for PCC members to meet during the coming year and produce the guidance paper needed to inform PCAS of the likely research needs. In the event that it was not possible to meet before the 14th ICPWS in Japan in August 2004, A Zeijseink would convene a workshop meeting of PCC members to discuss the topics and produce the guidance paper. Action A Zeijseink to convene appropriate meeting, and progress production of guidance paper.

9. Technical presentations/progress reports

The following papers were presented. Copies of the papers and further information can be obtained from the authors.

Monitoring			
E. MAUGHAN	On-line monitoring, technologies available and		
S. UCHIDA	the do's and don'ts. Water Chemistry Data Acquisition, Processing, Evaluation and Diagnostic Systems in Light Water Reactors - Latest Experiences with Japanese LWR Plants -		
Organics			
T. PETROVA - Dsc, prof. (MPEI (TU)) SONIYA VIDOIKOVICH – PhD	The effect of organic species on the contamination of saturated steam with sulphate and fluoride		
R.R. HARRIES	The distribution of organic matter in the steam/water cycle. Early condensate measurements in Staudinger Power Plant.		
R. SVOBODA			
Corrosion			
G. BIGNOLD	Corrosion Risk Assessments - How do other ions such as sulphate, bromide, acetate and formate compare with chloride?		
R. SVOBODA	Fluoride in power cycles.		
M. ZMITKO	Water chemistry and corrosion process monitoring during hot functional tests of		
STASTNY M., BLAHOVA O., SIMUNEK D.	Mochovce and Temelin NPPs. Copper Deposition and Surface Structure of the Steam Turbine Blades.		
Phosphate treatment M. BALL B. HUGHES	Some thoughts on Phosphate Treatment. Plant measurements leading up to the accurate calculation of sodium phosphate ratios.		

Thursday 28 August 2003

10. 14th ICPWS Proposed Programme Titles for 2nd Announcement

A Zeijseink had been requested by the IAPWS President to review the PCC related titles in the 1st Announcement and redefine them so that there were less topics listed. It would be essential that the topic titles were meaningful and recognisable to potential authors. The suggested new titles were as follows:

- 1 Power Cycle Chemistry in Conventional, Combined and Advanced Cycles.
- 2 Power Cycle Chemistry in Nuclear Cycles.
- 3 Water Purification and Other Plant Auxiliary Systems.
- 4 Steam chemistry, Condensation and Deposition.

It was further suggested that the title 'Properties of Aqueous Systems of Industrial and Geochemical Interest' should be amended to 'Properties of Aqueous Systems of Industrial and Geochemical Interest including Geothermal Energy'. PCC members pointed out that under the present IAPWS scope of work they had 'difficulty' including Renewable Energy within the titles. It was also considered that the title General Topics on Water, Steam and Aqueous Systems should be identified to include Chemical Monitoring Instrumentation and Chemical Analysis. In connection with the above titles the PCC members suggested the names of potential speakers. A Zeijseink noted the names and will pass them onto the Organising Committee. Action A Zeijseink In regard to Ultra Supercritical Power Plant issues there was a suggestion that a Workshop (with a structured programme) could be incorporated into the 14th ICPWS Meeting. In this way informed input on USC issues could be made and the Task Force would be 'brought up to speed'. No commitment was made to this suggestion, which A Zeijseink will put to the Organising Committee.

11. Conclusion on "Future of IAPWS"

R Svoboda reported back from his meeting with the group working on the proposals for the Future of IAPWS. He advised the PCC meeting that there would be four new Committees set up to formulate input on the following issues: -

- 1 Nuclear Power
- 2 Fuel cells
- 3 Effectiveness of ICRNs
- 4 IAPWS Awards

In addition there would be five task groups namely as follows: -

- 1 Properties and Formulations for High Temperature Aqueous Systems
- 2 Electrochemical Processes in High Temperature Aqueous Systems
- 3 Education and Outreach
- 4 Environmental Issues
- 5 Metastability, Nucleation, Early condensation, Droplet sprays and Cavitation

R Svoboda advised that members of these committees and groups would be sought from the various IAPWS Working Groups and outside experts possibly coopted.

12. Process for Priority List

J Bellows presented the proposed Process for the Priority List and Development of ICRNs. The document is attached to these minutes as Attachment A. The PCC members reviewed the stages in the proposed process and accepted that this was a suitable document, which the PCC should apply to future issues. It was recognised that in the use of the document some fine-tuning of the process would be applied as necessary.

13. Guideline from EBA, discussion of draft water chemistry guideline

K Daucik advised the meeting that several PCC members were involved in the drafting of the guideline alongside boiler and turbine manufacturers' nominees. Progress was being made and he expected the guideline would be available for issue in 2004. The organisation producing the guideline was now known as European Power Plant Suppliers Association. Members expressed the view that they would like to gain some knowledge of other countries guidelines.

14. Topics for next year's PCC meeting

A Zeijseink advised members that he wished to encourage members to come to the IAPWS Meetings and contribute both to the tasks set to meet identified issues and to participate in Technical Presentations. K Daucik pointed out that at the ICPWS meeting the time allocated to the Working Groups would be limited and it was likely that the PCC Meeting would be reduced to dealing with organisational matters only. The members generally agreed that in future PCC Meetings there should be a limited number of presentations focussed on a particular topic or set of related topics.

15. Membership

A Zeijseink advised members that he would write to those PCC members who had not attended a PCC Meeting in the previous three years and ask them to confirm their interest in remaining a member of PCC. After new attendees had attended two meetings in a three-year period they would be invited to become members of PCC. Action A Zeijseink

16. Election of Officers

There was no requirement to elect officers at this meeting.

17. Preparation of the Report to EC

A Zeijseink will prepare a report on the PCC activities for presentation to the Executive Committee meeting on Friday 29 August. **Action A Zeijseink**

18. Miscellaneous and Adjournment

There was no further business. A Zeijseink thanked the presenters of the papers at this meeting of the PCC. He expressed his thanks to all the members for attending and the assistance given to work on the tasks, which had been requested by the Executive Committee on Monday at the Opening Session. A Zeijseink declared the meeting closed.

PCC Attachment A

Process for Priority List

Using information available at meeting

- Problem suggestion [Monday]
- First screening—define problem more carefully
 - Is the problem widespread?
 - Is there a known root cause or most probable cause?
 - What is already known and who knows it?
- First task group (usually PCC only)

(Now on tentative (PCC private) priority list)

- o Will usually include suggester
- Problem redefinition based on screening
- What information do we really need?
- What is the case for going forward (return on investment)?
- What is (are) the best way(s) to tackle the problem?
- What is the technology gap? What are the technology options?
- What are the remaining questions?
- Second task group [Wednesday]
 - Now includes members of other working groups (usually but not necessarily PCAS)—found by first task group with aid of chairmen of other working groups
 - o Sketch research plan
 - Evaluate practicality and possible effort level required for a solution
 - o Plan ICRN's
- Review by working groups [Thursday]

(Now on priority list)

Using best information:

- Create ICRN's [Monday of next year] and lobby for funding
- Do research
 - o Midstream value review if more than one year long
- Publication with view of application
 - Patents if appropriate (must be exercised)
 - o Journal articles
- Closure of item by report to working groups
 Includes evaluation of cost and probable value
- ➢ No action in 3(?) years => drop off priority list
- > Priority list agenda item includes progress reports on the current priority items

CURRENT IAPWS RELEASES AND SUPPLEMENTARY RELEASES (September 2003)

- Supplementary Release: "Backwards Equations for the Functions *T*(*p*,*h*), *v*(*p*,*h*) and *T*(*p*,*s*), *v*(*p*,*s*) for the Region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam". (August 2003).
- "Revised Release on the IAPS Formulation 1985 for the Viscosity of Ordinary Water Substance". (August 2003). (This release is a revision of the corresponding release of 1997, which replaced the original release of 1985).
- Supplementary Release: "Backwards Equations for Pressure as a Function of Enthalpy and Entropy *p*(*h*,*s*) to the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam". (September 2001).
- Revised Release: "IAPS Formulation 1985 for the Thermal Conductivity of Ordinary Water Substances". (September 1998). (This release replaces the corresponding release of November 1985).
- "Release on the Refractive Index of Ordinary Water Substance as a Function of Wavelength, Temperature and Pressure." (September 1997) (This release replaces the corresponding release of 1991).
- "Release on the Static Dielectric Constant of Ordinary Water Substance for Temperatures from 238 K to 873 K and Pressures up to 1000 MPa.". (September 1997). (This release replaces the corresponding release of 1977).
- "Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam." IAPWS –IF 97. (September 1997) (This release replaces the 1967 IFC Formulation for Industrial Use).
- "Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use." (September 1996) (This release replaces the corresponding release of 1984).
- Release: "IAPWS Skeleton Tables 1985 for the Thermodynamic Properties of Ordinary Water Substance". (September 1994). (This is a revision of the 1985 Release).
- Release: "Surface Tension of Heavy Water Substance". (September 1994). (This is a revision of the 1985 Release).
- Release: "Surface Tension of Ordinary Water Substance". (September 1994). (This is a revision of the 1976 Release).
- "Release on the Pressure along the Melting and Sublimation Curves of Ordinary Water Substance". (September 1993). (This is a revision of the 1989 Release).
- IAPS Supplementary Release: "Saturation Properties of Ordinary Water Substance". (September 1992). (This is a revision of the 1986 Release).
- Release: "Values of Temperature, Pressure and Density of Ordinary and Heavy Water Substances at their Respective Critical Points". (September 1992) (This is a revision of the 1983 Release).
- Release: "IAPS Formulation 1984 for the Thermodynamic Properties of Heavy Water Substance". (September 1984).
- Release: "Viscosity and Thermal Conductivity of Heavy Water Substance". (September 1982. Revised February 1984).
- Release: "Ion Product of Water Substance". (May 1980).

CURRENT IAPWS GUIDELINES (September 2003)

- Guideline: "Tabular Taylor Series Expansion (TTSE) Method for Calculation of Thermodynamic Properties of Water and Steam Applied to IAPWS-95 as an Example". (August 2003).
- Guideline: "The Use of Fundamental Physical Constants and Basic Constants of Water". (September 2001).
- Guideline: "IAPWS Formulation 2001 for the Thermodynamic Properties of Ammonia-Water Mixtures". (September 2001).
- Guideline: "The Critical Locus of Aqueous Solutions of Sodium Chloride". (September 2000).
- Guideline: "Equilibrium Constant for the Distribution of Gaseous Solutes between Steam and Water". (September 1998)
- Guideline: "Equilibrium Constant for the Distribution of Gaseous Solutes between Steam and Water". (September 1998).
- Guideline: "Solubility of Sodium Sulfate in Aqueous Mixtures of Sodium Chloride and Sulfuric Acid from Water to Concentrated Solutions, from 250°C to 350°C". (September 1994). (This is a revision of the 1990 Guideline).
- Guideline: Solution of Simple Apolar Gases in Light and Heavy Water at High Temperature. (September 1993).
- Guideline: "Electrolytic Conductivity (Specific Conductance) of Liquid and Dense Supercritical Water from 0oC to 800°C and Pressures up to 1000 MPa". (May 1990).

CURRENT IAPWS ADVISORY NOTES (September 2003)

•

Advisory Note No. 1: "Uncertainties in Enthalpy for the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use (IAPWS-95) and the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (IAPWS-IF97)". (August 2003).

IAPWS CERTIFIED RESEARCH NEEDS (ICRNS) (AUGUST 2003)

- 1. Evaluation of Binary Nucleation Models. Issued September 1993. Needs Revision to extend to September 2004. IAPWS Contact: F. Sigon.
- 2. Solubility of Sodium Sulphate in Superheated Steam. Issued September 1993. Expired September 2001. IAPWS Contact: K. Daucik. Closing Statement, October 2001.
- Solubility of Spinels in the Chemical Conditions of Nuclear Reactors. September 1993. Issued September 1993. Expired September 1996. Closing statement prepared. IAPWS Contacts: D. You.
- Interaction Between Sodium Salts (Phosphates, Sulfates, Silicates, Borates) and Transition Metal Oxides. Issued September 1993. Closed September 1996. IAPWS Contact: J. Stodola.
- 5. Origin, Behaviour, and Fate of Organics in the Power Cycle. Issued September 1993. Needs Revision to extend to September 2004. IAPWS Contact: R. Gilbert.
- 6. Thermophysical Properties of Ammonia-Water Mixtures. Issued June 1994. Closed September 2002. IAPWS Contact: W. Parry. Closing Statement, July 2002.
- 7. Carryover Coefficients of Salts and Metal Contaminants in Boiler Water. Issued June 1994. Expired June 1997. Closed September 1999. IAPWS Contact: P. Tremaine.
- 8. Development of an Accurate External Reference Electrode for Use in High Temperature and High Pressure Aqueous Solutions. Issued August 1994. Expired August 1997. Closed September 1998. IAPWS Contact: S. Lvov.
- Thermodynamic Models for Transition-Metal/Water Systems under Steam Generator Conditions. Issued September 1994. Closed September 2000. IAPWS Contact: P. Tremaine
- 10. pH Measurements and Potentiometric Studies of Supercritical Aqueous Solutions. Issued May 1996. Extended to September 2002. IAPWS Contact: S. Lvov.
- 11. Properties of Salts in Steam. Issued May 1996. Closed September 2001. IAPWS Contacts: D. Palmer and R. Fernandez-Prini. Needs Closing Statement.
- 12. Kinetics of the Oxygen and Hydrogen Electrode Reactions in Subcritical and Supercritical Aqueous Systems. Issued September 1998. Closed September 2001. IAPWS Contacts: S. Lvov and D. Macdonald. Needs Closing Statement.
- 13. Surface Tension of Aqueous Solutions. Issued September 1998. Needs Revision to extend to September 2004. IAPWS Contacts: F. Sigon and F. Gabrielli.
- 14. Thermophysical Properties of Humid Air and Combustion-Gas Mixtures. Issued July 2002. Expires September 2005. IAPWS Contacts R. Span and F.L. Blangetti.
- 15. Thermodynamic Properties of Metastable Steam. Issued July 2002.Expires September 2005. IAPWS Contact: B. Rukes.

IAPWS Collaborative Grant Proposal

An experimental study of *PVTx* properties for the system ammonia + water at high temperatures and pressures

IAPWS Sponsors

Dr. Allan H. Harvey

Prof. Alexsei A. Alexandrov

Theory and Modeling Group Physical and Chemical Properties Division NIST, Boulder, CO 80305, USA Phone (303) 497 3555 Fax: (303) 497 5224 e-mail: aharvey@boulder.nist.gov Moscow Power Institute Krasnokazarmennaya 17 Department TOT Moscow E-250, Russia Fax: 7-095-362-7171 e-mail: petrova@twt.mpei.ac.ru

Senior Investigators

Prof. Ilmutdin M. Abdulagatov

Head of the Thermophysical Division of the DSC RAS Division Makhachkala, Dagestan, Russia USA Phone (303) 497 4027 Fax: (303) 497 5224 e-mail: ilmutdin@boulder.nist.gov

Dr. Joseph W. Magee

Leader Experimental Group Physical & Chemical Properties NIST, Boulder, CO 80305,

Phone (303) 497 3298 Fax: (303) 497 5224 e-mail: magee@boulder.nist.gov

Visiting Young Scientist

(Dr. Emil A. Bazaev, or colleague to be named) Institute for Geothermal Research of the Dagestan Scientific Center of the Russian Academy of Sciences, 367003 Makhachkala, Shamilya Str. 39A, Dagestan, Russian Federation

August 25, 2003

49

This proposal will have four principal outcomes: it will strengthen collaborations between the Thermophysical Division of the Dagestan Scientific Center of the Russian Academy of Sciences (DSC RAS) and the National Institute of Standards and Technology (NIST) in the US; it will enable a young scientist to travel from the DSC RAS to NIST for training in best practices for calibrations, measurements and data evaluation; it will provide the IAPWS community with new measurements of PVTx properties for the aqueous system ammonia + water in wide ranges of temperature and pressure, including near-critical and supercritical regions; and, it will initiate a broad program of measurements and models for the ammonia + water system.

An IAPWS Certified Research Need [1] indicated a need for properties for ammonia + water mixtures at temperatures to 866 K (593°C) at pressures up to 35 MPa, covering the complete range of composition. In spite of research activity from 1997 to 2002 that was reported in the Closure Statement for this ICRN, data are still very limited in high-temperature regions for ammonia + water mixtures.

The primary reasons for the scarcity of data are experimental difficulties related to the fact that this system is corrosive, toxic, potentially flammable, and has a high relative volatility. Special materials, safety procedures, special equipment and a knowledge of their proper use are all required. Only a handful of labs, including NIST, have been able to make sufficient investment in training and materials to make such measurements.

Accurate *PVTx* data are essential to the development of an accurate equation of state. New experimental data are particularly needed [2] at temperatures T > 523 K, which is the present upper limit of reported measurements. Both the Physical and Chemical Properties Division of NIST and DSC RAS have extensive experience and capabilities in accurate *PVTx* measurements covering wide ranges of temperature and pressure. We have reported [3-6] *PVTx* data for aqueous systems (H₂O + alcohol, H₂O + hydrocarbon, and H₂O + D₂O) in the near-critical and supercritical regions. For reasons mentioned earlier, the labs of DSC RAS and NIST are among the few research facilities in the world with capabilities for H₂O + ammonia *PVTx* measurements in the near-critical and supercritical regions, as documented at a Workshop on Properties of H₂O + Ammonia [7].

Under other funding, Prof. Abdulagatov's team in the Dagestan Labs will investigate PVTx properties in a temperature range from 300 to 673 K (27 to 400°C) at pressures up to 35 MPa. The measurements will be for a fixed composition of 0.5 mole fraction ammonia, with an uncertainty in density of 0.1 %. This investigation will provide reliable PVTx properties by using a high-temperature and high-pressure constant-volume piezometer [3-6].

Following the experiments, we plan to bring a younger Dagestan Labs scientist to the Boulder Labs of NIST for 3 to 4 months. Dr. Emil Bazaev will be our top choice, since his PhD was granted in 2000 for a dissertation on PVTx properties. Dr. Bazaev will assist Joseph Magee and his team in the Boulder Labs with the following tasks: (1) additional PVTx measurements with a high-temperature corrosion-resistant direct-weighing PVTx apparatus [8], at temperatures up to 1000 K; (2) analysis of the PVTx data; and, (3) comparison with published measurements and models, especially the IAPWS Formulation 2001 for the Thermodynamic Properties of Ammonia-Water Mixtures. As an additional educational component of his visit, we will conduct detailed discussions and comparisons of the experimental PVTx techniques used in the Dagestan Labs with those used in the Boulder Labs (isochoric gas expansion, direct-weighing isochoric, vibrating-tube densimeter and dual-sinker densimeter), methods for precise gravimetric mixture preparation, a propagation of uncertainties analysis, round-robin measurement comparisons, and establishing a chain of traceability to national and international standards.

The proposed *PVTx* measurements for IAPWS are to be carried out on a 0.5 mole fraction ammonia + 0.5 mole fraction water mixture at the conditions:

- Temperatures from 373 K to 673 K
- Pressures from 0.1 MPa to 50 MPa
- Measurements will be carried out in the liquid phase, vapor phase, and the supercritical fluid regions of the mixture.

The measurements will be compared to other experimental densities and all will be compared with the formulation in the current IAPWS Guideline.

Other funding will be sought for additional gas-phase PVTx measurements in a new apparatus, from 373 K to 1000 K, at pressures from 0.1 MPa to 20 MPa, and also specific heat, viscosity, and thermal conductivity.

Budget

We propose a total budget of \$10,000 for this project and a period of performance of one year. This would pay for the travel expenses and visit for Dr. Emil Bazaev or other young DSC RAS scientist for his work in Boulder with the US-based research team. A project report will be prepared and submitted to IAPWS by the next annual meeting.

Leveraging of the IAPWS Support

The research team has planned a comprehensive research project on the ammonia + water system, involving partnerships with university-based researchers. To leverage the support from IAPWS, we will seek additional support from other agencies. Toward the end of the proposed one-year IAPWS project, one or more proposals will be prepared to support the following tasks: (1) additional measurements of thermodynamic properties (a) *PVTx* data for two other compositions of the ammonia + water system and (b) C_V data with a constant-volume adiabatic calorimeter (Dagestan) at temperatures to 673 K; (2) measurements of transport properties (a) viscosity with a new oscillating-wire viscometer (Boulder), for which new high-temperature electrical feeds have been developed and (b) thermal conductivity with a tantalum transient hot-wire apparatus (Boulder); (3) development of new models for (a) thermodynamic properties – a Helmholtz fundamental equation and a crossover model for the critical region and (b) for transport properties – viscosity and thermal conductivity.

References

- IAWPS Certified Research Need ICRN #6. Thermophysical Properties of Ammonia-Water Mixtures, Issued by International Association for the Properties of Water and Steam, June 1997.
- 2. R. Tillner-Roth and D.G. Friend, J. Phys. Chem. Ref. Data. 27, 63 (1998).

- Rabezkii, M.G., Bazaev, A.R., Abdulagatov, I.M., Magee, J.W., Bazaev, E.A. PVTx Measurements for Water + Toluene Mixtures in the Near-Critical and Supercritical Regions. J. Chem. Eng. Data, 2001. V.46. P.1610-1618.
- Bazaev A.R., Abdulagatov I.M., Magee J.W., Bazaev E.A., Ramazanova, A.E., PVTx Measurements for H₂O+D₂O Mixtures in the Near-Critical and Supercritical Regions, J. Supercritical Fluids. 2003, V.26. P.115-128.
- Abdulagatov, I.M., Bazaev, E.A., Bazaev, A.R., Rabezkii, M.G. PVTx Measurements for Dilute Water+N-Hexane Mixtures in the Near-critical and Supercritical Regions. J. of Supercritical Fluids. 2001. V.19. P.219-237.
- Bazaev, A.R., Abdulagatov, I.M., Magee, J.W., Bazaev, E.A., Ramazanova, A.E., PVTx Measurements for (0.64 mol frac.) H2O+(0.36 mol frac.)Methanol Mixture in the Sub-Critical and Supercritical Regions, Int. J. Thermophys. 2003, in review.
- D.G. Friend and W.M. Haynes, NIST Report of the Workshop on Thermophysical Properties of Ammonia/Water Mixtures, 1996. Boulder, Colorado, USA.
- Magee, J.W., Abdulagatov, A.I. Direct–Weighing Corrosion–Resistant High– Temperature Isochoric PVT Apparatus, Fifteenth Symposium on Thermophysical Properties, Boulder, Colorado, USA. 2003.

PRESS RELEASE FOR IAPWS ANNUAL MEETING IN VEJLE, DENMARK

August 2003

Fifty-nine scientists and engineers from thirteen countries attended the annual meetings of the International Association for the Properties of Water and Steam (IAPWS), August 24-29, 2003 in Vejle, Denmark. IAPWS provides standards for steam and water properties and serves as a forum where engineers from the power industry and academic scientists can communicate problems and solutions to each other. IAPWS has traditionally concentrated on the science underlying the thermodynamics and chemistry in steam power plants, but is broadening into other aspects of power generation and high temperature aqueous systems.

In 1997, IAPWS adopted a formulation for industrial calculations IAPWS-IF97. It includes both defining equations and backward (closely approximating inverse) equations to promote speed of calculation. This year IAPWS approved supplementary backward equations, with pressure and enthalpy or pressure and entropy as the input variables, that significantly enhance the speed of computation for calculations using IAPWS-IF97. IAPWS expects to enhance IAPWS-IF97 further with additional backward equations. IAPWS also approved the "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". This guideline describes a method to do fast calculations based on the Release on the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use. An advisory note on the Uncertainties in Enthalpy for the IAPWS Formulation 1995 for the Thermodynamic Properties of Water and Steam (IAPWS-95) and the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (IAPWS-95) and the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (IAPWS-1F97) has also been released.

The working group on Power Cycle Chemistry exchanges information on the chemical problems in steam power plants world wide. Highlights of this exchange were a workshop on pH measurement in high purity water and at working temperatures up to 300°C. A series of talks on plans for the new ultrasupercritical plant with steam temperatures of 760°C led to considerable discussion of the chemical issues such a plant would face. Work on research plans to solve those issue will progress through the coming year.

Simulation of thermophysical properties of water continues to be an interest of IAPWS. The IAPWS Helmholtz Award lecture this year, "New Techniques for the determination of Phase Properties of Aqueous Systems via Computer Simulations," by E. Luijten of the University of Illinois, provided additional insights into ways to understand phenomena that occur in experimentally difficult regions.

A joint project between Aristotle University (Greece) and NIST (USA) to develop a new formulation for the viscosity of water furthers both science and the important IAPWS goal of international cooperation in developing formulations. Other major projects in progress include a critical compilation of high temperature experimental techniques and data on a variety of properties of aqueous systems, a proposed joint project between IAPWS and IUPAC for the hydration properties of selected organic solutes, and a monograph The Physical and Chemical Properties of Aqueous Systems at Elevated Temperatures and Pressures: Water, Steam and Hydrothermal Systems, due out early in 2004.

The next IAPWS meeting will be the 14th International Conference on the Properties of Water and Steam: Water, Steam and Aqueous Solutions for Electric Power—Advances in Science and Technology. It will be held August 29-September 3, 2004 in Kyoto, Japan. The deadline for abstracts for this conference is December 15, 2003. The IAPWS working groups and executive committee will meet before the conference on August 29, 2004. Details of the meeting will be available through links from the IAPWS website at www.iapws.org. Minutes of the 2003 meeting will appear on the website shortly.

People interested in IAPWS documents and activities should contact the chairman of their IAPWS National Committee (see website [or fill in information]) or the IAPWS Executive Secretary, Dr. Barry Dooley, EPRI, 3412 Hillview Ave, Palo Alto, California 94304, USA.

BIAPWS Report to IAPWS for 2003

BIAPWS has continued its programme of providing co-ordination of information to the sponsor companies. This year an expanded format consisting of a symposium with associated workshops was introduced. This event took place in May 2003. The programme was as set out in Attachment A to Attachment 12. Although support was less strong than in previous years, BIAPWS has made the commitment to continue to support such events on a regular basis.

Where possible BIAPWS is encouraging the publication of the material presented at its symposia in PowerPlant Chemistry.

The BIAPWS Prize

BIAPWS has also introduced a prize for the best University undergraduate project in fields of relevance to IAPWS interests. The Prize of £1000 has just been awarded to Miss Lindsay Plant from the University of Manchester for a research project report entitled "Third Phase Formation in the Purex Process".

BIAPWS Sponsors

Support for BIAPWS activities has proved more difficult to sustain during the last year because of economic pressures on the sponsor companies.

Despite these pressures, BIAPWS retains the active support of the following companies: *ABB Automation, Alstom Power, British Energy, ESB, Innogy, Powergen, PX Limited and Scottish Power*

G J Bignold 23 August 2003

Attachment A to Attachment 12

<u>Workshop 1 – 6 May 2003</u>

Use of Alternative Boiler Water and Feedwater Treatment Chemicals

- Facilitator - Richard Harries, Powergen

Steam Purity requirements for Unit Start-up

- Facilitator – Mr. Ken McGrath

Wednesday 7 May

Symposium on Power Plant Chemistry and Corrosion Issues

Session 1 - Chemistry and materials issues for steam/water circuits

Avedøre 2 – a Multi-fuel Concept. – J. P. Jensen, Energi E2, Denmark.

Environmental cracking processes in power plant materials: Electrochemical Interactions – J. D. Atkinson, Sheffield Hallam University, U.K.

Fundamental aspects of oxidation processes for engineering materials in steam. –

S. Osgerby, NPL, UK.

Corrosion of stainless steels – Interaction with Carbon Dioxide. E. Maughan - College of Knowledge, and J. Rau. Dockweiler, Germany.

Session 2 Corrosion Issues in Steam Water Circuits

Long time stress corrosion testing of steam turbine rotor and disc steels -

S. R. Holdsworth and B. W. Roberts - Alstom Power Ltd, U.K.

Electrochemical Corrosion Monitoring in a Low Pressure Steam Turbine – G. Quirk, British Energy, U.K

Interpretation of Corrosion Monitoring Data in terms of Steam Turbine Operation – G. Bignold, Innogy, U.K.

Workshop 2 - Thursday 8 May

Power Cycle Chemical Control - Facilitator – Patrick Colman, ESB Materials Selection issues and implications for Power Plant Chemistry - Facilitator – Geoff Bignold, Innogy

The Czech National Committee

International Association for the Properties of Water and Steam

REPORT on IAPWS related activities – July 2002 / August 2003

Submitted to the EC Meeting of IAPWS, Vejle – August 2003.

National Committee Contacts:

CZ NC PWS - Institute of Thermomechasnics, Dolejskova 5, 182 00 Prague 8, Czech Republic

Fax: + 420 2 858 4695, E-mails: <u>sifner@it.cas.cz</u>; <u>secr.czncpws@it.cas.cz</u> Prof. R.Mareš, Fax: + 420 377 638 102, E-mail: <u>maresr@kke.zcu.cz</u>

- 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 (ICHT-IE) and Department of Physical Chemistry (ICHT-IPCh), Technická 5, CZ-166 28 Prague 6
- **University of West Bohemia** (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, Ministry of Industry and Trade, and IAPWS.

- Prof.Mares (UWB) and Dr.Sifner (IT) prepared a paper on temperature conversion and recalculation of the thermal conductivity Ref. [1].
- Prof.Mares (UWB) solved a problem of measurements of heat when the supplying medium is wet steam and presented at the Conference Power Engineering-2003 organized by University of West Bohemia, Ref. [2].
- Prof.Marsik (IT) with co-authors modified and finished the manuscript of the Chapter 7: Binary Homogeneous Nucleation in Selected Aqueous Solutions for the ATLAS, Ref. [3]. The modifications respected recommendations of Dr.Palmer, Dr.Harvey, and reviewers. The further results of investigations into condensation, evaporation, and cavitation are presented in Refs. [4 to 9].
- Doc. Sedlbauer (TUL) collaborated with Profs. Majer and Wood on preparing the final version of Chapter 4: Calculation of Standard Thermodynamic Properties of Aqueous Solutes in a Wide Range of Temperatures and Pressures for the ATLAS Ref. [10]. In further research the

group (CZ-Fr cooperation) developed and applied the contribution method for standard thermo-dynamic properties (namely air-water distribution constants) of hydrocarbons in a wide range of temperature and pressure Refs. [11 to 15].

- Research activities at the CTU in Prague, Dept. of Fluid Dynamics and Power Engineering headed by Prof. Petr have continued during the period 7/2002 – 8/2003 in further improving our knowledge on the droplet nucleation process occurring in LP steam turbines by means of
 - analysis of realised diagnostics of wet steam in 1000 MW nuclear and 210 MW fossil steam turbines
 - tests with the expansion chamber for controlled heterogeneous droplet nucleation of steam.

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 and moisture level
- electrostatic charge of the droplet population
- chemical impurities in the steam.

The expansion chamber was found to be suitable test equipment for prediction of still unknown initial size and concentration of the heterogeneous impurities that could participate in the nucleation process. The data obtained in the mentioned turbine and the expansion chamber tests have been used in improving computational model of the droplet nucleation in LP steam turbines. Information on the research activities can be found in Refs. [16, 17].

 ICT-IE is concerned with power cycle chemistry, which is divided into water treatment for fossil and nuclear power plants, problems of electrochemistry and questions of material and corrosion. Typical behavior of organic compounds in steam/water cycle is studied. The results of this research team are published in Refs. [18 to 28]

• ICT-IE organized "The 4th International Power Cycle Chemistry Conference" (CHEOS 4) in September 3-5, 2002 in Prague under the auspices of the CZ NC PWS.

- Dr.Hnedkovsky (ICT-IPC) with collaborators investigated properties of organic solutes in water. The solute vapor absorption technique was applied at measurement of aqueous solubility of hydrophobic volatile organic compounds. Solution and transfer processes were modelled in non-polar solutes in water and aqueous solutions. Published articles are under Refs. [29 to 38].
- Stastny (SKODA ENERGO) with co-workers studied effects of deposits on the blades of HP and MP parts of steam turbine in fossil power station by chemical analysis, investigated degradation of steam turbine blade surfaces by deposits of chemicals, tested numerical models of the water steam flow with condensation in nozzles, and developed an advanced numerical model with entropy calculation. Refs. [39 to 43].

Reactor services division of Nuclear Research Institute Řež plc. has been engaged mainly in loop experiments and material testing in the research reactor LVR-15. Investigation of an effect of simultaneous influence of irradiation, water chemistry and high parameters (pressure, temperature) on behaviour of nuclear power plants structural materials and components is the main goal of the experimental programmes. The irradiation projects in progress are focused currently on the following research areas:

- investigation of fuel rod cladding materials (eg. Zircaloy-4 alloy) corrosion behaviour at specific VVER water chemistry conditions,
- investigation of an effect of water chemistry on radionuclides transport and radioactivity build-up in the reactor primary systems (eg. effect of ammonia and hydrazine),

 investigation of an effect of water chemistry, stress level and irradiation on irradiation assisted stress corrosion cracking (IASCC) of reactor pressure vessel and in-core structures materials.

A significant share of their effort was devoted to co-operation with nuclear power plants (NPPs), mainly in field of water chemistry, corrosion problems and radiation control. The following activities were carried out:

- A passivation procedure of the primary system inner surfaces during hot functional tests was developed and applied at unit 1 and 2 of NPP Temelín. Surveillance samples (coupons) were placed into the primary circuits and subsequently analysed to obtain information about characteristics of the developed passive film (morphology, chemical and phase composition).
- Primary and secondary water chemistry guidelines for VVER-440 and VVER-1000 units was prepared and issued for NPPs operated by the Czech Utilities (CEZ a.s.). Main principles of the guidelines reflect current status of knowledge and operational experience obtained in NPPs.

Young Scientists IAPWS Fellowships:

EC IAPWS granted a fellowship to T. Němec on the basis of the Proposal for the Young Scientists IAPWS (CZ-US) Project "Thermodynamic of Binary Homogeneous Nucleation in Superheated Steam". The scientific cooperation proceeds under supervising Prof.Maršík, Dr.Hrubý (both Czech Republic) and Dr.Palmer and Dr.Simonson (both U.S.A). The subject of the project consists in preparation a database of nucleation-relevant thermodynamic properties for several water-admixture binaries relevant to power cycles and to employ this database in a nucleation simulation program, solving the kinetic equations of nucleation. Final report of the project will be submitted by the end of 2003, brief information will be given at the WG-PCSA meeting in Denmark.

• References:

- [1] Mares R., Sifner O.: *Temperature conversion of the coefficient of thermal conductivity*, Proceedings of the University of West Bohemia in Pilsen, Pilsen, 2002, pp 65-70.
- [2] Mares R.: *Measurement of heat supplied by wet steam*, Proceedings of the Conference "Power Engineering 2003", Pilsen 2003, pp 79-84 (in Czech).
- [3] Marsik F., Hruby J., Demo P., Kozisek Z., Petr V., Kolovratnik M.: Chapter 7. Homogeneous Nucleation in Selected Aqueous Solutions (prepared for ATLAS The Physical and Chemical Properties of Aqueous Systems at Elevated Temperatures and Pressures: Water, Steam and Hydrothermal Solutions, Editors: Palmer D.A., Fernandez-Prini R., Tremaine P.)
- [4] Maršík F., Delale C.F., Sedlář M.: Condensation and Cavitation in Water and Water Mixtures, Archives of Thermodynamics, Vol. 24 (2003), No.1, pp.3-16
- [5] Delale C.F., Hruby J., Marsik F.: Homogeneous bubble nucleation in liquids: The classical theory revisited. J. Chem. Phys. Vol.118, No.2 (2003) 792-806.
- [6] Zima P., Maršík F., Sedlář M.: Cavitation Rates in Water with Dissolved Gas and Other Impurities, pp.268-273
- In: Aerothermodynamics of Internal Flows VI, Proceedings of the Sixth International Symposium on Experimental and Computational Aerothermo-dynamics of Internal Flows, Volume 2, Shanghai, 2003
- [7] Maršík F., Zima P., Sedlář M.: Estimation of Boiling and Cavitation Rates Based on Thermodynamic Fluctuations. In: Boiling Heat Transfer, Proceedings of the 5th International Conference ICBHT 2003, Montego Bay, 2003
- [8] Zima P.: *Cavitation Rates and Bubble Dynamics in Gas-Contamined Water*, PhD Thesis, Czech Technical University in Prague, Faculty of Mechanical Engineering, Prague, 2003

- [9] Hošek J.: *Optical Apparature for Studies of Aerosol Growth*, Czech Technical University in Prague, Faculty of Mechanical Engineering, PhD Thesis, Prague, 2003 (in Czech)
- [10] Majer V., Sedlbauer J., Wood R.H.: Chapter 4. Calculation of Standard Thermodynamic Properties of Aqueous Solutes in a Wide Range of Temperatures and Pressures, (prepared for ATLAS The Physical and Chemical Properties of Aqueous Systems at Elevated Temperatures and Pressure: Water, Steam and Hydrothermal Solutions, Editors: Palmer D.A., Fernandez-Prini R., Tremaine P.)
- [11] Sedlbauer J., Bergin G., Majer V.: Group Contribution Method for the Henry's Law Constant of Aqueous Hydrocarbons, AIChE J., 48, 2936-2959 (2002).
- [12] Sedlbauer J.: Semi-Empirical Models for Standard State Properties of Aqueous Non-Electrolytes, The 6th Liblice Conference on the Statistical Mechanics of Liquids, Špindlerův Mlýn, 2002.
- [13] Majer V., Sedlbauer J., Roux-Desgranges G., Ballerat K.: Thermodynamic Modeling of Biochemical Reactions at Extreme Conditions; Experiments and Predictions for Aqueous Organic Compounds, 17th IUPAC Conference on Chemical Thermodynamics, Rostock, 2002.
- [14] Sedlbauer J., Bergin G., Majer V.: Group Contribution Method for the Henry's Law Constant KH(T, p) of Aqueous Hydrocarbons, 16th European Conference on Thermophysical Properties, London, 2002.
- [15] Sedlbauer J., Bergin G., Majer V.: Software for Calculating the Henry's Law Constant of Aqueous Hydrocarbons at High Temperatures, 19-th European Seminar on Applied Thermodynamics, Santorini, 2002.
- [16] Petr V., Kolovratník M.: Diagnostics of Wet Steam in LP Steam Turbines, In: Proceedings 5th European Conference on Turbomachinery – Fluid Dynamics and Thermodynamics, Prague, 2003, pp.687-698.
- [17] Petr V., Kolovratník M., Hanzal V.: Instrumentation and Tests on Droplet Nucleation in LP Steam Turbines. In: Proceedings 7th International Conference on Cycle Chemistry in Fossil Plants, Houston, 2003.
- [18] Kučera P., Novotný R., Sajdl P., Macák J.: *Elektrochemical Noise in Corrosion Studies*, Conference on *Power Plant Chemistry CHEO4*, Prague, 2002 (in Czech).
- [19] Trapl K., Kučera P., Novotný R., Sajdl P., Macák J.: Accoustic Emission in Corrosion Of Brass, Conference on Power Plant Chemistry CHEO4, Prague, 2002 (in Czech).
- [20] Macák J., Růžičková M., Sajdl P.: The Use Of Zirkonium Alloys in Nuclear Industry, Conference on Power Plant Chemistry - CHEO4, Prague, 2002 (in Czech).
- [21] Růžičková M., Macák J., Sajdl P., Novotný R: In-Situ Study OF Zirkonium Alloy Corrosion, Conference on Power Plant Chemistry CHEO4, Prague, 2002 (in Czech).
- [22] Sajdl P., Matocha K., Vošta J., Novotný R., Macák J., Jiříček I.: Effect of Copper Ions on Stress Corrosion Cracking Of Steel, Conference on Power Plant Chemistry - CHEO4, Prague, 2002 (in Czech).
- [23] Machníková E., Jiříček I., Vošta J., Macák J.: Turbine Steel Passivity and Its Protection by PVD Coatings, Conference on Power Plant Chemistry CHEO4, Prague, 2002 (in Czech).
- [24] Jiříček I., Kalivodová J., Machníková E., Macák J., Vošta J.: Organic Compounds Balance in Steam Water Cycle, Conference on Power Plant Chemistry CHEO4, Prague, 2002 (in Czech).
- [25] Kalivodová J., Jiříček I., Machníková E., Novotná M.: Turbine Deposit Composition in CZ Powerhouses, Conference on Power Plant Chemistry CHEO4, Prague, 2002 (in Czech).
- [26] Hubálek R., Macák J., Vošta J., Novotná M., Jiříček I: Iron Oxide Characterisation by EIS, Conference on Power Plant Chemistry CHEO4, Prague, 2002 (in Czech).
- [27] Dohnálková M., Dudr V., Sajdl P., Novotný R.: Distribution of Disolved Gas Concentration in Systems with Temperature Gradient, Conference on Power Plant Chemistry CHEO4, Prague, 2002 (in Czech).
- [28] Novotná M., Macák J., Jiříček I., Kalivodová J.: Application of IR Spectroscopy in Surface Analysis of Metals, Conference on Power Plant Chemistry CHEO4, Prague, 2002 (in Czech).
- [29] Hynčica P., Hnědkovský L., Cibulka I.: Partial Molar Volumes of Organic Solutes in Water. VII. Oand p-aminobenzoic Acids at Temperatures T = 298 K to 498 K and o-diaminobenzene at Temperatures T = 298 K to 573 K and Pressures up to 30 MPa, The Journal of Chemical Thermodynamics 34, 861-873 (2002)

- [30] Hovorka Š., Roux A.H., Roux-Desgranges G., Dohnal V.: Limiting Partial Molar Excess Enthalpies of Selected Organic Compounds in Water at 298.15 K, Journal of Chemical and Engineering Data 47, 954-959 (2002)
- [31] Hovorka Š., Dohnal V., Roux A.H., Roux-Desgranges G.: Determination of Temperature Dependence of Limiting Activity Coefficients for a Group of Moderately Hydrophobic Organic Solutes in Water, Fluid Phase Equilibria 201, 135-164 (2002)
- [32] Hnědkovský L., Hynek V., Majer V., Wood R.H.: A New Version of Differential Flow Heat Capacity Calorimeter; Tests of Heat Loss Corrections and Heat Capacities of Aqueous NaCl from T = 300 K to T = 623 K, Journal of Chemical Thermodynamics 34, 755-782 (2002)
- [33] Majer V., Hynek V., Coxam J.-Y., Ballerat-Busserolles K.: Flow Methods for Measurements of Calorimetric and Volumetric Data of the Aqueous Systems, 3eme Forum de la Technologie des Hautes Pressions, Cologne-la-Rouge, 2002
- [34] Hnědkovský L., Wood R.H.: Electrical Conductivity of Aqueous Solutions: A New Method for Evaluation of Primary Experimental Data, 17th IUPAC Conference on Chemical Thermodynamics, Rostock, 2002
- [35] Hnědkovský L., Cibulka I.: Group Contributions for an Estimation of Partial Molar Volumes at Infinite Dilution for Aqueous Benzene Derivatives at Extended Ranges of Temperature and Pressure, 17th IUPAC Conference on Chemical Thermodynamics, Rostock, 2002
- [36] Fenclová D., Laštovka V., Dohnal V., Vrbka P.: Temperature Dependence of Limiting Activity Coefficient of 2-methyl-2-propanol in Water, 15th International Congress of Chemical and Process Engineering CHISA 2002, Praha, 2002
- [37] Dohányosová P., Dohnal V., Fenclová D.: A New Generator Column Apparatus to Determine the Temperature Dependence of Aqueous Solubility of Polynuclear Aromatic Hydrocarbons, 15th International Congress of Chemical and Process Engineering CHISA 2002, Praha, 2002
- [38] Dohnal V.: Air-Water Partitioning of Organic Compounds of Environmental Interest, 15th International Congress of Chemical and Process Engineering CHISA 2002, Praha, 2002
- [39] Šťastný M., Šejna M.: Numerical Modeling of the Steam Flow with Condensation in Nozzles, IAPWS Annual Meeting, Buenos Aires, 2002.
- [40] Šťastný M.: Effect of Deposits in HP Part on Steam Turbine Parameters, Proceedings of 16th Seminar on Turbomachinery 2002, Dresden, 2002.
- [41] Šťastný M.: Surface Degradation of Steam Turbine HP Blades, Conference on Power Plant Chemistry CHEO4, Prague, 2002 (in Czech).
- [42] Vaibar R., Nejedlý J., Brandner M., Míka S., Šťastný M.: Numerical Modeling of Two-Phase Wet Steam Flow With Homogeneous and Heterogeneous Condensation, Conference on Multiphase Flows in Industrial Applications, Dresden, 2003.
- [43] Šťastný M., Bláhová O., Šimůnek D.: Changes of Surface Roughness connected with Copper Deposition on the Steam Turbine Blades, IAPWS Annual Meeting, Vejle, 2003.

Danish National IAPWS Committee - DIAPWS

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

20 February 2003

IAPWS REPORT 2002

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

Part of the investigation of solubility of salts in superheated steam finished in 1999 were published in Power Plant Chemistry.

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, which improves its fit to the experimental data.

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

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

Publications in 2002:

J.P.Jensen, K.Daucik; Solubility of Sodium Chloride in Superheated Steam, Power Plant Chemistry 4 (2202), No. 11, p. 653 - 659

J.P.Jensen, K.Daucik; Solubility of Sodium Sulfate and Sodium Hydroxide in Superheated Steam, Power Plant Chemistry 4 (2202), No. 12, p. 735 – 740

Research Activities on the Thermodynamic Properties of Water Substance in Germany 2002/2003

In the period named above the following work has been done:

University of Applied Sciences of Zittau and Görlitz

Prof. Dr.-Ing. habil. H.-J. Kretzschmar

- 1. Supplementary backward equations T(p,h), v(p,h), and T(p,s), v(p,s) for region 3 of IAPWS-IF97
- The backward equations T(p,h), v(p,h), and T(p,s), v(p,s) for region 3 of IAPWS-IF97 were successfully evaluated by IAPWS. During the evaluation process, further comparison and test calculations were carried out.
- The Draft of "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 completed
- 2. Supplementary backward equations p(h,s) for region 3 of IAPWS-IF97
 - The backward equations p(h,s) for region 3 were completed and successfully tested in process modelling.
 - In addition, equations of h and s for the region boundaries and an equation $T_{sat}(h,s)$ for wet steam were developed. The equations can be used in combination with the Industrial Formulation IAPWS-IF97.
 - The Draft of "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 formulated and submitted to the IAPWS Working Groups "Industrial Requirements and Solutions" and "Thermophysical Properties of Water and Steam"
- 3. Supplementary backward equations v(p,T) for region 3 of IAPWS-IF97
 - The investigations regarding the achievable accuracy close to the critical point and the division of region 3 into subregions were completed.
 - First equations were developed for the subregions.
- 4. Supplementary backward equations p(h,s) for regions 1 and 2 of IAPWS-IF97
- The comprehensive publication:
 Kretzschmar, H.-J., Cooper, J. R., Dittmann, A., Friend, D. G., Harvey, A., Gallagher, J.,
 Knobloch, K., Mareš, R., Miyagawa, K., Stöcker, I., Trübenbach, J., Wagner, W., and
 Willkommen, Th., "Supplementary Backward Equations for Pressure as a Function of Enthalpy
 and Entropy *p*(*h*,*s*) to the Industrial Formulation IAPWS-IF97 for Water and Steam"
 was completed and submitted to the Journal of Engineering for Gas Turbines and Power.
- 5. Investigations on Thermodynamic Properties of Humid Air Part of the project "Advanced Adiabatic Compressed Air Energy Storage" (AA-CAES) of the European Union
- A property data base for humid air was set up
- Comparison calculations of different models for calculating thermodynamic properties of humid air were started

- 6. Implementation of the Industrial Formulation IAPWS-IF97 on pocket calculators
- The program FluidCASIO for Casio ALGEBRA 2.0 was completed.
- The program FluidTI for the model voyage 200 of Texas Instruments was prepared.
- 7. Property libraries for water and steam, combustion gas mixtures, and humid air for education
 - The versions for students of the programs
 - Add-In FluidEXL for Excel[®]
 - FluidMAT for Mathcad[®]

were revised.

_

Ruhr-Universität Bochum

Prof. Dr.-Ing. W. Wagner

1. Uncertainties in Enthalpy for the IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use (IAPWS-95) and the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (IAPWS-IF97).

These investigations resulted in the IAPWS Advisory Note No. 1 that is ready to be adopted by IAPWS at its annual meeting in Vejle, Denmark, 2003.

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, Vejle - August 2003

National Committee Contact: Prof. Marc J. Assael, Chemical Engineering Department, Aristotle University 54124 Thessaloniki, Greece Tel. +302310.996163, Fax. +30231.996190, EMail. assael@auth.gr

SCIENTIFIC WORK

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

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

2) Work under IAPWS Collaborative Grant "Formulations for the Viscosity and Thermal Conductivity of Water and Heavy Water: Evaluated Experimental Database and Initial Correlations"

The task of developing updated formulations for the viscosity and thermal conductivity of water is a very high priority within the Working Group on Thermophysical Properties of Water and Steam. The international effort on this project involves researchers from Russia, United Kingdom, Germany, and Japan, as well as from Greece and the United States. Considerable progress has been made on the task (see, e.g. M.J. Assael, E. Bekou, D. Giakoumakis, D.G. Friend, M. Killeen, J. Millat, and A. Nagashima, "Experimental Data for the Viscosity and Thermal Conductivity of Water and Steam," J. Phys. Chem. Ref. Data 29 (2), 141-166, 2000; A.A. Aleksandrov and A.B. Matveev, "Equation of Dynamic Viscosity in the Region of Existence of the Liquid and Gaseous Phases of Water: Method of Derivation," High Temp. (Russ.) 36, 885-890, 1998; M.J. Assael, V.K. Tsalmanis, N.K. Dalaouti, D. Giakoumakis, and A. Nagashima, "Transport Properties of D₂O: Data Survey & Comparisons," in Steam, Water and Hydrothermal Systems: Physics and Chemistry Meeting the Needs of Industry, Proc. 13th Int. Conf. on the Properties of Water and Steam, NRC Research Press, Ottawa, 2000, P.R. Tremaine, P.G. Hill, D.E. Irish, and P.V. Balakrishnan, eds., pp. 72-79) however a substantial amount of work remains.

Under this specific project, a Greek young scientist, Ms. Metaxa, spent 4 months at NIST. Her tasks included updating databases (incorporating new temperature conversion, as appropriate; searching current literature; introducing uncertainties in all variables; performing additional evaluation); working with NIST statisticians in developing/evaluating formal schemes to achieve consensus values; collecting, re-optimizing and evaluating existing formulations and approaches for viscosity of water; developing and implementing structural optimization algorithms for viscosity; and working with team members to incorporate terms for critical-region behavior. Substantial progress in all of these areas was achieved and a separate report describing these activities is available.

3) 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 is hoped that a new improved formulation for the viscosity of water will be proposed at the ICPWS Meeting in Kyoto 2005. The new formulation for the viscosity, η , will have a better theoretical form, which is described by the following equation

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

where, η_0 , is the viscosity at the dilute gas limit, η_1 , the initial density dependence, η_{ex} , the excess viscosity, and η_c , the viscosity in the critical region.

a) Viscosity at the Dilute Gas Limit

Following the 4-month stay of Ms Metaxa in NIST, 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.

- resulting proposed equation has a 1.6% uncertainty at the 95% confidence limit.
- Initial density dependence contribution Work is under way in cooperation with Prof. E. Vogel (Germany). It should be concluded by end of September 2003.

c) Excess Viscosity and Critical Contribution Work in these areas will start after completion of the previous task.

4) New Formulation for the Viscosity of Heavy Water

Following the above procedure for the viscosity of water, work is under progress to develop a new formulation for the viscosity at the Dilute-Gas Limit.

NON-SCIENTIFIC WORK

Work is still under progress in forming a full National Committee. Although some industries and institutions have responded positively, no National Committee has as yet been appointed. Nevertheless, it is hoped that a committee will be appointed before Christmas 2003.

Current Status of Research Activities in Japan Submitted to the Executive Committee Meeting, IAPWS, Vejle, Denmark, August 2003

by

Japanese National Committee International Association for the Properties of Water and Steam c/o The 139th 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 on the preparation of the forthcoming 14th ICPWS to be held in Kyoto, from August 29 through September 3, 2004. Your positive submission of abstracts and participation are highly appreciated. Please do visit the Website (http://14icpws.iapws.jp/).

The following research projects on the thermophysical and physico-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. Infrared and near infrared measurements of water-aromatic hydrocarbon mixtures in the temperature range 473 - 648 K and the pressure range 10 - 35 MPa have been performed. By analyzing these experimental results, π -hydrogen bonding between water and aromatic hydrocarbons at high temperatures and pressures has been discussed on the basis of a charge transfer theory [*J. Chem. Phys.*, **117** (2), 751 (2002)]. Anomalously large volume expansion for mixing of water and benzene has been found in the vicinity of the critical region of the mixtures [*J. Chem. Phys.*, **117** (4), 1682 (2002)]. Similar phenomena have been observed for mixtures of water with toluene and ethylbenzene [*Fluid Phase Equilib.* (2003) in press], and the anomalous volumetric behavior is considered to be common to hydrophobic hydrocarbons in the vicinity of the critical region. [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 new project on IASCC (Irradiation Assisted Stress Corrosion Cracking) of BWR core internals as a part of studies on life management of aged nuclear power plants. The effects of hydrogen peroxide on 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. The characterization results of oxide films confirmed that the oxide film formed under the H_2O_2 environment consists mainly of hematite (α -Fe₂O₃), while that under the O₂ environment consists of magnetite (Fe₃O₄). Furthermore oxidation at the very surface of the film is much more enhanced under the H_2O_2 environment than that under the O₂ environment. It was speculated that metal hydroxide plays an important role in oxidation of stainless steel in the presence of H_2O_2 . The difference in electric resistance of oxide film causes the difference in anodic polarization properties. Theoretical approaches to understand crack tip water chemistry under gamma and neutron irradiations are also promoted. The paper (1) was awarded the 2001 Preeminent Monograph Award by Atomic Energy Society of Japan. [Latest publication: (1) Y. Murayama, et al., J. Nucl. Sci. Technol., 39, 1199-1206 (2002), and (2) T. Satoh, et al., J. Nucl. Sci. Technol., 40, 334-342 (2003)] [contact: Prof. S. Uchida; E-mail: shunsuke.uchida@qse.tohoku.ac.jp].

At the Graduate School of Environmental Studies, Tohoku University, Sendai, Profs. N. YAMASAKI, H. ENOMOTO, K. TOHJI, Assoc. Prof. TSUCHIYA, and their group are studying the hydrothermal preparation of advanced materials such as diamond, stratified material 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. [contact: Prof. N. Yamasaki; e-mail: yamasaki@igt.earth.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 nano particles, 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. [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, 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 7×10^{-8} 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 in the SI units [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., 52 (2003), 646-651]. The data are being used for the next adjustment of the fundamental physical constants recommended by the CODATA Task Group on Fundamental Constants. Using the silicon density standard densities of standard liquids are being calibrated by a magnetic suspension density meter developed at NMIJ. A relative standard uncertainty of 6×10^{-6} has been achieved in the density measurement of organic liquids that are used as Certified Reference Materials (CRMs) for calibrating vibrating-tube densimeters. In his group a new absolute viscosity measurement using a falling ball method is in progress. Nanotechnologies 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 National Metrology Institutes. A new density-of-water table that has a specified isotopic abundance was proposed by the WG-Density and recently 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, 38 (2001), 301-309]. This new table is recommended as a metrological standard for the density of SMOW [contact: Dr. K. Fujii, Section Chief, Density and Viscosity Standards, NMIJ; Email: fujii.kenichi@aist.go.jp].

At the Division of Environmental Materials & Energy, Dept. Environmental Science & Technology, Faculty of Engineering, Shinshu University, Nagano, Prof. H. Takaku works since Feb. 1 of 2000, and previously worked at Central Research Institute of Electric Power Industry (CRIEPI). In the simulated geothermal waters containing the mixed corrosive chemicals such as chlorides, sulfides, carbon dioxide and others, he and coworkers are studying the corrosion of the steam turbine materials for

geothermal power plants and also that of Ti-Ni base shape memory alloys for geothermal engine actuators. They are studying the on-line corrosion monitoring of boiler materials in fossil power plants, using mainly the electrochemical methods. [Latest publications: (1) N. Kawai, H. Takaku, et al, *Zairyo-to-Kankyo (J. Corrosion Eng. 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] [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 thermodynamic properties of water substance and other fluid. In the IAPWS meeting in Buenos Aires in 2002, it was decided that the TTSE method should be accepted as an IAPWS guideline entitled "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". Following the decision, he submitted a draft of the guideline to the Editorial Committee. The draft has been distributed by Executive Secretary to National Committees for postal vote. Mr. Miyagawa is developing a new version of TTSE programs that calculates transport properties with high speed and high accuracies. This version will be useful to analyze

transient phenomena in heat transfer and fluid mechanics. [contact: Mr. K. Miyagawa; E-mail: miyagawa.kiyoshi@nifty.ne.jp]

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 oxidation on freezing of supercooled water, and finding that the oxidation of the surface restrain the supercooled water on the surface from freezing [Int. J. Refrigeration, 25 (6) (2002), 25, 5, 514-520]. They are also studying the melting phenomenon of porous material by direct contact melting [12th Int. Heat Transf. Conf., (in CD-ROM), (2002)], 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; Email: sokawa@ mech.titech.ac.jp].

At the Energy Materials Science Department (former, the Department of Surface Science), Central Research Institute of Electric Power Industry (CRIEPI), Yokosuka, Tokyo, Dr. M. Domae and his coworker are engaged in a national research project, "Fundamental R&D on Water Chemistry of Supercritical Pressure Water under Radioactive Environment". Within the program, they are in charge of Raman spectroscopy and zeta potential measurement of metal surfaces in sub- and supercritical water. They also worked a concept of metal separation technique in SCW using change in solubility. [contact: Dr. M. Domae; E-mail: domae@criepi.denken.or.jp]

At the Energy & Mechanical Engineering Department, Central Research Institute of Electric Power Industry (CRIEPI), Yokosuka, Kanagawa, Mr. E.KODA and Mr. T.TAKAHASHI are advancing the improvement of the computer software to analyze the heat and mass balance of power generation systems. In this study, IAPWS-IF97 was enhanced so as not to indicate the abnormal value also outside the range of validity, and built into the program. And the development of the computational method of inverse functions to improve the computation time and accuracy is advanced. [contact: Mr. E.KODA; E-mail: kouda@criepi.denken.or.jp]

At the Center for Mechanical Engineering and Applied Mechanics, Keio University, Yokohama, Prof. M. UEMATSU and his group are constructing an apparatus for measuring PVT properties of aqueous ammonia mixtures for temperatures to 800 K at pressures up to 200 MPa. The measurements of thermodynamic properties for methanol + water mixtures in a temperature range from 320 K to 420 K at pressures up to 200 MPa were published in the *Journal of Chemical Thermodynamics* 35 (2003) 813-823. The measurements of thermodynamic properties of ammonia + water mixtures in a temperature range from 310 K to 400 K at pressures up to 17 MPa were published in the *Journal of Chemical Thermodynamics* 34 (2002) 807-819 + 1045-1056. [contact: Prof. M. Uematsu; E-mail: uematsu@mech.keio.ac.jp].
At the Department of System Design Engineering, Prof. A. NAGASHIMA and coworkers are studying measurement of transport properties of liquids including aqueous solutions and correlations of fluids properties of environmental concern. [contact: Prof. A. Nagashima; E-mail: nagasima@sd.keio.ac.jp].

At the Department of Mechanical Engineering, Keio University, Yokohama, Dr. K. YASUOKA and his group are studying the molecular dynamics simulation to clarify the mechanism for the dissociation and formation of methane hydrate. They started the molecular dynamics simulation for the adosorption and desorption of ethanol molecules to liquid-vapor water suface. [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⁻³ to 989 kg m⁻³, and compositions up to 0.10 mol% of ammonia including pure water, focusing their attentions on the maximum density phenomena. Some of their results were presented at the 15th Symposium on Thermophysical Properties held in Boulder in 2003. [contact: Prof. K. Oguchi; E-mail: oguchi@me.kanagawa-it.ac.jp].

At the Research Center for Computational Science, Okazaki National Research Institutes, Prof. S. OKAZAKI and his group started quantum-classical molecular dynamics calculation for vibrational relaxation of solute in supercritical water. They are interested in understanding relaxation machanism in terms of time-dependent couplings between solute and solvent in supercritical fluids. They also published their calculation of dielectric constant of supercritica water [T. Mikami and S. Okazaki, J. Chem. Phys., 119 (2003), 4790-4797]. [contact: Prof. S. Okazaki; E-mail: okazaki@ims. ac.jp].

At the Department of Applied Chemistry, Ritsumeikan University, Shiga, Prof. S. SAWAMURA is measuring the solubility of aromatic hydrocarbons and amino acids in water at high pressures up to 400 MPa and the visicosity of aqueous elecrolyte solution at high pressures [see: H. Matsuo, Fluid Phase Equilibria 20 (2002), 227-238. Sawamura, S. et al., J. Phys. Chem. B105 (2001), 2429-2436]. At the same department, Prof. Y. TANIGUCHI and Assoc. 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, Dr. 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, Raman spectroscopy, and computer simulation. Their current focus are (1) the thermodynamics, structure, and dynamics of aqueous solutions over a wide range of thermodynamic conditions ["Theory of solutions in the energy representation. II. Functional for the chemical potential", N. Matubayasi and M. Nakahara, J. Chem. Phys. 117, 3605-3616 (2002)] and (2) the molecular mechanism of noncatalytic reactions in hydrothermal conditions ["Noncatalytic Cannizzaro-type Reaction of Acetaldehyde in Supercritical Water", Y. Nagai, C. Wakai, N. Matubayasi, and M. Nakahara, Chem. Lett. 32, 310-311 (2003)]. [contact: Prof. M. Nakahara; E-mail: nakahara@scl.kvoto-u.ac.jp]

At the department of Molecular Science and Technology, Doshisha University, Kyotanabe, Prof. M. UENO and his group are studying the conductivities of electrolytes in water and methanol at high temperatures and pressures to disclose the general trends of the density dependence of ionic mobilities at medium and low densities. They are trying to measure the critical micelle concentration at high temperatures and pressures by the conductivity method. In addition, the densities and viscosities of formamides-water mixtures at 25°C under high pressure up to 200 MPa have been reported and discussed in terms of the hydrogen bonding between water and amide molecules and the hydrophobic hydration

[Rev. High Press. Sci. Technol., **13** (2003), 134-140]. [Contact: Prof. M. Ueno; E-mail: mueno@mail.doshisha.ac. jp]

.

At the Department of Mechanical Engineering 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, which includes those of water substances. This software is available free of charge to any non-profit organizations, and some functions of which are demonstrated at <u>http://www2.mech.nagasaki-u.ac.jp/PROPATH/</u>. [contact: Prof. Y. Takata; E-mail: takata@mech.kyushu-u.ac.jp/].

At Mitsubishi Heavy Industries, Ltd., Nagasaki R&D Center, Mr. T. MORIMOTO and his coworkers are studying the oxygenated water treatment for super- and sub-critical thermal power plants and Mr. M. TATEISHI and his coworkers are studying the hydrothermal decomposition of organic compounds such as poly-chlorinated bi-phenyl (PCB) and Dr. J. IZUMI and his coworkers are studying the water treatment for geothermal plants, studying the solubility of hydroxy- and fluoro-apatite in hot water for radioactives storage, and also studying the molecular simulation to assume the solubility of inorganic compounds in hot water [contact: Dr. J. Izumi; E-mail: junizumi@ngsrdc.mhi.co.jp].

REPORT OF RUSSIAN NATIONAL COMMITTEE (2002 – 2003)

LIST OF PUBLICATIONS

- 1. Kostrikina E.Yu., Modestova T.D., Uliyanenko B.I. *et.al.*: An Experience of Boiler Lay-up with the Less Toxic Inhibitor. Energetik, 2002, No.9.
- 2. Elov A.I., Reshetov A.L., Lopatkin B.V., Gerasimov V.A.: The Automatic Control System of Water Treatment Technological Processes at Yuzhnouralskaya GRES. Elektricheskie Stantcii, 2002, No. 11.
- Valyashko V.M., Urusova M.A.: Solubility of Sodium Carbonate in the System Na₂CO₃ - NaCl - H₂O at Elevated Temperature and Pressure. Journal of Inorganic Chemistry, 2002, Vol. 47, No. 10, pp. 1723-1727.
- 4. Valyashko V.M.: Derivation of Complete Face Diagram for Ternary Systems with Immiscibility Phenomenon and Salt Liquid Equilibrium. Pure Appl. Chem., 2002, No. 10, pp. 1871-1884.
- 5. Man'kina N.N., Zhuravlev L.S., Kirilina N.N. *et al.*: The Practical Results of the Application of Oxygen-Steam Cleaning and Passivation of the Boilers with Natural Circulation. Elektricheskie Stantcii, 2002, No. 9.
- 6. Larin B.M., Bushuev E.N., Kosyulina E.V.: Increasing the Information Content in Monitoring the Water Chemistry of the Condensate–Feedwater Path of Power Units. Teploenergetika, 2003, No. 7, p. 2-9.
- 7. Prozorov V.V., Lysenko A.A.: Mechanisms for Protecting Oxide-Coated Steels in Anodic Inhibitor Solutions and When Conducting Neutral-Oxygen Water Chemistry. Teploenergetika, 2003, No. 7, p. 9-13.
- 8. OchkovV.F., Pilshikov A.P., Solodov A.P., Chudova Yu. V.: Analysis of Ion-Exchange Isotherms Using the Mathcad Software Package. Teploenergetika, 2003, No. 7, p. 13-19.
- 9. Bogachev A.F., Ostrovskaya M.V.: Analyzing the Water Chemistry and the Condition of the Heating Surfaces of the Heat-Recovery Boilers after the Experimental and Commercial Operation of the PGU-450 Combined-Cycle Power Unit at the Severo-Zapadnaya Thermal Power Station. Teploenergetika, 2003, No. 7, p. 19-23.
- 10. Dubrovsky I.Ya., Eskin N.B., Tugov A.N., Anikeev A.V.: The Adsorption of Octadecylamine on Boiler Steels under Conditions of a Once-Through Subcritical Pressure Boiler, Teploenergetika, 2003, No. 7, p. 23-24.
- 11. Yurchevsky E.B., Komarova I.V., Galkina N.K., YakovlevA.V., Anfilov B.G., Kiseleva S.A.: Predicting the Performance of Countercurrent Ion Exchangers Using a Mathematical Modeling Technique. Teploenergetika, 2003, No. 7, p. 24-29.
- 12. Veselovskaya E.V.: The Protection of Ion-Exchange Filters of Water Treatment Installations against Organic Impurities of Anthropogenic Origin. Teploenergetika, 2003, No. 7, p. 29-35.
- 13. Endrukhina O.V., Voronov V.N.: Mathematical Modeling of the Water Chemistry of a Thermal Power Station under Unsteady Conditions. Teploenergetika, 2003, No. 7, p. 60-63.
- 14. Nevedrov A.V., Ushakov G.V.: The Comparative Analysis of the Physical Methods of Water Treatment for the Decreasing of Scale Formation. Teploenergetika, 2003, No. 11, p. 62.

- 15. Petrova T.I., Ryzhenkov V.A., Kurshakov A.V., Zroichikov A.A., Chernov V.F., Galas I.V.: An Application of Film Forming Amine for the Lay-up of Heat Engineering Equipment at Thermal Power Station-23 OAO Mosenergo. Teploenergetika, 2003, No. 9, p. 56.
- 16. Khodyrev B.N., Fedoseev B.S., Korovin V.A., Sherbinina S.D., Schukina M.Yu., Suslov S.Yu.: Standardization of Organic Impurities Contents in the Water - Steam Circuit of Power Units Working on Neutral Oxygen Water Chemistry. Elektricheskie Stantcii, 2003, No. 8, p.16.
- 17. Rubashov A.M., Balaban-Irmenin Yu.V.: New Estimation Procedure of the Intensity of Inner Corrosion of Heat Network Pipelines Metal. Energetik, 2003, No.3, p.30.
- 18. Zhgenti Yu.V., Palmer D.A., Benezeth P., Wesolowski D.J., Anovitz L.M.: An Experimental Investigation of Borate/Lithium Adsorption from Solution onto Zirconium Dioxide Surfaces. 9th annual International Scientific and Technical Conference of Under-graduate and Post-Graduate Students "Radio-Electronics, Electrical and Power Engineering" REEPE-2003, 4-5 March, 2003, Moscow, Vol. 3, pp.113-114.
- 19. Makrushin V.V., Perova T.I.: The Factors Influenced on Deposits Formation Processes in Boilers Tubes. 9th annual International Scientific and Technical Conference of Under-graduate and Post-Graduate Students "Radio-Electronics, Electrical and Power Engineering" REEPE-2003, 4-5 March, 2003, Moscow, Vol. 3, pp.122-123.
- 20. Furunzhieva A.V., Petrova T.I.: Studying of the Polyamines Influence on the Corrosion Rate of Brass and Carbon Steel at Temperatures Under 100 ^oC. 9th Annual International Scientific and Technical Conference of Under-graduate and Post-Graduate Students "Radio-Electronics, Electrical and Power Engineering" REEPE-2003, 4-5 March, 2003, Moscow, pp. 129-130.
- 21. Furunzhieva A.V., Petrova T.I.: About he Using of Polyamines at Power Establishments. 9th Annual International Scientific and Technical Conference of Under-graduate and Post-Graduate Students "Radio-Electronics, Electrical and Power Engineering" REEPE-2002, February 28-March 1, Moscow: Vol. 3, pp. 130.
- 22. Starikova O.V., Ryzgenkov V.A.: An Investigation of Anticorrosion Properties of Abrasion-Resistant Ion-Plasmous Coatings at Conditions of High Aggressive Mediums. 9th Annual International Scientific and Technical Conference of Undergraduate and Post-Graduate Students "Radio-Electronics, Electrical and Power Engineering" REEPE-2002, February 28-March 1, Moscow: Vol. 3, pp. 128-129.
- Valyashko V.M., Urusova M.A.: Solubility and Behavior Ternary Water Salt Systems at Sub – and Super Critical Conditions. Monat. Chem., 2003, Vol. 134, pp. 679-692.

For more Russian Journal information, please see the following websites:

TEPLOENERGETIKA issued in English under the name "Thermal Engineering" <u>http://www.maik.ru</u>

ENERGETIK (POWER ENGINEER), issued in Russian

http://www.energy-journals.ru/energetic/index.htm

VODOSNABZGENIE I SANITARNAYA TEHNIKA (WATER SUPPLY AND SANITARY ENGINEERING), issued in Russian

http://www.vstmag.ru

ELEKTRICHESKIE STANTCII (*POWER STATIONS*), issued in Russian <u>http://www.energy-journals.ru/electr_st/index.htm</u>

VESTNIK MEI (BULLETIN of MOSCOW POWER ENGINEERING INSTITUTE), issued in Russian, abstracts are in English http://www.mpei-publishers.ru/vestnik.asp

Dr. Petrova T.I. consisting of creative group was rewarded with the First Degree Diploma and the Gold Medal at 51th Worldwide Salon of Innovation of Scientific Developments and New Technologies Brussels – Eureka - 2002 for the development of method of decreasing corrosion rate of power equipment.

Head of RNC

Aleksandrov A.A.

US National Committee Progress Report

Vejle, Denmark, Aug. 2003

The ASME Subcommittee on Properties of Steam (which is also the U.S. National Committee to IAPWS) completed an update (Version 1.1) to the ASME Steam Properties software based on IAPWS-IF97.

Physical and Chemical Properties Division (838), NIST, Boulder, CO.

D.G. Friend, A.H. Harvey, E.W. Lemmon, J.W. Magee, I. Metaxa, I.M. Abdulagatov, M.M. Aliev

In collaboration with theoretical chemists in England, we have continued our work on development of intermolecular pair potentials for aqueous systems and calculation of second virial coefficients. In the past year, we completed our first system with a diatomic gas: water/hydrogen. As with previous systems, second virial coefficients for the water/gas pair were considered more accurate than those available from experiment.

A new correlation has been developed (A.H. Harvey and E.W. Lemmon, J. Phys. Chem. Ref. Data, in press) for the second virial coefficient B(T) of ordinary water. Compared to the best previous correlation (Hill and MacMillan, 1989), the new correlation makes use of some new data and covers a larger temperature range.

In collaboration with researchers in Argentina, high-temperature solubility data have been analyzed for 14 solutes in H2O and 7 solutes in D2O. These data, expressed both in terms of Henry's constant and the vapor-liquid distribution coefficient, have been correlated to expressions that exhibit the theoretically correct behavior as the critical temperature of the solvent is approached. This work has been published in J. Phys.Chem. Ref. Data.

Work is continuing on the joint IAPWS and IUPAC efforts to update the formulations for the transport properties of water and steam. I. Metaxa from Greece spent 3 months in Boulder on an IAPWS grant and made significant progress on the low-density viscosity.

NIST played the leading role in organizing the 15th Symposium on Thermophysical Properties, held in Boulder in June of 2003. There were five special sessions on Properties of Aqueous Systems, and material relevant to IAPWS was also presented in sessions on Environmental Applications and Molecular Simulation. See http://symp15.nist.gov for details.

We are continuing to collaborate with the Dagestan Scientific Center of the Russian Academy of Sciences (DSCRAS) in the area of thermophysical properties measurements, largely on aqueous systems. In the past year, papers were completed on experimental studies of methanol + water mixtures with calorimeters at NIST and at the DSCRAS; part of this work (visit to Boulder by Mr. Aliev, a doctoral candidate at the DSCRAS) was supported by IAPWS.

Research Directions and Key Publications: 2002-2003

The Energy Institute Electrochemical Laboratory The Pennsylvania State University, University Park, PA, 16802

Professor S.N. Lvov (814-863-8377, lvov@psu.edu), Program Coordinator

High Temperature Electrochemistry - General

- Lvov S.N. Electrochemistry of High Temperature Subcritical and Supercritical Aqueous Systems, Volume 5 in "Encyclopedia of Electrochemistry" (D.D. Macdonald, Ed.) Wiley-VCH, 2003 (in press).
- 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, Ed.s), Wiley, 2003 (in press).

High Temperature Proton Exchange Membrane Fuel Cells

- Fedkin M.V., Zhou X.Y., Hofmann M.A., Chalkova E., Weston J.A., Allcock H.R., Lvov S.N. Evaluation of Methanol Crossover in Proton-Conducting Polyphosphazene Membranes, Materials Letter, 2002, v. 52, 192-196.
- Chalkova E., Zhou X.Y., Ambler C.M, Hofmann M.A., Weston J.A., Allcock H.R., and Lvov S.N. Sulfonimide Polyphosphazene-Based Hydrogen/Oxygen Fuel Cells, Electrochemical and Solid State Letters, 10, 2002, 221-223.
- Hofmann M. A., Ambler C. M., Maher A. E., Chalkova E., Zhou X. Y., Lvov S. N., Allcock H. R. Synthesis of Polyphosphazenes with Sulfonimide Side Groups. Macromolecules, 35, 2002, 6490-6493.
- Allcock H. R., Hofmann M. A., Ambler C. M., Lvov S. N., Zhou X. Y., Chalkova E., Weston J. Phenylphosphonic Acid Functionalized Poly[aryloxyphosphazenes] as Proton-Conducting Membranes for Direct Methanol Fuel Cells. J. Membrane Science, 202, 2002, 47-54.
- Zhou X. Y., Hofmann M. A., Weston J.A., Chalkova E., Allcock H. R., and Lvov S.N., High Temperature Methanol Crossover in Proton-Conducting Polyphosphazene Membranes: In Direct Methanol Fuel Cells, Narayanan, S., Zowodzinski, T. and Gottesfeld, S., Eds.; The Electrochemical Society Proceedings Series: Pennington, NJ, 2002, 34-41.
- 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 Potentiometery and pH measurements

1. Lvov S.N., Zhou X.Y., Fedkin M.V., Zhou Z., Kathuria A., and Barnes H.L. Advanced Electrochemical Studies of Hydrothermal Systems, Geochmica et Cosmichimica Acta, **202**, 2002, A467.

- Seneviratne D.S., Papangelakis V. G., Zhou X.Y., and Lvov S.N. (2003) 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. (2003) Progress on the Yttria-Stabilized Zirconia Sensors for Hydrothermal pH Measurements, Chemical Geology, 198, 2003, 141-162.

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. (2003) High Temperature Microelectrophoresis Studies of the Rutile/Aqueous Solution Interface, Langmuir, 19, 2003, 3797-3804.

IAPWS-related activities at the University of Maryland 2002-2003

A chapter on "Near-Critical Behavior of Aqueous Systems" by M.A. Anisimov, J.V. Sengers, and J.M.H. Levelt Sengers was completed for the forthcoming IAPWS Handbook on The Physical and Chemical Properties of Aqueous Systems at Elevated Temperatures and Pressures: Water, Steam and Hydrothermal Solutions.

Jan V. Sengers participated in the meeting of the task group on the transport properties of H2O which was held in conjunction with the 15th Symposium on Thermophysical Properties, held in Boulder, CO, June 2003.

IAPWS Mee	eting in Dei	1mark 24-30	August, 200	3 – List	of Particip	ants
	ing m Dei	$mar \times 2 = 50$	Tugust, 200	5 List	or r ar ticip	anus

Marc Assael Aristotle Univesity Greece	Malcolm Ball United Kingdom	James Bellows Siemens Westinghouse USA
Geoff Bignold Innogy plc United Kingdom	Rudolph Blum Elsam Denmark	Jeff Cooper Queen Mary University London United Kingdom
Karol Daucik Elsam Denmark	Barry Dooley EPRI USA	Daniel G. Friend NIST, Physical and Chemical Properties Division USA
Ada Garcia Technical University of Denmark Denmark	Søren Hansen Energi E2 Denmark	Richard Harries Harries Power Chemistry United Kingdom
Allan Harvey NIST USA	John Barry Hughes Enron Power Operations United Kingdom	Jørgen Peter Jensen Energi E2 Denmark
Katja Knobloch University of Applied Sciences of Zittau and Goerlitz Germany	Terunori Kobayashi Chubu Electric Power Co., Inc. Japan	Ivan Kodl Skoda Energo s.r.o. Czech Republic
Petr Konas University of West Bohemia in Pilsen Czech Republic	Hans-Joachim Kretzschmar University of Applied Sciences of Zittau and Goerlitz Germany	Bernard Le Neindre LIMHP France
Erik Luijten University of Illinois USA	Serguei Lvov Pennsylvania State University USA	Vladimir Majer Blaise Pascal University France
Radim Mares University of West Bohemia in Pilsen Czech Republic	Frantisek Marsik Institute of Thermomechanics CAS Czech Republic	Eric Maughan College of Knowledge Germany
Ken McGrath United Kingdom	Kiyoshi Miyagawa Japan	Masahiko Nagai Mitsubishi Heavy Industries Japan

IAPWS Meeting in Denmark 24-30 August, 2003 – List of Participants

Masaru Nakahara Kyoto University, Institute for Chemical Research Japan	Tomas Nemec Institute of Thermomechanics CAS Czech Republic	Kosei Oguchi Kanagawa Institute of Technology Japan
Nobuo Okita Toshiba Corporation Japan	Leonard Olavessen Buckman Laboratories International USA	Aksel Olsen AKOL-engineering Denmark
Donald A. Palmer Oak Ridge National Laboratory USA	William T. Parry General Electric USA	Lars Storm Pedersen Energi E2 Denmark
Tamara Petrova Moscow Power Engineering Institute Russian Federation	Johanna Levelt Sengers NIST USA	Oldrich Sifner Institute of Thermomechanics CAS Czech Republic
Erik Smitshuysen Elsam Denmark	Miroslav Stastny Czech Republic	Robert Svoboda Alstom Switzerland
Svend-Erik Therkildsen Energi E2 Denmark	Kaj Thomsen Technical University of Denmark Denmark	Shunsuke Uchida Tohoku University Japan
Masakatsu Ueno Doshisha University Japan	Vladimir M. Valyashko Kurnakov Institute of General and Inorganic Chemistry Russian Federation	Sonia Vodoikovich Serbian Power Generation, Power Plant Nikola Tesla A Yugoslavia
Wolfgang Wagner Ruhr-Universität Bochum Germany	Koichi Watanabe Keio University Japan	Ingo Weber Siemens Westinghouse Power Corporation USA
Kenji Yasuoka Keio University Japan	Andre Zeijseink KEMA The Netherlands	Yulia Zhgenti Moscow Power Engineering Institute Russian Federation
Milan Zmitko Nuclear Research Institute Rez plc Czech Republic		