

BIAPWS Report to the IAPWS Meeting, Doorwerth, Netherlands, September 2009

1. BIAPWS Committee

BIAPWS committee meetings are held three times a year, and the attendance at these has been very good, typically around 15, helped by the introduction of technical presentations and discussions into the meeting agenda. The discussions provide a useful forum for updating information and exchanging views on a number of topics. Sponsor's representatives are able to bring a colleague to the meeting to benefit from and contribute to the discussions.

In October 2008, the BIAPWS committee meeting was held in Dublin, a change from the usual venue of Birmingham. This temporary change of venue was made in acknowledgement of the support received from BIAPWS members in Ireland, and the meeting was followed by a morning of technical presentations to BIAPWS members and representatives from the power plant chemistry community in Ireland. The meeting was very successful and BIAPWS were grateful to ESB for hosting the meeting. BIAPWS aims to continue to hold meetings in Birmingham as the default, but to consider meetings at alternative venues, such as Dublin, on occasions.

In 2008, BIAPWS considered how to be most effective in its dual roles of UK & Irish national committee of IAPWS and representative body for power plant chemistry in the UK & Ireland. As a result, the BIAPWS statutes have been revised, principally to better reflect the role of BIAPWS as the representative body for power plant chemistry in the UK & Ireland. At the same time the committee is approaching academic specialists about becoming corresponding members of BIAPWS, in the hope that this will enable BIAPWS to better represent the UK & Ireland in areas of interest to the IAPWS working groups Thermophysical Properties of Water & Steam (TPWS), Industrial Relations and Solutions (IRS) and Physical Chemistry of Aqueous Systems (PCAS).

Finally, there was an election of officers in 2008, and BIAPWS would like to express its gratitude to Dr. Richard Harries and Mr. Malcolm Ball, who have stepped down from their roles as Chairman and Secretary respectively, for their time and dedication to the organisation of BIAPWS.

2. BIAPWS Award

The BIAPWS Award is given annually by BIAPWS to qualifying students as a means of promoting awareness of the topics of interest to BIAPWS. In 2008 the BIAPWS award was co-sponsored by E.ON Engineering. The award recipient was Joe Hook, who is studying for a Masters Degree in Physics at the University of York. The Award is given in the form of contributory funding by BIAPWS for a work experience placement for the student. Joe spent three months working on a project to assess technologies for post combustion carbon capture at E.ON's Technology Centre at Ratcliffe-on-Soar near Nottingham. Joe gave an excellent presentation on his work at the BIAPWS Symposium in April 2009.

Both Joe and the 2007 BIAPWS Award winner, Rochelle Green, have since gone on to full time employment in the power plant industry, both with BIAPWS sponsors, demonstrating a significant success for the Award in attracting high calibre individuals into the power generation industry.

BIAPWS has also supported a further educational initiative in 2008, sponsoring and judging prizes for energy related projects at a schools science fair in Hinckley, Leicestershire.

3. BIAPWS Symposium

The 11th BIAPWS Symposium, 'Progress in Environmental and Cycle Chemistry', took place at the Village Hotel, Nottingham, on 22 April 2009. This was preceded by a half day workshop on 21 April. Two sessions were held in the Symposium: 'Environmental Issues in Power Plants' and 'Flexibility in Cycle Chemistry', whilst two sessions were also held in the workshop, both on chemical aspects of flexible operation. This proved to be another successful meeting, with around seventy delegates attending the Symposium and thirty delegates attending the workshop. A summary report of the meeting was published in Power Plant Chemistry earlier this year.

4. BSI Representation

BIAPWS continues to represent the power industry on the BSI committee dealing with standards for power cycle chemistry, i.e. BS-EN 12952:12 and BS-EN12953:10. BIAPWS has taken a lead on behalf of European members of IAPWS to coordinate representations to CEN to get these standards reviewed.

In 2008, BIAPWS also joined the BSI committee with responsibility for the administration of ISO 5667 – Water Quality, Sampling. BSI has joined this committee with the aim of supporting a revision to Part 7 of this standard: 'Guidance on sampling water and steam in boiler plants'. BIAPWS is liaising with IAPWS PCC working group in this activity.

5. IAPWS Activities

BIAPWS has continued to support IAPWS through its formal membership and participation in IAPWS activities. A number of BIAPWS committee members are represented on IAPWS working groups, in particular Power Cycle Chemistry (PCC), and BIAPWS was especially proud that one of its members, Jeff Cooper, completed his second year as IAPWS President in 2008. BIAPWS members of the PCC working group have also supported the production of a new suite of IAPWS Technical Guidance Documents that are expected to provide a valuable resource to those involved power cycle chemistry.

The 15th International Conference on the Properties of Water and Steam (ICPWS) was held in Berlin in September 2008, and a number of BIAPWS members participated. At the meeting BIAPWS was invited to host the next ICPWS. Following an internal review, BIAPWS has agreed to host the 16th ICPWS, expected to be held in 2013. A BIAPWS sub-group has been formed to take the organisation of this conference forward.

6. Overview

This has been another successful year for BIAPWS. Membership remained strong and the BIAPWS symposium and BIAPWS Award have both been successful. The introduction of technical discussions into committee meetings is resulting in increased interest and participation in BIAPWS activities. The agreement by BIAPWS to host the 16th ICPWS presents a long term challenge for BIAPWS, but also provides an opportunity to show the UK & Ireland in a positive light.

Dr. Andy Rudge
Chair, British & Irish Association for the Properties of Water and Steam
September 2009

CANADIAN NATIONAL COMMITTEE INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM (IAPWS)

IAPWS-Related Research in Canada 2009

SUMMARY OF ACTIVITIES

1.0 National Workshop

On 2009 May 11th and 12th, the Canadian National Committee of IAPWS organized a workshop in Toronto for researchers, applied scientists and practising engineers in water-related areas to describe their work and discuss priorities for the future. The CANDU Owners Group was the sponsor and its staff were key in ensuring an efficient organization. About 50 people attended and participated in lively discussions after the presentations. In the final session, breakout groups focused on important issues arising from the areas of: process chemistry; deposition/precipitation; corrosion in confined regions and concentrated solutions; and, radiation chemistry. The findings of the groups are presented in Appendix 1.

Favourable comments were received after the event. This workshop will be held every two years and is seen as an important vehicle for bringing together Canadian researchers and practitioners and for promoting collaborations and funding support.

2.0 International Certified Research Needs

The Canadian National Committee has considered ICRNs and suggests the following for discussion:

- Sampling from high-temperature water and steam systems (specifically, the interaction of the sample with the sampling system walls).
- Chemical thermodynamics and kinetics of electrolytes and organics in subcritical and supercritical water (300 to 450 °C)
- Materials performance under supercritical steam-generator conditions (nuclear and thermal)
- Radiolysis models for high-temperature water at in-core reactor conditions.

3.0 International Collaborations

3.1 Czech Republic and Canada:

PhD student Jana Ehlerova (Supervisor Dr. Josef Sedlbauer, University of Liberec) completed a 1-year IAPWS collaborative project with Dr. Tremaine (University of Guelph) entitled *"Euilibrium Constants and Speciation of Aqueous Transition Metal Chloro-complexes over a Wide Range of Temperatures and Pressures"*. During this period Dr. Sedlbauer also spent 3 weeks at Guelph working with Dr. Tremaine and Dr. Trevani on data interpretation. A full report will be presented at the IAPWS 2009 Meeting in the Netherlands.

3.2 Denmark, Switzerland and Canada

The PhD student Piti Srisukvatananan, supervised by Derek Lister at the University of New Brunswick (UNB) in Canada, presented the results of the IAPWS-sponsored collaboration on the CFD modeling of systems for sampling high-temperature water and steam at the Berlin meeting of IAPWS in 2008. Subsequently, the collaboration involving UNB, Dong Energy in Denmark (Karol Daucik) and Alstom in

Switzerland (Bobby Svoboda) was extended and with support from Dong Energy undertook a further CFD study of sampling. The results are summarized in a presentation at the IAPWS 2009 meeting in the Netherlands.

4.0 Proposed IAPWS Meeting in 2010

The Canadian National Committee is prepared to host the 2010 IAPWS Meeting and Niagara Falls, Ontario, is proposed as a convenient venue.

It has been suggested holding it either the week before or the week after the International Conference on the Water Chemistry of Nuclear Reactor Systems (NPC2010), which is being held in Quebec City on October 3rd – 7th. However, it is recognized that this is rather late and may inconvenience several members; earlier in the summer may be better. IAPWS will be informed very soon about the decision.

Appendix 1. Findings of Workshop Discussion Groups

A1.1 Process Chemistry

- Diagnostics/Sensor Development for the study of chemistry processes in high temperature water at sub- and super-critical conditions.
 - In the study of water chemistry at high temperatures, on line diagnostic tools are required in the short term both for understanding the chemistry prevailing at these conditions and in the longer term to control processes that will take advantage of these high temperatures e.g. SCWR and SCWO.
 - Progress in these studies is hampered by the unavailability of high integrity diagnostic tools such as pH and redox potential measuring probes able to cover a wide temperature range from 200°C up to supercritical water conditions (350-400°C)
- Modelling High Temperature and Supercritical Water Chemistry
 - HKF models predicting the species in solution only utilize data below 300°C.
 - There is a need to generate more data at higher temperatures up to and beyond the supercritical point and then refine models to fit the data.
 - Paul's comment – are there models utilized in the hydrometallurgy industry that can be utilized in the nuclear industry to model hydrous return that are better than the current industry standard – Multeq?

A1.2 Deposition / Precipitation Processes

Significant Issues

1. Morphology of deposits and how the thermal conductivity is affected.
2. Mechanics of the deposition process
3. Deposition rate and temperature dependence
4. Solubility data in SCW and other thermodynamic properties
5. Mechanical properties of the deposits and heat flux
6. Nucleation issues
7. What is the actual structure of SCW?

Actions

1. Examine different NRCan coupons in SCW and study the subsequent corrosion. Perhaps set up a round-robin of tests?
2. Solubility of corrosion products in SCW, e.g., magnetite
3. Transport of deposits
4. The cladding materials should also be examined, e.g., ZrO₂ ceramics

N.B. Some of the work should also be done under subcritical as well as SCW conditions.

Non-Power-Plant Issue

1. Heat-exchanger fouling
2. Synthesis of new alloys, nonmetal materials and coatings

A1.3 Corrosion in Confined Regions / Concentrated Solutions

- Broad issue of significance:

Properties of water in confined space and how it affects to corrosion

- Specific research action needed:

Although a significant amount of work has been completed on the effect of water properties on corrosion of materials in general, additional work on the effect of water properties on corrosion in confined spaces would seem to be warranted. In particular there are still essentially no results for the key transport properties (viscosity, thermal conductivity, cell concentration and diffusion) for confined space.

- Non-power-plant aspects of the issue:

Many other industries experience and deal with corrosion in confined spaces. These industries include the hydrometallurgical, chemical, and petrochemical industries. Any advances made in relation to power plants would benefit these industries and vice-versa.

- Knowledge management:

It was emphasized that it is important to involve technical experts from industry to provide input and feedback to ensure direct relevance of the theoretical work to practice.

A1.4 Radiation Chemistry

Needs:

1. A better water radiolysis model for application to reactor systems. In the shorter term this would involve better inputs and model benchmarking so that we fully understand in-reactor-core processes. In the longer term we need to have models available that can be applied by non-experts.
2. A wider database for impurity degradation in radiation fields. In addition to prediction of hydrogen generation etc, we need to be able to understand the degradation pathways to look for undesirable products (e.g. oxalate, and organic goo).
3. Supercritical water. Understanding in-core radiolysis in SCW will be key to defining the correct chemistry regime for a SCW cooled reactor. Measurement of reliable radiolysis parameters in SCW should lead to some of the improvements in high temperature data described in point 1. Better knowledge of SCW radiolysis will also be of benefit in the application of SCW to waste treatment processes.

Appendix 2. Canadian Researchers

A2.1. University Research

Alan Anderson, St. Francis Xavier University
Synchrotron Measurements on Supercritical Fluids

Willy Cook, University of New Brunswick
Materials and Corrosion Product Behavior under CANDU-SCWR Conditions

Janusz Kozinski, University of Saskatchewan
Supercritical Water Chemistry in Materials and Energy Research

Derek Lister, University of New Brunswick
Power System Coolant Chemistry and Corrosion

Vladimiro Papangelakis, University of Toronto
Measurements and Modelling of Metal Solubility in Hydrometallurgical Processes

Paul Percival, Simon Fraser University
Muons as a Tool for Probing Supercritical Water Chemistry

Steve Rogak, University of British Columbia
Supercritical Water Material Testing and Electrochemical Measurements

Igor Svishchev, Trent University

Computer Simulations of Supercritical Aqueous Fluids and Particle Formation Processes

Peter Tremaine, University of Guelph

Deuterium Isotope Effects on Chemical Reactions under CANDU Operating Conditions and Gen IV Supercritical Water Reactor Chemistry

Clara Wren, University of Western Ontario

Radiolysis in CANDU Coolant and its Effect on Chemistry and Materials

A2.2 Industrial/Government Research

Dave Guzonas, Atomic Energy of Canada Ltd

Chemistry and Materials Challenges in Generation IV Supercritical Water Reactors

Gabriel Nicolaides, Ontario Power Generation

OPG WTP Performance / Trends in High Purity Water Treatment

Otto Herrmann and Teresa Switzer, Kinectrics

Determination of Metals by ICP-MS

Ken Sedman, Bruce Power

Stress Corrosion Cracking and Intergranular Attack of Steam Generator Tubing

Craig Stuart, Atomic Energy of Canada Ltd

Radiolysis in Reactor Coolant Systems

Dan Wright, Bedford Institute of Oceanography

Scientific and Industrial Formulations for the Properties of Seawater

Peter King, B&W Canada

Steam Generator Chemistry and Materials Degradation

The Czech National Committee

International Association for the Properties of Water and Steam

REPORT on IAPWS related activities – August 2008 / August 2009

Submitted to the EC Meeting of IAPWS, Arenhem, NL – September 2009.

National Committee Contacts:

CZ NC PWS, Institute of Thermomechanics AS CR, v.v.i., Dolejškova 5, 182 00 Prague 8,
Czech Republic, Fax: + 420 2858 4695, E-mail: secr.czncpws@it.cas.cz
Head: Dr. Jan Hruby, E-mail: hruby@it.cas.cz

Following Institutions participated in the research into the thermophysical properties and chemical processes:

Institute of Thermomechanics (IT) AS CR, v.v.i., 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, Technicka 4, CZ-166 07 Prague 6.

Technical University Brno (TU), Faculty of Mechanical Engineering, Energy Institute, Department of Power Engineering and Department of Thermodynamics and Environmental Engineering, Technicka 2, CZ-616 69 Brno.

Institute of Chemical Technology Prague (ICT), Power Engineering Department (ICT-IE) and Department of Physical Chemistry (ICT-IPC), Technicka 5, CZ-166 28 Prague 6.

University of West Bohemia (UWB), Faculty of Mechanical Engineering, Department of Power System Engineering, Univerzitni 8, CZ-306 14 Plzen.

SKODA POWER, Plzen, 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.

SIGMA Research and Development Institute (SIGMA), Jana Sigmunda 79, CZ-783 50 Lutín.

Activities were sponsored by the Grant Agency of the Academy of Sciences and Grant Agency of the Czech Republic, SKODA POWER Plzen, Ministry of Education, Youth and Sport of the Czech Republic, and Ministry of Industry and Trade of the Czech Republic.

Change in the board of the CZ NC Committee for the period 2010-2013:

Dr. J. Hruby, Prof. R. Mares, Dr. T. Nemec, Prof. P. Safarik, and Doc. J. Sedlbauer.

- In the 15th ICPWS in Berlin participated 13 workers from CR with 12 papers, Refs. [1 to 12]. The Workshop on Homogeneous Vapor-Liquid Nucleation in Water, organized the head of CZ NC PWS, Dr. J. Hruby, was a part of the 15th ICPWS and 11 contributions were presented and discussed.
- The 12 CD containing Proceedings of 15th ICPWS has been hand over to technical libraries in Czech Republic.
- A brief commentary has been published on web sites of CZ NC PWS to the new documents adopted and authorized by IAPWS.
- A new joint project IT AV ČR and WBU Plzen has been elaborated and accepted in the Research and Development Contest of the Ministry of Education, Youth and Sports of the ČR, which enabled cooperation with IAPWS for the next four years.

- Workers of the Institute of Chemical Technology, Prague, Faculty of Environmental Technology and Institute of Energetics (ICT-IE) organized in September 2008 the 7th International Power Cycle Chemistry Conference - CHEO-7 – dealing with water treatment for power and environment, corrosion in energetics and renewable energy sources. Selection of published articles, Refs. [13 to 22].
- Dr. Hruby (IT) participated in the evaluation of the formulations of the properties of seawater and ice, resulting in publication Ref. [23].
- Dr. Hruby (IT) with his collaborators, in collaboration with A. Harvey of NIST (USA), developed a formulation of thermophysical properties of liquid water at atmospheric pressure. The formulation was described in a draft of a Supplementary Release and was adopted in Berlin 2008, Ref. [24]. A background-paper for Supplementary Release on Properties of Liquid Water at 0.1 MPa was published, Ref. [25].
- Prof. Mares (UWB) with his collaborators took part at development a new international formulation for the viscosity of water and steam, Refs.[26 and 27] and took part in publication of supplementary backward equations, Ref.[28], contributed on behaviour of super-cooled water, Refs.[5 and 6, 29 and 30], on density of water substance at ambient pressure, Refs.[31 and 32], and on thermodynamic properties of water and steam. Ref. [7].
- Prof. Marsik (IT) coordinated research in the electrolyte membrane and efficiency of fuel cells, Ref. [33], and the metastable states, nucleation and development of a new model of cavitation erosion potential. Refs. [4, 34 to 40].
- Doc. Sedlbauer (TUL) and his team did research works on subject of chemistry of aqueous systems. Refs. [1, 11, 41 and 42]
- Doc.Sedlbauer (TUL) collaborated with team of Prof. Tremaine (Canada) and investigated the ionization constants of aqueous nitrophenols and the speciation of aqueous transition metal chloro-complexes. Refs. [10 and 43].
- Research activities at the (CTU) continued in further improvement of the current knowledge on the following subjects: determination of the heterogeneous particles in the superheated steam in turbines, Ref. [44], heterogeneous condensation seeds in expanding steam, Ref. [4 and 45], electrostatic charge of droplets in expanding wet steam, Ref. [46], hydrogen technologies, Ref. [47].
- The SIGMA Research and Development Institute (SIGMA) solved problems of erosion effects of cavitation bubbles on the blades of water pumps and the problems of the effect of water properties on cavitation phenomena. Refs. [4, 36 to 38, 48].
- Dr. Jiricek (ICT-IE) with collaborators investigated corrosion processes, renewable power sources and chemical effects in water and steam systems of power plants. Refs. [12, 13 to 22].
- Dr. Hnedkovsky (ICT-IPC) with collaborators investigated properties of organic solutes in water. Published articles and conference contributions are under Refs. [49 and 50].
- Prof. Stastny (SKODA POWER) with co-workers studied surface structure of the roughness on turbine blades, developed and applied numerical model of the water steam flow in nozzles and turbine blade cascades with NaCl binary nucleation and condensation, and collaborated in frame of the IAPWS ICRN 22. Refs. [2, 51 to 53].

Young Scientists IAPWS Fellowships

Information on the Young Scientists IAPWS Fellowship Projects.

- Ing. Ehlerova handed over the Final Report finished in the frame of the Young Scientists IAPWS Fellowship Project 2008 „Equilibrium Constants and Speciation of Aqueous Transition Metal Chlorocomplexes over a Wide Range of Temperatures and Pressures”. The report was assigned to the Executive Secretary of IAPWS. A brief summary will be presented on negotiations of WG PCAS at IAPWS Meeting 2009. The results will be published in journals and her dissertation thesis.

- Prof. R. Mares (CZ) and Prof. M. A. Anisimov (USA) (WG TPWS) prepared a Proposal for Young Scientist IAPWS Project 2010 for J. Kalova “*Thermophysical Properties of Supercooled Water*”. Proposed project has following research steps:
 - Overview and critical evaluation of existing experimental data for supercooled water, not only at ambient pressure, and critical evaluation.
 - Analysis of Widom line (experimental limits of stability, computer simulations).
 - Experimental data on amorphous ice can be used to constrain the thermodynamics functions of water at temperatures below 155 K.
 - Extrapolation of IAPWS 95 and other formulations of properties in the supercooled temperature range.
 - Recalculation of coefficients in the scaled equation including the second critical point parameters.
 - Finding the background functions for specific thermophysical properties of water.
 - Evaluation of the scaled equation and comparison with IAPWS 95 and with experimental data.

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51. Stastny M., Sejna M.: Effects of Chemistry on the Condensation of Flowing Steam in a Nozzle, Computational Mechanics, Pilsen, 2008
52. Stastny M., Sejna M. Condensation of Water-Steam with and without NaCl Impurity in a Nozzle, Power Plant Chemistry, No.9, 2008
53. Tajc L., Bednar L., Hoznedl M., Stastny M., Blahova O., Lorenc B., Valenta R. Benetka J.: Losses in Steam Turbine Stages with Increased Surface Roughness of Blades, pp.1267-1276, In: Proceedings of the 8th European Conference on Turbomachinery – Fluid Dynamics and Thermodynamics, Graz, 2009

German National Committee to IAPWS

Research Activities on the Thermodynamic Properties of Water and Steam

Report "Research in Progress 2009"

Baltic Sea Research Institute, Warnemünde, Germany, Dr. rer. nat. habil. R. Feistel

1. Preparation of the Revised Release on the Equation of State 2006 for H₂O Ice Ih
2. Preparation of the): Supplementary Release on a Computationally Efficient Thermodynamic Formulation for Liquid Water for Oceanographic Use
3. other Publications:

Feistel, R., Wright, D.G., Jackett, D.R., Miyagawa, K., Reissmann, J.H., Wagner, W., Overhoff, U., Guder, C., Tchijov, V., Feistel, A. and Marion, G.M.: Numerical implementation and oceanographic application of the thermodynamic potentials of water, vapour, ice, seawater and air. Part I: Background and Equations, Ocean Sci., 2009, *in preparation*.

Wright, D.G., Feistel, R., Jackett, D.R., Miyagawa, K., Reissmann, J.H., Wagner, W., Overhoff, U., Guder, C., Tchijov, V., Feistel, A. and Marion, G.M.: Numerical implementation and oceanographic application of the thermodynamic potentials of water, vapour, ice, seawater and air. Part II: The Library Routines, Ocean Sci., 2009, *in preparation*.

Feistel, R., Kretzschmar, H.-J., Span, R., Hagen, E., Wright, D.G., Herrmann, S.: Thermodynamic Properties of Sea Air. Ocean Science 2009, submitted

Feistel, R., Weinreben, S., Wolf, H., Seitz, S., Spitzer, P., Adel, B., Nausch, G., Schneider, B., Wright, D.G.: Density and Absolute Salinity of the Baltic Sea 2006-2009. Ocean Science Discussion 6, 1757-1817, 2009

Safarov, J., Millero, F., Feistel, R., Heintz, A., Hassel, E.: Thermodynamic properties of standard seawater: extensions to high temperatures and pressures. Ocean Science, 5, 235-246, 2009, Internet: www.ocean-sci.net/5/235/2009/

Feistel, R.: Extended equation of state for seawater at elevated temperature and salinity Desalination 2009, in press

McDougall, T.J., Feistel, R., Millero, F.J., Jackett, D.R., Wright, D.G., King, B.A., Marion, G.M., Chen, C.-T.A., Spitzer, P., Seitz, S.: IOC Manuals and Guides No. xx, 2010: The International Thermodynamic Equation Of Seawater 2010 (TEOS-10): Calculation and Use of Thermodynamic Properties, UNESCO (English) 2009, 150pp. Internet: www.teos-10.org

Marion, G.M., Millero, F.J., Feistel, R.: Precipitation of solid phase calcium carbonates and their effect on application of seawater S_A-T-P models. Ocean Science 5, 285-291, 2009. Internet: www.ocean-sci.net/5/285/2009/

Feistel, R., Wright, D.G., Miyagawa, K., Harvey, A.H., Hruby, J., Jackett, D.R., McDougall, T. J., Wagner, W.: Mutually consistent thermodynamic potentials for fluid water, ice and seawater: a new standard for oceanography. Ocean Science 4, 275-291, 2008. Internet: www.ocean-sci.net/4/275/2008/

University of Applied Sciences Zittau/Görlitz, Faculty of Mechanical Engineering,
Department of Technical Thermodynamics, Prof. Dr.-Ing. habil. H.-J. Kretzschmar

1. Supplementary Backward Equations $v(p,T)$ for Region 3 of IAPWS-IF97 (IAPWS-IF97-S05)
 - The comprehensive article on the backward equations $v(p,T)$ was published in the "Journal of Engineering for Gas Turbines and Power"
2. Development of Fast Property Algorithms Based on Spline Interpolation
 - The algorithms for fast spline-interpolation methods were developed and applied to the calculation of thermodynamic properties of steam and carbon dioxide.
3. Thermodynamic Properties of Humid Air
 - The research project RP-1485 "Thermodynamic Properties of Real Moist Air, Dry Air, Steam, Water, and Ice" of the American Society of Heating, Refrigerating, Air-Conditioning Engineers (ASHRAE) was completed.
 - Two comprehensive articles on the properties of moist air were prepared for the Journal "HVAC&R Research" and the "Journal of Engineering for Gas Turbines and Power".
 - The property library LibHuAirProp for calculating thermodynamic and transport properties of real moist Air was prepared.
4. Thermodynamic Properties of Seawater
 - The property library LibSeaWa for calculating thermodynamic and transport properties of seawater was completed.
 - A comprehensive article on the properties of sea air was prepared for the Journal "Ocean Science".

Recent Publications

- Kretzschmar, H.-J., Harvey, A.H., Knobloch, K., Mareš, R., Miyagawa, K., Okita, N., Span, R., Stöcker, I., Wagner, W., and Weber, I.: Supplementary Backward Equations $v(p,T)$ for the Critical and Supercritical Regions (Region 3) of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam. Journal of Engineering for Gas Turbines and Power, Vol. 131 (2009) pp. 043101-1
- Herrmann, S., Kretzschmar, H.-J., Teske, V., Vogel, E., Ulbig, P., Span, R., Gatley, D.P.: Determination of Thermodynamic and Transport Properties of Humid Air for Power-Cycle Calculations. Report PTB-CP-3 (2009), ISBN 1614-953X
- Herrmann, S., Kretzschmar, Gatley, D.P.: Thermodynamic Properties of Real Moist Air, Dry Air, Steam, Water, and Ice. Final Report ASHRAE RP-1485 (2008). Available from <http://www.ashrae.org>
- Kretzschmar, H.-J., Stöcker, I.: Mollier $h-s$ Diagram for Water and Steam (Pressure in MPa). Springer, Berlin (2009), ISBN 978-3-642-03321-6
- Kretzschmar, H.-J., Stöcker, I.: Mollier $h-s$ Diagram for Water and Steam. Siemens Energy Sector, Erlangen (2009)
- Kretzschmar, H.-J., Kraft, I.: Kleine Formelsammlung Technische Thermodynamik (Small Formula Collection of Technical Thermodynamics), third edition. Carl Hanser, Munich (2009)

Ruhr University Bochum, Germany, Faculty of Mechanical Engineering,
Department of Thermodynamics, Prof. Dr.-Ing. W. Wagner

1. Formulating a Revised Release on the IAPWS-95 formulation

This revised release is identical to the original release issued by IAPWS in 1996, except for inclusion of the calculated triple-point pressure, improved values for coefficients n_1^0 and n_2^0 in Table 1 to more accurately match the arbitrary conventions for the zeros of energy and entropy, and corrections in the last digits of a few calculated values in Tables 6-8. Calculations for physically measurable quantities are unchanged. Some minor editorial corrections and updates to references have also been made.

2. Editorial changes for the Revised Release on the Industrial Formulation IAPWS-IF97

Editorial changes were made for the correction of printing errors, a more exact value for the lowest pressure for the validity of Eq. (22) was given, and References [2a] and [10] were updated.

3. Steam Tables for the VDI-Heat Atlas 2010

The Section D2.1 “Properties of Water and Steam” of the VDI-Heat Atlas 2010 was written and corresponding steam tables were calculated based on the Industrial Formulation IAPWS-IF97. These steam tables are the main part of this section. Prof. H.-J. Kretzschmar is co-author of this contribution.

Current Status of Research Activities in Japan
Submitted to the Executive Committee Meeting, IAPWS, Doorwerth,
The Netherlands, September 2009

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

At the Nuclear Science and Engineering Directorate, Japan Atomic Energy Agency, Tokai-mura, Dr. S. UCHIDA made his effort to promote development of evaluation method on flow-induced vibration and corrosion of components in two-phase flow by combined analyses of flow dynamics and corrosion [Innovative and Viable Nuclear Energy Technology Development Project of the Ministry of Economy, Trade and Industry]. 1) A FAC (flow accelerated corrosion) wall thinning rate evaluation model based on combined analyses of a static electrochemistry model and a dynamic oxide layer growth corrosion model has been developed to predict wall thinning rates in PWR secondary piping [1]-[3], [5], [7], [9]-[11]. 2) Other efforts on water chemistry have been put on planning Road Maps on Research and Development Plans for Water Chemistry of Nuclear Power Systems in Japan and arranging Japan Industrial Standards for analytical procedures of water chemistry in PWR plants [4], [6], [8]. [Latest publication: [1] M. Naitoh, S. Uchida, S. Koshizuka, H. Ninokata, N. Hiranuma, K. Dosaki, K. Nishida, M. Akiyama and H. Saitoh, "Evaluation Methods for Corrosion Damage of Components in Cooling Systems of Nuclear Power Plants by Coupling Analysis of Corrosion and Flow Dynamics Analysis (I), Major targets and development strategies of the evaluation methods", *J. Nucl. Sci. Technol.*, 45, 1116-1128 (2008). [2] S. Uchida, M. Naitoh, Y. Uehara, H. Okada, N. Hiranuma, W. Sugino and S. Koshizuka, "Evaluation Methods for Corrosion Damage of Components in Cooling Systems of Nuclear Power Plants by Coupling Analysis of Corrosion and Flow Dynamics Analysis (II), Evaluation of corrosive conditions in PWR secondary cooling system", *J. Nucl. Sci. Technol.*, 45, 1275-1286 (2008). [3] S. Uchida, M. Naitoh, Y. Uehara, H. Okada, N. Hiranuma, W. Sugino, S. Koshizuka and Derek H. Lister, "Evaluation Methods for Corrosion Damage of Components in Cooling Systems of Nuclear Power Plants by Coupling Analysis of Corrosion and Flow Dynamics Analysis (III), Evaluation of Pipe Wall Thinning Rate with the Coupled Model of Static Electrochemical Analysis and Dynamic Double Oxide Layer Analysis", *J. Nucl. Sci. Technol.*, 46, 31-40 (2009). [4] S. Uchida, "Corrosion of Structural Materials and Electrochemistry in High Temperature Water of Nuclear Power Systems", *Power Plant Chemistry*, 10, 630-649 (2008). [5] D. H. Lister, L. Liu, A. D. Feicht, M. Khatib, W. G. Cook, K. Fujiwara, E. Kadoi, T. Ohira, H. Takiguchi and S. Uchida, "A Fundamental Study of Flow-Accelerated Corrosion in Feedwater Systems", *Power Plant Chemistry*, 10, 659-667 (2008). [6] S. Uchida, T. Satoh, Y. Satoh and Y. Wada, "Electrochemical sensor array for in situ measurements of hydrogen peroxide concentration in high temperature water", *Energy Materials*, 3, 104-112 (2008). [7] S. Uchida, M. Naitoh, Y. Uehara, H. Okada, S. Koshizuka and D. H. Lister, "Evaluation of Flow Accelerated Corrosion of PWR Secondary Components by Corrosion Analysis Coupled with Flow Dynamics Analysis", *Proc. International*

Conference on Water Chemistry of Nuclear Reactor Systems, NPC'08, Sep. 15 – 18, 2008, Berlin, Germany, VGB Power Tech (2008) (in CD). [8] S. Uchida, Y. Katsumura, H. Ikoma, K. Takamori, E. Kadoi and K. Ishigure, "Road Maps on Research and Development Plans for Water Chemistry of Nuclear Power Systems in Japan", Proc. International Conference on Water Chemistry of Nuclear Reactor Systems, NPC'08, Sep. 15 – 18, 2008, Berlin, Germany, VGB Power Tech (2008) (in CD). [9] S. Uchida, M. Naitoh, Y. Uehara, H. Okada, S. Koshizuka and D. H. Lister, "Evaluation of Flow Accelerated Corrosion of PWR Secondary Component by Corrosion Analysis Coupled with Flow Dynamics Analysis", Proc. 16th Pacific Basin Nuclear Conference, PBNC-16, Oct. 14-17, 2008, Aomori, Japan, Atomic Energy Society of Japan (2008) (in CD). [10] D. H. Lister, W. G. Cook, A. D. Feicht, K. Fujiwara, E. Kadoi, M. Khatibi, . Liu, T. Ohira, H. Takiguchi and S. Uchida, "A laboratory Study of Flow Accelerated Corrosion in Feedwater Systems", Proc. 16th Pacific Basin Nuclear Conference, PBNC-16, Oct. 14-17, 2008, Aomori, Japan, Atomic Energy Society of Japan (2008) (in CD). [11] S. Uchida, M. Naitoh, Y. Uehara, H. Okada, S. Koshizuka and D. H. Lister, "Evaluation of Flow Accelerated Corrosion of PWR Secondary Piping by Coupling Analysis of Corrosion and Flow Dynamics", Corrosion 2009, Paper No.09468, Mar. 23-26, Atlanta, GA, National association of Corrosion Engineers, 1-15 (2009)] [contact: Dr. S. Uchida; E-mail: uchida.shunsuke@jaea.go.jp].

The research center of Supercritical Fluid Technology, Graduate School of Engineering, Tohoku University has performed decomposition of polymers such as PC and PET in high temperature-high pressure water. They have also found the chemical recycling of polycarbonate in high pressure vapor. Even in the vapor phase, hydrolysis of polycarbonate successfully proceeded and high monomer yield was achieved. The results suggest that a high density of liquid water was not suitable for polycarbonate hydrolysis in high pressure water system due to the monomer instability at that conditions [ISHA2008 (September 2008, Nottingham, England) M. Watanabe, T. Matsuhita, Y. Matsuo, H. Inomata]. Decomposition rate and product selectivity were evaluated and utilized to estimate the reaction mechanism/kinetics. Sugar conversion could be controlled by temperature and pressure in high pressure high temperature water. They also revealed that microwave heating was effective for catalytic conversion of sugar into a furan compound. In the case of fructose reaction, 5-hydroxymethylfurfural was obtained with 90% of yield and 90% of selectivity by an ionic resin as catalyst by microwave heating in some organic mixture solvent. The effect of microwave on the formation of furan from sugar was observed in a water and water-organic mixture solvent [Green solvent 2008 (September 2008, Friedrichshafen, Germany) X. Qi, M. Watanabe, T. M. Aida, R. L. Smith, Jr.]. For the presentation, they won one of the poster presentation awards. They have also studied that sugar conversion could be controlled by temperature and pressure in high pressure high temperature water. The center has tried to clarify the effect of pressure on the sugar conversion in supercritical water by focusing on role of water on the reaction. Dehydration of intermediate was also conducted and found that high pressure (namely water density) promote dehydration of the intermediate [J. Supercrit. Fluids, 50 (2009) 257-264].

At the Institute of Multidisciplinary Research for Advanced Materials at Tohoku University, Prof. M. KAKIHANA and his group developed an original water-soluble and stable compound of silicon. The peculiar chemical properties of the new compound made it possible to elaborate a hydrothermal gelation method for synthesis of multicomponent silicon containing functional materials. The series of rare-earth and manganese activated phosphors containing silicon such as $(Y,Ce,Gd)_2SiO_5$, $Ca_3Sc_2Si_2O_{12}:Ce^3$ and $Zn_2SiO_4:Mn^{2+}$, which were prepared by use of the new water-soluble silicon compound, exhibited remarkably improved fluorescence brightness and color purity compared to the materials synthesized by the conventional approaches. The same group has continued to design and search for the stable water soluble titanium complexes. By utilizing the new peroxo-EDTA complex of Ti and directional application of the additives acting as surface modifiers the synthesis of pure nanocrystalline brookite with the highly controlled particles morphology was demonstrated for the first time. The partial nitridation of brookite TiO_2 during the hydrothermal synthesis resulted in the improved light absorption in the visible range, which, in the combination with the improved morphology, led to increased photocatalytic activity of such materials in terms of NO decomposition. [Y.Suzuki, M. Kakihana, J. Physics: Conf. Series: Mater. Sci. Eng., 1, 012012 (2009); Y.Suzuki, M. Kakihana, J. Cer. Soc. Japan, 117, 330 (2009); Y. Morishima, M. Kobayashi, V.

Petrykin, S. Yin, T. Sato, M. Kakihana, K. Tomita, *J. Cer. Soc. Japan* **117**, 320 (2009); M. Kobayashi, V. Petrykin, M. Kakihana, K. Tomita, *J. Am. Cer. Soc.* **92**, S21 (2009).]. Profs. T. SATO and S. YIN with co-workers studied on the panoscopic assembling of ceramic materials applicable for environmental clean-up, energy saving, preventing the healthy damage, etc. by solvothermal reactions. They successfully prepared visible light responsive photocatalysts such as $\text{TiO}_{2-x}\text{N}_y$ and $\text{SrTiO}_{3-x}\text{N}_y$ with controllable phase compositions and morphologies [S. Yin, M. Komatsu, B. Liu, R. Li, Y. Wang, T. Sato, *J. Mater. Sci.*, **43**, 2240 (2008); K. Tomita, M. Kobayashi, V. Petrykin, S. Yin, T. Sato, M. Yoshimura, M. Kakihana, *J. Mater. Sci.*, **43**, 2217 (2008); I. Kangl, Q. Zhang, Y. Shu, T. Sato, F. Saito, *Smart Processing Technology*, **2**, 137-140 (2008); I. Kangl, Q. Zhang, Y. Shu, T. Sato, F. Saito, *Environ. Sci. Technol.*, **42**, 3622 (2008); S. Yin, B. Liu, T. Sato, *Functional Materials Letters*, **1**, 173 (2008); S. Yin, B. Liu, P. Zhang, T. Morikawa, K. Yamanaka, T. Sato, *J. Phys. Chem.*, **112**, 12425-12431 (2008); J. Wang, H. Li, H. Li, S. Yin, T. Sato, *Solid State Phenomena*, **147-149**, 851 (2009); J. Wang, H. Li, S. Yin, T. Sato, *Solid State Sciences*, **11**, 182 (2009), U. Sulaeman, S. Yin, T. Suehiro, T. Sato, *Mater. Sci. Eng.*, (2009), **1**, 012017, 1 (2009); Y. Morishima, M. Kobayashi, V. Petrykin, S. Yin, T. Sato, M. Kakihana, K. Tomita, *J. Cer. Soc. Japan* **117**, 320 (2009)], and ceria-based new inorganic UV-shielding materials with excellent safety, comfort and transparency in the visible light region [A. M. El-Toni, S. Yin, T. Sato, *J. Mater. Sci.*, **43**, 2411-2417 (2008); T. Sato, A. M. El-Toni, S. Yin, T. Kumei, *Synthesis and Reactivity in Inorganic, Metal-Organic, and Nano-Metal Chemistry*, **38**, 335 (2008); *Phosphors Res. Bulletin.*, **22**, 17 (2008); Y. Minamidate, S. Yin, T. Sato, *Mater. Sci. Eng.*, **1**, 012003, 1 (2009); X. Liu, S. Yin, T. Sato, *Mater. Sci. Eng.*, **1**, 012013, 1 (2009)]. They also synthesized ZnO thin films with different superstructures such as nanorods, nanoscrews, nanodisks etc. [S. Yin, K. Ihara, R. Li, T. Sato, *Res. Chem. Intermed.*, **34**, 393 (2008); T. Long, S. Yin, K. Takabatake, P. Zhang, T. Sato, *Nanoscale Res. Lett.*, **4**, 247 (2009); T. Long, K. Takabatake, S. Yin, T. Sato, *J. Crstal Growth*, **311**, 576 (2009)], rare earth oxide nanoparticles with controlled morphology and excellent fluorescence properties [S. Yin, S. Akita, M. Shinozaki, R. Li, T. Sato, *J. Mater. Sci.*, **43**, 2234 (2008); M. K. Devaraju, S. Yin, T. Sato, *Mater. Sci. Eng.*, **1**, 012011, 1 (2009); M.K. Devaraju, S. Yin, T. Sato, *J. Crstal Growth*, **311**, 580 (2009)], Ag/ γ - Al_2O_3 nanocomposites possessing excellent DeNO_x catalytic activity [T. Sato, S.o Goto, Q. Tang, S. Yin, *J. Mater. Sci.*, **43**, 2247-2253 (2008)], a new compound, pyrochlore-type $\text{Sn}_{1.24}\text{Ti}_{1.94}\text{O}_{3.66}(\text{OH})_{1.50}\text{F}_{1.42}$ [Y. Xie, S. Yin, H. Yamane, T. Hashimoto, H. Machida, T. Sato, *Chem. Mater.*, **20**, 4931 (2008)] and porous SiC granules [H. Morino, H. Yamane, T. Yamada, S. Yin, T. Sato, *Mater. Trans.*, **49**, 1929 (2008)]. The relationship between morphologies and photo-chemical properties of inorganic materials was mainly investigated in detail. Profs. A. MURAMATSU and K. KANIE with co-workers have been studied the synthesis of monodispersed particles and their formation mechanism in liquid and/or solution phase. The Gel-sol method is originated and novel procedure to prepare the particles precisely controlled in size, shape, structure, and composition with rather higher productivity, based on the well controlled nucleation and growth via selective chemical reaction such as a forced hydrolysis, selective reduction, and selective sulfurization. Now, it has been applied to the formation of ITO particles as a transparent conductive film component, BaTiO_3 as dielectrics and/or piezoelectric material, ferric oxides as a magnetic material and so on. Also, they have been making their maximum efforts on the hybridization of monodispersed particles with organic material such as liquid crystals, in order to obtain multifunctional materials. In addition to these original methods, the Liquid-Phase Selective Deposition has also been developed as a novel preparation method of heterogeneous catalysts for industrial use in dilute solution of metal precursory complexes. [*Journal of Materials Science*, **43**(7), 2367-2371 (2008); *Catalysis Today* **132**, 81-87 (2008); *Chemistry Letters*, **37**(12), 1278-1279 (2008); *Chemical Communications*, **33**, 3382-3384 (2008); *Chemistry Letters*, **38**(6), 562-563 (2009); *Chemosphere*, **76**(5) 638-643 (2009); *Applied Catalysis B* **87**(3) 239-244 (2009)]. Adschiri laboratory, they regard supercritical water as a green solvent for biomass conversion and materials synthesis. So far, it has been demonstrated that cellulose could be dissolved and hydrolyzed in sub and supercritical water. Recently, it was found that a mixed solvent of supercritical water and phenolic compounds could convert lignin into valuable chemicals. [*Bioresource Tec.*, **99**, 1846 (2008)] Adschiri laboratory used a supercritical hydrothermal method to synthesize variety of nanocrystals by using supercritical hydrothermal synthesis. [*Phys. Rev. B*, **79**, 144411 (2009), *Cryst. Growth & Design*, **8**, 2814 (2008)] Recently, they proposed a new method to synthesize organic-inorganic hybrid nanocrystals by using supercritical method. In the supercritical state, organic molecules and metal salt

aqueous solution forms a homogeneous phase, and water molecule works as a catalyst for promoting organic –inorganic reactions. Thus, just by introducing organic molecules during the hydrothermal synthesis, hybrid nanoparticles are synthesized. Adschiri laboratory has challenged to synthesize variety of hybrid nanomaterials. [Dalton Transactions, **48**, 7038 (2008), J. Supercrit. Fluids, **44**, 441 (2008), J. Mater. Sci., **43**, 2393 (2008)] Previous research results for the supercritical hydrothermal synthesis method was summarized as review papers. [J. Mater. Sci., **43**, 2083 (2008). Adv. Drug Deliv. Rev., **60**, 299 (2008)] [contact: Prof. T. Adschiri; ajiri@tagen.tohoku.ac.jp]

At the Research Center for Compact Chemical Process, National Institute of Advanced Industrial Science and Technology (AIST), Dr. S. –I. KAWASAKI, Dr. K. HATAKEDA, Dr. A. SUZUKI, and co-workers are studying the supercritical water reaction system using a high performance microreactor. The microreactor made by the metal (Inconel 625 or SUS316), it can be used for high temperature and high pressure conditions. In addition, the specific microreactors and tubes lined the corrosion resistant materials (titanium or tantalum) were developed for the acid environment reaction. The corrosion resistant microreactor can be used many applications for safety process establishment. In the organic reactions, the nitration reaction of aromatic hydrocarbon such as benzene or naphthalene under subcritical water and diluted nitric acid conditions were achieved under non-catalytic environment. The systems were consisted by the titanium lined microreactor and tubes. In the nanoparticle production by the hydrothermal synthesis, the nanoparticle characteristics were affected by the mixing performance the starting solution and sc-H₂O. T-shape microreactor, swirl microreactor, central collision microreactor were developed for the hydrothermal synthesis. The CFD simulation was applied to improve the microreactor configuration. The homogeneous nanoparticles were synthesized by the microreactor systems. [K. Hatakeda, Y. Wakashima, A. Suzuki, T. Yokoyama, S. –I. Kawasaki, C. Wako, K. Arai, Proceeding of 5th International Workshop on Micro Chemical Plants, Kyoto, (2006); S. –I. Kawasaki, Y. Xiuyi, K. SUE, Y. Hakuta, A. Suzuki and K Arai, J. Supercrit. Fluids, 50 (2009) 276-282; Y. Wakashima, A. Suzuki, S. Kawasaki, K. Matsui, Y. Hakuta, J. Chem. Eng. JPN, 40 (2007) 622-629; S. –I. Kawasaki, Y. Wakashima, A. Suzuki, K. Sue, Y. Hakuta, K. Arai, Proceeding of 11th European Meeting on Supercritical Fluids, Barcelona, 2008, May, P_PR_36]. In the same research center, Dr. H. KAWANAMI and co-workers are studying organic synthesis and organic reaction using in high-pressure and high-temperature water with microreactors. Their reaction system can be applied many organic reactions, for example, C-C coupling, acylation, nitration, halogenations, etc. All these reactions were accelerated efficiently and were finished within few min at least leading very high yields and high selectivities. They further investigate the conversion of variety of saccharides using their water-based reaction method which is environmentally benign and develop the selective decomposition of polysaccharides to the valuable compounds selectively. [H. Kawanami, M. Sato, N. Otabe, T. Tuji, K. Matsushima, M. Chatterjee, T. Yokoyama, Y. Ikushima and T. M. Suzuki, *Green Chem.*, **11**, (2009), 763; H. Kawanami, K. Matsushima, M. Sato, Y. Ikushima, *Angew. Chem., Int. Ed.*, **46**, (2007), 6284; H. Kawanami, M. Sato, K. Matsushima, Y. Ikushima, *Angew. Chem., Int. Ed.*, **46**, (2007), 5129; K. Matsushima, H. Minoshima, H. Kawanami, Y. Ikushima, M. Nishizawa, A. Kawamukai, K. Hara, *Ind. & Eng. Chem. Res.*, **44**, (2005) 9626.]

At the department of material and environmental chemistry, Utsunomiya University, Dr. T. SATO and co-workers developed a new flow-type system combined the supercritical water gasification system and steam reforming system with membrane reactor to recover fuel gases especially hydrogen from biomass. In their study, the hydrogen permeable palladium-silver membrane was used for the improvement of the hydrogen recovery by selective removal of hydrogen from reaction field to shift the equilibrium of steam reforming into the favorable direction for hydrogen formation. The gas formation from glucose was carried out at 673 K and at 10 MPa for supercritical gasification and from 0.1 to 0.5 MPa of reaction pressure. The experiments changing the order of catalytic bed and Pd-Ag membrane in the membrane reactor for steam reforming revealed that the elevated high pressures and hydrogen removal before catalytic steam reforming are advantageous for high hydrogen recovery [Chem. Eng. Sci., in press].

At the Material Properties and Metrological Statistics Division, National Metrology Institute of Japan (NMIJ, formerly NRLM), National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, a section lead by Dr. K. FUJII is working on the density, viscosity, and refractive index standards. A determination of the Avogadro constant is being conducted in this section as an international project organized by the Comité International des Poids et Mesures (CIPM). This project continues through 2004 to 2010 with participants of eight National Metrology Institutes (BIPM, NMI-Australia, IMGC, IRMM, NIST, NMIJ, NPL, and PTB). The target of this project is to replace the present definition of the kilogram with a new definition based on fundamental physical constants. For the fundamental reduction of uncertainty, a 5 kg of ^{28}Si crystal was grown in 2007 under the cooperation with Russian and German institutes, and two 1 kg spheres were polished from the crystal in 2008 for density measurement. The density of the crystal has been determined with a relative standard uncertainty of 3×10^{-8} [N. Kuramoto and K. Fujii, "Improvement in the volume determination for the Si spehders with an optical interferometer," *IEEE Trans. Instrum. Meas.*, 2009, Vol. 58, No. 4, pp. 915-918]. Using the silicon crystals as a solid density standard, density standard liquids and PVT properties of fluids are calibrated by the magnetic suspension densimeter developed at the NMIJ. In his group a new absolute viscosity measurement by the 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 % [Y. Fujita, N. Kuramoto, Y. Kurano, and K. Fujii, "A new project at NMIJ for an absolute measurement of the viscosity by the falling ball method," *Proc. 14th ICPWS*, Kyoto, 2004, 112-115]. Dr. K. FUJII is working as a chairman of the WG-Density, CCM (Consultative Committee for Mass and Related Quantities) to organize the research activities on the density standards at the National Metrology Institutes. In April 2008, the CCM WG-Density meeting was held at the BIPM, and an idea for clarifying the roles of CIPM and IAPWS standards for the density of water has been discussed in the meeting, and approved both by the CCM and the IAPWS [A. H. Harvey, R. Span, K. Fujii, M. Tanaka and R. S. Davis, "Density of water: roles of the CIPM and IAPWS standards," *Metrologia*, 2009, Vol. 46, pp. 196-198]. For details, contact Dr. K. Fujii, Chief, Fluid Properties Section, NMIJ (E-mail: fujii.kenichi@aist.go.jp).

At Materials Science Research Laboratory, Central Research Institute of Electric Power Industry (CRIEPI), Yokosuka, Kanagawa, Dr. M. DOMAE and his co-workers study development of alternative reductant for hydrogen in the primary coolant of pressurized water reactors. Screening of candidates of hydrogen alternative resulted in the conclusion that methanol was the most promising. Type 304 stainless steel specimens were immersed at 593 K in the presence of dissolved hydrogen (DH) or methanol. Electrochemical corrosion potential of the specimens was measured during the immersion tests. After the immersion tests, oxide film formed on the specimens was analyzed. It is concluded that corrosion environment in the presence of DH is identical with that in the presence of methanol. [17th International Conference on Nuclear Engineering, No. 75551, Brussels, Belgium, (2009)].
[contact: Dr. M. Domae; E-mail: domae@criepi.denken.or.jp]

At the Department of Mechanical Engineering, Keio University, Yokohama, Prof. K. YASUOKA and his group are studying the molecular dynamics (MD) simulation to clarify the nucleation phenomena. For heterogeneous vapor-liquid nucleation, which is the cluster nucleation, the molecular dynamics simulation for sulfuric acid-water vapor mixture is performed. [H. Matsubara, T. Ebisuzaki, K. Yasuoka, *J. Chem. Phys.*, **130**, 104705(2009).] They also reported the coexistence and transition between Cassie and Wenzel state on pillared hydrophobic surface.[T. Koishi, K. Yasuoka, S. Fujikawa, T. Ebisuzaki, and X. C. Zeng, *PNAS*, 106, 8435(2009).] To accelerate the calculation of the molecular dynamics simulation they try to use GPU (Graphic Processing Unit).[Yokota, R., Narumi, T., Sakamaki, R., Kameoka, S., Obi, S., Yasuoka, K., *Comput. Phys. Commun.*, in press.; Narumi, T., Yasuoka, K., Taiji, M., Höfinger, S., *J. Comput Chem.*, in press.; Narumi, T., Kameoka, S., Taiji, M., and Yasuoka, K., *SIAM Journal on Scientific Computing*, 30, 3108-3125(2008).]
[contact: Prof. K. Yasuoka; E-mail: yasuoka@mech.keio.ac.jp].

At the Kanagawa Institute of Technology, Atsugi, Dr. K. OGUCHI has completely finished his experimental works concerning pVT Properties of fluids, and is now continuing the analytical and theoretical works such as correlating the equation of state for ammonia + water mixtures, especially focusing on the maximum density phenomena. [contact: Dr. K. Oguchi; E-mail: oguchi@kait.jp]

At the Department of Mechanical Systems Engineering, National Defense Academy, Yokosuka, Prof. N. KAGAWA and his group developed a twin-cell type adiabatic calorimeter for water + alcohol and water + ammonia mixtures. By the apparatus, isochoric heat capacities of water are currently being measured for temperatures from 220 to 520 K and pressures to 30 MPa. [contact: Prof. N. Kagawa; E-mail kagawa@nda.ac.jp]

Prof. H. TAKAKU was retired from Faculty of Engineering of Shinshu University in Nagano City at the end of March of 2006. However, at present he is entrusted by Shinshu University as a Professor in charge of education, and also has a lecture for graduate students of Energy Engineering Field in Tokai University. He has been working as a part-time technical adviser at Naigai Chemical Products Co., LTD. in Tokyo since May of 2006. He and his coworkers who are engaged in Shinshu University, electric power companies and water treatment makers are conducting R&D on the corrosion of steam turbine materials for geothermal power plants, the oxidation behavior of steam line materials in the high temperature-pressure steam for conventional thermal and combined cycle power plants, and other subjects on corrosion and water chemistry for power plants. The main publications; (1) H.-F. Zhan, H. Takaku, Y. Sakai, et al. "Electrochemical Corrosion Behavior of Steam Turbine Materials for Geothermal Power Plants", *Power Plant Chemistry*, **9**, 490-498 (2007), (2) H. Takaku "Essentials of the Revised Guideline-Water Conditioning for Boiler Feed Water and Boiler Water in Japan-(JIS B 8223:2006)", *Power Plant Chemistry*, **9**, 663-667 (2007). [Contact: Prof. H. Takaku; E-mail: takaku06@ybb.ne.jp]

At the Institute for Chemical Research, Kyoto University, Uji, Kyoto, Prof. M. NAKAHARA, Prof. N. MATUBAYASI, Dr. C. WAKAI, and their coworkers study the structure, dynamics, and reactions in super- and subcritical water by means of multinuclear NMR (nuclear magnetic resonance) spectroscopy and computer simulation. Their current focus are (1) the structure of low-density supercritical water studied by neutron scattering and the determination of all the O-O, O-H, and H-H radial distribution functions ["Partial Pair Correlation Functions of Low-Density Supercritical Water Determined by Neutron Diffraction with the H/D Isotopic Substitution Method", T. Otomo, H. Iwase, Y. Kameda, N. Matubayasi, K. Itoh, S. Ikeda, and M. Nakahara, *J. Phys. Chem. B* **112**, 4687-4693 (2008)] and (2) the kinetics and equilibrium of C1 and C2 chemical reactions in hot water toward the tuned control of C-C bond formation and disproportionation ["Hydrothermal C-C Bond Formation and Disproportionation of Acetaldehyde with Formic Acid", S. Morooka, N. Matubayasi, and M. Nakahara, *J. Phys. Chem. A* **112**, 6950-6959 (2008)]. [contact: Prof. M. Nakahara; E-mail: nakahara@scl.kyoto-u.ac.jp]

At the Department of Molecular Chemistry and Biochemistry, Doshisha University, Kyo-Tanabe, Kyoto, Prof. M. UENO, Prof. IBUKI and their group have been studying the electric conductivities of 1:1 electrolytes in liquid alcohol (methanol and ethanol) at temperatures up to about 240 °C under high pressure ["Density effect on the electric Conductivities of monovalent ions in methanol along the liquid-vapor coexistence curve", M. Ueno, T. Hoshina, N. Tsuchihashi, and K. Ibuki, *Rev. High Press. Sci. Tech.* **18**, 147-153 (2008)]. In collaboration with Dr. M. Kanakubo (AIST, Sendai) and Dr. Harris (University of New South Wales, Australia), the effect of pressure on the transport properties of the ionic liquid has been studied ["Effect of pressure on the transport properties of the ionic liquid: 1-alkyl-3-methylimidazolium salts", K. R. Harris, M. Kanakubo, N. Tsuchihashi, K. Ibuki, and M. Ueno, *J. Phys. Chem. B*, **112**, 9830-9840 (2008)]. [Contact: Prof. M. Ueno; E-mail: mueno@mail.doshisha.ac.jp]

At the Department of Mechanical Engineering, Kyushu University, Prof. Y. Takata and their group have released the new version of a program package for thermophysical properties of fluids: PROPATH Version 13.1. The package contains 78 pure substances, moist air, binary mixtures

and ideal gases. Information on this package is available through the website:
<http://www2.mech.nagasaki-u.ac.jp/PROPATH/>.
 [contact: Prof. Y. Takata; E-mail: takata@mech.kyushu-u.ac.jp]

At the Department of Applied Chemistry and Biochemistry, Kumamoto University, Kumamoto, Prof. M. GOTO, Assoc. Prof. M. SASAKI, and their group are studying kinetics and mechanism for reactions of biomass related materials in sub- and supercritical water. Chemical compounds such as phenolic compounds were recovered from lignocellulosics by using a batch reactor [Wahyudiono, M. Sasaki and M. Goto, *Fuel*, **88**, 1656-1664 (2009); Wahyudiono, Mitsuru Sasaki and Motonobu Goto, *Chemical Engineering Processing*, **47**, 1609-1619 (2008); M. Sasaki, Wahyudiono, H. Kawanabe, T. Saito and M. Goto, Proceeding of 9th International Symposium on Supercritical Fluids 2009, Arcachon, France (2009); Wahyudiono, M. Sasaki and M. Goto, Proceeding of 15th Regional Symposium on Chemical Engineering 2008, Kuala Lumpur, Malaysia (2008)]. The liquefaction of bitumen and the decomposition of its model compounds were carried out at 673 K and 723-773 K. These results suggest that supercritical water can be an effective solvent for the extraction and decomposition of them [Wahyudiono, T. Shiraiishi, K. Iwata, M. Sasaki and M. Goto, Proceeding of 9th International Symposium on Supercritical Fluids 2009, Arcachon, France (2009); Wahyudiono, M. Sasaki and M. Goto, Proceeding of AIChE Annual Meeting 2008, Philadelphia, PA (2008)]. Pigment and nutraceutical compounds were extracted from *Chlorella vulgaris* using scCO₂ and water in hydrothermal condition. Biological active compounds from other waste biomass were also extracted using scCO₂ and hot water. Furthermore, the antioxidant and antibacterial of extracts were analyzed [K. Kitada, S. Machmudah, M. Sasaki, M. Goto, Y. Nakashima, S. Kumamoto and T. Hasegawa, *J. Chemical Technology and Biotechnology*, **84**, 657-661 (2008); Y. Kawahito, M. Kondo, S. Machmudah, K. Sibano, M. Sasaki and M. Goto, *Separation and Purification Technology*, **61**, 130-135 (2008); K. Kitada, S. Machmudah, M. Sasaki, M. Goto, Y. Nakashima, S. Kumamoto and T. Hasegawa, *Separation Science and Technology*, **44**, 1228-1239 (2009)]. We are also studying various natural materials in collaboration with The University of Basque Country (Spain) [T. Kamogawa, S. Machmudah, M. Sasaki and M. Goto, Proceeding of 15th Regional Symposium on Chemical Engineering in Conjunction with 22nd Symposium of Malaysian Chemical Engineers (2008); S. Machmudah, T. Kamogawa, M. Sasaki and M. Goto, Proceeding of 9th International Symposium on Supercritical Fluids, Arcachon, France (2009)] and companies [R. Askin, M. Goto and M. Sasaki, *J. Food BioProd. Process*, (2009) (in press); R. Askin, M. Sasaki and M. Goto, Proceeding of the 11th European Meeting on Supercritical Fluids, Barcelona (2008)]. We overviewed the current state of the science and technology of supercritical fluids. The principal objective is to acquaint the reader with the unusual properties of supercritical fluids, and with the ways some basic principles are essential in understanding the supercritical fluid extraction (SFE) technique and the independence of relevant process parameters that are exploited for a variety of applications in cases of both SFE and supercritical fluid chromatography (SFC) in the food industry [R. Askin, M. Goto and M. Sasaki, Supercritical Fluid Extraction in Food Analysis, in S. Otles. (Ed), *Handbook of Food Analysis Instruments*, CRC Press, Chapter 3, p. 25 (2008)]. Hydrothermal electrolysis of many organic compounds especially glycerol was done by using batch reactor and the possible reaction mechanism and the effects of current on the decomposition of organic materials were examined [A. Yuksel, H. Koga, M. Sasaki and M. Goto, *Journal of Renewable and Sustainable Energy*, **1**(3), (2009) (in press); A. Yuksel, H. Koga, M. Sasaki and M. Goto, Proceedings of 9th International Symposium on Supercritical Fluids, Arcachon, France (2009)]. Particular phenomena (such as polymerization, exchange reaction, etc.) with discharged arc like plasma was investigated using aromatic compounds as initial materials in sub- and supercritical fluids (such as water, carbon dioxide, etc.) without catalyst [M. Mitsugi, A. Yoshida, T. Kiyari, M. Takade, K. Miyaji, T. Namihira, Y. Kuwahara, H. Akiyama, M. Hara, M. Sasaki, M. Goto, Proceeding of the 15th Regional Symposium on Chemical Engineering in Conjunction with 22nd Symposium of MALAYSIAN Chemical Engineers (2008); M. Goto, M. Sasaki, T. Kiyari, T. Fang, B. C. Roy, T. Namihira, H. Akiyama, M. Hara, Proceeding of Joint 21st AIRAPT and 45th EHPRG int. Conf. on High Pressure Science and Technology (2008)]. [contact: Prof. M. Goto; E-mail: mgoto@kumamoto-u.ac.jp, Assoc. Prof. M. Sasaki; E-mail: msasaki@kumamoto-u.ac.jp]

Russian National Committee 2009 Report

RNC meeting (18 June 2009) - changes in RNC:

new chairperson Tamara Petrova petrova@twi.mpei.ac.ru
new secretary Denis Smetanin SmetaninDS@mpei.ru

Publications:

Petrova T.I., Voronov V.N. Water chemistry at fossil and nuclear power plants: textbook for students. MPEI, 2009, P. 290. (Rus)

Petrova T.I., Repin D.A. Factors affecting cooling systems operation at fossil power plants // Vestnik MEI, # 1, 2009, pp 106-111 (Rus)

Bushuev E. N. Mathematical simulation of ionic equilibriums of water coolant using electrical conductivity and pH measurements // Thermal engineering, Vol. 56, # 7, 2009, pp 546-552

Ochkov V.F., Chudova Yu.V., Minaeva E. A. "Cloud computations" for chemical departments of power stations // Thermal engineering, Vol. 56, # 7, 2009, pp 553-559

Valyashko V.M. (editor) Hydrothermal properties of materials: Experimental data on aqueous phase equilibria and solution properties at elevated temperatures and pressures. 2008, John Wiley & Sons, Ltd.

Larin B.M., Larin A.B., Oparin M.Yu., Vinogradov V.N. Field experience with a new installation for countercurrent ion-exchange treatment of low-mineralized natural water with high content of organic impurities // Thermal engineering, Vol. 56, # 6, 2009, pp 506 - 509

Mulev Yu.V., Mulev A.Yu. Ultra-high-frequency method of diagnostics of two-phase state of a water coolant // Thermal engineering, Vol. 56, # 4, 2009, pp 316 - 319

The 2-nd International water chemistry forum (Moscow, April 2009) – problems discussed:

- water chemistry
- water chemistry automation
- water make-up systems
- waste water treatment

U.S. National Committee to IAPWS 2009 Report on Activities of Potential Interest to IAPWS

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

A collaboration is continuing with Prof. Richard Wheatley at the University of Nottingham, developing intermolecular pair potentials for aqueous systems for the quantitative calculation of second virial coefficients. Results for the water-carbon-monoxide binary have been obtained and a publication is in press. Similar results are almost complete for the water-CO₂ binary, which is the last item needed to complete a theory-based model for the thermodynamics of humid gases.

Reference: Wheatley, R.J., and Harvey, A.H., Intermolecular potential energy surface and second virial coefficients for the nonrigid water-CO dimer, *J. Chem. Phys.*, in press.

In collaboration with workers in Greece and Germany and at the University of Maryland, work is continuing on the joint IAPWS and IUPAC efforts to update the formulations for the transport properties of water and steam. The correlating surface for viscosity has been completed and a paper has been published in *J. Phys. Chem. Ref. Data*. For the thermal conductivity, the form of the critical enhancement has been worked out, and a preliminary low-density function and preliminary background function have been generated.

Reference: Huber, M.L., Perkins, R.A., Laesecke, A., Friend, D.G., Sengers, J.V., Assael, M.J., Metaxa, I.N., Vogel, E., Mareš, R., and Miyagawa, K., New International Formulation for the Viscosity of H₂O, *J. Phys. Chem. Ref. Data* **38**, 101 (2009).

In NIST's Process Measurements Division (Gaithersburg, MD), a new gravimetric hygrometer has been developed for direct measurement of humidity in gases. Initially it is being used to validate the performance of humidity generators, but with further refinements it could also be used to measure enhancement factors for the equilibrium solubility of liquid water or ice in air or other gases in order to obtain thermodynamic data for these mixtures.

Reference: Meyer, C.W., Hodges, J.T., Hyland, R.W., Scace, G.E., Valencia-Rodriguez, J., and Whetstone, J.R., A Second-Generation NIST Gravimetric Hygrometer, *Metrologia*, to be submitted.

NIST's Experimental Properties of Fluids group has built apparatus for two projects to measure thermophysical properties of aqueous gas mixtures at high temperatures. One apparatus is a high-temperature (up to 770 K) magnetic-suspension densimeter, which will be used to measure H₂O-N₂ and H₂O-CO₂ mixtures of interest for understanding the thermodynamics of combustion gases. A high-temperature thermal conductivity apparatus (using the transient hot-wire technique) has been converted to alternating-current operation (needed for polar fluids like water) in order to measure the thermal conductivity of H₂O-N₂ and H₂O-CO₂ mixtures at similar conditions. The thermal conductivity apparatus has completed measurements for the H₂O-N₂ binary and its two pure components from 500 K up to 740 K.

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

An article "Thermal diffusivity of H₂O near the critical point" by J.V. Sengers, R.A. Perkins, M.L. Huber, and B. Le Neindre was completed and will appear in the *International Journal of Thermophysics*.

The group at the University of Maryland is in the process of formulating a theoretically based equation for the critical locus of NaCl+water solutions. Progress of this research will be reported at the 2009 IAWPS meeting under item 15 of the agenda of the Working Group on Thermophysical Properties of Water and Steam.

Communicated from OLI Systems, Morris Plains, NJ:

Work is continuing on developing thermodynamic and transport property models for multicomponent, multiphase electrolyte systems. In 2008-2009, work was focused on (1) a new comprehensive model for thermal conductivity of aqueous and mixed-solvent electrolyte systems; (2) developing thermodynamic model parameters for systems containing Fe, Ni, Zn, Li, B, and H₂ within the framework of a speciation-based thermodynamic model at temperatures up to 350 °C; (3) developing, in collaboration with Professor Vladimiro Papangelakis of the University of Toronto, thermodynamic model parameters for

systems of interest in hydrometallurgy and (4) extension of speciation-based thermodynamic models to systems related to CO₂ sequestration.

References: Wang, P., Anderko, A., Modeling Thermal Conductivity of Concentrated and Mixed-Solvent Electrolyte Systems, *Ind. Eng. Chem. Res.* **47** 5698-5709 (2008); Wang, P., Anderko, A., Springer, R.D., Kosinski, J.J., and Lencka, M.M., Modeling Chemical and Phase Equilibria in Geochemical Systems Using a Speciation-Based Model, *J. Geochemical Exploration*, in press.

Communicated from the Energy Institute Electrochemical Laboratory, Penn State Univ.:

The Energy Institute Electrochemical Laboratory (S.N. Lvov) continues working on a number of electrochemistry related projects. In the past year of 2008-09, the research was focused on topics associated to high-temperature aqueous system such as electrophoresis of metal oxide particles, mineral-water electrical double layer, pH measurements, electrochemical corrosion of metals, zirconia coatings, proton exchange membrane fuel cells, and CuCl/HCl electrolysis for CuCl thermochemical cycle. The main outcomes can be found in the following publications:

1. Balashov V.N., Fedkin M.V., Lvov S. N., Experimental System for Electrochemical Studies of Aqueous Corrosion at Temperatures above 300 °C, *J. Electrochem. Soc.*, 2009, 156, C209-C213.
2. Rodriguez-Santiago V., Fedkin M.V., Wesolowski D.J., Rosenqvist J., and Lvov S. N., Electrophoretic Study of the SnO₂/Aqueous Solution Interface up to 260 °C, *Langmuir*, 2009, 25, 8101–8110.
3. Jankovic Z, Papangelakis V.G., Lvov S.N., Effect of nickel sulphate and magnesium sulphate on pH of sulphuric acid solutions at elevated temperatures, *J. Appl. Electrochem.*, 2009, 6, 751-759.
4. Rodriguez-Santiago V., Fedkin M.V., Vidojkovic S., Wesolowski D.J. and Lvov S. N. Nanoelectrophoresis studies of magnetite and silica in hydrothermal environments *Geochim. et Cosmochim. Acta*, 73, A1111-A1111.
5. Wesolowski D.J., Bandura A.V., Cummings P.T., Fenter P.A., Kubicki J.D., Lvov S. N., Machesky M.L., Mamontov E., Predota M., Ridley M.K., Rosenqvist J., Sofo J.O., Vlcek L., and Zhang Z., Atomistic origins of mineral-water interfacial phenomena and their relation to surface complexation models, *Geochim. et Cosmochim. Acta*, 73, A1429-A1429.
6. Zhang Z. C., Chalkova E., Fedkin M., Wang C., Lvov S. N., Komarneni S., and Chung T.-C. M., Synthesis and Characterization of Poly(vinylidene fluoride)-g-sulfonated Polystyrene Graft Copolymers for Proton Exchange Membrane, *Macromolecules*, 2008, 41, 9130-9139.
7. Zhou Z. F., Chalkova E., Lvov S. N., and Chou P. H., Hydrothermal deposition of zirconia coatings on pre-oxidized BWR structural materials, *J. Nuclear Materials*, 2008, 378, 229-237.
8. Rodriguez-Santiago V., Fedkin M. V., and Lvov S. N., Electrophoresis system for high temperature mobility measurements of nanosize particles. *Rev. Scientific Instr.*, 2008, 79, 093302.
9. Rodriguez-Santiago V., Fedkin M. V., Rosenqvist J., Machesky M. L., Wesolowski D. J., and Lvov S. N., Surface properties of nanosize oxides by high temperature electrophoresis, *Geoch. Cosmoch. Acta*, 2008, 72, A802.
10. Balashov V. N., Fedkin M. V., Lvov S. N., and Dooley R. B., Experimental System for Studying Interfacial Electrochemistry at Temperatures Above 300 °C, *ECS Trans.*, 2008, 11, 27-38.
11. Rodriguez-Santiago V., Fedkin M. V., and Lvov S. N. Study of the Electrochemical Step of Novel Active Metal Alloy Thermochemical Cycles for Hydrogen Production, *ECS Trans.*, 2008, 11, 133-142.
12. Fedkin M. V., Chalkova E., Wesolowski D. J., and Lvov S. N., Understanding the Water Retention of Composite Proton Exchange Membranes Based on Surface Chemistry of Inorganic Fillers, *ECS Trans.*, 2008, 11, 189-198.
13. Wang C., Chalkova E., Lute C., Fedkin M. V., Komarneni S., Chung T. C. M., and Lvov S. N., Proton Conductive Inorganics for Composite Membranes in PEM Fuel Cells, *ECS Trans.*, 2008, 16, 1451-1459.
14. Zhou Z. F., Chalkova E., Balashov V.N., Chou P. H., and Lvov S. N., Interfacial Chemistry of Hydrothermal Deposition of Zirconia on Metal Substrates, *ECS Trans.*, 2008, 11, 181-188.

15. Machesky M. L., Wesolowski D. J., Ridley M.K., Palmer D. A., Rosenqvist J., Lvov S. L., Fedkin M. V., Predota M., and Vlcek L., The Protonation Behavior of Metal Oxide Surfaces to Hydrothermal Conditions, *ECS Trans.*, 2008, 11, 151-166.