# **IAPWS Canadian National Committee**

### Annual Report 2010

*Executive:* David Guzonas (Chair), Peter Tremaine (Past Chair), Derek Lister (Secretary Treasurer), Willy Cook (Member at Large), Ian Hey (CANDU Owners Group Representative)

### 1: Canadian National Committee

Dues for the Canadian National Committee of IAPWS are supported by the National Research Council of Canada. This arrangement requires support and participation by a national association representing industry. In 2004, this role was taken on by the CANDU Owners Group (COG) on a trial basis. In 2007, COG agreed to accept this responsibility for a five-year term, to provide travel support for the CNC, and to organize an annual meeting aimed at providing liaison with the electric power industry. COG has been proactive in supporting the CNC since this arrangement was put in place.

### 2: IAPWS Annual Meeting

Canada hosted the 2010 Annual Meeting in Niagara Falls, 2010 July 18-23. The full details can be found in the minutes of the annual meeting.

### 3: IAPWS Collaborations

# 1) <u>ICRN 19: Improved Coolant Sampling and Analysis of Low Concentration Metals (Fe, Cu, Co, etc.)</u>

ICRN 19 was issued in September 2006 as an effort to address inadequate sampling techniques that all too often give rise to uncertainties in the constituents and composition of water and steam cycles. Sampling was the overarching theme of 2010 IAPWS Annual Symposium, Niagara Falls, Canada. ICRN 19 expired in September 2009, but at the 2010 meeting it was recommended that this ICRN be extended to 2012.

The ICRN was the subject of an IAPWS International Collaboration among: UNB, Canada; University of Tokyo, Japan; Alstom, Switzerland and Dong Energy, Denmark (2009); a student from Japan will visit UNB twice in 2010/2011 to investigate the interaction between hot sample streams and typical sample system materials.

### Publications:

A CFD Study of Corrosion Product Collection Efficiency of Sampling Nozzles under Power Plant Conditions (2009). P. Srisukvatananan, D.H. Lister, R. Svoboda and K. Daucik. The 9thIntl. Conf. on Cycle Chemistry in Fossil and Combined Cycle Plants with HRSGs, Boston, USA.

A CFD Study of Corrosion Product Collection Efficiency of Sampling Nozzles under Power Plant Conditions, P. Srisukvatananan, D.H. Lister, R. Svoboda and K. Daucik, Power Plant Chemistry, 11(10) (2009).

### 2) Canada-Czech Collaboration

The CNC has completed an international collaboration with the Czech National Committee (Tremaine and Sedlbauer). A Czech PhD. student, Jana Ehlerova, worked at the University of Guelph from 2008 July to 2009 June. The results of this and her previous IAPWS project were published as:

Spectrophotometric Determination of the Ionization Constants of Aqueous Nitrophenols at Temperatures up to 225°C, J. Ehlerova, L.N. Trevani, J. Sedlbauer and P. Tremaine, J. Solution Chem. **37**, 854-857 (2008).

Complexation in the Cu(II)-LiCl-H2O System at Temperatures to 423 K by UV-Visible Spectroscopy, L.N. Trevani, J. Ehlerova, J. Sedlbauer and P. Tremaine, Int. J. Hydrogen Energy, **96**, 117-124 (2009).

### 4: Research into the Properties of Water and Steam at Canadian Universities

### a) <u>University Network of Excellence in Nuclear Engineering (UNENE)</u>

In 2004, the Canadian government and nuclear industry cofounded an initiative to create a number of NSERC University Research Chairs to form a research network, and a common post-graduate MSc program in nuclear engineering. The industrial participants are Atomic Energy of Canada Limited (AECL), Ontario Power Generation (OPG), Bruce Power, and COG. The chairs relevant to the mission of IAPWS are listed below, along with related NSERC Industrial Chairs that form part of the network, with one-on-one funding by industry:

- **Roger Newman (University of Toronto):** Corrosion, materials performance, electrochemistry in the primary and secondary coolants.
- Dave Shoesmith (University of Western Ontario): Electrochemistry, materials performance and corrosion for high-level nuclear waste repositories.
- Clara Wren (University of Western Ontario): Radiolysis and radiation chemistry in irradiated reactor systems (primary coolant, moderator) and reactor accident scenarios.
- Derek Lister (University of New Brunswick, Associate Member of UNENE): Primary and secondary coolant chemistry, activity transport, corrosion.

Canadian researchers are also involved with UNENE as members of universities that are associate members in UNENE:

**Peter Tremaine (University of Guelph, Associate Member):** Solution thermodynamics, phase relations, and solubility in sub-critical and supercritical water, D<sub>2</sub>O isotope effects and CANDU primary water conditions.

### b) Other University Research in Areas of Interest to IAPWS

Generation IV Supercritical Water-cooled Reactors:

Canada has established a National Program to perform research and development in support of the concept of a CANDU Supercritical Water-cooled Reactor (SCWR). The research being carried out focuses primarily on key technology areas such as materials, chemistry, thermal-

hydraulics, safety, physics, and hydrogen production. Natural Resources Canada (NRCan), along with the Natural Sciences and Engineering Research Council of Canada (NSERC) and AECL established the NSERC/NRCan/AECL Generation IV Energy Technologies Grant Program, focusing on these four key areas of research for the Supercritical Water-cooled Reactor (SCWR) system. This grant program is co-funded by NSERC and NRCan's Office of Energy Research and Development, with in-kind contribution from AECL to guide and supervise research activities. Canadian academic researchers, in collaboration with AECL and NRCan scientists, receive grant funds to undertake specific research in support of Generation IV Energy Technologies. The following researchers are involved in chemistry-related projects of potential interest to IAPWS in this program:

- Igor Svischev (Trent University): Molecular simulations of high temperature aqueous systems.
- **Paul Percival (Simon Fraser University):** Muonium ion chemistry and radiolysis in subcritical and supercritical water using the TRIUMF cyclotron national facility.
- Alan Anderson (St. Francis Xavier University): Solubility and phase relations in supercritical water using diamond anvil cell methods.
- Cory Pye (St. Mary's University): Ab initio calculations on ionic hydration and complexation.
- Willy Cook (University of New Brunswick): Corrosion, water chemistry and corrosion product transport in nuclear reactor systems, including supercritical water.
- Jean-Paul Jay-Gerin (University of Sherbrooke): Computational studies of radiolysis in high temperature water.

**D. Guzonas (AECL)** provides guidance on program direction as well as advice related to the reactor design concept.

Other Canadian researchers with active programs in high-temperature water chemistry include:

• Vladimiros Papangelakis (University of Toronto): Hydrometallurgy of pressure-leach processes involving nickel, cobalt, copper, and zinc ores.

### 5. Other Publications of Interest to IAPWS

Chemistry Control Challenges in a Supercritical Water-cooled Reactor, D. Guzonas, P. Tremaine, J.-P. Jay-Gerin, Power Plant Chemistry, **11**, 284-291 (2009).

Research and Development Initiatives in Support of the Conceptual Design for the CANDU Supercritical Water-Cooled Reactor, D. Brady, D. Guzonas, W. Zheng, L. Leung, 31<sup>st</sup> CNS Annual Conference, Montreal, Canada, May 2010.

Enhancing University R&D Capabilities in Support of Generation-IV Nuclear Reactor Development, D. Brady, D. Guzonas, L. Leung, W. Zheng, J. Poupore, T. Anderson, CNS Conference on Nuclear Education and Outreach (NEO-2010), June 20-22, 2010, University of Calgary, Calgary.

# The Czech National Committee

### International Association for the Properties of Water and Steam

## **REPORT on IAPWS related activities – August 2009 / July 2010**

Submitted to the EC Meeting of IAPWS, Niagara Falls, Canada – July 2010.

#### 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 in 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.
- **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.

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

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

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.

### The board of the CZ NC PWS for the period 2010-2013:

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

- In the 2009 IAPWS Meeting in Doorwerth, Nederlands participated 13 workers from CR and some of their papers are in Refs. [1 to 4].
- Brief information has been published on web sites of CZ NC PWS to the new documents adopted and authorized by IAPWS.
- A joint project IT AV ČR and WBU Plzen sponsored by the Ministry of Education, Youth and Sports (MEYS, MŠMT in Czech) enables cooperation with IAPWS for the next four years, till 2012 inclusive.
- Dr. Hruby (IT) investigated properties at homogeneous and heterogeneous nucleation and at heat transfer, Refs. [5 and 6].
- Prof. Mares (UWB) with his collaborator investigated a new international formulation for the viscosity of water and steam, Ref. [7], contributed on behavior of super-cooled water, Ref. [8], and on thermodynamic properties of steam, Ref. [9].

- Prof. Marsik (IT) coordinated research in nucleation and cavitation processes, Refs. [33], and the metastable states, nucleation and development of a new model of cavitation erosion potential. Refs. [10 to 17].
- Doc. Sedlbauer (TUL) and his team continued in the research on chemistry of aqueous systems. Refs. [18 and 19]
- Doc. Sedlbauer (TUL) collaborated with the team of Prof. Tremaine (Canada) and investigated the Cu(II)–LiCl–H<sub>2</sub>O system by UV-Visible spectroscopy. Ref. [20].
- Doc. Sedlbauer (TUL) coordinated IAPWS-IUPAC Joint Project: Establishing recommended data on thermodynamic properties of hydration for selected organic solutes and gases.
- 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, heterogeneous condensation seeds in expanding steam and hydrogen technologies.
- The SIGMA Research and Development Institute (SIGMA) was engaged in the problems of hydrodynamic cavitation in water, erosion effects of cavitation bubbles on solid surfaces and nucleation processes during cavitation. Refs. [2, 14 to 17].
- Dr. Jiricek (ICT-IE) with collaborators investigated renewable power sources and chemical effects in water and steam systems of power plants. Refs. [21 to 24].
- Dr. Hnedkovsky (ICT-IPC) with collaborators investigated properties of organic solutes in water. Published articles are under Refs. [25 and 28].
- 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, Refs. [2, 29 and 30], and collaborated on the IAPWS ICRN 22. Ref. [4].

# Young Scientists IAPWS Fellowships

Information on the Young Scientists IAPWS Fellowship Project.

• J. Kalova performs her Young Scientist IAPWS Fellowship Project (CZ-USA) Project "Thermophysical Properties of Supercooled Water" under supervising of Prof. R. Mares, and Prof. M.A. Anisimov. The purpose of the collaborative project is to analyze a critical behavior of water near the liquid – liquid critical point, to calculate second critical point parameters, and to describe properties of supercooled water by means of existing experimental data and data form IAPWS formulations.

Preliminary results will be presented and discussed at the 2010 IAPWS Meeting in Niagara Falls, Canada. The Final Report of the Project will be finished by the end of the year 2010.

### **References:**

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- 2. Sedlar, M., Zima, P., Muller, M., Marsik, F.: Numerical and Experimental Investigation of Hydrodynamic Cavitation in Water, Presentation IAPWS Annual Meeting 2009, Doorwerth, 2009.
- 3. Stastny M., Sejna M.: Condensation of Water-Steam with NaCl Impurity Flowing in a Nozzle and in a Turbine Cascade, Presentation IAPWS Annual Meeting, Doorwerth, 2009.
- 4. Stastny M., Rudge A: IAPWS Certified Research Need ICRN 22, Presentation on IAPWS Annual Meeting, Doorwerth, 2009.

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- 6. Peukert P., Hruby J.: Experimental Heat Exchanger with a Corrugated Capillary tube. In: Experimental Fluid Mechanics 2009, Proceedings of the International Conference, pp.286-289, Liberec, 2009
- Mares, R., Kalova, J.: A New International Formulation for Viscosity of Water and Steam at Industrial Calculations, (in Czech). In: 8th Conference with international participation on Power System Engineering, Thermodynamics & Fluid Flow, Plzeň, 2009.
- 8. Kalova, J., Mares, R.: Application of Excel at Calculation of Pressure of Saturated Steam of Supercooled Water, Littera Scripta, České Budějovice, 2009. (in Czech).
- 9. Kalova, J., Mares, R.: Linear Expansion of Ideal Gas, Littera Scripta, České Budějovice, 2009. (in Czech).
- 10. Nemec T., Marsik F.: The Classical Multicomponent Nucleation Theory for Cavitation in Water with Dissolved Gases, 7th International Symposium on Cavitation, Ann Arbor, 2009.
- 11. Nemec T., Marsik F.: Microscopic Surface Tension in the Classical Nucleation Theory, 18th International Conference on Nucleation and Atmospheric Aerosols, Prague, 2009.
- 12. Nemec T.: The Classical Nucleation Theory and Modeling of Cavitation Processes, In: Experimental Fluid Mechanics 2009, Proceedings of the International Conference, Liberec, 2009.
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- 14. Sedlar, M., Zima, P., Muller, M.: CFD Analysis of Cavitation Erosion Potential in Hydraulic Machinery. In: Proceedings of the 3rd IAHR International Meeting of the Workgroup on Cavitation and Dynamic Problems in Hydraulic Machinery and Systems, (pp.205-214), Brno, 2009.
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- Zima, P., Sedlar, M., Muller, M.: Erosive Potential of Traveling Bubble Cavitation in a Water Pump - CFD & Experiment. In: Experimental Fluid Mechanics 2009. Proceedings of the International Conference. pp.432-442, Liberec, 2009.
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- 19. Sedlbauer J.: Air-Water Partition of Organic Chemicals in a Wide Range of Environmental Conditions. In: 12th EuCheMS International Conference on Chemistry and the Environment, Stockholm, 2009.
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# **Danish National IAPWS Committee - DIAPWS**

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

03 March 2010

### IAPWS report 2008 and 2009

The Danish research activities in 2008 and 2009 in the field of properties of water and steam were mainly concentrated at the Technical University of Denmark, Copenhagen. The main task was the modelling of multicomponent aqueous electrolyte systems and application of models to the carbon capture and storage (CCS) processes for treatment of flue gas.

The research at the utilities has concentrated on development of guidelines for sampling of particulate contaminants (corrosion products) in water/steam cycle. An international collaboration project (Canada, Switzerland and Denmark) supported by IAPWS was successfully elaborated in two stages (one each year). Furthermore, the effect of decomposition products from ion exchangers on the water/steam cycle, as well as the condensate polishing plant design, was subject for investigation.

Publications:

Victor Darde; Kaj Thomsen; Willy J.M. van Well; Erling H. Stenby, Chilled ammonia process for CO2 capture, Energy Procedia, 1(2009)1035-1042(issue 1)

Leila Faramarzi; Georgios M. Kontogorgis; Kaj Thomsen; Erling H. Stenby, Thermodynamic modeling of the solubility of CO2 in aqueous alkanolamine solutions using the extended UNIQUAC model application to monoethanolamine and methyldiethanolamine, Energy Procedia, 1(2009)861-867(issue 1)

Leila Faramarzi, Georgios M. Kontogeorgis, Kaj Thomsen, Erling H. Stenby, Extended UNIQUAC model for thermodynamic modeling of CO2 absorption in aqueous alkanolamine solutions, Fluid Phase Equilibria, 282(2009)121–132

P.Srisukvatananan, D.H.Lister, R.Svoboda, K.Daucik, Corrosion Product Sampling in Power Plants under Water/Steam Cycle Conditions, Proc. 15.Int Conf. On Properties of Water and Steam, Sept.7-11 2008, Berlin/Germany, ISBN 978-3-931384-64-7.

K.Daucik, Significance of leachable from ion exchange resin for the purity of water/steam cycle, Second Int. Conf.: Interaction of Organics and Cycle Treatment Chemicals with Water, Steam, and Materials, 4-6 November 2008, Luzerne, Switzerland.

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Philip Loldrup Fosbøl, Erling Halfdan Stenby, Kaj Thomsen, "The chilled ammonia process -Evaluation of the energy requirements", Internal report (2008)

Victor Camille Alfred Darde, Kaj Thomsen, Erling Halfdan Stenby, "Chilled ammonia process for CO2 capture", Internal report (2008)

# **German National Committee to IAPWS**

# Research Activities on the Thermodynamic Properties of Water and Steam Report "Research in Progress 2010"

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

- 1. Preparation of the Guideline on an Equation of State for Humid Air in Contact with Seawater and Ice, Consistent with the IAPWS Formulation 2008 for the Thermodynamic Properties of Seawater (with H.J. Kretzschmar, A.H. Harvey, M. Miyagawa)
- 2. Preparation of the Revision of the Revised Release on the Pressure along the Melting and Sublimation Curves of Water (with W. Wagner, A.H.Harvey)
- 3. Proposal for Renewal of ICRN 16 on Thermophysical Properties of Seawater
- 4. other Publications:

Wright, D.G., Pawlowicz, R., McDougall, T.J., Feistel, R., Marion, G.M.: Absolute Salinity, "Density Salinity" and the Reference-Composition Salinity Scale: Present and Future Use in the Seawater Standard TEOS-10. Submitted to Ocean Science on 30 May 2010

Seitz, S., Feistel, R., Wright, D.G., Weinreben, S., Spitzer, P., de Bievre, P.: Metrological Traceability of Oceanographic Salinity Measurement Results. Submitted to Ocean Science on 28 May 2010

Feistel, R., Marion, G.M.M., Pawlowicz, R., Wright, D.G.: Thermophysical Property Anomalies of Baltic Seawater. Ocean Science, submitted 26 May 2010

Feistel, R.: Stochastic Ensembles of Thermodynamic Potentials. Accreditation and Quality Assurance, submitted 20 May 2010

Feistel, R., Labrenz, R.: Neuer Internationaler Meerwasserstandard. Schiff & Hafen, April 2010, Nr.4, 66-67

Wright, D., Pawlowicz, R., McDougall, T., Feistel, R.: Progress Report for the SCOR/IAPSO Working Group 127 on "Thermodynamics and Equation of State of Seawater" CNC/SCOR Newsletter, 49, March 30, 2010, p.1-4 http://www.cmos.ca/scor/NL49Mar2010.pdf

Wright, D., Pawlowicz, R., McDougall, T., Feistel, R.: Progress Report for the SCOR/IAPSO Working Group 127 on "Thermodynamics and Equation of State of Seawater". CMOS Bulletin, submitted 26 March 2010

Marion, G.M., Millero, F.J., Camoes, F., Spitzer, P., Feistel, R. Chen, C.-T.A.: pH and Acidity of Natural Waters. Marine Chemistry, submitted 19 Feb 2010

Wright, D.G., Feistel, R., Reissmann, J.H., Miyagawa, K., Jackett, D.R., Wagner, W., Overhoff, U., Guder, C., 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. Discuss., 7, 649-708, 2010. www.ocean-sci-discuss.net/7/649/2010/

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Feistel, R., Wright, D.G., Kretzschmar, H.-J., Hagen, E., Herrmann, S., Span, R.: Thermodynamic Properties of Sea Air. Ocean Science, 6, 91-141, 2010. http://www.oceansci.net/6/91/2010/

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Feistel, R.: Extended equation of state for seawater at elevated temperature and salinity. Desalination 250, 14–18, 2010.

McDougall, T.J., Feistel, R., Wright, D.G., Pawlowicz, R., Millero, F.J., Jackett, D.R., King, B.A., Marion, G.M., Seitz, S., Spitzer, P., Chen, C.-T.A. (proposers): IOC, SCOR and IAPSO: The international thermodynamic equation of seawater - TEOS-10: Calculation and use of thermodynamic properties. Intergovernmental Oceanographic Commission, Manuals and Guides No. 56, UNESCO (English), 182 pp., Paris, 2010. www.teos-10.org

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

1. 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.
- An algorithm for the generation of data grids with optimized data density for the user requirements range of state and accuracy is being developed.

- 3. Thermodynamic Properties of Humid Air
  - The results of the research project RP-1485 "Thermodynamic Properties of Real Moist Air, Dry Air, Steam, Water, and Ice" for the American Society of Heating, Refrigerating, Air-Conditioning Engineers (ASHRAE) were published in the journal "HVAC&R Research".
  - A comprehensive article on the properties of moist air was prepared for the "Journal of Engineering for Gas Turbines and Power".
  - The property library LibHuAirProp for calculating thermodynamic and transport properties for real moist Air, steam, water and ice was completed.
- 4. Thermodynamic Properties of Seawater and Sea Air
  - 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**

- Herrmann, S.; Kretzschmar, H.-J.; Gatley, D.P.: Thermodynamic Properties of Real Moist Air, Dry Air, Steam, Water, and Ice. HVAC&R Research, 15 (2009), pp. 961-986
- Feistel, R.; Kretzschmar, H.-J.; Span, R.; Hagen, E.; Wright, D. G.; and Herrmann, S.: Thermodynamic Properties of Sea Air. Ocean Sci. (2010) 6, pp. 91-141
- Herrmann, S.; Kretzschmar, H.-J.; Gatley, D.P.: Table 2 Thermodynamic Properties of Moist Air at Standard Atmospheric Pressure Table 3 Thermodynamic Properties of Water at Saturation In: 2009 ASHRAE HANDBOOK FUNDAMENTALS, Chapter PRINCIPLES, SI and I-P Editions, ASHRAE (2009), ISBN 978-1-933742-55-7

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

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

Editorial changes were made for the correction of the "Notes" in the subsections "Range of validity" for Eq. (7) [region 1 of IAPWS-IF97], page 9, and for Eq. (15) [region 2 of IAPWS-IF97], page 17. In the current Notes, the range of validity of IAPWS-IF97 in the temperature range between 273.15 K and 273.16 K is not correctly described and was correspondingly corrected. In addition, in Section 12 "Estimates of uncertainties" a hint is given where to find estimates of the uncertainty in enthalpy, namely in the IAPWS Advisory Note No. 1 given as Ref. [15].

2. Editorial changes for the Revised Release on the IAPWS-95 Formulation

In Section 6 "Estimates of uncertainties" a hint is given where to find estimates of the uncertainty in enthalpy, namely in the IAPWS Advisory Note No. 1 given as Ref. [9].

3. Revision of the Revised Release on the Pressure along the Melting and Sublimation Curves of Ordinary Water Substance

The revision refers to a new estimation of the uncertainty in sublimation pressure. This new estimation is based on a comprehensive physically founded consideration performed by Rainer Feistel with input from Allan Harvey and Wolfgang Wagner.

4. Steam Tables for the VDI-Heat Atlas 2010

The work on Section D2.1 "Properties of Water and Steam" of the VDI-Heat Atlas 2010 was finished 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, Ontario, Canada, July 2010

by

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

The Japanese National Committee to the IAPWS is countinuing to play an active function as the 139th Committee on Steam Properties chaired by Professor Masaru Nakahara, Kyoto 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 Japan Atomic Energy Agency, Dr. S. UCHIDA made his effort to promote development of evaluation method on flow-accelerated-corrosion (FAC) of components in nuclear power plants and mitigation of stress corrosion cracking of core internals of BWRs. He also promotes the national project on FAC of PWR supported by Nuclear and Industrial Safety Agency as a visiting researcher of the University of Tokyo. A FAC wall thinning rate evaluation model based on combined analyses of a static electrochemical analysis and a dynamic oxide layer growth analysis has been developed to predict wall thinning rates in PWR secondary piping [1], [2], [5] -[12]. 2) Other efforts on water chemistry have been put on evaluating and mitigating corrosive conditions against IGSCC. [3], [4]. [Latest publication: [1] M. Naitoh, S. Uchida, Y. Uehara, H. Okada and S. Koshizuka, "Evaluation of wall thinning rate due to flow accelerated corrosion with the coupled models of electrochemical analysis and double oxide later analysis", Proc. PVP2009, 2009 ASME Pressure Vessel and Piping Division Conference, July 26-30, 2009, Prague, Czech Republic, PVP2009-77583 (2009), [2] S. Uchida, M. Naitoh, Y. Uehara, H. Okada, S. Koshizuka and D. H. Lister, "Evaluation of Wall Thinning Rate due to Flow Accelerated Corrosion with the Coupled Models of Electrochemical Analysis and Double Oxide Layer Analysis", Proc. 14th Int. Conf. Environmental Degradation of Materials in Nuclear Power Systems - Water Reactors, Virginia Beach, VA, Aug. 22-27, 2009, ANS, 2009 (in CD), [3] S. Uchida, T. Satoh, T. Tsukada, T. Miyazawa, Y. Satoh and K. Ishii, "Evaluation of the Effects of Oxide Film on Electrochemical Corrosion Potential of Stainless Steel in High Temperature Water", ibid., [4] T. Satoh, Y. Miwa, T. Tsukada and S. Uchida, "A new concept sensor for determination of oxygen and hydrogen peroxide concentrations in nuclear reactor coolant", ibid., [5] Tomonori Satoh, H. Ugachi, T. Tsukada and S. Uchida, "Effects of alloy composition of carbon steel on the flow accelerated corrosion and oxide film properties in neutral water condition", ibid., [6] H. Okada, S. Uchida, Y. Uehara, M. Naitoh and S.

Koshizuka, "Evaluation of Local Wall Thinning of Piping due to Liquid Droplet Impingement by Coupled Analysis of Corrosion and Flow Dynamics", Proc. the 13th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-13), 2009 (Kanazawa City, Japan), N13P1177 (in CD), [7] M. Naitoh, S. Uchida, H. Okada, Y. Uehara and S. Koshizuka, "Evaluation of Flow Accelerated Corrosion by Coupled Analysis of Corrosion and Flow Dynamics (I) Major Features of Coupled Analysis and Application for Evaluation of Wall Thinning Rates", ibid., [8] Y. Uehara, S. Uchida, H. Okada, M. Naitoh and S. Koshizuka, "Evaluation of Flow Accelerated Corrosion by Coupled Analysis of Corrosion and Flow Dynamics (II) Comparison of LES and k-e Models for Evaluating Mass Transfer Coefficients", ibid., [9] S. Uchida, H. Okada, Y. Uehara, M. Naitoh and S. Koshizuka, "Evaluation of Flow Accelerated Corrosion by Coupled Analysis of Corrosion and Flow Dynamics (III)Relationship of Oxide Film Thickness, Hematite/Magnetite Ratio, ECP and Wall Thinning Rate", ibid., [10] S. Uchida, H. Okada, Y. Uehara, M. Naitoh, S. Koshizuka and D. H. Lister, "Effects of Water Chemistry on Flow Accelerated Corrosion and Liquid Droplet Impingement", Proc. Symposium on Water Chemistry and Corrosion in Nuclear Power Plant in Asia 2009, Nagoya, Japan, Oct. 28-29, 2009, Atomic Energy Society of Japan (2009) (in CD), [11] S. Uchida, M. Naitoh, H. Okada, Y. Uehara, S. Koshizuka, R. Svoboda and D. H. Lister, "Effects of Water Chemistry on Flow Accelerated Corrosion and Liquid Droplet Impingement Accelerated Corrosion", Power Plant Chemistry, 11, 12, (2008) 704-716, [12] S. Uchida, M. Naitoh, Y. Uehara, H. Okada, T. Ohira, H. Takiguchi, W. Sugino and S. Koshizuka, "Evaluation of Flow Accelerated Corrosion of PWR Secondary Components by Corrosion Analysis Coupled Flow Dynamics Analysis (IV), Comparison of Wall Thinning Rates Calculated with the Coupled Model of Static Electrochemical Analysis and Dynamic Double Oxide Layer Analysis and Their Values Measured at a PWR plant", Journal of Nuclear Science and Technology, 47 [2], (2010) 184-196.] [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 heavy oil in supercritical water. It was revealed that the effect of water on bitumen reaction was mainly extraction solvent for lighter fraction in the bitumen and the yield of coke was promoted because the condensed heavy hydrocarbons combined together to form coke [WCCE8 (August 2009, Montréal, Ouebec, Canada) M. Watanabe, S. Kato, S. Nozoe, R. L. Smith; Masaru Watanabe, Shin-nosuke Kato, Satoshi Ishizeki, Hiroshi Inomata, Richard Lee Smith Jr. "Heavy oil upgrading in the presence of high density water: Basic study" The Journal of Supercritical Fluids, Volume 53, Issues 1-3, June 2010, Pages 48-52]. They continued to study on polycarbonate decomposition in high pressure steam [Masaru Watanabe, Yasuaki Matsuo, Takashi Matsushita, Hiroshi Inomata, Toshiyuki Miyake, Katsuhiko Hironaka "Chemical recycling of polycarbonate in high pressure high temperature steam at 573 K" Polymer Degradation and Stability, Volume 94, Issue 12, December 2009, Pages 2157-2162]. The center has tried to clarify the effect of temperature and pressure (sometimes with an additive) on sugar and sugar-related compound conversion in high pressure high temperature water [Naota Torii, Atushi Okai, Kazuaki Shibuki, Taku M. Aida, Masaru Watanabe, Masayuki Ishihara, Hiroichi Tanaka, Yoshiyuki Sato, R.L. Smith Jr. "Production of d-glucose from pseudo paper sludge with hydrothermal treatment" Biomass and Bioenergy, Volume 34, Issue 6, June 2010, Pages 844-850]. They also studied the effect of additive on sugar into a furan compound with microwave heating [Xinhua Qi, Masaru Watanabe, Taku M. Aida, Richard L. Smith Jr. "Sulfated zirconia as a solid acid catalyst for the

dehydration of fructose to 5-hydroxymethylfurfural" Catalysis Communications, Volume 10, Issue 13, 25 July 2009, Pages 1771-1775]. The center has recently started to study on biomass combustion in high pressure water media to recover the energy in the biomass as a heat [Kunio Arai, Richard L. Smith Jr., Taku M. Aida "Decentralized chemical processes with supercritical fluid technology for sustainable society" The Journal of Supercritical Fluids, Volume 47, Issue 3, January 2009, Pages 628-636]. The center also performed to synthesize the fluorescent material (ZnSiO4:Mn) in supercritical water [Masafumi Takesue, Atsuko Suino, Yukiya Hakuta, Hiromichi Hayashi, Richard L. Smith Jr." Crystallization trigger of Mn-doped zinc silicate in supercritical water via Zn, Mn, Si sources and complexing agent ethylenediamine tetraacetic acid" Materials Chemistry and Physics, Volume 121, Issues 1-2, 15 May 2010, Pages 330-334; Kazuaki Shibuki, Masafumi Takesue, Taku M. Aida, Masaru Watanabe, Hiromichi Hayashi, Richard L. Smith Jr. "Continuous synthesis of Zn2SiO4:Mn2+ fine particles in supercritical water at temperatures of 400-500 °C and pressures of 30-35 MPa" The Journal of Supercritical Fluids, In Press, Corrected Proof, Available online 21 May 2010] and they have tried to reveal the formation mechanism of the material during the heating process with the assist of Spring-8 [Masafumi Takesue, Kenji Shimoyama, Kazuaki Shibuki, Atsuko Suino, Yukiya Hakuta, Hiromichi Hayashi, Yasuo Ohishi, Richard Lee Smith Jr. "Formation of zinc silicate in supercritical water followed with in situ synchrotron radiation X-ray diffraction" The Journal of Supercritical Fluids, Volume 49, Issue 3, July 2009, Pages 351-355].

At the Institute of Multidisciplinary Research for Advanced Materials at Tohoku University, Prof. M. KAKIHANA and his group developed a panel of stable, non-toxic and water-soluble compounds of Si, V, Ti and Ta. These compounds can be utilized for the synthesis of oxide materials by solution based processes, which are based on the hydrothermal processing or which include a hydrothermal treatment as one of the key synthesis steps. The unique chemical properties of these complexes were used to synthesize new photocatalytic materials for water splitting that involve both Ti and Ta. The combination of hydrothermal process with post-synthetic treatment allowed for the first time to obtain highly crystalline  $TiO_2(B)$  materials. The new water-soluble compound of Si was applied for preparation of the series of rare-earth and manganese activated phosphors containing silicon such as (Y,Ce,Gd)<sub>2</sub>SiO<sub>5</sub>,  $Ca_3Sc_2Si_2O_{12}$ : Ce<sup>3</sup> and Zn<sub>2</sub>SiO<sub>4</sub>: Mn<sup>2+</sup>, which exhibited remarkably improved fluorescence brightness and color purity compared to the materials synthesized by the conventional approaches. Finally, water soluble complex of V was used in the synthesis of nano-crystalline YVO<sub>4</sub>:Eu<sup>3+</sup> phosphors by the solvothermal process in the mixed alcohol-water solvents under sub-critical conditions, and it yielded  $YVO_4$ nanoparticles with the unique raspberry-like morphology. The peculiar shape of the phosphor particles resulted in the remarkable enhancement of fluorescent intensity due to the favorable particles shape for the more efficient absorption of excitation radiation. [Y. Suzuki, and M. Kakihana, J. Cer. Soc. Japan, 117, 330 (2009); K. Yamamoto, K. Tomita, K. Fujita, M. Kobayashi, V.Petrykin, and M. Kakihana, J. Crystal Growth, 311(3), 619 (2009); K. Yamamoto, H. Shimoita, K. Tomita, K. Fujita, M. Kobayashi, V. Petrykin, and M. Kakihana, J. Cer. Soc. Japan, 117, 347 (2009); S. Kaowphong, V. Petrykin, S. Thongtem, and M. Kakihana, J. Cer. Soc. of Japan, 117, 273 (2009); S. Kaowphong, K. Nakashima, V. Petrykin, S. Thongtem, M. Kakihana, J. Am. Cer. Soc., 92, S16 (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, UV/NIR shielding, preventing the healthy damage, etc. by solvothermal reactions. They

successfully prepared visible light responsive photocatalysts with controllable phase compositions, morphologies, together with excellent visible light induced deNO<sub>x</sub> activity. They also researched on the synthesis of multifunction thin films with UV/NIR shielding property, photocatalytic activity and superhydrophobicity or superhydrophilicity. The relationship between morphologies and photo-chemical properties of inorganic materials was investigated in detail. In addition, environmental friendly synthesis of lead-free dielectric ceramic materials, ceria-based inorganic UV-shielding materials with excellent safety, comfort and transparency in the visible light region; rare earth oxide nanoparticles with controlled morphology and excellent fluoresence properties,  $Ag/\gamma$ -Al<sub>2</sub>O<sub>3</sub> nanocomposites with excellent deNO<sub>x</sub> catalytic activity, were carried out. [Solid State Sci., 11, 182-188 (2009);Solid State Phenomena, 147-149, 851-855(2009); Nanoscale Res. Lett., 4, 247-253(2009); J. Cryst. Growth, 311, 576-579 (2009); J. Cryst. Growth, 311, 580-584 (2009).; J. Ceram. Soc. Jpn. 117, 320-325 (2009); Appl. Catal. B, 89,118-122 (2009); Mater. Chem. Physics.116, 269-272 (2009); Solid State Sci., 11, 988-993 (2009); Mater. Lett., 63, 1583-1585 (2009); J. Colloid Interface Sci., 336, 150-254 (2009); Crystal Growth Des., 9, 2944-2949 (2009); Nanotechnol. 20, 305302 (2009); J. Molecular Catal. A: Chem., 309, 50-56 (2009); J.Mater.Sci., 44, 4834-4839 (2009); Mater.Chem.Phys., 116, 421-425 (2009); Mate. Sci.Eng.: C, 29, 1849-1854 (2009); Solid State Sci. 11, 1703-1708 (2009); Nanotechnol. 20, 405606 (2009); Appl. Mater. Interfaces, 1, 2649-2698 (2009); Eur. J. Inorg. Chem., 29-30, 4441-4445 (2009) J.Am.Ceram.Soc., 92, 3125-3128 (2009); Appl. Clay Sci., 46, 363-368 (2009); Func. Mater.Lett., 2, 157-161 (2009); Dyes & Pigments, 84, 237-241 (2010); Appl.Catal.B., 93, 299-303 (2010).; J.Euro. Ceram. Soc., 30, 699-704 (2010); J.Mater.Sc., 45, 725-732 (2010); Mater. Res. Bull., 45, 275–278 (2010); J.Nanosci.Nanotechnol. 10, 731-738 (2010); J.Cryst. Phys.Chem., 1(1), 11-30 (2010); Res. Chem. Intermed., 36, 61-67 (2010); Res. Chem. Intermed., 36, 69-75 (2010); J.Nanosci.Nanotechnol., 10, 4619–4623 (2010); J.Ceram.Soc.Jpn., 118, 555-557 (2010); Surf. Rev. Lett., 17, 147-152 (2010)]. The relationship between morphologies and photo-chemical properties of inorganic materials was mainly investigated in detail. Profs. A. MURAMATSU and K. KANIE with coworkers 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 multi-functional 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, recently, proposed a new method to synthesize organicinorganic hybrid nanocrystals by using supercritical hydrothermal 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, including CO<sub>3</sub>O<sub>4</sub> and CeO<sub>2</sub> nano crystals.[ PHYS. REV. B, **79**,144411(2009), CRYS. GROWTH & DES., 9 ,5297(2009).]

At the Energy Technology Research Institute, National Institute of Advanced Industrial Science and Technology, Drs. T. Takanohashi, M. Morimoto and S. Sato have succeeded in determining the conditions of supercritical water which have good miscibility with heavy oils, through comparisons of dielectric constant ( $\varepsilon$ ) and Hansen solubility parameter (HSP) of supercritical water with those of typical solvent. They found that the required conditions of supercritical water was  $2.2 \ll \varepsilon \ll 10.4$  and HSP for hydrogen bonding,  $\delta_{h}$ ,  $< 10.0 \text{ MPa}^{0.5}$ . Validity of the optimum conditions estimated was confirmed by some experimental results [Morimoto, M., Sato, S. and Takanohashi, T., *Journal of the Japan Petroleum Institute*, 53, 61-62 (2010)]. [contact: Dr. T. Takanohashi; E-mail: toshi-takanohashi@aist.go.jp, Dr. M. Morimoto; E-mail: m.morimoto@aist.go.jp]

At the department of material and environmental chemistry, Utsunomiya University, Dr. T. SATO and co-workers studied heavy oil upgrading with formic acid in supercritical water at 723 K. In supercritical water, water gas shift reaction between CO and supercritical water gives active hydrogen that proceeds hydrogenation of heavy oils. Formic acid is one of the intermediate of water gas shift reaction. The reaction under pyrolysis condition and supercritical water was also conducted. The supercritical water and formic acid system gave highest conversion of asphaltene and lowest amount of coke among these systems, which indicated that both the solvent power of supercritical water and active species derived from decomposition of formic acid promoted the conversion of hyavy oil (bitumen) to lower molecular weight side. The supercritical water and formic acid mixture can be the effective system for upgrading of heavy oil. [T. Sato et al., Proc. 8th World Congress of Chemical Engineering, Montréal, 2009, 01335].

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 2011 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 <sup>28</sup>Si crystal was grown in 2007, and two 1 kg spheres were polished from the crystal in 2008 for density measurement [P. Becker, H. Friedrich, K. Fujii, W. Giardini, G. Mana, A. Picard, H.-J. Pohl, H. Riemann and S. Valkiers, "The Avogadro constant determination via enriched silicon-28," Meas. Sci. Technol., 2009, Vol. 20, 092002]. The density of the crystal has been determined with a relative standard uncertainty of  $3 \times 10^{-8}$  [N. Kuramoto and K. Fujii, "Improvement in the volume determination for the Si spehers 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 [Y. Kano, Y. Kayukawa, K. Fujii, and H. Sato, "A new method for correcting a force transmission error due to magnetic effects in a magnetic levitation densimeter," Meas. Sci. TEchnol., 2007, Vol. 18, pp. 659-666]. 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 have been developed for providing reference data for 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, Kvoto, 2004, 112-115]. Based on the viscosity of water, calibration of the viscosity standard liquids is being conducted in a range 1 mPa s to 500 Pa s [Y. Fujita, Y. Kurano and K. Fujii, "Evaluation of uncertainty in viscosity measurements by capillary master viscometers," Metrologia, 2009, Vol. 46, pp. 237–248]. Calibration service for non-Newtonian liquid has also started in 2009 using a new falling cylinder method. 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 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. They reported urea-water binary droplets on the flat and pillared hydrophobic surfaces. [T. Koishi, K. Yasuoka, X. C. Zeng and S. Fujikawa, Faraday Disc., in press (2010), DOI: 10.1039/b926919c] They also reported how mercury inhibits water permeation through aquaporin-1. [Y. Hirano, N. Okimoto, I. Kadohira, M. Suematsu, K. Yasuoka, and M. Yasui, Biophys. J., 98, 1512 (2010).] They reported phase diagram of Lennard-Jones fluid confined in the slit pores [T. Kaneko, T. Mima, K. Yasuoka, Chem. Phys. Lett., 490, 165 (2010).] [contact: Prof. K. Yasuoka; E-mail: yasuoka@mech.keio.ac.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. The thermometers of the apparatus are being replaced to improve the measurement uncertainty. By the modified apparatus, isochoric heat capacities of water will be 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 in Energy Engineering School of Tokai University. He has been working as a temporary technical adviser at Naigai Chemical Products Co., LTD. in Tokyo since May of 2006. He and his coworkers engaged in Shinshu University, Naigai Chemical Products Co., the electric power companies and turbine manufacturer are conducting researches on the corrosion of materials for steam turbines in geothermal power plants, for boiler tubes and low pressure steam turbines in the conventional thermal and combined cycle power plants, and other subjects on corrosion and water chemistry for power plants. The latest papers; (1) T. Nakane, L.-B. Niu, Shuji Oishi and H. Takaku, "Influence of Organic Acids on Corrosion Behavior of Boiler Tube Materials in Simulated AVT Waters Coexisted with Chloride Ions ", *J. Japan Inst. Metals*, Vol. 74, No.9 (2010), (Accepted for printing). (2) L.-B. Niu, T. Goto, T. Nakane, H. Takaku and Yoshihiro Sakai, "Effect of Cl<sup>-</sup> and SO<sub>4</sub><sup>2-</sup> on Pitting Corrosion Susceptibility for Materials of Low-Pressure Steam Turbines in Power Plants", *J. Japan Inst. Metals*, Vol. 74 (2010 or 2011), (Accepted for printing). (3) T. Nakane, L.-B. Niu, S. Oishi and H. Takaku, "Electro-chemical Corrosion Behaviors and Formed Film Characteristics of Boiler Tube Steel Weldments in Simulated AVT Waters", *Journal of The Japanese Society for heat Treatment (NETSU SHORI)* (contributed and in review). (4) T. Nakane, L.-B. Niu and H. Takaku, "Effect of Chloride and Sulfate in Simulated AVT Waters on Electrochemical Corrosion Behaviors and Film Characteristics of Low Pressure Steam Turbine Materials", *PowerPlant Chemistry*, (contributed and in review). [Contact: Prof. H. Takaku; E-mail: takaku06@ybb.ne.jp]

At the Department of Mechanical Systems Engineering, Toyama Prefectural University, Toyama, Dr. H. MIYAMOTO and their group have been studying the various thermodynamic properties including the PVTx, critical locus, and saturation properties at temperatures up to 600 K and at pressures up to 200 MPa. [S. Muromachi, H. Miyamoto, and M. Uematsu, " $(p, \rho, T, x)$  Properties for {x NH<sub>3</sub> + (1-x) H<sub>2</sub>O} mixtures at T = (450, and 500) K over the pressure range from (10 to 200) MPa", J. Chem. Thermodyn., 2008, 40, pp. 1594-1599] [A. Sakabe, D. Arai, H. Miyamoto, and M. Uematsu, "Measurements of the critical parameters for {xNH<sub>3</sub> + (1 - x)H<sub>2</sub>O} with x = (0.9098, 0.7757, 0.6808)", J. Chem. Thermodyn., 2008, 40, pp. 1527-1530] Most of our apparatuses for higher pressure ranges had been developed by the Uematsu Laboratory in Keio University. After Uematsu retired from working at Keio Univ., he provided us most of his measurement apparatuses in 2008. Therefore, we aim to clarify the mixing effects of various mixtures in wider ranges of temperatures and pressures. We are also trying to measure the vapor-liquid equilibrium properties for natural substance mixtures using the new apparatus. [Contact: Dr. H. Miyamoto; E-mail: miyamoto@pu-toyama.ac.jp]

At the Institute for Chemical Research, Kyoto University, Uji, Kyoto, Prof. M. NAKAHARA, Prof. N. MATUBAYASI, Dr. C. WAKAI, and their coworkers study the structure, dynamics, and reactions in super- and subcritical water and related systems such as ionic liquids by means of multinuclear NMR (nuclear magnetic resonance) spectroscopy and computer simulation. Their current focus are (1) the translation dynamics of water and organic solvents in supercritical states and the elucidation of the effect of hydrogen bonding ["Self-diffusion coefficients for water and organic solvents in extremely low-density supercritical states", K. Yoshida, N. Matubayasi, and M. Nakahara, *J. Mol. Liq.* **147**, 96-101 (2009)] and (2) the environmental effect on the chemical shift of the diluted water and its usage in purification of ionic liquids ["Water as an In-situ NMR Indicator for Impurity Acids in Ionic Liquids", Y. Yasaka, C. Wakai, N. Matubayasi, and M. Nakahara, *Anal. Chem.* **81**, 400-407 (2009)]. [contact: Prof. M. Nakahara; E-mail: nakahara@scl.kyoto-u.ac.jp & Prof. N. Matubayasi; E-mail nobuyuki@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 high-temperature alcohols (methanol and ethanol) ["Electric conductivities of 1:1 electrolytes in high-temperature ethanol along the liquid-vapor coexistence curve. I. NaBr, KBr, and CsBr", *J. Chem. Phys.*, **132** (11), 114501 1-10 (2010)]. In our laboratory, the molecular dynamics simulations have been also studied ["Molecular dynamics simulations of partially diffusion-controlled reaction between mono- and diatomic molecules", *J. Mol. Liq.*, **147** (1-2), 30-36 (2009); "Molecular dynamics simulations of aqueous LiCl solutions at room temperature through the entire concentration range", *J. Mol. Liq.*, **147** (1-2), 56-63 (2009)]. [Contact: Prof. M. Ueno; E-mail: mueno@mail.doshisha.ac.jp]

At Department of Applied Chemistry & Bioengineering, Osaka City University, Dr. N. KOMETANI and his co-workers have studied the TiO2 photocatalysis in high-temperature high-pressure water. They revealed that TiO2 exhibits high photocatalytic activity even under sub- and supercritical conditions [N. Kometani, K. Sugimoto, A. Fujita, Y. Yonezawa, "Photocatalytic Activity of TiO2 Nanoparticles in Hydrothermal and Supercritical Water", J. Chem. Eng. Jpn., Vol.40, pp.463-467 (2007)]. Based on this finding, the hybrid process in which hydrothermal and photocatalytic techniques are combined has been developed. It was demonstrated that such hybrid process could be applied to the treatment of waste water containing organochloride compounds such as chlorobenzene [A. Shimokawa, N. Kometani, Y. Yonezawa, "Degradation of chlorobenzene by the hybrid process of supercritical water oxidation and TiO2 photocatalysis", Sep. Sci. Tech., in press (2010)] as well as the effective gasification of glucose [A. Nakatani, N. Kometani, "Photocatalytic Effect of TiO2 on the Hydrothermal Gasification of Glucose", J. Phys.: Conf. Seri., Vol.215, 012091 (2010)]. The same group also examined the hydrothermal synthesis of size-controlled silver nanoparticles [N. Kometani, T. Teranishi, Y. Yonezawa, "Development of the Metal Nanoparticle Synthesis Method by means of the Hydrothermal Technique", J. Soc. Mater. Sci. Jpn., Vol.58, pp. 481-485 (2009)]. [contact: Dr. N. Kometani; kometani@achem.eng.osaka-cu.ac.jp]

At the Department of Mechanical Engineering, Kyushu University, Prof. Y. TAKATA and their group are continuously developing a program package for thermophysical properties of fluids: PROPATH. The current version is 13.1 and 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/. In addition, his research group is studying thermophysical properties of hydrogen at ultra-high pressures. They are measuring PVT relation ["Review of the Thermodynamic Properties of Hydrogen Based on Existing Equations of State", N. Sakoda, et al., Int. J. Thermophysics, 31-2, 76-296(2010)], viscosity and thermal conductivity of hydrogen up to 100MPa. ["A Procedure for Application of the Three-Omega Method to Measurement of Gas Thermal Conductivity", E. Yusibani, et al., J. Thermal Sci. and Tech., 4-1,146-158(2009); "An Accelerated Two-Dimensional Unsteady Heat Conduction Calculation Procedure for Thermal-Conductivity Measurement by the Transient Short-Hot-Wire Method", P. L. Woodfield, et. al., Int. J. Thermophysics, 30-3, 796-809(2009); "End Effects in the Three-Omega Method to Measure Gas Thermal Conductivity", E. Yusibani, et al., Int. J. Thermophysics, 30-3, 833-850(2009); "Techniques for Accurate Resistance Measurement in the Transient -Short-Hot-Wire Method Applied to High Thermal-Diffusivity Gas", P. L. Woodfield, et. al., Int. J. Thermophysics, 30-6, 1748-1772(2009)] [contact: Prof. Y. Takata; E-mail: takata@mech.kyushu-u.ac.jp]

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 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. Biomass and its model compounds such as phenolic compounds and carbohydrates were recovered from lignocellulosic biomass with a batch reactor [Wahyudiono, M. Sasaki and M. Goto, Fuel, 88, 1656-1664 (2009); Wahyudiono, Mitsuru Sasaki and Motonobu Goto, accepted for publication in Journal of Material Cycles and Waste Management (2010); Mitsuru Sasaki, Wahyudiono, Hiroaki Kawanabe, Takashi Saito and Motonobu Goto, Proceeding of 9th International Symposium on Supercritical Fluids 2009, (CD-ROM), Arcachon, France (2009)]. 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. Shiraishi, K. Iwata, M. Sasaki and M. Goto, Proceeding of 9th International Symposium on Supercritical Fluids 2009, Arcachon, France (2009); Pradip C. Mandal, Tatsuya Shiraishi, Wahyudiono, Mitsuru Sasaki and Motonobu Goto, Proceeding of AIChE Annual Meeting 2009, Paper 81e, Nashville, TN, USA (2009)]. Pugment and nutraceutical compounds were extracted from *Chlorella vulgaris* using scCO<sub>2</sub> and water in hydrothermal condition. Biological active compounds from other waste biomass were also extracted using scCO<sub>2</sub> and hot water. Furthermore, the antioxidant and antibacterial of extracts were analyzed [Kiwa Kitada, Siti Machmudah, Mitsuru Sasaki, Motonobu Goto, Y. Nakashima, S. Kumamoto and T. Hasegawa, J. Chemical Technology and Biotechnology, 84(5), 657-661 (2009); Kiwa Kitada, Siti Machmudah, Mitsuru Sasaki, Motonobu Goto, Y. Nakashima, S. Kumamoto, T. Hasegawa, Separation Science and Technology, 44(5), 1228-1239 (2009); E. M. Suleimenov, Siti Machmudah, Mitsuru Sasaki, Motonobu Goto, Chemistry of Natural Compounds, 46(1), 140-141 (2010)] Yuzu oil was fractionated by semi-continuous supercritical CO<sub>2</sub> extraction column to recover sesquiterpenes [A. Terada, N. Kitajima, Siti Machmudah, Masahiro Tanaka, Mitsuru Sasaki, Motonobu Goto, Separation and Purification Technology, 71(1), 107-113 (2010)] and simultaneous extraction of coffee beans using supercritical  $CO_2$  and water was studied for recovering chlorogenic acid as a water soluble fraction and caffeine as a supercritical CO<sub>2</sub> soluble one [Siti Machmudah, Kiwa Kitada, Mitsuru Sasaki, and Motonobu Goto, accepted for publication in *Ind. Eng. Chem. Res.* (2010)]. They are also studying various natural materials in collaboration with universities [Siti Machmudah, Kiwa Kitada, Mitsuru Sasaki, Motonobu Goto, J. Munemasa, M. Yamagata, submitted for publication in Ind. Eng. Chem. Res. (2010); Siti Machmudah, T. Kamogawa, Mitsuru Sasaki and Motonobu Goto, Proceeding of 9th International Symposium on Supercritical Fluids, Arcachon, France (2009)] and companies [Ruhan Askin, Mitsuru Sasaki, Motonobu Goto, accepted for publication in Ind. Eng. Chem. Res. (2009); Ruhan Askin, Mitsuru Sasaki, and Motonobu Goto, accepted for publication in Journal of Food and Boproducts Pocessing (2009); Ruhan Askin, Mitsuru Sasaki, and Motonobu Goto, accepted for publication in Journal of Separation and Purification Technology (2009)] As a part of Kumamoto University Global COE program "Global Initiative Center for Pulsed Power Engineering", developments of an evolutional reaction / material processing methods were conducted. Electrospinning is one of the simple techniques to produce nanofibers and we challenged electrospinning of combined polymers in supercritical CO2 [Motonobu Goto, Kanako Murakami, Wahyudiono, Mitsuru Sasaki, Proceeding of 9<sup>th</sup> Conference on Supercritical Fluids and Their Applications, Sorrento, Napoli, Italy

(2010); Mitsuru Sasaki, Wahyudiono, Kanako Murakami, Motonobu Goto, Proceeding of International Seminar on Fundamental and Application of Chemical Engineering, Bali, Indonesia (2010)]. Pulsed laser ablation of various metals in supercritical CO<sub>2</sub> has been developed and morphology of ablated plates and generated nanoparticle were examined. Gold nanoparticles have been successfully generated by laser ablation in supercritical CO<sub>2</sub> [Yutaka Kuwahara, Takashi Saito, M. Haba, T. Iwanaga, Mitsuru Sasaki, and Motonobu Goto, J. Applied Physics, 48, 040207 (2009); Siti Machmudah, Yutaka Kuwahara, Mitsuru Sasaki, and Motonobu Goto, Proceeding of Supergreen 2009, Sendai, Japan (2009)]. [contact: Prof. M. Goto; E-mail: mgoto@kumamoto-u.ac.jp, Assoc. Prof. M. Sasaki; E-mail: msasaki@ kumamoto-u.ac.jp]

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

# **Report 2009-2010**

- 1. RNC active participation in organization of All-Russian theoretical and practical conference "Increasing reliability and efficiency of thermal power plants and energetic systems exploitation» 1-3 of June 2010, Moscow, MPEI (TU).
- 2. RNC active participation in organization of 3-rd Water-Chemistry Forum, April 2010, Moscow, MPEI (TU).
- 3. Two meetings of RNC have been held. Current problems are investigated. K. Orlov is elected as secretary of RNC.

### **Publications list**

- 1. Thermophysical properties of working substances of heat power engineering: reference book. A. Alexandrov, K. Orlov, V. Ochkov, Moscow, 2009. P. 224 [8]. ISBN 978-5-383-00405-0.
- 2. Improvement of water chemistry and chemistry contol at thermal power V. Voronov, T. Petrova. Thermal Engineering, #07, 2010, p. 2-6.
- 3. Selected questions on water chemistry monitoring systems developments V. Voronov, P. Gotovcev, O. Egoshina, D. Smetanin. Thermal Engineering, #07, 2010, p. 24-27.
- 4. Water chemistry and chemical control organization problems on thermal power plants T. Petrova, V. Voronov. All-Russian theoretical and practical conference "Increasing reliability and efficiency of thermal power plants and energetic systems exploitation» 1-3 of June 2010, Moscow.
- 5. Turbine condenser cooling systems water chemistry optimization D. Repin, T. Petrova. All-Russian theoretical and practical conference "Increasing reliability and efficiency of thermal power plants and energetic systems exploitation» 1-3 of June 2010, Moscow.
- 6. Water treatment new technologies investigation on thermal power plants B. Larin, A. Korotkov, M. Oparin, A. Larin. All-Russian theoretical and practical conference "Increasing reliability and efficiency of thermal power plants and energetic systems exploitation» 1-3 of June 2010, Moscow.
- 7. Using causes of infringement searching algorithms and mathematical models in water chemistry monitoring systems P. Gotovcev, D. Smetanin. All-Russian theoretical and practical conference "Increasing reliability and efficiency of thermal power plants and energetic systems exploitation» 1-3 of June 2010, Moscow.
- 8. T. Petrova, L. Seleznev, A. Isyanova. Assessing the impact of various parameters on the formation of deposits in boilers. New in the Russian electric-power industry, #3, 2010.
- 9. D. Smetanin, O. Egoshina, P. Gotovcev Prospects of water chemistry monitoring systems. New in the Russian electric-power industry, #8, 2009.
- 10. The problems of equipment corrosion at thermal power plants T. Petrova. 3-rd Water-Chemistry Forum, April 2010, Moscow.
- 11. V. Ochkov A New Reference Book for Power Engineers (9th conference on Power System Engineering, Thermodynamics & Fluid Flow ES 2010, June 17 18, 2010, Pilsen, Czech Republic)
- 12. V. Voloschuk, V. Ochkov, K. Orlov Thermodynamic optimization of a simple binary cycle CCGT with heat recovery boiler with the help of modern information technology // Bulletin of the National Technical University "Kharkov Polytechnic University, #2, 2010, p. 102-106.
- 13. K. Orlov, V. Voloschuk, V. Ochkov An interactive open calculation of gas turbine power plant // Automation and IT in the energetic, #2, 2010. p. 10-19.

# The Swiss National Committee

International Association for the Properties of Water and Steam

### **Report on IAPWS related activities – August 2009 / July 2010**

Submitted to the EC Meeting of IAPWS, Niagara Falls, CA - July 2010.

### National Committee Contacts:

SCPWS Swiss Committee for the Properties of Water and Steam Head: Dr. Robert Svoboda, E-mail: robert.svoboda@power.alstom.com

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

Prof.Dr. Kurt Heininger; University of Applied Sciences, Northwestern Switzerland; Windisch, E-mail: kurt.heiniger@fhnw.ch; web: www.fhnw.ch/technik/itfe

Prof.Dr. Horst-Michael Prasser; Institut für Energietechnik, Swiss Federal Institute of technology, Zürich, E-mail: hprasser@ethz.ch

Dr. Michael Hiegemann, Dr. Francisco Blangetti; Alstom, Baden, Switzerland, e-mail: michael.hiegemann@power.alstom.com, francisco.blangetti@ power.alstom.com Markus Bernasconi; Swan Analytical Instruments, Hinwil, E-mail: markus.bernasconi@swan.ch

### Research activities in the reporting period:

At the University of Applied Sciences, Northwestern Switzerland, a water test rig for 1000 MPa (10 kbar) pressure was set up. At this pressure, water is near the proximity of the liquidsolid phase border at ambient temperatures. This device is useful to study the properties of water for high-pressure cutting and for cleaning. Currently, there is no research project ongoing.

Another project by the University of Applied Sciences, Northwestern Switzerland, in cooperation with the Swiss Institute for Snow and Avalanches, Davos and supported by the Swiss government, was on the energy optimization at the production of artificial snow. Field tests performed during the past winters showed, that with an improved method for nuclei seeding, the energy requirements were reduced to 20% relative to the original design. Further improvements are ongoing.

### **Contributions to current IAPWS activities:**

Chairman Power Cycle Chemistry Working Group (PCC): R.Svoboda Vice-chairman of Subcommittee on Sea-Water: M.Hiegeman Initiation of ICRN 26 (Behavior of Aluminum in the Steam Water Cycle of Power Plants) Participation in the IAPWS International Collaboration on "Improved Sampling Techniques" for corrosion products in water / steam cycles. (Canada, Denmark, Japan, Switzerland) Informal international collaboration within PCC on technical publications (see "Recent Publications")

#### **Status of Associate Membership to IAPWS:**

Up to now, no team of sponsors to commit on mid- or long-term to a regular Swiss membership fee has yet been assembled. It is therefore requested to extend the Associate Membership for another term of three years.

#### **Recent Publications:**

- B. Elezi: "Inbetriebnahme einer 10kbar-Druckübersetzer-Pumpe", dissertation at University of Applied Sciences, Northwestern Switzerland,
- F. Kreitmeier, "Prof.George Gyrmathy and the wet steam turbine", memorial lecture for G. Gyarmathy (†24 Oct 2009), ASME Turbo Expo, Glasgow, June 2010
- B. Dooley, R. Svoboda, "Improving thermal cycle efficiency in advanced power plants: water and steam chemistry and materials performance" (Chapter 4 of "Advanced power plant materials, design and technology"). Woodhead 2010, (to be published).
- S. Uchida, M. Naitoh, H. Okada, Y. Uehara, S. Koshizuka, R. Svoboda, D.H. Lister, "Effects of Water Chemistry on Flow Accelerated Corrosion and Liquid Droplet Impingement Accelerated Corrosion", Power Plant Chemistry, 11 (2009) 12, pg 704-717

R.Svoboda, July 14, 2010

# U.S. National Committee to IAPWS 2010 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 published. Similar results are almost complete for the water- $CO_2$  binary, and the results have been incorporated into a software model for thermodynamics of moist gases.

<u>References</u>: Wheatley, R.J., and Harvey, A.H., Intermolecular potential energy surface and second virial coefficients for the nonrigid water-CO dimer, *J. Chem. Phys.* **131**, 154305 (2009); Wheatley, R.J., and Harvey, A.H., Intermolecular potential energy surface and second virial coefficients for the water-CO<sub>2</sub> dimer, *J. Chem. Phys.*, in preparation.

In collaboration with researchers in Greece and Germany and at the University of Maryland, work is continuing on the joint IAPWS and IUPAC efforts to update the formulation for the thermal conductivity of water and steam. The form of the critical enhancement has been worked out, and the low-density function and background function have been fitted to data and comparisons with data have been generated. The complete correlation is now ready for evaluation by IAPWS.

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. Also in the Process Measurements Division, the vapor pressure of ice has been measured over the temperature range 173 K to 273 K. These measurements were made using cavity ring-down spectroscopy to probe the output of a standard humidity generator which contains isothermal samples of ice. A preliminary analysis indicates better than 1% agreement over this temperature range between the measured ice vapor pressure and the correlation of A. Wexler, *J. Res. NBS* **81A**, 5 (1977).

<u>References</u>: Meyer, C.W, Hodges, J.T., Hyland, R.W., Scace, G.E., Valencia-Rodriguez, J., and Whetstone, J.R., The second-generation NIST standard hygrometer, *Metrologia* **47**, 192 (2010); Bielska, K., Havey, D.K., Scace, G.E., Lisak, D., and Hodges, J.T., Spectroscopic Measurement of the Vapor Pressure of Ice, *Int. J. Thermophys.*, 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 magnetic-suspension densimeter, which has been used to measure  $H_2O-N_2$  and  $H_2O-CO_2$  mixtures up to 620 K. 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) and used to measure the thermal conductivity of  $H_2O-N_2$  and  $H_2O-CO_2$  mixtures up to 740 K.

#### **Communicated from OLI Systems, Morris Plains, NJ:**

At OLI Systems, work was continued on various projects related to modeling thermophysical properties of aqueous electrolyte systems. In particular, our work in 2009-2010 was focused on:

- (1) Finalizing a comprehensive speciation-based thermodynamic model for aqueous systems containing Fe, Ni, Zn, Li, B, and H<sub>2</sub> at temperatures up to 350 °C
- (2) Revising a previously developed model for thermal conductivity of electrolyte solutions (P. Wang and A. Anderko, *Ind. Eng. Chem. Res.*, 47 (2008) 5698-5709) to introduce pressure dependence and to apply it to seawater

- (3) Developing a comprehensive model for surface tension of electrolyte solutions, including concentrated and mixed-solvent systems
- (4) Developing a phase equilibrium/reaction model for the sulfur-iodine thermochemical cycle for hydrogen production.
- (5) Initiating work on a thermodynamic model for interactions between carbon dioxide, natural brines, and minerals

Also, work is underway on developing an electrochemical model for predicting general and localized corrosion of copper in aqueous environments as a function of solution chemistry, temperature and flow conditions.

The following article has been published: P. Wang , A. Anderko, R. D. Springer, J. J. Kosinski, and M.M. Lencka, "Modeling Chemical and Phase Equilibria in Geochemical Systems Using a Speciation-Based Model", *J. Geochemical Exploration*, 106 (2010) 219-225.