

**BIAPWS Annual Report to IAPWS for 2006/07.**

**Summary.**

BIAPWS has increased its industrial sponsorship membership to 16 and is a power industry representative body for boiler steam and water chemistry in the British Standards organisation.

BIAPWS continues its role in technical education and outreach within the power generation industry. This past year has seen each BIAPWS committee meeting preceded by a technical seminar which is open to a wider audience from our industrial sponsors.

The BIAPWS Award scheme, modified to offer an undergraduate bursary for summer vacation work experience, was very successful in 2006 and has been repeated in 2007.

**Membership.**

BIAPWS membership of industrial sponsors has increased by three in the past year to now stand at 16 industrial members. This includes 11 power generation companies, 2 power plant manufacturers, 2 chemical instrument manufacturers and one technical support company. BIAPWS membership now includes almost all of the major electricity generating companies in the UK and Ireland (see footer for list).

BIAPWS links with the academic field remains as last year with only one active academic member on the committee. Two other universities are currently corresponding members, but are not active on the committee.

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

**Research.**

With all of the sponsors and a high percentage of the membership being drawn from the power generation industry, topics relevant to that industry have a higher priority than academic research in the BIAPWS agenda. Research is ongoing in the UK power industry but little is reported in the open scientific, engineering or technical press. The level of academic research into topics of interest to BIAPWS / IAPWS, appears to remain low in the UK. A list of recent publications that have been brought to the notice of BIAPWS is appended.

**British Standards Institute.**

BIAPWS acts as the UK generating industry representative body on the British Standards committee that is concerned with the design and operation of steam raising boilers, with particular reference to the steam and water chemistry requirements. BIAPWS has initiated discussion of the latest European standard in that area EN 12952 part 12 (water tube boilers) and EN 12953 part 10 (shell boilers) with the aim of instituting a major review of these standards. To this end, the European members of IAPWS will discuss EN 12952:12 in Luzern with the aim of producing a common position that will ensure effective revision of these standards.

**Education and Outreach.**

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

**BIAPWS Symposia.** The most recent BIAPWS Symposia was at the 2006 IAPWS International meeting, Witney. The next symposium is planned for spring 2008, when they will revert to an annual frequency at a fixed calendar period.

**BIAPWS Technical Seminars.** To enhance the value of BIAPWS membership regular technical seminars have been organised for the morning preceding each BIAPWS committee meeting. These have been opened to a wider audience from our industrial sponsors where active participation and discussion is encouraged, particularly by newer entrants to the power industry.

**BIAPWS Award.** In 2006 the BIAPWS Award was redefined as a co-sponsored undergraduate student bursary to enable a student to gain experience for at least 10 weeks working in an industry with relevance to the interests of IAPWS and BIAPWS. The co-sponsorship has been with one of BIAPWS industrial sponsors. In 2006 the Award went to a chemistry undergraduate from Nottingham University, co-sponsored by E.ON (UK). In 2007 the Award has been co-sponsored by Thames Power Services (Barking Power) with a chemical engineering undergraduate from Imperial College (London). The selected candidates have both been of high calibre and have benefited from their industrial experience.

**BIAPWS Future.**

BIAPWS remains committed to its role as a power industry representative body as well as developing further its role as the central point for co-ordinating and disseminating information on the properties of water and steam and their application to industry.

Richard Harries, Chairman BIAPWS  
August 2007.

Published Papers and Associated Work.

J Cooper and J Sengers have examined the effect on the values of properties calculated from the IAPS Release on the Viscosity and Thermal Conductivity of heavy water Substance 1982 using ITS-90 temperatures. A draft revised release has been produced for presentation to the IAPWS 2007 meeting.

The behaviour of ammonia, amines, carbon dioxide and organic anions during condensation in an air cooled condenser. Bignold GJ., 2006. *Power Plant Chemistry*. 8(2), 68-73.

Supercritical Carbon Dioxide in Water Emulsion Templated Synthesis of Porous Calcium Alginate Hydrogels. Darr J. A.; Partap, S. and Rehman, I.U., *Advanced Materials*. 18, 2006, 501 - 504.

Instant Nano-Hydroxyapatite; A Continuous and Rapid Hydrothermal Synthesis. Boldrin P.; Chaudhry, A.A.; Khalid, F.; Darr J. A. and Rehman, I.U., *J. Chem. Soc., Chem. Commun.* 2006, 2286 - 2288

Recent Developments in Processing and Surface Modification of Hydroxyapatite. Norton, J.; Malik, K.R.; Rehman, I.U. and Darr, J. A., *J. Adv. Appl. Ceram.*, 105, 2006, 113-139

## **The Czech National Committee**

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

### **REPORT on IAPWS related activities – August 2006 / August 2007**

Submitted to the EC Meeting of IAPWS, Luzern – August 2007.

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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  
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**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**, 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.

- Dr. Hruby (IT) investigated nucleation and measured surface tension of supercooled water. Refs. [1 to 4]. His research team investigated thermo-dynamic properties of water at pressure 0.1 MPa and dew point of combustion products (namely H<sub>2</sub>O-H<sub>2</sub>SO<sub>4</sub>).
- Prof. Mares (UWB) with his collaborators measured surface tension of super-cooled water and tested formulation IAPWS-IF97 in this region at ambient pressure. Ref. [5]. As the chairman of the Task Group he tested the new formulation for viscosity of water. Refs. [6 to 9].
- Prof. Marsik (IT) coordinated research in the metastable states. nucleation and lectured on thermodynamic modeling of fuel cells. Refs. [10 to 19].

- Prof. Sedlbauer (TUL) and his team collaborated with Prof. Majer (France) and investigated thermodynamic properties of selected aqueous solutes. Refs [20 to 26].
- Research activities at the (CTU) continued in further improvement of the knowledge on following subjects: Determination of the particles in the super-heated steam using a new sampling technique. The probe is designed for sampling superheated steam in the range of 170 to 400°C and 0.13 to 4 MPa. Ref. [1]. Thermodynamic analysis of hydrogen direct-fired Rankine steam cycle and hybrid H<sub>2</sub>/O<sub>2</sub> Solid Oxide Fuel Cell – Steam Turbine. Refs. [27 to 30].
- The activities of the SIGMA Research and Development Institute included solution of erosion effects of cavitation bubbles on the blades of water pumps and changes of the hydraulic machinery performance due to a cavitation. Refs. [10, 31]
- Dr. Jiricek (ICT-IE) with collaborators investigated corrosion processes and chemical effects in water and steam systems of power plants. Refs. [32 to 39].
- ICT-IE organized the 6<sup>th</sup> International Power Cycle Chemistry Conference (CHEO 6), held from 11<sup>th</sup> to 13<sup>th</sup> September 2006. Selected contributions are given in [40 to 55].
- Dr. Hnedkovsky (ICT-IPC) with collaborators investigated properties of organic solutes in water. Published articles and conference contribution are under Refs. [56 to 64].
- Prof. Stastny (SKODA POWER) with co-workers studied effects of deposits on the blades of HP steam turbine in fossil power plant by chemical analysis, measured degradation of steam turbine blade surfaces by deposits of chemicals and compared numerical models of the water steam flow in nozzles with NaCl binary nucleation and condensation. Refs. [32, 42, 65 to 67].
- Ing. Kodl (SKODA POWER) applied his own procedure for the evaluation of region 5 of IAPWS-IF97 enlarged up to 50MP; results were sent to Mr. Miyagawa the chairman of evaluation task group. He also tested the programming of the new formulation of viscosity.
- Dr. Zmitko (NRI) studied effects of simultaneous influence of irradiation, water chemistry at high pressures and temperatures on behavior of nuclear power plants structural materials and components and collaborated with nuclear power plants mainly on water chemistry, corrosion problems and radiation control. New research activities are turned to the role of the coolant chemistry and decontamination on formation of corrosion product deposits on the fuel cladding and on the out-of-core surfaces. Refs. [68 to 71]

#### **Young Scientists IAPWS Fellowships**

- O. Mican finished the 2006 Young Scientist IAPWS (CZ-US) Project “*Irreversible Thermodynamics of Fuel Cells Membrane Transport*” under supervising Prof. F. Marsik, and Prof. S. Lvov. The project was focused on four areas of interest in the advanced basic research:
  - preparation of a database of existing physical-chemical models describing transport and electrochemical processes, which occur in all components of MEA of PEM hydrogen/oxygen fuel cells,
  - formulation of an adequate physical-chemical model describing the influence of membrane material, including composite materials on the PEM fuel cell performance,
  - development of a computer program for numerical simulations of the model and investigation of the model behavior in a series of simulations,
  - comparison of the results of numerical simulations with available experimental results and possibly improve the original model, so that it will yield a better agreement with the experiment.

His Final Report is in Appendix 1. The publications of the fellowship holder are in Refs.[13,18].

- J. Ehlerova performed her Young Scientist IAPWS (CZ-Canada) Project “*Predictive Scheme for Standard Thermodynamic Properties of Aqueous Substituted Benzenes over a Wide Range of Temperatures and Pressures*” under supervising of Prof. J. Sedlbauer, and Prof. P. R. Tremaine. The project had two main objectives:
  - to develop the extended group contribution scheme by simultaneous treatment of all available standard thermodynamic data for nitro- and phenolate aqueous systems,
  - to supplement the existing scarce experimental results available on these aqueous systems at high temperatures by measurements of the ionization constants of isomeric nitrophenols to 250°C using hydrothermal indicators and UV-VIS spectroscopy.

Her Final Report of the Project will be finished by the end of the year 2007.

Preliminary results she will present at the 2007 IAPWS Meeting. Ref. [26].

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## **German National Committee to IAPWS**

### **Research Activities on the Thermodynamic Properties of Water and Steam**

#### **Report "Research in Progress 2007"**

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

1. „Release of an Equation of State of Ice Ih“ was issued by IAPWS in Witney 2006
2. IAPWS Certified Research Need „Thermophysical Properties of Seawater“, draft presented in Witney 2006, further edited for issue by IAPWS in Lucerne, 2007
3. Publication of R. Feistel, G.M. Marion: “A Gibbs-Pitzer Function for High-Salinity Seawater Thermodynamics”. *Progress in Oceanography*, 74 (2007) 515–539
4. Publication of R. Feistel, W. Wagner: “Sublimation pressure and sublimation enthalpy of H<sub>2</sub>O ice Ih between 0 and 273.16 K”. *Geochimica et Cosmochimica Acta* 71 (2007) 36–45
5. Publication of R. Feistel, F.J. Millero, T. J. McDougall: “Eine neue Zustandsgleichung für Meerwasser“. *DGM-Mitteilungen*, 2/2006, 19-21
6. Publication of F.J. Millero, R. Feistel, D.G. Wright, T.J. McDougall: “The Composition of Standard Seawater and the Definition of the Reference-Composition Salinity Scale”. *Deep-Sea Research*, submitted. To be presented in Lucerne 2007.
7. Certified Research and Development Need “Refractive Index of Seawater”. SCOR/IAPSO Working Group 127, Reggio di Calabria, May 2007
8. Publication of R. Feistel “A Gibbs Function for Seawater Thermodynamics for -2 °C to 80 °C and Salinity up to 120 g kg<sup>-1</sup>”. Draft presented at the WG127 meeting, Reggio di Calabria, May 2007. In preparation for submission.
9. Chairing the TPWS Taskgroups “Seawater”, “Metastable Liquid”, “Ideal Gas” and “Correlation Equations”
10. W. Wagner, R. Feistel: Draft “Revised Release on the Pressure along the Melting and Sublimation Curves of Ordinary Water Substance” for presentation in Lucerne 2007
11. R. Feistel: Draft “Release on the IAPWS Formulation for the Thermodynamic Properties of Seawater” for presentation in Lucerne 2007
12. Liaison with SCOR/IAPSO WG127 on Thermodynamics and Equation of State of seawater

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
  - The comprehensive article on the backward equations for the "Journal of Engineering for Gas Turbines and Power" was prepared.

2. Thermodynamic derivatives from IAPWS Formulations
  - The evaluation of the "Advisory Note No. 3 Thermodynamic Derivatives from IAPWS Formulations" was supported.
3. Development of fast property algorithms based on spline interpolation for non-stationary calculations of heat cycles and steam turbines
  - Different spline-interpolation methods and their implementation in Assembler programs were investigated.
4. Investigations on thermodynamic properties of humid air - part of the project "Advanced Adiabatic Compressed Air Energy Storage" (AA-CAES) of the European Union
  - The PTB Report "Determination of Thermodynamic and Transport Properties of Humid Air for Power-Cycle Calculations" was prepared.
5. Property libraries for water and steam, humid gases, and aqueous mixtures
  - The Add-On FluidMAT for MATLAB<sup>®</sup> was developed.
6. The homepage [www.iapws.de](http://www.iapws.de) of the German National Committee of IAPWS was hosted.

#### Recent Publications

- Kretzschmar, H.-J., Cooper, J. R., Dittmann, A., Friend, D. G., Gallagher, J. S., Harvey, A. H., Knobloch, K., Mareš, R., Miyagawa, K., Okita, N., Stöcker, I., Wagner, W., and Weber, I., Supplementary Backward Equations  $T(p,h)$ ,  $v(p,h)$ , and  $T(p,s)$ ,  $v(p,s)$  for the Critical and Supercritical Regions (Region 3) of the Industrial Formulation IAPWS-IF97 for Water and Steam, *Journal of Engineering for Gas Turbines and Power*, Vol. 129 (2007) No. 1, p. 294-303
- Kretzschmar, H.-J., Cooper, J. R., Dittmann, A., Friend, D. G., Gallagher, J. S., Harvey, A. H., Knobloch, K., Mareš, R., Miyagawa, K., Okita, N., Span, R., Stöcker, I., Wagner, W., and Weber, I., Supplementary Backward Equations  $p(h,s)$  for the Critical and Supercritical Regions (Region 3), Equations for the Region Boundaries, and an Equation for the Two-Phase Region of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam, *Journal of Engineering for Gas Turbines and Power*, Vol. 129 (2007) No. 7
- Kretzschmar, H.-J.; Stöcker, I.; Jähne, I.; Seibt, D.; Kunick, M.: Berechnung der thermodynamischen Zustandsgrößen und Transporteigenschaften von feuchten Verbrennungsgasen, feuchter Luft und Absorptionskältemittelgemischen in fortschrittlichen Energieumwandlungsprozessen (Calculation of the thermodynamic properties of humid air, humid combustion gases and absorption refrigerants in advanced power cycles). VDI-Berichte 1924 (2006) p. 417-423
- Knobloch, K.: Gleichungen für thermodynamische Umkehrfunktionen von Wasser und Wasserdampf im kritischen und überkritischen Zustandsgebiet für energietechnische Prozessberechnungen (Equations for thermodynamic backward functions of water and steam in the critical and supercritical regions for modelling power cycles. Fortschritt-Berichte VDI, Reihe 6, No. 542 (2006)

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

1. Basic equation for region 5 of IAPWS-IF97
  - A draft revised release on IAPWS-IF97 was prepared.
2. Equations for the melting pressure and the sublimation pressure of ice Ih
  - Development of new equations for the melting pressure and the sublimation pressure of ice Ih. The equations were not developed based on experimental data, but the input  $T$ - $p$  values were

calculated from IAPWS-95 and the equation of state for ice Ih by the application of the phase equilibrium condition.

- A draft revised release on the pressure along the melting and sublimation curves of ordinary water substance was prepared.

**Current Status of Research Activities in Japan  
Submitted to the Executive Committee Meeting, IAPWS,  
Luzern, Switzerland, August 2007**

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 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.

Dr. S. IKAWA, emeritus Prof. of Hokkaido University, Sapporo, conducted study on volumetric behavior of water-methanol mixtures in the vicinity of the critical region, in collaboration with Prof. P. Tremaine and his coworkers of University of Guelph, Canada. Densities of water-methanol mixtures at 573 and 588 K and at pressures in the 100-200 bar range have been measured with a vibrating-tube densimeter. A large negative-to-positive sigmoidal change of the excess molar volumes as a function of methanol mole fraction was interpreted on the basis of an estimated locus of the mixtures. The behavior of the water-methanol mixtures at the lower methanol mole fractions was discussed in terms of the local solute-solvent structure by estimating radial distribution functions and self-diffusion coefficients from molecular dynamics calculations. [Fluid Phase Equilib., **245**, 125 (2006)].  
[contact: Dr. S. Ikawa; E-mail: sikawa@sci.hokudai.ac.jp].

At the Nuclear Science and Engineering Directorate, Japan Atomic Energy Agency, Tokai-mura, Dr. S. UCHIDA has finished the second phase of the project on water chemistry of BWR, which has been supported by the Japan Society for the Promotion of Science (JSPS) [A Grant-in-Aid for Scientific Research: Subject No. 16360467 (2004-2006)] and then 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) The six year research project on hydrogen peroxide was rewarded as the 2006 Award for Distinguished Technology of the Atomic Energy Society of

Japan, “Establishment of Experimental Technology for the High Temperature High Pressure Hydrogen Peroxide Water Loop - Concentration Control of Hydrogen Peroxide in the High Temperature Water Loop and *In-situ* Measurements of Its Concentration and Effects on Corrosion Behavior”. 2) A model based on combined analyses of flow dynamics and corrosion has been developed to predict corrosive conditions in PWR secondary cooling system and pipe wall thinning due to flow accelerated corrosion. 3) Standard procedures were proposed to determine corrosive conditions in BWR primary cooling system based on combined analyses of water radiolysis and mixed potential models. [Latest publication: (1) T. Miyazawa, T. Terachi, S. Uchida, et al., “Effects of Hydrogen Peroxide on Corrosion of Stainless Steel (V) - Characterization of Oxide Film with Multilateral Surface Analyses“, *J. Nucl. Sci. Technol.*, 43, 884 (2006), (2) S. Uchida, T. Satoh, N. Kakinuma, et al., “An electrochemical sensor complex for in-situ measurements of oxide film electric resistance in high temperature water”, *ECS Transactions*, Volume 2, Issue 25, 37, 209th ECS Meeting, May 7-May 12, 2006, Denver, Colorado, Electrochemical Society (2006)., (3) S. Uchida, K. Otoha, and K. Ishigure, “Water Chemistry – One of the Key Technologies for Safe and Reliable Nuclear Power Plant Operation”, *Proc. the 15th Pacific Basin Nuclear Conference* (in CD), (2006), (4) S. Uchida, T. Satoh, T. Tsukada, et al., “Properties of Oxide Films on Stainless Steel Exposed to Hydrogen Peroxide and Oxygen in High Temperature Water”, *Proc. Int. Conf. Water Chemistry of Nuclear reactor Systems 2006*, Oct. 23-26, 2006, Jeju, Korea, Korean Atomic Energy Research Institute (2006). (in CD)., (5) T. Satoh, S. Uchida, T. Tsukada, et al., “Effects of Hydrogen Peroxide and Oxygen on Polarization Curves of Stainless Steel in High Temperature Pure Water”, *Proc. Int. Conf. Water Chemistry of Nuclear reactor Systems 2006*, Oct. 23-26, 2006, Jeju, Korea, Korean Atomic Energy Research Institute (2006). (in CD)., (6) E. Kadoi, H. Takiguchi, K. Otoha, et al., “Mitigation of Flow Accelerated Corrosion in Pure Neutral Water - Japan-Canada Collaboration Studies on FAC”, *Proc. Int. Conf. Water Chemistry of Nuclear reactor Systems 2006*, Oct. 23-26, 2006, Jeju, Korea, Korean Atomic Energy Research Institute (2006) (in CD), (7) S. Uchida, M. Naitoh, Y. Uehara, et al., “Evaluation Method of Corrosive Conditions in Cooling Systems of Nuclear Power Plants by Combined Analyses of Flow Dynamics and Corrosion”, *Power Plant Chemistry*, 9, 3, 143-156 (2007), (8) S. Uchida, Y. Morishima, T. Hirose, et al., “Effects of Hydrogen Peroxide on Corrosion of Stainless Steel (VI) - Effects of Hydrogen Peroxide and Oxygen on Anodic Polarization Properties”, *J. Nucl. Sci. Technol.*, 44, 758 (2007). (9) T. Satoh, Y. Shao, W. G. Cook,, et al., “Flow-Assisted Corrosion of Carbon Steel under PWR Secondary Water Conditions”, *Corrosion*, in press.

[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 been performed the density measurement of aqueous solutions at supercritical state of water. In these years, the densities of water-methanol and water-ethanol mixtures were measured with the laser-doppler type vibrating densimeter at 400 C in the pressure range of 25-40 MPa. The composition dependences of the excess molar volumes for both water-alcohol mixtures were estimated from the experimental values and fitted with the Redlich-Kister equation. The excess molar volumes of all mixtures were positive in the whole composition range at 400 C. The composition dependences of the excess molar

volumes showed maxima around 30-40 mol% of alcohol in water and the pressure dependences around 30 MPa at 400 C. [The Joint Meeting of ISHR-8 and ICSTR-7 (August 2006); T. Ono, T. Hoshina, T. Aida, M. Watanabe, Y. Sato, and H. Inomata AICHE 2006 Annual Meeting (November 2006) T. Hoshina, T. Ono, T. Aida, T. Matsushita, M. Watanabe, Y. Sato, R. L. Smith, Jr., and H. Inomata]

At the Institute of Multidisciplinary Research for Advanced Materials at Tohoku University, Prof. M. KAKIHANA and coworkers have discovered a series of new water-soluble, stable and non-toxic titanium complexes, which were proved to be very promising reagents from an environmental point of view for the preparation of titanium-containing functional materials using water-based synthesis methods. The hydrothermal treatment of these newly designed water soluble titanium complexes is one of the key synthesis techniques which allows the perfectly selective synthesis of nanocrystalline TiO<sub>2</sub> polymorphs including single phase brookite, anatase, rutile and TiO<sub>2</sub> (B). It was established that both brookite and TiO<sub>2</sub> (B) exhibited higher photocatalytic activities in NO decomposition reaction than commercially available anatase/rutile based TiO<sub>2</sub> photocatalysts.[K. Tomita, V. Petrykin, M. Kobayashi, M. Shiro, M. Yoshimura and M. Kakihana, *Angew. Chem. Int. Ed.* 45 (2006) 2378-2381.]. Prof. T. SATO and 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. Visible light responsive photocatalysts such as nitrogen-doped titania and strontium titanate nanoparticles, ceria based new inorganic UV-shielding materials showing low photocatalytic activity, high performance deNO<sub>x</sub> catalyst of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>/Ag nanocomposite, high performance rare earth oxide nanoparticle phosphors, zinc oxide film possessing superhydrophilicity and superhydrophobicity, etc. were synthesized by the solvothermal reactions using various alcoholic aqueous solutions as reaction media [*J. Photochem. Photobiol. A: Chem.*, 179, 105 (2006); *J. Mater. Sci.*, 41, 1433 (2006); *Chinese J. Process Eng.*, 6, 472 (2006); *J. Europ. Ceram. Soc.*, 26, 2735 (2006); *J. Photochem. Photobiol. A: Chem.*, 187, 72 (2007), *J. Oleo. Sci.*, 55, 249 (2006); *Appl. Surface Sci.*, 252, 5063 (2006). *Adv. Sci. Technol.*, 45, 668 (2006); *Adv. Sci. Technol.*, 45, 673 (2006); *Adv. Sci. Technol.*, 45, 679 (2006); *Adv. Sci. Technol.*, 45, 685 (2006); *Chinese J. Process Eng.*, 6, 633 (2006); *J. Photochem. Photobiol. A: Chem.*, 187, 72 (2007); *J. Luminescence*, 126, 427 (2007); *Key Engineering Materials*, 352, 293 (2007)]. Prof. A. MURAMATSU and 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<sub>3</sub> 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. [*Chemistry Letters*, 35(6), 570-571(2006), *Journal of Surface Science and Nanotechnology*,

4(1), 352-358 (2006), The Journal of Physical Chemistry B, 110 (12), 6224-6228 (2006), Catalysis, 48(4), 271-276 (2006)]. Prof. T. ADSCHIRI and co-workers studied on nano-bio reactions and organic-inorganic reactions at hydrothermal conditions. Recently Prof. Adschiri proposed a new method to synthesize organic-inorganic hybrid nanoparticles at supercritical hydrothermal conditions. By introducing organic species (aminoacids, carboxylic acids, amines, alcohols, aldehydes etc.) during supercritical hydrothermal synthesis, nanoparticles whose surface was modified with organic molecules were synthesized. This is due to the homogeneous phase formation for organic substance and aqueous solution at supercritical conditions. Particle size was in the range from 2 nm to 10 nm, and particle size dispersion is extremely narrow. Crystal shape can be controlled to be sphere, nano-cube, nano-ribbon etc. By selecting a proper modifier, particles could be dispersed perfectly in organic solvents or in aqueous solutions. By drying the colloid, we obtained self-assembly structure of nanocrystals. [Analytical Sciences, 22(11), 1417-1423 (2006.11), Chemistry Letters, 35, 636-637 (2006), Chemistry Letters, 35, 732-733 (2006), Combustion Science and Technology, 178, 509-536 (2006), Journal of Materials Science, 41, 1445-1448 (2006), Funtai Kogaku Kaishi, 43, 440-444 (2006)] [contact: Prof. T. Adschiri; [ajiri@tagen.tohoku.ac.jp](mailto:ajiri@tagen.tohoku.ac.jp)]

At the Graduate School of Environmental Studies, Tohoku University, Sendai, we have several laboratories which studies hydrothermal experiments in material and Earth sciences. Prof. K. IOKU published excellent papers: hydrothermal preparation of tailored hydroxyapatite (K. Ioku et al., J. Mater. Sci., **41** [5], (2006), 1341-1344). He also tried to analyze bio-phenomena of materials prepared by hydrothermal methods: the effect of the microstructure of  $\beta$ -tricalcium phosphate on the metabolism of subsequently formed bone tissue (Ioku et al., Biomaterials, **28**, (2007), 2612-2621). Prof. H. Ishida's group studied about mesoporous materials which were prepared by the hydrothermal process using metakaolinite, quartz and slaked lime (Maeda et al. J. Ceram. Soc. Jp., 114 (2006) 743-747). The mesoporous materials had a broad pore size distribution more than 3 nm, which contributes to humidity control in the middle humid range. The humidity change in the vessel with the mesoporous materials was suppressed by water vapor adsorption-desorption of the materials. Geofluid science research group (Prof. N. TSUCHIYA) is conducting water-rock interaction under sub- and supercritical condition, including multi-phase and multi-component solutions. They published experimental studies and new conceptual model of supercritical fluid in terms of chemical reactions (Tsuchiya and Hirano, Island Arc, 6 (2007), 6-15). Prof. N. Tsuchiya had an award on research of hydrogen production from  $H_2S$  by hydrothermal reaction in International Symposium of Renewable Energy 2006. Petroleum Engineering research group studies hydrothermal cracking for unconventional heavy crude oil such as tar sands to develop new on-site partial upgrading process with high temperature and high pressure water in supercritical region was performed. (Kishita et al., J. of Japan Petroleum Institute, 49 (4), (2006), 177-185). We are planning 5<sup>th</sup> International Workshop of WATER DYNAMICS in 25-27<sup>th</sup> September 2007 in Sendai International Center. WATER DYNAMICS is unique objectives covering very wide range of water and steam properties and utilization, which focused on the role of water in Earth processes, Life science and Material and Energy Process Design. The web site of WATER DYNAMICS is the follows: <http://geo.kankyo.tohoku.ac.jp/wd/wd5/index.html>. We



published workshop proceedings as AIP (American Institute of Physics) conference series (vol. 833 and 898)

[contact Prof. N. Tsuchiya; [tsuchiya@mail.kankyo.tohoku.ac.jp](mailto:tsuchiya@mail.kankyo.tohoku.ac.jp)]

At the Material Properties and Metrological Statistics Division, National Metrology Institute of Japan (NMIJ, formerly NRLM), National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, a section lead by Dr. K. FUJII is working on the density, 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. Most recent situation of this project is given in a paper [K. Fujii, A. Waseda, N. Kuramoto, S. Mizushima, P. Becker, H. Bettin, A. Nicolaus, U. Kuetgens, S. Valkiers, P. Taylor, P. De Bièvre, G. Mana, E. Massa, R. Matyi, E. G. Kessler, Jr., and M. Hanke, "Present state of the Avogadro constant determination from silicon crystals with natural isotopic compositions," *IEEE Trans. Instrum. Meas.*, 2005, 54, 854-859]. In 2007, the uncertainty of the density measurement of 1 kg silicon spheres has been reduced down to  $3.6 \times 10^{-8}$  [Kuramoto N., Fujii K., Azuma Y., Mizushima S., and Toyoshima Y., "Density Determination of Silicon Spheres using an Interferometer with Optical Frequency Tuning," *IEEE Trans. Instrum. Meas.* 2007, 56, 476-480]. Using the silicon crystals as a solid density standard, density standard liquids are calibrated by a magnetic suspension densimeter developed at the NMIJ [N. Kuramoto, K. Fujii, and A. Waseda, "Accurate density measurements of reference liquids by a magnetic suspension balance," *Metrologia*, 2004, 41, S84-S94]. A relative standard uncertainty of  $4 \times 10^{-6}$  has been achieved in the density measurement of organic liquids. A revised densimeter is being developed in this section as a joint research with the Keio University [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, 18, 659-666]. Review articles are given for the density standard [K. Fujii, "Present state of the solid and liquid density standards," *Metrologia*, 2004, 41, S1-S15] and for the hydrostatic weighing [K. Fujii, "Precision density measurements of solid materials by hydrostatic weighing," *Meas. Sci. Technol.*, 2006, 17, 2551-2559]. 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. [contact: Dr. K. Fujii, Chief, Fluid Properties Section, NMIJ; E-mail: [fujii.kenichi@aist.go.jp](mailto:fujii.kenichi@aist.go.jp)].

Mr. K. MIYAGAWA assessed the computing time of equations of the industrial formulation IAPWS-IF97 in the Release and Supplementary Releases adopted one after another from 1997 to 2005. The computing times of each release had been tested on the latest computing platforms at the time. The aim of the assessment was to compare them on the common and state-of-the-art platforms. It was found that the IAPWS-IF97 equations are 8.3 times as fast as the previous international formulation. Modern computer systems are optimized for “simple” computational operations and therefore favor the simple structure of IAPWS-IF97. Provision of “backward equations”, which are approximation of inverse equations, is one of the features of IAPWS-IF97. The backward equations showed much shorter computing times than iterative routines, which had been used to calculate with several independent variables. The results were published as a technical brief entitled “Assessment of the Computing Time for the IAPWS-IF97 Equations”, ASME Journal of Engineering for Gas Turbines, Volume 129, Issue 3, pp. 885-887, July 2007. [contact: Mr. K. Miyagawa; E-mail: miyagawa.kiyoshi@nifty.com]

At Materials Science Research Laboratory, Central Research Institute of Electric Power Industry (CRIEPI), Yokosuka, Kanagawa, Dr. M. DOMAE and his coworkers studies stability of chromium oxide in high temperature water up to supercritical region by *in situ* Raman spectroscopy and analyses after immersion tests. Experimental results of immersion tests of  $\text{Cr}_2\text{O}_3$  film formed by metal organic chemical vapor deposition on Pt were published [CORROSION2007, Paper 07411 (2007).]. At 623 K, stability of  $\text{Cr}_2\text{O}_3$  depends on redox conditions, and can be explained by oxidation of Cr(III). At 723 K, weight of  $\text{Cr}_2\text{O}_3$  film was reduced to some extent irrespectively of redox conditions, but cristalinity of  $\text{Cr}_2\text{O}_3$  increased. Stability of  $\text{Cr}_2\text{O}_3$  film formed on stainless steel substrate in high temperature water was measured by *in situ* Raman spectroscopy. Under all conditions of temperature and redox environment examined,  $\text{Cr}_2\text{O}_3$  was stable. The difference of  $\text{Cr}_2\text{O}_3$  stability between Pt and stainless steel substrates can be attirbuted to interaction of  $\text{Cr}_2\text{O}_3$  with oxide film formed on surface of stainless steel substrate.  
[contact: Dr. M. Domae; E-mail: domae@criepi.denken.or.jp]

At Energy Engineering Research Laboratory, Central Research Institute of Electric Power Industry (CRIEPI), Yokosuka, Kanagawa, Dr. NAKANO and his coworkers are studying on the efficiency improvement of geothermal power plant. They developed the software based on the heat and mass balance analysis, “General purpose program for analysis of thermal efficiency of power generation systems”. Using this software, they estimate the relationship between vacuum and power outputs, the influence that non-condensable gas extractor systems are replaced, and, the actual effects generated by repair of cooling tower.  
[contact: Dr. Nakao; E-mail: y-nakao@criepi.denken.or.jp]

At the Department of Mechanical Engineering, Keio University, Yokohama, Prof. M. UEMATSU and his group study the behavior of thermodynamic properties of water + ammonia mixtures by means of the PVTx measurements, and the critical parameter measurements. The PVTx properties of water +

ammonia mixtures is measuring in the temperature range from 450 K to 550 K at pressures up to 200 MPa by a metal-bellows variable volumometer. The critical parameter of water + ammonia mixtures is measuring by a metal-bellows variable volumometer with an optical cell. The Cp measurements of water + ammonia mixtures were finished in the temperature range from 280 K to 360 K at pressures from 0.1 MPa to 15 MPa by the thermal relaxation method. [I. Fujita, T. Suzuki, and M. Uematsu, Accepted for publication in the Journal of Chemical Thermodynamics] [contact: Prof. M Uematsu; E-mail: uematsu@mech.keio.ac.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 thermodynamic stability of structure-I, II, and H clathrate hydrate by estimating the free energy difference. [E. Sato, T. Miyoshi, R. Ohmura, K. Yasuoka, *Jap. J. Appl. Phys.*, in press.; T. Miyoshi, M. Imai, R. Ohmura, K. Yasuoka, *J. Chem. Phys.*, **126**, 234506 (2007).; T. Miyoshi, R. Ohmura, K. Yasuoka, *J. Phys. Chem. C*, **111**, 3799-3802 (2007).; T. Miyoshi, R. Ohmura, K. Yasuoka, *Mole. Simul.* **33**, 65-69 (2007).] They reported the supercritical phenomena on the 2D of liquid-vapor water surface and the cluster near the surface. [Y. Andoh and K. Yasuoka, *J. Phys. Chem. B.*, **110**, 23264-23273 (2006).; Andoh and K. Yasuoka, *Mole. Simul.* **33**, 139-145 (2007).] They reported the Spontaneous self-assembly process for threadlike micelles. [N. Arai, K. Yasuoka, Y. Masubuchi, *J. Chem. Phys.*, **126**, 244905 (2007).] [contact: Dr. K. Yasuoka; E-mail: yasuoka@mech.keio.ac.jp].

At the Department of Mechanical Engineering, Kanagawa Institute of Technology, Atsugi, Dr. K. OGUCHI and his group finished the measurements of the pVTx properties of ammonia + water mixtures. They are preparing to design the set-up for the iso-choric specific heat capacity of ammonia + water mixtures, and to correlate the equation of state for ammonia + water mixtures. [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 are developing a twin-cell type adiabatic calorimeter for water + alcohol and water + ammonia mixtures. By the apparatus, liquid isochoric heat capacities will be measured for temperatures from 220 to 520 K and pressures to 30 MPa including super critical region. One isochore of propane was measured from 310 K to 350 K preliminary. The data showed behavior similar to the previous measurements by another twin-cell type adiabatic calorimeter apparatus which had measured water + alcohol and hydrocarbon mixtures. But, the preliminary data were quieter than the previous. [contact: Prof. N. Kagawa; E-mail kagawa@nda.ac.jp]

Prof. H. TAKAKU was retired from Faculty of Engineering of Shinshu University at the end of March of 2006, but at present he is entrusted by Shinshu University as the Professor in charge of education. He and his coworkers, including also some researchers of Japanese utility and makers, are conducting the corrosion researches of steam turbine materials for geothermal power plants, the corrosion of boiler tube materials for fossil power plants, and other subjects related to the corrosion and water chemistry for both of the fossil and nuclear power plants. As the chairman of the committee, he contributed to the revision of JIS-B-8223 entitled on "Water conditioning for boiler feed-water and boiler water", and this revised JIS

(Japanese Industrial Standard) was published on October 20 of 2006. Their main publications are “Behavior of Organic Sulfate Ions of PWR plants; and also The Anticorrosive Magnetite Layer Formed by Amine-Carboxylate Aqueous Solution Treatment on Boiler Tubes; both papers presented at the International Conference on Interaction of Organics and Organic Cycle Treatment Chemicals with Water, Steam and Materials, organized by EPRI-Power Plant Chemistry, Oct.2-4 (2005)”, Stuttgart, Germany, “Water conditioning for boiler feed-water and boiler water; JIS B 8223-2006, published by Japanese Standards Association, Oct. 20 (2006), “Influence of Chloride and Carbon Dioxide on General and Crevice Corrosions of Steam Turbine Materials for Geothermal Power Plants, *Power Plant Chemistry*, **8** (2006), 558-565”, and so on. [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 thermodynamics, structure, and dynamics of supercritical aqueous solution over a wide range of thermodynamic conditions, especially the diffusion dynamics in very dilute region [“Self-diffusion of supercritical water in extremely low-density region”, K. Yoshida, N. Matubayasi, and M. Nakahara, *J. Chem. Phys.* **125**, 074307 (7 pages) (2006); **126**, 089901 (2 pages) (2007) (erratum)] and (2) the molecular mechanism of noncatalytic reactions in hydrothermal conditions in connection to next-generation hydrogen fuel technology. [“Kinetic and Equilibrium Study on Formic Acid Decomposition in Relation to the Water-Gas-Shift Reaction”, Y. Yasaka, K. Yoshida, C. Wakai, N. Matubayasi, and M. Nakahara, *J. Phys. Chem. A* **110**, 11082-11090 (2006)]. [contact: Prof. M. Nakahara; E-mail: nakahara@scl.kyoto-u.ac.jp]

At the Department of Molecular Science and Technology, 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) along the liquid-vapor coexistence curve up to about 240 °C to disclose the general trends of the density dependence of ionic mobilities at medium and low densities, and to examine the validity of the Hubbard-Onsager (HO) dielectric friction theory which is based on the continuum model. We found that ionic mobilities decrease with decreasing the density in the region of the relative density  $\rho_r (= \rho / \rho^0) < 2.0$ , and that the HO theory does not work in the region. We also study the Computer simulations: Application of Fokker-Planck-Kramers equation treatment for short-time dynamics of diffusion-controlled reaction in supercritical Lennard-Jones fluids over a wide density range [K. Ibuki and M. Ueno, *J. Chem. Phys.*, **124**, 134506 1-11 (2006)], and Analysis of short-time transient dynamics of a diffusion-controlled reaction in a hard-sphere fluid based on Fokker-Planck-Kramers equation [K. Ibuki and M. Ueno, *Bull. Chem. Soc. Jpn.*, **79**, 1509-1518 (2006)]. In collaboration with Dr. M. Kanakubo, AIST, Sendai, the effect of pressure on transport properties (self-diffusion coefficients and electrical conductivities) of the ionic liquid 1-Butyl-3-methylimidazolium Hexafluorophosphate has been investigated [M. Kanakubo, K. R. Harris, N. Tsuchihashi, K. Ibuki, and M. Ueno, *J. Phys. Chem. B*, **111**, 2062-2069 (2007)]. [Contact: Prof. M. Ueno; E-mail: mueno@mail.doshisha.ac.jp]

At the Department of Applied Chemistry, Ritsumeikan University, Shiga, Prof. S. SAWAMURA studies the solubility of NaCl and amino acids in water and that of fullerene C<sub>60</sub> in toluene under high pressure up to 400 MPa [S. Sawamura, N. Fujita, Carbon, 45, 965-970 (2007); S. Sawamura, N. Egoshi, Y. Setoguchi, H. Matsuo, Fluid Phase Equilibria, 254, 158-162 (2007); S. Sawamura, Pure and Applied Chemistry, 79, 861-874 (2007).] and found a high-pressure crystal of leucine as a residue of saturated mixture. [M. Yamashita, S. Inomata, K. Ishikawa, T. Kashiwagi, H. Matsuo, S. Sawamura, and M. Kato, Acta Cryst. E63, o2762-o2764 (2007).] [contact: Prof. S. Sawamura; E-mail: sawamura@se.ritsumei.ac.jp]

## International Association for the Properties of Water and Steam

### *Russian National Committee*

#### Report of Russian National Committee (2007)

##### *List of Publications*

1. Voronov V.N., Gotovcev P.M., Smetanin D.S. Building of Water Chemistry Mode Diagnostic Method Complex on the Base of Experimental Plant Monitoring System. // Thermal Engineering, vol. 7, pp. 2-6
2. Petrova T.I., Kashinsky V.I., Verkhovsky A.E., Nikolaev P.A., Repin D.A., Chernichov E.V., Bogdanov S.L. The Study of Influence Phosphate Concentration in Drum Water on Conductivity and pH.// Thermal Engineering, vol. 7, pp. 6-10
3. Boglovsky A.V., Chernozubov V.B., Chernih N.E., Gorbunov A.V., Birdin R.H. The Organization of Water Chemistry Mode of Thermal Water Purification Plant// Thermal Engineering, vol. 7, pp. 15-20
4. Smetanin D.S. Optimization Chemistry Monitoring System by Using Technology Algorithm.// Thermal Engineering, vol. 7, pp. 20-25
5. Egochina O.V., Voronov V.N., Nazarenko P.N. The Development of Automatic Control System for Hydrazine Dosation.// Thermal Engineering, vol. 7, pp. 25-28
6. Alexandrov A.A. Orlov K.A. The Thermodynamic Properties of Humid Air under High Temperature and Pressure// Thermal Engineering, vol. 7, pp. 36-40
7. Evsutin A.V., Boglovsky A.V. The Application of Aluminium Oxichloride for Coagulation Water with High Organic Impurities Concentration and Lower Alkalinity.// Thermal Engineering, vol. 7, pp. 67-71
8. Nikolaev P.A. The Influence of Liquid Film Contamination in the Turbin Blade on the Metall Corrosion// Energoberezhenie i Vodopodgotovka, 2007, № 1, pp. 67-68
9. Matsko T.V. The Application of Film-forming Combinations for Water Correction Treatment in Heat Supply Systems. //Vestnik MEI, 2007, № 1, pp. 29-31
10. Alexandrov A.A., Ochkov V.F., Orlov K.A., Ochkov A.V. Thermophysical properties of water and steam: information in Internet// Industrial energetics, 2007, No 2, P. 29-35

## U.S. National Committee to IAPWS 2007 Report on Activities of Potential Interest to IAPWS

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

The Energy Institutes' Electrochemical Laboratory at Penn State University continues to work in fundamental and applied areas on a variety of electrochemical and materials science studies related to traditional and renewable energy generation systems. We lead interdisciplinary studies on electrochemistry of high-temperature aqueous systems in a number of scientific areas including corrosion and protective coatings, proton exchange membrane and solid oxide fuel cells, surface electrochemistry and chemistry, etc. The main research directions and key publications in 2006-2007 are as follows:

#### (1) High-Temperature Thermodynamics of Aqueous Solutions

Bandura A. V., and Lvov S.N. The Ionization Constant of Water over Wide Ranges of Temperature and Density, *J. Phys. Chem. Ref. Data*, 2006, **35**, 15-35.

#### (2) High-Temperature Aqueous Electrochemistry

Lvov S.N. Electrochemical Techniques for Studying High-Temperature Subcritical and Supercritical Aqueous Solutions, in "*Encyclopedia of Electrochemistry*", Eds. A.J. Bard and M. Stratmann, Vol. 5. Electrochemical Engineering, Eds. D.D. Macdonald and P. Schmuki, 2006, Wiley-VCH, p. 725-747.

#### (3) High-Temperature Surface Chemistry

Machesky M.L., Wesolowski D.J., Palmer D.A., Ridley M.K., Benezeth P., Lvov S.N., and Fedkin M.V., Ion Adsorption into the Hydrothermal Regime: Experimental and Modeling Approaches. Chapter 12, in "Surface Complexation Modeling" (J. Lutzenkirchen, Ed.), 2006, Elsevier, Amsterdam, pp. 324-358.

#### (4) High-Temperature Surface Electrochemistry

Fedkin, M.V.; Chalkova, E.; Komarneni, S.; Wesolowski, D.J.; Lvov, S.N., "Surface Electrochemistry of Composite Materials for High-Temperature PEM Fuel Cells," *ECS Trans.* 2006, **1**, 215-225.

#### (5) High-Temperature Proton Exchange Membrane Fuel Cells

Chalkova, E.; Rybka, G.; Fedkin, M.V.; Wesolowski, D.J.; Roelofs, M.; Lvov, S.N., "Nafion/TiO<sub>2</sub> Composite Membranes for PEM Fuel Cells Operating at Elevated Temperature and Reduced Relative Humidity," *ECS Trans.*, 2006, **3**, 73-82.

Chung M., Komarneni S., Chalkova E., Lvov S.N. Proton Conductive Composite Materials with Co-continuous Phases Using Silane Functionalized and Crosslinkable PVDF Polymers, 2006, *ECS Trans.* **3**, 83-90.

Chalkova, E., Fedkin, M.V., Komarneni, S., and Lvov, S.N., Nafion/Zirconium Phosphate Composite Membranes for PEMFC Operating at up to 120°C and down to 13% RH, *J. Electrochem. Soc.*, **154**, B288-B295.

Gong Y., Yeboah Y.D., Lvov S.N., Balashov V., and Wang Z., Fe Modified Pt Based Cathodic Electrocatalysts for Oxygen Reduction Reaction with Enhanced Methanol Tolerance, *J. Electrochemical Soc.*, (in press).

#### (6) High-Temperature Solid Oxide Fuel Cells

Zhou Z.F., Kumar R., Thakur S.T., Rudnick L.R., Schobert H., and S.N. Lvov, Direct oxidation of waste vegetable oil in solid oxide fuel cells. *J. Power Sources*, 2007, in press.

#### (7) High-Temperature Aqueous Corrosion and Protective Coatings

Zhou Z.F., Chalkova E., Lvov S.N., Chou P., and Pathania R. Development of a Hydrothermal Deposition Process for Applying Zirconia Coatings on BWR Materials for IGSCC Mitigation. *Corrosion Science*, **49**, 830-847.

### Communicated from The University of Delaware, Newark, DE:

The research group of R.H. Wood produced the following work on high-temperature aqueous electrolyte systems:

“Potentials of Mean Force of Sodium Chloride in Supercritical Water as a Function of Density and an Equation for Dissociation Constant from 600 K to 1073K and 0 to 9 g/cm<sup>3</sup>,” by Wenbin Liu, Robert H. Wood, and Douglas J. Doren, in preparation.

“Structure of an accurate *ab initio* Model of the aqueous Na<sup>+</sup> ion at high Temperatures,” by Haitao Dong, Wenbin Liu, Robert H. Wood, and Douglas J. Doren., in preparation.

“Structure of an accurate *ab initio* model of the aqueous Cl<sup>-</sup> ion at high temperatures,” by Haitao Dong, Wenbin Liu, Douglas J. Doren, and Robert Wood. *J. Phys. Chem. B*, 2006, 110, 18504-18514.

“Dissociation constants and speciation in aqueous Li<sub>2</sub>SO<sub>4</sub> and K<sub>2</sub>SO<sub>4</sub> from measurement of electrical conductance to 673 K and 29 MPa,” by Andrei V. Sharygin, Brian K. Grafton, Caibin Xiao, Robert H. Wood, and Victor N. Balashov, *Geochim. Cosmochim. Acta* 2006, 70, 5169-5182.

**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-nitrogen and water-oxygen binaries have been published in the past year. These results, along with previous results for water-argon, have allowed a purely predictive calculation of the second virial coefficients for water with “air,” which is consistent (with similar uncertainties) with precise data from the humidity community but covers a much larger temperature range. This result should be useful for humidity standards, atmospheric applications, and the energy industry. The next system to be covered in this manner is water with carbon monoxide, which is important for synthesis gases in advanced power cycles.

References: Tulegenov, A.S., Wheatley, R.J., Hodges, M.P., and Harvey, A.H., 2007. “Intermolecular potential and second virial coefficient of the water–nitrogen complex,” *J. Chem. Phys.*, 126, 094305; Wheatley, R.J., and Harvey, A.H., 2007. “The water-oxygen dimer: first-principles calculation of an extrapolated potential energy surface and second virial coefficients,” *J. Chem. Phys.*, 127, 074303; Harvey, A.H., and Huang, P.H., 2007. “First-Principles Calculation of the Air-Water Second Virial Coefficient,” *Int. J. Thermophys.*, 28, 556.

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 refitted and is ready for evaluation by IAPWS. Work has started on the low-density portion of the thermal conductivity.

NIST’s Experimental Properties of Fluids group has begun apparatus design for two projects to measure thermophysical properties of aqueous gas-phase mixtures at high temperatures. One apparatus will be a high-temperature (up to 770 K) magnetic-suspension densimeter, which will be used to measure H<sub>2</sub>O-N<sub>2</sub> and H<sub>2</sub>O-CO<sub>2</sub> mixtures of interest for understanding the thermodynamics of combustion gases. An existing high-temperature thermal conductivity apparatus (using the transient hot-wire technique) is being converted to alternating-current operation (needed for polar fluids like water) in order to measure the thermal conductivity of H<sub>2</sub>O-N<sub>2</sub> and H<sub>2</sub>O-CO<sub>2</sub> mixtures at similar conditions (up to 750 K).

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

Jonas, Inc. is working on the following projects related to IAPWS interests:

1. Fusion Reactor ITER/Tokamak: water radiolysis and hydrogen water chemistry, Zn treatment, corrosion and activation of corrosion products (316L, 430ss, CuCrZr, Cu, borated ss)
2. Atmospheric corrosion: influence of cooling tower plumes, seawater for cooling towers, critical relative humidity (salt zone), seashore air, gas turbine compressors, ...
3. Rapid Response Corrosimeter and Surface Conductivity: general corrosion, FAC, steam piping, buried piping
4. On Line Moisture Monitor: % moisture, enthalpy, continuous monitoring
5. Low pressure steam turbine surface chemistry: on-line monitoring of early condensate, moisture drying, deposits, and corrosion.