BRITISH AND IRISH ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM (BIAPWS)

A Member of the International Association for the Properties of Water and Steam
www.biapws.org

BIAPWS Annual Report to IAPWS for 2005/06.

BIAPWS continues with a strong membership, with 13 Industrial Sponsors, all of whom are associated with the power generation industry. BIAPWS maintains links, through corresponding members, with academic institutions but has only one active academic member of the committee. Currently, BIAPWS has no active links with any research based institution.

BIAPWS has recently become a member of the British Standards Institute, representing the power generation industry on aspects of steam and water chemistry in the power cycle relative to recently issued European standards on boiler water chemistry.

The BIAPWS Award scheme has been modified to offer an undergraduate bursary for summer vacation work experience in a suitably relevant industry.

Membership.

There has been one additional industrial sponsor of BIAPWS in the past year. The sponsors of BIAPWS are currently: power generation companies (8); power plant manufacturers (2); chemical instrumentation suppliers (2); and technical support organisations (1).

The academic support 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

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BIAPWS is a member of the British Standards Institute.

BIAPWS is sponsored by: Alstom Power Ltd; ABB Ltd; Amec NNC Ltd; British Energy Generation Ltd.; EDF Energy plc; ESB (Eire); E.ON UK plc; PX Ltd; Hach Ultra Analytics Ltd; Rolls-Royce plc; RWE-npower plc; Scottish Power plc; Thames Power Services Ltd.

Chairman: Dr R R Harries, Power Chemistry Consulting, 6, Montague Drive, Loughborough, Leics. LE11 3SB., UK.
Secretary: Mr M Ball, 48, Leconfield Road, Loughborough, Leics. LE11 3SQ., UK.
Treasurer: Mr E G Huff, Plush Hill, All Stretton, Shropshire, SY6 6JP., UK

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. The level of academic research into topics of interest to BIAPWS/IAPWS, appears to remain low in the UK. However, with IAPWS expanding its sphere of interest into environmental areas the scope for research may increase.

British Standards Institute.

BIAPWS has been invited to become a member of the British Standards Institute, the body responsible for issuing British Standards and European Standards in Britain. BIAPWS will represent the power industry views in the area of steam and water chemistry as applied to power generation cycles.

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.

A large number of alternative schemes have been raised and discussed by BIAPWS.

BIAPWS Symposia.

BIAPWS continues to organise regular symposia on topics of interest to power plant operators and suppliers. This theme is continued in 2006 with the BIAPWS Symposium incorporated into the IAPWS Annual Meeting on the topic “Advances in power plant chemistry; current trends and future developments”. This has an environmental bias as well as addressing traditional water and steam cycle chemistry issues.

BIAPWS Award.

The BIAPWS Award was conceived 4 years ago, offering a cash prize to undergraduates for submission of final year project reports on topics relevant to the measurement or application of the properties of water and steam. For various reasons the award has only been made once. The quality of the (few) submissions was not high and there appeared to be a clear problem in accessing UK academic institutions, although chemistry, chemical engineering and mechanical engineering departments were all circularised.

There is an implication that BIAPWS (and IAPWS) does not have a high profile in UK universities and attempts to open dialogue with learned institutions on the possibility of joint awards have also foundered.

BIAPWS Student Bursary.

To overcome some of the above problems 2006 has seen BIAPWS institute a student bursary, initially for one undergraduate student, where BIAPWS jointly funds a summer vacation placement with one of its industrial sponsors. The first such placement, with the technical and engineering department of a power generation company, has been very successful. The candidate gained an appreciation of the wide application of chemistry of water and steam in power plants as well as gaining skills in research tools and report writing.

BIAPWS Future.

BIAPWS will continue to act as the central point for co-ordinating the properties of water and steam and their application to industry, particularly power generation in the UK and Ireland.

BIAPWS will continue to seek ways to widen the knowledge of the properties of water and steam and their industrial applications, particularly through financial support to undergraduate students and other appropriate initiatives.

Richard Harries
Chairman BIAPWS
September 2006.

IAPWS CANADIAN NATIONAL COMMITTEE

Annual Report 2006

Executive: *Peter Tremaine (Chair); David Guzonas (Secretary Treasurer); Igor Svischev (Past Chair); Derek Lister (Member at Large); Candu Owners Group Representative (TBD).*

1. Canadian National Committee: Dues for the Candian National Committee are supported by the National Research Council, which requires an industrial partner. Three years ago, the Canadian Electrical Association withdrew as the industrial partner for IAPWS, and it has been replaced by the Candu Owner's Group ("COG") on a three year trial basis. The Canadian Committee must submit a proposal this fall for continued participation and funding. Interest from the thermal industry has fallen, but the creation of ("UNENE") has created a vibrant research climate in nuclear R&D and we are optimistic..

2. University Nework of Excellence in Nuclear Engineering (UNENE). The Canadian government and nuclear industry are co-funding an initiative to create a number of NSERC University Research Chairs which will form a research network, and common postgraduate MSc program in nuclear engineering. Companies are: Atomic Energy of Canada Ltd. Ontario Power Generation, Bruce Power, CANDU Owners Group. Some of the Chairs relevant to IAPWS are listed below:

Roger Newman (University of Toronto): Corrosion, materials performance, electrochemistry.in primary secondary coolant

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 radiochemistry under nuclear reactor primary-coolant conditions, and reactor accident scenarios.

Three Canadian IAPWS National Committee Members are involved with UNENE, as sponsoring industrial participants or as`members of universities who are`are associate members in UNENE are:

Derek Lister: (University of New Brunswick, Associate Member of UNENE) Primary and secondary coolant chemistry, activity transport, corrosion.

Peter Tremaine: (University of Guelph, Associate Member): Solution thermodynamics, phase relations, and solubility in sub-critical and super-critical water; also D_2O isotope effects under CANDU-PHW conditions.

Dave Guzonas (Atomic Energy of Canada Ltd.) Section Leader, Reactor Chemistry Group. Materials performance and chemistry control in primary and secondary coolant circuits.

3. Other Research Relevant to IAPWS

Other researchers with active progrms in high-temperature water chemistry are:

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

Paul Percival (Simon Fraser University): Muonium ion chemistry and radiolysis in sub-critical and super-critical 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.

Proposals to fund a 1.5 M$ experimental laboratory for high-pressure, high-temperature water chemistry at the University of Guelph, and a $300,000 supercritical autoclave loop at the University of New Brunswick are under review by the Canadian "CFI" program.

A new program to fund research on a Generation IV super-critical water reactor is expected to be announced in early 2007.

THE CZECH NATIONAL COMMITTEE
INTERNATIONAL ASSOCIATION FOR THE PROPERTIES OF WATER AND STEAM

REPORT on IAPWS related activities – August 2005 / August 2006

Submitted to the EC Meeting of IAPWS, Witney – September 2006.

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

Institute of Thermomechanics (IT) AS CR, Department of Thermodynamics, Dolejskova 5, CZ-182 00 Prague 8

Czech Technical University in Prague (CTU), Faculty of Mechanical Engineering, Department of Fluid Mechanics and Power Engineering, Technicka 4, CZ-166 07 Prague 6

Technical University Brno (TU), Faculty of Mechanical Engineering, Department of Thermomechanics and Nuclear Energetics and Department of, Technicka 2, CZ-616 69 Brno

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

University of West Bohemia (UWB), Faculty of Mechanical Engineering, Department of Theory and Design of Power Plants, Univerzitní 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, Sigmunda, 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 properties of supercooled water and surface tension. He was the chairman of IAPWS team for evaluation of formulation of thermodynamic properties of ice. Refs [1, 2].

- Prof. Mares (UWB) was charged with chairmanship of the IAPWS task group on evaluation of a new formulation for viscosity of water. Ref. [3].

- Prof. Mares (UWB) with his collaborators measured surface tension of supercooled metastable water and extrapolated the Formulation IAPWS-95 to region of the supercooled metastable liquid down to -37°C. Refs [4 to 6].

- Prof. Mares (UWB) prepared extension of the region 5 of the formulation IAPWS-IF97. Ref. [7].
- Prof. Marsik (IT) coordinated research in the metastable states and nucleation and lectured on modeling of fuel cells. Refs. [8 to 11].

- Prof. Sedlbauer (TUL) and his team collaborated with Profs. Majer (France) and Wood (U.S.A.) and investigated thermodynamic properties of hydration for selected organic solutes. Refs [12 to 16].

- Dr. Patek (IT) prepared formulation of the thermodynamic properties of LiBr-H_2O solutions. Ref. [17].

- Research activities at the (CTU) have continued during the period 8/2005 – 6/2006 in further improvement of current knowledge on the following subjects:
  - Diagnostics of wet steam i.e. measurement of droplet size spectra and steam quality. The tests were carried out in the fossil (210 MW) and (360 MW) LP steam turbines with optical extinction probe.
  - Prediction of initial size and concentration of heterogeneous impurities that could participate in the droplet nucleation process in steam. The measurements were realized in the nozzle and in the new special sampling line supplied both with the laboratory steam.

- Research activities at the (TU) were oriented to:
  - Development of interactive graphical software "Moist Air" with IAPWS equations for application for heating, ventilation and air conditioning, Ref. [18].
  - Development of software for interferogram evaluation of refractive index and temperature fields in water with the IAPWS equations, Refs [19 to 22].
  - Measurements of bulk viscosity and speed of sound in water, Ref. [23]

- In SIGMA Research and Development Institute the activities included experimental and numerical modelling of bubble nucleation and cavitation in pumps as well as the investigation of the effect of water properties on these phenomena, Ref. [24].

- Dr. Jiricek (ICT-IE) with collaborators investigated corrosion processes and chemical effects in water and steam systems of power plants. Refs [25 to 27]. ICT-IE will organize the 6th International Power Cycle Conference (CHEO 6), held from 11th to 13th September, 2006.

- Dr. Hnedkovsky (ICT-IPC) with collaborators investigated properties of organic solutes in water. Published articles and conference fulltexts are under Refs [28 to 38].
- Prof. Stastny (SKODA POWER) with co-workers studied effects of deposits on the blades of MP parts of steam turbine in fossil power station, measured degradation of steam turbine blade surfaces by deposits of chemicals, and compared numerical models of the water steam flow with hetero-homogeneous condensation in nozzles and in blade cascade, Refs [39 to 43].

- Dr.Kodl (SKODA POWER) prepared information on application of IAPWS data in calculation in SKODA, Ref.[44].

- 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. Following activities were carried out:
  - monitoring and evaluation of primary water chemistry and radiation situation at units 1 and 2 of the Temelín Nuclear Power Station, Refs [45,46]
  - investigation of fuel rod cladding materials (eg. Zircaloy-4 alloy, Zr-1%Nb alloy) corrosion behavior at specific VVER water chemistry conditions.
  - investigation of the effect of water chemistry on radionuclides transport and radioactivity build-up in the VVER reactor primary systems (e.g. effect of different levels of ammonia, hydrogen dosing).

Young Scientists IAPWS Fellowships

- T. Nemec, the fellowship holder of the 2003 Young Scientists IAPWS (CZ-US) Project *"Thermodynamics of Binary Homogeneous Nucleation in Superheated Steam "* under supervising Prof. Maršík, Dr. Hrubý, Dr. Palmer, and Dr. Simonson, submitted his PhD. thesis. Ref. [11]. His new publications are in Refs [8, 9, 11].

- O. Mican performs his Young Scientist IAPWS (CZ-US) Project "*Irreversible Thermodynamics of Fuel Cells Membrane Transport*" under supervising Prof. F. Marsik, and Prof. S. Lvov. The project is 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 of the Project will be finished by the end of the year 2006.
  Preliminary results he will present at the 2006 IAPWS Meeting. Ref. [10].

- Prof. J. Sedlbauer (CZ) and Prof. P. R. Tremaine (Canada) (WG PCAS) prepared a Proposal for Young Scientist IAPWS Project for J. Ehlerova "*Predictive Scheme for Standard Thermodynamic Properties of Aqueous Substituted Benzenes over a Wide Range of Temperatures and Pressures*". The project has 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.

The CZ NC PWS fully recommends this project to the EC IAPWS to support it.

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8 February 2005

IAPWS REPORT 2004 AND 2005

The research activities in 2004 and 2005 in Denmark in the field of properties of water and steam were mainly concentrated at the Technical University of Denmark, Copenhagen:
- Modelling of multicomponent aqueous electrolyte systems and application of models to the recycling process for fertilizer from straw ash residues.
- Measurements and modelling of density and viscosity of multicomponent aqueous electrolyte solutions are in progress. The aim is to predict the scaling in hydrogeological systems. Pressure parameters are added to the Extended UNIQUAC model presented by Thomsen and Rasmussen (1999). The improved model is used for correlation and prediction of solid-liquid equilibrium of scaling minerals ($CaSO_4$, $CaSO_4.2H_2O$, $BaSO_4$ and $SrSO_4$) at temperatures up to 300C and pressures up to 1000 bar. The results show, that the Extended UNIQUAC model with the proposed pressure parameters is able to represent binary, ternary and quaternary solubility data within the experimental accuracy in the temperature range from –20 to 300C, and the pressure range from 1 to 1000 bar.
- Modelling of ion exchange processes, particularly with focus on removal of vanadium from effluent waters.

The research at the utilities have concentrated on new methods for monitoring of carbon dioxide in water/steam cycle.

Publications:
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Karol Daucik, Solubility of Sodium Sulphate in Steam in the Vicinity of the Critical Point, 14. ICPWS, Kyoto, Japan, Aug 29 – Sept. 3, 2004.
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GERMAN NATIONAL COMMITTEE TO IAPWS

Research Activities on the Thermodynamic Properties of Water and Steam

Report "Research in Progress 2006"

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

1. Final preparation of the „Release of an Equation of State of Ice Ih“, expected to be issued by IAPWS in 2006
2. Publication of “A New Equation of State of Ice Ih” by R. Feistel and W. Wagner, in J. Phys. Chem. Ref. Data, 35, 2 (2006) 1021-1047
3. New correlation equations of the sublimation pressure and the sublimation enthalpy of ice Ih between 20 K and 273.16 K, paper by R. Feistel and W. Wagner, accepted at Geochimica et Cosmochimica Acta, 2006.
4. New correlation equations of the melting pressure and the melting enthalpy of ice Ih between 0.1 MPa and 210 MPa, unpublished, to be presented at the IAPWS meeting in Witney.
5. A “Gibbs-Pitzer Function for High-Salinity Seawater Thermodynamics” by R. Feistel and G. M. Marion, valid for –7 to 25°C, 0.1 to 100 MPa, 0 to 110 g/kg salinity, submitted to Progress in Oceanography in Dec 2005

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 $p(h,s)$ for regions 1 and 2 of IAPWS-IF97
   - The comprehensive article on the backward equations $p(h,s)$ appeared in the "Journal of Engineering for Gas Turbines and Power" in 2006.
2. Supplementary backward equations $T(p,h)$, $v(p,h)$, and $T(p,s)$, $v(p,s)$ for region 3 of IAPWS-IF97
   - The comprehensive article on the backward and boundary equations will appear in the "Journal of Engineering for Gas Turbines and Power" in September 2006.
3. Supplementary backward and boundary equations $p(h,s)$ for region 3 of IAPWS-IF97
   - The comprehensive article on the backward and boundary equations for the "Journal of Engineering for Gas Turbines and Power" was prepared.
4. Thermodynamic derivatives from IAPWS Formulations
   - The Advisory Note No. 3 was prepared.

5. Investigations on thermodynamic properties of humid air - part of the project "Advanced Adiabatic Compressed Air Energy Storage" (AA-CAES) of the European Union. –

   - Comparison calculations of different models for calculating thermodynamic properties of humid air were carried out.

6. Property libraries for water and steam, humid gases, and aqueous mixtures
   - The property library LibAmWa for Ammonia/Water mixtures was developed.
   - The Add-In FluidEXL for Excel® and the Add-On FluidMAT for Mathcad® were extended.
7. The download "Steam Tables on Pocket Calculators" were prepared for the IAPWS website.
8. The homepage www.iapws.de of the German National Committee of IAPWS was prepared.

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
   - Development of a new basic equation for region 5 of IAPWS-IF97 that covers a pressure range up to 50 MPa.
   - A draft revised release on IAPWS-IF97 was prepared.
2. Investigations of the current IAPWS equations for the heat conductivity
   - The differences between the industrial equation and the scientific equation for the heat conductivity were investigated.

CURRENT STATUS OF RESEARCH ACTIVITIES IN JAPAN
Submitted to the Executive Committee Meeting, IAPWS, Witney, U.K., September 2006

by

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

The Japanese National Committee to the IAPWS is countinuing to play an active function as the 139th Committee on Steam Properties chaired by Professor Koichi Watanabe, Keio University, at the Japan Society for the Promotion of Science (JSPS), Tokyo.

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

At the Division of Chemistry, Graduate School of Science, Hokkaido University, Sapporo, Prof. S. Ikawa and coworkers conducted spectroscopic measurements of water and water-hydrocarbon mixtures at high temperatures and pressures. Infrared absorption of binary mixtures of water with hexane and decane were measured at temperatures and pressures in the 473-648 K and 70-350 bar ranges, respectively, and the anomalous volumetric behavior of the aqueous mixtures in the vicinity of the critical region was discussed [J. Chem. Phys., **122**, 204506 (2005)]. Near-infrared and ultraviolet spectra of water-NaCl-benzene mixtures were measured in the 473-573 K and 100-400 bar range, and it has been found that addition of NaCl in the aqueous phase suppresses transfer of water into the benzene-rich phase. The salting-out constant for the water-NaCl-benzene system increased significantly with increasing temperature. These facts seem to be explained by ion-induced electrostriction of the aqueous phase [J. Chem. Phys., **123**, 214504 (2005)]. Molecular dynamics study of anomalous volumetric behavior of water-benzene mixtures in the vicinity of the critical region was performed also [J. Chem. Phys., **123**, 244507 (2005)].
[contact: Prof. 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 is promoting a 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)]. In order to evaluate

the effects of H_2O_2 on corrosive conditions, static and dynamic responses of stainless steel exposed to H_2O_2 and O_2 in high temperature pure water were evaluated by analyzing ECP (electrochemical corrosion potential), FDCI (frequency dependent complex impedance), APP (anodic polarization properties) and CER(contact electric resistance) data. At the same time, multilateral surface analyses were carried out to determine characteristics of oxide film on the specimens. The following points were experimentally confirmed. 1) H_2O_2 resulted in a much higher ECP than O_2 with the same level oxidant concentration. ECP of the specimens exposed to 100 ppb H_2O_2 was as high as ECP of specimens exposed to 10 ppb H_2O_2 and it was not affected by co-existing O_2. 2) The cathodic currents of the specimens exposed to H_2O_2 were determined by the H_2O_2 redox reaction, the anodic ones were determined mainly by H_2O_2 oxidation, and both were determined by $[H_2O_2]$. ECP was saturated against $[H_2O_2]$ and this resulted from the compensation of $[H_2O_2]$ dependences of anodic and cathodic currents. 3) Oxide layers were divided into inner and outer layers: Outer layers exposed to 100 ppb H_2O_2 consisted of larger corundum type hematite particles, while inner layers consisted of very fine Ni rich magnetite. Outer layers exposed to 200 ppb O_2 consisted of larger magnetite mixture particles, while inner layers consisted of fine Cr rich magnetite. 4) Particle density and size were changed by oxidant concentration. The average diameter of the particles decreased with $[O_2]$ and $[H_2O_2]$. A larger dissolution rate at higher $[H_2O_2]$ resulted in a thinner oxide film with smaller particles and larger hematite particles. 5) A sensor complex consisting of ECP and FDCI sensors was proposed as a $[H_2O_2]$ monitor in operating power plants. [Latest publication: (1) S. Uchida, "Latest Experience with Water Chemistry in Nuclear Power Plants in Japan", *Power Plant Chemistry*, 2006, 8 (5), (2) S. Uchida, T. Satoh, Y. Morishima, *et al.*, "Effects of Hydrogen Peroxide and Oxygen on Corrosion of Stainless Steel in High temperature water", *Proc. 12th Int. Conf. Environmental Degradation of Materials in Nuclear Power Systems – Water Reactors*, Snowbird, Aug. 15-18, 2001, TMS, (2005) (CD), (3) S. Uchida, T. Satoh, T. Miyazawa, *et al*., "Dissolution of Oxide Film on Stainless Steel Surface in High Temperature H_2O_2 Water", *Proc. Symp. Water Chemistry and Corrosion of Nuclear Power Plants in Asia, 2005,* 145, Gyeonhju, Korea, Oct. 11-13, Korean Atomic Energy Research Institute (2005) (CD)]
[contact: Prof. S. Uchida; E-mail: uchida.shunsuke@jaea.go.jp].

At the Graduate School o Environmental Studies, Tohoku University, Sendai, Profs. N. Yamasaki and H. Enomoto were retired in March 2006, but they are still active. Prof . N. Yamasaki was back to Kochi (his hometown) and he had established private company on science and technology on water. Prof N. Yamasaki keeps excellent research on use of dry steam for material and environmental processing, and he is conducting research project on refinement of asbestos. Profs. H. Ishida and K. Ioku, they are covering development of new material by hydrothermal treatment. They published excellent papers: porous hydroxyapatite with tailored crystal surface was prepared bythe hydrothermal method (K. Ioku et al., Key Eng. Mater., 284-286, (2005), 353-356). They also tried to prepare high performance bioceramics: novel

bioceramics of calcium phosphates composed of rod-shaped particles were prepared by the hydrothermal method (K. Ioku et al., J. Hard Tissue Biology, 14 (2005), 136-137). 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 field observation on hydrothermal reaction of geomaterials. (Hara and Tsuchita, Geofluids, 5 (2005),251-26; Batkhisg et al., Resource Geology ,55(2005), 1-8). We organized 3rd workshop of WATER DYNAMICS in 16-17th November 2005 in Sendai International Center, which focused on the role of water in Earth processes, Life science and Material and Energy Process Design. The workshop was unique objectives covering very wide range of water and steam properties and utilization. We are planning 4th workshop of WATER DYNAMICS in 7-8th November 2006 in Matsushima (sightseeing place close to Sendai and University campus). The web site of WATER DYNAMICS is the follows: http://geo.kankyo.tohoku.ac.jp/events/WD4/index.html. We can provide 1st and 2nd workshop proceedings, and proceedings of 3rd workshop was published as AIP (American Institute of Physics) conference series (vol. 833). [contact Prof. N. Tsuchiya; 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 and viscosity standards. Absolute density measurements of silicon crystals for a determination of the Avogadro constant by the x-ray crystal density (XRCD) method are being conducted in this section as an international project organized by the Comité International des Poids et Mesures (CIPM). This project is scheduled to continue 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 the Avogadro constant. 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]. The data from the NMIJ and PTB were used for finding the best set of fundamental physical constants most recently recommended by the CODATA Task Group on Fundamental Constants. In 2006, the uncertainty of the density measurement of 1 kg silicon spheres has been reduced down to 3.6×10^{-8}, being close to the final target of the uncertainty for replacing the kilogram Using the silicon crystals as a density standard, densities of standard liquids are calibrated by a magnetic suspension density meter developed at the NMIJ [N. Kuramoto, K. Fujii, and A. Waseda, "Accurate density measurements of reference liquids by a magnetic suspension balance," Metrologia, 2004, 41, S84-S94]. A relative standard uncertainty of 4×10^{-6} has been achieved in

the density measurement of organic liquids. A review article on the density standards is given in a paper [K. Fujii, "Present state of the solid and liquid density standards," Metrologia, 2004, 41, S1-S15]. 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]. Preliminary data on the falling velocity measurement are being obtained at the NMIJ. 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].

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. He tested the computing times of 43 IAPWS-IF97 equation programs and compared them with those of 66 reference programs on 7 modern PC environments. 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. For users who still require iterative routines for inverse equations to achieve very high numerical consistency, the backward equations give good initial guess for iteration process. IAPWS-IF97 is faster than the equations of IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use (IAPWS-95) by factors of 70 to 200. The results will be presented at the IAPWS annual meeting in 2006. [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 *in situ* Raman spectroscopy of solid sample, in order to understand corrosion of metals and steels in high temperature water up to 673 K. The Raman spectroscopy system enables continuous *in situ* observation for several hundred hours [J. Nucl. Sci. Technol., **43**, 675-680 (2006).]. They are also conducting immersion tests under several redox conditions in high temperature water at 623 K and 723 K, to evaluate stability of chromium oxide. The samples are Pt plates coated with

chromium oxide, which is artificially formed by metal organic chemical vapor deposition. After the immersion tests, weight loss and [contact: Dr. M. Domae; E-mail: domae@criepi.denken.or.jp]

At the Center for Multiscale Mechanics and Mechanical Systems, Keio University, Yokohama, Prof. M. UEMATSU and his group study the behavior of thermodynamic properties of aqueous mixtures by means of the PVT measurements, isobaric specific heat capacity measurements, and the critical parameter measurements. The UEMATSU group measures the PVT properties of aqueous ammonia mixtures in the temperature range from 350 K to 600 K at pressures up to 200 MPa by a metal-bellows variable volumometer. The preliminary results were presented at the ICCT-2006 held in Boulder, Colorado, USA by Dr. N. Sakoda. The Cp measurements of water + methanol 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. The results were also presented at the ICCT-2006 by I. Fujita. The calorimeter, principle, and results to confirm the reliability of the apparatus were described in Review of Scientific Instruments, 77-3 (2006) 035110. The apparatus for the critical parameter measurements by a metal-bellows variable volumometer with an optical cell is reconstructed in order to measure the critical properties of aqueous ammonia mixtures. We proposed a new method to determine the critical point by image analysis which is available on line 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, Dr. K. YASUOKA and his group are studying the molecular dynamics (MD) simulation to clarify the thermodynamic stability of structure-H clathrate hydrate by estimating the free energy difference. [Y. Okano and K. Yasuoka, *J. Chem. Phys.* **124**, 024510 (2006)] They adopt the MD simulation for the adosorption and desorption of ethanol molecules to liquid-vapor water surface. They reported the supercritical phenomena on the 2D of liquid-vapor water surface and the cluster near the surface. [Y. Andoh and K. Yasuoka, Langmuir, **21**, 10885-10894 (2005); Y. Andoh and K. Yasuoka, *J. Phys. Chem. B.*, in press.] They estimated the nucleation rate, critical nucleus, and formation free energy for the bubble nucleation process of water. The reported the phenomena of "Nanoscale Hydrophobic Interaction and Nanobubble Nucleation". [T. Koishi et al., *Phys. Rev. Lett*, **93**, 185701 (2004).; T. Koishi et al., 123, 204707 (2005).] [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 are measuring the *pVTx* properties of ammonia + water mixtures. They have already measured new 49 points of the *pVTx* properties of aqueous solutions of ammonia along four isochors in the range of temperatures from 295 K to 308 K, pressures

from 0.29 MPa to 17.17 MPa, densities from 818 kg/m^3 to 825 kg/m^3, and compositions from 0.5036 mol /mol to 0.5221 mol/mol. [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. This apparatus was designed based on results by another twin-cell type adiabatic calorimeter which had measured water + alcohol and hydrocarbon mixtures. The new one will measure liquid isochoric heat capacities of these mixtures for temperatures from 220 to 420 K and pressures to 30 MPa including super critical region. [contact: Prof. N. Kagawa; E-mail kagawa@nda.ac.jp]

At the Institute for Chemical Research, Kyoto University, Uji, Kyoto, Prof. M. NAKAHARA, Prof. N. MATUBAYASI, Dr. C. WAKAI, and their co-workers 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 hydration over a wide range of thermodynamic conditions ["A new high-temperature multinuclear-magnetic-resonance probe and the self-diffusion of light and heavy water in sub- and supercritical conditions", K. Yoshida, C. Wakai, N. Matubayasi, and M. Nakahara, J. Chem. Phys. 123, 164506 (10 pages) (2005)] and (2) the molecular mechanism of noncatalytic reactions in hydrothermal conditions. ["Hydrothermal Carbon-Carbon Bond Formation and Disproportionations of C1 Aldehydes: Formaldehyde and Formic Acid", S. Morooka, C. Wakai, N. Matubayasi, and M. Nakahara, J. Phys. Chem. A 109, 6610-6619 (2005)]. [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 studied the electric conductivities of tetraalkylammonium bromides (R4NBr) in liquid methanol along the liquid-vapor coexistence curve up to about 180 °C to examine the validity of the Hubbard-Onsager (HO) dielectric friction theory. The translational friction coefficients z of relatively small ions, Me4N+ and Et4N+, were remarkably smaller than the prediction of the HO theory at high densities and low temperatures. However, the negative deviation from the HO theory gradually disappears with decreasing density and increasing temperature. For relatively large ions, Pr4N+ and Bu4N+, the experimental friction coefficients lay in the validity range of the HO theory in all the conditions studied here [T. Hoshina, K. Tanaka, N.Tsuchihashi, K. Ibuki, and M. Ueno, J. Chem. Phys., 122, 104512 1-8 (2005)]. [Contact: Prof. M. Ueno; E-mail: mueno@mail.doshisha.ac.jp]

U.S. NATIONAL COMMITTEE TO IAPWS
2006 REPORT ON ACTIVITIES OF POTENTIAL INTEREST TO IAPWS

Communicated from Arizona State University, Tempe, AZ:

It is shown that the corresponding-states correlations exist for families of similar compounds between the reduced values of the infinite dilution solute – water direct correlation function integrals (DCFI) when plotted against water density over the density ranges 500-1000 $kg \cdot m^{-3}$. The value of DCFI for a solute is calculated from its partial molar volume and thermophysical properties of pure water. The reduced DCFI is defined as the ratio of the DCFI at some T and water density to its value at 298 K and atmospheric pressure. The following classes of aqueous solutes are separated: simple fluids (Ar, CH_4,…), nonpolar compounds (CO_2, C_2H_4, aliphatic hydrocarbons,…), polar organic and inorganic compounds, and compounds with chemically bonded water (water itself, H_3BO_3, aqueous silica, …). It is expected that neutral hydroxides of metals and nonmetals belong to the last class, and the partial molar volumes of these solutes in water at elevated T and P can be estimated using the proposed correlations.

Reference: Plyasunov A.V., Shock E.L., O'Connell J.P. (2006) Corresponding-states correlations for estimating partial molar volumes of nonelectrolytes at infinite dilution in water over extended temperature and pressure ranges. *Fluid Phase Equil.*, **247**, 18-31.

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

The Energy Institutes' Electrochemical Laboratory at Penn State University strives to be at the front edge of fundamental and applied research in a variety of electrochemical and materials science technologies. The Laboratory aims to promote and facilitate the use of electrochemical methods in the areas of science and technology related to traditional and renewable energy generation systems. We lead interdisciplinary studies on electrochemistry of high temperature aqueous systems in a variety of scientific areas including corrosion and protective coatings, proton exchange membrane and solid oxide fuel cells, thermochemical hydrogen production, etc. The main research directions and key publications in 2005-2006 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*, 2005, **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*", v. 5, A. Bard, M. Stratmann, and D. Macdonald, and Patrick Schmuki, Eds., 2006, Wiley-VCH); **(3) High-Temperature Surface Electrochemistry** (Lvov S.L., Chalkova E., Fedkin M. V., Komarneni S., and Wesolowski D. J., Surface Electrochemistry of Composite Materials for High-

Temperature PEM Fuel Cells, *ECS Transactions*, 2006, v. 1, p. 215-225); **(4) High-Temperature Proton Exchange Membrane Fuel Cells** (Chalkova E., Fedkin M. V., Wesolowski D. J., and Lvov S.L. Effect of TiO_2 Surface Properties on Performance of Nafion-Based Composite Membranes in High Temperature and Low Relative Humidity PEM Fuel Cells, *J. Electrochem. Soc.*, 2005, **152**, A1742-A1747, Chalkova E., Pague M.B., Fedkin M.V., Wesolowski D.J., and Lvov S.N. Nafion/TiO_2 Proton Conductive Composite Membranes for PEM Fuel Cells Operating at Elevated Temperature and Reduced Relative Humidity, *J. Electrochem. Soc,* 2005, **152**, A1035-A1040); **(5) High-Temperature Aqueous Corrosion** (Z.F. Zhou, E. Chalkova, S.N. Lvov, P. Chou, and R. Pathania, Development of a hydrothermal deposition process for applying zirconia coatings on BWR materials for IGSCC mitigation, *Corrosion Science*, 2006, in press).

Communicated from The University of Delaware, Newark, DE:

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

"Conductance of Aqueous Na_2SO_4, H_2SO_4, and their mixtures: Limiting Equivalent Ion Conductances, Dissociation Constants, and Speciation to 673K and 28 MPa," by Lubomir Hnedkovsky, Robert H. Wood, and Victor N. Balashov, *J. Phys. Chem. B*, 2005, 109, 9034-9046; "Conductance study of association in aqueous $CaCl_2$, $Ca(CH3COO)_2$, and $Ca(CH3COO)_2$.nCH3COOH from 348 to 523 K at 10 MPa," by Lucila P. Méndez De Leo and R. H. Wood, *J. Phys. Chem. B*, 2005, 109, 14243-14250; "Multiple ion association and sulfate ion mobility in aqueous Li_2SO_4 and K_2SO_4 from measurement of conductance at temperatures from 523 to 673K," by Victor N. Balashov, Andrei V. Sharygin, Robert H. Wood, Brian K. Grafton, and Caibin Xiao. Accepted *Geochim. Cosmochim. Acta*; "Structure of an accurate *ab initio* model of the aqueous Cl^- ion at high temperatures" By Haitao Dong, Wenbin Liu, Douglas J. Doren, and Robert Wood. Accepted *J. Phys. Chem*.

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

A collaboration is continuing with Richard Wheatley at the University of Nottingham, developing intermolecular pair potentials for aqueous systems for the quantitative calculation of second virial coefficients. This approach produces second virial coefficients that for the most part have smaller uncertainties than those obtained by experiment. Water with nitrogen has been completed, and preliminary results have been obtained for water with oxygen. Calculations for water with "air" based on a combination of these results look promising. A similar collaboration with the University of Delaware has produced similar results for water with methane.

References: Akin-Ojo, O., Harvey, A.H., and Szalewicz, K., 2006. "Calculations of the cross second virial coefficient with quantum corrections for the methane—water system using an *ab initio* potential energy surface," *J. Chem. Phys.* 125, 014314; Tulegenov, A.S., Wheatley, R.J., Hodges, M.P., and Harvey, A.H., 2006. "Intermolecular potential and second virial coefficient of the water—nitrogen complex," *J. Chem. Phys*., submitted.; Wheatley, R.J., and Harvey, A.H., 2006. "Intermolecular potential and second virial coefficient of the water—oxygen complex," *J. Chem. Phys*., in preparation; Harvey, A.H., and Huang, P.H., 2006. "First-Principles Calculations for Humidity Standards: The Air-Water Second Virial Coefficient," *Int. J. Thermophys.*, in preparation.

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.

Communicated from Oak Ridge National Laboratory, Oak Ridge, TN:

The solubilities of cupric and cuprous oxides were measured in water over the range 25 to 350 °C in the presence of various chemical agents (NaOH, NH_3, $B(OH)_3$, H_3PO_4, $(OHCH_2)_3CNH_2$, $(OHCH_2)_3CN(OHCH_2CH_3)_2$, HF_3CSO_3, HNO_3 and mixtures thereof) as a function of pH, and in steam to 400 °C as a function of pressure. Large discrepancies exist between the various experimental studies, especially at high temperatures for cuprous oxide, where the current solubilities are orders of magnitude lower. The solubilities of both oxides in water are highly pH dependent exhibiting unexpected changes in the speciation of dissolved copper with temperature, but are virtually pH independent in steam.