To: Professor F Marsik, Chairman of IAPWS
From: Dr R R Harries, Chairman of BIAPWS
Cc: Dr B Dooley, International Secretary, IAPWS

June 2005

A REVIEW OF THE CURRENT STATUS OF BIAPWS IN 2005

Overview

BIAPWS is a joint association within the United Kingdom and the Republic of Ireland. BIAPWS is in healthy position, both financially and with respect to active membership. It has twelve corporate sponsors, one member with academic links, five associate members who are in consultancy or are retired from the power generation industry and three corresponding members (two in academia and one in a professional institution).

BIAPWS has an active role in promoting research and disseminating information within appropriate industries and academic areas. This is achieved through organisation of seminars and workshops and through the BIAPWS Award for final year undergraduate students.

Membership

Since 2004 there has been an increase in corporate sponsors from nine to twelve. Each corporate sponsor is a full member of BIAPWS and the representation is split as follows:

Power generation companies (8 members),
Power plant manufacturer (1 member)
Power plant chemical instrumentation manufacturer (2 members).
Power plant related research and technical consultancy (1 member)

There are currently two further enquiries about membership from an additional power generation company and power plant research / technical support consultancy.

The academic support has reduced in the last few years. There is now 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 five 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.

It is inevitable, that 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. It has proved difficult to determine the level of academic research into topics of interest to BIAPWS / IAPWS, but there is a general feeling that little research of specific interest is currently being conducted within the UK.

All corporate sponsors are required to pay an annual membership fee as a condition of continued membership. These fees allow BIAPWS to pay its IAPWS dues, to fund a delegate to the annual IAPWS international meeting, to organise symposia and workshops within the UK and, more recently, to sponsor the BIAPWS award.

Education and Outreach

BIAPWS sees 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.

This is achieved by regular committee meetings, at which representatives from the major UK and Irish power generation companies can meet and exchange views in a neutral environment. They can also interact with equipment suppliers and with academic institutions.

The second area of education and outreach is the regular organisation of technical symposia. Eight symposia have been held since 1995, initially annually, but latterly at 18 month intervals. The major topic is linked to power plant steam and water chemistry, and BIAPWS provides the only UK and Irish national forum for a regular symposia on power plant chemistry. As such it achieves a very important function and has regularly attracted attendances of 80 people, including speakers and attendees from other European countries. These symposia are a very effective way of raising awareness of BIAPWS and IAPWS within the UK and Ireland.

Following the initiative, in May 2003, of combining workshop sessions with a technical symposia, the pattern was repeated in December 2004, when a one day symposium on Power Plant Chemistry was preceded by a half day workshop on related topics. The workshop was oversubscribed and the increased numbers produced a master class environment rather than a true interactive workshop.

Both the workshop and symposium were well attended with around 30 for the workshop and 75 for the symposium.

The third initiative has been the BIAPWS Award, started in 2002 and first awarded in 2003. Its aim is to raise the awareness of undergraduates about research and careers in areas and industries associated with the properties of water and steam. It offers a prize of £1000 ($1800US) for a dissertation based on a final year undergraduate project with suitable association to the aims, ideals and topic areas of IAPWS. Despite contact with a large number of Universities the response has been extremely disappointing. The single entry in 2004 was not awarded the prize, for lack of technical merit. In 2005 the response has been similarly disappointing, but entries have not yet been reviewed.

The BIAPWS Award has been discussed at recent committee meetings. The decision whether to reformulate it or abandon it has yet to be taken.

The future

- BIAPWS will aim to continue to expand its membership with appropriate companies and institutions.

- BIAPWS will seek to find further ways of bringing awareness of the topics of steam and water, its scientific properties and its technical applications and challenges to a wider audience.
- BIAPWS will host the 2006 IAPWS International meeting in September 3 – 8th, in Oxfordshire, England.

Richard Harries
Chairman, BIAPWS.

The Czech National Committee

International Association for the Properties of Water and Steam

REPORT on IAPWS related activities – August 2004 / July 2005

Submitted to the EC Meeting of IAPWS, Santorini, Greece – July 2005.

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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, Technicka 2, CZ-616 69 Brno

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

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

Application Engineering, SKODA POWER, s.r.o., 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, J. Sigmunda 79, CZ-783 50 Lutín

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

- Dr. Sifner (IT) prepared information about history of international cooperation in research of thermophysical properties of water and steam. Ref.[1] and an

information on “Formulations and Steam Tables“ for interested persons from industry (9 pgs).

- Mr. Klomfar issued Molliér h - s diagram of water and steam based on IAPWS - IF97. Diagrams p - h, and t - s are enclosed. Ref.[2]

- Prof. Mares (UWB) prepared an information about thermal conductivity of ordinary water. Ref.[3, 4].

- Prof. Mares (UWB) with collaborators prepared an information about surface tension of supercooled water. Ref.[5,6].

- Prof. Marsik (IT) with his research team carried out investigations into metastable state of water and steam, condensation, evaporation, and cavitation. Refs.[7 to 10].

- Prof. Sedlbauer (TUL) collaborated with Profs. Majer (France) and Wood (U.S.A.) and investigated thermodynamic properties of aqueous solutions, Refs. [11 to 16].

- Dr. Hruby (IT) performed tests in the shock tube for atmospheric nucleation studies, experimental studies of water/nonane droplet growth in pressurized methane, constructed an experimental apparatus for measurements of the surface tension in supercooled water, and developed theoretical model for thermodynamic bulk and surface properties of supercooled water. Refs. [17-19].

- The research activities at the CTU in Prague, Department of Fluid Mechanics and Power Engineering, Division of Power Engineering, have continued during the period 8/2004 – 7/2005 in the further improvement of current knowledge on the droplet nucleation in LP steam turbines:
  - ♦ Diagnostics of wet steam i.e. measurement of droplet size spectra and electrostatic charge of the droplets. The tests were carried out in the nozzle (C/D) and in the fossil (210 MW) and nuclear (1000 MW) LP steam turbines with combined optical extinction and charge probe. Refs. [20, 21].
  - ♦ 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 expansion chamber supplied both with laboratory and with power plant (210MW) steam. Ref. [22].
  - ♦ Improvement of computational model of the droplet nucleation in LP steam turbine employing both mentioned test data. Ref. [20].

  Advanced thermal cycles of gas and steam turbines:

- ♦ Mathematical model and thermodynamic analysis of the GT cycle (simple and regenerative) with wet compression i.e. with compressor interstage water injection. Ref. [23].
- ♦ Thermodynamic analysis of evaporative GT cycle (EvGT). Ref. [24].
- ♦ Thermodynamic analysis of hydrogen direct – fired Rankine steam cycle with isothermal HP steam turbine. Ref. [25].

The analysis of all considered cycles suggests considerable increase in thermal efficiency and specific output, thus supporting further development of these promising advanced concepts. In connection with these studies the extension of moist air and steam properties is highly recommended up to (10MPa, 1000°C) and (50 MPa, 1800÷2000°C), respectively.

- In SIGMA Research and Development Institute two types of problems were studied during the last period:

  - ♦ Erosion effects of cavitation bubbles on the blades of water pumps. Ref. [7]. The erosion driving forces were evaluated for multiple collapses of wide spectrum of cavitation bubbles. The effects of flow rate fluctuations as well as the influence of blade surface changes on bubble collapses. Ref. [10].

  - ♦ The problem of head-drop and efficiency-drop of water pumps due to bubble cloud creation inside impeller passages have been studied using means of CFD and then compared with experimental data obtained in SIGMA Research and Development Institute Refs. [26, 27].

- Dr. Jiricek (ICT-IE) with collaborators investigated corrosion processes and chemical effects in water systems of power plants. ICT-IE organized the 5th International Power Cycle Conference (CHEO 5), September 1-3, 2004. Ref.[28 to 54].
- Dr. Hnedkovsky (ICT-IPC) with collaborators investigated properties of organic solutes in water. Published articles are under Refs [55 to 69].
- Prof. Stastny (SKODA ENERGO) with co-workers studied effects of deposits on the blades in LP part of steam turbine in fossil power plant by chemical analysis; measured degradation of steam turbine blade surfaces by deposits of chemicals; compared numerical models of the steam flow with hetero-homogeneous condensation in nozzles with experiments, and tested numerical model of the steam flow in nozzles with binary nucleation. Refs [70 to 72].
- Zmitko (NRI) collaborated with the nuclear power plants mainly in the fields of water chemistry, corrosion problems and radiation control. Following activities were carried out :

- investigation of fuel rod cladding materials (e.g. Zircaloy-4 alloy, Zr-1%Nb alloy) corrosion behavior at specific VVER water chemistry conditions, Refs [73, 74]
- 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), Ref. [75]
- investigation of the effect of water chemistry, stress level and irradiation on irradiation assisted stress corrosion cracking (IASCC) of reactor pressure vessel and in-core structures materials, Refs. [73 to 75]
- monitoring and evaluation of primary water chemistry and radiation situation at units 1 and 2 of the Temelín Nuclear Power Plant, Ref. [76]
- data processing technologies and system for diagnostics for water chemistry and corrosion control in Nuclear Power Plants (DAWAC), Ref. [77].

Young Scientists IAPWS Fellowships:

O. Mican submitted his Proposal for Young Scientist IAPWS 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.

The CZ NC PWS fully recommends this project to the EC IAPWS to support it. The proposal with attached Curriculum Vitae of Mr.O.Mican is in Appendix 1.

- **Nomination for 2005 Honorary Fellow of the IAPWS**

  The US NC IAPWS, CZ NC PWS, and Mr. Ingo Weber collaborated in preparation of the proposal to nomination Dr. Bert Rukes for 2005 Honorary Fellow of the IAPWS.

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German National Committee to IAPWS

Research Activities on the Thermodynamic Properties of Water and Steam
Report "Research in Progress 2005"

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) will appear in the "Journal of Engineering for Gas Turbines and Power" in 2005.

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 was prepared and submitted to the "Journal of Engineering for Gas Turbines and Power".
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" is being prepared.
4. Supplementary backward equations v(p,T) for region 3 of IAPWS-IF97
   - The evaluation of the "Supplementary Release on Backward Equations for Specific Volume as a Function of Pressure and Temperature v(p,T) for region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" was supported.
5. Thermodynamic differential quotients of the Scientific Formulation IAPWS-95 and the Industrial Formulation IAPWS-IF97 for Water and Steam
   - The Proposal for a guideline was prepared.
6. Investigations on thermodynamic properties of humid air - part of the project "Advanced Adiabatic Compressed Air Energy Storage" (AA-CAES) of the European Union
   - The property data base for humid air was completed.
   - Comparison calculations of different models for calculating thermodynamic properties of humid air were carried out.
7. Property libraries for water and steam, humid gases, and aqueous mixtures
   - The property library LibWaLi for water/lithium bromide mixtures was developed.
   - The Add-Ins
     FluidEXL for Excel®
     FluidMAT for Mathcad®
     were extended .
8. Implementation of the industrial formulation IAPWS-IF97 on pocket calculators

- The program FluidTI for the model TI 84 of Texas Instruments was prepared.

The Hellenic National Committee
International Association for the Properties of Water and Steam

REPORT on IAPWS related activities

On the 15th of June 2005, the Greek National IAPWS Committee (GIAPWS) was officially formed by the Hellenic Association of Chemical Engineers, as

Head	Prof. Marc J. Assael	Chemical Engineering Department Aristotle University of Thessaloniki (assael@auth.gr)
Members	Mr Nikos Karnabos	Hellenic Petroleum SA
	Mrs Argyro Kastanaki	Head of Environmental & Chemical Technology Department Division of Power Generation Exploitation Public Power Corporation (rkastan@otenet.gr)
	Mr Panagiotis Tsiambas	Head of Environmental & Chemical Technology Department Megapolis S.E.S., Public Power Corporation (pitsiamp@aias.gr)
	Mr Dimitris Sotiropoulos	Head of Environmental & Chemical Technology Department Agios Dimitrios S.E.S., Public Power Corporation

The first task of GIAPWS was the organization of the Seminar “Applied Water Treatment Processes for Power Plant Cycles” which successfully took place in the 2005 IAPWS Meeting, July 3-8, in Santorini island.

The Head of GIAPWS was responsible for the organization of the 2005 July 3 - 8 IAPWS Meeting in Santorini island in Greece.

Research carried out by GIAPWS during this year, involved

- the completion of the new Viscosity correlation for water. The correlation will be submitted for approval and send to the evaluation group.
- At the same time work for a new correlation for the Thermal Conductivity of water started.

Work on the Chapters of Viscosity and Thermal Conductivity of Aqueous Solutions at high Temperatures and High Pressures has progressed (book edited by V. Valyashko)

The www site of GIAPWS will soon be available in the internet.

It is expected that with the involvement of Greek Public Power Corporation, new areas of research will be activated.

Current Status of Research Activities in Japan
Submitted to the Executive Committee Meeting, IAPWS, Santorini, Greece, July 2005

by

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

The Japanese National Committee to the IAPWS is playing an active function as the 139th Committee on Steam Properties chaired by Professor Koichi Watanabe, Keio University, at the Japan Society for the Promotion of Science (JSPS), Tokyo. The Committee is pleased to report that the 14th ICPWS held in Kyoto from August 29 through September 3, 2004 was a great success with 267 participants from 19 countries. The Proceedings of the 14th ICPWS, entitled "Water, Steam, and Aqueous Solutions for Electric Power" (Editors: Masaru Nakahara, Nobuyuki Matumayasi, Masakatsu Ueno, Kenji Yasuoka and Koichi Watanabe, ISBN4-621-07596-9, 770 pp with CD-ROM) was pubblished from Maruzen Publishing, Co., Ltd., Tokyo in March, 2005. Those who wish to purchase any extra copies of the Proceedings are kindly requested to contact Dr. Kenji Yasuoka, one of the editors and the Secretary of the Japanese National Committee for the IAPWS (Assoc. Prof. Kenji Yasuoka, Dept. of Mechanical Engineering, Keio University, 3-14-1, Hiyoshi, Yokohama 223-8522, Japan; phone: +81-45-566-1523, fax: +81-45-566-1495, e-mail: yasuoka@mech.keio.ac.jp). It should be noted that full papers included in the Proceedings of the 14th ICPWS are now downloadable by accessing to the home page of our National Committee (http://www.iapws.jp).

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

At the Division of Chemistry, Graduate School of Science, Hokkaido University, Sapporo, Prof. S. IKAWA and coworkers are engaged in spectroscopic measurements of water and water-hydrocarbon mixtures at high temperatures and pressures. From near-infrared and ultraviolet measurements of water-benzene mixtures in the 373-673 K and 50-400 bar ranges, mutual solubilities were obtained. It has been found that the solubility of benzene in water is an order of magnitude smaller than that of water in benzene throughout the two-phase region, and the effect of pressure on solubilities is opposite between water in benzene and benzene in water. These solubility properties were discussed on the basis of a cavity-based solvation model [*J. Chem. Phys*., **122**, 024509 (2005)]. In collaboration with Drs. VIGASIN and PAVLYUCHKO, analyses of infrared and near-infrared band shapes of steam at high temperatures and pressures were performed and a state of molecular aggregation in the steam was discussed [*J. Mol. Struct*., 742, 173 (2005)].
[contact: Prof. S. Ikawa; E-mail: sikawa@sci.hokudai.ac.jp].

Prof. S. UCHIDA, who promoted a second phase of the project on water chemistry of BWR at the Department of Quantum Science and Energy Engineering, Graduate School of Engineering, Tohoku University, Sendai, has moved form Tohoku University to Japan Atomic Energy research Institute. The

effects of hydrogen peroxide on corrosion and IGSCC of stainless steel in high temperature pure water have been examined by using the high temperature high pressure hydrogen peroxide water loops with controlled hydrogen peroxide concentrations and lower possible oxygen concentrations at JAERI. By changing concentrations of H_2O_2 and O_2, in situ measurements of electrochemical corrosion potential (ECP) and frequency dependent complex impedance (FDCI) of test specimens were carried out and then characteristics of oxide film on the specimens were determined by multilateral surface analyses, i.e., laser Raman spectroscopy (LRS), scanning electron microscope (SEM-EDX), secondary ion mass spectroscopy (SIMS), and scanning transmission electron microscope (STEM-EDX) (XPS). As a result of experiments, the following points were confirmed. 1) The ECP and FDCI data of the specimens exposed to 100 ppb H_2O_2 were not affected by co-existing O_2 with the same level oxidant concentration and they were also not affected by pre-exposure to 200 ppb O_2. From the viewpoint of ECP, this meant that corrosive conditions of hydrogen water chemistry were the same as those of normal water chemistry. 2) Combination of ECP and FDCI sensors might be a hopeful candidate to determine the corrosive conditions in the BWR primary coolant at elevated temperature.
3) The hematite ratio in the oxide films of the specimens exposed to H_2O_2 was expressed as a logarithmic function of $[H_2O_2]$. The hematite ratio was measurable for 8 ppm O_2, but negligibly small for 200 ppb O_2.
4) H_2O_2 exposure led to thicker oxide layers than O_2 exposure and Cr depletion did. The oxide film thickness first increased as $[H_2O_2]$ decreased from 100 ppb to 10 ppb and then it decreased. [Latest publication: (1) N. Yamashiro, et al., *J. Nucl. Sci. Technol.*, **41**, (2004), 890-897, (2) S. Uchida,et al., *J. Nucl. Sci. Technol.*, **41**, (2004), 898-906, (3) J. Sugama, et al., *J. Nucl. Sci. Technol.*, **41**, (2004), 880-889, (4) S. Uchida, et al., *J. Nucl. Sci. Technol.*, **41**, (2005), 66-74 (5) T. Miyazawa, et al., *J. Nucl. Sci. Technol.*, **41**, (2005), 233 241, (6) S. Uchida, et al., Water, Steam and Aqueous Solutions for Electric Power – Advances in Science and Technology, 551, Maruzen Co. Ltd. (2005) , (7) T. Satoh, et al., Water, Steam and Aqueous Solutions for Electric Power – Advances in Science and Technology, 561, Maruzen Co. Ltd. (2005)]

At the Graduate School o Environmental Studies, Tohoku University, Sendai, Profs. N. YAMASAKI, H. ENOMOTO, K. TOHJI, H. ISHIDA, N. TSUCHIYA, and their group are covering wide field related to hydrothermal Material Science, Geofluid Science (Earth Science). Material research group developed several kinds of advanced and functional materials such as synthetic diamond, stratified materials on carbon nano-tube using hydrothermal process (Y. Sato et al., Chemical Physics Letters, 385, (2004), 323-328), and the liquefaction and gasification of heavy oil, the SCWO of rice husk for production of sodium acetate (ICPWS, (2004), 85, 186), the separation and extraction of useful materials from bio-mass using superheated steam, and the formation of organic materials by the hydrothermal reduction of carbon dioxide (N. Yamasaki et al., Material Science Letters, 58, (2004), 768-771). Geofluid science research group is conducting water-rock interaction under sub- and supercritical condition, including multi-phase and multi-component solutions. (G. Bignall et al., GEOTHERMICS, 33, (2004), 615-635), (Sekine et al., GEOTHERMICS, 33, (2004), 775-793). They organized 1st and 2nd international workshop on WATER DYNAMICS (1st workshop:17-19th March 2004, 2nd workshop: 11-12th November, 2004), which focused on the role of water in Earth processes, Life science and Material design. The workshop was unique objectives covering very wide range of water and steam properties and utilization. They are planning 3rd workshop of WATER DYNAMICS in 16-17th November 2005 in Sendai International Center. They can provide 1st and 2nd workshop proceedings, please contact N. Tsuchiya (chair of program committee of WATER DYNAMICS)
[contact Prof. N. Tsuchiya; tsuchiya@mail.kankyo.tohoku.ac.jp]

At the Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Prof. T. ADSCHIRI and his group are developing a new hybrid nanomaterial from organic, inorganic and bio materials at various reaction conditions. For organic/inorganic nanomaterials, the supercritical hydrothermal synthesis of nanoparticles they invented is advanced, so that metal oxide nanoparticles with a organic monolayer is synthesized in a homogeneous phase of hydrophilic and hydrophobic fluids under the sub/supercritical condition (Tahereh et al. submitted). Hydrophilic or hydrophobic nature of the nanoparticles can be controlled by the organic modification on the surface of the particles, which paves a way to various applications of nanoparticles for materials, electronics, and life science. At room temperature, his group has synthesized ZnO nanoparticles using a peptide with affinity for ZnO (Umetsu et al. submitted). To our knowledge, there have been no reports for room-temperature

synthesis of ZnO nanoparticles. The peptide can also assist in the homogeneous assembly of the ZnO nanoparticles into unique flower-like morphologies. Adschiri's group shows the potential of peptide for fabrication of unique structure. The techniques of patterning and synthesizing ZnO at room temperature are potentially useful for the orientation of ZnO in or on heat-labile or pH-sensitive organic compounds. [contact: Prof. T. Adschiri; e-mail: ajiri@tagen.tohoku.ac.jp]

At the Material Properties and Metrological Statistics Division, National Metrology Institute of Japan (NMIJ, formerly NRLM), National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, 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, CSIRO, 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. 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 used for calibrating the vibrating-tube densimeters. 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. Nano-technologies 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," Water, Steam and Aqueous Solutions for Electric Power – Advances in Science and Technology, 112, Maruzen Co. Ltd. (2005)]. 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. A new density-of-water table having a specified isotopic abundance was recommended by the WG-Density and endorsed by the CCM and CIPM [M. Tanaka, G. Gerard, R. Davis, A. Peuto, and N. Bignel, "Recommended table for the density of water between 0 °C and 40 °C based on recent experimental reports," Metrologia, 2001, 38, 301-309]. This new table is recommended as a metrological standard for the density of SMOW. In April 2005, WG-density and CCM meetings were held at the BIPM (Bureau International des Poids et Mésures), where the CCM and IAPWS standards for the density of water were discussed for clarifying their roles, and publishing the clarification in a form of cooperation with the IAPWS was agreed and approved at the meetings. [contact: Dr. K. Fujii, Chief, Fluid Properties Section, NMIJ; E-mail: fujii.kenichi@aist.go.jp].

At the Dept. of Environmental Science & Technology, Faculty of Engineering, Shinshu University, Nagano City, Prof. H. TAKAKU works since Feb. of 2000, and previously worked at Central Research Institute of Electric Power Industry (CRIEPI) in Japan. In the simulated geothermal waters containing the corrosive chemicals such as chlorides, sulfides and others, he and coworkers are studying the corrosion of the steam turbine materials for geothermal power plants and also the corrosion of the Ti-Ni base shape memory alloys for the heat engine actuators. They are also studying on the corrosion behavior of materials for the heat exchanger, and boiler and steam turbine of conventional fossil power plants. [Latest publications: [1] M. Kurashina, H. Takaku, et al, On-line Analysis of ETA and Organic Acids in Secondary Systems of PWR Plants, *Power Plant Chemistry*, **7** (4), p.219, 2005. [2] M. Hirano, H. Takaku, et al, Accelerated Corrosion Behavior due to Alternating Dry-Wet Conditions for LP Steam Turbine Materials of Fossil Power Plants, *ISIJ International*, **45** (3), p.373, 2005. [3] M. Hirano, H. Takaku, et al,

Corrosion Behavior of Boiler Materials during Long-Term Lay-up of a Fossil Unit, *Power Plant Chemistry*, **7** (1), p.16, 2005. [4] H. Takaku, Y. Sakai, et al, Corrosion Behavior of Steam Turbine Materials for Geothermal Power Plants, *Proc. of the 14th International Conference on the Properties of Water and Steam*, p.718, 2004] [Contact: Prof. H. Takaku; E-mail: takakuh@gipwc.shinshu-u.ac.jp]

Mr. K. MIYAGAWA investigated 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 those times. The aim of the investigation was to compare them on the common and state-of-the-art platforms. The test results showed that the today's platforms were more favorable for IAPWS-IF97 than for the previous industrial formulation IFC-67. Test results also showed that the "backward" equations of IAPWS-IF97 were much faster then those of iterative processes to solve inverse equations. The results will be presented at the IAPWS annual meeting in 2005. [contact: Mr. K. Miyagawa; E-mail: miyagawa.kiyoshi@nifty.com]

At the Department of Mechanical Sciences and Engineering, Tokyo Institute of Technology, Tokyo, Prof. A. SAITO, Assoc. Prof. S.OKAWA and their group are studying the effect of various properties of solid surface on nucleation of supercooled water using Molecular Dynamics Method, [See Int. J. of Refrigeration to be published and 14th Int. Conf. on the Properties of Water and Steam, Aug. 29 - Sep. 3, 690-695, (2004).]. They are also studying the effect of loading on fluid permeability and porosity of ice/water mixture, [See IIR Int. Conf. Vicenza (Italy) 2005 to be presented] and the effects of shapes of electrodes on freezing of supercooled water in electric freeze control [See Int. J. of Refrigeration, 28, 389-395, (2005)]. [contact: Dr. S. Okawa; E-mail: sokawa@mech.titech.ac.jp]

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, in order to understand corrosion of metals and steels in high temperature water up to 673 K. In air-saturated water at 673 K and 25 MPa, a unique Raman spectrum was observed for a pure titanium sample. They started immersion tests in high temperature water, using metals and steels on which corrosion-resistant metal oxides were coated. [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 are measuring the PVT properties of aqueous ammonia mixtures in the range of temperatures from 350 K to 650 K at pressures to 200 MPa. Isobaric specific heat capacities of water + methanol mixtures are being measured for temperatures from 250 K to 400 K at pressures to 20 MPa. The calorimeter was reported at the 14th ICPWS held in Kyoto, 2004. [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, Proceeding of the Fifth International Conference on Gas Hydrates (ICGH 2005), Trondheim, Norway, June 2005.] 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. [Y. Andoh and K. Yasuoka, Water, Steam and Aqueous Solutions for Electric Power – Advances in Science and Technology, 144, Maruzen Co. Ltd. (2005)] They also evaluated the water model contained in HIV-1 Protease.[T. Aramaki et al., Water, Steam and Aqueous Solutions for Electric Power – Advances in Science and Technology, 208, Maruzen Co. Ltd. (2005)] 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).] [contact: Dr. K. Yasuoka; E-mail: yasuoka@mech.keio.ac.jp].

At the Department of Mechanical Engineering, Kanagawa Institute of Technology, Atsugi, Prof. K. OGUCHI and his group are continuing to measure the *PVTx* properties of ammonia + water mixtures. They have measured the *PVTx* properties of aqueous dilute solutions of ammonia in the range of temperatures from 265 K to 305 K, pressures up to 16 MPa, densities from 975 kg□m^{-3} to 989 kg□m^{-3}, and compositions up to 0.10 mole fraction of ammonia including pure water, focusing their attentions on the maximum density phenomena, and also in the range of temperatures from 298 K to 309 K, pressures up to 15.6 MPa, densities from 810 kg□m^{-3} to 823 kg□m^{-3}, and compositions up to 0.5133 mole fraction and 0.5357 mole fraction of ammonia. Some of their results were presented at the 14th ICPWS. [contact: Prof. K. Oguchi; E-mail: oguchi@kait.jp].

At the Department of Mechanical Systems Engineering, National Defense Academy, Yokosuka, Prof N. KAGAWA and his group have constructed a twin-cell type adiabatic calorimeter for water + alcohol mixtures. Isochoric heat capacities (c_v) of water, methanol, ethanol, 1-propanol and their aqueous solutions were measured for temperatures from 280 to 420 K and pressures to 30 MPa. Liquid density information was also obtained on the basis of the sample mass and the volume of the calorimetric cell. The experimental results and a theoretical approach to the anomalous behavior of c_v data for the water + alcohol mixtures were presented at the 14th ICPWS. [H. Kitajima, N. Kagawa, and H. Endo, Water, Steam, and Aqueous Solutions for Electric Power -Advanced in Science and Technology-, 107-111 (2005)] [contact: Prof. N. Kagawa; E-mail kagawa@nda.ac.jp]

At the Department of Computational Molecular Science, Institute for Molecular Science, Prof. S. OKAZAKI and his group study quantum-classical molecular dynamics calculation for vibrational relaxation of solute in supercritical fluid of non-polar molecule and in supercritical water. They are interested in understanding relaxation machanism in the supercritical fluids in terms of the isolated binary collision model popularly used to describe the relaxation in gas phase. [see: M. Sato and S. Okazaki, J. Chem. Phys., (2005), in press and M. Sato and S. Okazaki, J. Chem. Phys., (2005), in press]. [contact: Prof. S. Okazaki; E-mail: okazaki@ims.ac.jp].

At the Department of Applied Chemistry, Ritsumeikan University, Shiga, Prof. S. SAWAMURA studies the solubility of hydrophobic compounds and amino acids under high pressure up to 400 MPa and the visicosity of H_2O and D_2O in the high-pressure and low-temperature region. [See: Seiji Sawamura, AIP Conf. Proc. (Amer. Inst. Phys.) 716, 175-182 (2004)]. At the same department, Prof. Y. TANIGUCHI and Prof. M. KATO are measuring the infrared, Raman, and NMR spectra for biological compounds at high pressures. (contact: Prof. Sawamura, S.; sawamura@se.ritsumei.ac.jp).

At the Institute for Chemical Research, Kyoto University, Uji, Kyoto, Prof. M. NAKAHARA, Prof. N. MATUBAYASI, Dr. C. WAKAI, and their coworkers study the structure, dynamics, and reactions in super- and subcritical water by means of multinuclear NMR (nuclear magnetic resonance) spectroscopy, computer simulation, and Raman spectroscopy. Their current focus are (1) the thermodynamics, structure, and dynamics of aqueous solutions over a wide range of thermodynamic conditions ["A quantum chemical approach to the free energy calculations in condensed systems: The QM/MM method combined with the theory of energy representation", H. Takahashi, N. Matubayasi, M. Nakahara, and T. Nitta, *J. Chem. Phys.* **121**, 3989-3999 (2004)] and (2) the molecular mechanism of noncatalytic reactions in hydrothermal conditions. ["NMR Spectroscopic Evidence for an Intermediate of Formic Acid in the Water-Gas-Shift Reaction", K. Yoshida, C. Wakai, N. Matubayasi, and M. Nakahara, *J. Phys. Chem. A* **108**, 7479-7482 (2004)]. [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 KBr and KI in liquid methanol along the liquid-vapor coexistence curve up to the critical temperature to examine the validity of the Hubbard-Onsager dielectric friction theory. The translational friction coefficients ζ of the halide ions (Cl^-, Br^-, I^-) in methanol were well reproduced by the HO theory at the density $\rho > 2.0\rho_c$, where $\rho_c = 0.2756$ g cm^{-3} is the critical density of methanol, compared with those in water [T. Hoshina, K. Tanaka, N.Tsuchihashi, K. Ibuki, and M. Ueno, J. Chem. Phys., **121**, 9517-9525 (2004)]. They have also measured the NMR spin-lattice relaxation times of ^2H of the deuterided solvents (CDCl, C_6D_6, and C_6D_{12})

at various temperatures under atmospheric pressure, and determined the NMR *B* coefficients of the solutes (Me_4Si, Et_4Si, Pr_4Sn, Bu_4Sn, and Pen_4Sn) to study the solvent motions in dilute nonaqueous solutions. It has been found that the local effect on the rotation of solvent molecules in nonaqueous nonelectrolyte solutions is much smaller than that in aqueous solutions [K. Yoshida, N. Tsuchihashi, K. Ibuki, and M. Ueno, J. Mol. Liq., **119**, 67-75 (2005)]. Theories for diffusion-controlled reaction dynamics based on the diffusion equation and the Fokker-Planck-Kramers equation have also been reviewed, and the validity of the theories has been examined in the picosecond time region by comparing them with computer simulations in liquid Ar [K. Ibuki and M. Ueno, Rev. High Press. Sci. Tech., **14**, 20-29 (2004)]. [Contact: Prof. M. Ueno; E-mail: mueno@mail.doshisha.ac.jp]

At the Thermofluid Physics Laboratory, Deaprtment of Mechanical Engineering Science, Kyushu University, Fukuoka, Prof. Emeritus T. ITO and Prof. Y. TAKATA have released the 12.1 version of the Computer Program Package for Thermophysical Properties of Fluids, PROPATH. Its new version is now under developement and will be released new future. This software consists of 5 subsets. Four programs for light water substances with different formulations and for heavy water substance are available. By using E-PROPATH, one of 5 subsets, one can calculate properties as functions of MS-EXCEL software.
[contact: Prof. Y. Takata; E-mail: takata@mech.kyushu-u.ac.jp
or http://gibbs.mech.kyushu-u.ac.jp/propath/index.html]

At Toshiba Corporation, Isogo Engineering Center, Dr. NARABAYASHI and his coworkers are developing steam injector (SI) system with Dr. MORI and Dr. OHMORI, R&D Center, Tokyo Electric Power Company. SI is a simple, compact and passive pump and also acts as a high-performance direct-contact compact heater. This provides SI with capability to serve also as a direct-contact feedwater heater that heats up feedwater by using extracted steam from the turbine. To develop high performance compact feedwater heater, it is necessary to quantify the characteristics between physical properties of the flow field. Its performance depends on the phenomena of steam condensation onto the water jet surface and heat transfer in the water jet due to turbulence on to the phase-interface. The analysis was conducted by using CFD code embedded separate two-phase flow models and confirmed that the steam has a high-performance direct-contact heater that was suitable for compact feedwater heater. As it is compact equipment, SI is expected to bring about great simplification and materials-saving effects, while its simple structure ensures high reliability of its operation, thereby greatly contributing to the simplification of the power plant by replacing all low-pressure feedwater heaters with the four-stage SI system, having steam extraction pressures equal to those for the existing ABWR system. In a recent paper, development of SI system for simplified nuclear power plant has been reported [13th International Conference on Nuclear Engineering, May 16-20, 2005, Beijing, China] and it was awarded by JSME (Japanese Society of Mechanical Engineering). [Contact: Dr. Narabayashi, tadashi.narabayashi@toshiba.co.jp]

Report of Russian National Committee (2004-2005)

List of Publications

1. L.G. Vasina, V.L. Menshikova, L.s. Krylova, and A.V.Evsyutin, “Effect of Coagulant Base Index and Water Stability in Selection of Optimum Coagulation Mode,” Proceedings of the International Conference on Water Treatment “Tekhnovod-2004”, Novocherkassk, Russia, 2004, pp. 136-140.

2. A.V. Boglovsky, Yu.V. Balaban-Irmenin, L.G. Vasina, and A.M. Rubashov, “ Regularities of Scale Formation in Hot Water Equipment of Heat Supply Systems,” Energosberezhenie I Vodopodgotovka, 2004, No. 3, pp. 10-16.

3. A.S. Sedlov, A.V. Boglovsky, K.A. Dunin, and A.A. Zonov, “ Corrosion of Steel at Operating Conditions of Evaporation Units,” Energosberezhenie I Vodopodgotovka, 2004, No. 1, pp. 86-88.

4. T.I. Petrova and A.V. Furunzhieva, “Use of Helamin and Fossil Power Plants with Drum-Type Boilers,” Energosberezhenie I Vodopodgotovka, 2004, No. 1, pp. 3-9.

5. T.I. Petrova, S. Vidojkovic, A.A. Zonov, and A.Y. Petrov, “Effect of Acetic Acid on the Contamination of Saturated Steam by Sulfates and Fluorides,” Thermal Engineering, 2004, vol. 51, No. 7, pp. 526-529.
6. D.S. Smetanin, “Evaluation of Water Chemistry Condition at Power Plants with Water Chemistry Quality Index,” Novoye v Elektroenergetike, 2004, No. 12.

7. T.I. Petrova, O.A. Povarov, V.N. Semenov, V.I. Kashinsky, A.N. Troitsky, A.Y. Petrov, R.B. Dooley, “Effect of Cycle Chemistry on Corrosion Processes in Steam Turbines,” Paper presented at the 14th ICPWS, August 29 – September 03, 2004, Kyoto, Japan.

8. T.I. Petrova and A.V. Furunzhieva, “The Influence of Acetic Acid on Mass Transfer of Copper Corrosion Products in Power Plant Cycle,” Paper presented at the 14th ICPWS, August 29 – September 03, 2004, Kyoto, Japan.

U.S. National Committee to IAPWS
2005 Report on Activities of Potential Interest to IAPWS

Communicated from Arizona State University, Tempe, AZ:

- Group concentrated its efforts on evaluation of properites of aqueous organic compounds at 298 K, 0.1 MPa and on development of predictive group contribution schemes. This information is expected to be important for many applications dealing with organic compounds in water, so it may be of interest for IAPWS as well. One of the recent projects concerns the development of methods to estimate activity coefficients of organic compounds in water at room termperatures in the framework of the Savage-Wood model. Several publications, including

Plyasunov A.V. and Shock, E.L. Prediction of the Krichevskii parameter for volatile nonelectrolytes in water. Fluid Phase Equil., **222-223C,** 19 (2004)

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

- *High Temperature Thermodynamics of Aqueous Solutions*

1. Bandura A. V., and Lvov S.N. The Ionization Constant of Water over Wide Ranges of Temperature and Density, *J. Phys. Chem. Ref. Data*, **34**, 2005, (in press).

- *High Temperature Aqueous Electrochemistry*

1. Lvov S.N. and Palmer D.A., Electrochemical Studies of High-Temperature Aqueous Systems, Chapter 11, in "*The Physical and Chemical Properties of Aqueous Systems at Elevated Temperatures and Pressures: Water, Steam and Hydrothermal Solutions*" (D.A. Palmer, R. Fernandez-Prini and A.H. Harvey, Eds.), 2004, Wiley, p. 377-408.

2. Zhou Z.-F., Lvov S.N., Thakur S., Zhou X., Chou P., and Pathania R. Hydrothermal Deposition of Zirconia Coating on BWR Materials for IGSCC Protection. In Proceedings of "International Water Chemistry Conference", San Francisco, October 2004, p. 602-624.

3. Lvov S.N., Zhou X.Y., Ulyanov S.M., Zhou Z.F., Papangelakis V.G., and Jankovic Z.D. In-situ pH Monitoring of High Concentration Acidified Geothermal Brines and Acidic Sulphate Solutions at Elevated Temperatures, In Proceedings of The Pressure Hydrometallurgy 2004 Conference, Canadian Institute of Mining, Montréal, Quebec, 2004, p. 561-576.

4. Lvov S.N. Electrochemistry of High Temperature Subcritical and Supercritical Aqueous Systems, Volume 5 (D.D. Macdonald, Vol. Ed.), in "*Encyclopedia of Electrochemistry*" (M. Stratmann and A. Bard, Eds.), 2005, Wiley-VCH, (in press).

- *High Temperature Electrokinetic Studies of Solid Oxide/Water Interface*

1. Zhang Z., Fenter P., Cheng L., Sturchio N. C., Bedzyk M. J., Predota M., Bandura A., Kubicki J. D., Lvov S.N., Cummings P.T., Chialvo A.A., Ridley M.K., Benezeth, P., Anovitz L, Palmer D.A., Machesky M.L., and Wesolowski D.J. Ion Adsorption at the Rutile-Water Interface: Linking Molecular and Macroscopic Properties, *Langmuir*, **20**, 2004, 4954-4969.

- *Elevated Temperature Proton Exchange Membrane Fuel Cells*

1. 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, in press).

2. 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.*, (2004, in press).

3. Lvov S.N., Fedkin M.V., Chalkova E., Jayabalan D.K., and Wesolowski D.J. Surface Chemistry of Solid Oxides for Developing High Temperature Proton Exchange Membranes, In: The 204th ECS Meeting Proceedings, Orlando, Florida, ECS, (2005, in press).

- *High Temperature Solid Oxide Fuel Cells*

1. Zhou Z.F., Gallo C., Pague M.B., Schobert H., and Lvov S.N., Direct Oxidation of Jet Fuels and Pennsylvania Crude Oil in a Solid Oxide Fuel Cell, *Journal of Power Sources*, **133**, 2004, 181-187.

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

- Under IAPWS support, Mr. Magomed Aliev, a PhD candidate in Physics from the Dagestan Scientific Center (Russian Academy of Sciences) visited NIST (Boulder) as a Guest Researcher from October to December, 2004 to work with Drs. Joseph Magee and Ilmutdin Abdulagatov on the project "An Experimental Study of *PVTx* Properties for the System Ammonia + Water at High Temperatures and Pressures." A separate report has been furnished.
- The collaboration of the Thermophysical Division of the Dagestan Scientific Center (Russian Academy of Sciences) and the Experimental Properties of Fluids Group of the Physical and Chemical Properties Division of NIST continues to thrive. In the past year, manuscripts were published on experimental *PVTx* studies of water + methanol mixtures at high temperatures and pressures and also on *PVTx* measurements and an equation of state for the water + hexane binary system.
  1) Bazaev, A. R., Abdulagatov, I. M., Magee, J. W., Bazaev, E. A., Ramazanova, A. E., and Abdurashidova, A. A., "*PVTx* Measurements for a H_2O + Methanol Mixture in the Subcritical and Supercritical Regions," Int. J. Thermophysics 25: 805-838 (2004).
  2) Abdulagatov, I. M., Bazaev, A. R., Magee, J. W., Kiselev, S. B., and Ely, J. F., "*PVTx* Measurements and a Crossover Equation of State of Pure n-Hexane and Dilute Aqueous n-Hexane Solutions in the Critical and Supercritical Regions," Ind. Eng. Chem. Res. 44: 1967-1984 (2005).
- The Physical and Chemical Properties Division (Boulder and Gaithersburg) of NIST is carrying out experimental studies of room-temperature ionic liquids (liquids composed entirely of ions) that are meant to establish reference systems, methods and data. The ionic liquids studied have both scientific and practical engineering interests. Three manuscripts were published which explore thermophysical behavior of dilute (water + ionic liquid) mixtures.
  1) Widegren, J. A., Laesecke, A., and Magee, J. W., "The Effect of Dissolved Water on the Viscosities of Hydrophobic Room-Temperature Ionic Liquids," Chem. Commun. 1610-1612 (2005).
  2) Widegren, J. A., Saurer, E. M., Marsh, K. N., and Magee, J. W., "Electrolytic Conductivity of Four Imidazolium-Based Room-Temperature Ionic Liquids and the Effect of a Water Impurity," J. Chem. Thermodynamics 37: 569-575 (2005).
  3) Archer, D. G., Widegren, J. A., Kirklin, D. R. and Magee, J. W., "Enthalpy of Solution

of 1-Octyl-3-methylimidazolium Tetrafluoroborate in Water and in Aqueous Sodium Fluoride," J. Chem. Eng. Data 50: (published in Web edition, 2005).

- Richard Wheatley, a theoretical chemist at the University of Nottingham, spent part of a sabbatical in Boulder to further the collaborative effort on development of intermolecular pair potentials for aqueous systems and calculation of second virial coefficients that have smaller uncertainties than those obtained by experiment. Work is nearly complete on water with nitrogen, and water with oxygen is underway. Completion of these two systems will allow improved calculations for water with "air" which is essential for humidity standards.
- 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, including a new form for the critical enhancement, has been completed and is ready for evaluation by IAPWS.
- A model has been developed for the effect of dissolved air on the density and refractive index of liquid water. The density effect is of interest in metrology, and the refractive-index effect is of interest for a technology called immersion lithography, which is being developed for manufacturing computer chips. Collaborators at NIST-Gaithersburg measured the refractive-index effect and obtained good agreement with the model.

Communicated from the Oak Ridge National Laboratories, Oak Ridge, TN

In collaboration with other members of the ORNL High-Temperature Aqueous and Geochemistry group, research work was completed from August 2004 to July 2005 or is ongoing or will begin soon in the following areas.

- Solubility studies of minerals to high temperatures including: lead oxide, dawsonite, zinc ferrite (stoichiometric and nonstoichiometric), zinc silicate, and nickel and zinc oxides in the presence of chloride ions.

- Isopiestic studies of binary aqueous solutions (60 – 170oC) containing combinations of the ions of Na, K, NO3, Cl, SO4 to very high concentrations. Isopiestic measurements were completed at 25 and 50 oC on the system: Fe3+-Fe2+, H+, SO42-.

- Thermodynamic studies of liquid films and the projected solutions existing in actively corroding crevices on canister surfaces containing high-level radioactive waste at the proposed Yucca Mountain repository site in Nevada were begun late last year. These include studies of deliquescent behavior, solute volatility and solution pH and well as modeling and speciation studies.

- Work was initiated on testing certain metal/metal oxide pH sensing electrodes for accurate and reliable measurements to at least 200 oC for use in oxidizing environments where hydrogen electrodes are unsuitable.

- Experimental measurements of designed to follow the dissolution and precipitation kinetics of metal oxide and hydroxide phases in aqueous solutions continued at a modest level with a draft of the first paper being prepared.

- The activities associated with being the editor-in-chief of the Journal of Solution Chemistry and coauthor of a chapter on potentiometry for the IAPWS Databook continued throughout this period.