To:Professor K Watanabe, Chairman of IAPWSFrom:Dr. R R Harries, Chairman of BIAPWSCc:Dr. B Dooley, International Secretary, IAPWS

28 July 2004

A REVIEW OF THE CURRENT STATUS OF BIAPWS IN 2004

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 nine corporate sponsors, three members with academic links and four associate members who are in consultancy or are retired from the power generation industry.

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

Membership

The nine corporate sponsors are full members of BIAPWS and represent the power generation industry (7 members), power plant manufacturer (1), technical support and consultancy (1) and power plant chemical instrumentation manufacturer (1). BIAPWS continues to encourage membership from other power plant generators and related industries as well as academia.

The academic support has reduced in the last few years, but three universities are currently associate members, with two actively engaged with 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 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 establish 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. At these meetings they also interact with equipment suppliers and with academic institutions.

The second area of education and outreach is the regular organisation of technical symposia. Seven 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 within the UK and Ireland.

At the last symposium, in May 2003, a new initiative was started, whereby BIAPWS organised half-day workshop sessions on the days before and after the symposium, with two power plant related topics in each workshop. The first workshop was reasonably successful, the second was less well attended. This was believed, partly, to be due to the poor economic state of the UK power generation industry. For the 2004 symposium, planned for autumn 2004, it is proposed to have only one half-day workshop session with three or four topics, some of which will be linked to papers presented in the main symposium. The symposium itself will be targeted at power plant operators. It is hoped this "added value" will attract attendees to both the workshop and 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. In 2003 the winning dissertation was on the topic of "Third Phase formation in the Purex Process". It was awarded to Ms Lindsay Plant of Manchester University.

Currently two members of the BIAPWS committee are active on a committee set up by the European Power Plant Suppliers Association in determining a common set of boiler chemistry and steam purity guidelines for new power plants supplied by these European companies. BIAPWS is currently co-ordinating responses from members on the recently issued European Standard EN 12952 – 12: 2003 "Water Tube Boilers and Auxiliary Installations – Part 12: Requirements for Boiler Feedwater and Boiler Water Quality".

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, particularly through developing an interest by undergraduates and pre-university students in science and engineering associated with water and steam.

Richard Harries, Chairman BIAPWS

The Czech National Committee

International Association for the Properties of Water and Steam

REPORT on IAPWS related activities – July 2003 / August 2004

Submitted to the EC Meeting of IAPWS, Kyoto – August 2004.

National Committee Contacts:

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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, Technická 4, CZ-166 07 Prague 6
- **Technical University Brno** (TU), Faculty of Mechanical Engineering, Department of Thermomechanics and Nuclear Energetics, Technická 2, CZ-616 69 Brno
- **Institute of Chemical Technology Prague** (ICT), Power Engineering Department (ICT-IE) and Department of Physical Chemistry (ICT-IPC), Technická 5, CZ-166 28 Prague 6
- **University of West Bohemia in Pilsen** (UWB), Faculty of Mechanical Engineering, Department of Power System Engineering, Univerzitní 8, CZ-306 14 Plzen
- SKODA ENERGO, Turbines, Plzeň, 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.

Activities were sponsored by the Grant Agency of the Academy of Sciences and Grant Agency of the Czech Republic, SKODA ENERGO-Turbines, Plzen Inc., 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 and results of the research into thermophysical properties of water and steam in Czechoslovakia and Czech Republic. /for use by CZ NC/ [1,2,3].
- Prof. Mares (UWB) prepared an information about Aleksandrov's equation for viscosity of ordinary water and with collaborators investigated wet steam flow [4,5,6].
- Prof. Marsik (IT) with co-authors finished and sent to press the manuscript of the Chapter 7: "Binary Homogeneous Nucleation in Selected Aqueous Solutions", in the frame of the ATLAS Project [7].
- Prof. Marsik (IT) with his research team carried out investigations into metastable state of water and steam, condensation, evaporation, and cavitation [8 to 14].
- Prof. Sedlbauer (TUL) with Profs. Majer and Wood finished and sent to press the manuscript of Chapter 4: "Calculation of Standard Thermodynamic Properties of Aqueous Electrolytes and Nonelectrolytes", in the frame of the ATLAS Project [15].

- Prof. Sedlbauer (TUL) with Prof. Wood developed a new model for simultaneous description of thermodynamic properties of aqueous ions at extreme conditions. The model is based on the Sedlbauer-O'Connell-Wood equation for standard part of the chemical potential and Mean Spherical Approximation for the excess part of the property [16 to 20].
- Dr. Hruby (IT) performed experimental and theoretical investigation of homogeneous nucleation of dropplets of pure water and water solutions from superheated steam/vapor mixtures and studied properties of subcooled water [21, 22].
- Research activities at the CTU have continued during the period 8/2003 8/2004 in further improving our knowledge on the droplet nucleation process occurring in LP steam turbines by means of analysis of realized diagnostics of wet steam in 1000 MW and 210 MW steam turbine of nuclear and fossil power station, respectively.

The diagnostics of wet steam at the exit of L-0 turbine stage (from the root to the blade tip) consisted in prediction of droplet size spectra, moisture level, and electrostatic charge of the droplet population.

Combined extinction and charge probe developed at the CTU was found to be suitable equipment for measurement of separate contributions of the fine and coarse droplets in the wet steam charge density. The data obtained in the mentioned turbine tests have been used in improving computational model of the droplet nucleation in LP steam turbines [23].

- Dr. Jiricek (ICT-IE) with collaborators evaluated deposits from steam turbine buckets on the basis of elemental analysis and spectroscopic examination. Compounds responsible for underlying steel corrosion brought by steam carry-over were identified [24].
- Dr. Jiricek (ICT-IE) studied corrosion inhibition in runway deicers based on potassium acetate. In the new formulation, toxic triazoles are avoided and optimized additives gave the fluid with low impact on aircraft materials measured by standard tests for aircraft maintenance chemicals [25, 26].
- Dr. Hnedkovsky (ICT-IPC) with collaborators investigated properties of organic solutes in water. Published articles are in [27 to 43].
- Prof. Stastny (SKODA ENERGO) 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 with experiments [44, 45].
- Dr. Zmitko (NRI) collaborated with nuclear power plants mainly in the fields of 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.
 - data processing technologies and system for diagnostics for water chemistry and corrosion control in Nuclear Power Plants (DAWAC). [46 to 48].

Young Scientists IAPWS Fellowships:

Mr. T. Nemec finished the IAPWS Young Scientists Project (CZ-US) "Thermodynamics of Binary Homogeneous Nucleation in Superheated Steam " under supervising Prof. Maršík, Dr.Hrubý, Dr. Palmer, and Dr. Simonson. The project was focused on three areas of interest in the binary homogeneous nucleation research:

- preparation of a database of nucleation-relevant thermodynamic properties for several water-admixture binaries relevant to power cycles,
- to employ this database in a nucleation simulation program,
- solving the kinetic equations of nucleation.

His Final Report for the IAPWS Young Scientists Fellowship is in Appendix 1.

The new publications of the fellowship holder are in [8, 9, 49].

IAPWS Certified Research Needs

Ad item 1.11 from the Minutes of EC IAPWS, Veile, DK, 2003

- a) Members of the CZ NC PWS interested in PCC problems, looked through the proposal of the new procedure for development of ICNRs (PCC Attachment A, pg.44 in Minutes) and agree with the proposal.
- b) They reviewed the priority list ICRNs accepted on September 25, 2003 in Veile and recommend to continue namely in solving
 - Copper Depositions
 - Nucleation and Condensation in Steam Turbines
 - Physical and Chemical Processes of Concentration and Deposition in the Power Cycle

and recommend for discussion and inclusion of three new tasks:

- A) Improving of the Heat Transfer of the Condenser Tubes in Power Plants. (Improving the Thermic Efficiency of Clausius-Rankine Cycle)
- B) Properties of Supercritical Water (SCW), Solubility of Salts, Corrosion Products and Oxide Protection Layers.
- C) Protection of alloys by coatings, hot corrosion in molten salts.

The deputy of the CZ PCC group (Dr.Zmitko) is prepared to give explanation for the proposed tasks under points A through C).

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THERMODYNAMICS OF BINARY HOMOGENEOUS NUCLEATION IN SUPERHEATED STEAM – YOUNG SCIENTISTS IAPWS PROJECT – FINAL REPORT

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BACKGROUND

Nucleation, a physical phenomenon which is closely connected to the nature of the world around us, is the area of interest of this project. Even though we focus on its special case only, the vapor – liquid nucleation, we can follow more than a century of scientific investigations of this problem. The broad area of application makes the nucleation very important nowadays; the two following cases are discussed mainly. The formation of aerosols in the atmosphere is very important in the study of various atmospheric processes. And the condensate creation in power cycles gives some restrictions on the power cycle design and efficiency.

Let me mention the most important milestones in the nucleation theory development. The early works of Gibbs [1] are usually referenced as the first attempt to describe the nucleation process. The nucleation theory development was started by Becker and Döring [2]. Their unary nucleation theory was fine-tuned later by Zeldovich [3]. The next big step into the field of binary nucleation was done by Reiss [4]. Then Stauffer [5] derived a proper expression for the binary nucleation rate and Trinkaus [6] generalized the theory to multicomponent mixtures. This approach to the nucleation problem is usually called the Classical Nucleation Theory (CNT).

Of course, the development of the nucleation theory was pushed forward by the enhancements and improvements of experimental nucleation techniques. Unfortunately, the results of these nucleation experiments (nucleation rate, size and composition of the critical cluster) showed significant deviations from the values predicted by the CNT. Many scientists tried to remove the discrepancies by introducing various revisions or consistency enhancements of the CNT, but these modifications were applicable to a specific small set of mixtures only, never reaching a general validity.

Our mission is to review the framework of the CNT. Evaluating the nucleation properties based on the CNT for a wide set of mixtures, and comparing them with available experimental results can help us to pinpoint the weaknesses of the CNT.

RESULTS

There is an obvious choice for the systems suitable for our purpose – aqueous binary systems. The nucleation of water with various admixtures has been investigated experimentally in many studies, especially in connection with the atmospheric aerosol formation and the power cycle condensation. Moreover, the properties of aqueous systems necessary for accurate evaluation of the nucleation properties using the CNT have been measured in most cases already. The only bottleneck in nucleation calculations remains the availability of thermodynamic properties of the investigated mixtures. Luckily, the aqueous chemistry group at ORNL, where I spent almost 5 months (March – July 2003) under the supervision of Don A. Palmer during this project, turned out to be the most suitable place for finding the necessary thermodynamic data and getting help with their representation.

We have studied several types of aqueous mixtures, introducing different thermodynamic models. Water with alcohols (methanol, ethanol, propanol) served for comparison with experiments. Other dissociative admixtures were implemented $(H_2SO_4, HNO_3, HCl, NaOH, NaCl)$ with a slightly different approach. Ammonia which can be described either by a non-dissociative model or by a dissociative one was very useful for calibrating our two nucleation models. As a result, I have developed an easy-to-use windows-based program called Conan. It calculates all the nucleation properties of the above mentioned systems at given temperature, pressure and composition. Moreover, it evaluates the sensitivity of the results to the errors in thermodynamic properties used throughout the calculations. The Conan software is available upon request.

The comparison of the Conan results and available experimental nucleation rates (e.g. Mirabel [7], Flageollet [8], or Wyslouzil [9]) shows a systematic deviation mentioned earlier. But we can follow the nature of these differences for a wide set of distinct aqueous systems. This gives us some ideas how to solve this problem; the CNT enhancement based on these results will be the next step in our research. Later, we will focus on multicomponent systems.

A short summary of this project was presented at the annual IAPWS Meeting in Vejle, Denmark, 24 - 30 August 2003.

COLLABORATIVE PROJECTS

Some of the results of this research will appear in the chapter "Binary Homogeneous Nucleation in Selected Aqueous Vapor Mixtures" of the upcoming ATLAS book edited by Don A. Palmer.

BUDGET

Living expenses (\$9000) in Oak Ridge were covered by the IAPWS Fellowship. Air tickets and health insurance (\$1000) were covered by the grant no. 60251 of the Grant Agency of the Academy of Sciences of the Czech Republic.

ACKNOWLEDGEMENTS

I would like to acknowledge the indispensable help of both my supervisors D. A. Palmer and F. Maršík, and important comments from M. Gruszkiewitz, A. Chialvo, and J. M. Simonson (ORNL), and A. H. Harvey (NIST). Finally, I would like to thank IAPWS for making this fruitful research possible.

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IAPWS REPORT 2003

The research activities in 2003 in Denmark in the field of properties of water and steam were mainly concentrated on continuation of activities started in the 2002. Due to the difficult economic situation new research has not been initiated.

Measurement of the solubility of sodium sulphate in steam in the vicinity of the critical point was made as a collaborative project supported by the EU.

Mathematical modelling of thermodynamic properties of ammonia / water mixtures is in progress at the Technical University of Denmark, Copenhagen. The model takes the chemical interaction between ammonia and water into account improving its fit to the experimental data.

Measurements and modelling of density and viscosity of multicomponent aqueous electrolyte solutions are in progress at the Technical University of Denmark, Copenhagen. The aim is to the predict the scaling in hydrogeological systems.

Modelling of multicomponent aqueous electrolyte systems and application of models to the recycling process for fertilizer from ash residues is in progress at the Technical University of Denmark, Copenhagen.

Modelling of ion exchange processes has started at the Technical University of Denmark, Copenhagen.

Publications in 2003:

Søren Gregers Christensen and Kaj Thomsen, "Modeling of Vapor-Liquid-Solid Equilibria in Acidic Aqueous Solutions", Ind. & Eng. Chem. Res. 42(2003)4260-4268, issue 18

Svend-Erik Therkildsen, "Water Chemistry Control and Monitoring Concept for Avoiding Chemistry-Related Failures in Small Combined Heat and Power Plants", Power Plant Chemistry, Vol. 5 (2003) No.9, p. 553-560.

German National Committee to IAPWS

Research Activities on the Thermodynamic Properties of Water and Steam Report "Research in Progress 2004"

- 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) in regions 1 and 2 was finished and finally accepted by the "Journal of Engineering for Gas Turbines and Power".
- 2. Supplementary backward equations *T*(*p*,*h*), *v*(*p*,*h*), and *T*(*p*,*s*), *v*(*p*,*s*) for region 3 of IAPWS-IF97
 - In addition to the backward equations T(p,h), v(p,h), and T(p,s), v(p,s), equations $p_{sat}(h)$ and $p_{sat}(s)$ for the region boundary between region 3 and wet-steam region 4 were developed.
 - The Draft of "Revised Supplementary Release on Backward Equations for the Functions T(p,h), v(p,h), and T(p,s), v(p,s) for region 3 of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" was prepared.
 - The evaluation of the revised release was supported.
 - The comprehensive article on the backward and boundary equations was prepared.
- 3. Supplementary backward and boundary equations p(h,s) for region 3 of IAPWS-IF97
 - The evaluation of the "Supplementary Release on Backward Equations p(h,s) for Region 3, Equations as a Function of *h* and *s* for the Region Boundaries, and an Equation $T_{sat}(h,s)$ for Wet Steam of the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" was supported.
- 4. Supplementary backward equations v(p,T) for region 3 of IAPWS-IF97
 - The development of backward equations v(p,T) in region 3 was completed.
 - The Draft of "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 prepared.

- 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 performed.
- 6. Property libraries for water and steam, combustion Gas mixtures, and humid air
 - The program libraries FluidEXL for Excel[®] FluidMAT for Mathcad[®]

were extended .

- 7. Implementation of the industrial formulation IAPWS-IF97 on pocket calculators
 - The program FluidTl for the model TI 83 of Texas Instruments was prepared.

Zittau, August 25, 2004

H.-J. Kretzschmar

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

REPORT on IAPWS related activities

Submitted to the EC Meeting of IAPWS, Kyoto - August 2004

National Committee Contact: Prof. Marc J. Assael, Chemical Engineering Department, Aristotle University 54124 Thessaloniki, Greece Tel. +302310.996163, Fax. +30231.996190, EMail. assael@auth.gr

SCIENTIFIC WORK

The work concentrated in the area of transport properties. More specifically:

1) Maintenance of the Water & Heavy Water Viscosity & Thermal Conductivity Data Bank

As part of a joint project between the International Association for the Properties of Water and Steam and the International Association for Transport Properties (formerly known as Subcommittee on Transport Properties of the International Union of Pure and Applied Chemistry Commission I.2 on Thermodynamics), all available and reliable experimental data on the viscosity and thermal conductivity of ordinary water and steam, as well as heavy water, have been collected and converted to the current temperature scale (ITS-90) and a common set of units. The data are grouped according to state into four regions: liquid phase (excluding data at 0.101 325 MPa), steam (vapor) phase, supercritical phase ($T > T_c$ for any pressure), and liquid at ambient pressure (0.101 325 MPa) between the triple point temperature and the normal boiling point temperature. Moreover, in the case of water, for each point with measured temperature and pressure (or at specified saturation conditions) a density has been computed with the current scientific standard thermodynamic formulation (IAPWS95), and each experimental datum has been compared with the viscosity or thermal conductivity calculated from the current standard formulations for these properties.

Fluid	Property	No of Points	Temperature range (K)	Maximum Pressure (MPa)
Water	Viscosity	4181	254 - 1316	346
	Thermal Conductivity	5111	255 - 1072	785
Heavy Water	Viscosity	1244	277 - 779	468
	Thermal Conductivity	2380	277 - 1043	250

The data bank is kept updated.

2) New Formulation for the Viscosity of Water

Work in this area is presently progressing fast with the cooperation of Dr D. Friend and Prof. J. Sengers (USA), Prof. E. Vogel (Germany), and A. Nagashima (Japan). It was hoped that a new improved formulation for the viscosity of water would have been ready to be proposed at the

ICPWS Meeting in Kyoto. However, this was slightly delayed, due to the measurement of new data by Prof. E. Vogel, which had to be added.

The new formulation for the viscosity, η , will have a better theoretical form, which is described by the following equation

 $\eta = (\eta_0 + \eta_1 + \eta_{ex})\eta_{cr}$

where, η_0 , is the viscosity at the dilute gas limit, η_1 , the initial density dependence, η_{ex} , the excess viscosity, and η_c , the viscosity in the critical region.

- a) Viscosity at the Dilute Gas Limit
 Following the 4-month stay of Ms Metaxa in NIST in 2003, the work on the viscosity of water
 vapor at the dilute gas limit, has successfully been concluded with the cooperation of Dr Dan
 Friend at NIST (USA), and Prof. E. Vogel (Germany). Thus, a modified form of the IAPWS
 1997 formulation is proposed for the viscosity of water vapor at the dilute gas limit.
 In order to derive this form, more data than the existing correlations, were employed. The
 data were evaluated using an extension of the international recommended procedure for Key
 Comparison Reference Values with the cooperation of the Statistics Division at NIST. The
 resulting proposed equation has a 1.6% uncertainty at the 95% confidence limit.
- b) Initial density dependence contribution Work is now completed by Ms Metaxa in cooperation with Prof. E. Vogel (Germany). The resulting correlation was sent to Dr Dan Friend (NIST) who will carry out the formulation of the excess viscosity and critical contribution in cooperation with Prof. S.V Sengers (USA)
- *c) Excess Viscosity and Critical Contribution* Work in these final areas of the formulation, is near each end.

3) New Formulation for the Viscosity of Heavy Water

Following the above procedure for the viscosity of water, a new formulation for the viscosity at the Dilute-Gas Limit was developed.

NON-SCIENTIFIC WORK

Work is still (Oh yes indeed!!) under progress in forming a full National Committee (This is going to be the longest-time-taken-to-be-formed National Committee in the history of IAPWS!). Although some industries and institutions have responded positively, no National Committee has as yet been appointed. The Hellenic Association of Chemical Engineers, which is the body representing Greece, is still thinking about it. Nevertheless, it has been agreed that in December 2004 the full fees will be paid and Greece will become a full member.

Current Status of Research Activities in Japan Submitted to the ExecutiveCommittee Meeting, IAPWS, Kyoto, Japan, August 2004

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 extensively concentrating every effort to organize the 14th ICPWS to be held in Kyoto, from August 29 through September 3, 2004. We are expecting more than 230 participants from 20 countries worldwide and 195 papers to be presented at the 14th ICPWS.

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-hydrocarbon mixtures at high temperatures and pressures. Near-infrared absorption spectra of water and water-benzene mixtures were measured at temperatures and pressures in the ranges of 373-673 K and 20-400 bar, respectively. Enthalpy for dimerization of water molecules in the gas and gaslike phase has been estimated to be 15 . . kJ/mol from a pressure-temperature dependence of the molar absorption intensity [*J. Chem. Phys.*, 119 (23), 12432 (2003)]. Anomalously large volume expansion on the mixing of water and benzene has been found in the region enclosed by an extended line of the three-phase equilibrium curve and the one-phase critical curve of the mixtures, and the gas-liquid equilibrium curve of water. It becomes as large as 7 times expansion at 573 K and 100 bar and at molar fraction of benzene of 0.18 [*J. Chem. Phys.*, 121 (6), 2694 (2004)]. [contact: Prof. S. Ikawa; E-mail: sikawa@sci.hokudai.ac.jp].

At the Department of Quantum Science and Energy Engineering, Graduate School of Engineering, Tohoku University, Sendai, Prof. S. Uchida is promoting a second phase of the project on water chemistry of BWR. 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. By changing concentrations of H₂O₂ and O₂, 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., X-ray diffraction (XRD), laser Raman spectroscopy (LRS), Rutherford back scattering spectroscopy (RBS), secondary ion mass spectroscopy (SIMS), and X-ray photoelectron spectroscopy (XPS). The ECP and FDCI data of the specimens exposed to 100 ppb H₂O₂ were not affected by co-existing O₂ with the same level oxidant concentration and they were also not affected by pre-exposure to 200 ppb O₂. From the viewpoint of ECP, this meant that corrosive conditions of hydrogen water chemistry were the same as those of normal water chemistry. Smaller oxide dissolution resistance and larger electric resistance of the oxide film were obtained for the specimens exposed to 100 ppb H_2O_2 . H_2O_2 exposure led to thicker oxide layers than O_2 exposure and Cr depletion did. The hematite ratio in the oxide films of the specimens exposed to H₂O₂ was expressed as a linear function of $[H_2O_2]$. The hematite ratio was measurable for 8 ppm O₂, but negligibly small for 200 ppb O₂. As a result of theoretical approaches to understand crack tip water chemistry under gamma and neutron irradiations, Mr. Tomonori Satoh (a doctor course student) got a 2003 Award for Emerging Technology of the Atomic Energy Society of Japan. [Latest publication: (1) S. Uchida, et al., Proc 11th Int. Conf. on Environmental Degradation on Materials in Nuclear Power Systems; Water Reactors, Aug. 10-14, 2003, Stevenson, Washington, American Nuclear Society (2003) (CD). (2) T. Satoh, et al., ibid. (3) H. Takiguchi, et al., J. Nucl. Sci. Technol., 41, 214 (2004). (4) S. Uchida, et al., Proc. the 14th Pacific Basin Nuclear Conference (2004) (CD). (5) T. Satoh, et al., J. Nucl. Sci. Technol., 41, 610 (2004). (6) H. Takiguchi, et al., J. Nucl. Sci. Technol., 41, 601 (2004)] [contact: Prof. S. Uchida; E-mail: shunsuke.uchida@gse.tohoku.ac.jp].

At the Graduate School of Environmental Studies, Tohoku University, Sendai, Profs. N. Yamasaki, H. Enomoto, K. Tohji, N. Tsuchiya, and their group are covering wide field related to hydrothermal material science and geofluid science. Material research group developed several kinds of advanced and functional materials [Yamasaki et al., J. Ceram. Soc. Jpn., 111,221-225(2003)], such as synthetic diamond, stratified materials on carbon nano-tube using hydrothermal process, and the liquefaction and gasification of heavy oil, the SCWO of rice husk for production of sodium acetate, 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(ex. [Liu et al., Energy Conversion and Management, 44, 1399-1410 (2003)]). Geofluid science research group is conducting water-rock interaction under sub- and supercritical condition [Tsuchiya et al., Geothermal Resources Council Trans., 27, 111-114 (2003)], including multi-phase and multi-component solutions. We organized 1st international workshop on WATER DYNAMICS (17-19th March 2004, Sendai), 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.

We are planning 2nd workshop of WATER DYNAMICS in 11-12th November 2004 in Sendai International Center.

[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 process of supercritical hydrothermal synthesis of nano particles. Specific features of this method have been found: (i) nano particle formation, (ii) single crystal formation, (iii) ability to control particle morphology to some extent with pressure and temperature, and (iv) ability to provide homogeneous reducing or oxidizing atmospheres by introducing gases or additional components (O2, H2). The method can be used for various applications, including magnetic material (BaO6Fe2O3), phosphor (Tb:YAG), metallic Ni nanoparticles, Li ion battery material (LiCoO2, LiMn2O4). For the rational design of this process, they developed a simulation method of supercritical hydrothermal synthesis, based on the fluid dynamics at supercritical conditions, kinetics, solubility estimation, nucleation, particle growth, and particle coagulation. Recently, they demonstrated that by using the supercritical hydrothermal synthesis, organic-inorganic hybrid nanoparticles could be synthesized due to homogeneous phase formation under the conditions. 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. [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 with a relative standard uncertainty of better than 1×107 and a determination of the Avogadro constant by the X-ray crystal density (XRCD) method are conducted for replacing the present definition of the kilogram [K. Fujii, A. Waseda, N. Kuramoto, S. Mizushima, M. Tanaka, S. Valkiers, P. Taylor, R. Kessel, and P. De Bièvre, "Evaluation of the molar volume of silicon crystals for a determination of the Avogadro constant," IEEE Trans. Instrum. Meas., 2003, 52, 646-651], resulting in the Avogadro constant of 6.022 $1375(12) \times 10^{23}$ mol¹. The data from the NMIJ were used for finding the best set of the fundamental physical constants most recently recommended by the CODATA Task Group on Fundamental Constants. Using the silicon 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. 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 %. 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 that has a specified isotopic abundance was recommended by the WG-Density and approved by the CCM [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 [contact: Dr. K. Fujii, Chief, Fluid Properties Section, NMIJ; E-mail: fujii.kenichi@aist.go.jp].

At the Division of Environmental Materials & Energy, Department of Environmental Science & Technology, Faculty of Engineering, Shinshu University, Nagano City, Prof. Hiroshi Takaku works since Feb.1, 2000. Previously, he worked approximately for 31 years at Central Research Institute of Electric Power Industry in Japan (CRIEPI) where he engaged in the study of the field of the corrosion, material properties and water chemistry both in nuclear and fossil power plants. In the simulated geothermal waters containing the mixed corrosive chemicals such as chloride, sulfide, carbon dioxide, hydrogen sulfide and others, he and his coworkers are studying the corrosion of the steam turbine materials for the geothermal power plants, and Ti-Ni base shape memory alloys for the heat engine actuator. They are also studying the corrosion of boiler materials and other equipments materials. [Latest publications: (1) N. kawai, H. Takaku, et al, Zairyo-to-Kankyo (J. of Corrosion Engineering in Japan), 49 (2000) 612-618, (2) T. Sakuma, H. Takaku, et al, Transactions of Materials Research Society of Japan, 26 (2001), 167-170, (3) H. Takaku, et al, Materials Transactions, 43 (2002), 840-845, (4) H. Sakai, H. Takaku, et al, Proc. International Conference on Power Engineering (ICOPE-03, ASME-JSME-CSPE), Vol.3 (2003), 297-302, (5) Y. Horiuchi, H. Takaku, et al, Transactions of Materials Research Society of Japan, 29 (2003)] [contact: Prof. H. Takaku; E-mail: takakuh@gipwc.shinshu-u.ac.jp]

Mr. K. MIYAGAWA is developing Tubular Taylor Series Expansion Method (TTSE) for rapid calculation of thermophysical properties of water substance and other fluid. In the IAPWS meeting in Vejle, Denmark in 2003, the IAPWS guideline "Guideline on the Tabular Taylor Series Expansion (TTSE) Method for Calculation of Thermodynamic Properties of Water and Steam Applied to IAPWS-95 as an Example" was adopted. Mr. Miyagawa is developing a new version of TTSE programs that calculates transport properties with high speed and high accuracies. It will be useful to analyze transient phenomena in heat transfer and fluid mechanics. He will present it at the 14th ICPWS in Kyoto, Japan in August 2004. [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 the shape of fallen particles on heterogeneous nucleation of water using Molecular Dynamics Simulaiton, and finding that the small projection on the surface influences the freezing. [Trans. JSRAE, 20, 2, 135-142, (2003) in Japaneses] They are also studying the effect of the difference in lattice constant of particle on freezing [Trans. JARAE, 20, 2, 155-162, (2003) in Japanese], and the effect of various kinds of external forces on freezing of supercooled water [6th ASME-JSME Thermal Engineering Joint Conference, (in CD-ROM), (2003)] [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 constructed a Raman spectroscopic system for solid sample in high temperature water up to 400 °C, as a part of a national research project, "Fundamental R&D on Water Chemistry of Supercritical Pressure Water under Radiation Environment". They measured Raman spectra of several metal oxides in high temperature water, finding that alumina is stable in air-saturated water of 250 °C. [contact: Dr. M. Domae; E-mail: domae@criepi.denken.or.jp]

At the Center for Mechanical Engineering and Applied Mechanics, Keio University, Yokohama, Prof. M. UEMATSU and his group have constructed PVT apparatus for aqueous ammonia mixtures in the range of temperatures to 800 K and pressures to 20 MPa. Isobaric specific heat capacities for water + methanol mixtures are being measured by new calorimeter for temperatures from 250 K to 400 K at pressures to 20 MPa. [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 mechanism for the dissociation and formation of clathrate hydrate. They adopt the MD simulation for the adosorption and desorption of ethanol molecules to liquid-vapor water surface. They have got the results, nucleation rate etc., for the bubble nucleation process. They started to evaluate the water model contained in HIV-1 Protease. These four topics are presented in 14th ICPWS. [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 measuring 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@me.kanagawa-it.ac.jp].

At the Department of Computational Molecular Science, Institute for Molecular Science, Prof. S. Okazaki and his group analyzed dissipation mechanism of excess vibrational energy of the solute molecules in ambient and supercritical water based upon mixed quantum-classical molecular dynamics calculation. Dynamics of coherence between vibrational states has also been investigated starting from a certain coherent initial state based upon path integral influence functional theory. [M. Sato and S. Okazaki, J. Mol. Liq. in press, M. Sato and S. Okazaki, Mol. Simul. in press, and T. Mikami and S. Okazaki, J. Chem. Phys. 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 hydrophobic hydration under high pressure up to 400 MPa in the stand point of the partial molar volume and the visicosity of H2O and D2O in the high-pressure and low-temperature region [see: H. Matsuo, Fluid Phase Equilibria **20** (2002), 227-238. Sawamura, S., Rev. High Press. Sci. Tech. 13, (2003) 157-164]. 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 [see: W. Dzwolak, et al, Biochim. Biophys. Acta **1595** (2002), 131-144; K. Fumino, et al. J. Mol. Liq. **100** (2002), 119-128; R. Kitahara, et al., Protein Science, 12. 207-217 (2003); Y. Shiratori, et al., Bull. Chem. Soc. Jpn, **76** (2003), 501-507.] [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 ["NMR Study on the Reorientational Relaxation in Supercritical Alcohol", T. Yamaguchi, N. MATUBAYASI, and M. NAKAHARA, J. Phys. Chem. A 108, 1319-1324 (2004)] and (2) the molecular mechanism of noncatalytic reactions in hydrothermal conditions. ["Hot Water Induces an Acid-Catalyzed Reaction in Its Undissociated Form", Y. Nagai, N. Matubayasi, and M. Nakahara, Bull. Chem. Soc. Japan 77, 691-697 (2004)]. [contact: Prof. M. Nakahara; E-mail: nakahara@scl.kyoto-u.ac.jp]

At the Department of Molecular Science and Technology, Doshisha University, Kyotanabe, Kyoto, Prof. M. UENO, Prof. IBUKI and their group have studied the electric conductivities of NaCl, KCl, and CsCl 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, and compared the results with those in water [T. Hoshina, N.Tsuchihashi, K. Ibuki, and M. Ueno, J. Chem. Phys., **120**, 4355-4365 (2004)]. They have also measured the NMR spin-lattice relaxation times of ²H and ¹N nuclei in acetonitrile-water mixtures at 30°C under high pressure up to 300 MPa together with density and viscosity measurements to investigate the rotational motion of water and acetonitrile molecules in the mixtures [in press, M. Ueno, S. Ueyama, S. Hashimoto, N. Tsuchihashi, and K. Ibuki, J. Solution Chem., **33**, 823-842 (2004)]. Computer simulations have been carried out to test a new theory of the dynamics of diffusion-controlled reactions based on the Fokker-Planck-Kramers equation [K. Ibuki and M. Ueno, J. Chem. Phys., **119**, 7054-7064 (2003)]. [contact: Prof. M. Ueno; E-mail: mueno@mail.doshisha.ac.jp]

At the Department of Mechanical Enginnering 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, PROPATH. Its new version is now under development. This software consists of 5 subsets. The water substances with different formulations are available. By using E-PROPATH, one of the 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, Keihin Product Operations, Dr. T. Tanuma and his coworkers are studying the application of the nonequilibrium wet steam CFD analysis for steam turbine blade design as a collaborative program with Professor S. Yamamoto, Department of Mechanical Engineering, Tohoku University, Japan and Professor X. Yuan, Department of Thermal Engineering, Tsinghua University, China. The research results indicate that the CFD method for compressible viscous wet steam flows in steam turbines is useful for optimization of blade designs (profile geometry, surface pressure distributions, blade exit angles, blade throat, etc.) in nonequilibrium wet steam conditions including rotor blade flow paths which are affected with passing stator blade wakes in real turbine stages. In a recent paper, the application results of nonequilibrium wet steam flow through steam turbine stages have been reported [The Proceedings of the 13th Pacific Basin Nuclear Conference October 21-25, 2002,

Shenzhen, China], [contact: Dr. T. Tanuma, tadashi.tanuma@toshiba.co.jp].

International Association for the Properties of Water and Steam Russian National Committee

Report of Russian National Committee (2003 – 2004) List of Publications

- 1. Bogachev A.F., Ul'yanov V.V., Yurkov V.A., Prutskova A.V. Diagnostics of the Period Between Washings in the Operation of High-Pressure Drum Boilers on the Basis of Temperature Inserts and Indicators of the Quality of Water Chemistry Conditions. Thermal engineering. 2004, Vol. 51, № 7, p. 511.
- 2. Grishin A.A., Larin B.M., Malakhov I.A., Fedoseev B.S. An Investigation of the Sorbtion–Desorbtion of Organic Impurities of Natural Waters on Anionite Filters. Thermal engineering. 2004, Vol. 51, № 7, p. 517.
- Man'kina N.N., Karkarin A.P., Kirilina A.V., Zagretdinov I.Sh., Kir'yanov I.I., LyspakA.I. The Results of the Introduction of Oxygenated Steam–Water Cleaning, Passivation, and Preservation of the Flow Path of the Type PK-38 Boiler st. no. 6 of the Krasnoyarsk GRES-2 District Power Station. Thermal engineering. 2004, Vol. 51, № 7, p. 522.
- Petrova T.I., Vidoikovich S., Zonov A.A., Petrov A.Yu. Effect of Acetic Acid on the Contamination of Saturated Steam by Sulfates and Fluorides. Thermal engineering. 2004, Vol. 51, № 7, p. 526.
- 5. Malakhov I.A., Askerniya A.A., Borovkova I.I., Malakhov G.I. Technological Aspects of Choosing Optimal Feedwater-Demineralization Schemes for Steam Generators of Thermal Power Stations and Industrial Enterprises. Thermal engineering. 2004, Vol. 51, № 7, p. 530.
- Dubrovskii I.Ya., Eskin N.B., Tugov A.N., Anikeev A.V. Experimental Investigations of the Behavior of Octadecyl Amine in Superheated Steam and on Metals Coming into Contact with It. Thermal engineering. 2004, Vol. 51, № 7, p. 544_
- Petrova T.I., Ryzhenkov V.A., Kurshakov A.V., Zroichikov N.A., Chernov V.F., Galas I.V. Using Film-Forming Amine for Conservation of Process Equipmentat the Mosenergo Cogeneration Station TETs-23. Thermal engineering. 2003, Vol. 50, № 9, p. 760.
- 8. Petrova T.I., Furunzhiyeva A.V. Use of chelamine at fossil power plants with drum boilers. Energosberezheniye i vodopodgotovka, 2004, №1, pp. 3 8.
- 9. Zaripov Z.I., Burtsev S.A., Bulaev S.A., Mukhamedzyanov G.Kh. Heat capacity and temperature conductivity of aqueous solutions of alkali metals in wide range of pressures. J.Phys. Chem. (Rus), 2004. Vol. 78. No. 5. P. 814 818.

- 10. Grigoriev E.B. Thermal conductivity of triple aqueous solutions of lantanium salts Teploenergetika. 2003. No. 6. P. 64 66.
- Bazaev A.R, Bazaev E.A. P,ρ,T,x -relation of gas mixtures water -hydrocarbon in wide range of parameters of state. Thermophys.of High Temperatures. 2004. Vol. 42. No. 1. P. 48 -57.
- Podmurnaya O.A., Gudkov O.I., Dubovikov A.A. Equilibrium concentration of mixtures of nitrogen with water at the pressures up to 10 MPa. J. Phys. Chem. (Rus). 2004. Vol. 78. No. 2. P. 373 -375.
- 13. Alexandrov A.A. The equations for thermophysical properties of aqueous solution of sodium hydroxide. Submitted to 14 ICPWS.

U.S. National Committee to IAPWS 2004 Report on Activities of Potential Interest to IAPWS

Communicated from Arizona State University, Tempe, AZ:

- Correlations and estimations for the second cross virial coefficients for interactions involving water. (Plyasunov A. V., Shock E. L. (2003) Second cross virial coefficients for interactions involving water. Critical data compilation; J. Chem. Eng. Data, 48, 808-821; Plyasunov A. V., Shock E. L., Wood R. H. (2003) Second cross virial coefficients for interactions involving water. Correlations and group contributions values. J. Chem. Eng. Data, 48, 1463-1470.)
- Correlations and estimations for the Krichevskii parameter for volatile nonelectrolytes in water. (Plyasunov A.V., Shock E.L. (2004) *Prediction of the Krichevskii parameter for volatile nonelectrolytes in water* Fluid Phase Equil., in press.)
- Correlations and estimations for the vapor-liquid distribution constants for volatile nonelectrolytes in water. (Plyasunov A.V., Shock E.L. (2003) *Prediction of the vapor-liquid distribution constants for volatile nonelectrolytes in water up to its critical temperature* Geochim. Cosmochim. Acta, 67, 4981-5009.)
- Additional work on high pressure equation of state for water. (Mark R. Frank, Yingwei Fei, Jingzhu Hu. (2004) *Constraining the equation of state of fluid H2O to 80 GPa using the melting curve, bulk modulus, and thermal expansivity of Ice VII* Geochim. Cosmochim. Acta, 68, 2781-2790; Evan H. Abramson, J. Michael Brown (2004) *Equation of state of water based on speeds of sound measured in the diamond-anvil cell* Geochim. Cosmochim. Acta, 68, 1827-1835)

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

- A new study of criticality in aqueous solutions was completed. It was concluded that the asymptotic critical behavior of aqueous electrolyte solutions is the same as in non-electrolyte solutions, but that the non-asymptotic crossover critical behavior is non-monotonic. An anomalous critical behavior in aqueous solutions of 3-methylpyridine and sodium bromide previously observed that was attributed to the formation of a micro-heterogeneous phase turned out to be caused by long-living non-equilibrium states. Further experimental studies showed the ubiquitous presence of mesoscopic non-equilibrium aggregates in electrolyte aqueous solutions. The physical and chemical variables that govern the appearance of long-living non-equilibrium structures are not yet understood. (A.F. Kostko, M.A. Anisimov, and J.V. Sengers, *On the nature of criticality in aqueous solutions of 3-methylpyridine and sodium bromide*, Phys. Rev. E, in press.)
- J.V. Sengers continued his collaboration with the Physical and Chemical Properties at the National Institute of Standards and Technology, Boulder, CO towards the development of a new formulation for the viscosity of water and steam.

Communicated from Jonas, Inc., Wilmington, DE:

- Low Temperature Corrosion Problems in Fossil Power Plants State of Knowledge: (Jonas, Inc. EPRI project with contributions by others) The objective of the project was to provide a basic understanding of common, low temperature (up to 150°C) corrosion problems in fossil fueled power plants, to present solutions currently applied to those problems, case histories, and available pertinent references. "Missing Knowledge" for each component. Emphasis was placed on those areas identified as severe problems by the participants of an informal survey. (Low Temperature Corrosion Problems in Fossil Power Plants State of Knowledge. EPRI, Palo Alto, CA: December 2003. 1004924).
- ChemExpert: Further development (network) and applications of the EPRI water chemistry control expert system. (O. Jonas, L. Machemer, and B. Dooley. "EPRI ChemExpert: Cycle Chemistry Advisor for Fossil Power Plants." *EPRI 6th International Conference on Cycle Chemistry in Fossil Plants*. June 27-29, 2000, Columbus, Ohio.)

- Experimental Investigation of Local Environments in a PWR LP Turbine; ETA + Boric Acid Water Treatment: Includes new instrument to collect early condensate, Converging-Diverging Nozzle, Deposit Collector/Simulator, and a Drying Probe. Joint EPRI - utility - Jonas, Inc. project. (Report pending)
- Stress Corrosion Cracking in PWR and BWR Component Cooling Water Systems: The purpose of this project was to identify the root cause(s) of the stress corrosion cracking which is occurring near carbon steel welds in the component cooling water systems of several nuclear pressurized water reactor (PWR) units and one boiling water reactor (BWR) unit. (Report Pending)
- Condition Monitoring for Damage Assessment: Two German PWRs, each instrumented at over 1000 points. Data used to evaluate fatigue, FAC, SCC, and other damage.
- Water Cooling of High Voltage Electrical Cables: Effort to replace oil cooling with water cooling; selection of water chemistry and corrosion testing.

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

- 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*, 2004, in press)
- High Temperature Aqueous Electrochemistry (Lvov S.N. and Palmer D.A. *Electrochemical Studies of High-Temperature Aqueous Systems*, Chapter 12, 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; 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., 2004, Wiley-VCH, in press).
- Elevated Temperature Proton Exchange Membrane Fuel Cells (Zhou X.Y., Weston J., Chakova E., Lvov S. N., Hofmann M., Ambler C. M., and Allcock H. R. *High Temperature Transport Properties of Polyphosphazene Membranes for Direct Methanol Fuel Cells, Electrochimica Acta,* 48, 2003, 2173-2180)
- High Temperature Solid Oxide Fuel Cells (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)
- High Temperature Potentiometery and pH measurements (Seneviratne D.S., Papangelakis V. G., Zhou X.Y., and Lvov S.N. Potentiometric pH Measurements in Acidic Sulfate Solutions at 250°C Relevant to Pressure Leaching, *Hydrometallurgy*, 68, 2003, 131-139; Lvov S. N., Zhou X. Y., Ulmer G. C., Barnes H. L., Macdonald D. D., Ulyanov S.M., Benning L. G, Grandstaff D. E., Manna M., and Vicenzi E. *Progress on the Yttria-Stabilized Zirconia Sensors for Hydrothermal pH Measurements*, Chemical Geology, 198, 2003, 141-162:Zhou X.Y., Lvov S.N., and Ulyanov S.M. "Yttria-Stabilized Zirconia Membrane Electrode", United States Patent # 6,517,694, February 11, 2003.)
- High Temperature Electrokinetic Studies of Solid Oxide/Water Interface: (Zhou X.Y., Wei X.J., M.V. Fedkin, Strass K.H., and Lvov S.N. A Zetameter for Microelectrophoresis Studies of the Oxide/Water Interface at Temperatures up to 200 °C. Rev. Sci. Instrum., 74, 2003, 2501-2506; Fedkin M.V., Zhou X.Y., Kubicki J.D., Bandura A.V., Lvov S.N., Machesky M.L., and Wesolowski D.J. High Temperature Microelectrophoresis Studies of the Rutile/Aqueous Solution Interface, Langmuir, 19, 2003, 3797-3804; 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).

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

- Magomed Aliev from the Dagestan Scientific Center (Russian Academy of Sciences) will visit NIST (Boulder) in October, 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* under IAPWS support.
- Collaborations between the Dagestan Scientific Center and NIST continue with a manuscript on experimental *PVTx* studies of light water + heavy water and a series of manuscripts on *PVTx* and *Cv* for the methanol + water system.
- Collaborations with the Japan National Defense Academy and Keio University continue with manuscripts on heat capacity measurements on alkanol (methanol, ethanol and 1-propanol) + water systems.
- Manuscripts have been completed on experimental enthalpies of dilution of salts in water, including the first such reported measurement for a room-temperature molten salt (C. S. Oakes, J. A. Rard and D. G. Archer, *Enthalpies of Dilution of NdCl₃(aq) at Temperatures from 297.89 K to 372.09 K and an Extended Pitzer Ion-interaction Model for the NdCl₃ + H₂O System, J. Chem. Eng. Data 49, 313-325, 2004; D. G. Archer, <i>Enth alpy of Solution of Potassium Tetrafluoroborate in Water and Aqueous Sodium Fluoride. Thermodynamic Properties of the Aqueous Tetrafluoroborate Anion and Potassium Tetrafluoroborate*, in review).
- Collaboration continues with theoretical chemists in England on development of intermolecular pair potentials for aqueous systems and calculation of second virial coefficients that have smaller uncertainties than those obtained by experiment. We expect this work to find application for humidity standards and for calculating thermodynamic properties of combustion gases. (Water/hydrogen M.P. Hodges et al., J. Chem. Phys. **120**, 710, 2004; water/nitrogen system is nearly complete)
- Work is continuing on the joint IAPWS and IUPAC efforts to update the formulations for the transport properties of water and steam; preliminary correlating surface for viscosity has been completed.

In collaboration with experimentalists at NIST/Gaithersburg, we have characterized the refractive index of liquid water in the far ultraviolet (193 nm) for a technology called immersion lithography, which is being developed for manufacturing computer chips. The project combined experimental work with modeling efforts to describe the variation of the index with temperature, pressure, and dissolved air.