Attachment 15

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

Report on IAPWS related scientific activities - September 2000-2001

Submitted to the Executive Committee Meeting, IAPWS
Gaithersburg, September 2001

National Committee address: CNEA, Av. Gral. Paz 1499, (1650) San Martín, Buenos Aires – Argentina.
National Representative: Dr. Horacio R. Corti. Tel. 5411-6772-7174, Fax: 5411-6772-7121 - e-mail: hrcorti@cnea.gov.ar

Unidad de Actividad Química, Comisión Nacional de Energía Atómica and INQUIMAE - Departamento de Química Inorgánica, Analítica y Química Física, Facultad de Ciencias Exactas y Naturales – Universidad de Buenos Aires

- The experimental spectrophotometric study of 4-methyl phenol weak acid in the range of 298 to 440 K has been completed and a paper has been submitted to J. Chem Thermodynamics. "Thermodynamics of 4-methylphenol dissociation in water at high temperature using UV-vis spectroscopy", Lucila Méndez De Leo, H.L.Bianchi and R.Fernández-Prini. A spectrophotometric study of ionic association in high temperature aqueous solutions has been started in the last month. The systems to be studied are $CrO_4^{=}$ + Mg^{2+} or Ca^{2+}. The same authors as previous study.

- In a close collaboration with A. Harvey (NIST), Jorge Alvarez and R.Fernández-Prini are reevaluating the gas solubility data in water at high temperature. This will be the main part of the formulation of Henry's constant and distribution constant for water over the complete range of steam-water coexistence. Moreover, this work will be submitted as a paper to J. Phys. Chem. Ref. Data. (R.Fernámdez Prini).

- A number of molecular dynamics studies related to aqueous systems are on progress:

- Equilibrium and dynamical aspects of excess electrons in aqueous reverse micelles
  using combined Path-Integral-MD techniques.

- Electron localization in supercritical states of polar solvents: water and ammonia.
- Solvation dynamics of water in the vicinity of lipidic monolayers
- Dynamical aspects of electronically excited I^- dissolved in aqueous nanoclustes. (D.H.Laría)

- The water sorption, ice crystallization kinetics and electrical conductivity of aqueous solutions of trehalose and sucrose containing NaCl, KCl, $MgCl_2$ and $CaCl_2$ have been studied. The conductivity of these solutions were measured over a wide range of viscosities, including the liquid and the supercooled region. An article has been submitted to the Phys.Chem.Chem.Phys. (H.R.Corti).

- Properties like refractive index, turbidity and salt solubility of several ionic aqueous systems have been studied experimentally, with the aim of understanding the characteristic of critical phenomena in ionic systems. (M.L.Japas)

- A procedure for transforming the NRTL excess Gibbs energy model to reproduce the universal scaling behavior in the vicinity of the consolute critical point has been improved. The corrected Crossover-NRTL model was succesfully applied to the description of binary liquid mixtures of different degree of asymmetry. (M.L.Japas)

- A new method for the synthesis of crystalline Ni(II)-Cr(III) layered hydroxides was developed. The procedure, based on homogeneous hydrolysis under hydrothermal conditions, resorts to the use of microwave reactors. The synthesis of other layered double hydroxides by this procedure is now being explored. Studies on the synthesis of metal oxide nanoparticles by precipitation in inverse micellar systems have also been undertaken. (A.E. Regazzoni)

- The chemisorption of bidentate ligands on titanium dioxide was studied. The different *surface complexes* were characterized by IR spectroscopy; the results indicate that binuclear-bidentate surface species predominates. (A.E. Regazzoni)

- In collaboration with the group of Prof. Richard G. Compton (University of Oxford) an experimental and theoretical study of the hydrodynamic characteristic of a flow wall-tube electrode under hydrothermal conditions is underway. Results of diffusion coefficients of $Fe(CN)_6^{4-}$ and $Ru(NH_3)_6^{3+}$ ions in aqueous solutions up to 350 K were reported using a high temperature channel flow cell heated by radio frequency radiation. (L.N.Trevani)

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Publications:

- J.L.Alvarez, R.Fernández-Prini and M.L.Japas
Aqueous nonionc Solutes at Infinite Dilution: thermodynamic description, including the near-critical region.
I&EC Research, 39, 3625-3630 (2000).

- D.P.Miller, S.Fucito, J.J. de Pablo and H.R.Corti.
Electrical conductivity of supercooled aqueous mixtures of trehalose with sodium chloride.
J.Phys.Chem. B, 104, 10419-10425 (2000).

- M. Matsuyoshi, R.T. Gettar, M.A. Blesa and A.E. Regazzoni.
Adsorption of Dicarboxylic Acids at the Titanium Dioxide/Aqueous Solution Interface.
Presented at the *X International Conference on Colloid*

- A.D. Weisz, A.E. Regazzoni and M.A. Blesa.
ATR-FTIR Study of the Stability Trends of Carboxylate Complexes Formed on the Surface of Titanium Dioxide Particles Immersed in Water.
Solid State Ionics, 143, 125, 2001.

- M. Jobbágy and A.E. Regazzoni.
Hydrothermal Synthesis of Mixed Ni(II)–Cr(III) Hydroxides Using Microwave Reactors.
Proc. Sixth International Symposium on Hydrothermal Reactions, K. Yanagisawa y Q. Feng (Eds.), Nishimura Tosha-Do Ltd., Kochi, Jpn., 2001, pp. 373-376.

- M.J.Moorcroft, N.S.Lawrence, B.A.Coles, R.G.Compton and L.N.Trevani.
High temperature electrochemical studies using a channel flow cell heated by radio frequency radiation.
J.Electroanal. Chem. 506, 28 (2001)

- D.Laria, J.Rodriguez, C.Dellago and D.Chandler.
Dynamical aspects of isomerization and melting transitions in $[H_2O]_8$.
J.Phys.Chem. A. 105, 2646 (2001)

- Jorge L. Alvarez, Roberto Fernández-Prini y M. Laura Japas
Description of infinite dilution thermodynamic properties of solutes in binary fluid mixtures, including the near-critical region.
LAAR, in press.

- M.F. Mazzobre, M.P. Longinotti, H.R. Corti and M.P. Buera.
Effect of salts on the properties of aqueous sugar systems, in relation to biomaterial stabilization. 1. Sorption behavior and ice crystallization/melting.
Cryobiology, in press.

- Aleidus van 't Hof, M. Laura Japas, Cor Peters.
Description of liquid-liquid equilibria including the critical region with the Crossover-NRTL model
Fluid Phase Equilibria, in press.

- Hugo L. Bianchi and M.L. Japas

Phase equilibria of a near-critical ionic system. Critical exponent of the order parameter

J. CHEM. PHYS., IN PRESS

- ANC in collaboration with B. Dias Baptista Filho, J. Baliño, M. Cegala, W. Bassel (Instituto de Pesquisas Energeticas e Nucleares - (IPEN) - San Pablo, Brazil), M. Veloso (Centro de Desenvolvimento de Tecnología Nuclear - CDTN, Belo Horizonte, Brazil), L. Guimaraes, M.Pinheiro Rosa (Instituto de Estudios Avanzados- Centro Técnico Aeroespacial, CTA, San Jose dos Campos, Brazil), J. Fiora (Instituto Nacional de Tecnología Industrial, Buenos Aires) and J.C. Petras (Central Puerto, Buenos Aires), is preparing a bilingual Portuguese/Spanish version of the Steam Tables IF-97, which is planned to be printed by July 2002.

Attachment 16

The British and Irish Association for the Properties of Water and Steam

Report to IAPWS 2001

Support

BIAPWS retains the active support of the following industrial sponsors: ABB Automation, Alstom Power, BNFL Magnox Generation, British Energy, ESB, Enron, NEL, Powergen and Scottish Power. The sponsors attend regular co-ordination meetings. The opportunity is taken, whenever possible, to review technical progress as presented at various conferences and meetings attended by the members and to debate technical issues.

Programme

The next event to be sponsored by BIAPWS is a symposium on Power Plant Chemistry to be held at Birmingham University Conference Centre on 18 October. The programme will include papers under the following titles:

Comparison of techniques for degassed cation conductivity,
A sensitive versatile monitor for the continuous measurement of CO_2 in steam water circuits,
Steam purity considerations for combined cycle power plants,
TOC – Practical experiences – A collection of case studies,
Chemistry policy management for power plant,
Practical experience of high efficiency reverse osmosis technology - Power plant experience.

For the future, BIAPWS is at the early stage of planning workshops on topics that will have a strong relevance for the sponsors and members.

Support for IAPWS Activities

Textbook

BIAPWS has confirmed the ability to provide a modest amount of financial support for the editorial effort towards production of the IAPWS textbook. This is in addition to contributions to the text from members.

Computer Simulation Task Group

BIAPWS is hoping to be able to support membership of an appropriate representative on this group.

G.J Bignold

Attachment 17

The Czech National Committee

International Association for the Properties of Water and Steam

REPORT on IAPWS related activities - September 2000 / 2001

Submitted to the EC Meeting of IAPWS, Washington, USA - September 2001.

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Prof. J. Kadrno_ka, Fax: + 420 5 4114 3345, E-mail: vesela@eu.fme.vutbr.cz

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

Institute of Thermomechanics (IT) AS CR, Department of Thermodynamics, Dolej_kova 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 and Department of Physical Chemistry, Technická 5, CZ-166 28 Prague 6

University of West Bohemia (UWB), Faculty of Mechanical Engineering, Department of Theory and Design of Power Plants, Univerzitní 8, CZ-306 14 Plze_

SKODA ENERGO, Turbines, Plze_, Inc., Tylova 57, CZ-316 00 Plze_

Nuclear Research Institute plc. (NRI), _e_, CZ-250 68.

Activities were sponsored by the Czech Grant Agency, Grant Agency of the Academy of Sciences, Czech Rep., SKODA ENERGO-Turbines, Plze_ Inc., Ministry of Education, Youth and Physical Training, and Ministry of Industry and Trade.

- CZ NC PWS organized a course for the technical public dealing with computation of thermophysical properties of water and steam according to the new and revised Releases of IAPWS. Proceedings included equations for all pertinent thermophysical quantities, tables, software and h-s diagram [1]. Software was developed by Prof. Mares (UWB).

- Mares (UWB). and Sifner (IT) prepared, after mail-exchange with Dr. Friend, a short information about temperature conversion and recalculation of the thermal conductivity for discussion in the TG on transport properties.

- Hruby (IT) sent a letter to Dr. Palmer with information on the change of the author team preparing the Chapter 6: Binary Nucleation in Selected Aqueous Systems in the ATLAS. The idea of the contents of this chapter was submitted as well.

  The study of condensation and evaporation performed by this working team Refs. [4 to 7] was spread by the study of cavitation, Refs. [2 and 3].

- *Research activities at the CZECH TECHNICAL UNIVERSITY IN PRAGUE. DEPARTMENT OF FLUID MECHANICS AND POWER ENGINEERING have continued during the period 9/2000 – 6/2001 in further improvement of the hetero-homogeneous nucleation model.*

  The unary homogeneous nucleation model of pure steam was used as a principal nucleation process. In addition, the influence of impure steam was taken into account by means of the heterogeneous condensation occurring on the seeds present in the inlet steam. The model was then fitted to the optical extinction test data, thus, predicting unknown concentration and initial size of the seeds.

  Reasonable agreement was obtained for both C/D nozzle experiments and LP steam turbine tests. The method and results can be found in Refs. [8 and 9].

- __astn_ and Ji_í_ek studied the copper composition's deposits on the blades of HP part of steam turbine.
  Numerical models of the flow with condensation through turbine cascade together with boundary layer calculation model were tested. The flow with condensation in first wet stage of LP part of 200MW turbine is analyzed with these numerical models by __astn_ in cooperation with _ejna. Refs.[10,11,12].

- Kodl from SKODA ENERGO finished TTSE tests based on calculation of 10 schemas (15 operations) of conventional power plants and combined cycles with or without regeneration, reheat and external extractions and for various operation parameters. The TTSE97 in both forms (real*8,real*4) were implemented in the heat balance code and calculations were carried out three times for IF97, TTSE97 real*8, TTSE97 real*4.

  Result is specific heat consumption (shc) and its following relative values

  shc shc shc
  (TTSE97_real*8 - IF97) / IF97 * 100
  (TTSE97_real*4 - IF97) / IF97 * 100

  for all operations.

  The detailed evaluation was sent to Mr. Miyagawa. From the report we excerpt:

  "Time consumption was slightly lower with TTSE against IF97 (about 10% lower)
  and it was difficult to catch reasonable unique value. I must appreciate very good user's comfort with implementation due to wide choice of functions working in all IF97 regions with the same independent variables and working also in the metastable region.
  Results are nearly the same for TTSE real*8 and real*4 in our tests.
  Time consumption of loading TTSE to the memory is low and may be simply increased by using of RAM disk in case of repeating calculations. At last, memory consumption with newer hardware is also negligible.
  My opinion as a common user is, that TTSE may be very good alternative to IF97
  in bid software and with regard to higher speed in critical cases is more general."

- At the POWER ENGINEERING DEPARTMENT OF THE ICT, studies of feed water treatment, behavior of corrosive organic chemicals in steam/water cycle, chemical cleaning of boilers and turbine deposit evaluation are being conducted. Published articles are under Refs. [13 to18].

- DEPARTMENT OF PHYSICAL CHEMISTRY OF THE ICT measured partial molar volumes of organic solutes in water. Published articles are under Refs. [24 to 32].

- Research activities of the NUCLEAR RESEARCH INSTITUTE _E_ plc - Power Cycle Chemistry Working Group (PCC WG) included:

Loop experiments and material testing in the research reactor LVR-15 belong to the main activities of Reactor services division of Nuclear Research Institute _e_ plc. Investigation of an effect of simultaneous influence of irradiation, water chemistry and high parameters (pressure, temperature) on behavior of nuclear power plants structural materials and components is the main goal of the experimental program. The irradiation projects currently in progress are focused on the following research areas:

- investigation of fuel rod cladding materials (eg. Zircaloy-4 alloy) corrosion behavior at specific VVER water chemistry conditions,
- investigation of an effect of water chemistry on radionuclides transport and radioactivity build-up in the reactor primary systems (eg. effect of ammonia and hydrazine),
- investigation of an effect of water chemistry, stress level and irradiation on irradiation assisted stress corrosion cracking (IASCC) of reactor pressure vessel and in-core structures materials.

A significant share of our effort was devoted to co-operation with nuclear power plants (NPPs), mainly in field of water chemistry and radiation control. The following activities were carried out:

- A procedure for passivation of the primary system inner surfaces during hot functional tests was developed and applied at unit 1 of NPP Temelín. Surveillance samples (coupons) were placed into the primary circuits and subsequently analyzed to obtain an information about characteristics of the developed passive film (morphology, chemical and phase composition).
- A necessity of revision of the primary and secondary water chemistry guidelines for VVER-440 and VVER-1000 units were discussed with the Czech Utilities and agreed for realization. Main principles of the revised guidelines reflecting current status of knowledge and operational experience obtained have been worked out.

Young Scientists IAPWS Fellowships:

_edlbauer continued on the project *" Correlation and Prediction of Standard Thermodynamic Properties of Aqueous Solutes over a Wide Range of Temperatures and Pressures"*. The project was focused on three areas of interest in the description of standard thermodynamic properties of aqueous solutions at elevated conditions:

- acquisition of experimental data for non-electrolyte organic aqueous solutes,
- testing and comparison of different models for correlation of standard thermodynamic properties and their extrapolation beyond the regions where experimental data were obtained,
- development of software tool for an easy calculation of standard thermodynamic properties in a wide range of conditions.

An integral part of the project is collaboration on preparing the chapter “Calculation of standard thermodynamic properties of aqueous solutes in a wide range of temperatures and pressures” (co-authored by V. Majer, J. Sedlbauer and R.H. Wood) for the “ATLAS”. Most of the results, databases and recommendations obtained in the course of this Fellowship are included in this chapter.

Activities and results in the second year

- Research visit (duration six weeks) of J. Sedlbauer at the Blaise Pascal University, France, May – June 2001. (*Costs:* $3000*)* resulted in the paper [20]
- The paper is focused on application of the standard derivative thermodynamic properties of aqueous solutes for predicting standard chemical potential in a wide range of conditions. An overview of recent sources of experimental data is given for non-electrolyte solutes and a set of tests is reported regarding the ability of several thermodynamic models to correlate and predict the standard chemical potential.
- A new group contribution scheme was proposed for calculating the standard thermodynamic properties of aqueous hydrocarbons (aliphatic, cyclic and aromatic). The

new scheme was implemented into a freeware tool. A paper summarizing these results is in preparation for AIChE Journal.

RESULTS ACHIEVED DURING THE FIRST YEAR OF THE FELLOWSHIP WERE PRESENTED AT TWO INTERNATIONAL CONFERENCES AND AT THE IAPWS ANNUAL MEETING IN PRAGUE. THEY ARE INCLUDED IN REFS.[21,22,23].

- Draft of the chapter for "ATLAS" will be presented in September at the IAPWS Annual Meeting in Gaithersburg by V. Majer.
- The project was prolonged for about six months: the last visit at UBP is planned in winter 2001/02. We expect to finalize the chapter for "ATLAS" and to work on required revisions of the paper for AIChE during this stay.

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Attachment 18

Danish National IAPWS Committee - DIAPWS

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

14 February 2001

IAPWS REPORT 2000

The research activities in 2000 in Denmark in the field of properties of water and steam were mainly concentrated on continuation of activities from the previous year.

The investigations of solubility of salts in superheated steam was continued throughout 2000. Measurements on sodium sulphate and sodium chloride are reported. Investigations on copper oxide were the main activity in this project. The work is performed as an international collaboration project with 5 participants.

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, which improves its fit to the experimental data.

Publications in 2000:

K.Daucik, Akumulacia ionovych necistot vo vodoparnom cykluse (Accumulation of ionic impurities in water/steam cycle), Proc. Conf. Chemie energetickych obehu 3, Prag 6-8 Sept., 2000. (Slovak)

Attachment 19

FRENCH National Committee

Report on the IAPWS related scientific activities
Gaithersburg, September 2001

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OBJECTIVES

(1) Determination of an empirical and accurate potential for simulated water.
(2) Comparison between molecular dynamics simulations and various experimental data; thermodynamics, structure, transport properties and dynamics, dielectric constant.
(3) Understanding supercritical water and supercooled water.

PRINCIPAL RESULTS, CURRENT PROJECTS

- A new water model for computer simulations taking into account the electronic penetration by the use of diffuse charges on O and H atoms.
- Evaluation of liquid -liquid equilibrium in aqueous solutions by the Gibbs ensemble method: investigation of reapparent phases.

RECENT PUBLICATIONS

How to build a better pair potential for wate
B.Guillot and Y.Guissani
J. Chem. Phys, 114, 6720 (2001)

Simulation of the liquid-liquid coexistence curve of tetrahydrofuran+water mixture in the Gibbs ensemble
I.brovchenko and B.Guillot
Proceedings of the 14th Symposium on Thermophysical Properties (Boulder,2000), Fluid Phase Equilibria, 46-48, 1 (2001)

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OBJECTIVES

1/ Chemical thermodynamics of aqueous solutions of electrolytes and nonelectrolytes at superambient conditions up to the critical region of water

2/ Development of instruments and techniques for data acquisition at high temperatures and pressures

3/ Experimental determination of volumetric and calorimetric properties over a wide range of temperatures and pressures (*T* between 273 and 723 K, *p* between 1 and 40 MPa), measurement of solubilities up to 200°C

4/ Correlation and prediction of standard state properties of aqueous nonelectrolytes as a function of state parameters up to the critical region of water

PRINCIPAL RESULTS, CURRENT PROJECTS

- Treatment of experimental data for heat capacities of aqueous hydroxy and aminoderivatives of benzene and toluene (phenol, cresols, aniline, toluidines, aminophenols, diaminophenols, dihydroxybenzenes) up to 350 °C and 30 MPa.

- Testing of models for correlating and predicting standard thermodynamic properties of aqueous organic nonelectrolytes, development of a group contribution method for predicting hydration properties of hydrocarbons (aq) up to 300°C and 100 MPa

- Developing methodology for determining solubility of highly hydrophobe nonelectrolytes in water by saturation column technique, new measurements for n-alkanes C12, C14, C16 and C18 up to 200°C were carried out in spring 2001 in collaboration with the Claude Bernard University, Lyon (prof. Jose), new investigation regarding solubility of mono and dihalogenated octanes started in summer 2001.

- Critical evaluation of thermodynamic data on aqueous polyaromatics and n-alkanes as a function of temperature (solubilities, temperatures and heats of fusion).

- Measurement of volumetric properties of aqueous solutions of highly polar nonelectrolytes using vibrating tube densimetry (inisitol up to 200°C, dimethysulfoxide up to 250°C, phosphoric acid up to 300°C)

RECENT PUBLICATIONS

Thermodynamics of aqueous acetic and propionic acids and their anions in a wide range of temperatures and pressures.
V. MAJER, J. SEDLBAUER, L. H NEDKOVSKY, R.H. WOOD
Phys Chem., Chem. Phys. 2000, 2, 2907-2917.

Heat capacity of aqueous solutions at superambient conditions by differential flow calorimetry
L. HNEDKOVSKY, V. HYNEK, V. MAJER, R.H. WOOD
In Steam, Water and Hydrothermal systems Eds. P. Tremaine, P.G. Hill, D. Irish, P.V. Balakrishnan. NRC Press, Ottawa 2000, pages 191-198.

Correlations and predictions of standard thermodynamic properties of aqueous organic solutes in a wide range of conditions.
J. SEDLBAUER, E. M. YEZDIMER, V. MAJER, R.H. WOOD
In Steam, Water and Hydrothermal systems Eds. P. Tremaine, P.G. Hill, D. Irish, P.V. Balakrishnan. NRC Press,
Ottawa 2000, pages 175-182.

Amino acids under hydrothermal conditions; apparent molar volumes and apparent molar heat capacities from 25 to 250°C and pressures up to 300 bars.

R.G. CLARKE, P. TREMAINE, L. HNEDKOVSKY, V. MAJER
In Steam, Water and Hydrothermal systems Eds. P. Tremaine, P.G. Hill, D. Irish, P.V. Balakrishnan. NRC Press, Ottawa 2000, pages 221-228.
Data and models for calculating the standard thermodynamic properties of aqueous non-electrolyte solute
under hydrothermal conditions.
J. SEDLBAUER, V. MAJER
Europ. J. Mineral. 2000, 12, 1109-1122

Amino acids under hydrothermal coditions: Apparent molar heat capacities of aqueous _-alanine, _-alanine, glycine, and proline at temperatures from 298 to 500 K and pressures up to 30.0 MPa.
R.G. CLARKE, L. HNEDKOVSKY, P.R. TREMAINE, V. MAJER
J. Phys. Chem. B 2000, 104, 11781-11793.

A new version of differential flow heat capacity calorimeter; heat capacities of aqueous NaCl from 303 to 623
K. L. HNEDKOVSKY, V. HYNEK, V. MAJER, R.H. WOOD. J. Chem. Thermodyn. in press.

Measurement of densities using vibrating bodies. V. MAJER and A. PADUA, in Experimental Thermodynamics
Volume VI, Measurement of the thermodynamic properties of single phases,
Editeurs K. Marsh, W.A. Wakeham, A.R.H. Goodwin, Elsevier Amsterdam under press (about 20 pages).

EDF/Research & Development Division / Materials Studies Department

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E-mail : luc.guinard@edf.fr

OBJECTIVES

1/ Research on release mechanisms on stainless alloys, in PWR primary circuit conditions:
- effects of surface condition, thermomechanical treatments, electropolishing...
- modeling of corrosion and release
- development of a loop for release measurement (sensibility of detection : 2 nanometers thick)

2/ Research on corrosion of zircaloy claddings:
- basic mechanisms, properties of build up in oxides (ionic transfer, structure, composition)
- effect of hydrogen pick up on corrosion rate

3/ Development of chemical decontamination process for nuclear power plants

4/ Chemistry in confined areas in the secondary circuit

CEA-DEN/DPC/SCCME

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E-Mail: dominique.you@cea.fr

OBJECTIVES

- Prediction of the behaviour of corrosion product (spinels solubility measurements) in the PWR primary coolant circuit.
- Understanding the formation of concentrated solutions in local crevices of PWR steam generators.

PRINCIPAL RESULTS, CURRENT PROJECTS

1/ Solubility behaviour of cobalt, zinc and nickel ferrites of different compositions was studied. A thermodynamic model was developped to obtain nickel release during shutdown and the chemical conditions of formation of metallic nickel in the primary circuit. The solubility data were used to obtain the thermodynamic functions. The new data has been extensively used in the PACTOLE code to predict formation, activation, migration and deposition of activated corrosion products.

2/ In local crevices of PWR steam generators, the formation of concentrated solutions is the precursor phenomena to corrosion and degradation of S.G. tubes. The concentration processes, due to the boiling phenomena and to the thermal gradient between the primary and the secondary temperatures, are strongly dependent on the mass transfer processes and also on the chemical equilibrium in the liquid phases and on the equilibrium between the liquid and the vapour phases. A special apparatus has been developed to study the evolution of crevice chemistry and of the chemical equilibrium during concentration processes (EVA device). In order to be able to interpret chemical equilibrium, concentration process is performed in EVA device at constant temperature and constant volume and the mass balance is calculated (isochore and isotherm concentration process).
This investigation is in progress on the concentration processes of sodium, aluminium and silicon with or without boron. The following main results are:
   - EVA facility appears to be a simple and good tool for crevice chemistry investigations (chemical equilibrium and thermodynamic purposes). Good agreement between mass balance calculations and direct chemical analyses on samples has been observed.
   - Simultaneous hideout of boron with aluminium, silicon and sodium leads to the following main observations:
      - boron, aluminium and sodium concentrate in the crevice liquid phase. The good hideout of boron leads to a limitation of the crevice pH, as expected;
      - silicon reacts with nickel of the apparatus to form a solid compound $Ni_3Si_2O_5(OH)_4$. It is needed to verify if the same compound is formed with nickel base alloy (alloy 600, 690 or 800);
      - differences appear between the EVA experimental results and code (MULTEQ®) data, mainly due to the fact that the precipitation of nickel silicon solid phase occurs during EVA tests, while a sodium alumina silicate compound is predicted by the code.

   Evolution of the EVA facility is needed to measure crevice pH and redox potentials, which are considered as the main parameters for IGA/IGSCC.

RECENT PUBLICATIONS

PACTOLE V3: a new code version to predict corrosion product contamination
VIIIth Int. Conf. of Water Chemistry of Nuclear Reactor Systems, Bournemouth (UK)
C. Marchetto, D. Tarabelli, D. You, C. Andrieu, A. Long, D. Zeitoun
SCECF 258/LECA 16944 (2000)/DECM 2113/

Attachment 19

INSTITUT DES SCIENCES DE LA TERRE D'ORLÉANS (ISTO) / CNRS

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E-Mail: gleb@cnrs-orleans.fr

OBJECTIVES

1/ Study of the identity, stoichiometry, and structure of aqueous and gaseous complexes of geochemically relevant metals and metalloids in high temperature geothermal fluids (to 500°C).

2/ Prediction of the stability, solubility and thermodynamic properties of minerals and aqueous/gaseous species in high temperature aqueous and mixed (H_2O-CO_2...) fluids; calculations of chemical equilibria between minerals and fluids, study of water-rock interactions.

3/ Development of special chemical reactors and optical spectroscopic cells (Raman, EXAFS) for study of metal speciation and solubility in high temperature vapours and low-density fluids.

PRINCIPAL RESULTS, CURRENT PROJECTS

- Experimental determination (partition coefficient measurements coupled with EXAFS spectroscopy) of the stoichiometry and stability of As gaseous species to 500°C. It was found that $As(OH)_3°$ is the main As-bearing complex in hydrothermal boiling systems, responsible for the As vapor/liquid fractionation during magmatic-to-hydrothermal fluid evolution and ore deposit formation.

- Experimental determination of arsenopyrite (FeAsS) stability and solubility in aqueous solution at temperatures from 300 to 450°C and pressures from 100 to 1000 bar. Results permitted to generate a consistent set of FeAsS thermodynamic properties, and to apply these data to predict As transport in natural hydrothermal fluids.

- EXAFS in situ study of arsenious (As^{III}) and arsenic (As^{V}) acids speciation and structure in supercritical aqueous solutions to 500°C and 1000 bar (in coll. with J.L. Hazemann, Laboratoire de Cristallographie/ESRF, Grenoble).

- Measurements of vapor/liquid (H_2O-NaCl) partition coefficients for Au, Ag, Cu, Sb and Zn at 350-450°C and saturation pressure of the system, using recently developed high T-P chemical reactors.

- Experimental study of gold solubility in the system Au-H_2O-H_2S-NaCl-As(III), and gold incorporation into arsenopyrite at hydrothermal conditions (300-500°C, 500 bar) (in coll. with J. Schott, Laboratoire de Geochimie, Toulouse)

- Measurements of molal heat capacities and volumes for $As(OH)_3°$(aq) and $AsO(OH)_3°$(aq) up to the critical point of water (in coll. with V. Mayer, Laboratoire de Thermodynamique des Solutions et Polymers, Clermont-Ferrand).

RECENT PUBLICATIONS

An X-ray absorption fine structure spectroscopy study of germanium-organic ligand complexes in aqueous solution
POKROVSKI G., MARTIN F., HAZEMANN J.-L., SCHOTT J. (2000).
Chemical Geology, 2000, 163, 151-165.

Arsenic speciation and the stability of arsenopyrite (FeAsS) in supercritical fluids and hydrothermal steams.
POKROVSKI G., ROUX J., ZAKIROV I.
In: "Steams, Water, and Hydrothermal Systems: Physics and Chemistry Meeting for the Needs of Industry" Eds. P.R. Tremain, P.G. Hill, D.E. Irish, and P.V. Balakrishnan, NRC Press, Ottawa, 2000, p. 686-693.

Raman spectroscopic study of aluminum silicate complexing at 20°C in basic solutions.
GOUT R., POKROVSKI G., SCHOTT J., ZWICK A.
Journal of Solution Chemistry, 2000, 29, 1173-1186.

Attachment 19

Stability and solubility of arsenopyrite in crustal fluids.
POKROVSKI G., S. KARA, ROUX J. submitted to Geochimica et Cosmochimica Acta (august 2001)

Attachment 20

Research Activities on the Thermodynamic Properties of Water Substance in Germany 2000/2001

The following institutions have been working in 2000/2001 on the field mentioned above:

Hochschule Zittau/Görlitz (Prof. H.-J. Kretzschmar)

1. Supplementary backward equations $p(h,s)$ for water and steam

- The test calculations of the Evaluation Task Group of IAPWS were supported. The Task Group has confirmed and recommended the equations as supplement to the Industrial Formulation IAPWS-IF97.
- The Draft of the "Supplementary Release on Backward Equations for Pressure as a Function of Enthalpy and Entropy $p(h,s)$ to the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam" was revised und completed.
  The Supplementary Release is ready for adoption by IAPWS at its annual meeting in 2001.
- The iteration variants for calculating $p\&T(h,s)$ from the basic and backward equations of IAPWS-IF97 were investigated.

2. Development of backward equations $T(p,h)$ and $T(p,s)$ for the critical and supercritical regions of water and steam

- The division of IAPWS-IF97 region 3 into subregions was investigated.
- First equations $T(p,h)$ and $T(p,s)$ for IAPWS-IF97 region 3 were developed.

3. Test of the TTSE method for calculating the thermodynamic properties of water and steam in process modelling
   - The accuracy of the TTSE functions was compared with IAPWS-IF97.
   - The numerical consistency of the TTSE functions was investigated.
   - The computing speed of the TTSE functions was compared with that of the IAPWS-IF97 equations

4. Preparation of program packages including the Industrial Formulation IAPWS-IF97 for the power industry
   - The property library LibHuAir for humid air calculated as ideal mixture of the real fluids air, steam, and water was set up. The air is calculated by the NIST standard of Lemmon at al. Water and steam are calculated by IAPWS-IF97.
   - The Add-In FluidEXL*Graphics* for Excel® including graphical representation of the calculated data in thermodynamic charts was improved.
   - The Library FluidMAT for Mathcad® 2001 was completed.
5. Implementation of the Industrial Formulation IAPWS-IF97 on pocket calculators
   - The program FluidHP for the model HP 49G of Hewlett Packard® was set up.
   - The program FluidTI for the models TI 92 and TI 89 of Texas Instruments® was expanded to calculate the properties of combustion gases and humid air.
6. Program FluidDIA for generating camera ready thermodynamic diagrams
   - The program FluidDIA was expanded to calculate and plot *h*,*x*-diagrams for humid air at variable pressures.
7. Property libraries including the Industrial Formulation IAPWS-IF97 for education
   - The Versions for students of the programs

     Add-In FluidEXL for Excel®

     FluidMAT for Mathcad®

     FluidTI for the pocket calculators TI 92 and TI 89

     FluidHP for the pocket calculator HP 49G

     FluidCASIO for the pocket calculator CASIO FX 880P

     were revised.

Attachment 21

Current Status of Research Activities in Japan Submitted to the Executive Committee Meeting, IAPWS, Gaithersburg, MD, USA, September 2001

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 following research projects on the thermophysical and physico-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 is conducting a spectroscopic study of water-hydrocarbon mixtures at high temperatures and pressures. In a recent paper [*Bull. Chem. Soc*. *Japan*, (2001), in press], infrared and near infrared measurements of water- aromatic hydrocarbon mixtures in the temperature range 473 – 648 K and the pressure range 10 – 35 MPa have been reported. Concentrations of the hydrocarbons were obtained from the integrated intensities of the near infrared absorption. The density of the hydrocarbon-rich phase of the mixtures has been estimated by use of the hydrocarbon concentrations and the previously obtained water concentrations [*J. Chem. Phys*., **113** (2000), 1942-1949, 8390 (E)]. It has been found that both the water concentration and the density show remarkable pressure dependence near an extended line of the three-phase coexistence curve of the mixtures [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 new project on crevice water chemistry (theoretical analysis and experiments on water radiolysis in crack tips under gamma ray irradiation) as a part of studies on life management of aged nuclear power plants. Two high temperature high pressure water loops with controlling hydrogen peroxide concentrations and lower possible oxygen concentrations are under construction to determine the effects of hydrogen peroxide on intergranular stress corrosion cracking (IGSCC) under BWR simulated condition. [Latest publication: Y. Wada, et al., *J. Nucl. Sci. Technol*., **37** (2000), 901-912, and Y. Wada, et al., *J. Nucl. Sci. Technol*., **38** (2001), 183-192] [contact: Prof. S. Uchida; E-mail: shunsuke.uchida @qse.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, a group of Dr. K. FUJII is working on the density and viscosity standards. An absolute density measurement of silicon crystals with a relative uncertainty of 1×10^{-7} and a determination of the Avogadro constant by the X-ray crystal density (XRCD) method for an atomic mass standard are conducted [K. Fujii, A. Waseda, and M. Tanaka, "Density measurements of silicon crystals by hydrostatic weighing," *IEEE Trans. Instrum. Meas.*, **36** (2001), 616-621]. Using this solid density standard the density of standard liquids are measured by a magnetic suspension density meter. A relative uncertainty of 4×10^{-6} has been

achieved in the density measurement of organic liquids that are used as Standard Reference Materials (SRMs) for calibrating vibrating-tube density meters. In his group a new absolute viscosity measurement using falling ball method is also in progress. Nanometer measurements of the falling distance and diameters of small silicon balls are performed for providing reference data of transport properties of liquid water with a relative uncertainty of 0.01%. Dr. M. TANAKA is working as a chairman of the WG-Density, CCM (Consultative Committee for Mass and Related Quantities), to issue a new density-of-water table [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), in press]. This new table will be used as a metrological standard for the density of SMOW [contact: Dr. K. Fujii, Group Leader, Density and Viscosity Standards, NMIJ; E-mail: fujii.kenichi@aist.go.jp].

At the Department of Environmental Science & Technology, Faculty of Engineering, Shinshu University, Nagano City, Prof. H. TAKAKU works since Feb. 1 of 2000, and previously worked at Central Research Institute of Electric Power Industry (CRIEPI). Recently, he has started to study mainly the corrosion of the steam turbine materials for the geothermal power plants, and also the corrosion of Ti-Ni type shape memory alloys for the thermal engine actuator using the geothermal energy [contact: Prof. H. Takaku; E-mail: takakuh@gipwc.shinshu-u. ac.jp].

Mr. K. MIYAGAWA is developing Tabular Taylor Series Expansion Method (TTSE) for rapid calculation of thermodynamic properties of water substance and other fluids. To evaluate the method, IAPWS established a task group. He developed three examples for the evaluation by the task group. The first one is a set of TTSE tables and subroutines based on IAPWS-95 using pressure and enthalpy as the independent variables. The second is similar with the first but based on IAPWS-IF97. The third is based on IAPWS-IF97 using density and enthalpy as the independent variables. The task group will test the examples using practical application programs for power industries [contact: Mr. K. Miyagawa; E-mail: miyagawa.kiyoshi@nifty.ne.jp].

At the Department of Mechanical Sciences and Engineering, Tokyo Institute of Technology, Tokyo, Assoc. Prof. S. OKAWA and Prof. A. SAITO are studying the effect of solid particles and metallic surface on the freezing of supercooled water, and finding the importance of the total surface area exposed to the water [*Int.J. Refrig.*, **24** (1) (2001), 108-117] and oxidation of the surface [To be published in *Int. J. Refrig.*]. They are also studying the directional dependency of solidification of water using molecular dynamics method [*Proc. 7th Int. Symp. on Thermal Eng. and Sci. for Cold Regions* (2001), 47-51] [contact: Dr. S. Okawa; E-mail: sokawa@mech.titech.ac.jp].

At the Department of Surface Science, Central Research Institute of Electric Power Industry (CRIEPI), Komae, Tokyo, Dr. H. HIRANO and his coworkers are conducting feasibility studies associated with the decomposition and extraction technology of fossil fuels and the separation of metal by supercritical fluid. The decomposition and extraction reactions of organic compounds and fossil fuels using supercritical fluid are being investigated. In this study, the in-situ measuring system to examine the decomposition and extraction reactions will be developed. They are also challenging the separation of metals making use of wide variation of dielectric constant of supercritical water (SCW). The stability of materials in SCW will be evaluated [contact: Dr. H. Hirano, Director; E-mail: hirano@criepi.denken.or.jp].

At the Energy & Mechanical Engineering Department, Central Research Institute of Electric Power Industry (CRIEPI), Yokosuka, Kanagawa, Messrs. E. KODA and T. TAKAHASHI are studying some new power generation systems. In one of these studies, they are trying to make an estimation method for thermophysical properties of mixture of steam and carbon dioxide which can cover the wide temperature range [contact: Mr. E. Koda; E-mail: kouda@criepi.denken.or.jp].

At the Center for Mechanical Engineering and Applied Mechanics, Keio University, Yokohama, Prof. M. UEMATSU and his group are measuring the thermodynamic properties of methanol + water mixtures in a range of temperatures up to 420 K and at pressures up to 200 MPa. The measurements of thermodynamic properties of ammonia + water mixtures have been completed and results will be published in the *Journal of Chemical Thermodynamics*. An apparatus for measuring isobaric heat capacity for aqueous mixtures in a wide temperature range at high pressures is constructed. A paper entitled "Prediction of *PVT* Properties for Dissociated Steam by Molecular Simulation" by K. Kinoshita and M. Uematsu was translated and published in *Heat Transfer - Asian Research*, **29** (3) (2000), 181-192 [contact: Prof. M. Uematsu; E-mail: uematsu@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 71 data points of *pVTx* properties of aqueous dilute solutions of ammonia along four isochores in the range of temperatures from 265 K to 305 K, pressures from 0.8 MPa to 16.2 MPa, and compositions from 0.047 to 0.064 mol% of ammonia, which will be presented at the 6th Asian Thermophysical Properties Conference this October [contact: Prof. M. Uematsu; E-mail: oguchi@me.kanagawa-it.ac.jp].

At the Department of Electronic Chemistry, Tokyo Institute of Technology, Yokohama, Prof. S. OKAZAKI and his group are calculating static and dynamic properties of supercritical water by molecular dynamics method. They have reproduced the dielectric constant of subcritical and supercritical water excellently based upon a polarizable potential model [N. Yoshii et al., to appear in *Chem. Phys. Lett.* (2001)]. Recently, in particular, they have been interested in molecular mechanism of vibrational relaxation of solute in supercritical water. The method is dynamic analysis based upon mixed quantum-classical molecular dynamics [T. Terashima et al., *J. Chem. Phys*., **114** (2001), 5663] [contact: Prof. S. Okazaki; E-mail:okazaki@echem.titech.ac.jp].

At the Department of Applied Chemistry, Ritsumeikan University, Shiga, Prof. S. SAWAMURA is measuring the solubility of anthracene, phenanthrene, and alkylbenzenes in water at high pressures up to 400 MPa and the visicosity of water and heavy water at low temperature and high pressure region [S. Sawamura et al., *J. Solution Chem*., **29** (2000), 369-376; S. Sawamura et al., *J. Phys. Chem*. **B105** (2001), 2429-2436]. At the same Department, Prof. Y. TANIGUCHI and Assoc. Prof. M. KATO are measuring the infrared, Raman, and NMR spectra for biological compounds at high pressures [M. Kato et al, *Appl. Spectrosc*., **54** (2000), 963-967; M. Kato et al, *Spectrochim. Acta*, Part A, **56** (2000), 1693-1701; M. Kato et al., *Applied Spectrosc*. **54** (2000), 963-967; M. Kato et al., *Biospectroscopy*, **62** (2001), 29-39] [contact: Prof. S. Sawamura.; E-mail: sawamura@se.ritsumei.ac.jp].

At the Institute for Chemical Research, Kyoto University, Uji, Kyoto, Prof. M. NAKAHARA, Dr. N. MATUBAYASI, and co-workers continue to study the structure, dynamics, and reactions in subcritical and supercritical water by applying multinuclear nuclear magnetic resonance spectroscopy, Raman spectroscopy, and computer simulation techniques. The papers published for the past one year include: (1) "^{19}F NMR Study of Molecular Aggregation of Lithium Perfluorooctylsulfonate in Water at Temperatures from 30 to 250 ˚C"; D. P. Bossev, M. Matsumoto, M. Nakahara; *J. Phys. Chem. B*, **104** (2000), 155-158, (2) "Tumbling and spinning diffusions of acetonitrile in water and organic solvents"; C. Wakai, H. Siato, N. Matubayasi, M. Nakahara; *J. Chem. Phys*., **112** (2000), 1462-1473, (3) "Super- and subcritical hydration of nonpolar solutes. I. Thermodynamics of hydration"; N. Matubayasi, M. Nakahara; *J. Chem. Phys*., **112** (2000), 8089-8109, (4) "Analysis of Concentration Dependences of Electrical Conductances for 1:1 Electrolytes in Sub- and Supercritical Water"; K. Ibuki, M. Ueno, M. Nakahara; *J. Phys. Chem. B*, **104** (2000), 5139-5150, (5) "Which carbon oxide is more soluble? Ab initio study on carbon monooxide and dioxide in aqueous solution"; H. Sato, N. Matubayasi, M. Nakahara, F. Hirata; *Chem. Phys. Lett.*, **323** (2000), 257-262, (6) "Association and Dissociation of Nonpolar Solutes in Super- and Subcritical Water"; N. Matubayasi, M. Nakahara; *J. Phys. Chem. B*, **104** (2000)**,**10352-10358, (7) "NMR Study of

Hydrothermal Reactions of Dichloromethane with and without Alkali"; Y. Yamasaki, H. Enomoto, N. Yamasaki, M. Nakahara; *Bull. Chem. Soc. Jpn*., **73** (2000), 2687-2693, (8) "Structural study of supercritical water. III. Rotational dynamics"; N. Matubayasi, N. Nakao, M. Nakahara; *J. Chem. Phys.,* **114** (2001)**,** 4107-4115 [contact: Prof. M. Nakahara; E-mail: nakahara@scl.kyoto-u.ac.jp].

At the Department of Molecular Science and Technology, Doshisha University, Kyotanabe, Prof. M. UENO and his group are studying the conductances of electrolyte solutions at high temperatures and pressures in collaboration with Prof. M. Nakahara, Kyoto University, Uji. The validity of the Hubbard-Onsager continuum dielectric friction theory for the limiting ionic conductance is examined by its application to LiCl, NaCl, and KCl in sub- and supercritical water [to be published in *J. Mol. Liq*.] [contact: Prof. M. Ueno; E-mail: tito@mech.kyushu-u.ac.jp].

At the Department of Mechanical Engineering Science, Kyushu University, Fukuoka, Prof. T. ITO and Dr. Y. TAKATA have released the newest 12.1 version of the Computer Program Package for Thermophysical Properties, PROPATH, which includes those of water substances [contact: Prof. T. Ito; E-mail: tito@mech.kyushu-u.ac.jp or http://propath.mech.kyushu-u.ac.jp/].

At Mitsubishi Heavy Industries, Ltd., Nagasaki R&D Center, Mr. T. MORIMOTO and his co-workers are studying the oxygenated water treatment for super- and sub-critical thermal power plants and Mr. TATEISHI and his co-workers are now studying the hydrothermal decomposition of organic compounds such as poly- chlorinated bi-phenyl (PCB) and Dr. J. IZUMI and his co-workers are studying the water treatment for geothermal power plants and also studying the molecular simulation to assume the solubility in hot water [contact: Dr. J. Izumi; E-mail: junizumi @ngsrdc.mhi.co.jp].

Attachment 22

Report of Russian National Committee (2000-2001)

List of Publications

1. Grigoriev E.B. The Heat Conductivity of Binary Aquaous Solutions of Prazeodium Salts. Teplofizika Vysokikh Temperatur, 2000, vol. 38, No. 11, pp. 60-62.
2. Magomedov U.B. The Heat Conductivity of Binary and Multicomponent Aqueous Solutions of Nonorganic Substances at High Parameters of State. Teplofizika Vysokikh Temperatur, 2001, vol. 39, No. 2, pp. 241 - 245.
3. Martynova O.I. Die Energieversorgung von Moskau. VGB Kraftwerkstechnik, 2000, vol. 21, No.9, s. 100-101.
4. Martynova O.I. Role of Water and Fuel Technology Department of Moscow Power Institute in Improvement of Water Treatment, Chemistry, and Monitoring at Fossil and Nuclear Power Plants. Proceedings of the MEI Conference on Water Treatment and Chemistry, Chemistry Monitoring at Fossil and Nuclear Power Plants, and Fuel Utilization, Moscow, Russia, December 14-15, 2000. MEI, Moscow, Russia, 2000, p. 6.
5. McLure I.A., Petrov A.Yu., Gordon D.H., Ball M., Dooley R.B. Interfacial Behavior at Above-Ambient Temperatures of Ionic and Non-Ionic Aqueous Solutions Important in Boiler Water Chemical Conditioning. Proceedings of the Sixth International EPRI Conference on Fossil Plant Cycle Chemistry, Columbus, OH, USA, June 27-29, 2000. - EPRI 1001363, Palo Alto, CA, USA, 2001, pp. 16.1-16.15.
6. MEI Conference "Water Treatment and Chemistry, Chemistry Monitoring at Fossil and Nuclear Power Plants, and Fuel Utilization". Abstracts compiled by Petrov A.Yu. Power Plant Chemistry, 2000, vol. 2, No. 11, pp. 672-675.
7. Palmer D.A., Benezeth P., Petrov A.Yu., Anovitz L.M., and Simonson J.M. Behavior of Aqueous Electrolytes in Steam Cycles. The Solubility and Volatility of Cupric Oxide. EPRI TR-1000455, Palo Alto, CA, USA, 2000.
8. Palmer D.A., Bénézeth P., Simonson J.M., Petrov A.Yu. The Transport and Chemistry of Copper in Power Plants as Determined by Laboratory Experiments. Proceedings of the Sixth International EPRI Conference on Fossil Plant Cycle Chemistry, Columbus, OH, USA, June 27-29, 2000. - EPRI 1001363, Palo Alto, CA, USA, 2001, pp. 38.1-38.8.
9. Petrov A.Yu, Xiao C., Palmer D.A. Use of Chemiliminescence Method for Determination of Microconcentrations of Copper. Proceedings of the MEI Conference on Water Treatment and Chemistry, Chemistry Monitoring at Fossil and Nuclear Power Plants, and Fuel Utilization, Moscow, Russia, December 14-15, 2000. MEI, Moscow, Russia, 2000, p. 22.
10. Petrova T.I. Effect of Cycle Chemistries on the Behavior of Impurities in Water and Steam Cycle of Heat Power Plants. Vestnik MEI, 2001, No. 1, pp. 62-64.
11. Petrova T.I. Increase in Operational Reliability of Copper-Based Equipment. Energosberezhenie I Vodopodgotovka, 2000, No. 4, pp. 69-72.
12. Petrova T.I. Ingress of Organic Impurities into the Water-Steam Cycle of Fossil Power Plant and Their Effect on Working Fluid Purity. Proceedings of the MEI Conference on Water Treatment and Chemistry, Chemistry Monitoring at Fossil and Nuclear Power Plants, and Fuel Utilization, Moscow, Russia, December 14-15, 2000. MEI, Moscow, Russia, 2000, pp. 13-14.
13. Petrova T.I. Optimization of Water Chemistry of Copper-Based Equipment. Novoye v Rossiyskoi Elektroenergetike, 2001, No. 1, pp. 47-50.
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Dr. A.A. Aleksandrov, Professor

RNC Chairman

Attachment 23

US Activities Report, 2001 IAPWS Meeting
NIST, Gaithersburg, MD 2001

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We presently are working on predictions of hydration free energies of Na+, Cl-, and the NaCl ion-pair at high temperatures using our ABC/FEP method based on ab initio calculations. Our first calculation at 573 K and 0.725 g/cm3 gave for the sum of hydration free energies of Na+ and Cl- = -657 kJ/mol versus the experimental value of -661 so we are very pleased with our accuracy. We are doing a grid of state points with the help of a supercomputer and hope to use this data to develope an equation of state that fits our data for the ions and the ion-pair.

We are just finishing a manuscript for J. Phys Chem. that treats conductance data for NaCl and KCl at high concentrations and comparing multi-ion association models with pair association only models.

We are also in the process of measuring the conductance of aqueaous HCl, H2SO4, and NaHSO4.

Selected recent papers:

Infinite dilution partial molar properties of aqueous solutions of nonelectrolytes. II. Equations for the standard thermodynamic functions of hydration of volatile nonelectrolytes over wide ranges of conditions including the subcritical Temperatures by A. V. Plyasunov, John P. O'Connell, Robert H. Wood, and Everett L. Shock, Geochim. Cosmochim. Acta, 2000, 64, 2779-2795

Exploring the ab initio/Classical Free Energy Perturbation Method: The Hydration Free Energy of Water, by Shiniche Sakane, Eric M.Yezdimer, Wenbin Liu, Jose A. Barriocanal, Douglas J. Doren, and Robert H. Wood, J. Chem. Phys. 2000, 113, 2583-259

Thermodynamics of aqueous acetic and propionic acids and their anions in a wide range of temperatures and pressures, by Vladimir Majer, Josef Sedlbauer, Lubomir Hnedkovsky, and Robert H. Wood, Phys. Chem. Chem. Phys., 2000, 2, 2907-2917

Conductivity measurements of dilute aqueous LiOH, NaOH, and KOH solutions to high temperatures and pressures using a flow-through cell, by Patience C. Ho, Donald A. Palmer, and Robert H. Wood, J. Phys. Chem. B, 2000, 104, 12084-12089

Tests of Equations for the Electrical Conductance of Electrolyte Mixtures: measurements of association of NaCl (aq) and Na2 SO4 (aq) at high temperatures, by Andrei V. Sharygin, Ilham Mokbel, Caibin Xiao, and Robert H. Wood, J. Phys. Chem. 2001, 105, 229-237

Accepted

Prediction of the Gibbs free energy and PVT properties of water at extreme conditions from Quantum mechanics with classical simulations, by Shiniche Sakane, Wenbin Liu, Douglas J. Doren, and Robert H. Wood, Geochim. Cosmochim. Acta, accepted

Semiempirical equation of state for the infinite dilution thermodynamic functions of hydration of nonelectrolytes over wide ranges of temperature and pressure, by A.V.Plyasunov, J.P. O'Connell, R.H.Wood, and E.L Shock. Fluid Phase Equlibria, accepted.

The Energy Institute's Electrochemical Laboratory
The Pennsylvania State University

DIRECTOR: PROF. S.N. LVOV (814-863-8377, LVOV@PSU.EDU)

(1) pH measurements in high temperature subcritical and super critical aqueous solutions
(2) development of high temperature electrochemical systems, electrodes and probes for industrial applications (geothermal systems, supercritical water oxidation technology, hydrometallurgy, etc.)
(3) dissociation/association constant measurements in high temperature subcritical and supercritical aqueous solutions
(4) electrochemical/hydrothermal coatings of metal surfaces using ceramic materials
(5) zeta potential measurements on oxide/water interface at elevated temperatures
(6) high temperature polymer electrolyte hydrogen and direct methanol fuel cells

National Institute of Standards and Technology, NIST, Boulder CO
Contributors: D. G. Friend, A.H. Harvey, E.W. Lemmon, J.W. Magee, L.A. Watts, I.M. Abdulagatov, M.M. Aliev

A project is underway (in collaboration with theoretical chemists at the University of Nottingham) in which intermolecular pair potentials are derived from quantum mechanics and used to calculate second virial coefficients for water/gas binaries; these interactions are difficult to measure experimentally. Thus far, the water-helium system has been examined, and the resulting second virial coefficients have much less uncertainty than the available experimental data. Ongoing work is moving toward gases (such as air components) of more practical interest for areas including humidity standards and combustion gases.

Data for the vapor pressure of heavy water have been thoroughly reviewed and converted to the ITS-90 temperature scale, and a new correlation for the vapor pressure has been produced. This work has been accepted for publication in the Journal of Physical and Chemical Reference Data.

The joint effort between IAPWS and IUPAC on transport properties of water and steam is continuing, with an emphasis on establishing and validating data for the viscosity of the dilute gas.

K. Knobloch of the University of Applied Sciences of Zittau and Gorlitz completed her visit to the Boulder laboratories, and work was finalized on the proposed supplementary backward equations, p(h,s), for IAPWS-IF97.

A collaborative project has been established between the Dagestan Scientific Center of the Russian Academy of Sciences (DSCRAS) and the Physical and Chemical Properties Division of NIST in the broad areas of thermophysical properties measurements and models. Recent financial support from IAPWS has served to strengthen our collaboration. Four papers have been published, or are currently in press, and a fifth has been submitted concerning our joint studies of aqueous systems. IAPWS awarded financial support for experimental studies of methanol + water mixtures with calorimeters at NIST and at the DSCRAS. Mr. Aliev, a doctoral candidate at the DSCRAS, is now completing a six-month visit to NIST during which he carried out heat capacity measurements in the NIST labs. This grant provided Dr. Magee with partial support for travel to Russia to meet with Drs. Abdulagatov, Polikhronidi, and Bazaev. The discussions focused on experimental apparatus, calibrations, lab practices, and propagation of uncertainties in the measured quantities. In addition, short and long-range research plans were discussed and agreed upon.

We are completing VLE and density measurements on the system water + acetone + isopropyl alcohol + sodium nitrate (including some binary, ternary, and quaternary systems) from about 308 to 348 K; these should be published in the next year.

Attachment 23

University of Maryland, Institute for Physical Science and Technology and Department of Chemical Engineering, College Park, MD.

M. A. Anisimov, and J. V. Sengers
Collaborators: Kh. S. Abdulkadirova, A. Kostrowicka Wyczalkowska, V. A. Agayan

Major activities:

A comprehensive analysis of the thermodynamic properties of mixtures of H_2O and D_2O, which was started as an IAPWS project, was completed.

A novel type of phase behavior in aqueous electrolyte solutions was discovered.

Publications:

1. "Thermodynamic Properties of H_2O and D_2O in the Critical Region", A. Kostrowicka Wyczalkowska, Kh. S. Abdulkadirova, M. A. Anisimov, and J. V. Sengers, J. Chem. Phys. 113, pp. 4985-5002 (2000).

2. "Experimental Evidence for Crossover to Mean-Field Tricritical Behavior in a Concentrated Salt Solution", M. A. Anisimov, J. Jacob, A. Kumar, V. A. Agayan, and J. V. Sengers, Phys. Rev. Lett. 85, pp. 2336-2339 (2000).

3. "Novel Phase-Transition Behavior in an Aqueous Electrolyte Solution", J. Jacob, M. A. Anisimov, A. Kumar, V. A. Agayan, and J. V. Sengers, Int. J. Thermophys. 21, pp. 1321-1338 (2000).

4. "Crossover Criticality in Ionic Solutions", K. Gutkowski, M. A. Anisimov, and J. V. Sengers, J. Chem. Phys. 114, pp. 3133-3148 (2001).

5. "Novel Phase-Transition Behavior near Liquid-Liquid Critical Points of Aqueous Solutions: Formation of a Third Phase at the Interface", J. Jacob, M. A. Anisimov, J. V. Sengers, A. Oleinikova, H. Weingärtner, and A. Kumar, Phys. Chem. Chem. Phys. 3, pp. 829-831 (2001)

6. "Thermodynamic Properties of Mixtures of H_2O and D_2O in the Critical Region", Kh. S. Abdulkadirova, A. Kostrowicka Wyczalkowska, M. A. Anisimov, and J. V. Sengers, J. Chem. Phys., to be submitted.