Attachment 13

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

Report on IAPWS related scientific activities - September 1999-2000

Submitted to the Executive Committee Meeting, IAPWS
Prague, September 2000

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Unidad de Actividad Química, Comisión Nacional de Energía Atómica.

- The possibility of describing the thermodynamics of inifinitely dilute nonionic solutes in water has been explored. The procedure is based upon the calculation of the Krichevskii function using as input values for a single property of the binary system which cover a wide range of T,p. A spectrophotometric study of the dissociation constant of p-cresol in water up to 473 K is well advanced (R.Fernández Prini).

- Dielectric relaxation times of SPC/E water have been simulated at several thermodynamic states above the critical temperature with densities ranging from 0.05 up to 1.0 $g.cm^{-3}$. The simulations were performed on the NVE ensemble using N=256 molecules placed in a cubic box with periodic boundary conditions. The total length of the simulations was between 1.5 and 2.5 ns, with typical time steps of 2-3 fs. The simulated results are found in good agreement with recent experimental data (K.Okada et al. J.Chem.Phys. 107, 9302 (1997), and 110, 3026 (1999)) for densities ρ=0.4 $g.cm^{-3}$, but the sharp increases in the experimental Debye time as ρ decreases is not reproduced.
  Molecular dynamic simulations were performed for the dissociation process of HNO3 in aqueous clusters containing up to n=124 water molecules. Ionic dissociation has a threshold cluster size between n=3 and n=10 (D. Laria).

- The viscosity and electrical conductivity of aqueous solutions of trehalose and other saccharides containing NaCl and LiCl have been measured at 25°C. The decrease in the molar conductivity of each of these electrolytes with increasing viscosity is less than that predicted by Walden's rule. Instead, the empirical relation $\Lambda\eta^{\alpha}$= constant, which has already been found for other glass-forming liquids, holds for these mixtures. The microscopic origin of the

deviation from the viscous friction model could be related to the presence of local heterogeneities in the distribution of water about the ions. This hypothesis is confirmed by the results of extensive molecular simulations performed by Conrad and de Pablo at the University of Wisconsin (USA). The temperature dependence of the Walden product of NaCl in aqueous trehalose mixtures indicates that this salt is fully dissociated close to the glass transition temperature (H.R.Corti).

- A hydrothermal, microwave-assisted, procedure for the synthesis of crystalline Ni(II)-Cr(III) layered hydroxide particles was developed. Nucleation is interpreted in terms of the fast formation of mixed-polynulear hydroxo tetramers; subsequent processes depend on thermodynamic and kinetic factors. The role of microwave radiation during nucleation seems crucial.
  Chemisorption of dicarboxylic acids on titanium dioxide was studied. Various possible *surface complexation* models have been analyzed. The most satisfactory, yet economic, description is offer by FFG isotherms. The established stability trends emphasize the role of complexing ability and ligand acidity. (A.E. Regazzoni)

Publications:

J.A.Kukuljan, J.L.Alvarez and R.Fernández Prini.
Distribution of $B(OH)_3$ between water and steam at high temperatures
J.Chem.Thermodynamics, 31, 1511 (1999)

J.L.Alvarez, R.Fernández-Prini and M.L.Japas
Aqueous nonionc Solutes at Infinite Dilution: thermodynamic description, including the near-critical region.
Ind. Eng. Chem. Res., in press.

D.P.Miller, J.J. de Pablo and H.R.Corti.
Viscosity and Glass Transition Temperature of Aqueous Mixtures of Trehalose with Borax and Sodium Chloride.
J.Phys.Chem. B, 103, 10243 (1999)

M.S.Skaf and D.Laría.
Dielectric relaxation of supercritical water: Computer simulations.
J.Chem.Phys. 113, 3499 (2000).

M.D.Elola, E.J.Marceca, D.Laría and D.A.Estrín.
Computer simulation study of HNO3 dissociation in aqueous clusters.
Chem.Phys. Lett. 326, 509 (2000).

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L.N.Trevani, E.Calvo and H.R.Corti.
Diffusion coefficients o iodide in high temperature aqueous solutions.
Electrochem.Comm. **2**, 312 (2000)

H.R.Corti, L.N.Trevani, D.L.Goldfarb and S.Fucito;
Transport properties in aqueous systems: from high temperature to supercooled solutions.
Proceedings of the 13th. International Conference on th Properties of Water and Steam, Toronto 1999, in press.

D.A.Palmer, H.R.Corti, A.Grotewold and K.E.Hyde.
Potentiometric measurements of the thermodynamics of cadmium chloride complexation to high temperatures.
Proceedings of the 13th. International Conference on th Properties of Water and Steam, Toronto 1999, in press.

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, in press.

M.A. Blesa, A.D. Weisz, P.J. Morando, J.A. Salfity, G.E. Magaz and A.E. Regazzoni.
The Complexation Chemistry of Solid Metal Oxides Immersed in Aqueous Solutions.
Coord. Chem. Rev, 196, 31(2000).

M. Jobbágy and A.E. Regazzoni.
Hydrothermal Synthesis of Mixed Ni(II)–Cr(III) Hydroxides Using Microwave Reactors.
Presented at the *Sixth International Symposium on Hydrothermal Reactions*, Kochi, Japan, July 2000.

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, in press.

Attachment 14

REPORT on IAPWS Related Activities in the Czech Republic from September 1999 to September 2000

Submitted to the EC Meeting of IAPWS, Prague, Czech Republic
September 3 - 8, 2000.

In the work of the Czech National Committee for the Properties of Water and Steam participated traditional Institutions.

In the **Institute of Thermomechanics AS CR** a considerable capacity was devoted to the organization of the IAPWS Meeting, Prague 2000, and to the preparation of information materials, which were published on our INTERNET pages www.it.cas.cz/iapws2000 and contemporary on www.iapws.org under item Meetings.

An article dealing with the 13th ICPWS was linked to the Cz NC PWS homepage. Another article to the 70 anniversary of the international cooperation in research and standardization of properties of water and steam was published in ENERGETIKA **49,** 12 (1999) 404-406. For the IAPWS homepage an information on Cz NC PWS was prepared.

In cooperation with the **West Bohemian University, Department of Theory and Design of Power Plants,** continued works on the software and on the preparation of the Second Symposium to inform the Czech technical public about the transport properties and other properties of ordinary water substance standardized by the IAPWS.

In the **Institute of Thermomechanics** continued the International Collaborative Project "Laboratory Impure Steam Nucleation by Shock Tube Technique", sponsored by the Grant Agency of the Czech Republic, Institute of Thermomechanics, AS CR, Czech Technical University in Prague, ŠKODA Turbines Ltd., Plzen, and ENEL S.p.A. Milano.

Experiments planned in the 2nd Stage of the project were finished and the results were partially published at the IAPWS Meeting in Toronto, Sept.1999. The methodology worked out last year in the 1st Stage has been used without substantial changes. The adaptation of the existing experimental apparatus is more difficult, due the high aggression of ammonia and formic acid. The measurement of nucleation rates and droplet growth for the ammonia-water mixture (+ argon as carrier gas) are now underway. The 3rd Stage , conclusion and final report, are planned for the end of the year 2000. The results will be published in the ATLAS Project as well.

For the 4th Japan-Central Europe Joint Workshop on "ENERGY and INFORMATION in NONLINEAR SYSTEMS" is prepared a paper by Maršík, Blaha, Hrubý and Zíma
" Condensation and Cavitation Rates in Water with Admixtures".

Another two papers, regarding nucleation in water vapor and related mixtures, by Hrubý, Hošek, Blaha and Maršík *"Nucleation Pulse Measurements for Water Vapor at Elevated Temperatures"*, and *"Experimental Determination of Molecular Content of Nuclei by Independent Variation of Activities"*, by Hrubý and Strey, were presented in August at the 15th International Conference on Nucleation and Atmospheric Aerosols, Rolla, MO, USA.

Research activities at the **Czech Technical University in Prague, Division of Power Engineering,** continued with measurements of the liquid phase occurring in the LP 200 MW steam turbine.

Distribution of droplet sizes and steam wetness was predicted along the blade length at the turbine outlet with use of the optical extraction probe. The data will be used in the improvement of the computational modeling of the hetero-homogeneous droplet nucleation process in the 4 and 3 stage LP steam turbine (200 and 250 MW). In addition distribution of the electric charge of the droplets along the blade length was obtained by means of the electrostatic probe.

Fundamental results concerning the hetero-homogeneous droplet nucleation in a multistage steam turbine were presented in "*Contribution to the Nucleation Process in Steam Turbines"* by Petr and Kolovratník, in Proceedings of the 13th ICPWS, Toronto Can., 1999.

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Štastný, Tejc, Petr and Kolovratník analyzed experiments with the influence of several gases on the steam condensation in the LP part of 200 MW turbine performed in 1999. Štastný and Šejna developed a two population numerical model for calculation of the flow with condensation through turbine cascade, and analyzed the flow with condensation in the first wet stage of LP part of 200 MW turbine with a numerical model. Two articles has been published: Štastný, Dooley, Jonas and Šejna: *" Hetero-homogeneous Condensation of Steam Flowing through Turbine Cascade*" Proceedings of the 13th ICPWS, Toronto, September 1999, and Štastný and Šejna: *"Analysis of Hetero-homogeneous Condensation of Steam Flow in a Turbine Cascade by Two Population Numerical Model"*, to be presented at the IAPWS Symposium, Prague 2000.

In the **Department of the Physical Chemistry of the Institute of Chemical Technology in Prague** were published following papers:

Hnedkovský, Hynek, Majer and Wood " *Heat capacities of aqueous solutions at Superambient Conditions by Differential Flow Calorimetry"*,

Clarke, Tremaine, Hnedkovský and Majer *"Amino Acids under Hydro-thermal Conditions: Apparent Molar Volumes and Apparent Molar Heat Capacities from 25 to 250 ºC and Pressures up to 300 bars"*, both in Proceedings of 13th ICPWS, Toronto, 1999,

Hnedkovský and Cibulka *"On the Temperature and Pressure Correlation of Partial Molar Volumes at Infinite Dilution for Aqueous Non-electrolytes"* 18th European Seminar on Applied Thermodynamics, Kutná Hora, Czech Republic, June 8-11, 2000 - poster presentation.

Workers of the **Department of Power Engineering of the Institute of Chemical Technology** presented following contributions on various meetings:

Bohmová V, Jirícek I., Olyšar: *Corrosion Resistance of PVD Coatings on Stainless Steel Substrate*, Sixth Sheffield ABS Days, Sheffield, UK, July 2000

Major A., Jirícek I. et all.: *Humics Thermolysis in Steam/Water Cycle*, Conference "Maintenance of SG NPS VVER", Ostravice, June 2000, pp. 1-7

Jirícek I., Kalivodová J.: *Turbine Deposit Composition and Effect on Blade Steel Material II*., RP 218-020/00 for Skoda, Energo, Pilzen, PED of ICT Prague, Feb. 2000, 40p.

Bohmová V., Jirícek I., and Vošta J.: *Ceramic Coatings on Blade Steel Material-Behavior in Saline Solution*, Conference AKI 99, Rožnov, Nov. 1999

Šedelbauer will submit at the PCAS meeting a progress report for the first year of the Young Scientists IAPWS Fellowship on *" Correlation and Prediction of Standard Thermodynamic Properties of Aqueous Solutes over a Wide Range of Temperatures and Pressures"*.

As a part of the project co-sponsored by IAPWS, heat capacities of several dilute aqueous derivatives of benzene were measured by Hnedkovský, Censký and Majer with the aid of a recently constructed flow calorimeter. The new data covered a range of temperatures from 300 to 623 K and together with previously obtained partial molar volumes significantly extended the database of thermodynamic properties of aqueous non-electrolytes at high temperatures. The results of the measurements were used to calculate partial molar heat capacities at infinite dilution. Data were further analyzed to see, how they are affected by the presence and the position of the functional groups on the benzene ring. Several correlation functions were also tested from the point of view of their ability to describe the temperature and pressure dependence of partial molar heat capacities.

In the Nuclear Research Institute REZ, pcl, following water chemistry and material testing works were underway:

Loop experiments, and material testing in the research reactor LVR-15, belong to the main activities of Reactor Services Division of the Nuclear Research Institute REZ. 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 programs. The irradiation projects focused on investigation of fuel rods cladding materials behavior, water

chemistry aspects of radionuclides transport and irradiation effect on structural material corrosion including irradiation assisted stress corrosion cracking (IASCC) were carried out.

- Project investigating Zinc injection effect on transport and contamination the inner surfaces by corrosion product radionuclides (Co60, Co58, Mn54, Fe59 etc.) has been performed in co-operation with AEA Technology (UK). Two single-purpose loops modeling water chemistry, thermal-hydraulic conditions, and structural material inventory of the PWR primary circuits have been irradiated in LVR-15 reactor. A wide-range post-irradiation examination has been performed at selected material samples.
- In the period covered a construction of new reactor water loop RVS-4 was finished, hot functional tests performed, and the primary system surfaces passivated. This loop will be used for the projects which are focused on Zircaloy-4 cladding corrosion behavior and effect of water chemistry on radionuclides transport under the VVER primary circuit conditions.
- Within the framework of the Czech Nuclear Regulatory Body (SÚJB) project, Zircaloy-4 cladding samples were pre-oxidized in a high-temperature autoclave for 18 months with the objective to prepare samples for the loop irradiation.

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, theoretical studies and mathematical modeling of physical-chemical processes and phenomena:

- A procedure for passivation of the primary system inner surfaces during hot functional tests was developed and applied at 1st and 2nd NPP Mochovce units, and 1st NPP Temelín unit. 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).
- As a contribution to Axial Offset Anomaly (AOA) issue, we have prepared for EPRI a study based on the loop experimental data on potassium and lithium influence on corrosion processes and crud deposition in VVER and PWR environments.
- A model describing dissolved gasses behavior and radiolytical processes at subcooled boiling conditions in pressurized water reactors was developed and verified in co-operation with Prague Institute of Chemical Technology.

The member dues to IAPWS were paid on May 30, 2000.

Ši: Report to EC 290800

Attachment 15

Danish National IAPWS Committee - DIAPWS

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

14. February 2000

IAPWS report 1999

1999 research activities in Denmark in the field of properties of water and steam were mainly concentrated on continuation of activities from previous year.

The investigations of solubility of salts in superheated steam was continued throughout 1999. Measurements on sodium sulphate are accomplished and reported together with the results on sodium chloride from 1998. Investigations on copper oxide and sodium hydroxide are scheduled for year 2000. The work is performed as an international collaboration project with 5 participants.

Equilibrium between carbon dioxide and ammonia in water/steam environment were studied at the Department of Chemical Engineering, the Technical University of Denmark. Resulting model for the thermodynamic properties was presented at the 13th International Conference on Properties of Water and Steam.

A simple method for prediction of activity coefficients in mixed electrolyte solutions was derived and presented at the 13th International Conference on Properties of Water and Steam.

Evaluation of operational data from an ultra supercritical unit resulted in a mathematical model for oxidation of steel on the basis of measurements of hydrogen concentration in steam. The model gives reasonable agreement with models based on investigation of tube samples. The work was presented at the 13th International Conference on Properties of Water and Steam.

Publications in 1999:

J.P.Jensen, P.Rasmussen; Prediction of Activity Coefficients in Aqueous Mixed Electrolyte Solutions, 13th Int. Conf. on Properties of Water and Steam, Toronto, Canada, 12 - 16 Sep. 1999.

K.Thomsen, P.Rasmussen; Thermodynamic model for the Ammonia-Water System, 13th International Conference on Properties of Water and Steam, Toronto, Canada, 12 - 16 Sep. 1999.

K.Daucik, J.P.Jensen, N.Henriksen; Supercritical Steam Oxidation of Steel Surfaces, 13th International Conference on Properties of Water and Steam, Toronto, Canada, 12 - 16 Sep. 1999.

K.Daucik; Steam/Water Cycle Chemistry of Ultra Supercritical Units, Power Plant Chemistry, **1,** 2 (Aug. 1999), p. 8 - 12 (eng.) p. 43 - 47 (ger.)

A.Bursik, J.P.Jensen; Comments on Carbon Dioxide Behavior in Power Plant Cycles, Power Plant Chemistry, vol.1, no.3, p.28-31.

K.Thomsen, P.Rasmussen; Modeling of vapor-liquid-solid equilibrium in gas-aqueous electrolyte systems, Chem.Eng.Sci. 54 (1999), 1787-1802.

Attachment 16

FRENCH National Committee

Report on IAPWS related scientific activities
Prague, September 2000

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OBJECTIVES, SUBJECTS

Prediction of the behaviour of radioelement (U) in water.

1/ Hydrolysis of uranyl (VI) in aqueous solution by spectroscopy (FTIR ATR, absorption UV-visible, and luminescence) at 25°C, 0.1MPa.
2/ Uranyl (VI) chloride complexes in aqueous solution by spectroscopy (FTIR ATR, absorption UV-visible, and Raman) at 25°C, 0.1MPa.
3/ Adsorption of uranyl (VI) onto goethite in aqueous solution at 25°C, 0.1MPa.

PRINCIPAL RESULTS, CURRENT PROJECTS

1/ Determination of characteristic antisymmetric stretching of linear uranyl ion of 8 uranyl hydroxides:
- $(UO_2)^{2+}$
- one dimer: $[(UO_2)_2(OH)_2]^{2+}$,
- five trimers $[(UO_2)_3(OH)_z]^{(6-z)}$ (z = 5,7,8,10, and 11), and
- one monomer $[(UO_2)(OH)_4]^{2-}$

over a large pH range 2 - 15, at 25□C, 0.1MPa.

2/ Determination of excitation spectra of three uranyl hydroxides:
- $(UO_2)^{2+}$
- $[(UO_2)_2(OH)_2]^{2+}$, and
- $[(UO_2)_3(OH)_5]^{+}$

over a pH range 2 - 5, at 25□C, 0.1MPa.

3/ Determination of characteristic antisymmetric stretching of linear uranyl ion and absorption UV-visible spectra of five uranyl chlorides of the type $[(UO_2)(Cl_x)]^{(2-x)}$ (x = 1-5) in acidic solutions (pH = 1.40), at 25°C, 0.1MPa.

4/ Quantitative adsorption of uranyl (VI) onto goethite in non complexing aqueous solution (NaClO4) (pH = 3-13) at 25°C, 0.1MPa

RECENT PUBLICATIONS

NGUYEN-TRUNG C., PALMER D., BEGUN G., PEIFFERT C., MESMER R. (2000) - Aqueous uranium complexes 1. A Raman Spectroscopic Study of the Hydrolysis of Dioxouranium (VI) Ion in Solutions of Trifluoromethanesulfonic Acid and Tetramethylammonium Hydroxide at 25°C, 0.1 MPa. J. Sol. Chem., 29, 2, pp. 101-129

NGUYEN-TRUNG C. , PALMER D.A., PEIFFERT C., and GIFFAUT E. (2000) - Experimental Study of the Solubility of amorphous and crystalline TcO2 in Aqueous Solution at 25°C, 0.1MPa. Submitted to Inorg. Chem..

PERRONE J., NGUYEN-TRUNG C., LAMBERT J. and EHRHARDT J.J. (2000) - Experimental study of the adsorption of uranyl (VI) onto synthetic goethite in NaClO4 solutions in a large pH range (3 - 13) at 25°C, 0.1MPa. Submitted to Radiochim. Acta.

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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

An accurate pair potential for simulated water
B.Guillot and Y.Guissani
In Steam, Water and Hydrothermal systems Eds. P. Tremaine, P.G. Hill, D. Irish, P.V. Balakrishnan. NRC Press, Ottawa 2000.

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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, to appear

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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 and excess properties as a function of state parameters up to the critical region of water

PRINCIPAL RESULTS, CURRENT PROJECTS

- Experimental determination of enthalpies of solution and densities for dilute solutions of three isomeric dimethylbenzenes and ethylbenzene in water between 250 and 350°C.
- 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
- Developing methodology for determining solubility of hydrocarbons in water, dynamic method for liquid and solid hydrocarbons, tests with polyaromatics(aq), dodecane(aq) and hexadecane(aq) up to 200°C, in collaboration with the Claude Bernard University, Lyon (Prof. Jose)
- Critical evaluation of thermodynamic data on aqueous polyaromatics and n-alkanes (solubilities, temperatures and heats of fusion)

RECENT PUBLICATIONS

New approaches to calculation of the Henry's constant of aqueous solutes at superambient conditions. V. MAJER.*
High Pressure Chemical Engineering, Proceedings of the International Meeting of GVC-Fachausschuss "Hochdruckverfahrentechnik", Karlsruhe 1999, pages 141-146.

Attachment 16

Temperature correlation of partial molar volumes of aqueous hydrocarbons at infinite dilution: test of equations.
V. MAJER, S. DEGRANGE, J. SEDLBAUER.*
Fluid Phase Equilibria, 1999, 158, 419-428.

Combined flow-mixing power compensation calorimeter and vibrating tube densitometer for measurements at superambient conditions.
V. HYNEK, S. DEGRANGE, M. POLEDNICEK, V. MAJER, J.R. QUINT, J-P.E. GROLIER.*
J Solution Chem., 1999, 28, 637-672.

Volumes of aqueous alcohols, ethers and ketones up to 523 K and 28 MPa.
M. SCHULTE, E. SHOCK., M. OBSIL, V. MAJER.*
J. Chem. Thermodyn., 1999, 31, 1195-1229.

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.

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.

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.

Data and models for calculating the standard thermodynamic properties of aqueous non-electrolyte solutes under hydrothermal conditions.
J. SEDLBAUER, V. MAJER
Europ. J. Mineral. in press.

Amino acids under hydrothermal conditions: Apparent molar heat capacities of aqueous α-alanine, β-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. submitted.

Heats of mixing of benzene and water at superambient conditions up to 563 K.
N. FAUCHER, J.-Y. COXAM, S. DEGRANGE, V. MAJER.
Int. El. J. Phys. Chem. Data, submitted.

Attachment 16

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. to be submitted to J. Chem. Thermodyn. in September 2000.

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OBJECTIVES

1/ Research on release mechanisms on stainless alloys, in PWR primary circuit conditions :
- effects of surface condition, thermomechanical treatments, electropolishing...
- modelling 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-CEREM/SCECF

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Fax: 33 (0)1 69 08 15 86
E-Mail: dominique.you@cea.fr

OBJECTIVES

- Prediction of the behaviour of corrosion product (spinels solubility measurements) in the PWR primary coolant circuit.
- Understand 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 were measured to determined solubilities. A thermodynamic model was develop 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 PACTOLE code to predicate the 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 of the mass transfer processes and also of the chemical equilibrium in the liquid phases and of 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 also at constant volume to perform mass balance calculations (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 have 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

A chemical study of concentration processes in steam generator crevices: influence of boron on the hideout of sodium, aluminium and silicon
Water Chemistry'98 - Kashiwazaki (Japan)
D. You, Y. Lefèvre, D. Féron
SCECF / LECA 16133

Attachment 17

Current Status of Research Activities in Japan
Submitted to the Executive Committee Meeting, IAPWS
Prague, September 2000

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)
5-3-1, Kohjimachi, 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 spectroscopic study of water-hydrocarbon mixtures at high temperatures and pressures. In a recent paper [*J. Chem. Phys*., **113** (2000), 1942-1949], infrared measurements of water-benzene mixtures at temperatures 473 – 648 K and at pressures 10 – 35 MPa have been reported. The OH stretching band intensity of HDO dissolved in benzene was obtained as a measure of water concentration. The temperature-pressure dependent change of the water concentration can be understood with the aid of a phase diagram of the water-benzene mixture. From coalescence of the hydrogen-bonded and hydrogen-bond-free OH stretching bands observed at higher temperatures, rotational dynamics of water molecules in a hydrogen-bonded water cluster has been discussed. (contact: Prof. S. Ikawa; E-mail: sikawa@sci.hokudai.ac.jp).

At the Department of Quantumn Science and Energy Engineering, Graduate School of Engineering, Tohoku University, Sendai, Prof. S. UCHIDA who has recently moved from Hitachi, Ltd. where he used to promote experimental studies on the effects of hydrogen peroxide on stress corrosion cracking of stainless steel in water at elevated temperatures, is going to carry out a new project on crevice 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 unclear power plants [see: Uchida, S. et al., *J. Nucl. Sci. Technol*., **37** (2000), 257-266]. (contact: Prof. S. Uchida; E-mail: shunske.uchida@qse.tohoku.ac.jp).

At the Hitachi Research Laboratory, Hitachi Ltd., Hitachi, H. YAMAUCHI and M. HIROTA are studying corrosion behaviors and corrosion prevention techniques for fossil power plants. Optimization of feed water conditions to mitigate corrosive environment for both a turbine and a boiler is one of the aims. Furthermore, searching new deoxygenating reagents instead of hydrazine and evaluating SCC susceptibility of turbine materials are conducted. (contact: H. Yamauchi, Senior Researcher; E-mail: hyamau@hrl.hitachi.co.jp).

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At the Thermophysical Metrology Department, National Research Laboratory of Metrology (NRLM), Tsukuba, a group of Dr. K. FUJII is working on the density and viscosity standards. Absolute density measurements based on solid density standards and a determination of the Avogadro constant by the X-ray crystal density method are conducted [see: Fujii, K., Tanaka, M., Nezu, Y., Nakayama, K., Fujimoto, H., De Bièvre, P., and Valkiers, S., *Metrologia*, **36** (1999), 455-464]. A new absolute viscosity measurement using falling ball method and an accurate measurement of sound velocity [Fujii, K. and Masui, R., *J. Acount. Soc. Am*., **93** (1993), 276-282] are also in progress for providing reference data of thermodynamic and transport properties of liquid water. Dr. M. TANAKA is working as one of the members of the WG-Density, CCM (Consultative Committee for Mass and Related Quantities), for compiling a new density-of-water table based on updated absolute measurements of the density of water at the NRLM [Masui, R., Fujii, K. and Takenaka, M., *Metrologia*, **32** (1995/96), 333-362] and at the CSIRO (Australia). (contact: Dr. K. Fujii, Group Leader, Density and Viscosity Standards, NRLM; E-mail: fujii@nrlm.go.jp).

At the Department of Environmental Science and Technology, Shinshu University, Nagano, Prof. H. TAKAKU is planning various kinds of studies on the corrosion and water chemistry in power plants, including the corrosion test of steam turbine materials in the simulated phase transition zone since February, 2000. (contact: Prof. H. Takaku; E-mail: takakuh@gipwc.shinshu-u.ac.jp).

K. MIYAGAWA is collaborating with Prof. P. G. Hill, University of British Columbia, Canada, on the development of Tabular Taylor Series Expansion Method (TTSE) for rapid calculation of steam properties. They will propose the method as a guideline of IAPWS. The background papers of the drafted guideline are: [(1) Miyagawa, K. and Hill, P.G., to appear in *J. of Eng. for Gas Turbine and Power, Trans. ASME* (2000); (2) Miyagawa, K. and Hill, P.G., *J. of Eng. for Gas Turbine and Power, Trans. ASME* **119** (1997), 485-491; (3) Hill, P.G., Miyagawa, K., and Denton, J.D., to appear in *J. Mech. Eng. Sci., Proc. I. Mech. E*. (2000)]. (contact: 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 the difference in ice structure on melting process under atmospheric pressure using molecular dynamics method. [see: *Int. J. Trans. Phenomena*, **2** (2000), 103-111]. They are also studying the effect of solid particles on the freezing of supercooled water, and finding the importance of the total surface area exposed to the water rather than the weight itself. [to be published in *Int. J. Refrigeration*]. (contact: Dr. S. Okawa; E-mail: sokawa@mech.titech.ac.jp).

At the Department of Surface Science, Central Research Institute of Electric Power Industry, Komae, Tokyo, Dr. H. HIRANO and his coworkers are studying the mechanism of scale adhesion at the inlet of flow hole between tube and tube supportplate under PWR secondary water chemistry conditions. For that purpose, they are trying to measure the zeta potentials of colloidal Fe304 particles and stainless steel in high temperature water. (contact: Dr. H. Hirano, Director; E-mail:hirano@criepi.denken.or.jp).

At the Department of Mechanical Engineering, Keio University, Yokohama, Prof. M. UEMATSU and his group are measuring the thermodynamic properties of methanol + water mixtures and ammonia + water mixtures in a range of temperatures up to 420 K at pressures up to 200 MPa. A paper on formulation of ammonia + water mixtures is publishued in *Nippon Kikai Gakkai Ronbunshu*, B Hen, **66**-649 (2000). (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 dissociation process of methane hydrate using molecular dynamics simulation [see: Yasuoka, K. and Murakoshi, S., *Ann. N. Y. Acad. Sci*., **912** (2000), 678-684]. They simulate the vapor-liquid nucleation phenomena. The nucleation rate and critical nucleus are estimated [see: Yasuoka, K. and Matsumoto, M., *J. Chem. Phys.*, **109** (1998), 8463-8470]. (contact: Dr. K. Yasuoka; E-mail: yasuoka@mech.keio.ac.jp).

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At the Department of Mechanical Engineering, Kanagawa Institute of Technology, Atsugi, Prof. K. OGUCHI and his group are measuring the *PVT* properties of ammonia + water mixtures along four isochores including pure water in the range of temperatures from 260 K to 380 K and pressures up to 17 MPa. They found the maximum density for mixture with 0.0591 mole fraction of ammonia at 271.12 K, 0.468 MPa and 982.3 kg/m^3.(contact: Prof. K. Oguchi; 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 based upon polarizable potential model [see: *Chem. Phys. Lett.*, **317** (2000), 414-420]. In particular, their recent results show that dielectric constant has been excellently reproduced for water from ambient state to sub- and supercritical states. (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 inorganic and organic compounds under high pressures up to 400 MPa and the viscosity of water at low temperature and high pressure region [see: Sawamura, S. et al., *J. Phys. Chem*., **103** (1999), 2981-2983; Sawamura, S. et al., *J. Sol. Chem*., **29** (2000), 369]. 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 [see: Taniguchi, Y. et al., *Biochim. Biophys. Acta*, **1433** (1993), 45; Taniguchi, Y. et al., *Spectrochim. Acta*, **A455** (1999), 2659]. (contact: Prof. S. Sawamura; sawamura@se.ritsumei.ac.jp).

At the Institute for Chemical Research, Kyoto University, Uji, Kyoto, Prof. M. NAKAHARA, Dr. N.. MATSUBAYASHI and coworkers are engaged in multi-nuclear magnetic resonance spectroscopic and computer simulation studies on water and aqueous solutions under sub- and supercritical conditions. In a recent paper ["Super-and subcritical hydration of nonpolar solutes.", *J. Phys. Chem*., (2000), in press], a comprehensive computer simulation study has been carried out in order to establish the molecular picture of the thermodynamics of hydrophobic solutes under the extreme conditions. The chemical potentials for methane and hard sphere solutes are computed as functions of temperature and density over a wide range. The cavity distribution in supercritical water has been analyzed and the applicability of the scaled-particle theory has been tested. Their analysis of electrolytic conductance and ion-pair formation in supercritical water has been published [see: Ibuki, K., Ueno, M. and Nakahara, M., *J. Chem. Phys*. B, **104** (2000), 5139-5150]. A NMR study of rotational dynamics of super- and subcritical water has been finished and submitted for publication. A variety of organic reactions in super- and subcritical water are being systematically studied in order to get insight into the bond-rearrangement mechanism. (contact: Prof. M. Nakahara; E-mail: nakahara@scl.kyoto-u.ac.jp).

At the Deaprtment 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. In a recent paper, the analysis of concentration dependence of electrical conductances for 1:1 electrolytes in sub- and supercritical water has been reported [see: Ibuki, K., Ueno, M. and Nakahara, M., *J. Chem. Phys*. B, **104** (2000), 5139-5150]. They are also engaged in NMR studies on aqueous solutions, paying attention to the temperature and pressure effects on the dynamics of water molecules in the vicinity of various solutes [see: Yoshida, K., Ibuki, K. and Ueno, M., *J. Chem. Phys*., **108** (1998), 1360-1367]. (contact: Prof. M. Ueno; E-mail: mueno@mail.doshisha.ac.jp).

At the Department of Mechanical Science and Engineering, Kyushu University, Fukuoka, Prof. T. ITO and Dr. Y. TAKATA have released the newest 11.1 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).

Attachment 18

Report of Russian National Committee (1999-2000)

List of Publications

1. Alexandrov A.A. The Temperature and Enthalpy of Boiling Aqueous Solutions of Sodium Chloride and Sodium Sulfate. Thermal Engineering, 2000, No. 6, pp.561-566.
2. Beketov V.G. Partial Pressure of Steam in Humid Air and Relative Humidity. High Temperature, 1999, vol. 37, No. 6, pp. 876–880.
3. Beketov V.G. The Results of Investigation of Ice and Water Solubility in Compressed Gases. High Temperature, 2000, vol. 38, No. 1, p. 137-146.
4. Dubrovsky I.Ya., Batalina L.N., Kurshakov A.V., Loshkarev V.A., Polevoi E.N., Ryzhenkov V.A., Anikeev A.V. On the Use of Octadecylamine in Thermal Engineering. Vestnik MEI, 2000, No. 2, pp. 79-82.
5. Filippov G.A., Kukushkin A.N., Saltanov G.A., Velichko E. V., Voronina M.P. Kurshakov A.V., Mikhailov V.A., Petrova T.I., Ryzhenkov V.A., Chempik E., Balayan R. S. Preservation of Thermal Power Equipment Using Reagents Based on Film-Forming Amines. Thermal Engineering, 1999, vol. 46, No. 9, pp. 789-794.
6. Fokin L.R., Kalashnikov A.N. Reference Data for Viscosity of Rare Steam at Temperatures up to 2000 –2500 K. High Temperature, 2000, vol. 38, No.2, pp. 242–248.
7. Grigoriev B.A, Grirориev E.B., Safronov G.A. Experimental Investigation of Thermal Conductivity of Binary Aqueous Solutions of Potassium Haloids. Thermal Engineering, 2000, No. 6, pp.564-560.
8. Kopylov A.S., Kulov V.E., Petrova T.I. Physico-Chemical Properties and Technologies of Solutions. In book: "Thermal and Heat Engineering". Vol. 1. Klimenko A.V. and Zorin V.M., Eds. - MEI, Moscow, Russia, 1999, pp. 263-314.
9. Magomedov U.B. The Viscosity of Aqueous Solutions of Electrolytes and Its Dependence on Density and Thermal Conductivity. High Temperature, 1999, vol. 37, No. 3, pp. 398–403
10. 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. Precedings of the Sixth International EPRI Conference on Cycle Chemistry in Fossil Plants. Columbus, OH, USA, June 27-29, 2000.
11. 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. Precedings of the Sixth International EPRI Conference on Cycle Chemistry in Fossil Plants. Columbus, OH, USA, June 27-29, 2000.
1. Petrova T.I., Petrov A.Yu., Vidojković S., Palei A.O. Distribution of Sodium Sulfate between Boiling Water and Equilibrium Saturated Steam. Vestnik MEI, 2000, No. 2, pp. 74-78.
13. Petrova T.I., Ryzhenkov V.A., Ermakov O.S., Verkhovskii A.E., Bodrov A.A., Chernyshev E.V., Petrov V.A. Studies of the Corrosion of Network Water Heaters at a Cogeneration Power Station and Ways for Reducing It. Thermal Engineering, 1999, vol. 46, No. 12, pp. 1007-1011.
14. Povarov O.A., Martynova O.I., Petrova T.I., Semenov V.N., Kashinsky V.I., Petrov A.Yu,. Dooley B, Jonas O. An Investigation into the Formation of Deposits in Steam Turbines. Thermal Engineering, 2000, vol. 47, No. 6, pp. 538-541.
15. Povarov O.A., Petrova T.I., Semenov V.N., Kashinsky V.I., Troitsky A.N., Petrov A.Yu,. Dooley R.B. Study of the Electrochemical Properties of Liquid Films Formed on Turbine Stages in the Phase Transition Region: Experimental Turbine Tests. Precedings of the Sixth International EPRI Conference on Cycle Chemistry in Fossil Plants. Columbus, OH, USA, June 27-29, 2000.
16. Rasulov S.M., Rasulov A.R. Experimental Investigation of Thermal Properties of Binary Mixture of n-Hexane–Water at High Temperatures and Pressures. High Temperature, 2000, vol. 38, No. 3, pp. 412–417.
17. Ryzhenkov V.A. The State of the Problem and Ways for Increasing the Wear Resistance of the Power Equipment at Thermal Power Stations. Thermal Engineering, 2000, vol. 47, No. 6, pp. 492-498.
18. Voronov V.N., Martynova O.I, Petrova T.I., Belosel'skii B. S, Vasina L.G., Nazarenko P.N., Ochkov V.F. Improvement of Chemical Technologies for Power Engineering. Thermal Engineering, 2000, vol. 47, No. 6, pp. 524-528.
19. Zorin V. M., Gorburov V. I. Organization of the Water Chemistry of Steam-Generating Units. Thermal Engineering, 2000, vol. 47, No. 6, pp. 519-523.

Attachment 19

US National Committee
Report to IAPWS

Prague, September 3-9. 2000

National Institute of Standards and Technology
Physical and Chemical Properties Division
Boulder, Colorado
D.J. Friend, A. H. Harvey, J.W. Magee

The U.S. National Committee for IAPWS has produced a book based on IAPWS-IF97. The book "ASME International Steam Tables for Industrial Use" (authors W.T. Parry, J.C. Bellows, J.S. Gallagher, and A.H. Harvey) was published by ASME Press in February 2000.

NIST released an updated version (Version 2.2) of its Standard Reference Database for computing water properties according to IAPWS standards for general and scientific use. The new version makes a number of additional properties (dielectric derivatives, Debye-Huckel slopes, refractive index) available through the graphical user interface.

Five sessions on aqueous systems (and four additional sessions on aqueous aspects of other areas such as computer simulation and critical phenomena) were organized for the 14th Symposium on Thermophysical Properties, held in Boulder in June 2000. Details on the program may be found under the Symposium website: symp14.nist.gov.

The project on the transport properties of water and steam is continuing as part of the joint effort between IAPWS and IUPAC. The data survey paper, "Experimental Data for the Viscosity and Thermal Conductivity of Water and Steam," by M.J. Assael, E. Bekou, D. Giakoumakis, D.G. Friend, M. Killeen, J. Millat, and A. Nagashima has been published in the Journal of Physical and Chemical Reference Data (29, 141, 2000).

K. Knobloch of the University of Applied Sciences of Zittau and Gorlitz has been visiting the Boulder laboratories, and work has been done on developing supplementary backward equations, p(h,s), for IAPWS-IF97.

Some measurements have been completed on the isochoric heat capacity of D2O and D2O+H2O as well as PVTx measurements of H2O + toluene, in conjunction with the Dagestan Scientific Center (with I.M. Abdulagatov). In addition, we have been involved in measurements of the isochoric heat capacity of H2O+methanol in a collaboration with N. Kagawa from Japan. Some VLE measurements on water-acetone, water-sodium nitrate, and the ternary water-acetone-sodium nitrate (including densities) have been completed. Additional measurements with isopropyl alcohol substituted for acetone are in progress. Models for these mixed aqueous solvent + electrolyte data are being developed and optimized to describe these data.

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The Thermodynamics Research Center, formerly at the Texas A & M University System, has been moved to NIST in Boulder. Although this data effort does not emphasize aqueous systems, the current database includes some information for 1330 binary systems and 422 ternary systems containing water. The data collection and evaluation is ongoing.

Physical and Chemical Properties Division (NIST, USA)
Thermophysical Division of the Dagestan Scientific Center of the Russian Academy of Sciences
(Makhachkala, Dagestan, Russia)

I. M. Abdulagatov, N.G. Polikhronidi, G.V. Stepanov, D.J. Friend, J.W. Magee, V. Valyashko, J.M.H. Levelt Sengers, S.B. Kiselev,

Experimental studies of the calorimetric (C_VVTx) and thermal (PVTx) properties for aqueous systems in wide ranges of temperature and pressure including the critical region and phase boundaries

A. Isochoric heat capacity measurements for pure D_2O and D_2O+H_2O mixture near the critical point in progress.
B. PVTx measurements for D_2O+H_2O, in the critical region (in preparation).
C. PVTx measurements for H_2O+Toluene near the critical point of pure water in progress.

Publications:

1. Valyashko V.M., Abdulagatov I.M., Levelt Sengers J.H.M. Vapor-Liquid-Solid Phase Transitions in Aqueous Sodium Sulfate and Sodium Carbonate From Heat Capacity Measurements Near the First Critical Endpoint: Part II. The Phase Boundaries, J. Chem. Eng. Data. 2000**.** (accepted).
2. Polikhronidi N.G., Abdulagatov I.M., Magee J.W., Stepanov G.V., Isochoric Heat Capacity Measurements for Light and Heavy Water Near the Critical Point. Int. J. Thermophys., 2000 (submitted).
3. Abdulagatov I.M., Magee J.W., Kiselev S.B., Friend D. J. A Isochoric Heat Capacity of Light and Heavy Water at Subcritical and Supercritical Conditions. Proc. of the 13th International Conference on the Properties of Water and Steam. Toronto, Canada. 2000. (accepted).

University of Maryland
Institute for Physical Science and Technology
College Park, MD

A. Anisimov, J.V. Sengers, A. A. Povodyrev, A. Kostrowicka Wyczalkowska, Kh. S. Abdulkadirova, J. Jacob, A.V. Agayan, J.P. Roseli.

Recent publications:

1. "Critical Locus of Aqueous Solutions of Sodium Chloride", A. A. Povodyrev, M. A. Anisimov, J. V. Sengers, W. L. Marshall, and J.M.H. Levelt Sengers, Int. J. Thermophys. 20, pp. 1529-1545 (1999).

2. "New Steam Properties Are Coming", J. C. Bellows, J. B. Sewell, D. G. Friend, A. H. Harvey, J.M.H. Levelt Sengers, W. T. Parry, J. V. Sengers and H. J. White, Jr., Proceedings of the 61st American Power Conference, Chicago, IL, Vol. II (1999), pp. 589-593.

3. "Crossover Critical Phenomena in Aqueous Solutions", M. A. Anisimov and J. V. Sengers, in "Steam, Water, and Hydrothermal Systems: Physics and Chemistry Meeting the Needs of Industry", Proceedings of the 13th International Conference on the Properties of Water and Steam, P. R. Tremaine, P. G. Hill, D. E. Irish, and P. V. Balakrishnan, eds. (National Research Council Press, Ottawa), in press.

4. "Critical Amplitudes of H2O and D2O in the Near Vicinity of the Critical Point", M. A. Anisimov, A. A. Povodyrev, J. P. Roseli, J. V. Sengers, S. B. Kiselev, and D. G. Friend, in "Steam, Water, and Hydrothermal Systems: Physics and Chemistry Meeting the Needs of Industry", Proceedings of the 13th International Conference on the Properties of Water and Steam, P. R. Tremaine, P. G. Hill, D. E. Irish, and P. V. Balakrishnan, eds. (National Research Council Press, Ottawa), in press.

5. "A Crossover Equation for the Thermodynamic Properties of Light and Heavy Steam in the Critical Region", A. Kostrowicka Wyczalkowska, Kh. S. Abdulkadirova, M. A. Anisimov, and J. V. Sengers, "Steam, Water, and Hydrothermal Systems: Physics and Chemistry Meeting the Needs of Industry", in Proceedings of the 13th International Conference on the Properties of Water and Steam, P. R. Tremaine, P. G. Hill, D. E. Irish, and P. V. Balakrishnan, eds. (National Research Council Press, Ottawa), in press.

6. "Thermodynamic Properties of H2O and D2O in the Critical Region", A. Kostrowicka Wyczalkowska, Kh. S. Abdulkadirova, M. A. Anisimov, and J. V. Sengers, J. Chem. Phys., in press.

7. "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., in press.

8. "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., submitted.

The Pennsylvania State University

Center for Electrochemical Studies
Pennsylvania State University, University Park, PA

Director: Prof. S.N. Lvov, lvov@psu.edu

RESEARCH RELATED TO THE IAPWS ACTIVITIES IN THE CENTER FOR ELECTROCHEMICAL STUDIES AT THE ENERGY INSTITUTE IS CURRENTLY CARRIED OUT AS FOLLOWS:

(1) Potential-pH diagrams of Cu-Ni-Zn alloys in water-ammonia power plant environments
(2) pH measurements in high temperature subcritical and super critical aqueous solutions
(3) development of high temperature electrochemical systems, electrodes and probes for industrial applications (geothermal systems, supercritical water oxidation technology, hydrometallurgy, etc.)

(4) dissociation/association constant measurements in high temperature subcritical and supercritical aqueous solutions
(5) electrochemical/hydrothermal coatings of metal surfaces using ceramic materials
(6) zeta potential measurements on oxide/water interface at elevated temperatures
(7) high temperature polymer electrolyte direct methanol fuel cells

High-Temperature Aqueous Chemistry Group

Chemical and Analytical Sciences Division

Oak Ridge National Laboratory
Oak Ridge, Tennessee

J. M. Simonson, D. A. Palmer, P. C. Ho, M. S. Gruszkiewicz, A. A. Chialvo, Y. S. Badyal
[R. E. Mesmer, H. F. Holmes, and W. L. Marshall, Consultants (retired)]

Over the past year this group has continued in its investigations of the thermodynamic and structural properties of water and aqueous solutions over extended ranges of temperature, pressure and solution composition. These investigations involve a number of experimental techniques including electrical conductance, electromotive force measurements, isopiestic and direct vapor pressure determinations, flow calorimetry and densimetry, and static and flowing measurements of phase behavior (primarily liquid-vapor and solid-liquid equilibria). Results of particular interest include: new direct measurements of vapor pressure were made over several very concentrated aqueous solutions at temperatures up to 250 □C; new experimental and simulation studies of the hydration structure of aqueous $NiCl_2$ solutions; measurements and simulations of the ion-pair association behavior of aqueous HCl at high temperatures; equilibrium solubility (and in one case the kinetic) behavior of such solids as CuO and Cu_2O, ZnO, Al(OH)O to temperatures as high as 350□C; and potentiometric measurements at high temperatures to determine the thermodynamics of hydrolysis reactions and the surface charge on metal oxides in contact with aqueous solutions.

Chialvo, A. A., P. T. Cummings, J. M. Simonson, and R. E. Mesmer, "Solvation in High-Temperature Electrolyte Solutions. I. Hydration Shell Behavior from Molecular Simulation," *J. Chem. Phys.* **110**, 1064-1074 (1999).*

Chialvo, A. A., P. T. Cummings, J. M. Simonson, and R. E. Mesmer,"Solvation in High-Temperature Electrolyte Solutions. II. Some Formal Results." *J. Chem. Phys.* **110**, 1075-1086 (1999).*

Bénézeth, P., D. A. Palmer, and D. J. Wesolowski, "The Solubility of Zinc Oxide in 0.03m Ionic Strength as a Function of Temperature with in situ pH Measurement," *Geochim. Cosmochim. Acta*, **63**, 1571-1586 (1999).*

Holmes, H. F. and R. E. Mesmer, "Isopiestic studies of H_3PO_4(aq) at elevated temperatures," *J. Solution Chem.* **28**, 327-340 (1999).

Ridley, M. K., D. J. Wesolowski, D. A. Palmer, and R. M. Kettler, "Association Quotients of Aluminum Sulphate Complexes in NaCl Media from 50 to 125□C: Results of a Potentiometric and Solubility Study," *Geochim. Cosmochim. Acta*, **62**, 459-472 (1999).*

Xiao, C., P. R. Tremaine, and J. M. Simonson, "Densities and apparent molar volumes of $Gd(CF_3SO_3)_3$(aq) at T = 373, 423, and 472 K and p = 7 and 26 MPa," *J. Chem. Thermodynamics*, **31**, 1055-1065 (1999).*

Ridley, M. K., D. J. Wesolowski, D. A. Palmer, and R. M. Kettler, "Association Quotients of Aluminum Sulphate Complexes in NaCl Media from 50 to 125□C: Results of a Potentiometric and Solubility Study," Geochim. Cosmochim. Acta, **62**, 459-472 (1999).

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Bénézeth, P., D. A. Palmer, and D. J. Wesolowski, "The Solubility of Zinc Oxide in 0.03m Ionic Strength as a Function of Temperature with in situ pH Measurement," Geochim. Cosmochim. Acta, **63**, 1571-1586 (1999).

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