The Czech National Committee

International Association for the Properties of Water and Steam

REPORT on IAPWS related activities – July 2010 / August 2011

Submitted to the EC Meeting of IAPWS, Plzeň, Czech Republic – September 2011.

National Committee Contacts:

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

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

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

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

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

SKODA POWER, Plzen, Inc., Tylova 57, CZ-316 00 Plzen.

Technical University of Liberec (TUL), Department of Chemistry, CZ-461 19 Liberec.

SIGMA Research and Development Institute (SIGMA), Jana Sigmunda 79, CZ-783 50 Lutin.

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

The board of the CZ NC PWS for the period 2010-2013:

Dr. J. Hruby, Prof. R. Mares, Dr. T. Nemec, Prof. P. Safarik, and Prof. J. Sedlbauer.

- In the 2010 IAPWS Meeting in Niagara Falls, Canada participated 7 workers from CzR. One of presented papers is in Ref. [1].
- Brief information has been published on web sites of CZ NC PWS to the new documents adopted and authorized by IAPWS.
- A joint project IT AV ČR and WBU Plzen sponsored by the Ministry of Education, Youth and Sports (MEYS, MŠMT in Czech) enables cooperation with IAPWS for the next two years, till 2012 inclusive.
- Dr. Hruby (IT) with his collaboratoers investigated properties of homogeneous and heterogeneous nucleation and heat transfer, Refs. [2 to 6].
- Prof. Mares (UWB) with his collaborator investigated a temperature dependence of the surface tension of water, Refs [7 and 8]
- Prof. Mares and Dr. Kalova (UWB) collaborated with Prof. M. A. Anisimov (USA) and investigated thermophysical properties of supercooled water, Ref.[9]

- Prof. Marsik (IT) with his research team studied condensation problems and cavitations processes, Refs. [1, and 10 to 12].
- Prof. Sedlbauer (TUL) and his team continued in the research into chemistry of aqueous systems. Refs. [13 and 14]
- Prof. Sedlbauer (TUL) coordinated IAPWS-IUPAC Joint Project: Establishing recommended data on thermodynamic properties of hydration for selected organic solutes and gases.
- Research activities at the (CTU) continued in further improvement of the current knowledge on the following subjects: determination of the heterogeneous particles in the superheated steam in turbines, Ref. [2], and development of correction in classical nucleation theory, Ref. [15].
- The problems studied in SIGMA Research and Development Institute (SIGMA) have been related mainly to the problems of nucleation processes and bubble dynamics during hydrodynamic cavitation and problems of cavitation instabilities in hydraulic machinery. Refs. [1 and 16].
- Dr. Jiricek (ICT-IE) with collaborators investigated renewable power sources and chemical effects in water and steam systems of power plants. Refs. [2, 17 to 21].
- Dr. Hnedkovsky (ICT-IPC) with collaborators investigated properties of organic solutes in water. Published articles are under Refs. [22 and 37].
- Prof. Stastny (SKODA POWER) with co-workers tested and applied the numerical model of the steam flow in nozzles and turbine blade cascades with NaCl binary nucleation and condensation, Ref. [38].
- ICT-IE organized 8th International Conference on Power Cycle Chemistry (CHEO8) from 7th to 8th September 2010 in Prague.
- Dr.Nemec worked with Dr.A.Harvey (USA) on some improvements to the IAPWS website that will increase the usability of the website.
- The CZ NC PWS collaborated with IT and WBU on the preparation and organization of the IAPWS Meeting 2011, Plzen.

Young Scientists IAPWS Fellowships

Information on the Young Scientists IAPWS Fellowship Projects.

- Dr. V. Vins performs his Young Scientis IAPWS Fellowship Project (CZ-Germany) "Development of Thermodynamic Models for Hydrates in Water – Carbon Dioxide Mixtures" under supervising of Dr. J. Hruby and Prof. R. Span. Preliminary results will be presented and discussed at the 2011 IAPWS Meeting in Plzen. The Final Report of the Project will be finished by the end of the year 2011.
- Dr. Kalova handed over the Final Report finished in the frame of the Young Scientists IAPWS Fellowship Project 2010 „Thermophysical Properties of Supercooled Water". A brief summary will be presented on negotiations of WG PCAS at the IAPWS Meeting 2011 in Plzen. The results will be published in proceedings and journals.

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18. Jiricek I., Zemlova T., Janda V.: Mixed Fuels Based on Straw, pp.125-129. In: Proceedings of CHEO8 Conference, Prague, 2010. (in Czech)

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German National Committee to IAPWS

Research Activities on the Thermodynamic Properties of Water and Steam

Report "Research in Progress 2011"

Baltic Sea Research Institute, Warnemuende
Dr. Rainer Feistel

Recent Publications

- W. Wagner, T. Riethmann, R. Feistel, A.H. Harvey (2011):
  New Equations for the Sublimation Pressure and Melting Pressure of H2O Ice Ih.
  J. Phys. Chem. Ref. Data, under review at NIST, to be submitted before the Pilsen meeting
- Feistel, R. (2011):
  Thermodynamic Properties of Seawater.
  EOLSS 2-03-07, submitted June 2011, http://www.eolss.net/
- Feistel, R. (2011):
  TEOS-10: A New International Oceanographic Standard for Seawater, Ice, Fluid Water and Humid Air.
  International Journal of Thermophysics, DOI: 10.1007/s10765-010-0901-y
  http://www.springerlink.com/content/p4834412420n5j61/
- Wright, D.G., Pawlowicz, R., McDougall, T.J., Feistel, R., Marion, G.M. (2011):
  Absolute Salinity, "Density Salinity" and the Reference-Composition Salinity Scale: Present and Future Use in the Seawater Standard TEOS-10.
  Ocean Science, 7, 1–26, www.ocean-sci.net/7/1/2011/, doi:10.5194/os-7-1-2011
- Seitz, S., Feistel, R., Wright, D.G., Weinreben, S., Spitzer, P., de Bievre, P. (2011):
  Metrological Traceability of Oceanographic Salinity Measurement Results.
  Ocean Sci., 7, 45–62. www.ocean-sci.net/7/45/2011/
- Feistel, R., Marion, G.M.M., Pawlowicz, R., Wright, D.G. (2010):
  Thermophysical Property Anomalies of Baltic Seawater.
  Ocean Sci., 6, 949-981, www.ocean-sci.net/6/949/2010/
- Feistel, R. (2011):
  Stochastic Ensembles of Thermodynamic Potentials.
  Accreditation and Quality Assurance, 16, 225-235
- Marion, G.M., Millero, F.J., Camoes, F., Spitzer, P., Feistel, R., Chen, C.-T.A. (2011):
  pH of Seawater.
  Marine Chemistry, doi:10.1016/j.marchem.2011.04.002, in press

Zittau/Goerlitz University of Applied Sciences, Faculty of Mechanical Engineering, Department of Technical Thermodynamics
Prof. Dr. Hans-Joachim Kretzschmar

1. Development of Fast Property Algorithms Based on Spline Interpolation
   - The algorithms for fast spline-interpolation methods are being developed and applied to the calculation of thermodynamic properties of different fluids.
   - An algorithm for generating spline-interpolation data grids with optimized data density for the user requirements 'range of state' and 'accuracy' is being developed.
2. Thermodynamic Properties of Humid Air
   - The property library LibHuAirProp of the American Society of Heating, Refrigerating, Air-Conditioning Engineers (ASHRAE) for calculating thermodynamic and transport properties for real moist air, steam, water and ice has been completed.
3. Property Libraries for Calculating Heat Cycles
   - The property library LibIF97 for steam and water has been extended to include sublimation and melting pressures and ice properties.
   - The property libraries for steam, water, ice, seawater, humid combustion gases, humid air, ammonia/water mixtures and water/lithium bromide mixtures have been connected to DYMOLA (Modelica) for non-stationary process calculations.

Recent Publications

- Wagner, W.; Kretzschmar, H.-J.:
  Chapter 2.1 Properties of Water and Steam.
  In: *VDI Heat Atlas*, 2nd ed., Springer (2010), ISBN: 978-3-540-77876-9
- Herrmann, S.; Kretzschmar, H.-J.; Teske, V.; Vogel, P.; Ulbig, P.; Span, R.; Gatley, D.P.:
  Properties of Humid Air for Calculating Power Cycles.
  Journal of Engineering for Gas Turbines and Power, 132 (2010), pp. 093001: 1-8
- Feistel, R.; Wright, D. G.; Kretzschmar, H.-J.; Hagen, E.; Herrmann, S.; Span, R.:
  Thermodynamic Properties of Sea Air.
  Ocean Science, pp. 91-141, 6 (2010)
- Kretzschmar, H.-J., Stöcker, I.:
  Mollier h,s-Diagramm von Wasserdampf (*Mollier h-s* Diagram for Steam).
  Annex in: Zahoransky, R.: *Energietechnik* (*Power Engineering*), 5th Ed.
  Vieweg Verlag, Wiesbaden (2010), ISBN 978-3-8348-1207-0

Ruhr University Bochum, Faculty of Mechanical Engineering,
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Prof. em. Dr. Wolfgang Wagner

1 Article "New Equations for the Melting Pressure and Sublimation Pressure of H2O Ice Ih"

The manuscript for the background article for the "IAPWS Revised Release on the Pressure along the Melting and Sublimation Curves of Ordinary Water Substance" was written. The reference for this article reads: *Wagner, W., Riethmann, T., Feistel, R., and Harvey, A. H.* New Equations for the Melting Pressure and Sublimation Pressure of H_2O Ice Ih. Submitted to *J. Phys. Chem. Ref. Data*.

2 Stoffwerte für Wasser und Wasserdampf (Steam Tables for Water and Steam),VDI Wärme Atlas 2012

Section D2.1 "Stoffwerte für Wasser und Wasserdampf" (Properties of Water and Steam) of the VDI-Wärme Atlas 2012 (VDI-Heat Atlas), 11th German Edition, is being worked on. The corresponding steam tables are calculated based on the Industrial Formulation IAPWS-IF97 and the current equations for the transport properties and other properties based on the corresponding IAPWS Releases. The reference for this publication reads: *Wagner, W. and Kretzschmar, H.-J.,* Stoffwerte von Wasser und Wasserdampf, VDI-Wärmeatlas, 11. Auflage, Abschnitt D2.1, pp. 1-15, Springer-Verlag, Berlin, 2012.

Current Status of Research Activities in Japan

Submitted to the Executive Committee Meeting, IAPWS, Plzeň, Czech Republic, September 2011

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

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

At the Nuclear Science and Engineering Directorate, Japan Atomic Energy Agency, Tokai-mura, Dr. S. UCHIDA is promoting research projects on the effects of hydrogen peroxide on stress corrosion cracking of stainless steel, which are going to be demonstrated at the in-pile loop experiments at JMTR, and has finished the first phase of the project on flow accelerated corrosion (FAC) in PWR, which has been supported by the Nuclear and Industrial Safety Agency (NISA). 1) The results of the six year research project on FAC, which were published in more than 15 technical articles, were awarded as the 2010 Award for Distinguished Technology of the Atomic Energy Society of Japan, "Development of Evaluation Methods for Pipe Wall Thinning by Coupled Analysis of Flow Dynamics and Corrosion" [(1)-(10)]. 2) Irradiation resistant high temperature sensors for electrochemical corrosion potential (ECP) measurement have been developed for applying them for in-pile SCC experiments[(11), (12)]. 3) Theoretical model based on a coupled model of water radiolysis and mixed potential analyses has been developed for evaluating corrosive conditions in BWR primary cooling system and in in-pile loop of JMTR. A collaborative project between NRL-Rez in Czech and JAEA-JMTRin Japan has been promoted for demonstrating applicability of the model[(13), (14)].

[Latest publication: (1) S. Koshizukam M. Naitoh, S. Uchida and H. Okada, "Evaluation Procedure for Wall Thinning due to Flow Accelerated Corrosion and Liquid Droplet Impingement", Proc. Int. Symposium on the Aging Management & Maintenance of Nuclear Power Plants (ISaG2010), Mitsubishi Research Institute, May, 27-28,Tokyo, Japan (2010), (2) M. Naitoh, S. Uchida, H. Okada, T. Ohira and S. Koshizuka, "Evaluation of Wall Thinning of PWR Feed Water Piping with the Coupled Model of Static Electrochemical Analysis and Dynamic Double Oxide Layer Analysis", Proc. PVP2010, 2010 ASME Pressure Vessel and Piping Division Conference, July 18-22, 2010, Bellevue, Washington, USA, PVP2010- 25517 (2010), (3) S. Uchida, M. Naitoh, H. Okada, S. Koshizuka, Taku Ohira and D. H. Lister, "Evaluation of FAC Simulation Code Based on Verification and Validation", Power Plant Chemistry, 12 (9), 550 (2010), (4) S. Uchida, M. Naitoh, H. Okada, Taku Ohira, S. Koshizuka and D. H. Lister, "Evaluation of Wall Thinning of PWR Feed Water Piping with the Coupled Model of Static

Electrochemistry Analysis and Dynamic Double Oxide Layer Analysis", Proc. Nuclear Plant Chemistry Conference 2010, NPC2010, Oct. 3-7, 2010, Quebec City, Canada, Canadian Nuclear Society, (2010) (in CD), (5) M. Naitoh, S. Uchida, H. Okada and S. Koshizuka, "Plant-Unique Procedures Applied to Mitigate Wall Thinning of PWR Feed Water Piping due to Flow Accelerated Corrosion", Proc. 8th Int. Meeting on Nuclear Thermal-Hydraulics, Operation and Safety (NUTHOS-8), NUTHOS0060, Oct. 10-14, 2010, Shanghai, China (in CD), (6) M. Naitoh, S. Uchida, H. Okada and S. Koshizuka, "Pipe Wall Thinning due to Flow Accelerated Corrosion and Liquid Droplet Impingement", Proc. 7th Korea-Japan Symposium on Nuclear Thermal-Hydraulics and Safety (NTHAS7), N7P0070, Nov. 14-17, 2010, Chuncheon, Korea (in CD), (7) D. H. Lister and S. Uchida, "Reflections on FAC Mechanisms", Power Plant Chemistry, 12 (10), 650 (2010), (8) H. Okada, S. Uchida, M. Naitoh, J. Xiong and S. Koshizuka, "Evaluation Methods for Corrosion Damage of Components in Cooling Systems of Nuclear Power Plants by Coupling Analysis of Corrosion and Flow Dynamics (V) Flow Accelerated Corrosion in Single and Two-phase Flow Conditions", J. Nucl. Sci. Technol., 48 [1], (2011) 65-75, (9) S. Uchida, M. Naitoh, H. Okada, Taku Ohira, S. Koshizuka and D. H. Lister, "Application of Coupled Electrochemistry and Oxide Layer Growth Models to Water Chemistry Improvement against Flow Accelerated Corrosion in the PWR Secondary System", Corrosion 2011, Paper No.09468, Mar. 14-17, Houston, TX, USA., National association of Corrosion Engineers (2011) 1-16, (10) D. H. Lister, A. Feicht, M. Khatibi, L. Liu, K. Fujiwara, T. Ohira and S. Uchida, "The Mitigation of Flow-Accelerated Corrosion in the Feedwater Systems of Nuclear Reactors – the Influence of Dissolved Oxygen under Different Operating Conditions", Power Plant Chemistry, 13 [4], (2011) 188-196, (11) S. Uchida, "Corrosion monitoring applications in nuclear power plants – a review", Edited by Stefan Ritter and Anders Molander, European Federation of Corrosion Publications, Number 56 (EFC 56): Corrosion Monitoring in Nuclear Systems, Maney Publishing, Leeds, UK (2010), 158-170, (12) S. Uchida, T. Satoh, Y. Wada and Y. Satoh, "An electrochemical sensor array for in-situ measurements of hydrogen peroxide concentration in high-temperature water", Edited by Stefan Ritter and Anders Molander, European Federation of Corrosion Publications, Number 56 (EFC 56): Corrosion Monitoring in Nuclear Systems, Maney Publishing, Leeds, UK (2010), 239-254, (13) S. Hanawa, T. Nakamura, S. Uchida, P. Kus, R. Vsolak and J. Kysela, "ECP Measurements Under Neutron and Gamma Ray in In-pile Loop and their Data Evaluation by Water Radiolysis Calculations", Proc. Nuclear Plant Chemistry Conference 2010, NPC2010, Oct. 3-7, 2010, Quebec City, Canada, Canadian Nuclear Society, (2010) (in CD), (14) P. Kus, R. Vsolak, J. Kysela, S. Hanawa, T. Nakamura and S. Uchida, "ECP Measurements in the BWR-1 Water Loop Relative to Water Composition Changes", Proc. Nuclear Plant Chemistry Conference 2010, NPC2010, Oct. 3-7, 2010, Quebec City, Canada, Canadian Nuclear Society, (2010) (in CD).]

[contact: Dr. S. Uchida; E-mail: uchida.shunsuke@jaea.go.jp].

The Research Center of Supercritical Fluid Technology, Graduate School of Engineering, Tohoku University is studying organic and inorganic reactions in sub- and supercritical water. Some projects are cooperative with Chinese Academy of Sciences (Kunming) and Tongji University (China). In 2010-2011, the following research areas were studied: density measurement, saccharide modification, polysaccharide depolymerization, formation of functional organic materials, formation of luminescent inorganic materials, formation mechanism of catalytic inorganic materials, and redox cycles for carbon cycling. The densities of methanol-water mixtures have been measured and analyzed via molecular dynamic simulation [Takumi Ono, Shunsuke Kobayashi, Taka-aki Hoshina, Yoshiyuki Sato and Hiroshi Inomata, "Volumetric Behavior and Solution Microstructure of Methanol-Water Mixture in Sub- and Supercritical State via Density Measurement and MD Simulation", Fluid Phase Equilibria, 302,(2011)55-59]. In Aida, Watanabe, and Smith et al. [T.M. Aida, N. Shiraishi, M. Kubo, M. Watanabe, R.L. Smith Jr, Reaction kinetics of d-xylose in sub- and supercritical water, Journal of Supercritical Fluids 55 (2010)

208-216.], the reaction pathway, reaction mechanism and reaction kinetics of D-xylose transformation at high temperatures (400 ^{o}C) and high pressures (100 MPa) are reported. Retro-Aldol reaction of D-xylose increased with increasing water density . Reaction of D-xylose to D-xylulose occurred by the Lobry de Bruyn-Alberta van Ekenstein (LBET) pathway. In Aida, Watanabe, and Smith et al. [T.M. Aida, T. Yamagata, M. Watanabe, R.L. Smith Jr, Depolymerization of sodium alginate under hydrothermal conditions, Carbohydrate Polymers 80 (2010) 296-302.], depolymerization of sodium alginate with hydrothermal treatment (180–240 ^{o}C) is studied. Alginate depolymerization occurs by releasing mannuronic acid preferentially first that is followed by the release of guluronic acid. In Fang and Smith et al. [Z. Fang, R.L. Smith Jr, J.A. Kozinski, T. Minowa, K. Arai, Reaction of D-glucose in water at high temperatures (410 °C) and pressures (180 MPa) for the production of dyes and nano-particles, Journal of Supercritical Fluids 56 (2011) 41-47.], reaction of D-glucose was studied at high temperatures (410 ^{o}C) and high pressures (180 MPa). By allowing the reaction to proceed and decompose, micron-sized particles and colored solutions could be produced by slow heating, while rapid heating resulted in the formation of dye-like substances with glucose-like structures. Near nano-size particles could be produced with the method In Takesue et al. [M. Takesue, A. Suino, Y. Hakuta, H. Hayashi, R.L. Smith, Crystallization trigger of Mn-doped zinc silicate in supercritical water via Zn, Mn, Si sources and complexing agent ethylenediamine tetraacetic acid, Materials Chemistry and Physics 121 (2010) 330-334.] decomposition of metal chelates in supercritical water was studied with the purpose to produce of Mn-doped zinc silicate, α-Zn_2SiO_4:Mn^{2+}, which is a practical industrial phosphor. The complexing agent used was ethylenediamine tetraacetic acid (EDTA) with various Zn and Mn sources. Remarkably, for the sulfate sources of Zn and Mn, addition of EDTA with Si source, tetraethoxyorthosilicate (TEOS) gave botryoidal druses of rod-like shaped α-Zn_2SiO_4:Mn^{2+}, which only occur in natural deposits (willemite) in La Calamine, Belgium (Moresnet). In Aida, Watanabe, Smith et al. [K. Kaseda, M. Takesue, T.M. Aida, M. Watanabe, H. Hayashi, R.L. Smith Jr, Restructuring mechanism of NbO_6 octahedrons in the crystallization of $KNbO_3$ in supercritical water, Journal of Supercritical Fluids (2011).], the mechanism of $KNbO_3$, which is a Pb-free piezoelectric material and alternate material to zirconate titanate, is studied in supercritical water. The material can form by two different crystallization routes that depend on the conditions of water. It was found that the restructuring of NbO_6 octahedrons is a primary factor in the crystallization mechanism. Namely, the rearrangement of edge-sharing NbO_6 octahedrons to corner-sharing NbO_6 octahedrons proceeds directly under homogeneous conditions and provides polygonal-shaped $KNbO_3$. In Jin and Smith et al. [F.M. Jin, Y. Gao, Y.J. Jin, Y.L. Zhang, J.L. Cao, Z. Wei, R.L. Smith, High-yield reduction of carbon dioxide into formic acid by zero-valent metal/metal oxide redox cycles, Energy & Environmental Science 4 (2011) 881-884.], hydrothermal conditions are used to reduce carbon dioxide to formic acid via oxidation of zero-valent fine particle metals. Reduction of the oxidized metal for recycle is accomplished by treatment with an organic compound. The cycle is demonstrated with zero-valent Fe, which gives 80 % formic acid yield. Recycle of the oxidized metal is by contact with glycerin, which gives lactic acid and essentially 100 % yield of zero-valent Fe.

At the Institute of Multidisciplinary Research for Advanced Materials at Tohoku University, Prof. M. KAKIHANA and his group have developed a panel of stable, non-toxic and water-soluble compounds of Si, V, Ti and Ta. These compounds can be utilized for the synthesis of oxide materials by solution based processes, which are based on the hydrothermal processing or which include a hydrothermal treatment as one of the key synthesis steps. Rutile- and brookite polymorphs of TiO_2 were selectively synthesized by a facile hydrothermal method using a novel titanium-picolinato complex as a precursor. Porous microspheres several micrometers in size, composed of a highly ordered arrangement of nanorods were synthesized in the presence of a picolinic acid additive. Hydrothermal treatment of a citratoperoxotitanate complex at high NH_3 concentrations resulted in the formation of agglomerated brookite particles with unusual snowflake-like shapes. Using the same method, the aspect ratios of the obtained rod-like brookite particles increased from 5 up to 20 with an increase of the NH_3 concentration. A new chemical route for synthesis of spherical agglomerations of titanic acid and titanium dioxide was developed on the basis of solvothermal treatments of a series of water-soluble titanium complexes in mixed solutions of water / amine. [M. Kakihana, M. Kobayashi, K. Tomita, and V. Petrykin, Bull. Chem. Soc. Japan, **83**, 1285 (2010). Q. Duc Truong, M. Kobayashi, H. Kato, and M. Kakihana, J. Ceram. Soc. Jpn., **119**, 513 (2011). K. Yamamoto, S. Matsushima, K. Tomita, Y. Miura, and M. Kakihana, J. Ceram. Soc. Jpn., **119**, 494 (2011).] Profs. T. SATO and S. YIN with co-workers studied on the panoscopic assembling of ceramic materials applicable for environmental clean-up, energy saving, UV/NIR shielding, preventing the healthy damage, etc. by solvothermal reactions. They successfully prepared visible light responsive photocatalysts with controllable phase compositions, morphologies, together with excellent visible light induced deNO_x activity. They also researched on the synthesis of multifunction thin films with UV/NIR shielding property, photocatalytic activity and superhydrophobicity or superhydrophilicity. The relationship between morphologies and photo-chemical properties of inorganic materials was investigated in detail. In addition, environmental friendly synthesis of lead-free dielectric ceramic materials, ceria-based inorganic UV-shielding materials with excellent safety, comfort and transparency in the visible light region; rare earth oxide nanoparticles with controlled morphology and excellent fluoresence properties, Ag/γ-Al_2O_3 nanocomposites with excellent deNO_x catalytic activity, were carried out. [Phosphorous Res. Bullet., **24**, 43-48(2010); Mater. Chem. Phys. **123**, 516–520(2010); Mater. Res. Bull., **45**, 1345-1350(2010); J.Solid State Chem., ***183, 1545-1549***(2010)*;* J.Nanomater., **2010**, 629727(6pages), (2010); Appl.Phys.Lett., **97**, 103102 (3pages) (2010); J.Mater.Chem.,**20**, 8227-8229(2010); Adv. Sci. Technol. **63**, 30-35(2010); Adv. Sci. Technol. **63**, 36-40(2010); Adv. Sci. Technol. **63**, 52-57(2010); Adv. Sci. Technol. **63**, 107-113(2010); J.Solid State Chem., **183**, 2456-2460(2010); Inter.J. Moden Phys. B, **24,** 3209-3214(2010); Appl. Clay Sci., **50**, 118-124(2010); J.Alloy Compd. **508**, L1-L4(2010); International J. Optics, **2010**, Article ID 261420, 6 pages (2010); J.Mater.Res., **25**, 2392-2400(2010); Nanoscale Res.Lett., **6**: 5(2011); *Appl. Catal. B. Chem.* **102**, 286-290(2011); *Appl. Catal. B. Chem.* **103**, 462-469(2011); J.Alloys Comp. **509**, 1482-1488(2011); CrystEngComm, **13,** 741-746(2011); J.Mater.Chem.,**21**, 5099-

5105(2011); *Res. Chem. Intermed.*, **37**, 319-327(2011); Nanosci. Nanotechnol. Lett. **3**, 413-416(2011); *Appl. Catal. B. Chem.* **105**, 206-210(2011); J.Cer. Soc.Jpn., **119**,445-450(2011); Phosphorus Res. Bull. **25**, 68-71(2011). Mater. Integration, **24**, No.2, 54-61(2011); J. Alloys Comd., **509**, 8581-8583(2011); *Appl. Catal. B:Environ.,* **106**, 586-591(2011); *ACS Applied Materials & Interfaces*, **3**, 2794-2799(2011); *Chem.Commun.*, **47**, 8853-8855(2011); Mater. Sci. Appl., **2** 757-763(2011)]. The relationship between morphologies and photo-chemical properties of inorganic materials was mainly investigated in detail. Profs. A. MURAMATSU and K. KANIE with co-workers have been studied the synthesis of monodispersed particles and their formation mechanism in liquid and/or solution phase. Recenty they have investigated preparation of ITO particles as a transparent conductive film component, $BaTiO_3$ as dielectrics and/or piezoelectric material, ferric oxides as a magnetic material and so on. Also, they have been making their maximum efforts on the hybridization of monodispersed particles with organic material such as liquid crystals, in order to obtain multi-functional materials. In addition to these original methods, the Liquid-Phase Selective Deposition has also been developed as a novel preparation method of heterogeneous catalysts for industrial use in dilute solution of metal precursory complexes. [Chemistry Letters, 38(6), 562-563 (2009); Chemosphere, 76(5) 638-643 (2009); Applied Catalysis B 87(3) 239-244 (2009); Materials Transactions, 50, 2808-2812 (2009); Chemistry Letters 39, 1080-1081 (2010); Chmeistry Lettrs, 39, 319-321 (2010); Journal of Materials Chemistry, 20, 8153-8157 (2010)]. Adschiri laboratory, recently, proposed a new method to synthesize organic inorganic hybrid nanocrystals by using supercritical hydrothermal method. In the supercritical state, organic molecules and metal salt aqueous solution forms a homogeneous phase, and water molecule works as a catalyst for promoting organic inorganic reactions.Thus, in the presence of organic capping agents in hydrothermal synthesis, hybrid nanoparticles are synthesized. Adschiri laboratory has challenged to synthesize variety of hybrid nanomaterials, includingTiO_2, CeO_2,$MgFe_2O_4$,Cu_2O,ZnO and $BaFe_2O_4$, [Zeitschrift fuer Naturforschung B-A J. CHEM. SCIE., 65*b,*1045-1050(2010) ; B. Jeyadevan, J. Supercrit. Fluids, 53(1-3)92-94(2010) ; MATER.LETT. 64(9),1049-1051 (2010) ; J.MATER. RES.,25(2), 219-223(2010)] .Since these nanoparticles has organic legands on the surface, affinitybetween nanoparticles and solvents can be controlled to have perfect dispersion. [Ind. Eng. Chem. Res., 49 (20), 9815–9821(2010);CHEM. LETT.,39(9), 961-963(2010) ; NANOSCALE,2(5),689-693(2010)]

At the Energy Technology Research Institute, National Institute of Advanced Industrial Science and Technology, Drs. M. MORIMOTO, Y. SUGIMOTO, S. SATO, and T. TAKANOHASHI have clarified the effect of supercritical water on upgrading reaction of oil sand bitumen. They comprehensively compared the yields and properties of products prepared in supercritical water and high-pressure nitrogen at 430 to 450°C and about 25 to 30 MPa. It was found that the dispersion effect of supercritical water led to intramolecular dehydrogenation of the heavier component and prevention of recombination reactions, and consequently gave the highest conversion. Also, the chemical effect of

supercritical water on the upgrading reaction of bitumen was stated to be almost negligible. [Morimoto, M., Sugimoto, Y., Saotome, Y., Sato, S. and Takanohashi, T., *Journal of Supercritical Fluids*, 55, 223-231 (2010)]. [contact: Dr. T. Takanohashi; E-mail: toshi-takanohashi@aist.go.jp, Dr. M. Morimoto; E-mail: m.morimoto@aist.go.jp]

At the department of material and environmental chemistry, Utsunomiya University, Dr. T. SATO and co-workers has been studying heavy oil upgrading through water gas shift reaction in supercritical water. They used formic acid as a model hydrogen source because formic acid is an intermediate of water-gas shift reaction in supercritical water. In supercritical water, formic acid reduced coke formation during the decomposition of bitumen especially in high water/oil ratio region. A reaction model was proposed and the model predicted that hydrogenation of the asphaltene core was important for the suppression of coke formation [Takafumi Sato, Shota Mori, Masaru Watanabe, Mitsuru Sasaki, Naotsugu Itoh, "Upgrading of bitumen with formic acid in supercritical water," J. Supercrit. Fluids, 55, 232-240 (2010)]. The gasification of biomass in supercritical water was studied. The production of hydrogen from the biogas obtained from the supercritical water gasification of glucose was improved. The apparatus combined the flow-type reactor for supercritical water gasification and the flow-type steam reforming rector with hydrogen permeable palladium membrane reactor was developed and found the hydrogen removal in membrane reactor enhance hydrogen recovery [Takafumi Sato, Takeyuki Suzuki; Mitsuhiro Aketa; Yasuyoshi Ishiyama; Kenichi Mimura; Naotsugu Itoh, "Steam reforming of biogas mixtures with a palladium membrane reactor system," Chem. Eng. Sci., 65, 451-457 (2010)] Gasification of bean curd refuse in high-temperature water with noble metal catalysts in supercritical water. In the case of Ru/C catalyst, bean curd refuse decomposed to intermediates and then intermediates were gasified to mainly methane and carbon dioxide. The sum of the yield of gases significantly increased with increase in water density. Water was effective hydrogen source in gasification [Takafumi Sato, Kentaro Inda, Naotsugu Itoh, "Gasification of bean curd refuse with carbon supported noble metal catalysts in supercritical water", Biomass and Bioenergy, 35, 1245-1251 (2011)]. [contact: Dr. T. Sato; E-mail: takafumi@cc.utsnomiya-u.ac.jp]

At the Material Properties Division, National Metrology Institute of Japan (NMIJ, formerly NRLM), National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, a section lead by Dr. K. FUJII is working on the density, viscosity, and refractive index standards. A determination of the Avogadro constant is being conducted in this section as an international project organized by the Comité International des Poids et Mesures (CIPM). This project continued through 2004 to 2011 with participants of eight National Metrology Institutes (BIPM, IMGC, IRMM, NIST, NMI-Australia, NMIJ, NPL, and PTB). The target of this project is to replace the present definition of the kilogram with a new definition based on fundamental physical constants. For the fundamental reduction of uncertainty in the Avogadro constant, a 5 kg of ^{28}Si crystal was prepared, and the final result of measurements was summarized in a paper [B. Andreas, Y. Azuma, G. Bartl, P. Becker, H. Bettin, M. Borys, I. Busch, M. Gray, P. Fuchs, K. Fujii, H. Fujimoto, E. Kessler, M. Krumrey, U. Kuetgens, N. Kuramoto, G. Mana, P. Manson, E. Massa, S. Mizushima, A. Nicolaus, A. Picard, A. Pramann, O. Rienitz,

D. Schiel, S. Valkiers, and A. Waseda, "Determination of the Avogadro Constant by Counting the Atoms in a ^{28}Si Crystal," Phys. Rev. Lett., 2011, Vol. 106, 030801]. Following this result, the redefinition of the kilogram will be discussed at the forth coming Conférence Générale des Poids et Mesures (CGPM) to be held in October 2011. In this project, the density of the crystal has been determined with a relative standard uncertainty of 3×10^{-8} [N. Kuramoto and K. Fujii, "Improvement in the volume determination for the Si spehers with an optical interferometer," IEEE Trans. Instrum. Meas., 2009, Vol. 58, No. 4, pp. 915-918]. Using the silicon crystals as a solid density standard, density standard liquids and PVT properties of fluids are calibrated by the magnetic suspension densimeter developed at the NMIJ [Y. Kano, Y. Kayukawa, K. Fujii, and H. Sato, "A new method for correcting a force transmission error due to magnetic effects in a magnetic levitation densimeter," Meas. Sci. Technol., 2007, Vol. 18, pp. 659-666]. In his group a new absolute viscosity measurement by the falling ball method is in progress. Nanotechnologies for measuring the falling distance and diameters of small silicon spheres have been developed for providing reference data for liquid water with a relative standard uncertainty of 0.01 % [Y. Fujita , N. Kuramoto, Y. Kurano, and K. Fujii, "A new project at NMIJ for an absolute measurement of the viscosity by the falling ball method," Proc. 14th ICPWS, Kyoto, 2004, 112-115]. Based on the viscosity of water, calibration of the viscosity standard liquids is being conducted in a range 1 mPa s to 500 Pa s [Y. Fujita, Y. Kurano and K. Fujii, "Evaluation of uncertainty in viscosity measurements by capillary master viscometers," Metrologia, 2009, Vol. 46, pp. 237–248]. Calibration service for non-Newtonian liquid has also started in 2009 using a new falling cylinder method. Dr. K. FUJII is working as a chairman of the WG-Density, CCM (Consultative Committee for Mass and Related Quantities) to organize the research activities on the density standards at the National Metrology Institutes. In May 2011, the CCM WG-Density meeting was held at the BIPM, and an idea for clarifying the roles of CIPM and IAPWS standards for the density of water has been confirmed [A. H. Harvey, R. Span, K. Fujii, M. Tanaka and R. S .Davis, "Density of water: roles of the CIPM and IAPWS standards," Metrologia, 2009, Vol. 46, pp. 196-198]. For details, contact Dr. K. Fujii, Chief, Fluid Properties Section, NMIJ (E-mail: fujii.kenichi@aist.go.jp).

At the Department of Mechanical Engineering, Keio University, Yokohama, Prof. K. YASUOKA and his group are studying the molecular dynamics (MD) simulation to clarify the nucleation phenomena. They reported nucleation phenomena with spherical seed. [D. Suh and K. Yasuoka, J. Phys. Chem. B., in press. DOI:10.1021/jp201964h] They also reported the thermodynamic properties of vapor/liquid coexistence for water and water/methane. [R. Sakamaki, A. K. Sum, T. Narumi, R. Ohmura, and K. Yasuoka, J. Chem. Phys., 134, 144702(2011). DOI : 10.1063/1.3579480 ; R. Sakamaki, A. K. Sum, T. Narumi, and K. Yasuoka, J. Chem. Phys., 134, 124708(2011). DOI : 10.1063/1.3574038] They reported contact angle hysteresis for droplets on Nanopillared surface and in cassie and wenzel states. [T. Koishi, T., K. Yasuoka, S. Fujikawa, and X. C. Zeng, ACS Nano, in press. DOI : 10.1021/nn2005393] They repoted non-gaussian fluctuations resulting from power-law trapping in a lipid bilayer. [T. Akimoto, E. Yamamoto, K. Yasuoka, Y. Hirano, and M. Yasui, Phys. Rev. Lett., in press.] They reported Size Dependent Phase Changes in Water Clusters. [T. Kaneko, T. Akimoto, K. Yasuoka, A. Mitsutake, and X.

C. Zeng, J. Chem. Theory Comput., in press.] [contact: Prof. K. Yasuoka; E-mail: yasuoka@mech.keio.ac.jp].

At the Department of Mechanical Systems Engineering, National Defense Academy, Yokosuka, Prof. N. KAGAWA and his group developed a twin-cell type adiabatic calorimeter for water + alcohol and water + ammonia mixtures. The thermometers of the apparatus are being replaced to improve the measurement uncertainty. By the modified apparatus, isochoric heat capacities of water and R 134a will be measured for temperatures from 220 to 520 K and pressures to 30 MPa. [contact: Prof. N. Kagawa; E-mail kagawa@nda.ac.jp]

Ret. Prof. H. TAKAKU was retired from Faculty of Engineering of Shinshu University in Nagano City at the end of March of 2006. He has been working as a temporary technical adviser at Naigai Chemical Products Co., LTD. in Tokyo since May of 2006. He and his coworkers engaged in Shinshu University, Naigai Chemical Products Co., the electric power companies and turbine manufacturer are conducting researches on the corrosion of materials for steam turbines in geothermal power plants, for boiler tubes and low pressure steam turbines in the conventional thermal and combined cycle power plants, and other subjects on corrosion and water chemistry for power plants, and so on. [The latest papers: (1) T. Nakane, L.-B. Niu, Shuji Oishi and H. Takaku, "Influence of Organic Acids on Corrosion Behavior of Boiler Tube Materials in Simulated AVT Waters Coexisted with Chloride Ions ", *Journal of Japan Institute for Metals*, 74 (9), 565-571 (2010); (2) L.-B. Niu, T. Goto, T. Nakane, H. Takaku and Yoshihiro Sakai, "Effect of Cl^- and SO_4^{2-} on Pitting Corrosion Susceptibility for Materials of Low-Pressure Steam Turbines in Power Plants", *Journal of Japan Institute for Metals*, 74 (10), 635-642 (2010); (3) T. Nakane, L.-B. Niu, S. Oishi and H. Takaku, "Electrochemical Corrosion Behaviors and Formed Film Characteristics of Boiler Tube Steel Weldments in Simulated AVT Waters", *NETSU SHORI* (*Journal of The Japanese Society for Heat Treatment)*, 50 (6), 614-619 (2010); (4) T. Nakane, L.-B. Niu and H. Takaku, "Effect of Chloride and Sulfate in Simulated AVT Waters on Electrochemical Corrosion Behaviors and Film Characteristics of Low Pressure Steam Turbine Materials", *Power Plant Chemistry*, 12 (7), 376-383; (5) T. Nakane, L.-B. Niu, H. Takaku and S. Oishi, "Evaluation of Corrosion Resistances and Characteristics of Films Formed on Boiler Tube Steels in Simulated AVT Water", *Zairyo -to- Kankyo (Journal of Corrosion Engineering of Japan)*, 60 (5), 265-270 (2011).] [Contact: Prof. H. Takaku; E-mail: takaku06@ybb.ne.jp]

At the Department of Mechanical Systems Engineering, Toyama Prefectural University, Toyama, Dr. H. MIYAMOTO and their group have been studying the various thermodynamic properties including the PVTx, critical locus, and saturation properties. ["The precise measurement of the (vapour-liquid) equilibrium properties for (CO_2 + isobutane) binary mixtures", Y. Nagata, K. Mizutani, and H. Miyamoto, J. Chem. Thermodyn., 2011, 43, pp. 244-247] ["(p, ρ, T, x) properties for CO_2/*n*-butane binary mixtures at T= (280 to 440) K and (3 to 200) MPa", T. Sugiyama, S. Orita, and H. Miyamoto, J. Chem. Thermodyn., 2011, 43, pp. 645-650]. Most of our apparatuses for higher pressure ranges had been

developed by the Uematsu Laboratory in Keio University. We aim to clarify the mixing effects of various natural substance mixtures (including aqueous solutions) at temperatures up to 600 K and at pressures up to 200 MPa. [Contact: Dr. H. Miyamoto; E-mail: miyamoto@pu-toyama.ac.jp]

At the Institute for Chemical Research, Kyoto University, Uji, Kyoto, Prof. M. NAKAHARA, Prof. N. MATUBAYASI, Dr. C. WAKAI, and their coworkers study the structure, dynamics, and reactions in super- and subcritical water and related systems such as ionic liquids and lipid membranes by means of multinuclear NMR (nuclear magnetic resonance) spectroscopy and computer simulation. Their current focus are (1) the accurate determination of the self-diffusion coefficients of water and organic solvents and the elucidation of the intermolecular-interaction effect ["Scaled Polynomial Expression for Self-Diffusion Coefficients for Water, Benzene, and Cyclohexane over a Wide Range of Temperatures and Densities", K. Yoshida, N. Matubayasi, Y. Uosaki, and M. Nakahara, *J. Chem. Eng. Data* **55**, 2815-2823 (2010)], (2) the rotational dynamics of benzene in ionic liquid and the effect of temperature and solvent charge ["Exploring the reorientation of benzene in an ionic liquid via molecular dynamics: Effect of temperature and solvent effective charge on the slow dynamics", Y. Yasaka, M. L. Klein, M. Nakahara, and N. Matubayasi, *J. Chem. Phys.* (Communication), **134**, 191101 (4 pages) (2011)], and (3) the diameter dependence of the lipid-membrane dynamics and the presence of multiple orders of dynamical time scale ["NMR-NOE and MD Simulation Study on Phospholipid Membranes: Dependence on Membrane Diameter and Multiple Time Scale Dynamics", M. Shintani, K. Yoshida, S. Sakuraba, M. Nakahara, and N. Matubayasi, *J. Phys. Chem. B **115**, 9106–9115 (2011)*]. [contact: Prof. M. Nakahara; E-mail: nakahara@scl.kyoto-u.ac.jp & Prof. N. Matubayasi; E-mail nobuyuki@scl.kyoto-u.ac.jp]

At the Department of Molecular Chemistry and Biochemistry, Doshisha University, Kyo-Tanabe, Kyoto, Prof. M. UENO, Prof. IBUKI and their group have been studying the electric conductivities of 1:1 electrolytes in high-temperature alcohols (methanol and ethanol) ["Electric conductivities of 1:1 electrolytes in high-temperature ethanol along the liquid-vapor coexistence curve. II. Tetraalkylammonium bromides", *J. Chem. Phys.*, **134** (12), 124509 1-8 (2011); "Electrical conductivities of 1:1 electrolytes in high-temperature methanol", *Netsu Sokutei*, **37** (2), 64-72 (2010)]. In our laboratory, the densities and viscosities of aqueous solutions have been also studied ["Pressure and temperature effects on the density and viscosity of DMF-water mixtures", *J. Physics: Conference Series*, **215**, 012074 1-4 (2010)]. [Contact: Prof. M. Ueno; E-mail: mueno@mail.doshisha.ac.jp]

At Department of Applied Chemistry & Bioengineering, Osaka City University, Dr. N. KOMETANI and his co-workers have studied the TiO_2 photocatalysis in high-temperature high-pressure water. They revealed that TiO_2 exhibits high photocatalytic activity even under sub- and supercritical conditions [N. Kometani, K. Sugimoto, A. Fujita, Y. Yonezawa, "Photocatalytic Activity of TiO_2 Nanoparticles in Hydrothermal and Supercritical Water", *J. Chem. Eng. Jpn.*, **40**, 463-467 (2007)]. Based on this finding, the hybrid process in which the hydrothermal and photocatalytic techniques are combined has been developed. It has been demonstrated that such hybrid process could be applied to the treatment of waste water containing organochloride compounds such as chlorobenzene [A. Shimokawa, N. Kometani,

Y. Yonezawa, "Degradation of chlorobenzene by the hybrid process of supercritical water oxidation and TiO_2 photocatalysis", *Sep. Sci. Tech.*, **45**(11), 1538-1545 (2010)] as well as the effective gasification of glucose [A. Nakatani, N. Kometani, "Photocatalytic Effect of TiO_2 on the Hydrothermal Gasification of Glucose", *J. Phys.: Conf. Seri.*, **215**, 012091 (2010)]. The same group also examined the hydrothermal synthesis of size-controlled metal nanoparticles [N. Kometani, T. Teranishi, Y. Yonezawa, "Development of the Metal Nanoparticle Synthesis Method by means of the Hydrothermal Technique", *J. Soc. Mater. Sci. Jpn.*, **58**, 481-485 (2009); N. Kometani, T. Teranishi, "Preparation of size-controlled silver nanoparticles by the hydrothermal method", *Phys. Stat. Soli. C*, **7**, 2644-2647 (2010)]. [Contact: Dr. N. Kometani; kometani@a-chem.eng.osaka-cu.ac.jp]

At the Department of Mechanical Engineering, Kyushu University, Prof. Y. Takata and their group are continuously developing a program package for thermophysical properties of fluids: PROPATH. The current version is 13.1 and the package contains 78 pure substances, moist air, binary mixtures and ideal gases. Information on this package is available through the website: http://www2.mech.nagasaki-u.ac.jp/PROPATH/. In addition, his research group is studying thermophysical properties of hydrogen at ultra-high pressures. They are measuring PVT relation up to 100MPa, viscosity and thermal conductivity of hydrogen up to 100MPa. ["A Capillary Tube Viscometer Designed for Measurements of Hydrogen Gas Viscosity at High Pressure and High Temperature", E. Yusibani, et al., *Int. J. Thermophysics*, 32-6, 1111-1124(2011); "Thermal Conductivity Measuremet of Gases by the Transient Short-Hot-Wire Method", S. Moroe, et. al., Experimental Heat Transfer, 24-2, 168-178(2011)]
[contact: Prof. Y. Takata; E-mail: takata@mech.kyushu-u.ac.jp]

The following research projects on the thermophysical and physicochemical properties of water substances including various aqueous systems of technological importance are currently in progress at several universities and institutions in Japan. At the Department of Applied Chemistry and Biochemistry, Kumamoto University, Kumamoto, Prof. M. GOTO, Assoc. Prof. M. SASAKI, Assistant Prof. Armando T. QUITAIN, and their group are working on reaction kinetics and mechanism of biomass-related materials in sub- and supercritical water. Biomass and its model compounds such as phenolic compounds and carbohydrates were reacted to obtain added-value chemical intermediates with a batch or semi-batch reactors [Wahyudiono, M. Sasaki and M. Goto, accepted for publication in *Journal of Material Cycles and Waste Management* (2010); T. Saito, Y. Yoshino, H. Kawanabe, M. Sasaki, M. Goto, *Separation Science and Technology*, **44**, 1228-1239 (2009)]. Electrochemical oxidation of biomass and its model compounds has been investigated under hydrothermal conditions for elucidating a reaction pathway for glucose, and for recovering added-value chemicals [M. Sasaki, T. Oshikawa, H. Watanabe, Wahyudiono, M. Goto, *Research on Chemical Intermediates*, **37**(2-5), 457-466 (2011); A. Yuksel, M. Sasaki, M. Goto, *Ind. Eng. Chem. Res.*, **50**(2), 2227-2235 (2011); M. Sasaki, Wahyudiono, A. Yuksel, M. Goto, *Fuel Processing Technology,* **91**(9), 1125-1132 (2010); A. Yuksel, H. Koga, M. Sasaki, M. Goto, *Ind. Eng. Chem. Res.*, **49**(4), 1520-1525 (2010)]. The metal removal from bitumen and its model compounds were carried out at temperatures of 673 K – 763 K. These results suggest that supercritical water have a capability to remove metals by decomposing them [P. C. Mandal, Wahyudiono, M. Sasaki and M. Goto. *Proceeding of*

International conference on Mechanical, Industrial and Energy Engineering, KUET, Khulna, Bangladesh (2010); P. C. Mandal, Wahyudiono, M. Sasaki, and M. Goto, *J. Hazard. Mater.* **187**, 600-603 (2011); P. C. Mandal, Wahyudiono, M. Sasaki, and M. Goto, *Fuel*, accepted on July 01, 2011; P. C. Mandal, Wahyudiono, M. Sasaki, and M. Goto, *Fuel Processing Technology*, accepted on July 9, 2011]. The results of sulfur removal from bitumen and its model compounds revealed that supercritical water can also be removed sulfur from bitumen and its model compounds. The manuscripts based on desulfurization of bitumen are being prepared to submit in international journals. The upgrading of bitumen and the decomposition of its model compounds were carried out in near- and supercritical water. These results suggest that supercritical water can be an effective on the visbreaking of bitumen and extraction of sulfer from bitumen or its model sulfer-containing compounds with supercritical water [T. Sato, S. Mori, M. Watanabe, M. Sasaki, N. Itoh, *The Journal or Supercritical Fluids,* **55**(1), 232-240 (2010); P. C. Mandal, T. Shiraishi, Wahyudiono, M. Sasaki, M. Goto, *J. Chem. Eng. Jpn.*, **44**(7), 486-493 (2011); Wahyudiono, T. Shiraishi, M. Sasaki, M. Goto, *Research on Chemical Intermediates*, **37**(2-5), 375-381 (2011)]. They are also studying about various natural materials in collaboration with universities and companies [M. Tanaka, A. Takamizu, M. Hoshino, M. Sasaki, M. Goto, *Food and Bioproducts Processing*, in press (2011); L. Qadariyah, M. Sumarno, M. Siti, Wahyudiono, M. Sasaki, M. Goto, *Bioresource Technology*, in press (2011); R. Askin, M. Sasaki and M. Goto, *Food and Bioproducts Processing*, 88(2-3), 291-297 (2010); M. Siti, K. Kitada, M. Sasaki, M. Goto, J. Munemasa, M. Yamagata, *Ind. Eng. Chem. Res.*, **50**(4), 2227-2235 (2010)] Application of microwave irradiation to hydrothermal extraction of bioactive compounds from natural resources such as marine algae and herbal plants were also carried out [T. Kai, Armando T. Quitain, M. Sasaki and M. Goto, *Proceedings of 2011 AIChE Annual Meeting* (2011); Tayyebeh Zohourian Haleh, Armando T. Quitain, M. Sasaki and M. Goto, *Separation Science and Technology*, *submitted for publication*]. Researches on microwave-assisted solvothermal synthesis of biofuels are also in progress. [Armando T. Quitain, S. Katoh and M. Goto; *Biofuels/Book 2*, in press (2011); Armando T. Quitain, S. Katoh, M. Sasaki and M. Goto, *Proceedings of 2011 AIChE Annual Meeting* (2011)] As a part of Kumamoto University Global COE program "Global Initiative Center for Pulsed Power Engineering", developments of an evolutional reaction / material processing methods were conducted. Electrospinning is one of the simple techniques to produce nanofibers and we challenged electrospinning of combined polymers in supercritical fluid [M. Goto, K. Murakami, Wahyudiono, and M. Sasaki, *Proceeding of 9th Conference on Supercritical Fluids and Their Applications*, Sorrento, Napoli, Italy (2010)]. Pulsed discharge plasma irradiation of various organic compounds in sub- and supercritical fluids has been investigated to synthesize valuable materials and chemical intermediates [M. Goto, M. Sasaki, Wahyudiono, K. Nagafuchi, H. Watanabe, T. Kiyan, T. Namihira, H. Akiyama, *Proceedings of AIChE Annual Meeting 2010* (2010); M. Sasaki, Wahyudiono, T. Kiyan, H. Akiyama, M. Goto, Y. Suga, W. Toshiyuki, *IEEE Region 10 Annual International Conference, Proceedings/TENCON*, art. No. 5686632, 2108-2112 (2010); M. Mitsugi *et al.*, *J. Physics: Conference Series*, 215, art. No 012088 (2010)] Pulsed laser ablation of various metals in supercritical fluid has been developed and morphology of ablated plates and generated nanoparticle were examined and some kinds of metal nanoparticles have been successfully generated by laser ablation in supercritical fluid [S. Machmudah, Wahyudiono, Y. Kuwahara,

M. Sasaki, M. Goto, *J. Supercrit. Fluids*, in press (2011); S. Machmudah, M. Goto, Wahyudiono, Y. Kuwahara, M. Sasaki, *Research on Chemical Intermediates*, **37**(2-5), 515-522 (2011); Y. Kuwahara, M. Morita, H. Endo, K. Yoshimori, T. Nagami, K. Kumamaru, T. Iwanaga, T. Sawada, M. Sasaki, M. Goto, *Materials Research Innovations*, **14**(1), 16-18 (2010)]. [contact: Prof. M. Goto; E-mail: mgoto@kumamoto-u.ac.jp, Assoc. Prof. M. Sasaki; E-mail: msasaki@ kumamoto-u.ac.jp, Assistant Prof. Armando T. Quitain; E-mail: quitain@kumamoto-u.ac.jp]

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

Report 2010-2011

1. RNC active participation in organization of 4-rd Water-Chemistry Forum, April 2011, Moscow, MPEI (TU).
2. Two meetings of RNC have been held. Current problems are investigated.

Publications list

1. Alexandrov A.A., Dzhuraeva E.V., Utenkov V.F. Temperature depression and solubility in aqueous solutions of sodium chloride. Novoe v rossiyskoy elektroenergetike (New in Russian elektroenergetiks), 2010, No 10, P. 24.
2. Alexandrov A.A., Dzhuraeva E.V., Utenkov V.F. The saturated steam pressure and surfase tension of aqueous solutions of the sodium sulfate. Vestnik MEI, 2011, No 3, P. 5.
3. Larin B.M., Larin A.B. Korotkov A.N., Oparin M.Y. Water chemistry of the cooling system of the electric generator stator on TPP. Thermal Engineering, #07, 2011, pp. 17-20.
4. Mulev Y.V., Belyaeva O.V., Mulev M.Y., Saplitsa V.V., Zayatc T.A. The dielectric constant as one of the main parameters controlling the state of the working fluid. Thermal Engineering, #07, 2011, pp. 36-40.
5. Ochkov V.F. Water chemistry for TPP and NPP – a new level of information support. Thermal Engineering, #07, 2011, pp. 76-77.
6. V.A. Voloschuk, V.F. Ochkov, K.A. Orlov. Thermodynamic optimization cycles of some gas turbines and CCGT using modern information technology (part 1)// // New in the Russian electric-power industry, #7, 2011, pp. 23-42.
7. V.A. Voloschuk, V.F. Ochkov, K.A. Orlov. Thermodynamic optimization cycles of some gas turbines and CCGT using modern information technology (part 2) // New in the Russian electric-power industry, #8, 2011, pp. 15-25.
8. V.F. Ochkov, E.E. Ustuzhanin, V.E. Znamenskiy, I.M. Abdulagatov, M. Frenkel. Information on the thermophysical properties of the Internet: problems and technologies. Abstracts of the 13th Russian Conference on Thermophysical substances. Novosibirsk, Russia, June 28–July 1, 2011, ISNB 978-5-89017-030-9, pp. 128 – 129
9. Ochkov V.F., Orlov K.A., Znamenskiy V.E. Thermal calculations based on the Internet functions on the properties of thermal power plants working fluids // New in the Russian electric-power industry, #6, 2011. pp. 40-49.
10. Voloshchuk V.A., Ochkov V., Orlov K. Thermodynamic optimization of cycles of some schemes of gas and gas-steam turbine power plants with the help of modern IT // Доклад на 10th conference on Power System Engineering, Thermodynamics & Fluid Flow - ES 2011, June 16 - 17, 2011, Pilsen, Czech Republic.
11. Ochkov V.F. , Ustuzhanin E.E. , Znamenskiy V.E. Analysis of Internet sites containing information on the thermophysical properties of working fluids // Proceedings of the Academenergo, #1, 2011, pp.110-123.
12. Voloschuk V.A., Ochkov V.F., Orlov K.A. Investigation of combined-cycle power plants using modern information technology // Aerospace engineering and technology. #5 (72), Kharkiv, HAI, 2010. pp. 71-76.
13. Ochkov V.F., Frenkel M., Khusnullin A.S. Interactive open thermotechnical network reference data: problems and solutions // Proceedings of the VII Summer School of young scientists and Academician V.E. Alimasova "Problems of heat and mass transfer and hydrodynamics in power, 15-17 September 2010, Kazan, Russia. pp. 281-284.
14. A.E.Verchovsky, D.G.Bucharov, A.A.Zonov at al.Automatization of Phosphate introducing in the high pressure boiler. New in Russia Electrical Power, 3, 2011, p.25-32.

U.S. National Committee to IAPWS
2011 Report on Activities of Potential Interest to IAPWS

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

In collaboration with Prof. Richard Wheatley at the University of Nottingham, a pair potential was developed for the water-CO_2 binary pair, and used for the quantitative calculation of second virial coefficients. Results from this and previous water/gas systems are being incorporated into a software model for thermodynamics of moist gases.

Reference: Wheatley, R.J., and Harvey, A.H., Intermolecular potential energy surface and second virial coefficients for the water-CO_2 dimer, *J. Chem. Phys.* **134**, 134309 (2011).

In collaboration with researchers in Greece and Germany and at the University of Maryland, a new formulation has been developed for the thermal conductivity of water and steam. The complete correlation, which covers a wider range of conditions than the existing IAPWS formulation and is consistent with IAPWS-95 and the new IAPWS viscosity correlation, was presented for evaluation by IAPWS.

In NIST's Chemical and Biochemical Reference Data Division (Gaithersburg, MD), the vapor pressure of ice has been measured over the temperature range 173 K to 273 K. These measurements were made using cavity ring-down spectroscopy to probe the output of a standard humidity generator which contains isothermal samples of ice in a nitrogen atmosphere. The measurement is relative to the known triple-point pressure, and is corrected for the enhancement factor. A preliminary analysis indicates good agreement over this temperature range between the measured ice vapor pressure and the new IAPWS formulation for the sublimation pressure.

Reference: Bielska, K., Havey, D.K., Scace, G.E., Lisak, D., and Hodges, J.T., Spectroscopic Measurement of the Vapor Pressure of Ice, *Proc. Royal Soc. A*, in press.

NIST's Experimental Properties of Fluids group has built apparatus for two projects to measure thermophysical properties of aqueous gas mixtures at high temperatures. One apparatus is a high-temperature magnetic-suspension densimeter, which has been used to measure H_2O-N_2 and H_2O-CO_2 mixtures up to 620 K. The cross second virial coefficients from this work agree reasonably well with those determined from theory as described above. A high-temperature thermal conductivity apparatus (using the transient hot-wire technique) has been converted to alternating-current operation (needed for polar fluids like water) and used to measure the thermal conductivity of H_2O-N_2 and H_2O-CO_2 mixtures up to 740 K.

Communicated from the University of Maryland

The thermodynamic behavior of supercooled water was investigated at the University of Maryland as a continuation of a previous project supported by IAPWS in 2010:

C.E. Bertrand and M.A. Anisimov, *The peculiar thermodynamics of the second critical point in supercooled water*, J. Phys. Chem. B, in press (doi: 10.1021/jp204011z).

J. Kalova, R. Mareš, M.A. Anisimov, and J.V. Sengers, *Scaled equation of state for supercooled water in the mean-field approximation*, Technical Report prepared for the International Association for the Properties of Water and Steam (September 2011).

V. Holten, C.E. Bertrand, M.A. Anisimov, and J.V. Sengers, *Thermodynamic modeling of supercooled water*, Technical Report prepared for the International Association for the Properties of Water and Steam (September 2011).

Communicated from Don Palmer

I thought that the PCC in particular *might* be interested in the three publications listed below. I have also been engaged with the OECD NEA Headquarters in Paris (TDB projects) together with many others in producing volumes on the thermodynamic properties of elements of prime importance in nuclear waste storage. A list of those already published is available on their Web site. We have after long delays almost finished the first book on iron (solids and solution species) which should go to press by the end of the year. Work on a second iron book has just started as has others on (aluminum, magnesium, calcium, iodine and other minor topics), as well as one on molybdenum in which I am not evolved. These books are an excellent source of recommended thermodynamic properties (as well as a source of the available literature) in which each paper is reviewed and critiqued in an Appendix and the values recalculated in a consistent and up to date manner.

D.A. Palmer, H. Gamsjäger, "Solubility Measurements of Crystalline β-$Ni(OH)_2$ in Aqueous Solution as a Function of Temperature and pH," *J. Coord. Chem*., **63**, 2888-2908 (2010).

D.A. Palmer, P. Bénézeth, C. Xiao, D.J. Wesolowski and L.M. Anovitz, Solubility Measurements of Crystalline NiO in Aqueous Solution as a Function of Temperature and pH", J. Solution Chem., 40, 680-702 (2011).

D.A. Palmer, "Solubility Measurements of Crystalline Cu_2O in Aqueous Solution as a Function of Temperature and pH," J. Solution Chem., 40, 1067-1093 (2011).

Communicated from Andre Anderko, OLI Systems

In 2010-2011, the work at OLI Systems was focused on:

(1) Finalizing a comprehensive model for surface tension of electrolyte solutions in wide ranges of concentrations and temperature
(2) Developing a thermodynamic model for predicting the behavior of mixtures composed of carbon dioxide and various salts containing the Na, K, Mg, Ca, Cl, SO4, and CO3 ions. Further, work was initiated on applying this model to predict the interactions between CO2-rich phases and minerals, which may be of interest for understanding the behavior of CO2 in sequestration environments
(3) Developing a thermodynamic model for aqueous systems containing various alkanolamines and carbon dioxide and hydrogen sulfide. This model combines phase and chemical equilibria and is designed for applications such as CO2 capture and gas processing.
(4) Developing an electrochemical model for predicting general and localized corrosion of copper and alloy CuNi9010 in a variety of aqueous environments as a function of solution chemistry, temperature and flow conditions. Currently, this model is being extended to alloy CuNi7030.
(5) Initiating the development of a model for predicting interfacial tension.

In the past year, the following two articles have been published:

P. Wang, A. Anderko and R.D. Young, "Modeling Surface Tension of Concentrated and Mixed-Solvent Electrolyte Systems", Ind. Eng. Chem. Res., 50 (2011) 4086-4098.

P. Wang and A. Anderko, “Modeling Chemical Equilibria, Phase Behavior, and Transport Properties in Ionic Liquid Systems”, Fluid Phase Equilibria, 302 (2011) 74-82.