Attachment 8

IAPWS Collaborative Grant Proposal

Formulations for the Viscosity and Thermal Conductivity of Water and Heavy Water: Evaluated Experimental Database and Initial Correlations

IAPWS Sponsors:

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Chemical Engineering Department
Aristotle University
54124 Thessaloniki, Greece

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National Institute of Standards & Technology
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U.S.A.

Young Investigator:

Ifigenia Metaxa
Chemical Engineering Department
Aristotle University
54124 Thessaloniki, Greece

Attachment 8

Executive Summary

Mrs. Ifigenia Metaxa is a junior research assistant in the Chemical Engineering Deprtment of the Aristotle University. She has been involved in the collection of papers as well as in the development and checking of the databases for the viscosity and the thermal conductivity of water and heavy water. Ms Metaxa is currently working toward her PhD in the area of the thermal conductivity of nanofluids.

The requested Collaborative Grant will allow Ms. Metaxa to travel to and stay at NIST (Boulder campus) for 4 months. This time is sufficient for the updating and evaluating the databases of experimental results, and setting the foundation for the development of the new correlations, with an emphasis on the viscosity of ordinary water.

Background and Outline of the Project

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

The water database contains 3993 points for viscosity in the range of temperatures from 254 K to 1316 K with pressures to 346 MPa and 5095 points for thermal conductivity in the range of temperatures from 255 K to 1072 K with pressures to 785 MPa. The heavy water database contains 1244 points for viscosity in the range of temperatures from 277 K to 779 K with pressures to 468 MPa, and 2380 points for thermal conductivity in the range of temperatures from 277 K to 1043 K with pressures to 250 MPa.

Both collections include all data considered for the current IAPWS formulations as well as measurements published since those were completed. The study has identified new data which were not available for the previous reviews of the transport properties of water, has identified regions in which the current standard transport property formulations can now be improved, and is intended to facilitate the development of new, more accurate, international formulations for the viscosity and thermal conductivity of water and steam and heavy water.

Current facets of the research involve further temperature conversions (with Czech collaborators), evaluation of Russian equation (with Czech collaborators), development of formal statistical methods to achieve correlations (at NIST), and theoretical calculation

of low-density viscosity (with British collaborators). The specific tasks that will involve Ms. Metaxa include updating databases (incorporating new temperature conversion, as appropriate; searching current literature; introducing uncertainties in all variables; performing additional evaluation); working with NIST statisticians in developing/evaluating formal schemes to achieve consensus values; collecting, re-optimizing and evaluating existing formulations and approaches for viscosity of water; developing and implementing structural optimisation algorithms for viscosity; and working with team members to incorporate terms for critical-region behavior. Although this ambitious program will not be completed in a 4-month visit, we anticipate substantial progress in all of these areas.

Justification

The task of developing updated formulations for the viscosity and thermal conductivity of water is a very high priority within the Working Group on Thermophysical Properties of Water and Steam. The international effort on this project involves researchers from Russia, United Kingdom, Germany, and Japan, as well as from Greece and the United States. Considerable progress has been made on the task (see, e.g. M.J. Assael, E. Bekou, D. Giakoumakis, D.G. Friend, M. Killeen, J. Millat, and A. Nagashima, "Experimental Data for the Viscosity and Thermal Conductivity of Water and Steam," J. Phys. Chem. Ref. Data 29 (2), 141-166, 2000; A.A. Aleksandrov and A.B. Matveev, “Equation of Dynamic Viscosity in the Region of Existence of the Liquid and Gaseous Phases of Water: Method of Derivation,” High Temp. (Russ.) 36, 885-890, 1998; M.J. Assael, V.K. Tsalmanis, N.K. Dalaouti, D. Giakoumakis, and A. Nagashima, “Transport Properties of D_2O: Data Survey & Comparisons,” in Steam, Water and Hydrothermal Systems: Physics and Chemistry Meeting the Needs of Industry, Proc. 13th Int. Conf. on the Properties of Water and Steam, NRC Research Press, Ottawa, 2000, P.R. Tremaine, P.G. Hill, D.E. Irish, and P.V. Balakrishnan, eds., pp. 72-79) however a substantial amount of work remains. The proposed international collaborative project will ensure a close working relationship between the Greek and U.S. efforts, and will give the young investigator a significant opportunity to interact with several team members that are active in this area of research.

Schedule and Budget

A possible starting date can be March 2003. We believe that four months will be sufficient time for the aforementioned work.

Return airfare, Thessaloniki to Denver	$ 1000 (US)
Living expenses in Boulder for four months	$ 6200 (US)
Total amount requested	$ 7200 (US)

Attachment 9

Proposal for Young Scientist IAPWS project

for the years 2003 in duration 5 month.

Applicant: **Tomáš Němec**, PhD student, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University Prague, CZ

Supervisors: František Maršík and Jan Hrubý, Institute of Thermomechanics CAS, Department of thermodynamics, Dolejskova 5, 182 00 Prague, CZ

D. A. Palmer, Oak Ridge National Laboratory, Chemical and Analytical Science Division, Oak Ridge, TN 37831-6110, USA

Thermodynamics of binary homogeneous nucleation in superheated steam.

The formation of the so-called early condensate is an important unknown in the design of reliable and efficient fossil and nuclear power plants. The mechanisms of formation of the early condensate are:

a.) heterogeneous nucleation, i.e. nucleation of droplets on solid particles (the matter which does dissolve in the superheated steam). Some of the particles can be charged.
b.) binary or multicomponent homogeneous nucleation.

In this project we focus on the second mechanism. Here the droplets grow from microscopic clusters, which are formed by random collisions water molecules and molecules of admixture(s). Although nucleation is a kinetic process, the applicability of contemporary theories depends mainly on thermodynamic data. The absence or insufficient quality of thermodynamic data in the range of interest is an important (if not the major) obstacle in achieving adequate predictions of nucleation rates. Needed data include:

- solubilities of admixtures in superheated steam,
- fugacity and activity coefficients,
- partial molar volumes, and
- surface tension as a function of concentrations.

The initial droplets represent a concentrated aqueous solution. Hence, the data must span from infinite dilution to concentrated solutions. Also the pressure-dependence is important, because it is necessary to extrapolate thermodynamic data to higher pressures (into the metastable region).

The expertise of the host Oak Ridge National Laboratory will be of great help for the applicant in assessing thermodynamic data, finding optimal ways of their representation, and, possibly, filling up a gap with original measurements. Measurement of high temperature solubilities

of aqueous electrolytes represents a core function of the "Aqueous Chemistry" group at ORNL led by J. M. Simonson. Moreover, during the ongoing compilation of the treatise on high temperature aqueous chemistry sponsored by IAPWS, data for the solubility of electrolytes and non-electrolytes in liquid water and steam are being evaluated that have direct application to the behavior of solutes in the nucleation of droplets in steam. Therefore, the timing for this collaboration is optimal from the standpoint of the state of knowledge at ORNL.

The aims of the project.

The project aims to prepare:

- the database of nucleation rates models,
- the database of needed thermodynamic properties for several water-admixtures (e.g., water solution of NaCl, Na_2SO_4, NaCOOH) relevant to power cycles,
- the report describing the improved nucleation model,

and to employ these databases in a nucleation simulation program, solving the kinetic equations of nucleation. The simplified phase transition kinetics formulation will be implemented into the used CFD codes for the simulation of the non-equilibrium two-phase flow.

The stay of Tomas Nemec at Oak Ridge National Laboratory, Chemical and Analytical Science Division, will be supervised by D. A. Palmer, who has expertise in the field of the aqueous electrolyte properties at higher temperatures. The proposed 5 month T. Nemec will spend in this laboratory. The beginning of the stage is planned to January 2003.

Budget: expenses 9000 USD.

Enclosed: Applicant Curriculum Vitae. Prague 6. February 2002

Attachment 9

Ing. Tomáš Němec

Date of birth: July 15th, 1977 **Nationality:** czech
Place of birth: Třebíč **Marital status:** single

Email: nemec.tomas@volny.cz

Education

March 2001 – present **Czech Technical University in Prague**
Faculty of Nuclear Sciences and Physical Engineering, Dept. of Mathematics
Doctoral degree programme, specialization Mathematical Modelling

September 1995 – – February 2001 **Czech Technical University in Prague**
Faculty of Nuclear Sciences and Physical Engineering, Dept. of Mathematics
Master's degree programme , specialization Mathematical Modelling
State final exam passed on *February 12th, 2001*.

September 1991 – – May 1995 **Grammar-school in Moravské Budějovice**
School-leaving exam passed on *May 30th, 1995*.

Praxis

January 1998 – present **Institute of Thermomechanics CAS –** Research assistent
Nucleation processes modelling, simulation software development

Languages

English	advanced	CTU exam passed on *June 12th, 1997*
German	advanced	CTU exam passed on *May 13th, 1997*
Russian	beginner	reading of scientific literature

Key skills

Mathematical applications in physics, natural sciences and engineering
Development and computer realization of mathematical models
Win32 platform programming in the Borland C++ Builder environment
Basic insight into the html, php, java, delphi, opengl and open inventor technologies

Interests

Computers, mathematical simulation, quantum physics, space exploration
Martial arts, windsurfing

References

Prof. František Maršík, DrSc. Institute of Thermomechanics CAS
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Ing. Jan Hrubý, CSc. Institute of Thermomechanics CAS
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IAPWS WEBSITE

- **http://www.iapws.org**
- Text of all Releases and Guidelines now available, more than half (including IF97 and IAPWS-95) can be copied and searched.
- Information about 2002 IAPWS meeting, link to local information.
- Minutes of 2000 and 2001 meetings
- About 15 000 “pages” per month
- 99 000 visits to “home” page since Jan. 2001
- Most popular items: Thermal conductivity Release (?), info on new formulations, IF-97 Release, IAPWS-95 Release, some FAQs.

IAPWS WEBSITE -- FUTURE

- Some Releases and Guidelines only scanned, can't search or copy coefficients. Lots of work (and some danger) to make "real" documents. Who can do it? Is it worth doing?
- Future Releases, Guidelines, ICRNs, etc. should be provided electronically (preferably PDF, Postscript or Word OK)
- Effort on FAQs has slowed down (suggestions from WGs?)
- Need to get text of current ICRNs on Web (and closing statements for expired ones?)

Attachment 11

Recommendations of IAPWS Task Group on Software/Legal Issues

JULY 2002

1. The main issue for decision is whether IAPWS will have software as a product (or part of a product). Whether the software is on the IAPWS Website, or some other website, or obtained from the Executive Secretary, does not affect the main issue, which is that of possible liability of IAPWS for its software products.

2. Because of the potential for problems, it is recommended that IAPWS should not make software available for products (releases, guidelines, etc.) where the software is not an integral part of the product.

3. For situations where software is judged to be an integral part of the product, lawyers at Siemens and Toshiba have advised that it should be possible to make software available from IAPWS in a way that minimizes risk to IAPWS (though the risk can never be made zero). This would involve adding appropriate language (to the website if the software were there, perhaps as comments with the code itself, etc.) saying that IAPWS made no warranty about the quality of the code, the user assumed all risk and responsibility, etc. It is also important in reducing the risk to IAPWS that the software be given away and not sold.

4. In order to satisfactorily reduce the risk to IAPWS, it is recommended that IF IAPWS decides to have software products, IAPWS must pay for a lawyer (with experience in software issues in the U.S.) to tell IAPWS exactly how to do this.

5. In case it was not clear, we stress that #3 and #4 above leave IAPWS with only two choices. IAPWS could decide not to have software as a product (this would reverse the decisions made about the TTSE in 2001). OR, IAPWS can obtain professional legal advice to properly minimize the risks to issuing software products. While a third choice would be to issue software and not worry about the risk, this Task Group recommends against that choice.

6. While it is not strictly in the mandate of this Task Group, we wish to bring to the attention of the EC the important issue of support and maintenance of the product. For traditional IAPWS products (releases and guidelines), the WG that produced the product is responsible for support and maintenance. But support and maintenance of software is much more difficult, and the WGs may not be able to do this.

ATTACHMENT

Committee on restructuring of IAPWS
Anneke Levelt Sengers, Jeff Cooper, Roberto Fernandez-Prini, and Koichi Watanabe

A. Questions addressed to the WG

1. Which product of your Working Group do you consider as the most valuable achievement of the past five years?

2. Please formulate a vision of the future directions of electric power generation, including new technologies and reduced environmental impact.

3. Could you envision alternative Working Group structures that would make IAPWS work more effectively and productively? Consider merging of exsisting WGs, creating new WGs, different ways of organizing the working week, and different spacings of the IAPWS Conferences, or any other constructive ideas.

B. REPLIES BY THE WG

TPWS/IRS:

1. Most valuable achievements: IAPWS-95 (TPWS)
IAPWS-IF97 (IRS)

2. Vision: Gas turbines with high moisture content
Fuel cells (microturbines)
Low-temperature heat sources (incl. geothermal)
Nuclear fission
Reduced CO_2 and other immissions, reduced environmental impact

3. Structure: TPWS/IRS satisfied with their existing structure.
Focus needs to be on providing products: high-quality information of value to industry, based on best science.
Tentative new name for TPWS (based on current activities): "Thermophysical Properties of Aqueous Fluids"
TPWS favors annual 1-hr plenary session in which WG communicate about directions for IAPWS
ICPWS: preference for 5-year cycle
More IAPWS involvement in education

PCAS

1. Most valuable achievement: IAPWS Monograph project

2. Vision: Deregulation has resulted in dwindling company support of R&D in general, and of IAPWS-related activities in particular.
Difficult for IAPWS attendees to find support for attending annual meetings. Somewhat easier to justify for ICPWS attendance.
See a role for IAPWS in educating power engineers, by workshops, training, and short courses.
Ultra-supercritical power cycles will require information on aqueous-system properties and chemistry from 300°C to 700°C.

3. Structure: PCAS is strongly in favor of 3-year cycle for ICPWS, with simplified Proceedings and Program Committee structure.
Several PCAS mmbers are in favor of coordinating the ICPWS with meetings of the international hydrothermal community.
PCAS plans to retain current work-week structure, with three half-day presentations: one jointly with TPWS, one with PCC, and one for PCAS alone.
PCAS plans to focus on products. It stablished a task group on pH, and one on ion pairing.

PCC

1. Most valuable achievements:
ICRNs on surface tension and on Na2SO4 distribution between water and steam.
IAPWS international collaboration projects on nucleation, and on solubilities in Steam.
Power Cycle sessions at ICPWS 13 (thermochemistry; power plant chemistry, case studies.)

2. Vision
Drivers: reduced emissions of CO_2, NOx, SOx; reduced water use; reduced cost, capital and production.
Plant maintenance: reduced staffing-automation and sophisticated monitoring; optimize economic life; maintain knowledge base; alternative chemistries.
Environmental: water recovery; CO_2 sequestration; zero liquid-discharge plants
Alternative fuels: Gas hydrates, biomass.
New types of power generation: intrinsically safe nuclear plants; fuel cells; high-P, high-T plants; combined-cycle plants.
Alternative technologies: integrated coal gasification; pulverized fluid-bed combustion; Start-stop load following; storage; membrane technology.

3. Structure: PCC should better define needs → more ICRNs.
PCC will use National Committees to be sure problems are of general nature before they are put on the Agenda.
PCC wants to establish topical task groups, including members of other WGs and outside experts, leading to, or addressing ICRNs.
PCC wants presentations of problems *prior* to their solution.
PCC wants workshops to be continued.
Study needed of chemical effects in leading-edge technologies.

C. SUMMARY

Intra-WGs – relatively minor changes in structure proposed.
Inter-WG – a desire was expressed for joint sessions, joint task groups, and more interaction.
ICPWS frequency - the issue of a 3 *vs.* 5-year cycle. The issue has not been resolved.
Several WG express an interest in an IAPWS role regarding education.

D. DISCUSSION

Name
"Properties of Water and Steam" covers only a fraction of the current activities.
Neither physical chemistry at high temperatures and pressures, nor power cycle chemistry, over half of IAPWS's interest, are recognized by the present IAPWS name.
Likewise, "TPWS" does not suggest the ongoing branching out to mixtures and to combustion gases. Name changes may have to be considered.

Directions
If IAPWS is considered an organization strongly linked to electric power generation, many new directions, to which IAPWS is beginning to contribute, such as gas combustion turbines and fuel cells, may not use water and steam, so that "PWS" does not cover our activities.

If IAPWS is considered a group of experts on properties of high-pressure, high-temperature aqueous systems, our natural allies are the geothermal, supercritical-water and hydrothermal communities, and "PWS" is too narrow.

IAPWS may not actually have to choose between these two directions. In fact, there is a great advantage to the IAPWS bridge function between these two communities. Nevertheless, some focusing may be needed to prevent IAPWS from becoming wide but shallow. On the other hand, the deep digging, the continual improvement of formulations, may have to be interrupted now and then for the sake of a taking a broader perspective.

Chemically reacting mixtures
This is the province of PCAS and PCC. By entering the field of combustion gases, however, TPWS members are producing the first models for chemically active gas mixtures. Thus it seems that the current separation: "TPWS is concerned with thermophysical properties of water and steam, PCAS with chemical properties of aqueous systems" is increasingly artificial and counterproductive. These two traditionally separate constituencies ought to find each other in the fascinating realm of supercritical fluids and reacting gases, and we should welcome and exploit the overlap of interest.

Education
Several WGs are groping for an educational role for IAPWS. They notice the need for more and better education of power engineers and students at engineering departments. They wonder whether IAPWS members could contribute by teaching short courses, or writing small monographs. The current FAQs section on the Web could be expanded, or transformed into a more formal teaching tool.

E. Power in 2020

(Jim Bellows' private thoughts, incomplete and subject to frequent change.)

Power in 2020 will not be monolithic with just central stations. Advances in small power generation devices will make a blend of central and distributed power the normal situation. The power for transportation will be integrated into the power for other purposes.

FUEL SOURCES

A blend of fuel sources will be used to provide power. These will include human power, largely for transportation, in the form of walking and bicycles. In order to use this power effectively, small communities with central facilities for everyday shopping will be the normal state. Larger cities will provide the extended functions, but going to the larger city will be a rarer event, perhaps a dozen time per year. Most automobiles will have a portion, or all of their power supplied electrically. The electric power will probably come from fuel cells. Hybrid automobiles with internal combustion engines, battery storage, and electric drive may be a bridge to largely electric vehicles.

Biomass and waste
Biomass and waste materials will be used to generate power, either by fermentation to methane or by direct combustion. If direct combustion is used, there will be considerable effort required to be certain that incomplete combustion does not produce polutants. It may well be that these materials will be converted to producer gas, which will be used as fuel for combustion turbines. The producer gas would then go through a very hot flame.

Natural gas
Natural gas, from sources common in 2002 and from fermentation of waste material, will continue to be a major fuel in 2020. It will certainly be used to power some combustion turbines, but large combustion turbines will be largely powered by secondary source fuels, such as producer gas. Issues of natural gas from permafrost need to be explored.

Coal
Coal will continue to be a significant primary source of energy. Most of the coal will be converted into other forms before final combustion. Some legacy coal plants will survive. Only the most efficient coal plants will be in use burning coal as primary fuel. They will have significant costs to clean the flue gas.
Nuclear
Nuclear must come back, if only as a source of hydrogen. I would think that nuclear might come back as a basic source and be used to generate hydrogen when demand is less than 100% for electricity.
Hydrogen
Hydrogen, if used, is a secondary source fuel. It has the advantage that its combustion product is water, which will not be a pollutant. However, it has two problems. First, hydrogen will evaporate from the surface of the atmosphere. Since it is relatively unreactive as a gas, most leaks will survive to reach the surface, hence be lost to the earth. Second, it is not easy to store and transport. It does not liquefy easily due to the low boiling point. Storage as sodium borohydride must be examined from a total energy efficiency. The explosion hazard is generally a false issue, since hydrogen dissipates so readily.
Oil
Petroleum is too valuable as a chemical feedstock to be used for fuel. Waste products from petroleum may be used as fuel in the facilities where they are generated, but the large scale burning of petroleum based fuels will cease.

GENERATION METHODS

Fuel Cells
Simple
Combined cycle fuel cells

Nuclear
Advanced cycles

One of the chief energy problems with nuclear power is the low efficiency. This is due, in major part, to the low steam conditions (1000 psia, 540°F = 66 bar, 282°C). About 2/3 of the nuclear energy is dumped into the environment as waste heat. To be very practical from an environmental perspective, nuclear power will need to raise the efficiency.
Cogeneration
One way to increase efficiency is to put a topping cycle on the nuclear turbine. A superheater fired by fossil fuel would have nearly 100% energy recovery (Check this point carefully before use.). Thus in a cogeneration configuration, a fossil-nuclear system could have very high fossil efficiency and reasonable average thermal efficiency.

Combustion turbines

Combined Cycle

Simple cycle

There will remain a need for fast startup systems of small size to fill peak demands. This is readily filled by combustion turbines in simple cycle configurations. The efficiencies are not remarkably high, but the amount of time that the plants are actually operating is small.

Ultrasupercritical Plants

Materials issues

Chemical issues

Ultrasupercritical plants will have a number of chemical issues. Ammonia will not be stable at the working temperatures. The usual plant chemistry will be neutral oxygen. Additionally at 700°C, compounds commonly tolerated in the cycle at 540°C will become highly corrosive to the alloys used because the ionic conductivity of the oxide layers will be higher, and some of the compounds (sulfate and phosphate) have eutectics below 700°C which will lead to corrosion analogous to the hot corrosion of combustion turbines. The usual turbine problems in the moisture transition region will persist, but organic materials in the cycle will probably be less of a problem, since the higher temperatures will promote destruction to CO_2. *The chemical and corrosive effects of CO_2 on power system components must be clearly known before this time.*

Distributed generation

Fuel Cells

Microturbines

Internal combustion

Uses not currently common

Automobile power

Bulk storage in automobile batteries

Electricity must be generated as it is needed. One method of peak shaving (covering peak load without additional generation capacity) would be to use automobile batteries as a temporary storage system. During peaks, the batteries would be drained. Off-peak, the batteries would be recharged. This has serious schedule concerns, but they are not insurmountable.

Information needs

Combustion gas properties

Combustion gas chemistry

High temperature corrosion by steam and impurities

Kinetic information on steam dissociation and recombination—how far from equilibrium do we operate?

Kinetic information on ammonia dissociation and recombination—how far from equilibrium do we operate?

Biomass conversion questions

Engineering needs

Higher steam conditions on nuclear power plant