“Live” Formulations of International Association for the properties of Water and Steam (IAPWS)

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Abstract. Online publication of IAPWS formulations for calculation of the properties of water and steam is reviewed. The advantages of electronic delivery via Internet over traditional publication on paper are examined. Online calculation can be used with or without formulas or equations printed in traditional publications. Online calculations should preferably free of charge and compatible across multiple platforms (Windows, Android, Linux). Other requirements include availability of multilingual interface, traditional math operators and functions, 2D and 3D graphic capabilities, animation, numerical and symbolic math, tools for solving equation systems, local functions, etc. Using of online visualization tools for verification of functions for calculating thermophysical properties of substances is reviewed. Specific examples are provided of tools for the modeling of the properties of chemical substances, including desktop and online calculation software, downloadable online calculations, and calculations that use server technologies such as Mathcad Calculation Server (see the site of National Research University “Moscow Power Engineering Institute”) and SMath (see the site of Knovel, an Elsevier company).

The first time an IAPWS formulation implemented “live” on the Internet was demonstrated by one of the authors of this paper at the meeting of IAPWS Task Forces in 2007 in Luzern (Switzerland). The formulation (Fig. 1) for computing water and steam ionization constant as a function of temperature and pressure was created in Mathcad (engineering calculations software by PTC https://www.ptc.com/en/engineering-math-software/mathcad) and supported online by Mathcad Calculation Server.

This calculation is quite simple. Yet, during development of online version, an error was found in the original, non-interactive (“static”) document. The error was caused by programming language used for creation of this formulation that, in contrast to Mathcad, couldn’t handle physical quantities and their units of measurement properly.

Thus, creating “live” versions of formulations could help eliminate calculations errors and misprints that may go unnoticed in “static” documents. These errors are quite frequently found in scientific and technical publications. Editors check the texts carefully, but the formulas often suffer from the lack of attention and/or proper background.

Fig. 2 shows a page from IAPWS website with formulations, released in 1997, for calculating thermodynamic properties of water and steam. This page has a reference to the official document

IAPWS in PDF format, its brief description, and references to online calculations for the following regions:

- Region 1–water
- Region 2–steam
- Region 3–near-critical
- Region 4–saturation
- Region 5–steam at high temperatures, etc.

An example in Fig. 3 shows some online calculations of thermodynamic properties of water (Region 1). The pressure and temperature are input with appropriate units. The value of dimensionless Gibbs free energy is calculated via polynomial of the 34th degree, along with the values of its partial derivatives by pressure and temperature, under specified conditions of water. From that, thermodynamic properties of water at a given temperature and/or pressure are calculated from the well-known formulas using partial derivatives of Gibbs free energy. The complete calculation can be found at http://twt.mpei.ac.ru/mcs/worksheets/iapws/IAPWS_IF97_Region1.xmcd. The authors have developed online calculations for all the regions of this basic IAPWS-IF97 formulation, as well as for some other formulations, e.g., for the transport properties of water and steam.

Putting formulations online is convenient for debugging applications for calculating the properties of water and steam during development by comparing the results of intermediate calculations. "Live" formulations can also be used as an online reference tool by inputting new values of pressure and temperature to obtain properties of a substance without seeing the intermediate results of calculations.

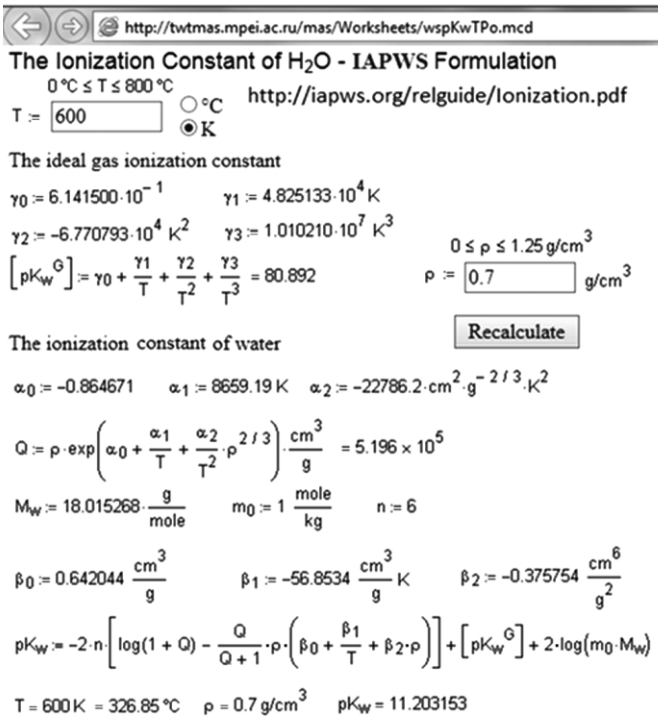

Fig. 1. "Live" calculation of the ionization constant of water as a function of temperature and density.

If intermediate results are not required, one can visit other websites created by the authors, e.g., http://twt.mpei.ac.ru/rbtpp (Fig. 4). There we have a graphic capability allowing us to display a family of curves or a surface to visualize properties of steam and water as functions of pressure, temperature, etc.

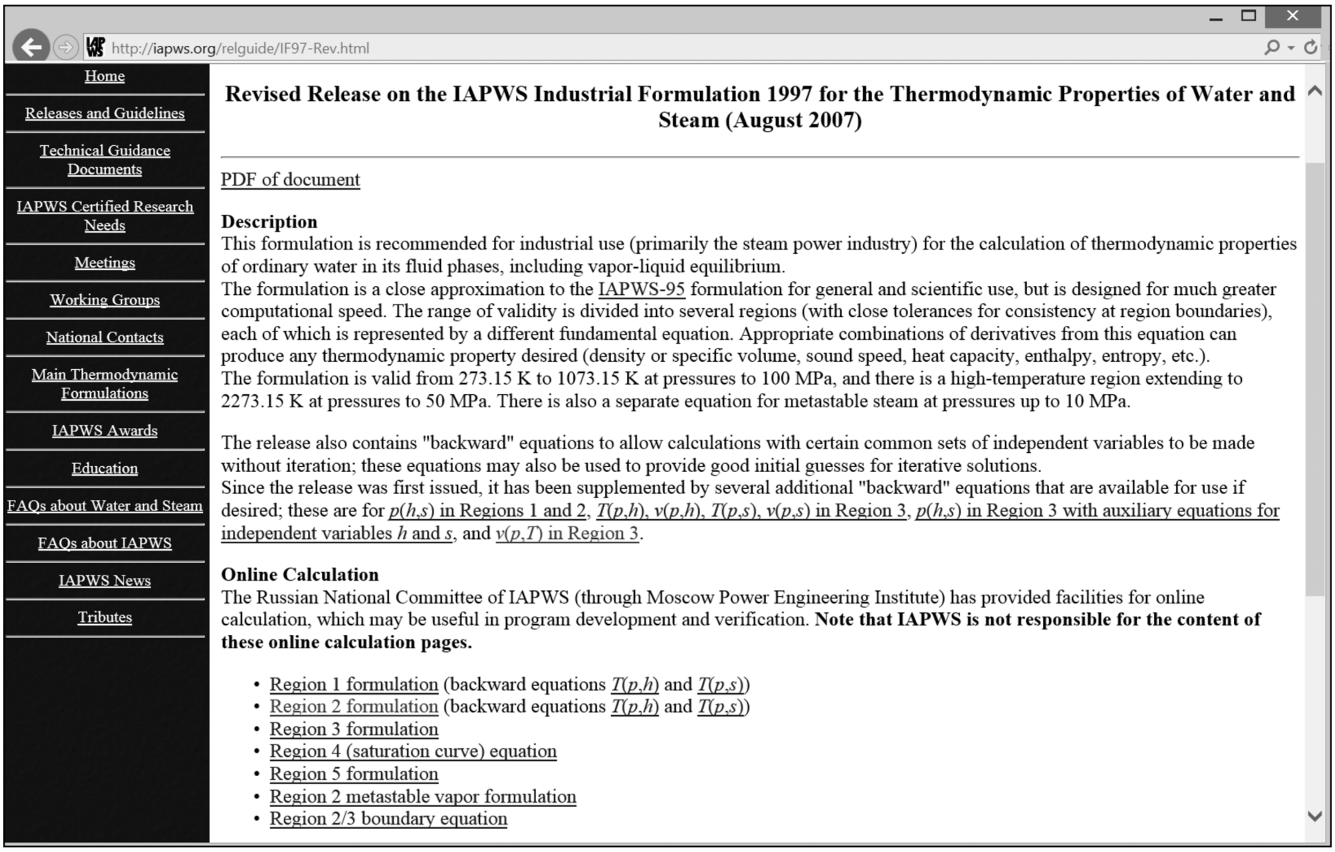

Fig. 2. Page from the IAPWS website with references to online calculations for thermodynamic properties of water and steam.

This website contains both, references to "static" formulations and online calculations similar to one shown in Fig. 1. It also allows downloading files for Mathcad (Mathcad 15 and Mathcad Prime versions) and SMath Studio (a Russian app similar to Mathcad, see www.smath.info). Fig. 4 shows the SMath function called wspD1PT, which returns the value of water density (*D*) (Region *1*) as a function of pressure (*p*) and temperature (*T*). The suffix wsp in the name of this and similar functions stands for Water/Steam Properties.

Fig. 4 shows does not show all the values of vectors *J* and *n* - coefficients of the polynomial of the 34th degree. As mentioned above, these are used for calculation of the dimensionless Gibbs free energy and its partial derivatives for a given pressure (π) and temperature (τ).

Similar freely distributed functions have been developed for other regions of the IAPWS-IF97 formulation and for other initial parameters. Users can insert these functions in their calculations to solve real-life problems, e.g., calculation of the steam turbine thermal cycle's efficiency. Even for the simplest cycle, without steam reheating, steam diversion from the turbine for heating feed water, and other efficiency measures, eleven wsp functions had to be inserted in this calculation.

In Fig. 4 this region is expanded. The functions are self-evident from their symbols (*H* - enthalpy, *P* - pressure, *T* - temperature, *S* - entropy, *W* - water, and *X* - steam quality).

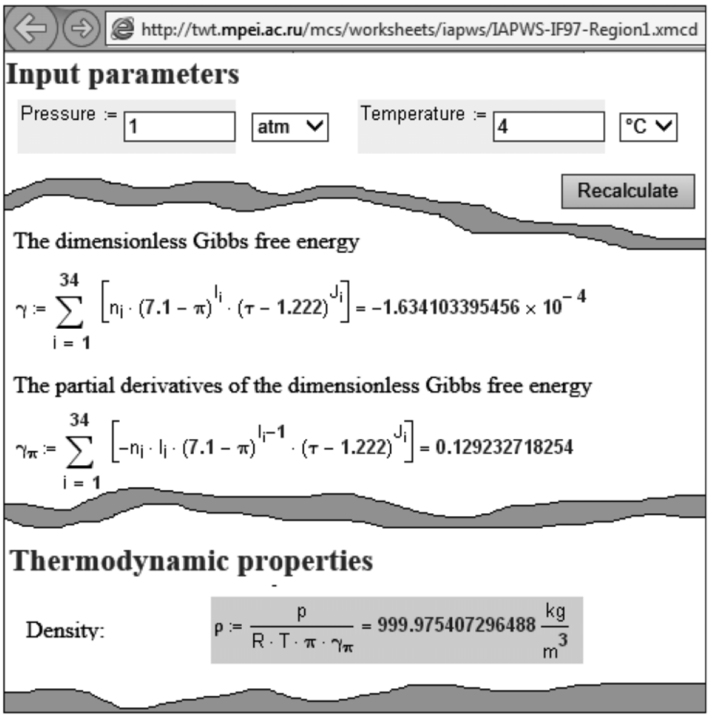

Fig. 3. "Live" calculation of the thermodynamic properties of water (Region 1, see Fig. 1).

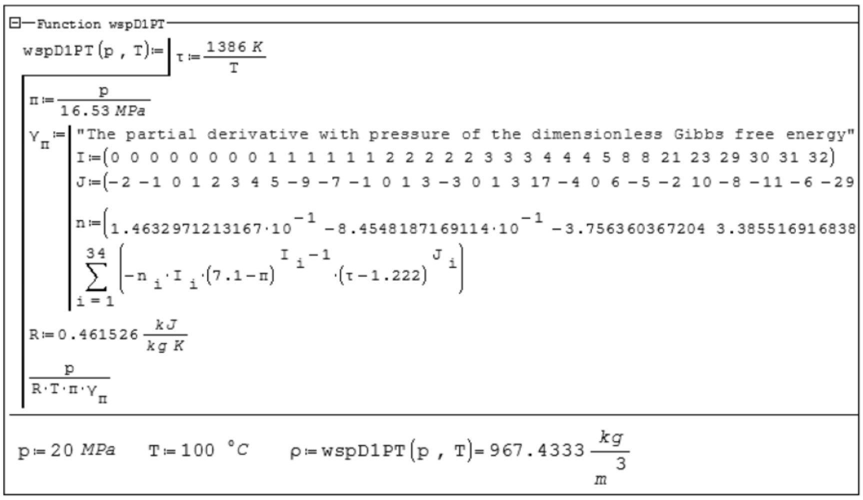

Fig. 4. Function returning water density in SMath.

One disadvantage of Mathcad is that its current Mathcad Prime version, in contrast to SMath, does not support interactive internet clients. That is way Elsevier, the world's largest electronic publishing house (www.elsevier.com), used SMath to develop Knovel Interactive Equations (https://app.knovel.com/ie/#welcome) for augmenting technical handbooks and databases published on Knovel website with *interactive calculations*. Knovel Interactive Equations product was developed by one of the authors. Access to it is free of charge. Visitors of the Elsevier website will be able not only to see and analyze "static" formulas in the electronic versions of books, handbooks, and papers, but also to carry out calculations by these formulas by inputting them online and "borrow" these formulas for their calculations. In addition, Knovel site has books with interactive tables and graphs, fully interactive and numerically searchable databases, including Knovel Steam Tables.

An example in Fig. 5 shows a calculation from Knovel Interactive Equations developed by one of the authors. To calculate pump power capacity, users have to know the density of pumped fluid (in this case, water) to calculate the volume flow rate from the mass flow rate of water. Calculation in Fig. 5 incorporates the equation returning the density of water as a function of pressure and temperature from Fig. 4. The calculation contains a reference to a source from ASHRAE (www.ashrae.org) with “static” formula for calculating pump power capacity, described in detail.

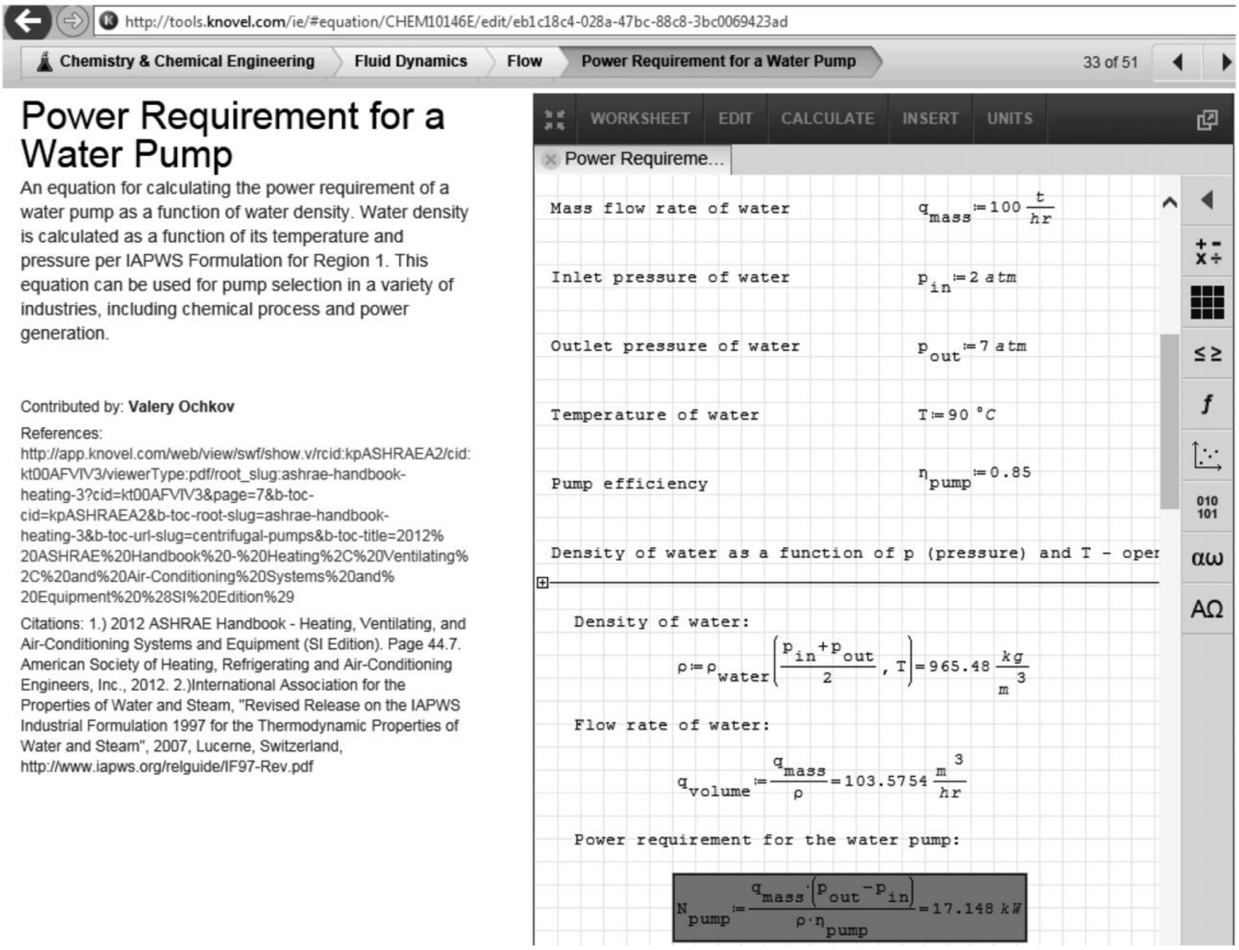

Fig. 5. Calculation of the pump power requirement.

References

1. Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (The International Association for the Properties of Water and Steam, Lucerne, Switzerland, August2007), www.iapw.org.
2. V F Ochkov, K A Orlov, A V Ochkov, V E Znamensky, and G I Kondakova, “Cloud water and steam functions for industrial applications,” in Proceedings of the 16th International Conference on the Properties of Water and Steam, September 1–5, 2013 (Univ. of Greenwich, London, UK, 2013), http://twt.mpei.ac.ru/ochkov/WSPHB/London