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REFERENCE MATERIALS

Properties of Water and Steam: Network, Open, and Interactive IT-Resources

V. F. Ochkov[a, b], K. A. Orlov[a, b], A. A. Aleksandrov[a], and A. V. Ochkov[a]

[a] *Moscow Power Engineering Institute National Research University, Krasnokazarmennaya ul. 14, Moscow, 111250 Russia*
[b] *Joint Institute of High Temperatures, Russian Academy of Sciences, Izhorskaya ul. 13, str. 2, Moscow, 125412 Russia*
e-mail: ochkov@twt.mpei.ac.ru

Abstract—New tendencies in publishing data on the thermophysical properties of substances are considered taking as an example water and steam, substances used as the main working fluid in thermal and nuclear power engineering. The advantages and shortcomings of both the traditional approach to publishing data on the properties of substances in hard printed form and the modern one, according to which the data are published in electronic form on Internet websites, are pointed out. The important requirements for publishing data in electronic form are described: the data must be presented in the form of network open and interactive calculations with examples of using them. A critical analysis of the relevant Internet resources is given. Some aspects of the work conducted by the International Association on the Properties of Water and Steam (IAPWS) are described. Particular examples of possible ways in which modern IT-resources on calculating the properties of substances can be set up are given: a hard printed handbook, a calculation program for being installed on a computer, calculation documents for downloading from a website, and using server calculations based on the technologies Mathcad Calculation Server on the website of the Moscow Power Engineering Institute National Research University and SMath on the website of the Elsevier electronic publishing house.

Keywords: thermophysical properties of substances, working fluids, and coolants used at thermal and nuclear power plants, thermal engineering calculations, Mathcad, SMath, Internet, IAPWS, Elsevier, Knovel

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Nowadays, in connection with very rapid development of information technologies, it is insufficient to have a description of thermophysical properties of substances in the form of "static" tables, graphs, or formulas (sets of formulas, tables, and graphs with manuals on using them, collectively called as formulations) published in journal articles, hard-printed handbooks, and on websites. At present, it is necessary that these databases were "live," (online) ones, i.e., *network, open, and interactive*. What does it mean?

Almost all computers of specialists who need data on the properties of substances are connected to the Internet. This is the present-day reality. And if a technician, engineer, or scientist needs information on the properties of one or another substance, including water and steam, his or her hand stretches not to the shelf with handbooks and journal articles, but to ... the computer mouse. Yes, the necessary information can be found in the Internet quite easily and promptly. Unfortunately, it should be borne in mind that the Internet also has the following uncomplimentary characterization: the Internet is a "worldwide free-for-all," and those who fill it with information frequently post everything there taking little care of how reliable the posted information is. However, it should be mentioned that many archeological excavations from the results of which we recreate the history of our civilization were carried out exactly at dumps that emerged near towns and settlements of ancient people. It can be conjectured that the future researchers will recreate the history, including the history of our mistakes and delusions, by delving exactly through the Internet archive.

It would not be out of place to point out that the terms "hard-printed" and electronic (Internet-based) are not quite unambiguously connected with the notion "faithful," because, alas, inaccurate information can also be found on paper carriers (in journal articles, handbooks, and other data carriers), even though these are rigorously peer-reviewed editions.

Nonetheless, there exist a number of quite reliable sources in the Internet, and it is exactly these sources that will be dealt with in this article.

At present, in publishing his or her data on the properties of substances, a researcher should take care of making sure that these data appeared in both hard-printed and electronic (network-based) forms. Hard-printed editions (journal articles, monographs, handbooks, various sorts of manuals, and regulatory documents) have their indubitable advantages. The point is that, with all promptness and accessibility of the Internet, the traditional technical book will remain in demand for quite a long time ahead. Such book (sewed together sheets with soft- or hard-cover binding) can be given as a gift to colleagues, friends, and dear ones; it can also be presented to a creativity competition (competitive selection for occupying a position in a higher school or research institute, for receiving a scientific degree, etc.). This hitherto cannot be done with a website, which nonetheless has its indubitable advantages. In particular, this technology offers the possibility of promptly rectifying errors and misprints and supplementing the existing data with new materials, color illustrations, 3D diagrams, animation, and, what is very important, and which is discussed below, "live" (online) calculations. Instead of disputing what is better—a book or a website, we will actively use the advantages of these two media products and try to avoid their drawbacks. One else argument that is commonly outspoken in favor of a hard-printed book (journal) is that such book (journal) can be read lying on a sofa, traveling along a road, etc. But at present, electronic books or tablet computers with good connection to the Internet have become available, which can also be dealt with lying on a sofa or traveling along a road. In addition, the user can additionally make electronic bookmarks in them and carry out an operative search and ... calculations.

As a rule, it is the journal publisher who takes care of the electronic (Internet) form of a publication. But in many cases it is the author himself (or herself) who does this by placing on the own website not only his or her articles or books, but also other auxiliary materials: reviews, early versions of articles, references to online calculations, etc. However, attempts of readers (users) to access these Internet-resources encounter difficulties in view of their being not free of charge and/or registration requirements. It should be noted that the access procedure itself, which involves the need of registration and transmitting personal data or data on the job place (including the data on the bank card) etc. to external servers, rather than the cost of granting access to one or another Internet-resource that holds off its potential users. This is one of aspects characterizing the *openness* of publications.

The notion *openness* implies the following. If a *calculation* is carried out based on the data on the properties of substances (for the notion *interactivity* see below), all *formulas* and intermediate results of calculations should be visible with estimating, as far as possible, the error (uncertainty).

Intermediate data are necessary not only for checking the correctness of calculations. They are also of importance for the site visitors who wish to develop their own program for calculating the properties of substances using the published formulas. Accessibility of intermediate data will help the user to quickly locate and rectify an error in the program being developed should it take place.

Interactivity as a characterization of modern databases implies the possibility of not only changing the initial parameters of a substance (pressure, temperature, density, etc.) by the website visitor, but also *attaching* the appropriate functional dependence to the visitor's software shell, as well as performing independent work with the function (procedure, template) downloaded from the website, its modification (refinement, correction of the permissible range of parameters, setting up nested and inverse functions, supplementing with comments, etc.). But what is most important, the term "interactivity" should be understood to mean the possibility of inserting the downloaded functions, procedures, and templates in the user's application calculations, in which these data on the properties of substances are required. And it is exactly these calculations for which such data are created, collected, analyzed, processed, and published...

The essence of the "network–open–interactive" triad is illustrated below taking as an example water and steam, which is one of the most widely used substances.

The International Association on the Properties of Water and Steam (IAPWS), www.iapws.org is the entity in charge for collection and generalization of thermophysical data of this sort, in the work of which the authors of this article take an active part. This noncommercial self-regulated organization holds annual working meetings, and once in 4–5 years it holds scientific conferences.[1]

At the IAPWS meetings, their participants discuss and confirm formulations on the properties of water and steam, which then become national and industry(-specific) standards applied in carrying out various calculations of processes, apparatuses, and technologies involving the use of this substance. There is no industry branch that would not use water as heat carrier/coolant, solvent, working fluid, etc. For example, what value has water density at atmospheric pressure and temperature equal to 80°C?! To answer this question, it is best to refer to the original source, namely, to take the relevant IAPWS formulation approved in 1997 and refined in 2007 for industrial use (the IAPWS-IF97) [1] and to carry out the appropriate calculations according to the formulas given in it. It is also possible to refer to tables of graphs prepared on the basis of these

[1] In 2014, such meeting was held in Moscow, see http://iapws.org/news/Press2014.pdf. In 2015, the IAPWS meeting will be held in Stockholm, and in 2016 it will be held in Dresden, see http://iapws.org/meetings.html. T.I. Petrova, a Professor at the Moscow Power Engineering Institute National Research University, in 2013–2014 was the Chairman of this authoritative organization.

calculations and published in various handbooks. The calculations presented in the formulations are rather cumbersome and as a rule are not suitable for manual calculations. Thus, for determining the density of water as a function of its pressure and temperature according to the IAPWS-IF97 formulation, it is necessary to calculate a polynomial of the 34th degree with coefficients having 14 digits in the mantissa (see Fig. 5 below). It should be noted that this formula is far from being the most complex and bulky one in the IAPWS-IF97 formulation, from which the properties of water and steam are calculated. For example, in the near-critical region (Region 3 of the IAPWS-IF97 formulation), the density of water as a function of pressure and temperature is calculated with subdividing this region into 24 subregions, and the density in each of them is calculated by individual formulas. Handbooks are published, and commercial and noncommercial computer programs are developed from IAPWS formulations after approving them.[2] The traditional formulations are a "static" document, which "does not respond to external inputs"—one cannot change the initial data in it and obtain a new answer. The formulations contain a detailed description of the calculation procedure and include tables with check calculation figures and calculation errors. A computer program is a "live" entity using which some calculations can be carried out, but one cannot call it a document because it does not contain a detailed description of the calculation procedure itself; in addition, it may contain computer errors (misprints in the computer program code). Efforts are presently taken by the IAPWS to remove this contradiction on the initiative and with active participation of the authors of this article.

Previously, IAPWS formulations were printed on typewriters, after which they were set up at print shops, sent to all interested organizations and persons, and were offered for free sale. Even now it is possible to find such old formulations on the IAPWS website in the form of scanned yellow typewritten pages with somewhat illegible letters. Texts and numerical constants cannot be copied from such a document by mouse clicks.

Later on, with development of information and computer technologies, formulations began to be published as text files, from which numerical constants could already be more or less easily copied for inserting them in the performed calculations and developed computer programs. Owing to these features, it became possible to accomplish the work on developing computer programs within an essentially shorter period of time and to reduce the risk of errors, which are unavoidable in manually (visually) transferring numbers from the formulation into the program being developed. The freely distributed shell Adobe Reader (www.adobe.com) became the means for publishing such formulations, and the formulations themselves were stored in pdf files, which can easily be generated using, e.g., the Word text processor, a program installed in almost each computer. However, the formulations still remained "static."

At the meeting of the IAPWS Task Forces that was held in 2007 in Luzern (Switzerland), one of the authors of this article demonstrated for the first time the "live" (online) formulation of a new technique in the Internet: calculation of water and steam ionization constant as a function of temperature and pressure. This online calculation was made in the Mathcad engineering calculator environment and published in the Internet using the Mathcad Calculation Server tool [2] (Fig. 1).

The calculation shown in Fig. 1 is quite simple. Nonetheless, an error was made in documenting this calculation in the form of "static" formulation, which was rectified in the course of developing the online calculation shown in Fig. 1. The point is that this formulation was prepared with orientation on programming languages that do not use the tools of physical quantities and their measurement units. On the contrary, the Mathcad package operates with these tools and does not allow "centimeters to be added with degrees," a feature that is very helpful in developing and debugging calculations.

The first conclusion that follows from what was said above is that formulations on the properties of substances shall be documented in the form of online calculations at least in order to reveal possible errors, misprints, and calculation inaccuracies, which may not be noticeable in "static" formulations. Unfortunately, such errors are quite frequently encountered in scientific-technical publications. Editors and correctors are very scrupulous in reading their texts, but the formulas often suffer from lack of such attention.

Initially, the IAPWS members met this first online calculation (see Fig. 1), which was proposed as a supplement to the traditional formulation, half-heartedly and even with vigilance. This can be attributed to the fact that according to one unspoken rule of the IAPWS, it is regarded inappropriate to single out or advertise one or another commercial computer program for calculations by the IAPWS formulations.

However, as time passed, after a number of reports that had been presented at regular working meetings and conferences of the IAPWS [3, 4], the technology of online calculations supplementing the "static" formulations was at last accepted and has become part of the IAPWS toolkit. Figure 2 shows one page of the IAPWS official website with the 1997 formula-

[2] The WaterSteamPro (www.wsp.ru) is an example of an author's computer program.

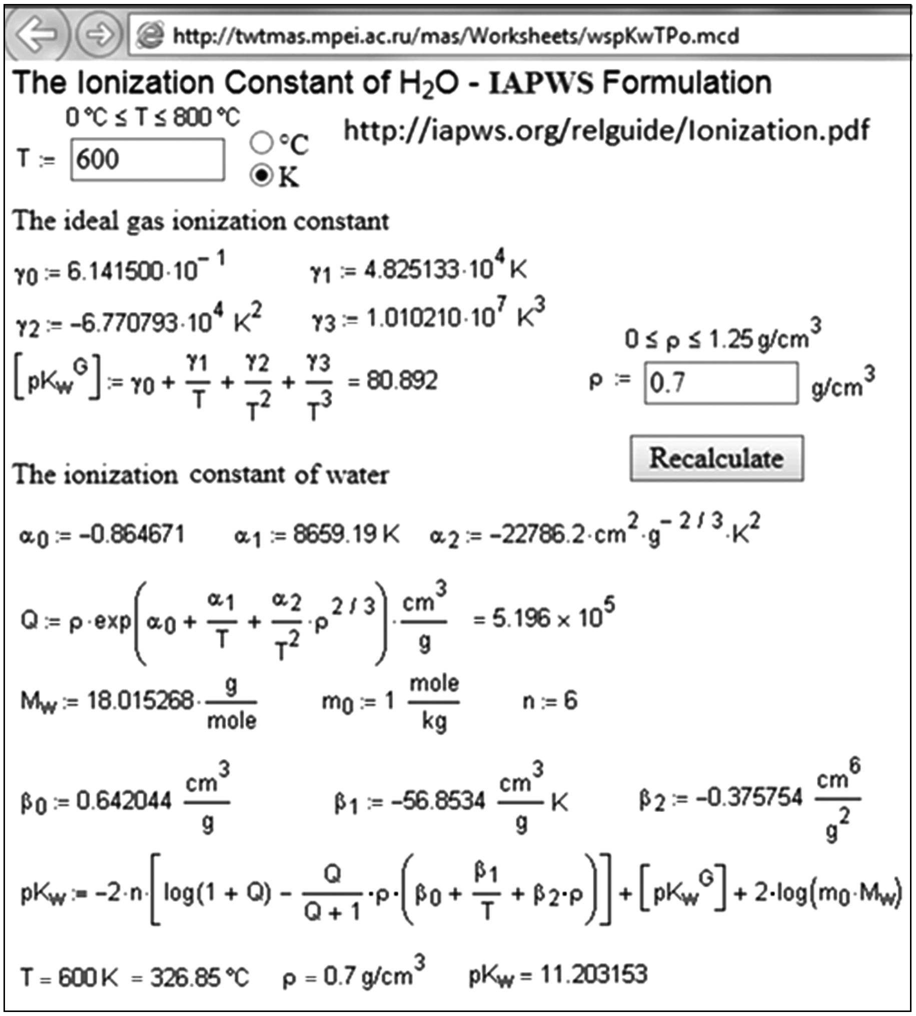


Fig. 1. "Live" calculation of the ionization constant of water as a function of temperature and density.

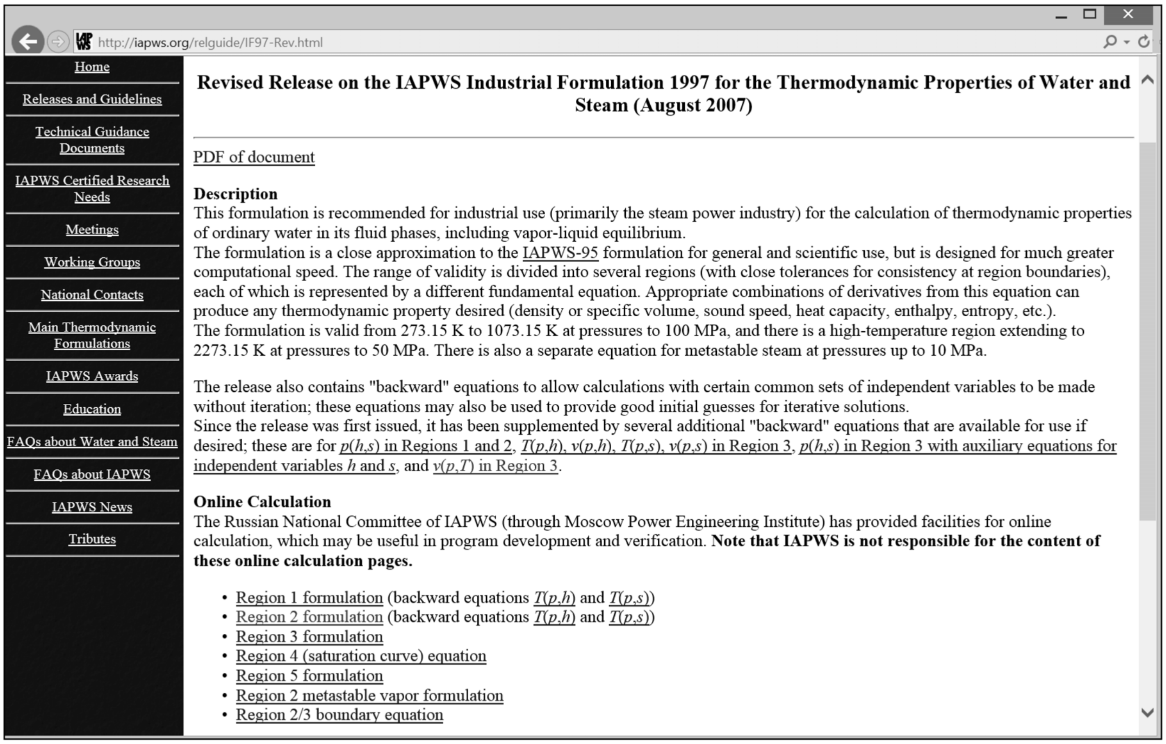
tions for calculating the thermodynamic properties of water and steam.

This page of the IAPWS website (see Fig. 2) contains a reference to the official pdf-document, its brief description, and references to online calculations in individual formulation regions:

- Region 1—water;
- Region 2—steam;
- Region 3—near-critical region;
- Region 4—saturation state;
- Region 5—steam at high temperatures, etc.

As an example, Fig. 3 shows fragments of the online calculation of the thermodynamic properties of water (Region 1): the pressure and temperature are entered (with selecting the necessary measurement units), the value of dimensionless Gibbs free energy is calculated (the already mentioned polynomial of the 34th degree), and the values of its partial derivatives by pressure (shown in Fig. 3) and temperature (not shown in Fig. 3) at the specified parameters of water. After that, the thermodynamic characteristics of water at the given point are calculated from the well-known formulas containing partial derivatives of Gibbs free energy by pressure and/or temperature: density (ρ), as well as (which is not shown in Fig. 3) specific inner energy (u), specific entropy (s), specific enthalpy (h), specific isochoric heat capacity (c_v), specific isobaric heat capacity (c_p), and sound velocity (w). The whole calculation is placed in the Internet on http://twt.mpei.ac.ru/mcs/worksheets/iapws/IAPWS-IF97-Region1.xmcd. The authors of this article have developed such online calculations also for other regions of the basic IAPWS-IF97 formulation, as well as for other formulations, e.g., on the transport properties of water and steam.

As was already pointed out, the online formulations are a very convenient tool for debugging an application computer program on calculating the properties of water and steam in the course of its


http://iapws.org/relguide/IF97-Rev.html

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Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam (August 2007)

PDF of document

Description
This formulation is recommended for industrial use (primarily the steam power industry) for the calculation of thermodynamic properties of ordinary water in its fluid phases, including vapor-liquid equilibrium.
The formulation is a close approximation to the IAPWS-95 formulation for general and scientific use, but is designed for much greater computational speed. The range of validity is divided into several regions (with close tolerances for consistency at region boundaries), each of which is represented by a different fundamental equation. Appropriate combinations of derivatives from this equation can produce any thermodynamic property desired (density or specific volume, sound speed, heat capacity, enthalpy, entropy, etc.).
The formulation is valid from 273.15 K to 1073.15 K at pressures to 100 MPa, and there is a high-temperature region extending to 2273.15 K at pressures to 50 MPa. There is also a separate equation for metastable steam at pressures up to 10 MPa.

The release also contains "backward" equations to allow calculations with certain common sets of independent variables to be made without iteration; these equations may also be used to provide good initial guesses for iterative solutions.
Since the release was first issued, it has been supplemented by several additional "backward" equations that are available for use if desired; these are for *p*(*h*,*s*) in Regions 1 and 2, *T*(*p*,*h*), *v*(*p*,*h*), *T*(*p*,*s*), *v*(*p*,*s*) in Region 3, *p*(*h*,*s*) in Region 3 with auxiliary equations for independent variables *h* and *s*, and *v*(*p*,*T*) in Region 3.

Online Calculation
The Russian National Committee of IAPWS (through Moscow Power Engineering Institute) has provided facilities for online calculation, which may be useful in program development and verification. **Note that IAPWS is not responsible for the content of these online calculation pages.**

- Region 1 formulation (backward equations *T*(*p*,*h*) and *T*(*p*,*s*))
- Region 2 formulation (backward equations *T*(*p*,*h*) and *T*(*p*,*s*))
- Region 3 formulation
- Region 4 (saturation curve) equation
- Region 5 formulation
- Region 2 metastable vapor formulation
- Region 2/3 boundary equation

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

development by comparing the results of intermediate calculations. Such formulation can also be used as a reference by interactively entering new values of pressure and temperature and obtaining the characteristics of this substance at the given point without paying attention to the intermediate results of calculations. If intermediate data are not needed at all, other similar websites of the authors can be visited (see http://twt.mpei.ac.ru/rbtpp), in which only the final result is returned, and the specified point can be additionally imaged in a family of curves or on a surface, which makes it possible to get a better idea on how the properties of steam and water depend on pressure, temperature, and/or other parameters.

The need to download files containing calculations on the properties of water and steam is satisfied through the website of the author's handbook on the thermodynamic properties of working fluids used in thermal power engineering: http://twt.mpei.ac.ru/rbtpp [5]; one of its pages is shown in Fig. 4.

The website shown in Fig. 4 contains not only references to "static" formulations and online calculations similar to the one shown in Fig. 1, but includes the additional possibility to download files for the mathematical computer programs Mathcad (the Mathcad 15 and Mathcad Prime versions) and SMath Studio (the Russian clone of Mathcad, see www.smath.info). The main advantage of the last computer program is that in many respects it repeats the philosophy and interface of the popular computer program Mathcad but is free of charge—in approximately the same way as is done with respect to the Adobe Reader computer program, which is mentioned above. Figure 5 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 other similar functions means Water/Steam Properties. Figure 5 shows only part of the values of vectors J and n, which are the coefficients of the polynomial of the 34th degree, from which, as was mentioned above, the dimensionless Gibbs specific energy and its partial derivatives with respect to pressure (π) and temperature (τ) are calculated.

Similar freely distributed functions have also been developed for other regions of the IAPWS-IF97 formulation and for other combinations of initial parameters, see Fig. 4. The users can insert these functions in their calculations and solve application problems, one of which, namely, calculation of the steam turbine thermal cycle's efficiency is shown in Fig. 6. This cycle is the simplest one: without steam reheating, without steam extractions from the turbine for heating feed water, and for other measures on improving the efficiency. Nonetheless, eleven functions with the suffix wsp had to be inserted in this calculation (see the reduced regions with the plus sign; in Fig. 5 such

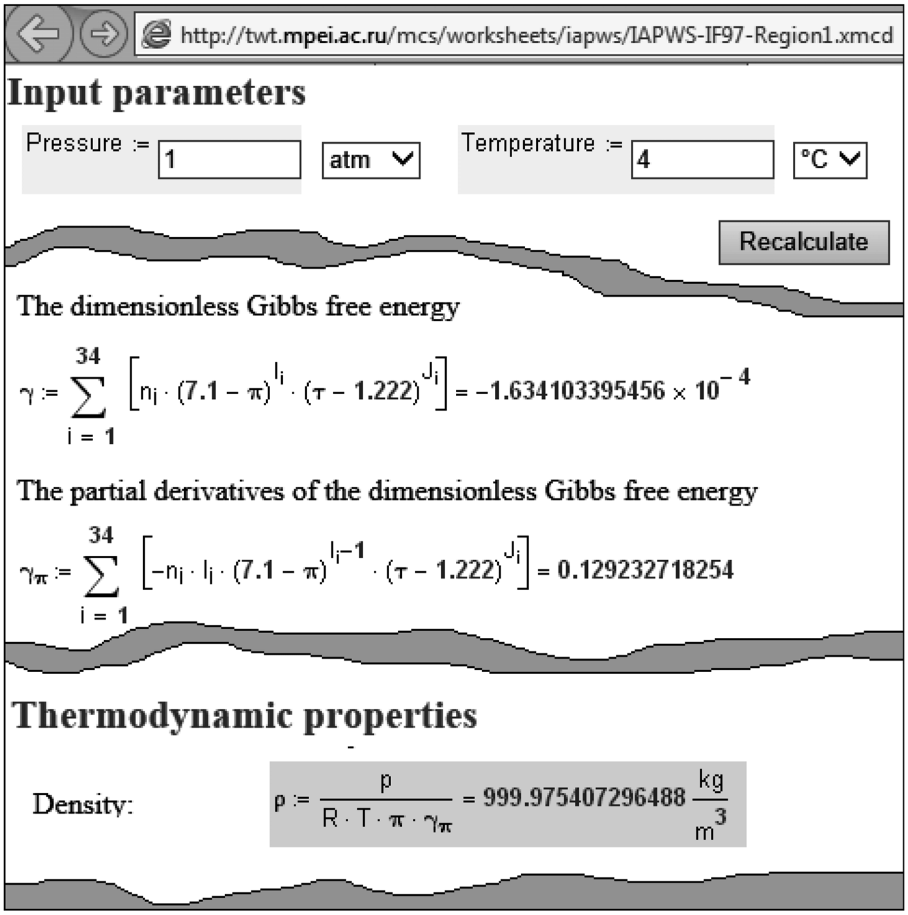
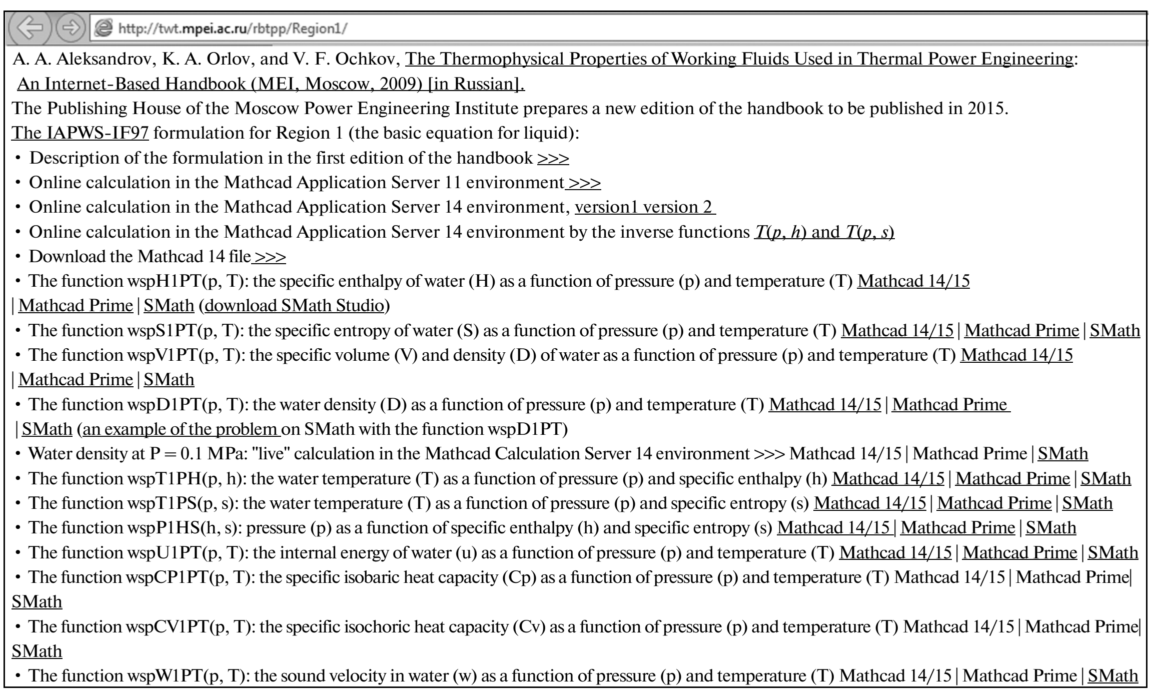


Fig. 3. "Live" calculation on the thermodynamic properties of water (Region 1, see Fig. 1).


http://twt.mpei.ac.ru/rbtpp/Region1/

A. A. Aleksandrov, K. A. Orlov, and V. F. Ochkov, The Thermophysical Properties of Working Fluids Used in Thermal Power Engineering: An Internet-Based Handbook (MEI, Moscow, 2009) [in Russian].

The Publishing House of the Moscow Power Engineering Institute prepares a new edition of the handbook to be published in 2015.

The IAPWS-IF97 formulation for Region 1 (the basic equation for liquid):

- Description of the formulation in the first edition of the handbook >>>
- Online calculation in the Mathcad Application Server 11 environment >>>
- Online calculation in the Mathcad Application Server 14 environment, version1 version 2
- Online calculation in the Mathcad Application Server 14 environment by the inverse functions *T*(*p*, *h*) and *T*(*p*, *s*)
- Download the Mathcad 14 file >>>
- The function wspH1PT(p, T): the specific enthalpy of water (H) as a function of pressure (p) and temperature (T) Mathcad 14/15 | Mathcad Prime | SMath (download SMath Studio)
- The function wspS1PT(p, T): the specific entropy of water (S) as a function of pressure (p) and temperature (T) Mathcad 14/15 | Mathcad Prime | SMath
- The function wspV1PT(p, T): the specific volume (V) and density (D) of water as a function of pressure (p) and temperature (T) Mathcad 14/15 | Mathcad Prime | SMath
- The function wspD1PT(p, T): the water density (D) as a function of pressure (p) and temperature (T) Mathcad 14/15 | Mathcad Prime | SMath (an example of the problem on SMath with the function wspD1PT)
- Water density at P = 0.1 MPa: "live" calculation in the Mathcad Calculation Server 14 environment >>> Mathcad 14/15 | Mathcad Prime | SMath
- The function wspT1PH(p, h): the water temperature (T) as a function of pressure (p) and specific enthalpy (h) Mathcad 14/15 | Mathcad Prime | SMath
- The function wspT1PS(p, s): the water temperature (T) as a function of pressure (p) and specific entropy (s) Mathcad 14/15 | Mathcad Prime | SMath
- The function wspP1HS(h, s): pressure (p) as a function of specific enthalpy (h) and specific entropy (s) Mathcad 14/15 | Mathcad Prime | SMath
- The function wspU1PT(p, T): the internal energy of water (u) as a function of pressure (p) and temperature (T) Mathcad 14/15 | Mathcad Prime | SMath
- The function wspCP1PT(p, T): the specific isobaric heat capacity (Cp) as a function of pressure (p) and temperature (T) Mathcad 14/15 | Mathcad Prime | SMath
- The function wspCV1PT(p, T): the specific isochoric heat capacity (Cv) as a function of pressure (p) and temperature (T) Mathcad 14/15 | Mathcad Prime | SMath
- The function wspW1PT(p, T): the sound velocity in water (w) as a function of pressure (p) and temperature (T) Mathcad 14/15 | Mathcad Prime | SMath

Fig. 4. Website for rendering information support to calculations on the thermodynamic properties of water.

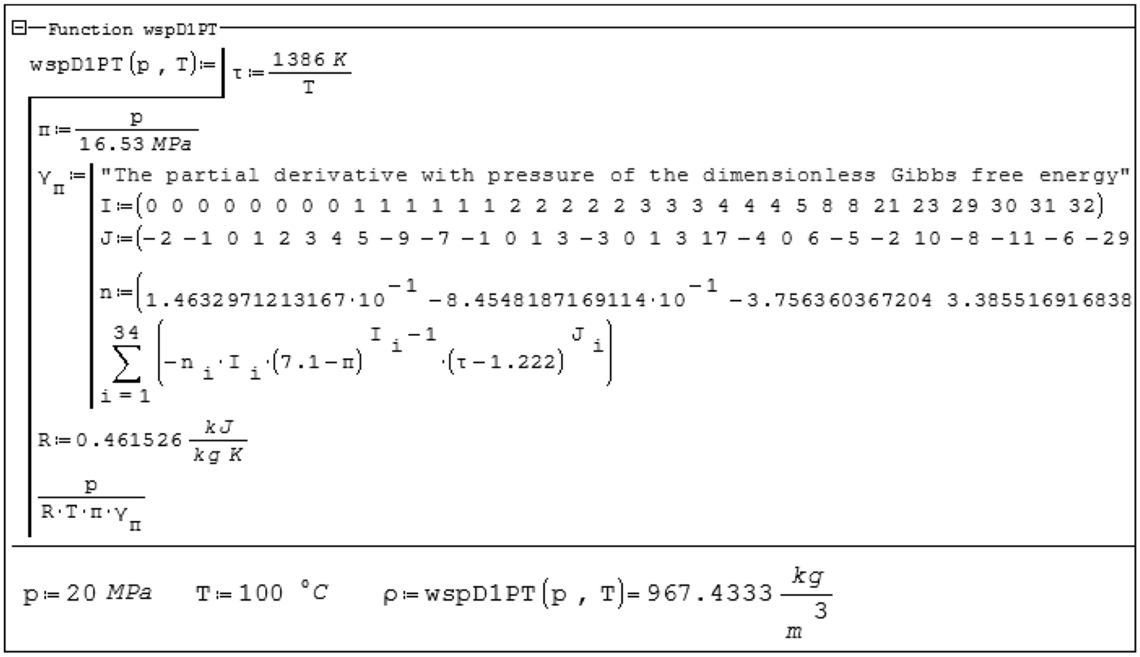


Fig. 5. Function returning water density set up in the SMath environment.

region is opened, and the plus sign has become the minus sign); the meaning of these functions can be understood from their abbreviation (*H* is enthalpy, *P* is pressure, *T* is temperature, *S* is entropy, steam, or saturation, *W* is water, and *X* is steam quality):

(1) *H2PT* is the specific enthalpy of steam as a function of pressure and temperature.

(2) *S2PT* is the specific entropy as a function of pressure and temperature.

(3) *TSP* is the temperature on the saturation line as a function of pressure.

(4) *SSWT* is the specific entropy of water on the saturation line as a function of temperature.

(5) *SSST* is the specific entropy of dry saturated steam as a function of temperature.

(6) *XTS* is the wet steam quality as a function of temperature and specific entropy (it was constructed with resting on the *SSWT* and *SSST* functions).

(7) *HSWT* is the specific enthalpy of water on the saturation line as a function of temperature.

(8) *HSST* is the specific enthalpy of dry saturated steam as a function of temperature.

(9) *HSTX* is the specific enthalpy of wet steam as a function of temperature and steam quality (it was constructed resting on the *HSWT* and *HSST* functions);

(10) *T1PS* is the temperature of water as a function of pressure and specific entropy.

(11) *H1PT* is the specific enthalpy of water as a function of pressure and temperature.

There is one more circumstance due to which the SMath computer program deserves close attention. The point is that Elsevier, which is the world's largest electronic publishing house (www.elsevier.com), has turned attention to this mathematical program and intends to use the SMath package as a tool for supplementing the technical handbooks and scientific-technical articles published on the Elsevier website for free or paid access with *interactive calculations*. The visitors of the Elsevier website will be able not only to see and analyze "static" formulas in the electronic versions of books, handbooks, and articles, but also to carry out calculations by these formulas and transfer these formulas in their calculations.

As an example, Fig. 7 shows one such calculation from the Elsevier website developed by one of the authors of this article.[3] For calculating the pump power capacity, it is necessary to know the density of pumped fluid (in the given case, water) for calculating the volume flow rate from the mass flow rate of water. The calculation shown in Fig. 7 incorporates the function returning the density of water depending on its pressure and temperature, which is reflected in Fig. 5. The website shown in Fig. 7 contains a reference to the authoritative source published by ASHRAE (see www.ashrae.org), in which the "static" formula itself for calculating the pump power capacity is presented and described in detail. The reader of this handbook

[3] This author has long been cooperating with the Knowel Company, which has become part of the Elsevier Publishing House.

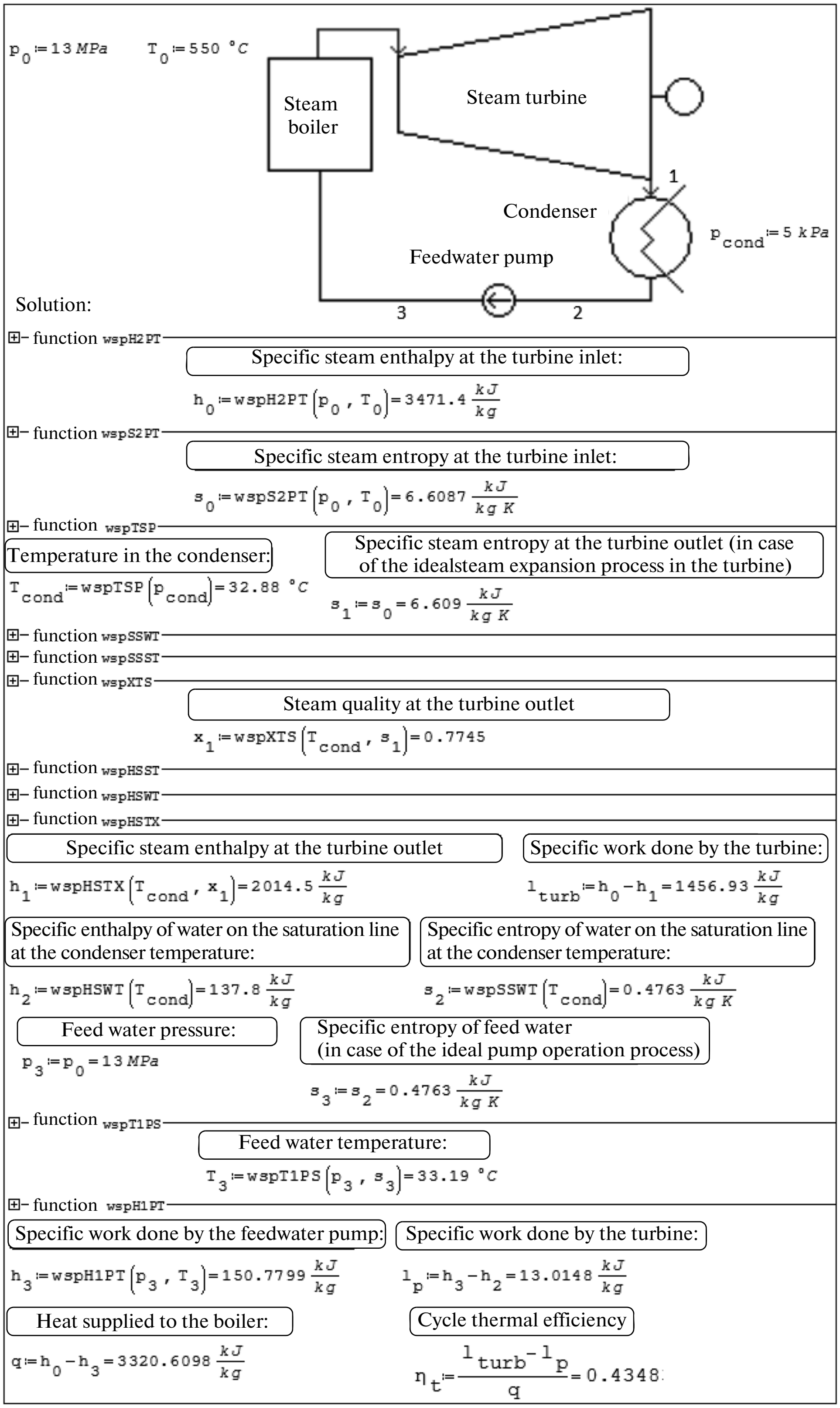


Fig. 6. Calculation of the thermal efficiency for the simplest steam-turbine cycle on superheated steam.

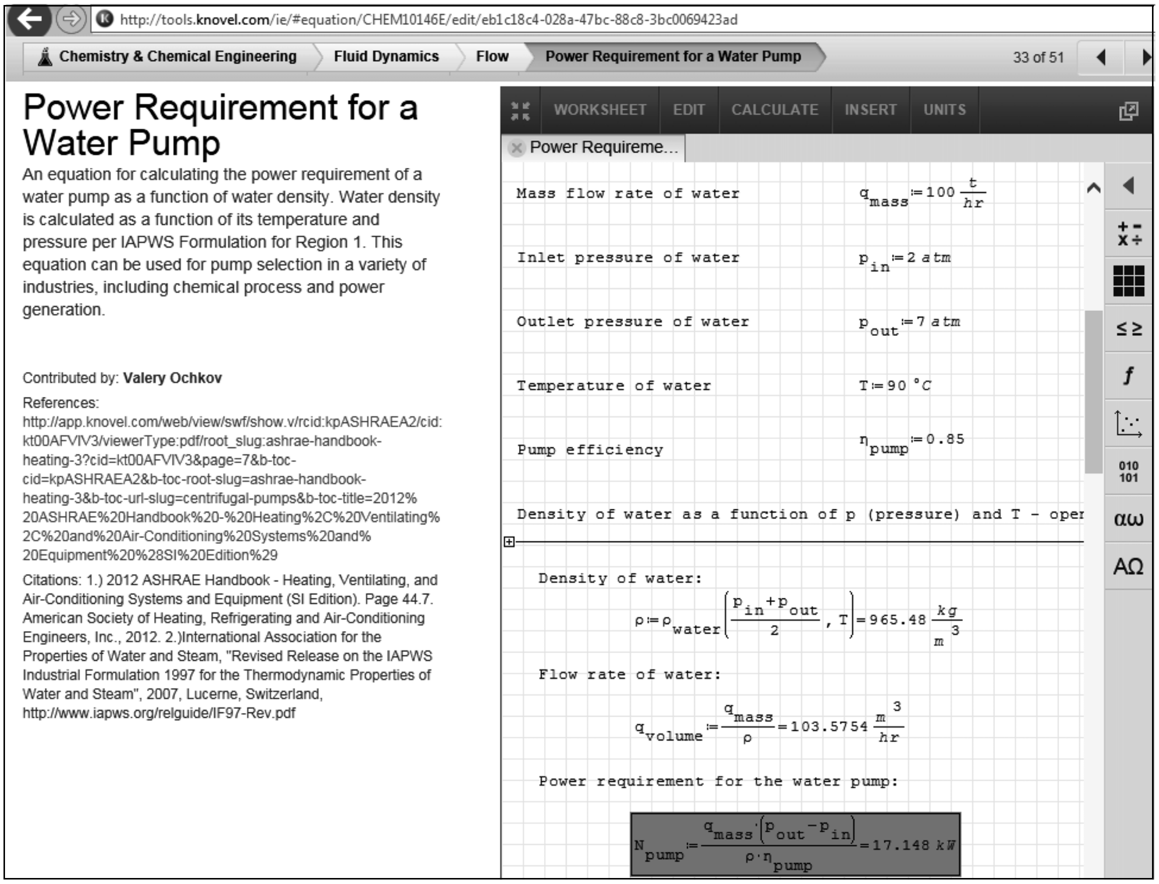


Fig. 7. Calculation of the pump power requirement.

(the visitor of the Elsevier website) can directly carry out calculation by these formulas and transfer there formulas into his or her application calculations [6–9].

The authors of this article have put forward a proposal about using the new information technology described above. It can be hoped that in the future, in parallel with publishing a new formulation on the properties of water and steam, the relevant functions will be posted in the IAPWS site, which can at once be transferred by the users to their application and scientific-technical calculations. The authors of this article have already prepared over 50 functions on the properties of water and steam, as well as a few practical calculations in which these functions are used. These functions will soon be tested and published. At present, these functions have been published only on the authors' site http://twt.mpei.ac.ru/rbtpp.

CONCLUSIONS

(1) The modern stage of the process through which data on the properties of substances are published must include a procedure of "animating" all graphs, tables, and formulas.

(2) In publishing an article, a monograph, or a handbook, the authors of data on the properties of substances should take care of making sure that all calculations were online ones and were supplemented with functions for downloading and inserting them into application computer programs.

(3) Given that the Adobe Reader text and formula processor is the standard for publishing "static" formulations on the properties of substances, the SMath mathematical computer program can become the standard for publishing online formulations.

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