Internet calculations of thermodynamic properties of substances: Some problems and results

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Abstract. Internet resources (databases, web sites and others) on thermodynamic properties \( R = (p, T, s, \ldots) \) of technologically important substances are analyzed. These databases put online by a number of organizations (the Joint Institute for High Temperatures of the Russian Academy of Sciences, Standartinform, the National Institute of Standards and Technology USA, the Institute for Thermal Physics of the Siberian Branch of the Russian Academy of Sciences, etc) are investigated. Software codes are elaborated in the work in forms of “client functions” those have such characteristics: (i) they are placed on a remote server, (ii) they serve as open interactive Internet resources. A client can use them for a calculation of \( R \) properties of substances. “Complex client functions” are considered. They are focused on sharing (i) software codes elaborated to design of power plants (PP) and (ii) client functions those can calculate \( R \) properties of working fluids for PP.

1. Introduction

Let us consider characteristics of the information that relates to thermodynamic properties, \( R = (p, T, s, h) \), of technologically important substances and posted on several web sites, where \( p \)—the pressure, \( T \)—temperature, \( s \)—the entropy, \( h \)—the enthalpy. We involve example No. 1 associated with a design of a power plant (PP). A client-designer should calculate the energy criteria \( Z \) including \( Z_1 \)—a gas turbine power, \( Z_2 \)—a thermal efficiency of the cycle, \( Z_3 \)—an input heat and other \( Z \) parameters of the cycle with respect to PP. The client uses its own program, which is referred to as Code1\((Z, R, Y)\), where \( Y = (Y_i, i = 1 \ldots N) \)—the set values including \((p_{t1}, T_{t1})\) those are the pressure and the temperature at the inlet of the first turbine, \( R = (p, T, s, \ldots) \) are the thermodynamic properties of the working body at predetermined points of the cycle.

This software is developed in Mathcad and often used in thermal power engineering. The above-mentioned \( R \) values are taken usually by the designer from an external source. Currently, a typical source of the information is the web site of one of organizations (including the National Institute of Standards and Technology (NIST) [1], the Joint Institute for High Temperatures of the Russian Academy of Sciences (JIHT RAS) [2–5], Standartinform (Russia), the Institute for Thermal Physics of the Siberian Branch of RAS). A client can choose the first type of \( R \) values from these web sites in the form of a text file. This name means that these \( R \) values has not got by a computer program or by an exe-file (the second type of \( R \) properties those are calculated by mathematical formulas or by an equation of state—EOS).
There is example No.2 that is associated with thermophysical calculations and connected with complex PP. A designer deals with a complex cycle in the case. This cycle includes many technical blocs and works with two substances. The designer has to operate with more complicated Code2\((Z, R, Y)\) that let us: (a) to work with a large number of \(Y\) set values and with many predetermined points of the cycle, (b) to fulfill an optimization procedure that consists of many steps and uses criterion functions, e.g. \(Z_1(Y_1, Y_2, \ldots)\).

The experience of the authors \([6–9]\) shows that there is a problem to produce a software which allows us: (i) to supply the designers with \(R\) data those have an analytical form and a high accuracy, (ii) to involve modern EOS’s in these calculations, (iii) to use IT possibilities in these calculations. We consider one more difficult problem to adopt accurate and complete EOS’s of working substances for a modernization that is connected with: (a) PP, (b) Code2\((Z, R, Y)\) and (c) an optimization procedure.

We have an aim to get a decision of these problems; we intend to develop a special technology and tools of creating a software that has a form of an open interactive (OI) Internet resource. There are several forms of OI resources those are connected with thermophysical calculations and discussed in the report (client functions, templates including resources (No.1, No. 2, No.3, No.4) see part 2) in a frame of the problem mentioned. One of the forms contains tabulated properties, \(R_t = (p, T, s, \ldots)\) of a substance (air, \(H_2O\), R134a, etc) with fixed arguments, for example \((p, T)\) — data those are placed in some area of values.

2. Open interactive Internet resources

Let us consider a method that is elaborated to build OI resource and to operate with tabulated properties, \(R_t = (p, T, s, \ldots)\), of a substance (air, \(H_2O\), R134a, etc). The first phase of OI resource creating includes Mathcad program development, for example, Code3\((\rho, Y)\). The code allows us to calculate \(\rho\) value of the air under boundary conditions \(Y = (p_1, T_1, \ldots)\) using \(R_t = (\rho, p, T)\) array which can be seen as a numerical table in figure 1. The air is a working substance of gas turbine engines. The code is based on a method that is connected with two-dimensional spline interpolation of \(R_t\) array. In the case, we use: (a) Mathcad function, \(\rho(p, T)\) (figure 1); (b) the values of \(p\) lying in the interval from 1 to 300 bar (figure 1); (c) \(t\) values in the range from \(-50\) to \(400^\circ\)C (the first row of \(R_t\) array, figure 1); (d) the values of \(\rho\); (e) a Mathcad function, csplain\((X, Z)\), performing a spline interpolation under \(Y\) conditions (figure 1). These \(Y\) conditions include: (a) \((p_1, T_1)\) parameters entered by an operator, (b) \((p, T)_{\text{max}}\) data and \((p, T)_{\text{min}}\) as border data, (c) other parameters.

Figure 1 shows a part of Code3\((\rho, Y)\) program. Here one can see the Mathcad function, \(\rho(p, t)\), which provides: (a) the choice of units, (b) the input \(Y\) values, for example \(Y = (p_1 = 250\text{ bar}, \ T_1 = 175^\circ\text{C})\), (c) formulas of \(\rho\) calculations and (d) the results of the calculations. There are two options for the values (European and American units) in figure 1. The proposed method gives an opportunity to use different units of measurement due to the positive features of Mathcad \([6,7]\).

OI resource No.1 is produced in the second phase of the method. We have used web site “Forum Mathcad” and its remote server to place the resource. OI resource No.1 includes a computing part \([6,8]\) or “Mathcad field” which is associated with formulas and used to calculate the density, \(\rho\), at input parameters, \(Y = (p, T)\). The Mathcad field (figure 2) is based on the program Code3\((\rho, Y)\). The resource contains an information part or “a text field” that represents a text information (references, comments on the mathematical formulas and comments on the method of calculations, etc). The third interactive part of the resource is related to the computer science and Internet technologies. This part gives us an ability to solve such tasks as: (a) to post the OI resource No.1 on a remote server, (b) to connect the personal computer (PC) with web site “Forum Mathcad” and (c) to implement a number of important options to the client. There are several options including: (a) to insert \(Y\) data and to calculate \(\rho\), (b) to read textual information, (c) to copy mathematical formulas or the code in general. These options can be
realized in the remote server (a cloud) and not in the PC. An important role plays some tools of Internet technologies those are used in the resource and related to the packages (“Mathcad Calculation Server”, “Microsoft Expression Web 3”) [6].

Using a “copy option”, a client can make a copy of the program Code2(ρ, Y) and simply insert it in his own code, for example, Code1(Z, R, Y). The client uses an ordinary method of his code modification in the case. We have got the following result: this variant of Code1(Z, R, Y) can automatically perform calculations of ρ properties for PP cycle under appropriate conditions Y = (p_i, T_i, i = 1..N), where N—a number of the cycle points. Using OI—resource No. 1, the client frees from an operation “the introduction of the properties of R = (ρ, p, T) to the loop points manually”. A “copy option” does not exist in known databases (JIHT RAS [2, 3], Standartinform (Russia) etc) those operate on closed programs (exe-files).

Along with these options, OI resource No. 1 provides additional features, for example, you can easily replace the array of (ρ, p, T)-data on the rectangular array if you are familiar with Mathcad in general. This array contains similar data connected with another substance. This option explains the term “template” which can be used with respect to OI resource No. 1. Due to the template a client can perform thermophysical calculations in a relation to PP. The values of ρ are calculated on the basis of a modern method in the case.

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\rho(250\text{bar},175^\circ\text{C}) = 174.755 \text{ kg/m}^3
\]
3. Some types of client functions

Let us consider another variant of OI resource named as No. 2. This client function is made in the following form: it is based on the program Code3(ρ, Y) and placed on a remote server owned by the National research university “MPEI” [9]. We have elaborated a following form to connect PC of a client with a web site [9] and with OI resource No. 2. On the first step, a designer introduces a service address or “Link” (http://twt.mpei.ac.ru/TTHB/Ro-p-t.xmcdz) in his own Code1(Z, R, Y). The link is related to OI resource No. 2. There is a part of Code1(Z, R, Y) in figure 2 where one can see the link of OI resource No. 2 or a client function ρ(p, T). On the second step, the client inserts Y parameters (p = 20 MPa, T = 350 °C) those can be seen at the top of figure 2. The resource provides a client with an option “to compute ρ” under Y conditions. The calculated density value, 103.016 kg/m^3, is placed too in figure 2.

Our technology involves the following algorithm: (i) the user accesses: (a) Y parameters, (b) a link associated with OI resource No. 2, (ii) the resource performs the following actions: (a) sending Y parameters to a remote server, (b) computing the value of ρ on this server using “cloud function ρ(p, t)”, (c) returning the value of ρ to PC. We remark firstly: due to OI resource No. 2 a client can convert these tabulated R data into: (a) values of ρ calculated with a help of the resource, (b) 2D graph (figure 2) or (c) 3D graph using Mathcad tools. These characteristics explain common terms: “live tables and live graphs” those are used for R data and for 2D graph (figure 2) connected with OI resource No. 2. Secondly, due to the resource a designer has get an opportunity to run ρ(p, t) calculations on the powerful remote server with the last version of Mathcad.

We have elaborated another variant of OI resource named as No. 3, which is developed in a relation to the so-called inverse functions. It is accepted that the client function, ρ(p, t), is known and available on the remote server in the case. This client function is discussed earlier and

![Figure 2. A part of Mathcad field connected with OI resource No. 2: 1–5—isobars.](image-url)
let us calculate a density of the air. Using OI resource No. 3, one can calculate the properties, \( R = (p, T) \) including the pressure, \( p \), at given arguments, \((\rho, T)\) as well as the temperature, \( T \), at given arguments, \((\rho, p)\). Figure 3 shows the Mathcad field related to resource No. 3. It can be seen a built-in Mathcad function, \( \text{root}(\rho(p, T) - \rho, p) \), which allows to calculate the inverse function, \( p(\rho, T) \), using the method of “half division” (position 1). The resource includes a Mathcad function, \( T(\rho, p) \), that computes parameter \( t \) using “secants method” (position 2).

We have created OI resource No. 4 that has following features: (a) it deals with a complex PP (example No. 2), (b) it uses Code_3\((Z, R, Y)\) that is familiar to Code_2\((Z, R, Y)\) but works with two substances (the air, the water), (c) it uses a big number of \( Y \) set values and (d) it operates with many predetermined points of the combined cycle. The combined PP includes: (a) several gas turbines and compressors (a gas turbine part), (b) several steam turbines, (c) a heat recovery boiler, etc. Code_3\((Z, R, Y)\) let us calculate \( Z \) criteria those include \( Z_1, Z_2, Z_3, Z_4 \)—the power of a heat recovery boiler, \( Z_5 \)—a steam turbine power, \( Z_6 \)—the thermal efficiency of a steam turbine and other criterions of the complex cycle [10]. The code involves modern EOS’s in the \( R \) calculations of the substances. In the case, we have adopted EOS that is related to the water [11] and has a form of the free energy, \( F(\tau, \omega) \), where \( \tau \)—a relative temperature, \( \omega \)—a relative density. The code contains near 100 coefficients. It let us build OI resource No. 4 to calculate \( R \) properties with a high accuracy. For example, an error, \( \delta h \), of the enthalpy is less than \( \delta h = 0.1\% \) when we determine \( Z_6 \) criterion, which depends on \((h_i)\) values of the cycle in our task. With a help of the resource, for example, a client can determine \( Z_6 \) values of a cycle that is related to the steam turbine part of PP.

In the case of Code_3\((Z, R, Y)\), we have adopted EOS of the arc [12] that has a form of the compressibility, \( z(\tau, \omega) \), and contains near 50 coefficients. The code let us calculate \( Z_2 \) values of a cycle that is related to the gas turbine part of PP in the case. For example, we have got \((Z_2, \pi_k, T_1)\) data those are calculated by Code_3\((Z, R, Y)\) and covered a wide area of arguments.
Figure 4. $Z_2(\pi_k, T_1)$ dependence of a cycle that is related to the gas turbine: 1—$T_1 = 1700 \, ^\circ C$, 2—$T_1 = 1600 \, ^\circ C$, 3—$T_1 = 1500 \, ^\circ C$, 4—$T_1 = 1400 \, ^\circ C$, 5—$T_1 = 1300 \, ^\circ C$, 6—$T_1 = 1200 \, ^\circ C$.

including $T_1 = (1200\ldots1700) \, ^\circ C$ (figure 4) at the pressures up to $p = 50 \, MPa$, where $\pi_k$—a relative pressure of the gas compressor, $T_1$—a temperature in the first gas turbine, $p$—the pressure in a gas compressor.

A row of client functions are elaborated for Internet calculations and inserted in OI resource No. 4. These functions are approved by the International association for properties of the water and the steam (IAPWS; http://www.iapws.org). The resource is placed in a server of the National research university “MPEI”. Due OI resource No. 4, we have solved a problem to share: (i) a software code that is used for PP design and (i) client functions those can calculate $R$ properties of working bodies on a base of accurate EOS’s.

The authors together with specialists from the National research University “MPEI”, JIHT RAS and LLC “Trier” have created a group of OI resources those can be used to calculate $R$ properties of some technologically important substances (the air, $H_2O$, $CH_4$, $R134a$, etc). There are some OI resources those enter in the group and use: (i) approximation methods and (ii) the spline–schemes mentioned in the report. A least squares method has been adapted to build polynomials, for example, a $\rho(t)$ function for the density on the saturation line of a substance mentioned. Some of these OI resources are placed in [11, 13].

4. Conclusion

We have discussed some client functions and templates those are connected with thermodynamic properties of technologically important substances and based on innovative Internet technologies. These functions have a form of OI resources (OI resource No. 1, OI resource No. 2, etc) and can be an effective software for PP design. OI resource No. 4 complements significantly traditional forms of an Internet information that is reflected, for example, in the classification [8]. These OI resources can be considered as a positive decision of the problems discussed in part 1 of the article.
Some of these OI resources are placed in [11, 14]. Interesting OI resources and a technology of OI resource development are considered too in [15]. One type of these resources is used successfully in e-trainers those are placed in power plants to train a personnel [16]. The authors have shown [14] some advantages of client functions those are discussed in the article and work much faster than a similar traditional software that calculates $R$ properties of the water in e-trainers. There has been a working IAPWS meeting in Moscow on July 10, 2014. The members of the meeting have adopted a IAPWS formulation that governs the usage of some client functions discussed above and focused on thermodynamic properties of the water.

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References
[1] Linström P J and Mallard W G 2005 *NIST Chemistry WebBook, NIST Standard Reference Database Number 69* (Washington, DC: National Institute of Standards and Technology)
[2] 2007 URL http://www.thermophysics.ru/triptych
[3] Levashov P R, Khishchenko K V, Lomonosov I V and Fortov V E 2004 *AIP Conf. Proc.* 706 87–90
[4] Levashov P R, Khishchenko K V and Lomonosov I V 2006 *AIP Conf. Proc.* 849 353–357
[5] Khishchenko K V, Levashov P R, Povarnitsyn M E and Zakharenkov A S 2009 *AIP Conf. Proc.* 1195 69–72
[6] Ochkov V F 2009 *Mathcad 14 dlya Studentov i Inzhenerov: Russkaya Versiya (Mathcad 14 for Students and Engineers: The Russian Version)* (Saint-Petersburg: BKhV-Peterburg)
[7] Ochkov V F 2002 *Fizicheskie i Ekonomicheskie Velichiny v Mathcad i Maple (Physical and Economic Quantities in Mathcad and Maple)* (Moscow: Finansy i Statistika)
[8] Ochkov V F 2007 *Internet-Versiya Spravochnika “Teploenergetika i Teplotekhnika: Instrumentalnye Sredstva Sozdaniya i Razutiya (Internet Version of the Reference Book “Heat Power and Heat Engineering: Instrumental Tools for the Creation and Development)* (Moscow: Moscow Power Engineering Institute)
[9] Ochkov V F, Orlov K A, Ochkov A V, Znamenskii V E, Voloshchuk V A and Chizhakova V Y 2013 *Vestn. Mezhdunar. Akad. Kholoda* 47 23–28
[10] Ochkov V F, Ustyuzhanin E E and Znamenskii V E 2011 *Trudy Akademenergo* 1 110–123
[11] 2002 URL http://www.wsp.ru
[12] Aleksandrov A A, Orlov K A, and Ochkov V F 2009 *Teplofizicheskie Svoistva Rabochikh Veshchestv Teploenergetiki: Internet-Spravochnik (Thermal and Physical Properties of Working Substances for Heat Power Engineering: Internet Reference)* (Moscow: Moscow Power Engineering Institute)
[13] URL http://ttw.mpei.ac.ru/TTHB/kyawkoko/
[14] Sychev V V, Vasserman A A, Kozlov A D and Spiridonov G A 1978 *Termodynamicheskie Svoistva Vozdukha (Moscow: Izdatebtsvo Standartov)*
[15] Kunick M, Kretzschmar II J, and Gampe U 2012 *Tagungsband der 13 Nachwuchswissenschaftler konferenz mitteldeutscher Fachhochschulen Gorlitz* (Honekamp, W. and Schindler, P.) p 209
[16] Ochkov V F 2009 *Trudy Akademenergo* 2 13–32