Thermophysical Databases: From Tables to Interactive Internet Resources and Cloud Templates

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Abstract—Internet resources with information on thermal–physical properties of technologically important substances are analyzed. 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, the Institute for Thermal Physics of the Siberian Branch of the Russian Academy of Sciences, etc.) are reviewed. Custom functions and cloud templates for the calculation of the thermal properties of substances and solutions to some applied problems are considered.

INTRODUCTION

Let us consider the characteristics of the information on the thermophysical properties of substances that has been published on several websites, for example, on the website associated with the design of the power plant (PP). In this example, the user-designer should calculate the values of energy criteria Z (the thermal efficiency, turbine power, heat input, and other parameters of the cycle) with respect to the PP using its own program, which is referred to as Code_1(Z, Y), where $Y = (y_i, i = 1...N)$ are set values including (p_{t1}, t_{t1}) that are the pressure and temperature at the inlet of the first turbine and thermodynamic properties of $R_{cycle} = (p, t, v, h, …)$, the working body at predetermined points of the cycle.

Let the program Code_1(Z, Y) be created in the Mathcad environment. The values of R_{cycle} are taken by the user usually from an external source. Currently, a typical source of information is the website of one of the organizations (e.g., the Joint Institute for High Temperatures of the Russian Academy of Sciences (JIHT RAS), Standartinform, the National Institute of Standards and Technology (NIST) [1], the Institute for Thermal Physics of the Siberian Branch of the Russian Academy of Sciences (ITP SB RAS) [2], etc.), on which the best-known resources with such text files are published. This choice means that the resource does not use a computer program or exe-file to calculate the properties by mathematical formulas. Resource files contain tabulated properties of $R_t = (\rho, h, s, …)$ for fixed arguments (p, t) for the working material (R134a, H_2O, etc.). Turning to the resource, the user receives tabular values of R_t focusing on Y parameters. In order to determine R_{cycle}, it is necessary to perform a multistep interpolation of table values R_t and multiple introduction of this information in the program.

The experience of the authors of [3–6] shows that it is relevant to search for software (SW) that makes it possible to adapt tabulated values of R_t for the PP design. Let us consider the recently created Internet resource based on the array $R_t = (\rho, p, t)$ of material density data in the gas phase (see Fig. 1).

In the first phase the program Code_2(ρ, Y) was developed. It makes it possible to calculate the value of ρ based on the method designed for the double spline interpolation of the array R_t and includes the following: (1) the Mathcad function $\rho(p, t)$, (2) values of p ranging from 1 to 300 bar (see Fig. 1), (3) values of the temperature t in the range from −50 to 400°C (the first row of the array, Fig. 1), (4) the table of density ρ, and (5) the Mathcad built-in function in the form of csplain(X, Z) (see Fig. 1) that performs spline interpolation in the specified boundary conditions.

The program Code_2(ρ, Y) includes boundary conditions $Y = (p, t, …)$, which are parameters (p, t) entered by the user, boundary arguments $(p, t)_{max}$ and $(p, t)_{min}$, and other parameters.

Figure 1 shows a part of the program Code_2(ρ, Y). Here, the Mathcad function $\rho(p, t)$ can be seen, which provides for the selection of measurement units, input of given values of U, e.g., $U = U$ ($p = 250$ bar, $t = 175$°C), calculation of ρ, and display of the results on the screen. Figure 1 shows two options, i.e., customary units of the United States and the metric system. The code makes it possible to select other measurement units, too. The proposed calculation method using the units is one of the positive features of Mathcad [3, 4] that greatly facilitates the calculations and eliminates possible errors.

$\rho(p,t) :=$ "Spline interpolation of table data"

$$M \leftarrow \begin{pmatrix} \text{"p, bar\textbackslash t, °C"} & -50 & 0 & 50 & 100 & 150 & 200 & 300 & 400 \\ 1 & 1.563 & 1.275 & 1.078 & 0.932 & 0.8226 & 0.7356 & 0.6072 & 0.517 \\ 50 & 83.79 & 65.2 & 53.96 & 46.25 & 40.57 & 36.18 & 29.8 & 25.37 \\ 100 & 175.6 & 131.4 & 107.1 & 91.13 & 79.66 & 70.92 & 58.37 & 49.71 \\ 200 & 340.3 & 253.7 & 205.4 & 174.3 & 152.2 & 135.6 & 111.8 & 95.41 \\ 300 & 449.3 & 350.8 & 288.6 & 246.7 & 216.4 & 193.4 & 160.3 & 137.4 \end{pmatrix}$$

$\left(x \leftarrow \dfrac{p}{\text{bar}} \, y \leftarrow \dfrac{t}{K} - 273.15 \text{ "Transformation of arguments to a dimensionless form"} \right)$

$(X \leftarrow \text{submatrix}(M,1,\text{rows}(M) - 1,0,0) \text{ "Stub column} - \text{p"})$

$[Y \leftarrow (\text{submatrix}(M,0,0,1,\text{cols}(M) - 1))^T \text{ "Table heading} - \text{t"}]$

return "p and/or t outside the range" if $x < \min(X) \lor x > \max(X) \lor y < \min(Y) \lor y > \max(Y)$

$(Z \leftarrow \text{submatrix}(M, 1, \text{rows}(M) - 1,1,\text{cols}(M) - 1) \text{ "Contents of the table} - \rho\text{" })$

$\begin{pmatrix} \text{for } i \in 0.. \text{ cois}(Z) - 1 & \text{"Formation of an additional line"} \\ \quad Zv_i \leftarrow \text{interp}(\text{cspline}(X,Z^{\langle i \rangle}), X,Z^{\langle i \rangle}, x) \end{pmatrix}$

$\text{interp}(\text{cspline}(Y,Zv), Y, Zv, y) \cdot \dfrac{\text{kg}}{\text{m}^3}$

$\rho(250\text{bar}, 175°\text{C}) := 178 \dfrac{\text{kg}}{\text{m}^3}$

Fig. 1. Mathcad field of OI resource no. 1.

INTERACTIVE PUBLIC INTERNET RESOURCES

At the second stage, open interactive (OI) Internet resource no. 1 was created using the website Mathcad Forum and a remote server. The computing part (Mathcad field), which is included in the OI resource, was based on the program Code_2(ρ, Y). In the general case, the methodological base of the OI resource no. 1 was the open interactive algorithm [6]. The authors developed a specific technology and used a number of tools for the creation of the OI algorithm (Fig. 2). The OI algorithm *1* contains the following components: part *2* associated with the formulas for the calculation of the density ρ by given parameters *U* and the corresponding Mathcad code *7*, text part *3* that includes support information on the density ρ of the material (the array of (ρ, *p*, *t*) data, the chemical formula of the material, notesn to mathematical formulas, and the description of the calculation of the density ρ, as well as other information), and part *4* related to computer and Internet technologies.

Note that OI resource no. 1 provides the client with a number of options, including calculation of the property ρ when entering data $\tilde{U}$, reading of the text information including the array of (ρ, *p*, *t*) data, and copying of the mathematical formulas or code in general. These options are executed on a remote server

rather than on the personal computer (PC) of the user. The packages Mathcad Calculation Server *8* and Microsoft Expression Web 3 *9* play an important role in the formation of the OI resource no. 1 (Fig. 2).

With the copying option, the client can make a copy of the program Code_2(ρ, Y), place it in an individual code Code_1(Z, Y), and then perform calculations of the density on the PC using $\rho(p, t)$. There is no copying option in the known databases (JIHT RAS [2], Standartinform, etc.), which operate closed programs (exe-files).

Along with the options considered, OI resource no. 1 provides additional features. Firstly, it is possible to construct a surface by the function of two arguments $\rho(p, t)$ using 3D graphics in the Mathcad environment. It is useful to build such a function graph not only for visual analysis of the behavior of the material when its parameters are changed but also in order to record possible errors and typos. Thus, a graph (Fig. 3) was constructed using a deformed matrix that was obtained by replacing 107.1 kg/m^3 (Fig. 1) with the shifted value 170.1 kg/m^3.

Secondly, users familiar with Mathcad in general can easily replace the array of (ρ, *p*, *t*) data included in the copy of the program Code_2(ρ, Y) with their own rectangular array containing similar data. As a result, the user can perform thermophysical calculations with

respect to the PP. In this case, the values of ρ will be calculated based on the mentioned method of spline interpolation and a modified array of (ρ, p, t) data.

OI resource no. 1 is classified as a client function. Since 2010, such functions have been placed not only on the Mathcad Forum but also on other websites related to thermophysical calculations.

INTERPOLATION VERSIONS OF CLIENT FUNCTIONS

Let us consider another option of OI resource no. 2, which was developed by the authors in the following form. This option was based on the program Code_2(ρ, Y), located on a remote server that belongs to the Moscow Power Engineering Institute (MPEI) and provides the user with a number of options including the "calculation of the ρ property" in the following form. If, in the previous example, it was necessary to calculate the density ρ(p, t) for input parameters $U(p = 20$ MPa, $t = 350°$C), here the user inserts a service address or a link (http://twt.mpei.ac.ru/TTHB/Ro-p-t.xmcdz) in the program Code_1(Z, Y). Figure 4 shows the Mathcad field of OI resource no. 2, where the parameters U, the calculated density, and the link to the cloud function ρ(p, t) are placed at the top. At the bottom of Fig. 4, there is a 2D graph built using the function ρ(p, t) for fixed values of U without the typo mentioned above. Under the graph there is an option for the temperature $t = 500°$C (this value is outside of conditions Y (Fig. 1)) and the corresponding error message "out of range."

Let us emphasize that the graphs (Figs. 3, 4) explain the common terms "live table" with respect to the table, which is an array of $R_t = $ (ρ, p, t) and is included in Code_2(ρ, Y), and "live books" in relation to e-books, which are equipped with OI resources in order to present tables from the book in the form of graphs.

The technology developed by the authors provides the following algorithm: the user accesses the link, and OI resource no. 2 automatically sends U parameters to a remote or cloud server, calculates the value of ρ on the remote server by cloud function ρ(p, t), and returns to the computer.

An option is proposed according to which the client uses a service password, and OI resource no. 2 gives them access to a Mathcad field similar to the field shown in Fig. 1. As a result, it is possible to copy other options, too.

As in the first option, the user can edit the copied Mathcad field (i.e., to use the resource as a template, which makes it possible, for example, to replace the original array of (ρ, p, t) data with an array R_t that contains similar data for other material and has a rectangular shape) and calculate the density ρ under the new boundary conditions.
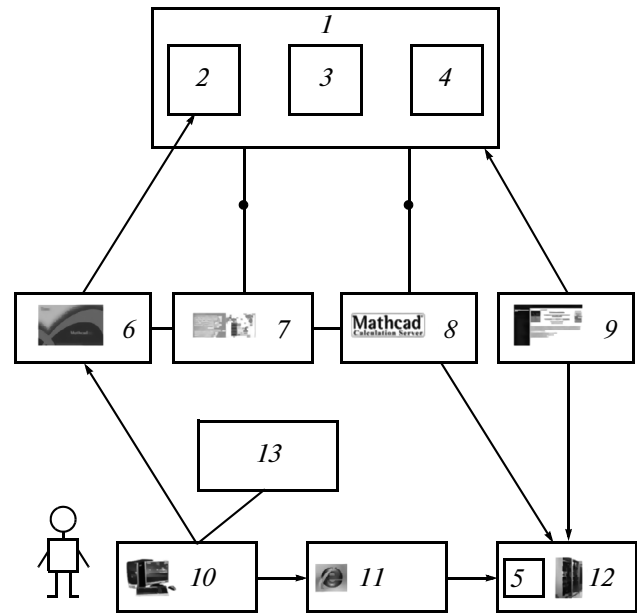
Fig. 2. Sources of information and tools used to create an open interactive algorithm: the OI algorithm (*1*), The Mathcad field of the algorithm (*2*), text (*3*), part associated with Computer Science and Internet technologies (*4*), the template (*5*), Mathcad-tools (*6*), Mathcad-program (*7*), Mathcad Calculation Server (*8*), package Microsoft Expression Web 3 (*9*), PC user (*10*), Internet (*11*), the remote server (*12*), and the individual user program (*13*).
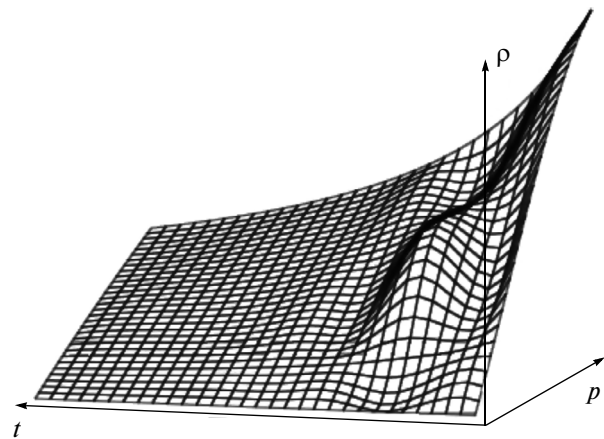

Fig. 3. Surface displacement ρ(p, t).

Note that the considered template presented in the form of a link (see Fig. 4) has certain advantages (availability over the Internet, a wide range of options, etc.) over information that has a traditional shape, is scattered over thermophysical databases, and belongs to a number of organizations (research and commercial companies and educational institutions). Traditional forms are quite varied (paper or spreadsheets, charts, formulas or computer programs, see the classification in [5]). Interested professionals involved in
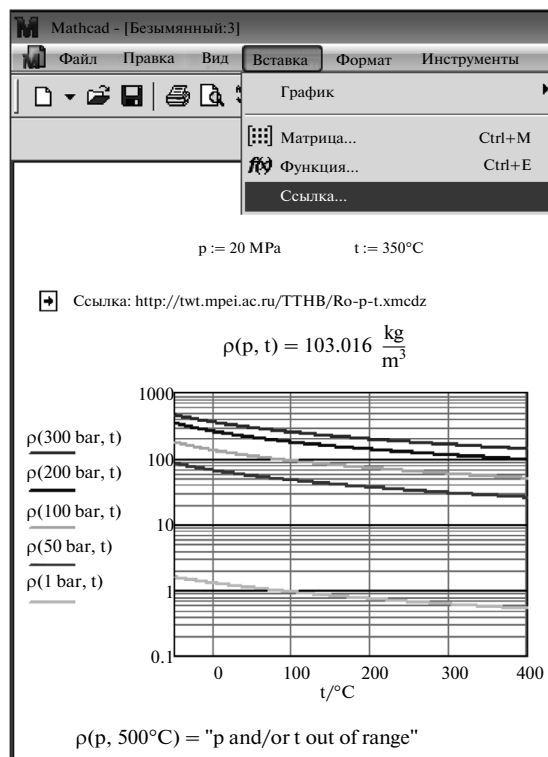
Fig. 4. The Mathcad field of OI resource no. 2 and 2D-graphics function $\rho(p, t)$.

▶ Function $\rho(p, t)$

$\rho(300 \text{ bar}, 100°C) := 247 \dfrac{\text{kg}}{\text{m}^3}$

Inverse function

1. $t(p, \rho) := \text{root}(\rho(p, t) - \rho, t, 223.15 \text{ K}, 673.15 \text{ K})$

$t\left(300 \text{ bar}, 247 \dfrac{\text{kg}}{\text{m}^3}\right) := 100°C$

2. $p(\rho, t) := \begin{vmatrix} \rho \leftarrow 100 \text{ bar} \\ \text{root}(\rho(p, t) - \rho, p) \end{vmatrix}$

$\rho\left(247 \dfrac{\text{kg}}{\text{m}^3}, 100°C\right) := 300 \text{ bar}$

Fig. 5. The Mathcad field of OI resource no. 3.

the PP design often cannot use these databases effectively. Firstly, it is necessary to find them. Secondly, it is necessary to ensure that they are of good quality and are certified. Thirdly, and most importantly, it is necessary somehow to connect the information included in this database to the working software environment. A typical situation is when a project organization is prohibited to enter external data on the properties of material manually into their own codes, although the information can be fresher and/or more precise than that preloaded into the computer database. The reason is that in the case of the manual input there might be a typo or measurement units could be confused.

Let us consider OI resource no. 3, which has been developed in relation to the so-called inverse functions that reflect the properties of R_t in cases where the function $\rho(p, t)$ is known (Fig. 1) or it is necessary to solve inverse problems, namely, to calculate the pressure by density and temperature, as well as to compute the temperature by pressure.

Figure 5 shows the Mathcad field of the OI resource no. 3 designed to find inverse functions $p(\rho, t)$. As in the case of OI resource no. 1, the built-in function $\text{root}(\rho(p, t) - \rho, p)$ was involved. This function makes it possible to retrieve the value of p for given boundary conditions using the bisection method (item 1). There is also a built-in function ($\text{root}(\rho(\rho, t) - \rho, p)$) for calculation of t using the secant method (item 2).

The function $\rho(p, t)$ (Fig. 4) is continuous and monotonic in the selected field of values of pressure and temperature. When dealing with more complex equations, inverse functions of which can have two or more values within the given boundary conditions, it is necessary to introduce an additional argument, the initial approximation in finding the inverse function. For example, in order to determine the water (water vapor) pressure by temperature and specific enthalpy, the desired point can lie in any single-phase region or in a two phase region (wet steam) [7].

These studies showed that it is possible to use a random number in a predetermined range as the first approximation in the calculation of the values of properties of R as the inverse function. This option has been tested in the development of OI resource no. 4, which builds a 2D graph that contains a set of curves $p(t, \chi)$ for water vapor provided that the isentropic exponent χ takes a number of constant values. Figure 6 shows the Mathcad field for OI resource no. 4 and the 2D graph for the set of curves $p(t, \chi)$. In this resource custom functions wspPTK(t, χ) and wspKPT(p, t) posted on the website WaterSteamPro were used [8]. These functions rely not on the tabulated raw data but on a single equation of the state of water [8]. The random number generator made it possible to build the required set of curves $p(t, \chi)$ of very complex form. The experience of the authors shows that in the Mathcad environment it is possible to construct inverse functions provided that the given direct function that describes the properties of R of the material and the tools used to solve the necessary equation or system of equations are consistent.

A large number of client functions and cloud templates on the calculation of thermophysical properties of working substances were created on the server by the authors in collaboration with experts of MPEI, JIHT RAS, and OOO Trieru (see http://www.trie.ru). The statistics of complaints received on this site indicates that user-defined functions and templates of this type are very popular. The work on the creation of live

tables from data published in papers, books, and on the Internet, as well as data on thermal properties of technologically important materials, was organized at the Department of Water and Fuel Technology of MPEI. Custom functions and templates were constructed based on mathematical formulas presented in the literature, graphs showing the properties of *R* and published in papers, and numerical data relating to the properties of *R* and stored on discs.

At the request of Mathcad users working in the field of thermal and industrial power engineering a number of cloud templates were constructed. With the participation of the authors, custom functions [6] were created for thermophysical properties of organic working bodies, which were used in the steam-turbine cycle, for example, with ethanol.

The OI resources specified are partly described in [9], and the technology of their development and method of use are considered in [10−12]. Many of these resources are focused on calculation of the properties of *R* in relation to the PP and have a much more complex form than OI resources nos. 1−3. For example, in OI resources related to the properties of water, formulas are programmed designed to calculate the properties of water. These formulas were approved by the International Association for the Properties of Water and Steam (see http://www.iapws.org). The equation of state and auxiliary formulas used in these client functions contain about 100 coefficients.

Similar software is popular in the design of refrigerators and heat pumps [10]. The user is also looking for numerical values of energy criteria *Z* (refrigerating factor, thermodynamic efficiency, compressor power, input and output heat, etc.) using their own program. In [10] OI resources devoted to *R* properties of organic compounds (ethanol and a number of refrigerants) and numerical data $R_t = (\rho, p, t)$ based on them were developed. Some arrays R_t were obtained using the code Refprop (developed by NIST).

For some OI resources, approximation methods were used including the linear least squares (LLS) method, which makes it possible to construct the approximating polynomial by tabulated (*R*, *t*) data. The analysis shows that OI resources that make it possible to calculate the density ρ based on the tabular (ρ, *i*) data and LLS have important practical applications. They successfully work in electronic simulators, which are used to train staff of thermal and nuclear power plants. This software provides calculation of *R* properties of working bodies with high speed and a small time step in the online mode. A small loss of accuracy is considered permissible. Under these conditions, calculations based on the interpolation of points of the original array are carried out faster than, for example, a similar calculation of the equation of state. Our experience shows that modern PCs have a fairly large amount of memory that makes it easy to install any source arrays. In addition, the task of the user who wants to enter known numerical data on all
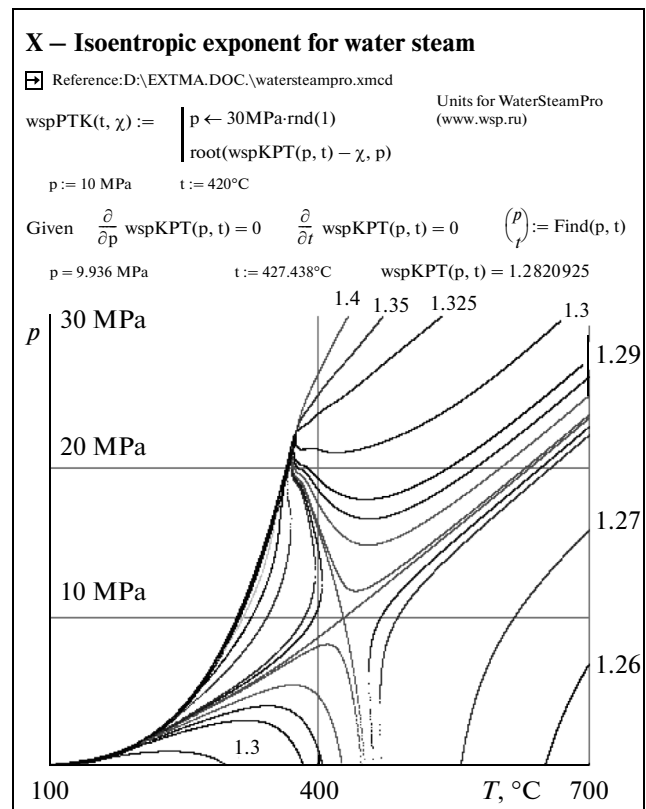

Fig. 6. The Mathcad field of OI resource no. 4 and the graph of the set of curves $p(t, \chi)$.

properties of all possible substances in the PC memory is impossible. The following approach is much more realistic: the reference information on the *R* properties should be placed in the form of client functions and cloud templates that users can easily access over the Internet and easily adapt, for example, to the PP design.

In this paper we considered the problem associated with the calculation of *R* properties based on the interpolation table $(R, p, t, …)_t$, while the region of existence is divided into parts by phase transition lines. In the selected table [9], there is a jump in values of properties at the phase transition. The table is not rectangular and can be partially filled. In [7, 12, 13] OI resources were proposed that were designed to solve this problem including calculation of $R(p, t, …)$ properties in a wide range of state parameters including solid, liquid, and gaseous phases. In [13] an OI resource was also considered that made it possible to interpolate the original table $(R, p, t, …)_t$, and a combined method of presenting certain areas/lines was proposed using vectors related to transition curves, partly filled matrices, and a set of equations. The development of such methods is being conducted in Germany [14].

CONCLUSIONS

Client functions and cloud templates were designed for the calculation of thermophysical properties. They are based on an innovative Internet technology and are effective software for the design and operation of energy and other facilities. The OI resources investigated significantly supplement those traditional forms of information, as reflected, for example, in the classification in [6]. An important problem is the development and installation of software in the form of cloud templates that make it possible to calculate the properties of $R(p, t, …)$ and are accessible on the Internet, greatly simplifying the work of designers of power plants, heat pumps, and refrigeration equipment.

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