1. Properties of working fluids, coolants and structural materials for thermal calculations

As we noted in the introduction, calculations of thermal processes are impossible without a proper knowledge of the properties of working bodies. We begin with the Etude by not focusing on the use of software tools such as WaterSteamPro (we will talk about this packages in different parts of the book). Instead, we will talk about some unique techniques associated with new information technologies.

1.1. About databases on the properties of substances for functions and templates in Mathcad

Some time ago in an internet forum about Mathcad (http://communities.ptc.com/community/mathcad - see also studies 6 and 12), the author saw a request by a stranger from a far-awway India for some help (see Table. 1.1).

	A	B	C	D	E	F	G	H	I
1	p, bar\ t, °C	-50	0	50	100	150	200	300	400
2	1	1,563	1,275	1,078	0,932	0,823	0,736	0,607	0,517
3	50	83,79	65,20	53,96	46,25	40,57	36,18	29,08	25,37
4	100	175,6	131,4	107,1	91,13	79,66	70,92	58,37	49,71
5	200	340,3	253,7	205,4	174,3	152,2	135,6	111,8	95,41
6	300	449,3	350,8	288,6	246,7	216,4	193,4	160,3	137,4

Table 1.1 Pressure, density and temperature of a substance

A stranger from a far-away India, which, after our conversation on the forum became the "a far-away Indian friend", asked visitors of the forum to create a function that would use as arguments the pressure ranging from 1 to 300 bar (see table 1.1, first column) and temperature ranging from -50 ° C to 400 °C (see the first row of the table) and then return the density of a substance in kg/m^3 (content of the table).

The author had a function for solving this problem at his fingertips, edited it a bit and then posted the solution on the forum - see Fig. 1.1. In Mathcad the first row/column is designated with the index 0. By using the built-in variable Origin, the user has the opportunity to change how to designate the first row/column. So, for example, if the the variable ORIGIN is set to 1,

you can call the first row/column with the index 1.

```
ρ(p,t) := | "Сплайн-интерполяция табличных данных"
          |
          |        ("p, bar \ 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 |
          | M ←    |  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 |
          |
          | ( x ← p/bar   y ← t/K − 273.15   "Приведение аргументов к безразмерному виду" )
          |
          | (X ← submatrix(M, 1, rows(M) − 1, 0, 0)   "Боковик таблицы - p" )
          |
          | [Y ← (submatrix(M, 0, 0, 1, cols(M) − 1))^T   "Шапка таблицы - t" ]
          |
          | return  "p и/или t вне диапазона"  if  x < min(X) ∨ x > max(X) ∨ y < min(Y) ∨ y > max(Y)
          |
          | (Z ← submatrix(M, 1, rows(M) − 1, 1, cols(M) − 1)   "Содержание таблицы - ρ" )
          |
          | ( for  i ∈ 0 .. cols(Z) − 1                    "Формирование дополнительной строки"
          |   Zv_i ← interp(cspline(X, Z^⟨i⟩), X, Z^⟨i⟩, x) )
          |
          | interp(cspline(Y, Zv), Y, Zv, y)·kg/m^3
```

$$\rho(250\text{bar}, 175\ °\text{C}) = 174.8\ \frac{\text{kg}}{\text{m}^3} \qquad \rho(2.2\text{ksi}, 175\ °\text{F}) = 9.004\cdot\frac{\text{lb}}{\text{ft}^3}$$

Figure 1.1 Spline-interpolation of tabular data (Mathcad 15)

In the program shown in Fig. 1.1 you can see how double- spline interpolation is used. What happens in the program? First, the arguments of the function ρ lose their units x ← p/bar and y ← t/K - 273.15. Without this the built-in function cspline in Mathcad 15 would not work. In the newest version, Mathcad Prime, you can also use cspline with units- see Fig. 1.1a. The last statement of the program (function shown in Fig. 1.1) is, because of the desired unit density. This is a common technique for empirical formulas - see Etude 2.

The built in function submatrix creates a matrix out of the matrix M - the outset (vector X) and "cap" (vector Y). The line with the return statement controls the arguments of the function ρ, so they remain within the specified pressure- and temperature range (see also paragraph 1.1.7 "extrapolation" in the Etude below). Hereinafter the same function generates a submatrix Z – it filters Table 1.1, so there will be a submatrix created without the "cap" and the outset. Next, out of the columns of the density matrix Z an additional line (vector Zv) for a given pressure will be generated by spline interpolation. Our "intermediate" in this example will have for p = 250 bar, following elements 403, 306, 249, 211, 185, 165, 136 and 116 kg/m³ for the temperatures -50, 0, 50, 100, 150, 200, 300 and 400 ºC, respectively (see "cap" table 1.1). Further in the program shown in Fig. 1.1 again spline interpolation is required for the density dependence on

temperature, absent of the "cap" of the table. Spline interpolation of two vectors is shown in Fig. 4.3.

In Fig. 1.1 the last two operators show how to call the generated function ρ(p, t) for different values of pressure (p) and temperature (t) and with various European and American units. Function ρ (p, t) returns the default density (ρ) with the basic SI units (kilograms and meters), but the user also may choose other units - pounds and feet, for example. Working with units (not just with the values and the physical quantities) - it is, we repeat, a unique feature of Mathcad, greatly facilitates calculations and prevents many errors [2], which we describe in more detail in the Etude 2.

Fig. 1.1a shows a program with double spline interpolation and English commentary (Mathcad Prime), where it becomes possible to use a matrix with different dimension. The function shown in Fig. 1.1a, does not depend on the value of the system variable ORIGIN. Again the "cap" and outset of the table in Fig. 1.1a have the units pressure and temperature. In order to save space the units of the table content (density) are not shown.

```
ρ(p, t) := | "Spline interpolation of tabular data"
           |  M ← [ "p \ t, °C"  −50 °C   0 °C   50 °C  100 °C  150 °C  200 °C  300 °C  400 °C ]
           |        [   1 bar     1.563   1.275  1.078  0.932   0.8226  0.7356  0.6072  0.517  ]
           |        [  50 bar    83.79    65.2   53.96  46.25   40.57   36.18   29.8   25.37  ]
           |        [ 100 bar   175.6    131.4  107.1  91.13   79.66   70.92   58.37  49.71  ]
           |        [ 200 bar   340.3    253.7  205.4  174.3   152.2   135.6   111.8  95.41  ]
           |        [ 300 bar   449.3    350.8  288.6  246.7   216.4   193.4   160.3  137.4  ]
           |  [P ← submatrix(M, 1+ORIGIN, rows(M)−1+ORIGIN, ORIGIN, ORIGIN)  "Outset of the table - pressure"]
           |  [T ← (submatrix(M, ORIGIN, ORIGIN, 1+ORIGIN, cols(M)−1+ORIGIN))^T  "Cap of the table - temperature"]
           |  if p<min(P) ∨ p>max(P) ∨ t<min(T) ∨ t>max(T)
           |     | return "p and / or t out of range"
           |  [R ← submatrix(M, 1+ORIGIN, rows(M)−1+ORIGIN, 1+ORIGIN, cols(M)−1+ORIGIN) · kg/m^3  "Content of the table"]
           |  [ for i ∈ ORIGIN .. cols(R)−1+ORIGIN   "Formation of an additional line in the table"
           |  [    | Rv_i ← interp(cspline(P, R^(i)), P, R^(i), p)                                ]
           |  interp(cspline(T, Rv), T, Rv, t)
```

$\rho(250\ bar, 175\ °C) = 174.8\ \frac{kg}{m^3}$ $\rho(2.2\ ksi, 175\ °F) = 9.004\ \frac{lb}{ft^3}$

Fig. 1.1a. Spline interpolation of tabular data (Mathcad Prime)

For a function with two arguments it is easy to construct the surface in Mathcad. Fig 1.2 shows that the function ρ (p, t) is smooth, increases with increasing pressure and decreases with increasing temperature.

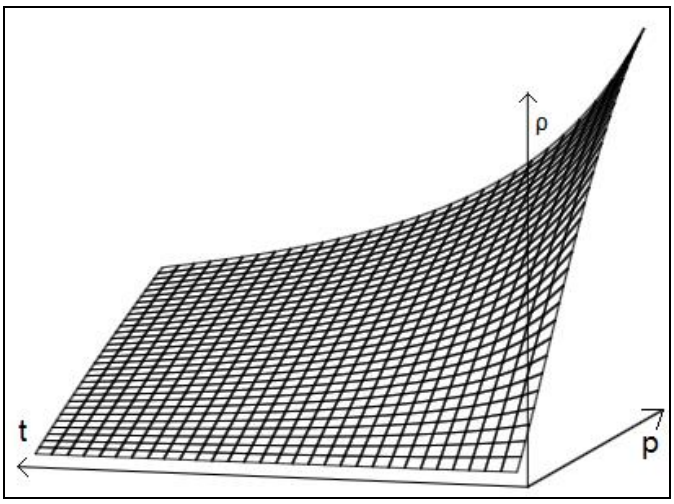


Fig. 1.2. Graphic display of a function (density) with two arguments - pressure and temperature

It (Fig. 1.2) shows typical "Thermophysical behavior" of many substances (gases) in the single-phase region. The graph of the function is not only useful for visual analysis of the behavior of matter, but also to fix possible errors and typos. Thus, if in the matrix shown in Fig. 1.1, intentionally or accidentally the density 107.1 kg/m3 (Table it. 1.1 allocated in the frame) is overwritten by 170.1 kg/m3 (a very common error when publishing numbers in magazines and books, and / or when manually entering numbers on a computer), the surface shown in Fig. 1.2, change its form - see Fig. 1.3. But this is not so simple. A splash on the chart may be not just a mistake, but maybe some anomalous behavior of substances. So, when seeing such a "mistake", you need first to check before correcting it – either it is a typo, or a scientific discovery. The graph is not created by interpolation (conducting the surface through the points) - it is just created by approximation (smoothing - conducting surface near points) of the table.

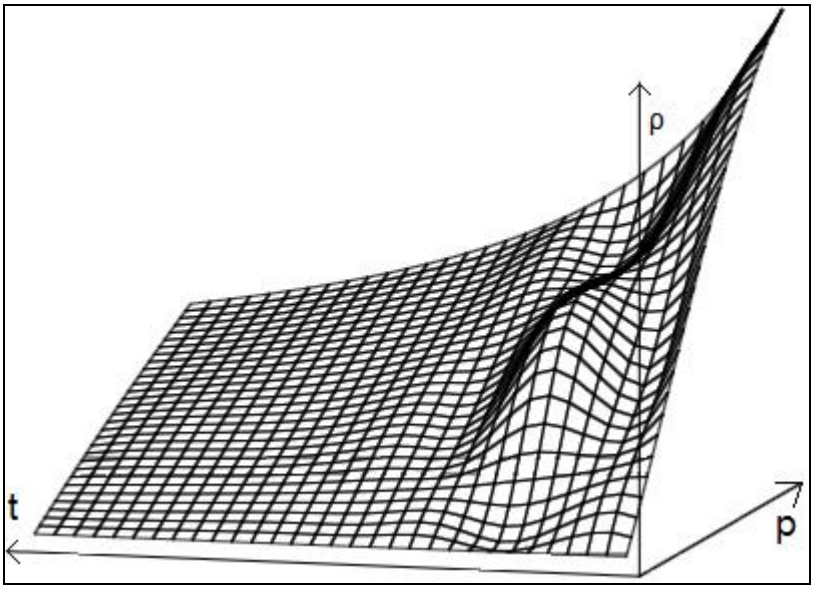


Fig. 1.3. Graphical display according to a possible error source data

Of course, you would have to immediately ask the "distant Indian friend" either what this substance (gas) is or if the formula is known. This rather ordinary episode of Mathcad problems raises a very important issue, which will be outlined in this etude.

Currently various scientific and educational (academic), as well as commercial organizations have accumulated a huge amount of databases on the properties of substances. These data are partially published on paper or electronic media in the form of tables (a typical example - Table. 1.1), graphs, formulations (sets of formulas and guidelines for their use) or computer programs. We just described such a program - see Fig. 1.1. But on the other hand, specialists, which are involved in research, design, development, operation and / or disposing of various "processes, devices and technologies“ cannot always effective use of these databases. Why? First, they must find them somewhere. Second, we must ensure that they are of adequate quality - that they are certified. Thirdly, and most importantly, you need to spend a lot of time and effort to somehow connect these databases to the working environment (Excel, Mathcad, Matlab, other programming languages and specialized programs, etc.). Often you can see this picture: a specialist working on a computer with expensive and powerful specialized programs is forced to use paper guides, the Internet or run separate programs to learn and tell the computer, for example, the density of a working fluid or any material of construction. Yes, some of these "special programs" have databases on the desired properties of substances, but usually they are quite primitive - contain only of constants and do not include, for example, the dependence of properties on some parameters (temperature, for example), do not work with new materials, or/and simply outdated. This is explained by the desire of companies to reduce the cost of developing programs. On the other hand, in many engineering organizations it is prohibited to "manually" enter external data on the properties of substances in specialized programs, despite the fact that they can be much more updated. This is done because of the fear, that manual inputs may include a trivial typo (compare Fig. 1.2 and 1.3) or wrong units - entering some values in °C (see Table. 1.1), although the computer is set to the Kelvin scale, or (U.S. program) the Rankine scale or Fahrenheit.

Ideally your computer, if you need some properties of some substances, should automatically synchronize itself over a computer network to a ("cloud") specialized and certified server with parameters of the needed substance and the server should return to the user's computer the needed properties.

How is it realized? A specific example: the Mathcad document shown in Fig. 1.1 is placed on the server http://twt.mpei.ac.ru/TTHB/Ro-pt.xmcdz. If the property you have to calculate is the density of the substance is a function of pressure and temperature, you only have to insert a link (Figure 1.4) to the desired Mathcad- document (shown in Fig. 1.1) and the function ρ (p, t) is visible in your calculation.

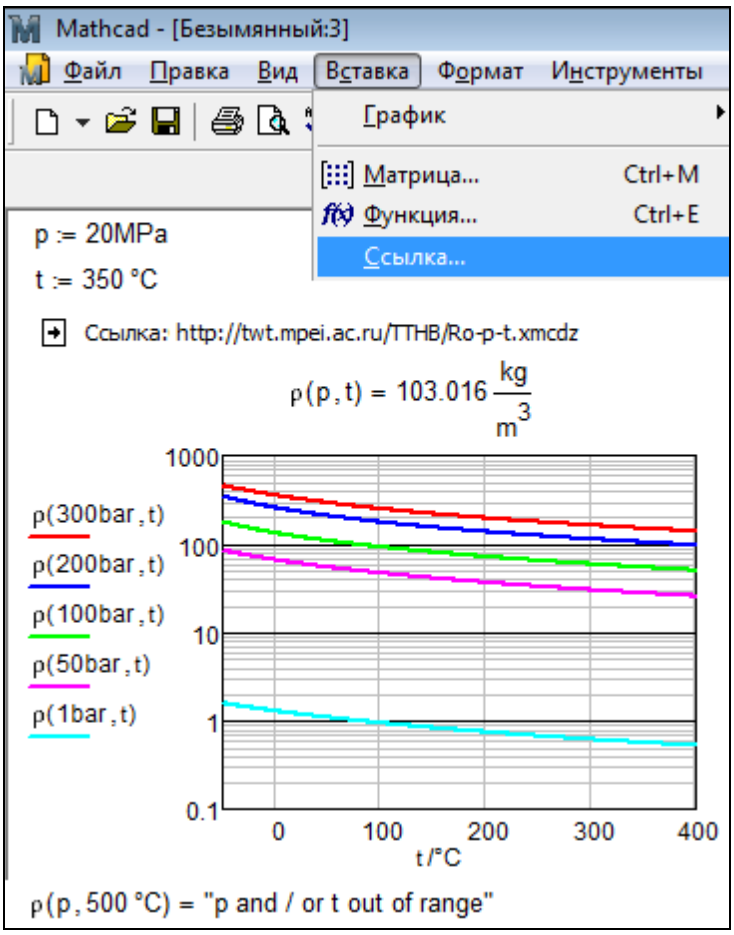


Fig. 1.4. Clickable link to external Mathcad- document

(Fig. 1.4) After the data entry of t and p and entering a reference to the file named Ro-pt, the "cloud" function ρ(p, t) becomes available. This function is here called with the parameters p = 20 MPa and t = 350 °C. This function is further visualized by some isobars. When entering t = 500 °C (this temperature is outside of the range covered by Table. 1.1), the function ρ (r, t) returns an error message.

On the current server, which is a collaboration of specialists from NIU "Moscow Energy Institute" (www.mpei.ru), Joint Institute for High Temperatures (www.jiht.ru) RAS and OOO "Trier" (see www.trie.ru), collected a large number of such "cloud" features. And their number is growing.

These functions are created for different reasons and in different ways.

First, if the author sees in a book or online a table similar to Table. 1.1, he instructs his students to "revive" it by using, for example, by the program shown in Fig. 1.1. Sometimes it is enough to insert it into a new matrix and make some other minor changes. If in the book or on the Internet the formulas, which are used to calculate the properties of substances, are shown, it is significantly easier. We have also developed a technology to transfer schedules to the "cloud"

function. All of these techniques are described in reference [3], which is released by RFBR grant fifth additional volume reference series. [4].

Second, these "cloud" features are customized for Mathcad for working in the field of thermal and nuclear power industry. Thus, for example, have been created and placed on the server functions on thermophysical properties of ethanol for calculation of steam turbine cycles with organic working fluids (ORC - organic Rankine cycle), for the calculation of refrigeration units [5] and other cycles. ORC posted at http://twt.mpei.ac.ru/MCS/Worksheets/PTU/Rankin-Ethanole.xmcd.

The main part of the "cloud" functions hosted on MEI - JIHT - Trier, are linked, of course, with properties of working fluids and coolants. These functions are described in reference [6], and the technology they use in the calculations in the papers [7, 8]. Functions related to water and steam (which is the main working body of domestic and foreign thermal and nuclear power), are based on the formulations approved by the International Association for Properties of Water and Steam (IAPWS - www.iapws.org; authors of this book it active). These formulations are not based on table data, and formulas. For example, the pressure and the saturation temperature of water in the range from the triple point to a critical point are associated with quadratic equations. But in practice very often calculation formulas are replaced by interpolation from individual points. That is why we pay special attention to this issue. This does not only apply for calculating the properties of saturated (a function of one argument), but also for individual single-phase regions and areas of subcooled liquid or superheated steam (a function of two arguments). Waiver of calculation formulas and the transition to working with tables can be considered a step backwards in the historical process of creating databases on the properties of substances. At the dawn of this process, such databases were published in the form of tables and/or graphs (visualized tables). Reading a table or graph without a computer or calculator is much faster than using the formulas. Loss of accuracy here was not so important. With the advent of electronic computing people slowly began to move away from tables, graphs and formulas and moved to computer programs, where these formulas are programmed. Formulation process of not yet fully investigated or newly synthesized compounds is being carried out as follows: create a table with the so called skeletal material properties through experimental measurements with various physical methods. Then out of these discrete tabular data one common function or a set of functions is generated by various mathematical methods for different areas or applications, and predicting possible errors for the primarily use on computer programs - this is called the formulation. But often there is only a table published without the mathematical processing. Having at hand powerful and convenient means of interpolation - such, for example, which are built in in Mathcad (e.g., Fig. 1.1), you can refuse to create complex equations of state, covering a wide range of parameters of the material, and limit the amount of tables. Interpolation replaces work with equations of state for another

reason. When you create, such programs for thermal and nuclear power plants and need to know the parameters of working bodies - water and steam, air, fuel, combustion products, etc., it is necessary for the calculations of properties of these substances, that they are carried out very quickly, even at the expense of a loss of accuracy. Often the interpolation requires polynoms with very high degrees, but for better understanding of the mathematical process and higher speed, polynoms with lower degrees are used. The problems with functions on the properties of substances, based on previously created databases can be described by an old "computer" situation. When there were only mechanical devices, before electronic devices, which facilitated calculations and reduced the costs, these devices could carry out only four basic arithmetic operations - addition, subtraction, multiplication and division. If, however, it was necessary to compute a more complex calculation, for example, the square root or sine of an angle, then you had to go away from computing and to use tables - search there for the desired rows and columns and if necessary to carry out interpolation. All this greatly hampers and slows down calculations and increasing the risk of errors in them.

Now a situation, which frequently occurs in calculations on properties of substances. Yes, these calculations are usually carried on computers, but you often have to break away from the computer and look in the directory - paper or electronic, to clarify the nature of a substance appearing in the calculation. All this "greatly complicates and slows down the calculations and increases the risk of errors in them."

Sinus problem and other elementary and special functions (Bessel functions, for example) are solved in electronic calculators by inserting these functions in these devices. Modern mathematical-, but also other programming languages can load extension packages, which include not only additional special functions (Bessel functions, for example), but also the means for specialized tasks - signal and image processing, solution of equations, statistical data processing, etc.. .

Embedding all functions on all properties of all substances in one modern calculating device is of course, unrealistic and not rational. You should be allowed to make visible only those functions that are needed at the moment. This information technology we did not only test on the Mathcad package, but also in other environments and it is described in this book.

And now we outline some of the nuances of this work.

1.2. Initial data standard configuration

The program shown in Fig. 1.1 is pretty easy due to the fact that the original rectangular matrix is full. If the matrix is square shaped, it will simplify the work. Spline interpolation on a square matrix in Mathcad is shown in Fig. 1.1. If you want to cover a wide range of parameters of a substance by interpolation, including solid, liquid and gaseous phases, the corresponding table of material properties (density, for example) will be "cracked" by lines of phase transitions. These tables are usually published in various reference books on the properties of substances, for example [6]. In these tables phase transition are marked by lines. Furthermore such tables are often only partially filled.

We have developed [9, 10], an effective interpolation technology for this type of data through their breakdown into separate areas (partially filled matrix), the boundaries of these are represented by pairs of vectors (curves, fixing phase transitions), separate equations, etc. This work is being done in Germany [11].

Fig. 1.5 shows an example of a partially filled matrix. Left - source matrix, right - matrix with added fictitious values for "smoothness" (enclosed in parentheses). These additional points are generated by extrapolating the values of the matrix. Having completed the matrix, it is easy to carry out the interpolation, for example, with the algorithm shown in Fig. 1.1. When you call the function created for two input arguments you have to make sure that the values of pressure and temperature are included in the scope of permissible values. Data shown in Fig. 1.5 - is a piece of a density table of a gas condensate (see http://twt.mpei.ac.ru/TTHB/2/GasCondensat.html). The missing elements of the matrix (see table on the left in Fig. 1.5) or values framed by brackets - this is area represents the phase transition.

"t, K \ p, MPa"	0.1	1	3	5
380	737.51	738.50	740.65	742.75
390	"-"	730.87	733.75	735.38
400	"-"	723.16	725.59	727.95
410	"-"	715.39	717.97	720.48
420	"-"	707.53	710.28	712.95
430	"-"	699.58	702.52	705.35
440	"-"	691.54	694.68	697.69
450	"-"	683.38	686.74	689.96
460	"-"	675.11	678.71	682.15
470	"-"	666.71	670.57	674.25
480	"-"	658.16	662.32	666.26
490	"-"	649.44	653.93	658.16
500	"-"	640.55	645.40	649.95
510	"-"	"-"	636.70	641.61
520	"-"	"-"	627.83	633.13
530	"-"	"-"	618.74	624.48
540	"-"	"-"	609.43	615.66
550	"-"	"-"	599.85	606.64

"t, K \ p, MPa"	0.1	1	3	5
380	737.51	738.50	740.65	742.75
390	(728.66)	730.87	733.75	735.38
400	(722.04)	723.16	725.59	727.95
410	(714.21)	715.39	717.97	720.48
420	(706.27)	707.53	710.28	712.95
430	(698.22)	699.58	702.52	705.35
440	(690.08)	691.54	694.68	697.69
450	(681.82)	683.38	686.74	689.96
460	(673.43)	675.11	678.71	682.15
470	(664.91)	666.71	670.57	674.25
480	(656.21)	658.16	662.32	666.26
490	(647.32)	649.44	653.93	658.16
500	(638.26)	640.55	645.40	649.95
510	(628.96)	(631.44)	636.70	641.61
520	(619.41)	(622.12)	627.83	633.13
530	(609.56)	(612.52)	618.74	624.48
540	(599.37)	(602.63)	609.43	615.66
550	(588.78)	(592.39)	599.85	606.64

Fig. 1.5. Not completely filled matrix with fictitious numbers

In the blank cells of the table you can put the system variable NaN (Not a Number) - see Fig. 1.6. In this case, spline interpolation cannot be carried out, but linear interpolation can be carried out, using the built-in Mathcad function linterp. Linear interpolation has the advantage over spline interpolation that in linear interpolation oscillations is not observed - see Fig. 1.7.

$\rho_{NaCl}(t, \omega) :=$

"Density of NaCl aqueous solution as function of temperature and mass ratiol - see the table as a picture at right"

"Density of NaCl aqueous solution at t=20C from one separate tablel"

$$\left(x \leftarrow \frac{t}{K} - 273.15 \quad y \leftarrow 100 \cdot \omega\right)$$

return "t or/and mass ratio is out of the range" if $x > 20 \vee x < -15$

return "t or/and mass ratio is out of the range" if $y > 25 \vee y < 10$

return "t or/and mass ratio is out of the range" if $x < -5 \wedge y < 15$

return "t or/and mass ratio is out of the range" if $x < -10 \wedge y < 19$

return "t or/and mass ratio is out of the range" if $x < -10 \wedge y > 24$

$M \leftarrow$

"t, °C / ω, %"	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
20	1071	1078	1086	1093	1101	1109	1116	1124	1132	1140	1148	1156	1164	1172	1180	1189
15	1075	1082	1089	1098	1103	1111	1119	1127	1134	1141	1151	1160	1168	1174	1184	1193
0	1078	1086	1093	1101	1108	1116	1124	1133	1141	1147	1158	1165	1174	1181	1191	1199
−5	1079	1089	1095	1102	1110	1117	1125	1134	1142	1148	1160	1168	1176	1183	1194	1202
−10	NaN	NaN	NaN	NaN	NaN	1119	1125	1135	1144	1149	1162	1169	1178	1185	1196	1204
−15	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	NaN	1151	1163	1171	1180	1187	1198	NaN

$X \leftarrow \text{reverse}(\text{submatrix}(M, 1 + ORIGIN, 6 + ORIGIN, ORIGIN, ORIGIN))$

$Y \leftarrow \text{submatrix}(M, ORIGIN, ORIGIN, 1 + ORIGIN, 16 + ORIGIN)^T$

$Z \leftarrow \text{submatrix}(M, ORIGIN + 1, ORIGIN + 6, 1 + ORIGIN, 16 + ORIGIN)$

for $i \in ORIGIN .. \text{cols}(Z) - 1 + ORIGIN$

$\quad Zv_i \leftarrow \text{linterp}\left(X, \text{reverse}\left(Z^{\langle i \rangle}\right), x\right)$

$\text{linterp}(Y, Zv, y) \cdot \frac{kg}{m^3}$

Fig. 1.6. Not completely filled matrix with NaN values and linear interpolation

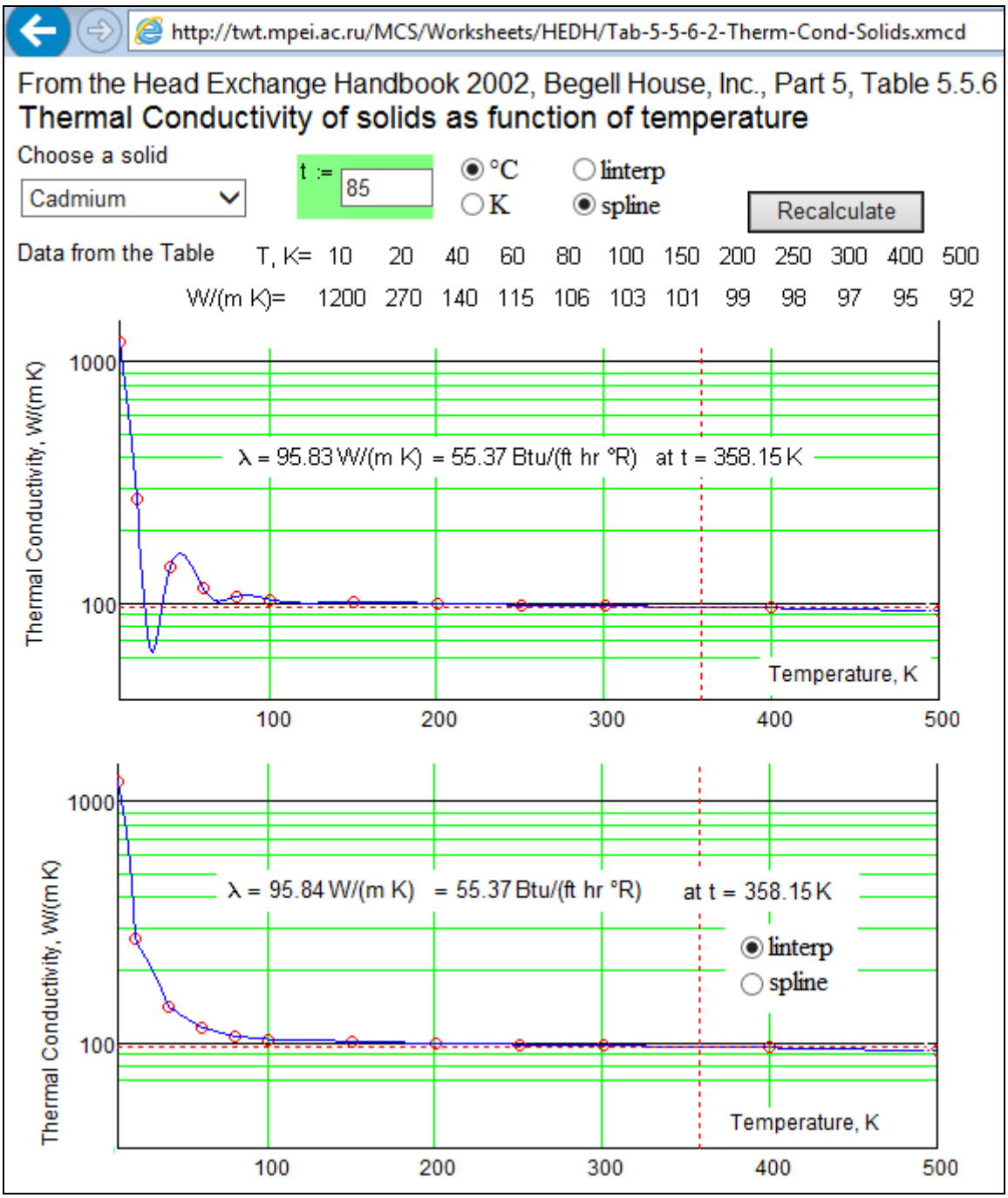


Fig. 1.7. Comparison of spline interpolation and linear interpolation: oscillation

Source data for tables can not only be taken from directories and the Internet, but also from other programs. Data on the properties of ethanol to calculate the above mentioned steam turbine cycle with organic working fluid (see separate study) and some refrigerants (see separate study), were taken from the program RefProp [12]. This program can be connected directly to Mathcad through the mechanism of DLL (Dynamic-Link Library). But this technology does not work with all versions of Mathcad, and only few can do it. Therefore (alternatively) the technology described in figures 1.1 and 1.5 is used. RefProp generates the desired vector or matrix, which will be inserted into a Mathcad function, which is similar to that which is shown in Fig. 1.1. You can obtain a function, which returns the desired property of a substance with the

right dimensions and has dimensional arguments, but does not work with equations of state, is hidden in the program RefProp, and can be viewed and edited if necessary. Fig. 1.8 displays the process of generating a matrix in the medium RefProp with two columns that hold the temperature and pressure of ethanol on the saturation line. In the table (she left in Fig. 1.8) it is sufficient to select the desired track and copy and paste it in Mathcad- document (right part of Fig. 1.8), in which the number will be converted to a string (character string enclosed in quotation marks, where we need to remove the commas and replace them by points, and then Mathcad- function str2num to translate it into numbers). Another way to obtain direct numbers in Mathcad-document from a program like RefProp – is to transfer data to a spreadsheet in Excel, which will be transferred to a Mathcad-document. Data source tables similar to that, which is shown in the left half of Fig. 1.8, can often be found on the Internet. They are easy to move in Mathcad- document with the methods described above. Here the main "fuss" is about the problem of "point - comma as decimal separator". Create a function on the table with two columns is not difficult, as shown in Fig. 4.3.

2: ethanol: V/L sat. T=260, to 510, K

	Temperature (K)	Pressure (MPa)
1	260,00	0,00061048
2	265,00	0,00089527
3	270,00	0,0012928
4	275,00	0,0018399
5	280,00	0,0025823
6	285,00	0,0035770
7	290,00	0,0048932
8	295,00	0,0066146
9	300,00	0,0088408
10	305,00	0,011690
11	310,00	0,015298
12	315,00	0,019826
13	320,00	0,025456
14	325,00	0,032394
15	330,00	0,040875
16	335,00	0,051162
17	340,00	0,063544
18	345,00	0,078343

$$M := \begin{pmatrix} \text{""} & \text{""} \\ \text{"Temperature"} & \text{"Pressure"} \\ \text{"(K)"} & \text{"(MPa)"} \\ \text{"260,00"} & \text{"0,00061048"} \\ \text{"265,00"} & \text{"0,00089527"} \\ \text{"270,00"} & \text{"0,0012928"} \\ \text{"275,00"} & \text{"0,0018399"} \\ \text{"280,00"} & \text{"0,0025823"} \\ \text{"285,00"} & \text{"0,0035770"} \\ \text{"290,00"} & \text{"0,0048932"} \\ \text{"295,00"} & \text{"0,0066146"} \\ \text{"300,00"} & \text{"0,0088408"} \\ \text{"305,00"} & \text{"0,011690"} \\ \text{"310,00"} & \text{"0,015298"} \\ \text{"315,00"} & \text{"0,019826"} \\ \text{"320,00"} & \text{"0,025456"} \\ \text{"325,00"} & \text{"0,032394"} \\ \text{"330,00"} & \text{"0,040875"} \\ \text{"335,00"} & \text{"0,051162"} \\ \text{"340,00"} & \text{"0,063544"} \end{pmatrix}$$

Fig. 1.8. Copying data from the program RefProp

The interval between two temperatures can be increased in order to save computer memory or decreased in order to increase the accuracy. Speaking of computer memory -

previously, it was one of the main limiting factors of calculations. Therefore interpolation was often refused, because of the required storage of large data sets on the computer memory, and the work on equations of state proceeded. Now this restriction is eliminated.

1.3. Create inverse functions

If there is a dependence of one parameter from another one, it is possible to create two functions - forward and backward. The establishment of a pair of functions is shown in Fig. 4.3. Built in Mathcad means of solving equations and finding zeros of functions make it easy to quickly create and inverse functions on the properties of substances with more complex (not only unique) dependence, as well as dependencies of three or more parameters). Now we return to our problem of the density of matter, depending on pressure and temperature (Fig. 1.1). In specific calculations we often have to solve the inverse problem - finding the pressure dependent on density and temperature or the temperature dependent on density and pressure. If the equation of state is known, you can try to solve analytically in this case and find its inverse function - modified equation of state. We can go another way - see Fig. 1.8.

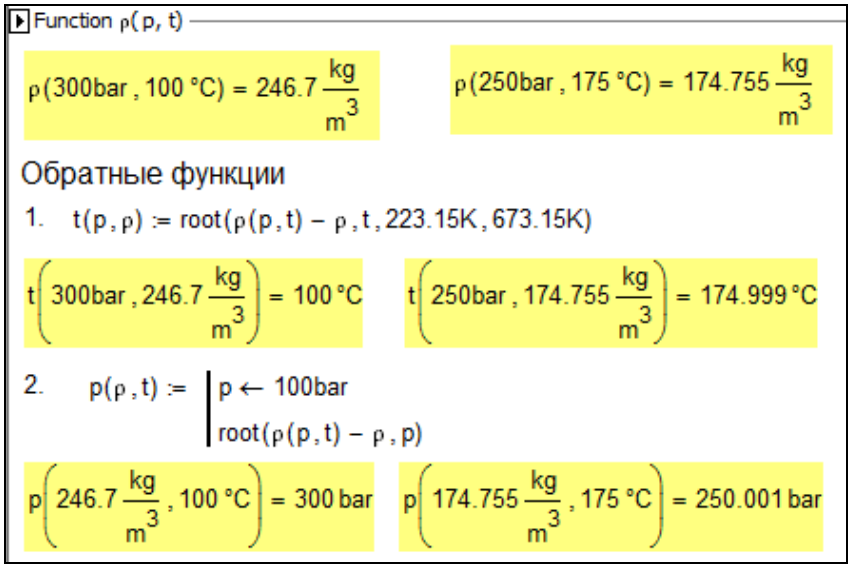


Fig. 1.9. Create inverse functions

Mathcad has a built-in function (root), which returns the zero value of analysed functions by using bisection method (see 1 in Fig. 1.9) or secant method (see 2 in Fig. 1.9). In the first case you need to specify the range of possible values of the desired parameters for the numerical solution of the problem - temperature, keep in mind if you claim 1 in Fig. 1.8, while the second - the guess value to the desired parameter - the pressure (see section 2 in Fig. 1.9).

Our function, the creation of this is shown in Fig. 1.1, is continuous and monotone dependent on each of the parameters in the selected range of pressure and temperature. When you work with more complex features state agents should be understood that for such functions or not there is an inverse or inverse functions somewhat (which all have the same domain, but

different value). In this case the given parameters need to know exactly what the inverse function we will seek and will need to be created in the inverse function to provide an additional argument - the initial approximation to the desired solution. If it is theoretically proved that in the defined area the inverse function is uniquely defined, we will get the same result for any approximation. For the existence and uniqueness of constructing the inverse function of one variable its strict monotony is sufficient. In general, the search for the inverse function is a complex mathematical problem.

A specific example: the water pressure and/or steam temperature, and the specific enthalpy can then be either determined in the 1-phase region (pressurized water) or in the two-phase region (wet steam). This situation is described in etude 5, wherein the compression curve is constructed in the T, h- diagram.

Sometimes it is useful as a first approximation to use a random numbers in a specified range as values of the inverse function. Fig. 1.10 illustrates the change of the pressure dependent on the temperature for different χ (χ - isobaric heat capacity, ratio for the isochoric heat capacity), for χ 1.26, 1,27... 1.4. The wspPTK function is based on function wspKPT, which is included in the package WaterSteamPro (see www.wsp.ru). The wspPTK function returns different values depending on the first approximation. Random number generator helped us to construct the required family of curves, although in fact they are not the curves, and the new family of points with discontinuities in those places where the package Mathcad could not find solutions function root.

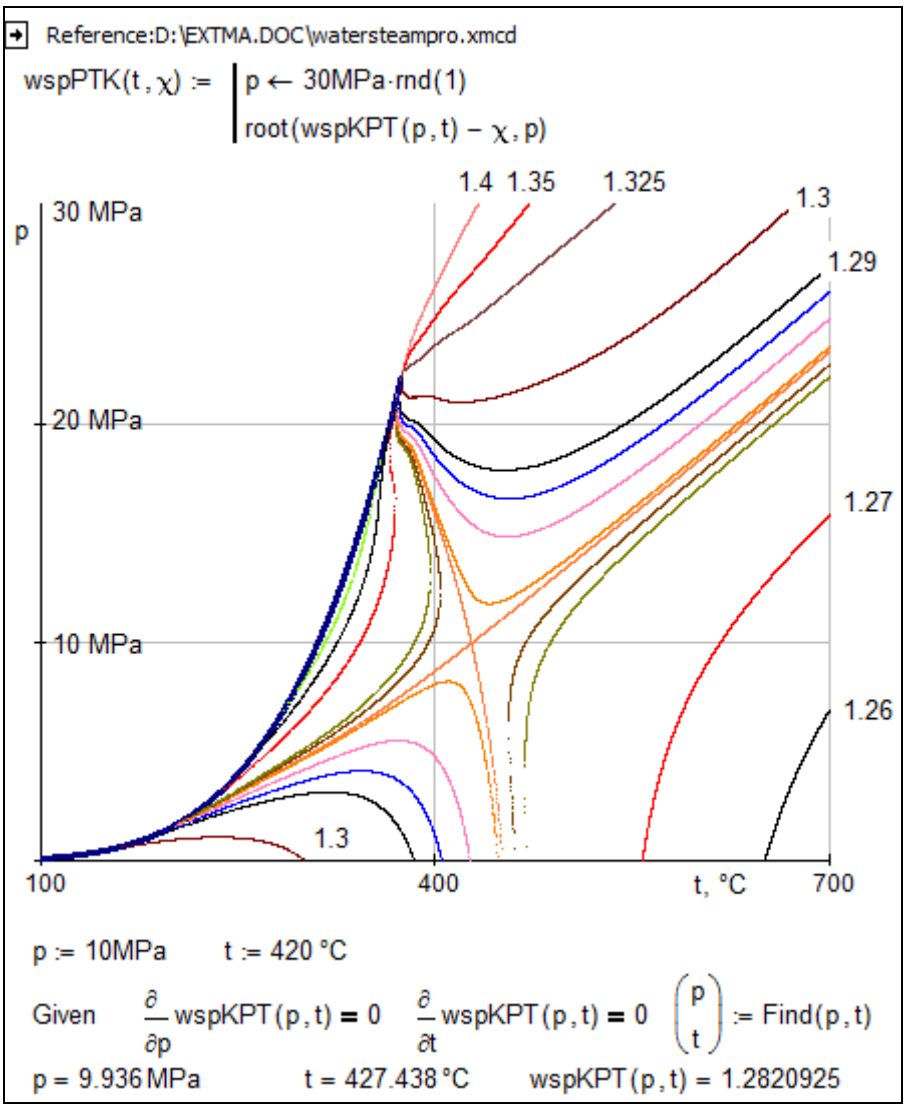


Fig. 1.10. Isentropic dependence

In Fig. 1.10, as well as in Fig. 1.9, we use to create the reverse function the built- in Mathcad function root. However, as a first approximation of the pressure we use a random value in the range of 0 to 30 MPa. This is done with the built- in Mathcad function rnd, which returns a random number in the range from zero to the value of its argument. In Fig. 1.10 you can also see a Given-Find block. There pressure and temperature is calculated at which the partial derivatives of wspKPT are equal to zero. In mathematics, this is called a saddle point.

About Fig. 1.10 an interesting story can be told. One of MPEI`s teachers promised his students, that he will give to the one, who can construct this family of curves using Mathcad, a six in the exam (not five – actually the best mark in Russia). The instructor was hundred percent sure, that this can be done only with the help of more powerful programs. Students were not able to do it, and asked the author of this book for some help. The problem was solved, but none of students received a six in the exam, because they asked for help from outside.

In Mathcad, with "direct" functions on the properties of materials and tools for solving equations and systems, you can understand the essence of this problem, it is easy to create inverse functions. We will show this in some etudes of this book.

The issue of creating inverse functions will continue in the etude 11.

1.4. extrapolation

The problem of creating inverse functions is closely related to the problem of extrapolation.

In the program shown in Fig. 1.1 the operator before the calculation checks either the inputs do fall within the specified range of pressure and / or temperature, or not. This is on the one hand good and on the other bad. Good because it cuts off any possible errors a user can do - either accidentally or deliberately entering invalid data and getting the wrong answer - the result of extrapolation, not interpolation. But on the other hand, such a restriction may interfere with the procedure of calculating the inverse functions (see above).

The implementation of numerical algorithms for searching zero function (see, e.g., 1.2 in Fig. 1.5) can go beyond the agreed limits of the function - intermediate iterations can reach higher/lower values than allowed in order to obtain a completely correct answer. In this regard, the "cloud" features on the properties of substances contain an optional argument, which allows or excludes extrapolation.

This technique is illustrated by following four figures.

Fig. 1.11 shows a table findedyuzhdennaya" from the Internet by keyword "density of the solution NaCl“. (Incidentally, in Fig. 1.11 in the table header is a link to the source [34], but actually you can find this table on the following website: http://thermalinfo.ru/publ/zhidkosti/voda_i_rastvory/teplofizicheskie_svojstva_vodnykh_rastvorov_khloristogo_natrija_i_kalcija/32-1-0-225) not established).

Зависимость плотности растворов хлористого натрия различной концентрации от температуры [34]					
Содержание соли, %	ρ (в *кг/м³*) при температуре, °C				
	15	0	—5	—10	—15
10	1075	1078	1079	—	—
11	1082	1086	1087	—	—
12	1089	1093	1095	—	—
13	1098	1101	1102	—	—
14	1103	1108	1110	—	—
15	1111	1116	1117	1119	—
16	1119	1124	1125	1125	—
17	1127	1133	1134	1135	—
18	1134	1141	1142	1144	—
19	1141	1147	1148	1149	1151
20	1151	1158	1160	1162	1163
21	1160	1165	1168	1169	1171
22	1168	1174	1176	1178	1180
23	1174	1181	1183	1185	1187
24	1184	1191	1194	1196	1198
25	1193	1199	1202	1204	—

Fig. 1.11. Table from the Internet

Fig. 1.13 shows the program Mathcad returning interpolated densities of an aqueous NaCl solution, depending on its concentration (rather, mass fraction (percent))and temperature. This table was scanned from paper books in order to be translated into "digital" form – an Excel spreadsheet or a matrix in Mathcad (see Fig. 1.13 below). This can be done by using the special software OCR. But if the quality of the original "pattern" is low or the table itself is not very voluminous, then such work can be also done "by hand". (The National Institute of Standards and Technology, which was already mentioned in this etude, engaged this summer a group of students for this handiwork. One student dictates the table, and the second enters the numbers into a computer. This first student alternates his eyes from the paper to the display in order to check the correctness of the input.)

The matrix M shown in Fig. 1.12 is not completely filled, as she repeats the data recorded in the table shown in Fig. 1.12. But it is not so - to "empty" areas of the matrix M are "fictitious" number

prescribed white on white. This technique works with non-standard data and is described in the following [9] (in Fig. 1.5 such data registered "black and white", but in brackets.)

```
ρNaCl(t, ω, Check) := | ( x ← t/K − 273.15   y ← ω/% )
if  Check
    | Err ← "t и/или ω вне диапазона"
    | return  Err  if  x > 15 ∨ x < −15 ∨ y < 10 ∨ y > 25
    | return  Err  if  x < −5 ∧ y < 15
    | return  Err  if  x < −10 ∧ y < 19
    | return  Err  if  x < −10 ∧ y > 24
```

$$M \leftarrow \begin{pmatrix} \text{"ω, \%t \ t, °C"} & 15 & 0 & -5 & -10 & -15 \\ 10 & 1075 & 1078 & 1079 & & \\ 11 & 1082 & 1086 & 1089 & & \\ 12 & 1089 & 1093 & 1095 & & \\ 13 & 1098 & 1101 & 1102 & & \\ 14 & 1103 & 1108 & 1110 & & \\ 15 & 1111 & 1116 & 1117 & 1119 & \\ 16 & 1119 & 1124 & 1125 & 1125 & \\ 17 & 1127 & 1133 & 1134 & 1135 & \\ 18 & 1134 & 1141 & 1142 & 1144 & \\ 19 & 1141 & 1147 & 1148 & 1149 & 1151 \\ 20 & 1151 & 1158 & 1160 & 1162 & 1163 \\ 21 & 1160 & 1165 & 1168 & 1169 & 1171 \\ 22 & 1168 & 1174 & 1176 & 1178 & 1180 \\ 23 & 1174 & 1181 & 1183 & 1185 & 1187 \\ 24 & 1184 & 1191 & 1194 & 1196 & 1198 \\ 25 & 1193 & 1199 & 1202 & 1204 & \end{pmatrix}$$

```
X ← reverse(submatrix(M, 0, 0, 1, 5)^T)
Y ← submatrix(M, 1, 16, 0, 0)
Z ← submatrix(M, 1, 16, 1, 5)
for  i ∈ 0 .. cols(Z) − 1
  Zv_i ← interp(cspline(Y, Z^⟨i⟩), Y, Z^⟨i⟩, y)
interp(cspline(X, reverse(Zv)), X, reverse(Zv), x)·kg/m^3
```

Fig. 1.12. Program spline interpolation

The function ρ(NaCl) checks for wrong input data and returns an error message, if the third argument of the function (Check) has a value of 1 (not zero). This is shown in Fig. 1.13.

$$\rho_{NaCl}(10\ °C, 10.5\%, 1) = 1080.78\ \frac{kg}{m^3}$$

$$\rho_{NaCl}(-15\ °C, 7\%, 0) = 507.47\ \frac{kg}{m^3}$$

$$\rho_{NaCl}(-15\ °C, 7\%, 1) = \text{"t и/или ω вне диапазона"}$$

Fig. 1.13. Calling a function with and without scrutiny

Fig. 1.13 shows three calls of the function ρ(NaCl): "normal" call, when the arguments of the function are within the acceptable ranges of temperature and concentration of the solution NaCl, "false", when the third argument (Check) is 0, and the function output of ρ(NaCl) is wrong, extrapolation value and clipping the wrong case, false answer.

Fig. 1.14 also shows how to create an inverse function on the basis of the function ρ(NaCl).

The new function ω(NaCl) returns the NaCl solution concentration depending on the temperature and the density (for example: in a NaCl solution a thermometer and hydrometer was inserted and now we want to know its concentration). If the function is enabled ρ(NaCl) check the source data, but the inverse function does not work.

$$\omega_{NaCl}(t, \rho) := \left| \begin{array}{l} \omega \leftarrow 20\% \\ \text{root}\left(\rho_{NaCl}(t, \omega, 1) - \rho, \omega\right) \end{array} \right.$$

$$\omega_{NaCl}\left(-10\ °C, 1185 \cdot \frac{kg}{m^3}\right) = \blacksquare$$

Значение должно быть скаляром или матрицей.

$$\omega_{NaCl}(t, \rho) := \left| \begin{array}{l} \omega \leftarrow 20\% \\ \text{root}\left(\rho_{NaCl}(t, \omega, 0) - \rho, \omega\right) \end{array} \right.$$

$$\omega_{NaCl}\left(-10\ °C, 1185\ \frac{kg}{m^3}\right) = 23\ \%$$

Fig. 1.14. Creating an inverse function

The created inverse function can be supplemented by operators in order to avoid wrong answers - see Fig. 1.15.

$$\omega_{NaCl}(t,\rho) := \left| \begin{array}{l} \omega \leftarrow \mathrm{root}\left(\rho_{NaCl}(t,\omega,0) - \rho, \omega, 10\%, 25\%\right) \\ \text{return error("t must be from -15 to 15°C")} \ \text{if} \ t > 15\,°C \vee t < -15\,°C \\ \text{return error("ω must be from 10 to 25%")} \ \text{if} \ \omega < 10\% \vee \omega > 25\% \\ \text{return error("ρ must be from 1075 to 1204 kg/m^3")} \ \text{if} \ \rho < 1075\,\frac{kg}{m^3} \vee \rho > 1204\,\frac{kg}{m^3} \\ \text{return } \omega \end{array} \right.$$

$$\omega_{NaCl}\left(10\,°C, 1100\,\frac{kg}{m^3}\right) = 12.971\,\%$$

$$\omega_{NaCl}\left(17\,°C, 1100\cdot\frac{kg}{m^3}\right) = \blacksquare\cdot\%$$

t must be from -15 to 15°C

Fig. 1.15. Inverse function to the control response

The function shown in Fig. 1.15, determines the concentration of NaCl in the solution depending on its temperature and density, without any limitation, since third argument of ρ(NaCl) is zero. But before the output response it is monitored, if the values of the function arguments of ω(NaCl) and the values of the function are in a reasonable range. The density value is controlled by checking whether the value does fall within the range of the minimum density (1075 kg/m3) and maximum (1204 kg/m3) density - see the table in Fig. 1.12 and the matrix in Fig. 1.13.

Remark. Two pitfalls can be noted in the function shown in Fig. 1.15. First, the root feature seeking functions are zero near the point (20 % - see Fig. 1.15, and in the range 10-25 %). Secondly, the function, the creation of which shown in Fig. 1.15, when erroneous data returns, not text message detailing the user response.

Speaking of extrapolation among Mathcad - functions with the root name spline (see Fig. 1.1) can have three preposition (prefix) - l (el), p and c: lspline, psline and cspline. These prefixes represent: linear (l), square (parabolic - p) and cubic (c) extrapolation. Inside the area of tabular data interpolation is conducted by cubic extrapolation.

1.5. People experiment on people and (d) experiment (th)

One of the authors of this book is often criticized that he "in his life has never spent a single measurement of properties of substances, and is only concerned with the fact that someone else takes the published experimental data, processes them, and puts it on his server in the form of online calculations or "cloud" functions." Sometimes this reproach is enveloped in a cruder form. They say: "hit the keys of the computer - every <one rather rude word> can, and you try to run an experiment here!" These criticisms can be continued. The persons conducting experiments on the stand and measure some properties of substances can blame the author for something like this: "to conduct experiments on the final stand - every <... > can. Did you try it

yourself here to collect and establish a similar stand!" And more. " Collect and organize stand on the properties of substances, based on the known techniques - every <... > can, and you try to come up here and implement a new method for the study of these properties ," and etc.

Since quite a long time and not only in manufacturing, but also in science occurs the process of division of labour. There are scientific organizations (like the already mentioned NIST, or for example, the National Institute of Standards and Technology in the U.S.), which along with the study of the properties of individual substances are gathering previously obtained data around the world from others, and create this way databases on properties of the substances (and also of course programs). A concrete example - the program RefProp (see above). Here, the main thing is not to give out wrong information and explain where you got this information from. But in reality it is not so easy to do. Why!? You can find in many books and directories tables of data on the properties of substances and integrate them in newly created programs and declare where they were taken from. Everything seems to be correctly. But then it turns out that in the handbook, to which you referred to, is said, that this table is taken from a different book, and in this "other book" is a new link to another source, etc. Sometimes it seems that certain widespread table properties of the substance filled the Creator himself when creating this substance.

The author of this book, by the way, did the following experiment at the beginning of his career - he collected a stand and held it experiences. But then the fate forced him to give serious attention to computer technology. This work is carried away and let him do something. When the writer hears the words that " every <... > can hit the keys of a computer", he answers (usually mentally to himself) something like that and at the ready, each laboratory bench can <... > work, and here you try to create a program that will be a success - and scientific and commercial - for example, the program RefProp [12], ThermoData Engine [13] or WaterSteamPro [14]. The scientific process of creating databases on the properties of substances and provide them to users in digital form involvs many different specialists. Everybody contributes an important part to this work! The main thing is that this work is carried out professionally and meets the principles of scientific ethics. You can not only learn about nature, but also about the "second" nature, in particular, the programs created by people.

A scientist, who wants to learn about the world, can not speak directly to the Creator - God or Nature, and should ask the questions to himself, ie, he must carry out an experiment.

A program has authors. Their names are not always listed on the boxes and documentations, but they exist. Consequently, any experiments on programs are unnecessary. Emerging questions should be addressed to either the documentation or the authors themselves. But, If a user, for example, need to clarify, either the argument of sine is measured in degrees or radians, he will not check the documentation, and just simply write x: = sin (30) and see what

result he gets for the variable x. Such experiments give users an option,i.e., checking the documentation only in severe cases (or not) and usually not finding the answer there. This appeals to the creator as problematic. On the hotlines do not sit the creators of the program – usually just some mildly skilled employees, and as the reader knows, it is not the same thing. Consultant firms are likely to ask you to call back in a couple of days during which they will perform some experiments with the program and try to find the answer. Yes, and according to the author, you often do nothing in the meantime, forget about the problem and will be fully absorbed to a new project. Even if it is not this case, then the author cannot remember all the details of his program after he calls back.

Because of this when working with programs the user often forgets that it is a product of the mind and human hands, i.e., which is the fruit of the work of anonymous persons, that cannot be reached via a hotline. Here, apparently, lies the philosophical explanation (but not in any way an excuse) for the widespread use of illegal copies of programs. Here we are talking about relatively honest people that put the program on your computer in order to get to know more about nature and pass on their knowledge, such as students.

We can assume that the Creator, throwing an apple on top and please them on the head of Newton, we opened one of the secrets of his Divine Plan. The merit of genius (Newton) - the ability to be in the right place at the right time. Program (and not only brilliant) would also like to fall on top of us, and there is no obligation for them to pay crazy money by Russian standards. Hence the idea of vitality and shareware, which oppose primarily sellers and not the authors of programs.

We can assume that God created from his own image and likeness, not only humans, but also the computer. Writing for a program - the inhalation of soul into a lifeless pile of iron, plastic and sand. Trading bodies (organ transplants, blood transfusions or, finally, prostitution) - is a reality of our days. Buying and selling of souls is found only in fairy tales and fiction (the story of Faust, for example). By purchasing the software, we buy only the "body" - disks, documentations, information and discounts on new versions, and most importantly - after-sales service.

Hence our conclusion: experiments with programs like RefProp [12], ThermoData Engine [13], WaterSteamPro [14] or Thermoflow (see Introduction) have the same right to life as classic experiments.

1.6. Once again why Mathcad?

Often you can hear the statement (another rebuke to the author) that, Mathcad is a "frivolous" program , designed only for pupils or students. Engineers and scientists need to work with more serious programs - like Matlab, for example.

What can I say?

First, Matlab - like it is mentioned in the Preface, is a programming language, or rather, a programming language for technical computing. It is no secret and the company itself developer MathWorks (www.Mathworks.com). Mathcad is primarily a scientific calculator with an interface as close as possible to the "interface" of calculations written down on paper, and then a programming tool.

In order to master the program Matlab, you actually need to master a second specialty – the specialty of a programmer. The situation in Mathcad: a scientific / technical worker or engineer, sitting at the computer for the first time with the program Mathcad, begins after a few hours to solve quite complex problems - calculating formulas (involving units; which Matlab, we repeat, not can), solving equations and systems of equations, building complex graphs and charts, etc. And all this without any loss of their qualification in their main speciality.

The program Matlab is without special courses or "thick" books very difficult to master. Because of this, often more than one person works with Matlab, usually two. The first level (an experimenter) forms the task, and the second (an expert in the package Matlab) translates this problem into the language of the computer. In such a chain are often glitches and inconsistencies. Of course there are exceptions of this rule, but they are isolated.

It is not needed to compare the programs Matlab and Mathcad. Nobody bothers specialist of applied work with Mathcad package and package Matlab. Moreover, when working with Mathcad, you can automatically send data to Matlab, where they are processed by using specialized tools in Matlab, and return the new data to Mathcad. Such technology, incidentally, works also with a spreadsheet program, like Excel - or another software environments, which are often used for scientific and technical calculations, although they are intended primarily for accounting calculations. Table 1.1, by the way, is a table from Excel - it is convenient to store and edit tabular data sets there.

The Mathcad package is very good for this kind of work, e.g., when you need to make certain estimates or rough calculation of a process. Here in interactive continuous interaction work knowledge and human intelligence and computer speed and accuracy. And if this process to mount the database on the properties of substances, such creative work is very productive in what we hope reader will see very soon.

1.7. Temperature scales

In the table, placed at the beginning Studies (Table. 1.1 and Fig. 1.2) the Celsius temperature scale was used. This is not a typical case. Usually these tables are based on the absolute temperature - on the Kelvin scale. Working with different temperature scales (Kelvin, Rankine, Celsius, Fahrenheit, and sometimes Reaumur) often leads to confusion and errors, when we work with tables. Mathcad greatly facilitates the work with its ability to work with units. In

addition, we must remember that old tables, graphs and formulas, which display the properties of substances, can rely on the temperature scale of 1968 (ITS- 68). Currently a new scale since 1990 - ITS- 90, is used. To set the "cloud" features on the properties of substances applied a pair of functions, providing for a new recount temperature (ITS- 90) and old (ITS- 68) scales, which eliminates possible errors in the use of old, but, nonetheless, demand data. The site http://twt.mpei.ac.ru/PVHB/pvhbeng.html - a web version of the book "physical quantity" (Energoatomizdat, 1991) in the "thermometer" the reader will find on-line recalculations on the temperature scale and corresponding functions for embedding them in Mathcad.

Fig. 1.16 shows the difference of the both temperature scales (ITS-90 and ITS-68). On the site you can also find links to functions for recalculations of metrological standards and description of these.

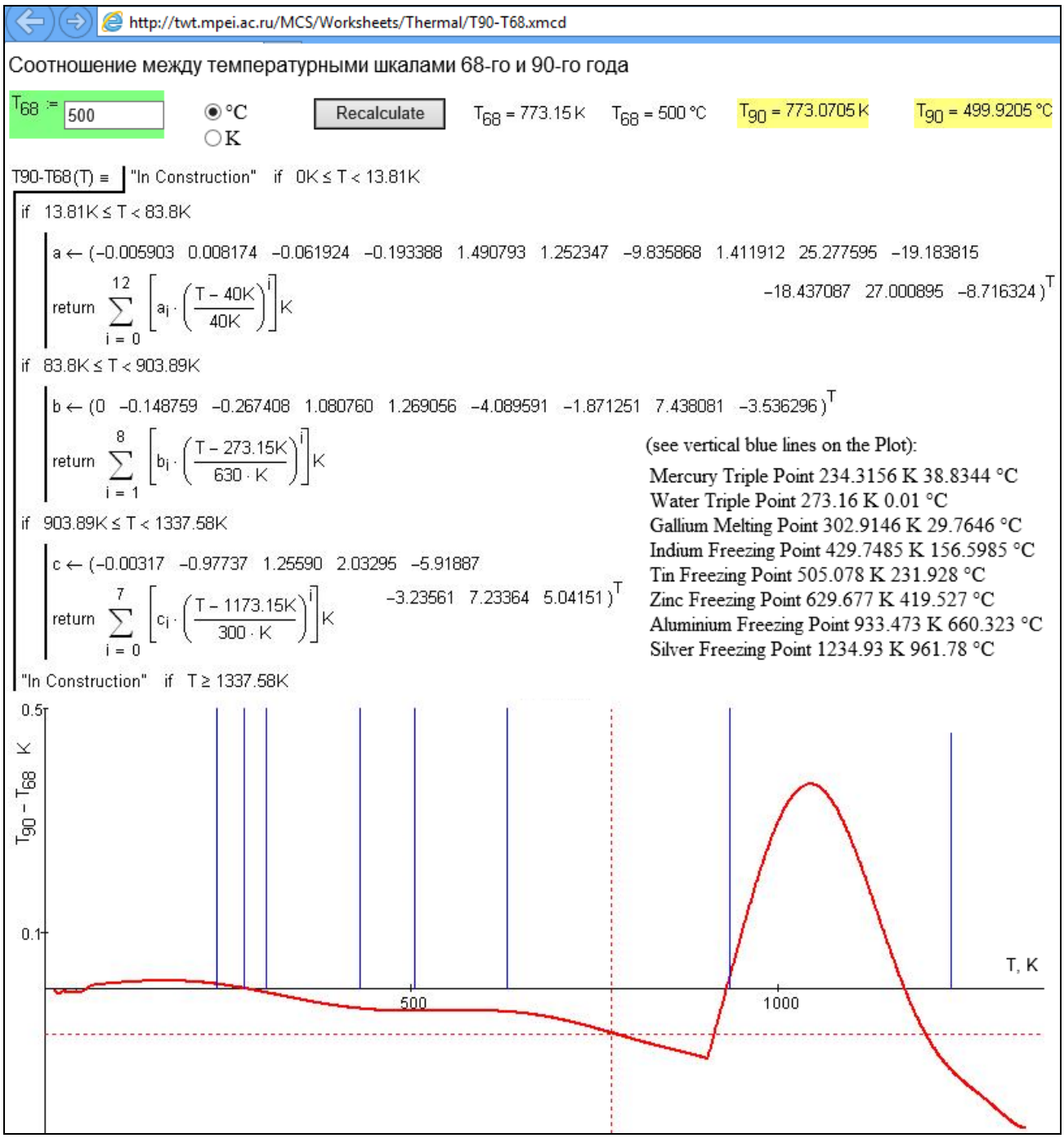


Fig.1.16. Difference between old and new temperature scales

In old Russian (Soviet) references, along with the old temperature scale can be (see above) to meet and outdated symbol of the unit of temperature, the temperature difference rather. The unit of thermal conductivity is watts divided by meter and degree Celsius - W / (m ° C) and the unit of specific heat - calories rms divided per kilogram and degree Celsius - cal / (kg ° C). In modern references replace Celsius by Kelvin, although not always. In U.S. references you can find as the unit of thermal conductivity - Btu / (hr ° ft ° F), while the specific heat has the unit (or unit specific entropy) Btu / (hr ° lb ° R). The author asked one of the authors of a handbook published by the National Institute of Standards and Technology (NIST), why they used degrees

Rankine in the unit of heat capacity, but degree Fahrenheit for heat conduction and entropy. The answer was - it's an American tradition of engineering and we can not change it. We can change the U.S. Constitution rather than the tradition.

In Mathcad, by the way, in support of this tradition two temperature units are introduced: Δ ° C and Δ ° F, numerically equal to Kelvin and degrees Fahrenheit, respectively.

1.8. Error

Many properties of substances given in databases come with a certain error. This error is fixed in various formulations on the properties of substances, but is not always shown in tables and graphs.

"Cloud" functions, for online calculations on the properties of substances, are described in this article. In these calculations, is not only the calculated value of the property given, but also the calculation error - the interval of admissible values (see Fig. 1.17).

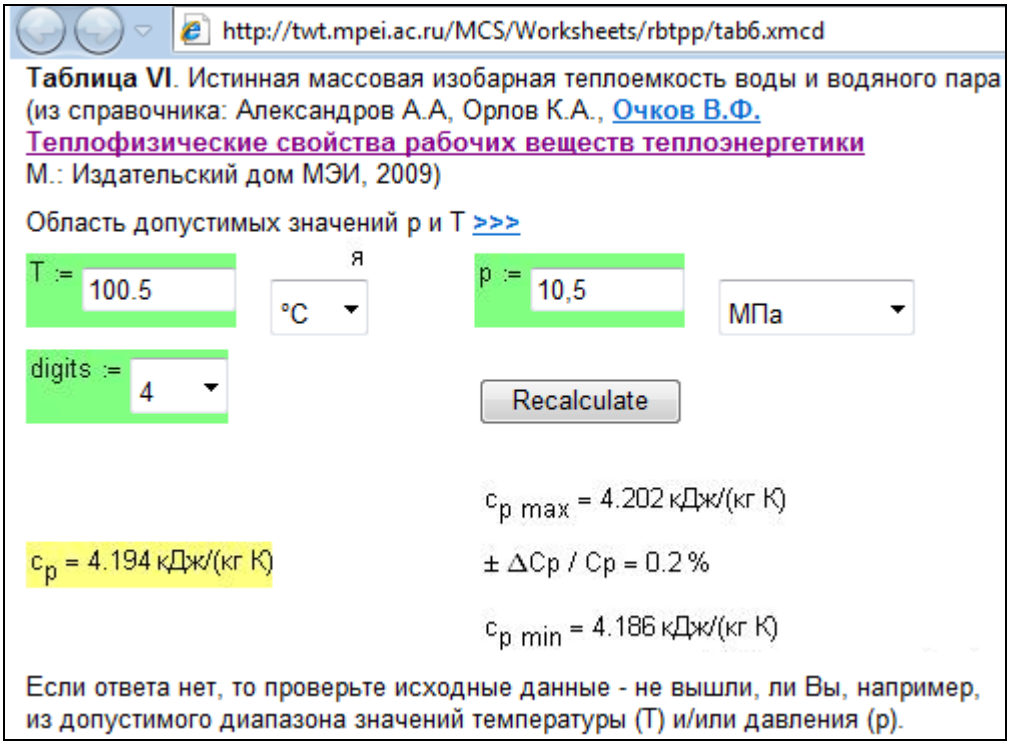


Fig. 1.17. Calculation of the specific isobaric heat capacity of water, indicating the error

If it is necessary, you can modify the "cloud"-function, which is discussed in the article, that it returns more than one value (scalar or vector) - the value of the substance itself, the error (absolute and / or relative), and the maximum and minimum value of the determined error.

1.9. IT- Security

Many "serious" organizations (research institutes, design bureaus, commissioning organizations) deny or restrict Internet access for end-users` computers. Internet access is often only available for the system administrator. This is done in order to guarantee 100% safety. These organizations can use cloud functions in this way: download them from the "cloud" and place them on the organization`s local server or end user's workstation. In etude 17, we show how the same problem can be solved by making a reference to cloud features (Fig. 17.8) and how to work with templates (Fig. 17.11).

But the benefits of working with cloud features are undeniable. First, these functions are always "fresh" - they are continually optimized, redefined, and extended. Secondly, it eliminates the problems associated with the loss of installed programs - by changing databases or the computer (operating system).

1.10. Templates

The problem of security (see above) is such an important aspect of information technology as the work with templates.

The fact that the technology options "cloud" function in Mathcad 15 - is, frankly, an undocumented trick that, like any other undocumented, developers were locked in a new version of Mathcad - Mathcad Prime. And it was done for security reasons. An alternative to the same references to the "cloud" function in an environment Mathcad Prime 3 are templates, including "cloud".

What is this template?

For us, the more familiar term is the term form, which goes back to typewriters and writing with a pen on paper. If we need to write a formal or informal letter, invitation or something else, we do this by using a form or template, as it is now more common to call. Such templates are used in almost all organizations. They have been inserted earlier in typewriters, and then in printers. But now we use more and more electronic forms. For paper forms for printers now usually resort to if the form color and the text on it is printed on black-and- white printer.

Blanks are integrated in many text editors. Thus Fig. 1.18 shows a part of the screen after starting Word 2013, with which, by the way, this book was written.

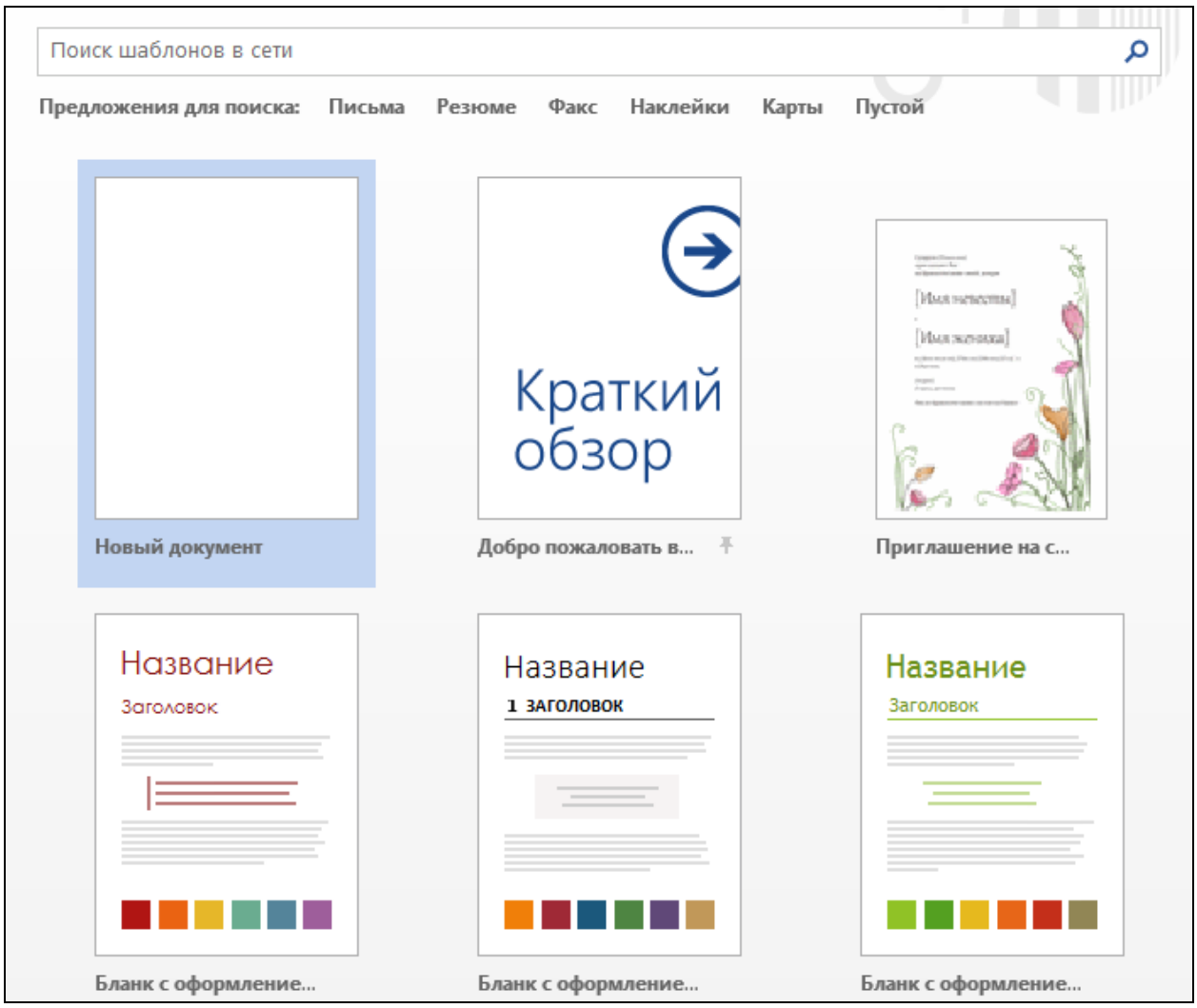


Fig. 1.18. Word templates

Fig. 1.18 shows how Word offers its users not to start writing on a blank sheet of paper (which, incidentally, is also a template, however, a primitive one), and to select the appropriate template.

The ready-made Word document (official letter, for example), we repeat, consist of two parts - a constant (name of organization, its details and so on.), which was in the template and a variable part – what we enter in the template (main part of the letter). All this significantly accelerates and simplifies the work, and reduces the risk of errors therein.

Mathcad also comes with a few templates. Usually they are rarely used when working with Mathcad due to the fact that after the launch of this program not a list of patterns (as in Word - see Fig. 1.18), and a blank document (the most primitive pattern) appear. If we press the small button next to the icon with the image of a new blank document in Mathcad and give the command "New" from the File menu (Mathcad 15), then the screen will display a list of templates, which are built into Mathcad - see Fig. 1.17.

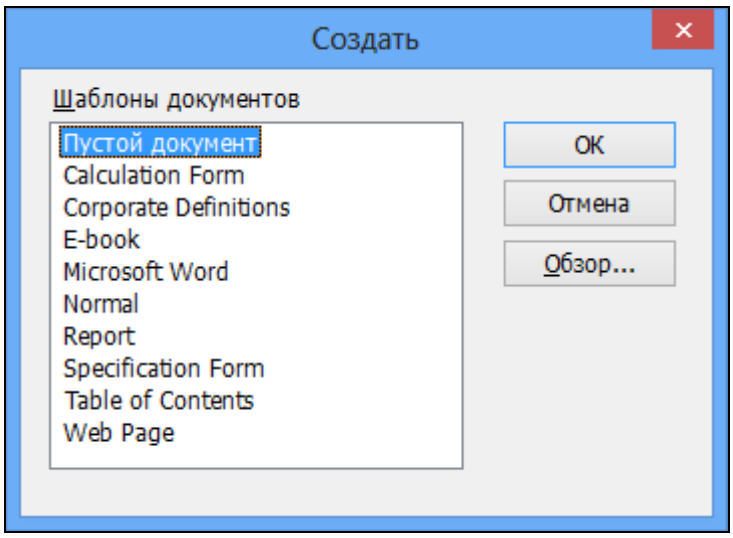


Fig. 1.19. Built-in templates in Mathcad 15

Not only built in templates can be used (see Fig. 1.19 and 1.20), but also user created ones. Creating a template is easy - you need to open a built-in template, change something in it and save it in the folder "template" with a new name and the ending *.hmct. The same operation can be also done with a finished document. Fig. 1.18 after adding a new template the user can use his own created template just like the built-in templates.

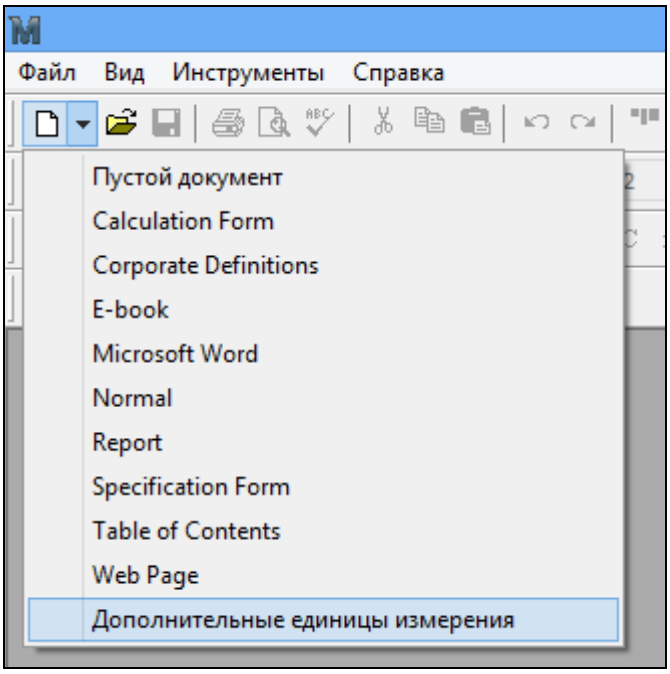


Fig. 1.20. List with custom template

If you open a custom template, as shown in Fig. 1.20, Russian units can be used in the Mathcad document (if Russian units have been introduced in this template), which are not built into Mathcad - see Fig. 1.21. (You can also make a reference to the "cloud" Mathcad document with full name http://twt.mpei.ac.ru/ochkov/units.xmcdz, and some additional Russian and

English units of measure become available. They are also used in the "cloud" document named http://twt.mpei.ru/tthb/H2O.xmcdz, to which we often refer in this book.)

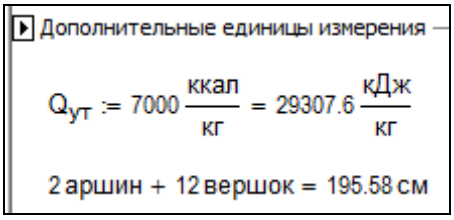


Fig. 1.21. Working with custom template

Custom pattern shown in Fig. 1.21, a built-in Mathcad standard template (Normal), which is inserted in an area named Additional units. In this area, the operators stored kJ: = 1000*J, g: = gm, etc., i.e. Binding Russian unit names to the built-in English counterparts.

Among Mathcad Prime 3.0 the opportunities to work with templates are expanded. In particular, you can not only use your own templates (My Templates - see Fig. 1.22), but also templates from all users of the local computer network (Shared Templates) and standard templates from the firm PTC - Developer Mathcad.

With the ability to share templates among all users in the network it is possible to replace Mathcad servers in those organizations, which for various technical reasons and/ or for security reasons do not have access to the Internet.

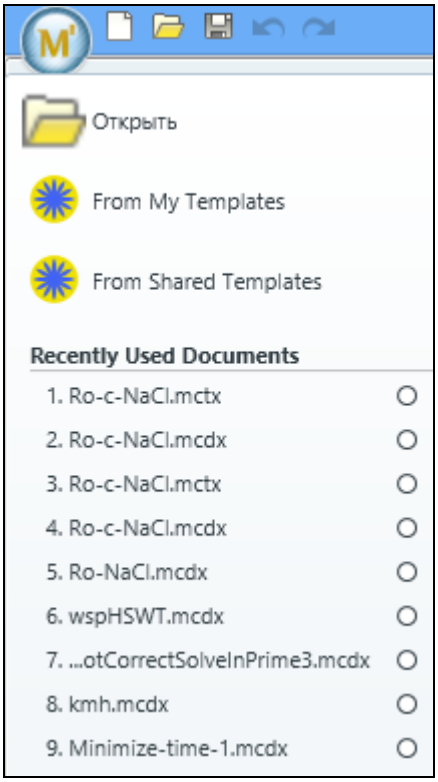


Fig. 1.22. Opening Templates in Mathcad Prime 3.0

Mathcad templates primarily contain no text (except heading, etc.) and calculation elements. Thus Fig. 1.23 shows a template for the use with aqueous NaCl (this will be described in detail in the etude 4). In this pattern are following functions integrated: a function that returns the density of NaCl in aqueous solution depending on the concentration, expressed in different ways - the weight percent (%), molality (mole / kg), molarity (mole / L) and the titer (g/mL), the inverse function (concentration of density), a scaling function of concentration depending on the function of the freezing point of the solution, and other useful functions. All this considerably simplifies and accelerates the calculation where this solution appears - for example, the calculation of air conditioning systems with this solution as a coolant or refrigerant.

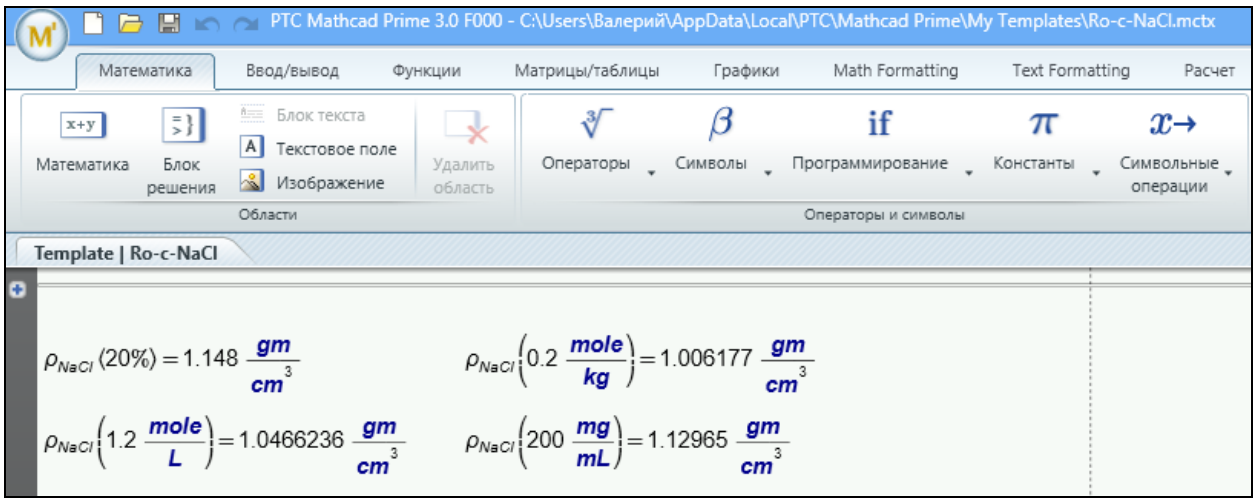


Fig. 1.23. Template with the properties of aqueous NaCl solution

Looking ahead, we can, say that a template for Mathcad 15 may contain links to cloud features on the properties of water and steam - the main working body in engineering sciences.

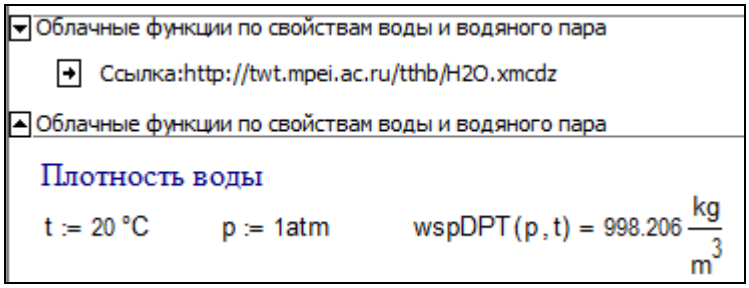


Fig. 1.24. Template with the properties of water and steam

Fig. 1.24 shows the calculation of the density of water for a given temperature and pressure with a function named wspDPT, which is stored in the "cloud" file named H2O.xmcdz. More details about this calculation are described in etude 6 "maximum density of water."

Working with templates can greatly simplify the calculations. Starting a new project does not require opening a new blank document and not be lazy and search the World Wide Web right template with the right functions. The used template can be edit and expanded- add to it, for

example, new functions and return it back to the Internet, providing new functions for other users. It is one possible way of communication about databases and calculations on properties of substances and CAD programs.

The free and shortened version of Mathcad Prime - Mathcad Express has not programming tools. In this connection, will be very useful to create functions that return the properties of substances, without programming. Fig. 1.25 shows three functions with different appearances but the same content. They return the solubility (weight percent) of sodium chloride in water depending on the temperature.

For Mathcad Prime

$$NaCl_1(T) := \left\| \begin{array}{l} \text{“Solubility: P - mass NaCl/mass water, ω - mass NaCl/mass solution”} \\ \text{if } T < 0\ °C \\ \quad \| \text{return error(“T must be >= 0°C”)} \\ \text{if } T > 100\ °C \\ \quad \| \text{return error(“T must be <= 100°C”)} \\ t \leftarrow \frac{T}{K} - 273.15 \\ P \leftarrow \left(35.71189 + 8.48019 \cdot 10^{-3} \cdot t + 3.17016 \cdot 10^{-4} \cdot t^2\right) \cdot 1\% \\ \omega \leftarrow \frac{P}{1+P} \end{array} \right.$$

For Mathcad Express

$$NaCl_2(T) := \text{if}\left(\frac{T}{K} - 273.15 < 0, \text{error(“T must be >= 0°C”)}, \text{if}\left(\frac{T}{K} - 273.15 > 100, \text{error(“T must be <= 100°C”)}, \frac{\left(35.71189 + 8.48019 \cdot 10^{-3} \cdot \left(\frac{T}{K} - 273.15\right.\right.}{1 + \left(35.71189 + 8.48019 \cdot 10^{-3} \cdot \left(\frac{T}{K} - 273\right.\right.}\right.\right.$$

$$NaCl_3(T) := \text{if}\left(T < 0\ °C, \text{error(“T must be >= 0°C”)}, \text{if}\left(T > 100\ °C, \text{error(“T must be <= 100°C”)}, 0.36975 - 8.31824 \cdot 10^{-4} \cdot \frac{T}{K} + 1.61596 \cdot 10^{-6} \cdot \left(\frac{T}{K}\right)^2\right)\right)$$

Fig. 1.25. Function solubility NaCl: two options

The dependence of the solubility of sodium chloride on the temperature is well described by a second degree polynomial. Many calculations about solubility are provided on the site: http://twtmas.mpei.ac.ru/mas/Worksheets/Chem/solutions.html. The calculations are based on the tables from the directory "Lurie on Analytical Chemistry" (Moscow: Khimiya, 1972). Fig. 1.26 shows such a calculation for an aqueous solution of NaCl.

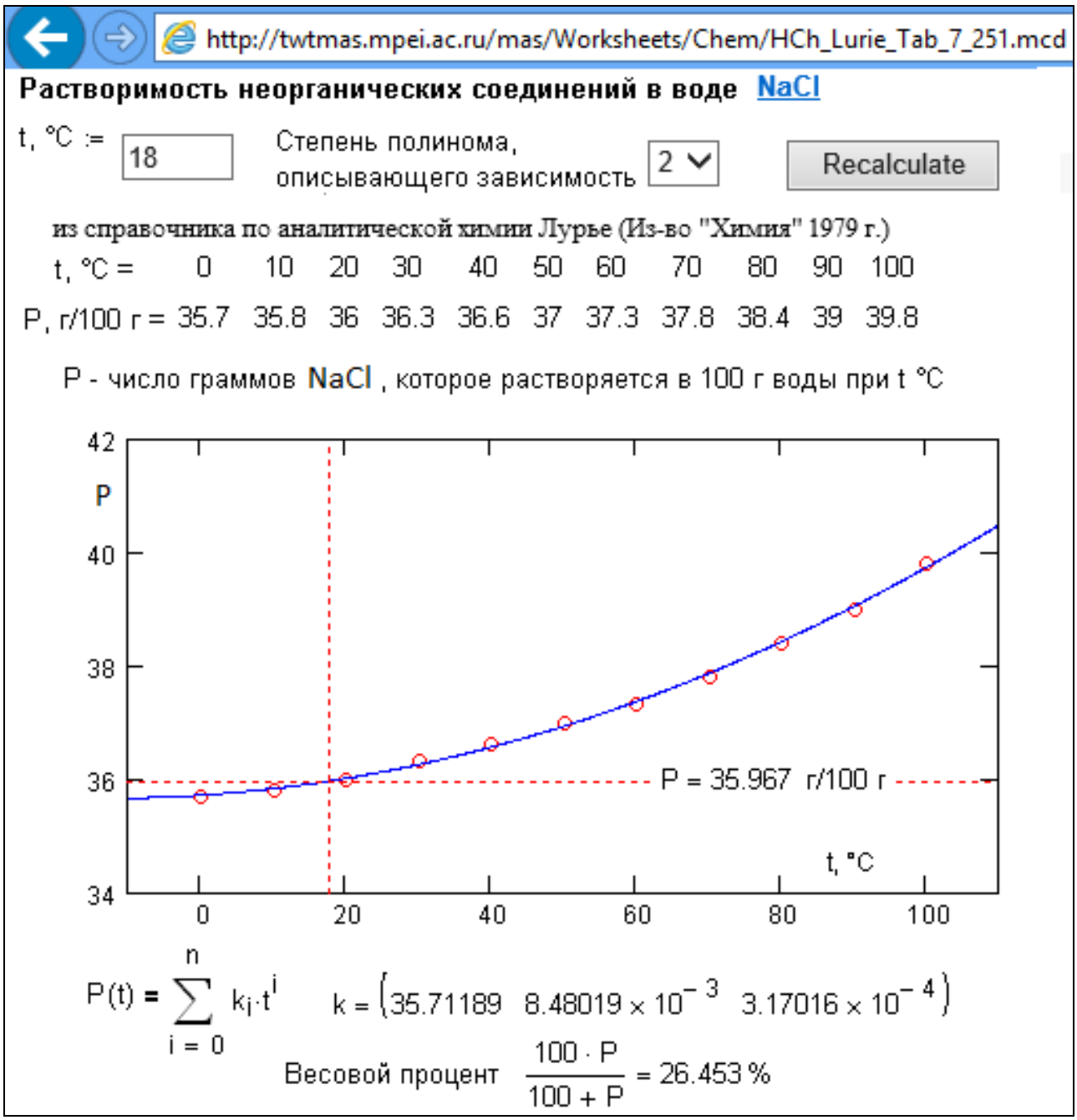


Fig. 1.26. Online calculation of the solubility of NaCl in water

In Fig. 1.25 we can see three functions named NaCl with the subscripts 1, 2 and 3, which return the solubility of sodium chloride depending on the temperature. The first of them is created using programming tools. The second function (only a part of it) uses only the built-in Mathcad function , that allows this function with the name of NaCl work as the full version of Mathcad Prime, and in its shortened version of Mathcad Express. Nevertheless the first function (with programming elements) is more transparent in terms of its understanding and provides more possibilities for editing. The third function is a simplification of the second function. It different polynomial coefficients because once the temperature considered Kelvin, Celsius, and not that

it outputs a value polynomial ω (mass ratio of solute to the mass of the solution), not P (ratio of the mass of solute to the mass of of water).

Related solution concentration will be devoted to study three books. Now it may be mentioned that in different books can be found widely differing data on thermophysical properties of fluids. This occurs in part because that some references realize the percentage ratio of the weight concentration of the solute in the bulk solution, to the other - the ratio of the mass of solute to the mass of solvent, and the third - the ratio of the amount of solute to solvent, etc.. So use this data with great care.

Another modern way to publish data about properties of substances is to create a website, which contains a code for specific programs. Thus in Fig. 1.27 you can see a website, which generates a code for engineering calculations with Matlab.

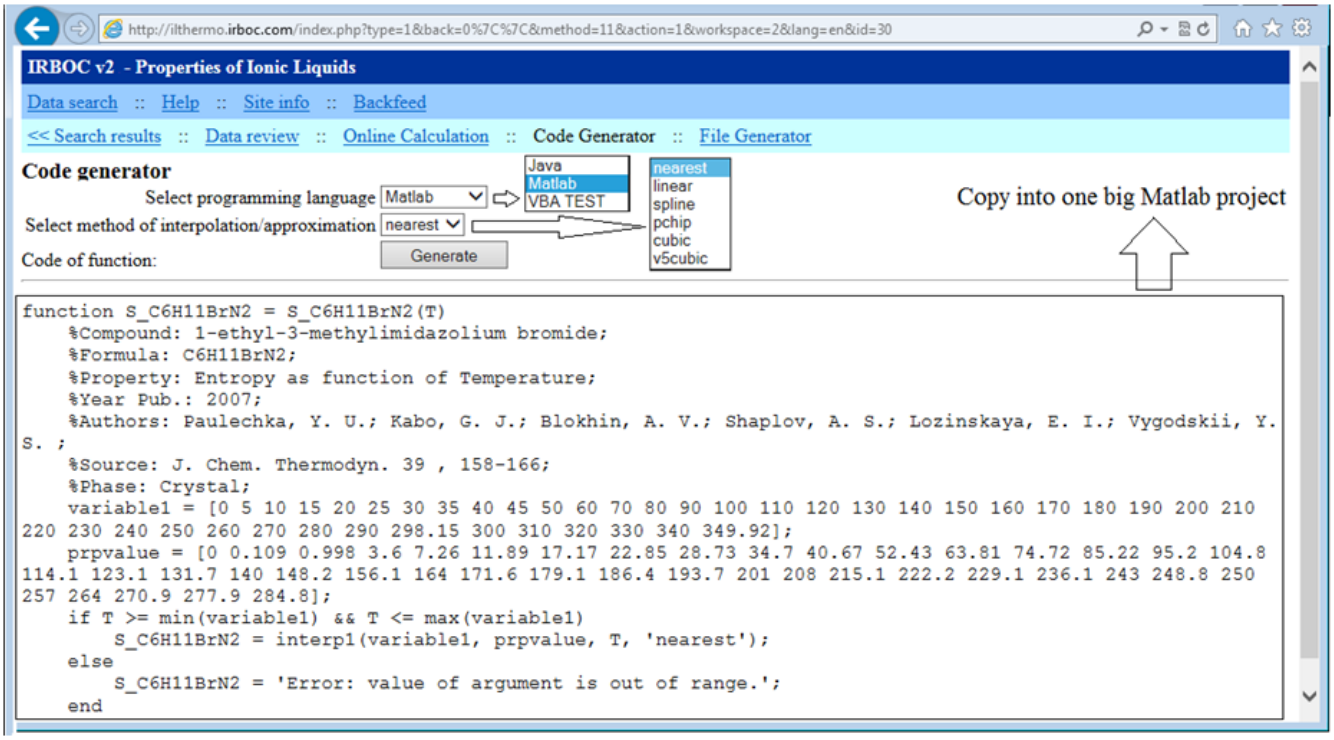
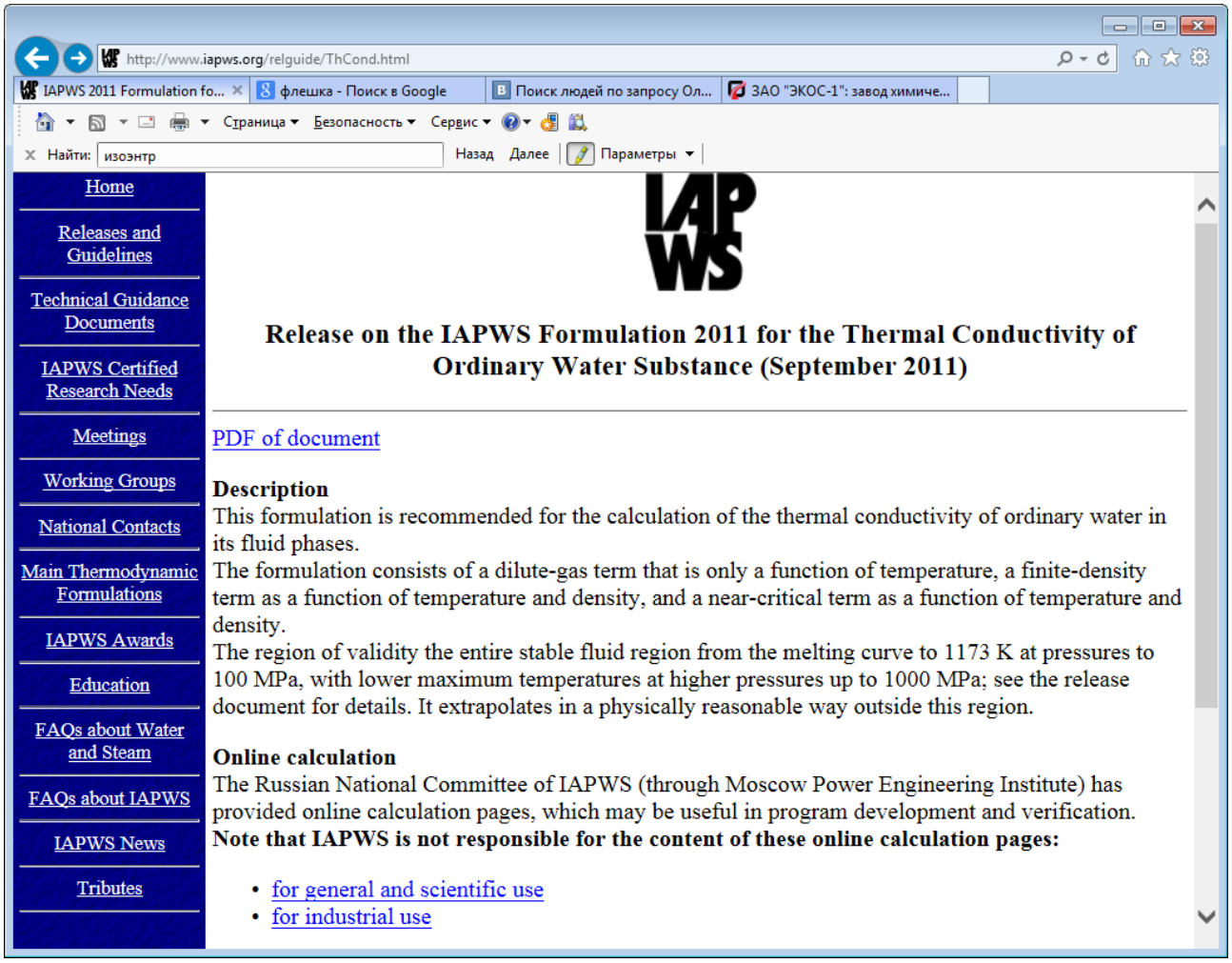


Fig. 1.27. Internet generation user functions on the properties of substances for Matlab

In conclusion we can say that the International Association for the Properties of Water and Steam uses for interactive website design calculations basic properties of this working fluid and material engineering (e.g., Fig.

1.28).



1. Fig. 1.28. Link to the online-payments website site IAPWS

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13. www.nist.gov/srd/nist23.cfm
14. http://trc.nist.gov/tde.html
www.wsp.ru