p V = T

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A new technology for working with temperature in computer calculations in the environments of physical and mathematical programs is discussed. The fundamental questions of physics related to systems of physical quantities are touched upon. Temperature is considered not as a basic, but as a derived physical quantity. A new 3D diagram is proposed that displays the IAPWS-IF97 formulation.

Attention! Three important warnings in the abstract!

1. This article is not about temperature as a physical quantity, but about the technology of working with temperature in the environment of modern physical and mathematical computer packages. Or rather so. This article primarily touches upon the issues of computer work with physical quantities, and secondly, the issues of physics, the system of physical quantities.

2. The article will most likely not be understood and appreciated by those who have never performed calculations using units of measurement in the environments of modern computer physics and mathematics packages such as Mathcad, Maple, Mathematica, SMath, etc. Moreover, such people will consider that the author is nothing does not understand in physics, in particular, in the physical essence of temperature and "climbs with his pig's snout into the Kalashny row".

3. The article does not call for radical changes in the technology of thermodynamic calculations. The article urges to look at them critically and take this criticism into account when improving the tools for working on a computer with physical quantities.

> *"Well, well, electricity and heat are one and the same, but is it possible to put one quantity instead of another in the equation for solving the problem? No. So, what then? The connection between all the forces of nature is already felt by instinct ..."*
>
> *Leo Tolstoy "Anna Karenina"*

The title of this article is doubly unusual. Firstly, it consists only of a short formula, and secondly, as the prescribed equation of state for an ideal gas (the Clapeyron-Mendeleev[1] equation) it is given without the traditional letter *R*—without a universal gas constant.

Imagine that you open a physics textbook and see the formula ***m a = k F***, with the explanation that this is a mathematical representation of Newton's second law, where *m* is mass, *a* is acceleration, *F* is force, and *k* is the universal force constant... You, of course, would be surprised and say that there should not be any letter *k* in this formula. But you would be answered in the sense that the constant *k* serves to translate the force expressed in kilograms-force (*the base force unit*) into newtons (*an auxiliary force unit*). People have long been accustomed to expressing force in kilograms-force (***kgf***),

[1] Or Mendeleev—Clapeyron. The authorship of this basic formula of classical thermodynamics has not been conclusively established. In many Western countries Mendeleev is not mentioned here. About the same story happened with the periodic table of chemical elements, which is named only in Russia (periodic table). Before Mendeleev, the ideal gas equation was different for each specific gas. Mendeleev combined them by introducing another quantity into the equation—the molar mass of a gas. The Germans in the question of the ideal gas equation remember their Rudolf Julius Emanuel Clausius (1822-1888). There is a lot of conjecture and politics in this business. As, however, in the international system of physical quantities, which will be discussed in the article.

and not in some “incomprehensible” newtons (***N***). That is why this formula contains the value *k*, called a universal force constant. Force can be expressed in other common units—in dynes, in pounds-force, and so on. But all of them would first have to be converted into kilograms-forces, and only then inserted into the formula ***m a = k F***.

But if we open a textbook on classical thermodynamics—one of the branches of physics, then in reality we will see a similarly "burdened" formula (the equation of state for an ideal gas) $p\ v = R\ T$, where *p* is pressure, *v* is specific molar volume, *T* is temperature, and *R* is a universal gas constant used to convert kilograms-force, sorry, degrees Kelvin, again sorry, kelvin[2] into the correct units of temperature. For which ones—see below.

To justify such an unusual title, we will not go into the physical essence of the concept of temperature (or rather, we will postpone it for later), but will compute the solution to a simple problem from the field of thermodynamics of ideal gases.

Task. You need to pump up the wheel of your bike. The question is how many strokes with a piston bicycle pump need to be done in order to raise the tire pressure from one atmosphere to five atmospheres. Figure 1 shows the diagram of the problem, and Figure 2 shows its solution, *modernized by the author,* as computed by Mathcad.

We make three assumptions. 1. The bicycle tube is a torus that does not change its volume when inflated (the tire is quite rigid—the process is isochoric). 2. The air temperature in the chamber and pump does not change. Due to heat exchange with the environment, the air has time to cool down to the ambient temperature at each pump stroke (isothermal process)[3]. To do this, you need to inflate the bicycle wheel very slowly and smoothly. 3. There is no air leakage from the pump.

[2] Note that for a scientist, the highest assessment of his merits will be that his surname will be written with an initial lowercase, rather than uppercase letter: Not Kelvin (Thompson, 1824—1907), but kelvin. In the article, for example, Blaise Pascal (1623—1662), who gave his name to the basic unit of pressure, is also mentioned. One can continue: volt, ampere, pendant, stokes ...—a whole string of basic and auxiliary units of measurement, named after famous scientists. It is also extremely honorable if the surname is reduced to one or two letters: not Kelvin, but K!

[3] I recall "Solo on Underwood" by Sergei Dovlatov. “One famous director had a heart attack. Having slightly recovered, the director again began to pursue young women. One of them delicately asked:

- Is IT possible for you?

The director replied:

- You can... But smoothly... "

If it were not a director, but a physicist (the famous Lev Landau from USSR, for example, is still that womanizer!), then he would say: “You can. But smoothly, isothermal!"

Now this behaviour is called harassment. In The Master and Margarita by Bulgakov, Fagot complained to Woland about the director of the variety show, Stepa Likhodeev: “in general, he has been terribly piggy lately. He gets drunk, touch women, using his position."

Fig .1. Scheme of the problem of pumping a bicycle wheel

Figure 2 shows the successive approximation procedure. The number of pump strokes n is set, which is corrected depending on the calculated value of the tire pressure p_n.

The calculation specifies the geometric dimensions of the bicycle tire and bicycle pump. A tire is a torus with a small radius r and a large radius *R*, and a pump is a cylinder with a diameter *d* and a height *H* (pump stroke). The entered values of *r, R, d* and *H* allow you to calculate the volumes of these geometric bodies (6.477 litres and 283 millilitres[4]). We can see that Mathcad works with units of physical quantities, which makes the calculations readable, eliminating many possible errors and ensuring you select the correct formulas [1]. The pressure p_0 and the ambient temperature T_0 are included in the calculation. The pressure is entered in physical atmospheres (1 atm = 760 mm Hg), which are immediately converted into pascals (the basic unit of pressure in SI, which Mathcad uses by default—see also footnote 2). The entered value of the variable *T* (18 degrees Celsius) is first converted to the Kelvin scale (absolute thermodynamic temperature 18 + 273.15 = 291.15—this is done directly by Mathcad), and then additionally multiplied by the universal gas constant *R* = 8.314 J/mol/K. The result (2421 J/mol) is printed by default, but the user has the right to replace this unit of temperature with the more familiar Kelvin, Celsius, Rankine, Fahrenheit...

The universal gas constant *R* has, as it were, moved from the ideal gas equation of state to a tool for entering the temperature calculation. This is not just a computational trick—it is the restoration of physical justice, so to speak. This will be discussed below.

[4] Rounding is carried out when the answer is printed. In the depths of the computer, these values are stored in cubic meters (the basic unit of volume in SI, to which the Mathcad package is oriented by default) and with a maximum precision of 15 significant digits.

$$r := 50\ cm \qquad R := 55\ cm$$

$$V_o := \frac{1}{4}\ \pi^2 \cdot (R+r) \cdot (R-r)^2 = 6.477\ L$$

$$p_0 := 1\ atm = \left(1.013 \cdot 10^5\right)\ Pa \qquad T_0 := 18\ °C\ = \left(2.421 \cdot 10^3\right)\ \frac{J}{mol}$$

$$p_0 \cdot \frac{V_0}{x_0} = T_0 \qquad x_o := p_0 \cdot \frac{V_o}{T_0} = 0.271\ mol$$

$$H := 40\ cm \qquad d := 3\ cm \qquad V_{pump} := \pi \cdot \frac{d^2}{4} \cdot H = 283\ mL$$

$$p_0 \cdot \frac{V_{pump}}{x_{pump}} = T_0 \qquad x_{pump} := p_0 \cdot \frac{V_{pump}}{T_0} = 0.012\ mol$$

$$n := 88 \qquad \Delta T := 10\ \Delta°C = 83.145\ \frac{J}{mole}$$

$$p_n \cdot \frac{V_0}{x_0 + n \cdot x_{pump}} = T_0 + \Delta T \qquad p_n := \frac{T_0 + \Delta T}{\dfrac{V_o}{x_o + n \cdot x_{pump}}} = 5.008\ atm$$

Fig. 2. Calculation of the process of inflating a bicycle wheel

After entering the initial data, the initial amount of air in the bicycle wheel chamber x_o, in moles, is calculated[5]. Further, the second assumption in the problem, that the process is isothermal, is something of a simplification. The temperature of the air during its compression will still rise by ten degrees Celsius (ten kelvin). After that, the pressure in the bicycle wheel chamber after 88 pump strokes is calculated through the "de-energized" ideal gas equation. And nowhere in the calculations is the value of *R*, the universal gas constant, visible. We note in passing that this speeds up the calculations—the *R* value is only used to enter the temperature value to convert kelvin to joules per mol.

But back to the physics of the problem.

The fact is that in life and in physics, there is no temperature, but there is the energy of molecules and other elementary particles, which is interpreted as temperature. In plasma physics, in elementary particle physics, for example, temperature is often measured by electron volts (one of the units of energy), implying that the amount of matter is a dimensionless quantity. Mathcad, by default, works in SI, where there are seven basic units of measurement, including temperature (kelvin) and amount of substance (mol). But physicists in their calculations prefer to work with the CGS system (CGS—centimetre-gram-second), where there are only three basic quantities (length, mass and time) and where the temperature and amount of the substance are “a flight of fancy”.

[5] We don’t need to say “mass in kilograms”, but simply say “mass”. But in the case of the amount of substance, it is necessary to clarify that this value is set in moles. Otherwise, the expression "amount of air" can be incorrectly interpreted as a mass of air or a volume of air.

Historically, it so happened that, first in life, and then in physics (in metaphysics), the empirical concept of temperature with different nominal degrees and scales appeared (Fahrenheit—1724, Reaumur—1730, Celsius—1742, etc.), and only later (1834—1874) a theoretical equation of state for an ideal gas was invented, which had to be adjusted to "degrees". This is where the mystery lurks about why temperature has become not just a separate physical quantity, but a basic physical quantity in SI. It should be an auxiliary value, which we have tried to show in this article. This is evidenced by the fact that until 1968 the kelvin was officially called the degree Kelvin. Degrees were widely excluded from metrology [3]. Yes, Kelvin degree has been renamed to kelvin. But this looks like the "metrology house" has not been completely cleaned up, but simply that the rubbish has been swept under the carpet. By the way, the Rankine degree (or Rankine—the transatlantic analogue of the Kelvin degree) has remained a Rankine degree: there are no rankines (temperature units) in metrology and none are expected.

For manual calculations and for calculations in software environments without tools for working with physical quantities (spreadsheets, programming languages), you can use the old ideal gas equation with four changes—with two thermodynamic quantities (pressure-volume-temperature) and one constant—a universal gas constant. The transition to calculations in the environments of modern physical and mathematical programs with tools for working with physical quantities (Mathcad, Maple, Mathematica, SMath, etc.) allows you to return true physics to calculations and finally exclude Kelvin degrees (kelvin) from calculations not formally ("sweeping garbage under the carpet"), but in essence. Users of these packages have the right to work with any unit of temperature—with the usual degrees or with the correct joules divided by mol (see Fig. 2). Or just with joules—see the title, where the uppercase letter *V* (volume) is spelled out, and not the lowercase letter *v* (specific molar volume). A joule is not just a unit of energy, but a person, we recall, who was the first to find a connection between mechanical (and electrical—see the epigraph below the title) work and thermal energy.

The SI unit system is, frankly, a complete mess. We have already written about the kelvin, undeservedly raised to the power of the basic unit. The basic unit of mass turned out to be a multiple of kilo. Multiples are just things like ten, dozen, hundred. The incomprehensible candela appeared, the units of value, the amount of information were left behind. The units of time remained non-decimal. Little-known, almost forgotten physicists were awarded with named units, and honored luminaries were bypassed with this distinction. Etc. etc. Exactly seven basic physical quantities (mass, length, time, current strength, amount of substance, luminous intensity and our temperature) are not some kind of physical rationale, but rather the magic of numbers: seven colors of the spectrum, seven notes of a scale, seven days of the week , seven wonders of the world, etc. In this article, the author has tried to rationalise at least the temperature.

"A complete mess"—this is of course is the author getting excited! Let's correct and say that the SI unit system is extremely imperfect. But our World is also extremely imperfect! In this regard, I recall an old anecdote about how one client waited a long time for the trousers he'd ordered and rebuked the tailor, saying that the Lord God created the world in seven days, but that the tailor had been busy with the trousers for a month. The tailor replied: "Look at this World and look at my trousers!"

If we are not talking about an ideal gas, but about real substances—gases and liquids, then to describe their properties, we can return the fourth variable to the equations of state: not $p\ v = T$, but $p\ v = k\ T$, where the variable k depends on pressure and temperature and changes from unity (ideal gas) to almost zero (incompressible liquid). The reciprocal of k is called the compressibility factor.

In Figure 3, the contour graph (lines of the same level) shows the dependence of compressibility on pressure and temperature. The graph was built in Mathcad using the author's program WaterSteamPro® (www.wsp.ru). The colors of the graph are from Mathcad's rainbow scheme: red represents large values of the k coefficient, close to one (ideal gas, water vapor with low pressure and high temperature), while purple represents small values close to zero (water under low pressure). In the middle of the figure, 3 lines of one level merge into one, forming the so-called saturation line of water and steam, extending from the triple point, where ice, water and water vapor are simultaneously present, then the critical point, where water ceases to differ qualitatively from water vapor.

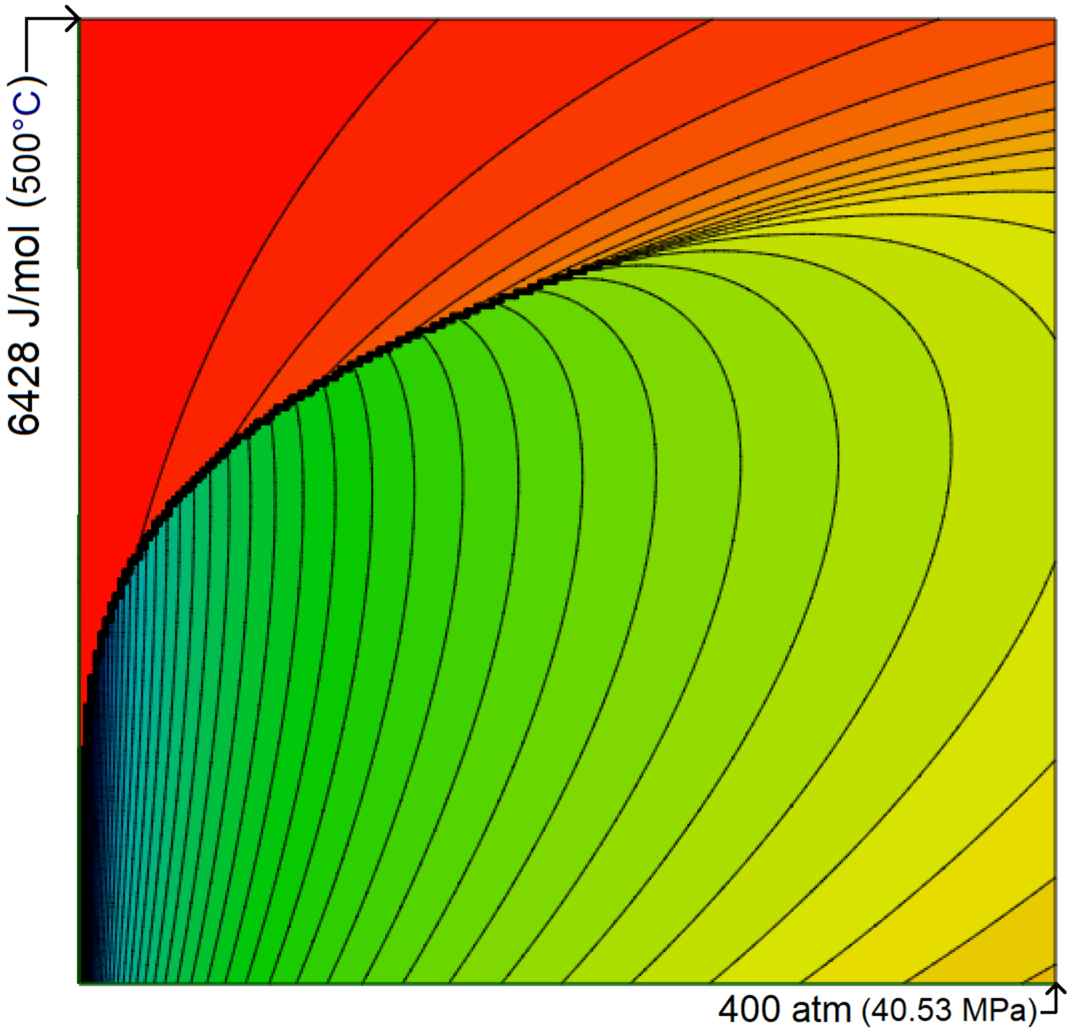

Fig. 3. Compressibility of water and steam depending on pressure and temperature

If you go to the right from the upper left corner of the diagram in Fig. 3 along the horizontal isotherm line to the right corner, then go down to the lower corner along the isobar line, and then go to the lower left corner, then the values of the f parameter will change as follows: 1, 0.625, 0.315 and... two values: a unit for water and zero for water vapor at the ends of the triple line.

The value of the coefficient *k* depends not only on pressure and temperature, but also on other factors. If, for example, in the subcritical region the temperature is raised isochorically, then the value of k when crossing the saturation line can increase not by a step, but by a kind of gentle "ramp". This phenomenon is associated with overheating of saturated water. If you go down and isochorically reduce the temperature of the superheated steam, then the process of supercooling of water vapor can be observed. And all this, as in the case of a bicycle pump, is determined by the rate of cooling or heating. If everything is done smoothly enough (remember the famous director and his ladies—see footnote 4), then there will be no unstable thermodynamic problems. The director and the physicist will not have a new heart attack either!

The diagram in Fig. 3 is based on the IAPWS-IF97 formulation developed by the International Association for the Properties of Water and Steam (www.iapws.org), in which the author has been working since 2007. This formulation includes separate formulations on the thermophysical properties of water and steam for the five regions shown in Fig. 4: water region (Region 1), steam region (2), near-critical region 3), saturation region (4) and high temperature steam (5). In the upper right part of Fig. 4, these areas are shown in the coordinates of pressure and temperature. To the left is shown the same diagram in the coordinates "expandability"—temperature, and below in the coordinates pressure—"expandability". The square in the diagrams marks the triple point, and the circle marks the critical point.

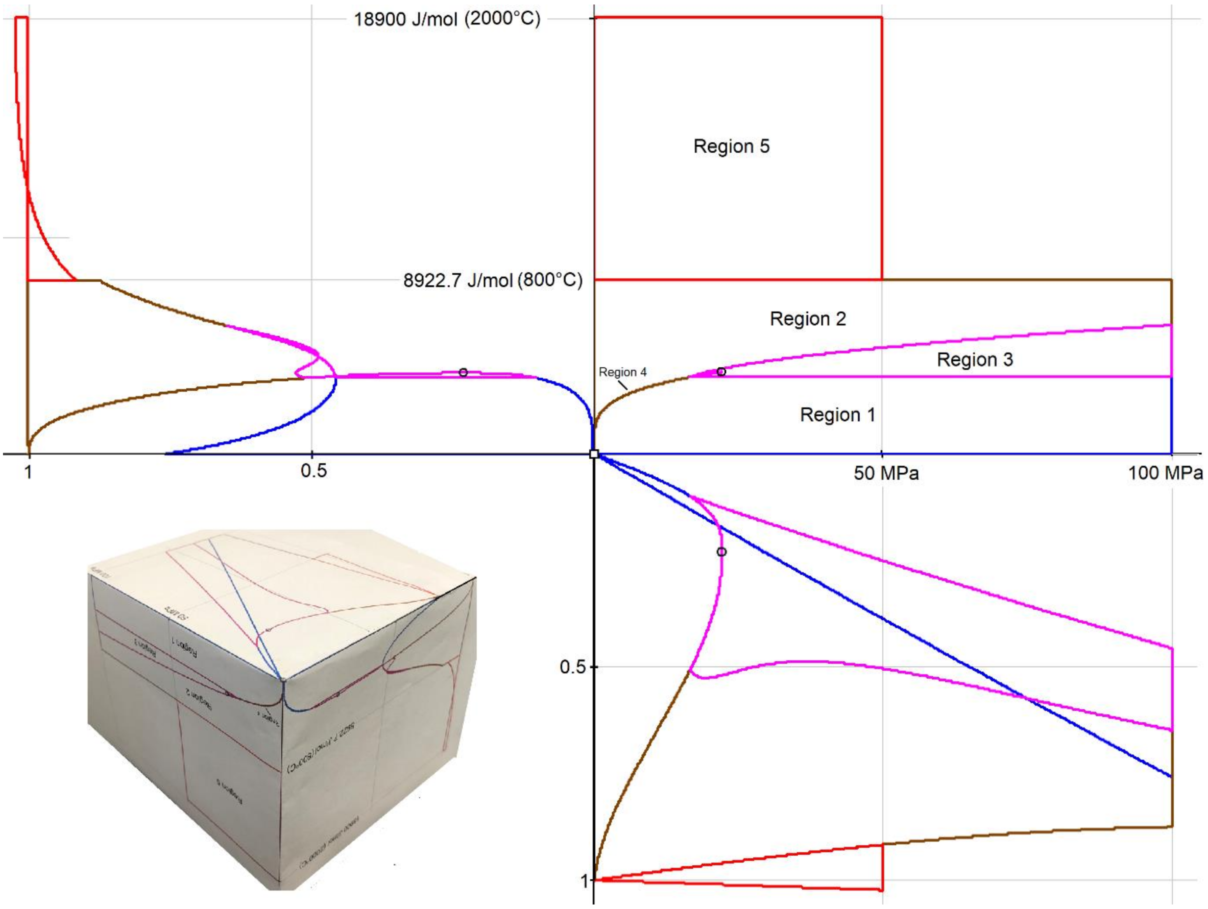

Fig. 4. Coefficient (factor) of "expandability" of water and steam depending on pressure and temperature in three coordinate systems

If the left and bottom diagrams in Fig. 4 "bend" upwards, you get a rectangular parallelepiped, on the six faces of which the lines shown in Fig. 4. And what can be seen inside this rectangular parallelepiped? This requires a good imagination and/or 3D computer graphics. On the edges of this rectangular parallelepiped, the pressure, temperature and "expandability" of water and steam will be measured. More precisely, it will be a large rectangular parallelepiped (0-100 MPa, 0-2000 ° C, 0-1), from which a small rectangular parallelepiped was removed (50-100 MPa, 800-2000 ° C, 0.759-1).

Note also that in region 5 (steam at high temperature and low pressure), the coefficient *k* (factor of "expansion") can be greater than 1.

Imagine that you are looking out of the house onto the street, and you notice such an “ideal” outdoor thermometer on the outside of the window—Fig. 5.

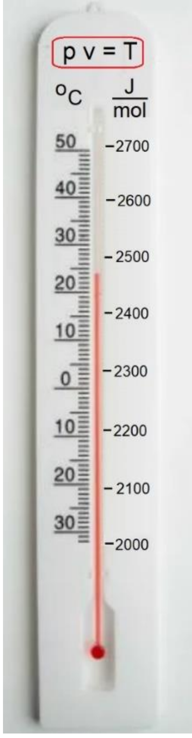

Fig. 5. Street thermometer with two scales: with the usual and correct.

In the USA there are many similar thermometers with one (left) scale for "aborigines" accustomed to the Fahrenheit scale, and on the other (right) for visitors from the Old World who perceive only Celsius degrees. Our thermometer in Fig. 5 is intended for some "temperature orthodox", to which the author refers himself. They only work with the correct temperature units, but they also allow auxiliary ones. It can be either Celsius (Fig. 5) or Fahrenheit for the New World. Degrees of Kelvin, sorry, kelvin is practically not needed by anyone here.

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