

Hybrid thermodynamic calculations

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Abstract. This report shows, the possibility of combining numerical and symbolic tools of modern computer mathematical programs for solving thermodynamics problems, in particular, for calculating thermodynamic cycles.

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Let's solve a simple thermodynamic problem using a computer: the pressure $p_1 = 1$ atm is known and the temperature $T_1 = 18$ °C of an ideal gas with a specific isobaric heat capacity $c_p = 7R / 2$ (a diatomic ideal gas, R is a universal gas constant). It is necessary to determine the temperature T_2 and the pressure p_2 of this gas after it was adiabatically compressed by a factor of 7 (n is the compression ratio). We thus calculate the first part of the ideal thermodynamic cycle of a four-stroke internal combustion engine. The second part of this cycle will be isochoric (Otto cycle), or isobaric (Diesel cycle) or mixed (Trinkler cycle) heat supply. The third stroke of the cycle will be the working stroke of the piston (another adiabat), and the fourth - isobaric heat removal, engine exhaust. The reader can, if desired, calculate the entire cycle [1], based on the methodology outlined below. We will calculate only the first part - compressing air or a fuel-air mixture.

Fig. 1 shows the solution of this problem in Mathcad, which is very popular among students, engineers and scientists, because it can work with dimensional values [2, 3]. It also incorporates the basic physicochemical constants - the universal gas constant R , for example. This greatly facilitates and accelerates the physicochemical and thermodynamic calculations, allows you to control the dimensions, enter and output quantities with units of measurements to which the user is accustomed, and not with those prescribed by different regulations and rules that do not always correspond to the real needs of engineering practice.

$$T_0 := 1 \text{ K} \quad p_0 := 1 \text{ Pa}$$

$$T_1 := 18 \text{ }^\circ\text{C} \quad p_1 := 1 \text{ atm} \quad c_p := \frac{7}{2} R = 29.101 \frac{\text{J}}{\text{mole} \cdot \text{K}}$$

$$v_1 := \frac{R \cdot T_1}{p_1} = 0.023891 \frac{\text{m}^3}{\text{mol}}$$

$$n := 7 \quad v_2 := \frac{v_1}{n} = 0.003413 \frac{\text{m}^3}{\text{mol}}$$

$$s_{12} := \int_{T_0}^{T_1} \frac{c_p}{T} dT - R \cdot \int_{p_0}^{p_1} \frac{1}{p} dp = 69.279 \frac{\text{J}}{\text{mol} \cdot \text{K}}$$

Guess Values

$$T_2 := 500 \text{ K} \quad p_2 := 10 \text{ atm}$$

Constraints

$$p_2 \cdot v_2 = R \cdot T_2 \quad s_{12} = \int_{T_0}^{T_2} \frac{c_p}{T} dT - R \cdot \int_{p_0}^{p_2} \frac{1}{p} dp$$

Solver

$$\begin{bmatrix} T_2 \\ p_2 \end{bmatrix} := \text{Find}(T_2, p_2) = \begin{bmatrix} 634.098 \text{ K} \\ (1.545 \cdot 10^6) \text{ Pa} \end{bmatrix}$$

$$T_2 = 360.948 \text{ }^\circ\text{C} \quad p_2 = 15.245 \text{ atm}$$

FIGURE 1. Numerical solution of the problem of compression of an ideal gas

A well-known formula of classical thermodynamics with two integrals is used to calculate the specific entropy of an ideal gas s_{12} , which will remain constant in the process of its compression. Its value is $69.279 \text{ J}/(\text{mol K})$. Then the system of two equations with two unknowns, T_2 and p_2 , is solved and the numerical answer is given: the temperature and pressure of the compressed gas in basic SI units (Kelvin and Pascal is the answer in square brackets of the vector) and in degrees Celsius and physical atmospheres that are more common in heat engineering. Here we used numerical solution, including that for integrals. But in thermodynamics, the numerical value of entropy or energy (Gibbs energy or Helmholtz energy, for example) has no physical meaning – the meaning is only the difference of energies and entropies. In Fig. 1, we calculated the entropy of the gas referenced to the standard state $T_0 = 1 \text{ K}$ and $p_0 = 1 \text{ Pa}$ (see the first line in Fig. 1). The answer will not change if the standard state is different. For water, for example, the standard parameters are triple point parameters. Similarly, in mechanics, the value of the potential energy of a body depends on the selected zero point: the level of the floor, the level of the ocean or the centre of the Earth. These values do not make any sense – only the values of the potential energy change are important.

In The second equation in the system (see Fig. 1) can be simplified - see Fig. 2. But in this case, the logarithms will include dimensional quantities - pressure and temperature. However, we have to remember that the difference between the logarithms of two quantities is the logarithm of the ratio of these quantities, to solve the problem: dimensionless quantities are the logarithm. It is possible to calculate the value of the specific entropy at T_2 and p_2 , if we set the "standard values" of T_0 and p_0 , which was done in the calculation in Fig. 1.

$$\int_{T_0}^{T_2} \frac{c_p}{T} dT - R \cdot \int_{p_0}^{p_2} \frac{1}{p} dp \rightarrow \left\| \begin{array}{l} \text{if } p_0 > 0 \wedge T_0 > 0 \vee p_0 > 0 > T_2 \vee T_0 > 0 > p_2 \vee 0 > p_2 \wedge 0 > T_2 \\ \left\| R \cdot (\ln(p_0) - \ln(p_2)) - c_p \cdot (\ln(T_0) - \ln(T_2)) \right. \\ \text{else} \\ \left. \left\| \text{undefined} \right. \right. \end{array} \right\|$$

FIGURE 2. Symbolic simplification of the formula for computing the specific entropy

The assertion that there cannot be a dimensional quantity in the logarithm is obsolete. And this is due to the development of computer calculation and transformation techniques, which are discussed in this report.

What is the decimal logarithm of pressure in a hundred pascals, for example? This is 2 plus a logarithm ... of one pascal: $\lg(100 \text{ Pa}) = \lg(100) + \lg(\text{Pa}) = 2 + \lg(\text{Pa})$. We have a hybrid answer, where both the number 2 and the symbol $\lg(\text{Pa})$ are present! Further, the chain of transformations cannot be transformed. What is the decimal logarithm of pressure in ten pascals? This is 1 plus the same logarithm of one pascal: $\lg(10 \text{ Pa}) = \lg(10) + \lg(\text{Pa}) = 1 + \lg(\text{Pa})$. What is the difference between these two logarithms? That is the dimensionless ratio of the pressure in a hundred pascals to the pressure of ten pascals. The answer is a unit: two plus the logarithm of Pascal minus one and the same logarithm of pascal: $2 + \lg(\text{Pa}) - 1 - \lg(\text{Pa}) = 1$. The Pascal logarithms are shortened and the required unit remains. Thermodynamic calculations of energy and entropy include this notorious "logarithm of Pascal" paired with the "logarithm of the kelvin". These logarithms are eliminated in numerical calculations by introducing the concept of a standard state, as shown in Fig. 1. But this cannot be done if we conduct ... hybrid calculations [4].

What are these calculations? Fig. 1 shows a numerical calculation - the Mathcad package uses the numerical values of variables converted into SI units: kelvin, not degrees Celsius, pascal, and not atmospheres. In Fig. 2 shows the analytical (symbolic) transformations, when the Mathcad package does not use the values of the variables, but uses the variables themselves. But these calculations can be combined. In Fig. 3 (Maple package plus manual conversions) shows a hybrid solution of our gas compression problem: numerical calculations are combined with symbolic transformations when the units of measurement do not have numerical values, and the logarithms of the dimensional physical quantities are reduced and are not present in the final numerical answer. This allowed us to eliminate the need to determine the numerical value of the specific entropy [5], which, we repeat, in classical thermodynamics, has no physical meaning. Moreover, these "phantom" values of energies and entropies often lead to errors when, for example, a binary thermodynamic cycle is calculated, for which two standard bodies have different standard states.

$$\begin{aligned}
&> R := 8.314472 \frac{J}{mole \cdot K} \\
&> c_p := \frac{7}{2} R \\
&> T_1 := (18 + 273.15) K \\
&> p_1 := 1 atm \\
&> v_1 := \frac{R \cdot T_1}{p_1} \\
&> solve(\{p_2 \cdot v_2 = R \cdot T_2, s = c_p \cdot (\ln(T_2) - \ln(T_0)) - R \cdot (\ln(p_2) - \ln(p_0))\}, \{T_2, p_2\}) \\
&\left\{ T_2 = e^{1.4 \ln(T_1) - 0.4 \ln(0.1428571428 T_1)} \quad p_2 = e^{1.4 \ln(T_1) - 1.4 \ln(0.1428571428 T_1)} atm \right\} \\
&> evalf(T_2) \quad 634.098 K \\
&> evalf(p_2) \quad 15.245 atm
\end{aligned}$$

FIGURE 3. Hybrid solution of the ideal gas compression problem

Note. In the calculation shown in Fig. 3, the original formula of the specific entropy with two integrals was simplified and its logarithmic version is used. It is simplistic, not equivalent. The point is that a simplified formula is obtained only if it is possible to assume that the values of pressures and temperatures are positive. The system of equations in Fig. 3 will not have hybrid solutions, if it contains a formula for the entropy with integrals.

One more important note. Authors, forming figure 3, have made a “collage”. The authors could not, in the Maple environment, convert the expressions for the variables T2 and p2 into numbers, specific values of temperature and pressure for compressed ideal gas. The evalf function (evaluation float) was extremely unstable. It produced a value in some cases, and in others it was an algebraic expression, where the numerical value of T1 stood in its place, while the other one was an algebraic expression and vice versa. Saving and reopening this file yielded new values. This was a consequence of the fact that numerical and symbolic computations were combined in the calculation, which contradicts modern mathematical programming and requires corrections. The authors reproduced the transformation of the expression for the variables T2 and p2 in Mathcad environment. This restored the stability of the calculation - see Fig. 4.

$$T_1 := 18 \text{ } ^\circ\text{C} = 291.15 \text{ } K$$

$$T_2 := e^{1.4 \cdot \ln(T_1) - 0.4 \cdot \ln(0.1428571428 \cdot T_1)} \xrightarrow{\text{simplify}} 634.09745558961695924 \cdot K$$

$$p_2 := e^{1.4 \cdot \ln(T_1) - 1.4 \cdot \ln(0.1428571428 \cdot T_1)} atm \xrightarrow[\text{float, 5}]{\text{simplify}} 15.245 \cdot atm$$

FIGURE 4. Work with the logarithm of the temperature in Mathcad

However,, the authors could not reproduce the Maple calculation, shown in Fig. 3, in the Mathcad environment. The authors worked, so to speak, in a hybrid environment, using both, Mathcad and Maple packages.

In the meantime, as a compromise, thermal engineering calculations can be carried out without "printing out" numerical values of enthalpy and entropy. Figure 5 shows the calculation of adiabatic air compression using cloud functions for the thermodynamic properties of substances [1]. The initial air parameters (pressure p_1 and temperature t_1) are given, as well as the pressure p_2 of compressed air. It is necessary to determine the temperature of the compressed air t_2 and the spent specific work.

After the reference (Reference) to Mathcad-document Gas.xmcd in the calculation shown in Fig. 5, the functions with names `wspgHGT`, `wspgSGPT`, `wspgTGPS` and `wspgVGPT` become visible and return the thermodynamic properties of air (Air) as a function of its parameters. Specific enthalpy h and entropy s are determined, but these values cannot be shown in the calculation, since these are hybrid values. Further calculations using these hybrid values are carried out without problems and the calculated values (temperature and specific work – the difference of specific enthalpy) are provided numerically.

☞ Reference:<http://twt.mpei.ru/tthb/Gas.xmcd>

$$p_1 := 1\text{atm} \quad t_1 := 18\text{ }^\circ\text{C} \quad p_2 := 10\text{atm}$$

$$h_1 := \text{wspgHGT}(\text{"Air"}, t_1) = \blacksquare$$

You cannot see this numeric value

$$s := \text{wspgSGPT}(\text{"Air"}, p_1, t_1) = \blacksquare$$

You cannot see this numeric value

$$t_2 := \text{wspgTGPS}(\text{"Air"}, p_2, s) = 284.6\text{ }^\circ\text{C}$$

$$h_2 := \text{wspgHGT}(\text{"Air"}, t_2) = \blacksquare$$

You cannot see this numeric value

$$\Delta h := h_2 - h_1 = 271.59 \frac{\text{kJ}}{\text{kg}}$$

$$\Delta h := \int_{p_1}^{p_2} \text{wspgVGPT}(\text{"Air"}, p, \text{wspgTGPS}(\text{"Air"}, p, s)) dp = 271.58 \frac{\text{kJ}}{\text{kg}}$$

FIGURE 5. Thermodynamic calculation with the inability to see the numerical values of enthalpy and entropy

ACKNOWLEDGMENTS

Modern mathematical programs allow conducting hybrid thermodynamic calculations while eliminating the need to calculate fake numerical values of entropies and energies. This simplifies the calculations and eliminates a number of errors, especially when binary thermodynamic cycles are calculated, the working bodies of which have different standard states.

Heat engineers and physicochemists will not abandon numerous tables with the enthalpy and entropy values for various working bodies and coolants, of course (for example, [6]). But hybrid calculations should push everyone to eliminate fake values.

Mathematical packages should be developed so that they can carry out the hybrid calculations described in the report. In the meantime, hybrid calculations can be conducted using different packages.

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