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A Thermophysical Property Databank for Technically Important Gases and Liquids[1]

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A thermophysical property databank for technically important gases and liquids has been created. It provides users with data for nearly 30 substances: monatomic and diatomic gases, air, water and steam, carbon dioxide, ammonia, some hydrocarbons, and refrigerants. The coefficients of the equations of state and equations for calculating transport properties, the ideal-gas functions, the saturated vapor pressure, and the melting pressure are provided for each substance. The system of programs allows the calculation of the compressibility factor, density, enthalpy, entropy, isochoric and isobaric specific heats, speed of sound, Joule–Thomson coefficient, viscosity, and thermal conductivity and some other properties. These values can be determined in the single-phase and two-phase regions and on the phase-equilibrium lines at temperatures from the triple point up to 500 to 1500 K and at pressures up to 100 MPa (for monatomic and diatomic gases, up to 2500 to 3000 K and 300 MPa). Properties can be calculated for the following nine combinations of independent variables: T, ρ; T, p; T, s; T, x; p, ρ; p, h; p, s; p, x; and h, s. The software of the databank has a modular structure and permits an increase in the number of substances, properties, and independent variables.

KEY WORDS: databank; gases; high pressures; liquids; thermophysical properties.

1. INTRODUCTION

Reliable data on the thermophysical properties of substances are necessary for many scientists, engineers, and students. For solving many practical

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tasks, these data should be presented at different independent variables and at various values of these variables. Therefore, the creation of a new type of information system—the databank—acquires special importance. In contrast to the usual information searching systems, the databank allows not only the storage of data but also the ability to get new results on the basis of equations, used in these databanks, with the help of logical and mathematical operations.

2. DATABANK

2.1. General Description

We created a thermophysical property databank for technically important gases and liquids. It provides users with data for nearly 30 substances: monatomic and diatomic gases, air, water and steam, carbon dioxide, ammonia, some hydrocarbons, and refrigerants. The information stored includes a set of program modules and blocks of numeric data. For calculating thermodynamic properties of a substance, most often a unified equation of state for gas and liquid is used. For a series of substances, side by side with the unified equations of state, the virial equations for the gaseous phase, which are valid at high temperatures (300 to 3000 K), are also used. In some cases, for greater reliability, two forms of equation of state can be applied, and users have the option to choose either of them. The dependences of viscosity and thermal conductivity on temperature and density are used for calculation of transport properties.

The coefficients of the equations of state and equations for the transport properties are stored for each substance. Parameters of the critical point and coefficients of equations for calculation of the ideal-gas functions, the saturated vapor pressure, and the melting pressure are also stored. For the majority of substances, reliable equations of state were employed that describe the experimental data with high accuracy. Most of these equations were used by their authors for calculating tables of reference data.

The system of programs consists of the following main functional blocks: a block of input initial data (for choosing the substance, the independent parameters, and the units of measurements); a block for choosing the mode of calculation (single calculation or step-wise calculations with a given number of steps); a block for calculating the properties of substances; a block for output of the results; a block for saving, editing, and printing the results; and a block for presenting the information in a graphical form.

The programs allow the calculation of the compressibility factor, specific volume, density, enthalpy, internal energy, entropy, isochoric and isobaric specific heats, speed of sound, Joule–Thomson coefficient, adiabatic exponent, volume expansion coefficient, thermal pressure coefficient, saturated vapor pressure, heat of vaporization, dynamic and kinematic viscosities, thermal conductivity, temperature conductivity, and Prandtl number. The values of properties can be determined in the single-phase region, on the phase-equilibrium lines, and in the two-phase region at temperatures from the triple point up to 500 to 1500 K and at pressures up to 100 MPa (for monatomic and diatomic gases, up to 2500 to 3000 K and 300 MPa; for some substances, up to higher pressures).

2.2. Equations

The difficulty of constructing the databank was due to the existence of different forms of empirical equations describing the experimental data for the thermophysical properties of substances. We used, in most cases, the equation of state having a polynomial form, which is convenient for fast calculation of various properties,

$$Z = 1 + \sum_{i=1}^{m} \sum_{j=0}^{s_i} b_{i,j} \frac{\omega^i}{\tau^j} \tag{1}$$

where $Z = pv/RT$ is the compressibility factor, $\omega = \rho/\rho_{\mathrm{cr}}$ is the reduced density, and $\tau = T/T_{\mathrm{cr}}$ is the reduced temperature.

The equations of state for gases valid in the high-temperature region have the same form as Eq. (1), but in these equations theoretically grounded virial coefficients are used. This circumstance ensures the extrapolation by means of these equations in the region where experimental data are absent.

For some well-investigated substances, so-called fundamental equations of state are also used. These equations have the form

$$\Phi = \frac{A}{RT} = \alpha_0(\omega, \tau) + \alpha(\omega, \tau) \tag{2}$$

where A/RT is the dimensionless Helmholtz energy, $\alpha_0(\omega, \tau)$ is the ideal-gas part of Φ, and $\alpha(\omega, \tau)$ is the real part of Φ.

The function $\alpha(\omega, \tau)$ may be represented in the form

$$\alpha(\omega, \tau) = \sum_{i=1}^{m} \sum_{j=0}^{S_i} b_{i,j} \frac{\omega^i}{\tau^j} + \exp(-\gamma\omega^2) \sum_{i=1}^{n} \sum_{j=1}^{r_i} c_{i,j} \frac{\omega^i}{\tau^j} \tag{3}$$

or in a more complicated form containing different powers of ω in the exponential terms. The advantage of Eq. (2) is the possibility for calculating all thermodynamic properties only by differentiation of the function $\Phi(\omega, \tau)$.

The equations describing the data for viscosity and thermal conductivity and data on ideal-gas functions and on the saturated vapor pressure and melting pressure have different forms for various substances. This circumstance was taken into account in the development of the programs for the databank. Finally, the databank was constructed with the use of equations of state of the form of Eq. (1) or (2), in the vast majority of cases, and various forms of equations, describing the transport properties, ideal-gas functions, and data on the saturation line. The literature sources from which the equations were taken are given in Table I. In this table, the intervals of temperature and maximum values of density and pressure for each equation are also indicated.

2.3. Calculation of Properties

In the development of algorithms and programs for the calculation of thermophysical properties, we took into account the specific demands which are connected with designing power and refrigerating plants. In the design of such plants, the properties are calculated repeatedly at different combinations of independent variables. Therefore, the main demand for the thermophysical property databank is reliability and internal agreement of calculated values of properties on all points of the thermodynamic surface

Table I. List of Substances, Sources of Equations, and Intervals of Parameters

Substance	Source of equations: For thermod. properties	Source of equations: For transport properties	Temperature range (K)	Max. density ($kg \cdot m^{-3}$)	Max. pressure (MPa)
Argon	[1]	[2]	84–1300	1500	100
	[3]		84–1200	1830	1000
	[4]		84–700	1830	1000
	[5]	[5]	373–3000	400	300
Helium	[6]		2–1500	300	100
		[7]	2–1000	300	100
Krypton	[8]	[2]	120–1300	2570	100
	[5]	[5]	273–3000	600	220
Neon	[2]	[2]	25–1300	1400	100
	[5]	[5]	200–3000	300	400
Xenon	[2]	[2]	161–1300	3100	100
	[5]	[5]	323–3000	600	120
Carbon monoxide	[5]	[5]	323–2250	600	220
Fluorine	[5]	[5]	300–1000	550	160

Table I. *(Continued)*

Substance	Source of equations: For thermod. properties	Source of equations: For transport properties	Temperature range (K)	Max. density ($kg \cdot m^{-3}$)	Max. pressure (MPa)
Hydrogen	[5]	[5]	273–2500	300	350
Nitrogen	[9]		65–1500	920	100
	[10]		63–1000	1600	2200
		[11]	65–1000	920	200
	[5]	[5]	273–2500	330	300
Nitrogen oxide	[5]	[5]	273–2000	400	280
Oxygen	[12]		55–1500	1350	100
	[13]		55–300	1340	80
		[14]	70–500	1340	100
	[5]	[5]	500–2500	300	280
Air	[15]		70–1500	1020	100
	[16]		60–2000	1650	2000
		[17]	150–1000	850	100
	[5]	[5]	323–2500	320	300
Ammonia	[18]		195–750	750	50
	[19]		195–700	850	1000
Carbon dioxide	[20]	[20]	220–1300	1300	200
	[21]		216–1100	1450	800
	[5]	[5]	573–2500	300	180
Water and steam	[22]		273–1073	1220	1000
	[23]		252–1273	2150	25000
n-Butane	[24]		135–700	750	100
Ethane	[25]		91–700	660	80
	[26]	[26]	90–600	660	70
Ethylene	[27]		110–600	700	300
	[28]		105–450	680	260
Methane	[29]		91–1000	480	100
	[30]		91–625	580	1000
		[31]	91–1000	480	100
Propane	[32]		100–700	720	100
R11	[33]		223–470	180	3
R12	[33]		173–453	960	18
R13	[33]		173–383	1070	10
R21	[34]	[34]	303–473	1400	20
R22	[34]	[34]	233–473	1340	20
R23	[34]	[34]	233–473	1340	20
R32	[35]		140–500	1420	70
R125	[35]		180–500	1680	70
R142	[33]		243–433	250	4
R502	[33]		173–423	1020	15

by different combinations of independent parameters. This demand was ensured by use of reliable equations of state and equations for calculating transport properties for each substance.

A great significance was placed on the speed of calculations and a minimum amount of used memory. The quick calculation of thermophysical properties is performed by the development of optimum algorithms as a whole and of separate procedures most often used in the calculations (e.g., the determination of reduced density for given values of temperature and pressure). For economy of memory, the modular principle of programming was taken with unified use of modules.

For calculating the working processes of chemical, power, and refrigerating plants, the values of thermophysical properties at different independent variables are necessary. Therefore, in the creation of the databank, great attention was paid to the compiling of programs for calculating the thermophysical properties using various combinations of independent variables, but not only as a function of temperature and pressure. Properties can also be calculated for the following nine combinations of independent variables: T, ρ; T, p; T, s; T, x; p, ρ; p, h; p, s; p, x; and h, s.

The problem of calculating thermophysical properties for different independent variables arises because, in the equations of state, the density and temperature have a degree more than three. Therefore, it is necessary to use iterative methods for determining the values of these parameters.

For calculating the properties for coordinates T, p and T, s, it is necessary first to determine the second independent parameter used in the equation of state (and in equations for transport properties), the density. To determine the density for coordinates T, p, Newton's method is used. This is very efficient in the entire field of state parameters except in the vicinity of the critical point. The necessary initial values of density are determined from the unified relations depending on the phase where the given point is located (gas or liquid). If the Newton method does not converge, the method of bisection is automatically used. The density for coordinates T, s is determined on the given isotherm by way of iteration. This ensures the agreement of the given value of s with the value calculated from the equation of state.

For calculating properties for coordinates T, x or p, x, the properties on the saturation line are first calculated. The necessary values of pressure (or temperature) and densities of the saturated vapor and liquid are calculated by means of the unified equation of state on the basis of Maxwell's rule.

For calculating the properties for coordinates p, ρ, it is first necessary to determine the temperature, and for coordinates p, h and p, s, both the independent variables of the equation of state, temperature and density, must be determined. Therefore, in the first case, a single iterative cycle is employed, and in the second case, a double iterative cycle. The temperature for coordinates p, ρ is determined by iteration on the given isochore by the method of bisection, for coordinates p, h and p, s, by the method of direct iteration on the isobar on the basis of known thermodynamic relations. The values of the density necessary for calculation of caloric properties (h or s) are determined for a given pressure, and the iterative temperature by means of the above-mentioned procedure of determining the density for coordinates T, p. The iterative calculations for determining T and ρ are repeated until admissible errors of density, enthalpy, and entropy are reached.

The coordinates h, s are the most complicated for defining the position of the calculated point on the thermodynamic surface. This happens because neither of the three thermal parameters connected with the equation of state is given in this case. Therefore, the algorithm for calculation of thermophysical properties in coordinates h, s is based on a relative comparison of given and calculated values of enthalpy on the given isentrope. According to this algorithm, the point of intersection of the isentrope with the saturation line is defined first. Then iterative calculations are made in the single-phase or two-phase region, depending on the given value of enthalpy.

The system of programs developed on the basis of the mentioned algorithms showed its efficiency. Calculations carried out for many substances that are used as working media in power and refrigerating plants showed not only coincidence of the calculated properties at different combinations of independent variables, but also their high internal agreement in the entire single-phase region, metastable states, and two-phase region. To ensure such agreement of properties, the following values of admissible errors were applied: density, 0.001%; enthalpy, $0.05\ \mathrm{kJ \cdot kmol^{-1}}$; and entropy, $0.005\ \mathrm{kJ \cdot kmol^{-1} \cdot K^{-1}}$. The time of calculations for a single set of properties depends upon the system of parameters and increases by 2 to 4 times for coordinates p, h and p, s and by 10 to 20 times for coordinates h, s in comparison with coordinates T, p. It should be noted that calculations of properties can also be made on the given isoline at a chosen increment of the second independent parameter and a chosen number of steps.

The software of the databank, having a modular structure, permits an increase in the number of substances, calculated properties, and independent variables. We are currently working on inclusion in our databank of the published experimental data on thermodynamic and transport properties of the above-mentioned substances and on equations for the calculation of thermophysical properties for new substances.

3. CONCLUSIONS

The described databank is effectively used for calculating processes in chemical, power, and refrigerating plants. Its possibilities are larger than those involved in the usual printed reference books. First, the high speed of receiving the information on properties of substances in different coordinates should be noted. The part of the system of programs can be used separately for constructing programs for specific aims, e.g., for calculation of the heat-exchange apparatus of air-separating installations. Therefore, with the help of this databank, the working place of a designer or a technologist can be rearranged.

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