DOI 10.34185/1562-9945-2-145-2023-01
UDK 533.6.013.14 : 629.1.025.3

O.L. Tokareva, O.D. Ihnatiev, O.V. Priadko

APPROXIMATION OF THE THERMOPHYSICAL PROPERTIES OF HIGH-TEMPERATURE GAS

Annotation. For the numerical study of high-temperature gas-dynamic processes, approximating dependences of the thermophysical properties of air on temperature are proposed. The approximation error averaged over the temperature series does not exceed 0.87%.
Air at high temperatures in terms of molecular transport properties is quite close to other loose multicomponent partially dissociated and ionized gas mixtures, such as products of rocket fuel combustion in a rocket engine nozzle.
The advantage of the approach to the development of approximating dependences of the physical properties of high-temperature gases is the possibility of their use in multifunctional software packages for numerical simulation and engineering analysis.
The approximating dependences of thermo physical properties were used to study by means of the ANSYS software package the processes occurring in the nozzles of rocket engines. The physical characteristics of the air, calculated according to the proposed dependences, ensured that the polytropic index corresponded to the data on the combustion products of a real rocket engine. A mechanism is proposed for matching data from different sources due to the deterioration of the approximation in the vicinity of the boundary. The use of the technique for well-consistent data is acceptable and does not lead to a noticeable decrease in the approximation quality near the boundary. An approach is proposed for approximating multiparameter dependencies.
Keywords: high-temperature gas-dynamic processes, thermophysical properties, approximation, multi-parameter approximation, data matching.

Introduction. The solution of practical problems arising in the study of high-temperature gas-dynamic processes occurring in multicomponent media involves the use of a large data array characterizing the thermophysical properties of gases in the operating range of temperatures and pressures. Modern algorithms for solving gas dynamics problems have high accuracy and the initial data on the physical properties of gases should not yield to the general requirements for the solving accuracy of the gas dynamics and heat transfer equations themselves.

© Tokareva O.L., Ihnatiev O.D., Priadko O.V., 2023

The thermophysical properties of substances are most often presented in the form of tabular dependencies on one (temperature or pressure) or two (temperature and pressure) parameters. The main tasks are to select analytical dependencies that can describe tabular data with satisfactory accuracy and to determine the parameters of these approximating dependencies. This approach helps to compress and to smooth (where necessary) the data. It also allows you to apply analytic differentiation.

The possibility of analytical setting of the physical properties of working bodies is integrated into the advanced multifunctional programs for numerical simulation and engineering analysis. Figure 1 shows the user interface window of the ANSYS program, demonstrating that, when using the program for numerical calculations, the properties of working bodies (the thermal conductivity of an ideal gas in Fig. 1) can be set by a constant value, piecewise linear, piecewise polynomial or polynomial law.

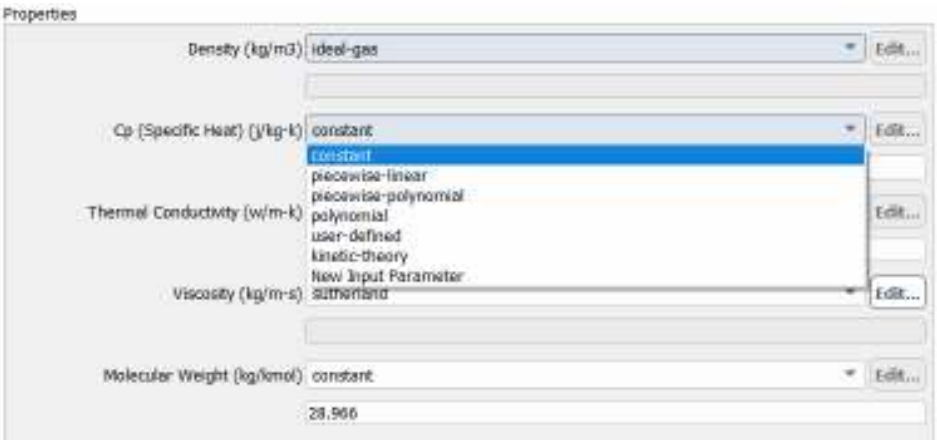

Figure 1 - Methods for setting thermal conductivity in the ANSYS software package

The optimal law for setting the values of the thermophysical properties of the working fluid allows you to speed up the calculation process and improve the results.

The purpose of this work is to develop a mechanism for constructing approximating formulas for complex temperature dependences, such as the thermophysical properties of multicomponent partially dissociated gas mixtures. To study high-temperature gas-dynamic processes using the ANSYS software package it's necessary to construct approximating temperature dependences for the thermophysical properties of air.

Despite the important role of air as an atmosphere and technical gas, there are quite a few direct definitions of the thermodynamic properties of air. Such charts and tables [1-9], which have been published, are limited to a range of temperature or

ISSN 1562-9945 (Print)
ISSN 2707-7977 (Online)

pressure, or both. Although there are convenient tables for air as an ideal gas [1,8], there are no published tables that contain a complete consistent value set for the thermodynamic properties of air, considered as a real gas, in the range of temperatures and pressures required in modern research and development.

Air at high temperatures in terms of molecular transport properties is quite close to other loose multicomponent partially dissociated and ionized mixtures of gases, such as, for example, combustion products of rocket fuel.

In the region below 1500°K, the air composition is assumed to be fixed, and corrections for gas defects are significant. Here, experimental state data and other relevant data are required for an adequate representation. At temperatures above 1500°K in this pressure range, the corrections for gas imperfections are small, and the dissociation degree of the air components has a predominant effect on the thermodynamic properties. In this area, the air properties are based on the contribution of each of the molecular and atomic varieties presenting in the equilibrium composition at each temperature and pressure [5, 6, 10].

Main research**.**

The thermophysical properties of air were approximated for numerical calculations by the ANSYS software package for the controlled supersonic gas flow in a rocket engine nozzle and for numerical experiments on the methods of perturbing the nozzle gas flow. Computational studies were carried out taking into account changes in the main thermophysical parameters depending on temperature and taking into account dissociation processes. The average calculated temperature was 3458°K, pressure 1 bar. The physical characteristics of the working gas ensured that the polytropic index corresponded to the data on the combustion products of a real rocket engine. The calculation results are verified by experimental data.

As a result of the analysis and generalization of the data [1 - 10] for the specific heat Cp (J/kg/K), thermal conductivity λ (W/m/deg) and viscosity μ (Pa·s), three analytical formulas depending on the temperature range were obtained.

The specific heat capacity is approximated with a reasonable degree of accuracy by the following polynomials:

– in the temperature range from 100°K to 1000 K

$$c_p = -1{,}5736 \cdot 10^{-17}T^7 + 6{,}5402 \cdot 10^{-14}T^6 - 1{,}1111 \cdot 10^{-10}T^5 + 9{,}9286 \cdot 10^{-8}T^4 - 5{,}035 \cdot 10^{-5}T^3 + 0{,}0149T^2 - 2{,}3688T + 1161{,}482;$$

– in the temperature range from 1000°K to 3000°K

$$c_p = 1{,}1123 \cdot 10^{-19}T^7 - 1{,}5655 \cdot 10^{-15}T^6 + 9{,}2375 \cdot 10^{-12}T^5 - 2{,}9367 \cdot$$

$$\cdot 10^{-8}T^4 + 5{,}4216 \cdot 10^{-5}T^3 - 0{,}058013T^2 + 33{,}70605T - 7069{,}814;$$

– in the temperature range from 3000°K to 3600°K

$$c_p = -3{,}0 \cdot 10^{-9}T^4 - 5{,}0 \cdot 10^{-5}T^3 - 0{,}2523T^2 - 579{,}39T + 491209.$$

The integration of the analytical specification of thermophysical properties into the ANSYS program is shown in Fig. 2, demonstrated the user interface window, in which the coefficients of the approximating formula for the heat capacity and the limits of its application are set

Figure 2 - Setting the approximating formula for thermal conductivity in the ANSYS software package

For the thermal conductivity of gaseous air at a pressure of 1 bar, according to the tables [2], the following polynomial dependences are defined for various temperatures.

– in the temperature range from 200°K to 1900°K

$$\lambda = -3{,}5 \cdot 10^{-15}T^4 + 2{,}0 \cdot 10^{-11}T^3 - 4{,}35 \cdot 10^{-8}T^2 + 9{,}0 \cdot 10^{-5}T + 0{,}0012;$$

– in the temperature range from 1900°K to 3000°K

$$\lambda = 8{,}625 \cdot 10^{-11}T^3 - 4{,}94 \cdot 10^{-7}T^2 + 0{,}0001T - 0{,}59;$$

– in the temperature range from 3000°K to 3600°K

$$\lambda = 5{,}035 \cdot 10^{-10}\mathrm{T}^3 + 4{,}689 \cdot 10^{-6}\mathrm{T}^2 - 0{,}0142\mathrm{T} + 14{,}3026.$$

The viscosity is approximated by the following polynomials:

– in the temperature range T= 200 K÷1000.00 K

$$\mu = 1{,}361 \cdot 10^{-14}T^3 - 4{,}199 \cdot 10^{-11}T^2 + 7{,}0 \cdot 10^{-8}T + 8{,}17 \cdot 10^{-7};$$

– in the temperature range T=1000 K÷2000 K

$$\mu = -8{,}0 \cdot 10^{-15}T^3 + 3{,}713 \cdot 10^{-11}T^2 - 2{,}9 \cdot 10^{-8}T + 4{,}235 \cdot 10^{-5};$$

– in the temperature range T=2000 K÷3600 K

ISSN 1562-9945 (Print)
ISSN 2707-7977 (Online)

$$\mu = 5{,}98 \cdot 10^{-16} T^3 - 2{,}95 \cdot 10^{-12} T^2 + 3{,}0 \cdot 10^{-8} T + 1{,}6 \cdot 10^{-5}.$$

Multi-parameter dependences of the substance properties are mainly presented in the form of tables for one of the parameters (let's call this parameter primary; as a rule, this is temperature) with a number of fixed rest values, secondary (for example, pressure). Approximation of such dependencies involves the initial stage of processing, which consists in choosing the smallest possible number of dependency types on the primary parameter that well approximates the data in all tables for a given property. Next, coefficients of approximating dependencies for each table are found. Usually, the number of these coefficients, as well as the number of tabular values of the secondary parameter, is small, and to calculate the desired property, the procedure that combines functional approximation with respect to the primary parameter with interpolation with respect to the secondary can be the most convenient.

A more consistent approach is to study and then functionally approximate the dependence of each of the coefficients on the secondary parameters. At the same time, since functions of a more general form are used than is necessary for each of the tables separately, interdependence of some coefficients is often found, which is clearly visible when one of them is varied in the vicinity of the optimal value. Such interdependence can manifest itself only in a certain subrange of changes in the secondary parameter and, in principle, is convenient for describing the dependences of the coefficients on the secondary parameter, and since at smoothing the data in the mentioned subrange, suboptimal solutions are obtained that are not much worse than the optimal one. According to this fact, the approximation of the coefficients should be carried out sequentially, refining the values of the remained ones.

In cases of inconsistency of data from different sources, an artificial matching of separately constructed dependences is performed due to the deterioration of the approximation in the vicinity of the boundary. Note that the use of this technique for well-consistent data is also quite acceptable and does not lead to a noticeable decrease in the approximation quality near the boundary.

Let us illustrate the method of data matching by the example of a parameter described by the function f(T, p) of two variables referred to the critical values of temperature T and pressure p. Let suppose the dependence $T_S(p)$ of temperature on pressure is known, for example, on the saturation line and the dependence of the parameter on saturated vapor pressure $f_S(p)$ (here and below, relative temperature and pressure are meant). For a smooth transition from data on the boundary to data inside the region of the function definition scopes f(T,p), one can use for $p < 1$ an auxiliary function of the general form:

$$f^*(T,p) = f(T,p) + [f_s - f(T_s,p)]\varphi(T - T_s),$$

where the values of f_S and T_S are determined at pressure p, and the weight function $\varphi(x)$, такая что $\varphi(0) = 1$, and rapidly tends to zero as x increases. As a function of φ the following dependence can be proposed:

$$\varphi(x) = \begin{cases} (1 - \frac{x}{T^* - T_s})^m, & T < T^*; \\ 0, & T \geq T^* \end{cases}, \quad \varphi(x) = exp\left(-\frac{kx}{T^* - T_s}\right), T^* > T_s.$$

The values of the parameters T*, m, k are selected empirically.

A more reliable method, albeit giving less smooth data matching, is a linear interpolation between the data at the boundary and at some point inside the region of the described property:

$$f^*(T,p) = \begin{cases} f_S + [f(kT_S,p) - f_S]\dfrac{T - T_S}{(k-1)T_S}, & T < kT_S; \\ f(T,p), & T \geq kT_S. \end{cases}$$

The coefficient k > 1 is chosen from the condition of the best approximation of the transition region and it can be a function of pressure or T_S.

Below there are graphical dependences of the gas constant of N_2O_4 vapors on pressure and temperature, constructed from tabular data, as well as the corresponding analytical dependences obtained using the developed tool.

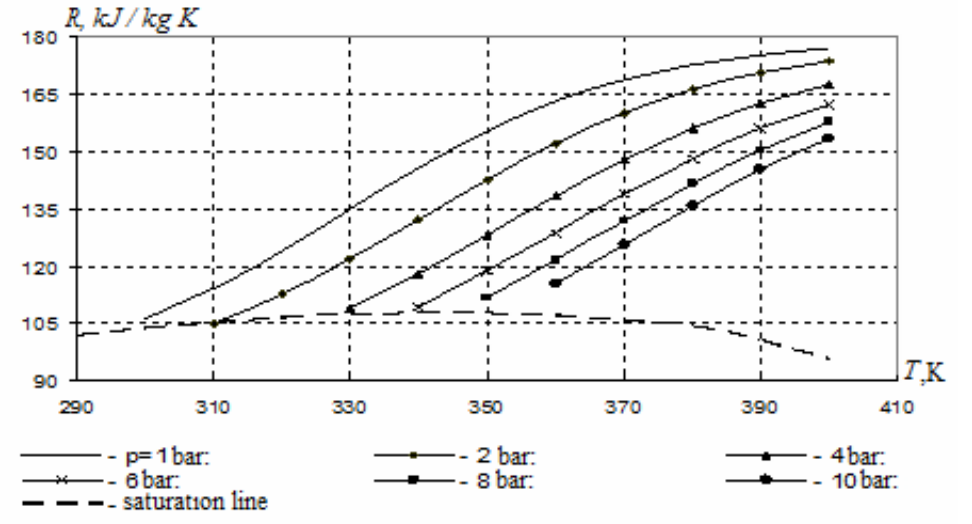

Figure 3 - Graphs of N_2O_4 gas constant versus pressure and temperature

The approximating function has the form
at $\bar{T} > 0$

$$R = R_s + R_1(\bar{T}) + R_2(\bar{T}),$$

ISSN 1562-9945 (Print)
ISSN 2707-7977 (Online)

where $R_2(\bar{T}) = R_s' T_{кр}(e^{-f_1\bar{T}/0{,}120721} - e^{-10\bar{T}})/10$,

$f_1 = (\bar{T}/0{,}120721)^{f_2-1}$; $f_2 = 3{,}50982 - 2{,}7909 T_s/T_{кр}$;

R_s and R_s' – the values of the gas constant and its derivative on the saturation line, respectively;

$\bar{T} = (T - T_s)/T_{кр}$.

For $\bar{T} < 0$ or $\bar{T} = 0$ we accepted $R = R_s$.

Conclusions. To study the high-temperature gas-dynamic processes occurring in the nozzles of rocket engines using the ANSYS software package, approximating temperature dependences for the thermophysical properties of air have been developed. The approximation error averaged over the temperature series does not exceed 0.87%.

The approach for approximating multiparameter dependencies is proposed.

A mechanism is proposed for matching data from different sources due to the deterioration of the approximation in the vicinity of the boundary. The use of this technique for well-consistent data is also quite acceptable and does not lead to a noticeable decrease in the approximation quality near the boundary.

REFERENCES

1. Wasserman A.A. Thermophysical properties of air and its components / A.A. Wasser-man, Ya. Z. Kazavchinsky, V. A. Rabinovich. - M .: Academy of Sciences of the USSR. Publishing house "Nauka", 1966. - 375 p.

2. Vargaftik N. B. Handbook of thermophysical properties of gases and liquids / N. B. Vargaftik. - M .: Publishing house "Nauka", 1972. - 720 p.

3. Aerodynamics in questions and tasks: textbook. manual for technical colleges / N. F. Krasnov, V. N. Koshevoy, A. N. Danilov and others; ed. N. F. Krasnova. - M .: Higher. school, 1985. - 759 p.

4. Thermophysical properties of technically important gases at high temperatures and pressures: reference book / V. N. Zubarev, A. D. Kozlov, V. M. Kuznetsov et al. - M.: Energoatom-izdat, 1989. - 232 p.

5. Sokolova I. A. Properties of molecular transfer of dissociated and ionized gas mixtures / I. A. Sokolova, G. A. Tirsky. - Moscow, 1973. - 183 p.

6. NACA. Review of the properties of thermodynamic, transport and chemical reactions of high-temperature air [Electronic resource]. – Access mode: https://www.comcol.ru.

7. D'Angola A. Thermodynamic and transport properties in equilibrium air plasmas in a wide pressure and temperature range / A. D'Angola, G. Colonna, C. Gorse, and M. Capitelli // Eur. Phys. J. – D 46.– 2008 .– P. 129 – 150.

DOI: 10.1140/epjd/e2007-00305-4.
8. Table_A_9_CC_Properties_of_Air.pdf [Електронний ресурс] . – Режим доступу: https://www.me.psu.edu/cimbala/me433/Links/Table_A_9_CC_Properties_of_Air.pdf.
9. Tables of Thermodynamic and Transport Properties of Air, Argon, Carbon Dioxide, Carbon Monoxide Hydrogen, Nitrogen, Oxygen, and Steam / By Joseph Hilsenrath, Charles W. Beckett, William S. Benedict, Lilia Fano, Harold J. Hoge Joseph F. Masi, Ralph L. Nuttall, Yeram S. Touloukian, Harold W. Woolley // National Bureau of Standards. – Circular 564 . – Issued November 1. – 1955
10. Hirschfelder J. Molecular theory of gases and liquids / J.Hirschfelder, C.Curtis, R. Byrd. - M., 1961. - 120 p.
11. Efficiency of rocket engine thrust vector control by solid obstacle on the nozzle wall / Genadii Strelnikov, Oleksandr Ihnatiev, Nataliya Pryadko, Katerina Ternova // Proc IMechE Part G: J Aerospace Engineering. – 2022. –Vol. 0(0). – P.1–10. IMechE 2022 DOI: 10.1177/09544100221083714.

Received 01.03.2023.
Accepted 03.03.2023.

Апроксимація теплофізичних властивостей високотемпературного газу

Для чисельного дослідження високотемпературних газодинамічних процесів запропоновано апроксимуючі залежності теплофізичних властивостей повітря від температури. Середня по температурному ряду похибка апроксимації не перевищує 0,87%. Перевагою даного підходу є їх використання у багатофункціональних програмних пакетах чисельного моделювання та інженерного аналізу. Апроксимуючі залежності теплофізичних властивостей використовувалися для дослідження засобами програмного пакету ANSYS процесів, що протікають у сопла ракетних двигунів. Запропоновано підхід для апроксимації багатопараметричних залежностей.

Токарева Олена Леонідівна – молодший науковий співробітник Інституту технічної механіки НАН України і ДКА України.
Ігнатьєв Олександр Дмитрович – старший науковий співробітник Інституту технічної механіки НАН України і ДКА України, к.т.н.
Прядко Олександр Валерійович – інженер 1 категорії Інституту технічної механіки НАН України і ДКА України

Tokareva Olena Leonidivna – junior researcher of Institute of Technical Mechanics NAS of Ukraine and SSA of Ukraine;
Ihnatiev Oleksandr Dmitrievich – senior researcher of Institute of Technical Mechanics NAS of Ukraine and SSA of Ukraine;
Priadko Oleksandr Valerievich – engineer of 1 category of Institute of Technical Mechanics NAS of Ukraine and SSA of Ukraine

ISSN 1562-9945 (Print)
ISSN 2707-7977 (Online)