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Information Systems and Technology of Using Substance Properties in Calculations

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Abstract

The article deals with the best known domestic and foreign computer-aided information systems that store data on the thermodynamic properties of substances and technology of using substance properties in calculations. It is shown that at the present level of computer technology development one of the most promising approaches to mathematical modeling of thermodynamic processes is to discontinue using the equations of state which are used in traditional models and replace them with the values obtained by interpolation of the experimental data for the individual substances of which the working fluid consists. This is especially true for the majority of processes with phase transitions at high operating pressures and temperatures for which there are no effective approaches to their modeling.

Keywords

Automated information systems; gases; liquids; phase equilibrium; thermodynamic properties;

Introduction

An approach to mathematical modeling of interrelated thermodynamic and hydrodynamic processes in real gases was proposed in [1]. A distinctive feature of the proposed approach is to discontinue using the equations of state which are used in traditional models and replace them with the values obtained by interpolation of the experimental data for the individual substances of which the working fluid consists. Thus, when modeling, only the basic laws of thermodynamics, the law of conservation of energy and experimental data are suggested to be used. The validity of such an approach is justified in this paper.

Computer-Aided Information Systems on Thermo-Physical Properties of Materials

Currently, various research, educational as well as commercial organizations have accumulated a great amount of information on the properties of substances, which are usually presented in a variety of reference books: in traditional paper media, such as a reference book by N.B. Vargaftik, which has been republished several times [2–4]; electronic databases on thermophysical properties of substances (databases surveys are given in [5–8]) and a variety of automated data-processing systems. The latter are the most attractive for a number of reasons: firstly, you do not need to look for them, because an access to them is open via the Internet; secondly, they tend to be certified; thirdly, they have an advanced service to search necessary data on the properties of substances and its processing. Table 1 provides a list of the most famous automated information-processing systems on thermophysical substance properties.

Let us consider the capabilities of these systems in more detail.

REFPROP program [7], http://www.nist.gov/srd/nist23.cfm, provides the calculation of thermophysical properties of technologically important materials, contains data on the constants of equations of state. It was developed by the National Institute of Standards and Technology (USA), which, along with the study

Table 1

Automated information-processing systems on thermo-physical properties of substances

System name	Developer	System description
REFPROP [5, 9]	NIST (Boulder, USA)	120 substances и 145 mixtures
Library GERG-2008 [10, 11]	Institute EMU, Ruhr University Bochum, Germany	For calculating mixtures of 21 natural gas components under pressures (up to70 MPa) and temperatures (from 60 to 700 K)
STARS [12]	LLC STE "Truboprovod" (Moscow)	1600 individual substances, oil fractions and mixtures
Information triptych of thermophysical substance properties [13]	Joint Institute for High Temperatures (**JIHT**), RAS; Moscow Power Engineering Institute (Technical University) (**MPEI** (**TU**))	A number of on-line programs for calculating substance properties in the range of parameters determined by the user
Simulis Thermodynamics [14]	French company "ProSim"	The calculation of a large set of thermodynamic and transport properties of the products by their molar or mass composition
Program WaterSteamPro [15]	MPEI (TU)	More than 300 functions for calculating the properties of water and steam from the formulas proposed by "International Association for the Properties of Water and Steam"
Trieru [14]	LC "Trieru-Soft" NRI MPEI, (Moscow)	One of the largest and most powerful computational servers

of the properties of individual substances, has been collecting from all over the world the previously obtained data, their processing and creating on their basis free or commercial software products – databases on properties of substances

System Version 9.1 released in May 2013 allows calculating thermophysical properties of liquid and gaseous products, as well as vapor-liquid equilibrium for 121 organic products (hydrocarbons, refrigerants, inert and cryogenic gases, etc.), 5 "pseudocomponents" (air and freon R404A, R407C, R410A, R507A), and their mixtures including up to 20 components.

Both thermodynamic properties and their derivatives and transport properties (viscosity, thermal conductivity, dielectric constant, higher and lower combustion heat values) are calculated.

For a number of pure products solid phase boundaries (melting and sublimation lines) are also calculated. The system also makes it possible to represent the thermodynamic processes in diagrams T, s; T, h; p, h.

This program can be directly connected to Mathcad using DLL (Dynamic Link Library) mechanism.

GERG-2008 Library [10, 11] is the author's realization of the thermodynamic library based on the GERG-2008 equation of state proposed by doctor-engineer Professor W. Wagner and his colleagues. This equation of state provides the most accurate (currently) assessment of the thermodynamic properties of natural gases and other mixtures of natural gas components. It can be used to calculate the mixtures of 21 natural gas components (12 alkanes, hydrogen, nitrogen, oxygen, carbon monoxide and dioxide, hydrogen sulfide, water, helium, and argon) in a very wide range of pressures (up to 70 MPa) and temperatures (from 60 to 700 K). At present more than 80 leading companies and universities as well as public research institutions in Germany, France, Norway, the United States and other countries are the users of this equation and software.

Simulis Thermodynamics made by the French company "ProSim" is a powerful modern software system for calculating thermophysical properties and phase equilibria (**TPP** and **PE**) for a wide range of products on up-to-date methodology base [14].

Simulis Thermodynamics is able to calculate a large set of thermodynamic and transport properties of products by their molar or mass composition: density, compressibility, isobaric and isochoric heat capacity, internal energy, enthalpy, entropy, speed of sound, Joule-Thomson coefficient of dynamic and kinematic viscosity, thermal conductivity, surface tension. At the same time the derivative of the calculated property with respect to pressure, temperature or the content of one of the components can be simultaneously defined and calculated.

If it is necessary, you can immediately perform the calculation of phase equilibrium, find phase compositions and determine the value of the desired properties of each of the phases. In addition, the system allows for the calculation of phase

equilibrium of two immiscible liquids, determining the compositions and phase content by temperature and pressure. Phase equilibrium coefficients and their derivatives are also calculated with respect to pressure, temperature or content of one of the components.

Information triptych of thermophysical properties of substances [13] is the information-analytical system for storing and distributing bibliographic and numerical data on the thermophysical properties of substances on www.thermophysics.ru portal.

It is an integrated medium that combines the capabilities of the three previously created products:

– an electronic reference-book on thermophysical properties of substances for heat power engineering [6];

– data-processing system "EPIDIF" (knowledge base), which provides calculation of the transport properties of rarefied gas mixtures;

– a guide to the thermophysical resources in the Internet network.

Also the server provides a series of on-line programs for calculating the properties of substances in the range of parameters defined by the user:

– a program for calculating the thermodynamic properties of water and steam in a saturated state and single-phase region;

– electrical conductivity of water in a single-phase region and at the saturation line;

– static dielectric constant of water and steam in a single-phase region;

– a program for calculating transport properties of water and steam in a single-phase region;

– the thermodynamic properties of substances in a single-phase region and a saturation curve (air, oxygen, nitrogen, carbon dioxide, methane, propane, ethane, ethylene). The program performs the calculation of thermodynamic properties (density, enthalpy, entropy, heat capacity and the speed of sound) for a given temperature and pressure based on "pseudovirial" equation of state;

– thermodynamic properties of steam li, na, k by the method of parent atoms for a given temperature and pressure of equation of state.

STARS System developed by LLC STE "Truboprovod" (Moscow).

STARS System [12] calculates TPP and the phase state of individual substances, oil fractions, mixtures, including the mixtures of hydrocarbons with oil fractions. It calculates the density, compressibility factor, enthalpy, isochoric and isobaric heat capacity, dynamic and kinematic viscosity, thermal conductivity, and a number of other properties of gases and liquids. The program also allows you to find some quantities relating to the problems of phase equilibrium. The database of reference constants contains information about 1600 individual substances and petroleum products.

The program successfully operates both independently (on-line), and in the form of a called library included in the technology programs of STE "Truboprovod" such as HYDROSYSTEM, PREDKLAPAN, POTOK1F [14].

In 2009 – early 2010 the library was supplemented by calculation of the entropy of products and isentropic expansion process (including two-phase mixtures), as well as by the updated calculation of throttling process at constant enthalpy.

WaterSteamPro program [15], http://www.wsp., is one of the most common and convenient programs for properties of working substances of power engineering (water and steam, air and flue gases) [16–18]. After downloading the program from the website and installing it on your computer in heat engineering calculations the relevant functions on properties of working substances become obvious. The software package defines approximately 300 functions for calculating the properties of water and steam. The calculations are performed according to the formulas designed by "The International Association for the Properties of Water and Steam" [19].

The advantage of the program WaterSteamPro is its flexibility in terms of its connecting to other software, such as Microsoft Excel, Mathcad, C++, Delphi and others.

On the basis of this package in the MPEI (TU) there was developed and submitted to the Internet [18] a set of programs to calculate the cycles of steam-turbine, gas-turbine and steam-gas plants, as well as internal-combustion engines taking into account the actual changes in the properties of working fluids in thermodynamic processes. Using this complex makes it possible to analyze the changes in the effectiveness of cycles depending on the operating parameters of the working fluid with the use of rigorous thermodynamics equations without using various simplifications. In particular, the reversible adiabatic processes, when the main work is generated and spent in cycles, are strictly calculated as processes with constant entropy (isentropic), rather than by approximate formulas.

Online Directories

In recent years, the most popular developments have been interactive online directories on heat power and heat engineering. The addresses of the existing directories are: www.vpu.ru/mas [20], http://twt.mpei.ac.ru/pvhb [21], http://twt.mpei.ac.ru/tthb [22], http://twt.mpei.ac.ru/gdhb [23], http://www.thermophysics.ru [24], www.teplota.org.ua [25] and others.

In 2009 the Publishing House of MPEI (http://mpei-publishers.ru) issued a new handbook "Thermophysical properties of working substances

of heat power engineering" http://twt.mpei.ac.ru/rbtpp/rbtpp.pdf [26]. This is a new type of reference book which includes a book and an Internet website. Unlike other existing directories which were created based on the technology: from a paper medium to an electronic one, this directory was created in the reverse order: first, the Internet site was created and only then the book was written.

The handbook provides information on: entropy, enthalpy, values of specific volume, isobaric heat capacity, speed of sound, ion product for water and steam, calculated by [19] for use in industrial calculations. The tables with thermodynamic properties data cover the range of temperature from 0 to 800 °C at pressures up to 100 MPa.

The handbook also presents the Internet sites with open access to information. The website visitors can download Mathcad-documents if necessary, and work with them in Mathcad.

The most important difference between a site and a paper table is that the site gives not only the required quantity (specific isobaric heat capacity of water and steam depending on temperature and pressure), but the quantity with an error, which is also a function of temperature and pressure. One of the errors concerns the water, the other – the superheated steam and the third one is in the close-to-critical region. In addition to error values, it gives the range of possible values of a certain property of water, determined by a certain error. The last updated electronic version of the handbook is presented on http://twt.mpei.ac.ru/rbtpp/index.html page.

Of particular note is the server of the Moscow Power Engineering Institute (www.mpei.ru) in which there was developed the Electronic Encyclopedia of Energy Engineering [26]) containing the Internet pages on which the calculation of thermophysical parameters of more than 3000 substances and mixtures of substances is carried out. The access to these pages is open on http://twt.mpei.ru/TTHB site.

Technologies of Using Substance Properties in Calculations

The above considered online resources of thermophysical parameters of substances use different technologies of data storing, processing and distributing to the user.

Downloading Technology. This technology is based on downloading programs from the Internet sites or from the disks and installing them on the user's computer. However, the technique has one major drawback: the programs for computers, in particular, programs for calculating the thermophysical properties of individual substances and mixtures are being continuously improved. This is due to the fact that, firstly, there appear new formulations prescribing the procedure for calculating the specific properties of specific substances, and, secondly, the existing programs are being constantly corrected of errors and inaccuracies, the scope of their application is expanding and their characteristics are being improved (operating speed, the amount of memory of the computer and others). The users of these programs do not always keep up with these changes and work with older versions.

The present level of development of computer technology provides direct access to them through the use of cloud servers [27]. Therefore, the aforementioned disadvantages can be easily overcome.

Cloud technology. The technology of cloud thermophysical calculations based on references to Internet-functions of the properties of working substances in heat power engineering rather than downloading was proposed in [28, 29]. One of the disadvantages of this approach to heat engineering calculations is the demand for a reliable connection of the computer on which they are carried out to the Internet.

Ideally, the user's work with databases must proceed in the following way. If the user requires the properties of some substance, the substance parameters are sent through a network to some "cloud" server, and the server, in its turn, returns the value of this property for given parameters to the user's computer.

An example of such a server is the calculation server, which was developed jointly by NRU MPEI, JIHT RAS and LLC "Trier" experts (see www.trie.ru) [30]. It has collected a large number of such "cloud" functions, and their number is continuously increasing. The main part of the "cloud" functions, hosted on MEI-JIHT-Trier server is concerned with the properties of working bodies and heat-transfer agents in power engineering.

The functions related to water and steam (the main working fluid in domestic and foreign thermal and nuclear power engineering) are based on the recommendations approved by the International Association for the Properties of Water and Steam [19]. These formulations are based on formulas rather than table data. For example, pressure and water saturation temperature in the range from the triple point to the critical point are associated with implicit quadratic equation.

The process of developing formulations on previously uninvestigated or newly synthesized substances proceeds as follows: first, the so-called skeletal table of substance properties is created by

means of experimental measurements by various physical methods on the experimental stands, and then by these discrete tabular data using various mathematical methods, a function or a set of functions are generated for different areas with the rules of their application and indicating errors for their use, primarily, in computer programs. Quite often only tables without their mathematical processing are still published.

Conclusion

1. At present time, there exists a huge number of databases on the properties of substances. These data are partly published in paper or electronic media in the form of tables, graphs, formulas or computer programs. The most promising of these are calculation servers operating with cloud computation. An example of such a server is the calculation server, which was developed jointly by NRU MPEI, JIHT RAS and LLC "Trier" experts [30] www.trie.ru.

2. Experimental data on the properties of substances are published both directly – without their mathematical processing – and in the form of various functions obtained by mathematical methods for different areas with the rules of their application and indicating errors of their use. For example, the recommendations approved by the International Association for Properties of Water and Steam [19] (www.iapws.org).

3. Mathematical modeling of the majority of thermodynamic processes is based on the use of thermodynamic functions for ideal gases and equations of state for real gases and liquids, which leads to large errors in the calculations, especially |it concerns the processes taking place with the change in phase composition, near phase equilibrium lines and critical points.

4. A large number of attempts have been made to derive a theoretically grounded equation of state, which holds true for a quite wide range of states of real gases (virial equations). However, the coefficients of virial equations can not be calculated by purely theoretical methods, and should therefore be determined by experimental data. This problem is often so complex that it is more rational to use the experimental data directly in the calculations.

5. For most processes with phase transitions under high operating pressure and temperature there are no effective approaches to modeling.

Therefore, the development of methodology [31] of mathematical modeling of thermodynamic processes with phase transitions under high operating pressure and temperature based on the use of tables with experimental data on the properties of real gases and vapors is not only relevant, but can also significantly improve the quality of mathematical modeling of complex thermodynamic processes.

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