Thermodynamic Database for Pure Substances IVTANTHERMO-Online

Igor Morozov [0000-0002-0122-9400]

Joint Institute for High Temperatures of RAS, Izhorskaya 13, bld 2, Moscow 125412, Russia
morozov@ihed.ras.ru

Abstract. Development of the IVTANTHERMO-Online information system is discussed including the corresponding thermodynamic database for pure substances, bibliographic database, user interface and supplementary software. In contrast to numerous thermodynamic databases for engineers, the IVTANTHERMO-Online is meant as a database for researchers, so that scientists from different institutions can contribute to the database extension and regular updates.

Keywords: thermodynamic properties, database, pure substances

1 Introduction

Thermodynamic databases play an essential role in a wide range of applications such as rocket engine engineering, nuclear power, chemical technology, metallurgy, resource usage, waste recycling, etc. The IVTANTHERMO information system [1] based on the reference book [2] has made a significant contribution to the accumulation of thermodynamic data. It has been developed since 1966 in the Institute of High Temperatures of the Academy of Sciences of the USSR. Initially it was focused at thermodynamics of the rocket fuel combustion products but later the area of its applicability was extended substantially. Nowadays the development is continued in the Laboratory for Thermophysical Databases of JIHT RAS.

The thermodynamic databases are being developed in many research centers [3–7]. Some of them are united into international organizations such as SGTE [8]. Typically, the information from these databases is not open and provided for a fee. The most well-known open web resource is the NIST WebBook [3, 9] which provides access to a part of information about thermodynamical properties, thermochemical data, energy spectra of ions, vibrational and rotational spectra of molecules, etc.

In the course of the IVTANTHERMO system development a set of requirements was formulated that any fundamental thermodynamic database or a reference book should fulfill [1]. Fitting to these requirements is used to distinguish between the “critical reference books” or “expert level databases” and the databases compiled from different sources and providing information “as is” without references, clear identification of the calculation procedures and evaluation of its reliability and accuracy. The goal of further IVTANTHERMO development is to keep adherence to the

requirements [1] using at the same time contemporary technologies to make the system more functional, user friendly and accessible by different kinds of researchers.

2 IVTANTHERMO Database Development

2.1 IVTANTHERMO-Online Project

The first version of the IVTANTHERMO ran on the HP3000 hardware system whereas the subsequent versions were implemented for PC as “INVATHERMO for DOS” and “INVATHERMO for Windows” software packages. The later was distributed since the end of 1990s [10]. Nowadays it includes information about more than 3400 substances, formed of 96 chemical elements, as well as supplementary software for analysis of experimental results, data fitting, calculation and estimation of thermodynamical functions and thermochemistry quantities.

Recently a next generation of the IVTANTHERMO database and related software is proposed called “IVTANTHERMO-Online” [11] (Fig. 1). It has the following main features:

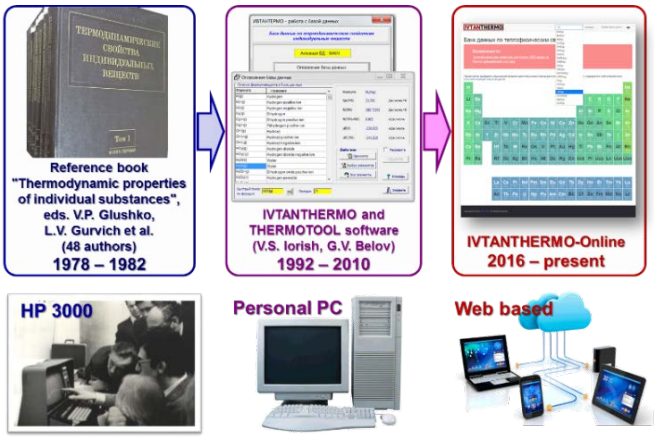

Fig. 1. Development of the IVTANTHERMO information system

- Modern user-friendly web interface with client-server architecture for remote access of users and contributors.
- Regular data updates with a full history of all changes.
- Two-level scheme of new data submission and assessment by an expert committee.
- Storing original tables of data (experimental or simulation results) with the information about data sources, methods of processing and fitting, fundamental constants.
- Detailed bibliography information for all data sources.
- Integration with the existing codes for calculation of the thermodynamical functions.
- Substance search by names, chemical elements, chemical formula, CAS and InChi numbers and substance categories.

- Extensible database design.
- Online calculation services (chemical composition, etc).

2.2 Revision Control System

One of the key features that can make the IVTANTHERMO-Online a collaboration platform is the ability to store multiple revisions of the thermodynamic data in the similar way that it is done in the contemporary version control systems such as Git, Subversion, etc. The data are slit into blocks, each block is an elementary unit for tracking revisions. The block can include, for instance, the thermodynamic properties of a particular substance in a given phase or basic properties of a molecule.

A user that can contribute to the database is called as an “expert”. The experts have additional rights to add or edit the data for a group of substances assigned by the site administrator. After adding or editing, a new block of data is created and marked as unchecked or preliminary (see Fig. 2). Then the expert can continue to edit the data creating, if needed, additional versions of the data block. Finally, the new data are submitted to the expert committee that checks the data and possibly accepts it as a new recommended version that becomes visible at the web site for all users.

As seen from Fig. 3 all the versions that have been recommended earlier are stored in the database and available for users. It allows users to find what has been changed, when the changes have been accepted, who was an expert and what was the reason for the changes (appearance of new experimental data, better approximation, etc).

Moreover, the database is designed to store additional metadata for each data block which may include comments, original experimental data, bibliography, full papers and preprints. Storage of these metadata increases usability and reproducibility of the main data and allows new experts to get full information of previous studies when the data is to be updated.

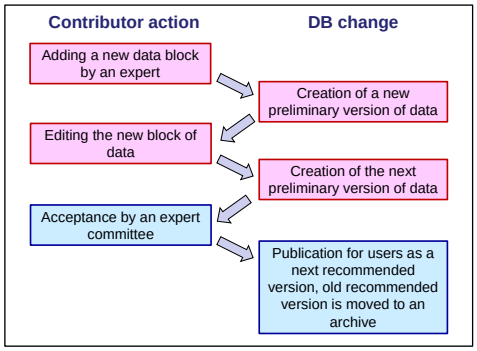

Fig. 2. Life cycle of a data block in the IVTANTHERMO-Online system

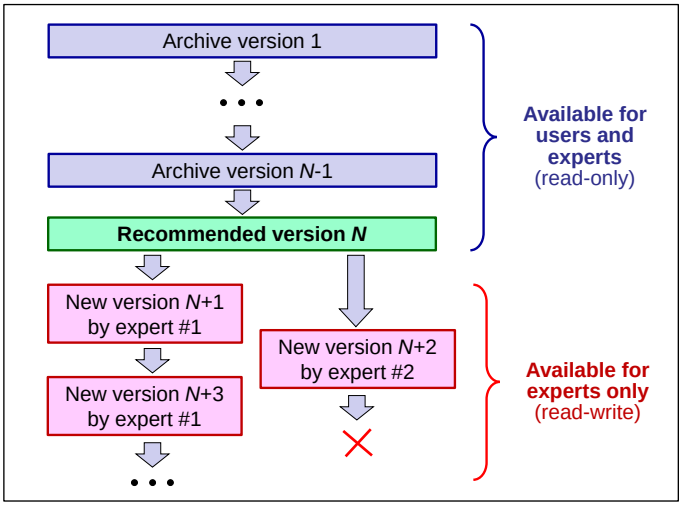

Fig. 3. Storing of multiple revisions of the same data block in the IVTANTHERMO-Online database

2.3 Supplementary Software for Experts

Traditionally the thermodynamic data for substances in the condensed and gaseous states are treated separately. The partition functions of a molecular gas can be obtained from either molecular constants or direct solution of the Schrödinger equation based on the interatomic potential calculated by quantum chemistry or other approaches [12, 13]. On the contrary, ab initio calculations of the thermodynamic properties of solid and liquid substances which provide reasonable accuracy are rather challenging and there are few of them in the literature. Therefore, assessment of the thermodynamic properties of a condensed matter is based typically on the statistical analysis of direct measurements of enthalpy increments and/or heat capacity including estimation of initial data error, robust statistics, examining phase transition areas and approximation of the measured values with appropriate analytical dependencies [14, 15].

Figs. 4 and 5 present the corresponding supplementary software packages that is being developed in JIHT RAS. These packages are to be used by experts for assessment of experimental or ab initio data and updating the database. They include comparison of different experimental measurements, weighted approximation, estimation of errors, etc. It is planed that the IVTANTHERMO-Online system will include the web version of these codes which will allow experts to perform the whole research cycle online storing the intermediate results and all the metadata in the same database and sharing them with each other.

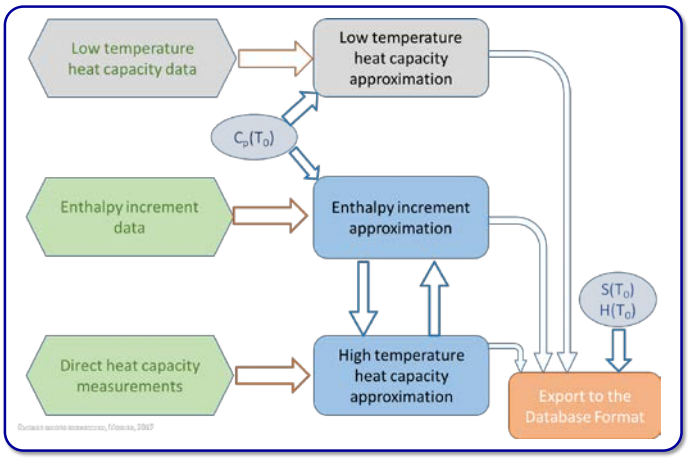

Fig. 4. CondensedThermoFit package [15] for assessment of the thermodynamic properties of substances in the condensed state

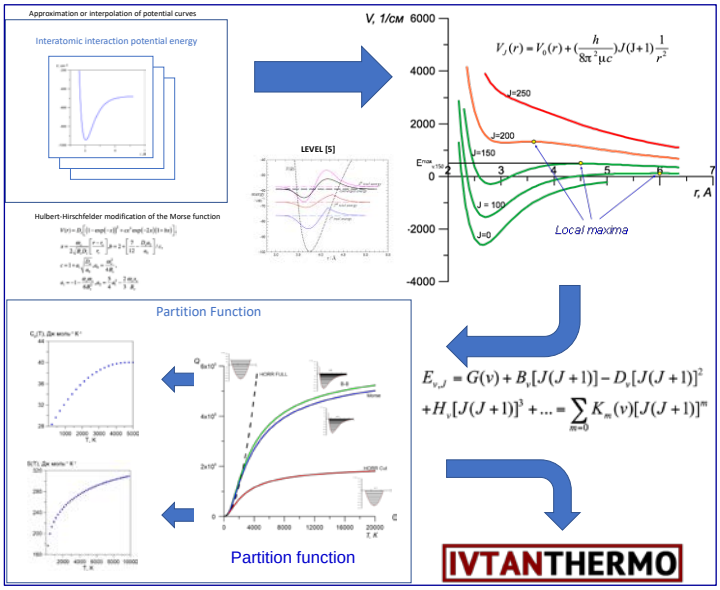

Fig. 5. Calculation of the thermodynamic properties of diatomic molecules in the gaseous state based on the interatomic potential

3 Conclusions

The IVTANTHERMO-Online thermodynamic database is discussed that continues the series of IVTANTHERMO information systems. It meets both the requirements to critical reference books and the standards of modern web-based systems. Opposed to

other thermodynamic databases it keeps track of the old versions of data, contains full information on data sources and methods of data processing. Supplementary thermodynamic data processing software should allow experts to add or update information in the database without using external codes.

References

1. Gurvich, L.V.: Reference books and data banks on the thermodynamic properties of individual substances. Pure Appl. Chem. **61**, 1027–1031 (1989).
2. Gurvich, L.V., Bergman, G.A., Veyts, I.V., et al.: Thermodynamic Properties of Individual Substances. Glushko V.P. (ed). New York, Hemisphere Publishing (1989).
3. Chemistry WebBook Homepage (NIST), http://webbook.nist.gov/chemistry/, last accessed 2019/08/26
4. Facility for the Analysis of Chemical Thermodynamics (FACT) Homepage, http://www.crct.polymtl.ca/fact/, last accessed 2019/08/26
5. Thermodata, France Homepage, http://thermodata.online.fr/, last accessed 2019/08/26
6. Thermo-Calc Software Homepage, http://www.thermocalc.com/, last accessed 2019/08/26.
7. Materials-oriented Little Thermodynamic Database (MALT) Homepage, http:// kagaku.com/malt/, last accessed 2019/08/26
8. Scientific Group Thermodata Europe (SGTE) Homepage, http://www.crct.polymtl.ca/sgte/, last accessed 2019/08/26
9. Linstrom, P.J. and Mallard, W.G.: The NIST Chemistry WebBook: A chemical data resource on the internet. J. Chem. Eng. Data 46, 1059–1063 (2001).
10. Belov, G.V., Iorish, V.S., and Yungman, V.S.: IVTANTHERMO for Windows – database on thermodynamic properties and related software. CALPHAD **23** (2), 173–180 (1999).
11. Belov, G.V., Dyachkov, S.A., Levashov, P.R., Lomonosov, I.V., Minakov, D.V., Morozov, I.V., Sineva, M.A., and Smirnov, V.N.: The IVTANTHERMO-Online database for thermodynamic properties of individual substances with web interface. J. Phys. Conf. Ser. **946**, 012120 (2018).
12. Maltsev, M.A., Kulikov, A.N., and Morozov, I.V.: Thermodynamic properties of vanadium and cobalt argide ions, VAr^+ and $CoAr^+$. J. Phys. Conf. Ser. **774,** 012023 (2016).
13. Maltsev, M.A., Morozov, I.V., and Osina, E.L.: Thermodynamic Properties of Ar_2^+ and Ar_2 Argon Dimers. High Temp. **57** (1), 37–40 (2019).
14. Aristova, N.M., Belov, G.V., Morozov, I.V., and Sineva, M.A.: Thermodynamic properties of condensed uranium dioxide. High Temp. **56** (5), 652–661 (2018).
15. Sineva, M.A., Morozov, I.V., Belov, G.V., Aristova, N.M., and Lavrinenko, Ya.: Simultaneous analysis of the enthalpy increment and heat capacity data measurements for updating the IVTANTHERMO database. J. Phys. Conf. Ser. (2019), in press.