THE ESSENTIAL FEATURES REQUIRED OF POOLED INTERNET THERMODYNAMIC DATABASE

Khodakovsky I.L., Victorov V.N. (University «Dubna»), **Sergeyeva E.I., Devina O.A.** (GEOKHI RAS)
ikhodakovsky@uni-dubna.ru; Phone: 8 (221) 228-03; (495) 137-57-42

Key words: website, thermodynamic database, radionuclides and toxic elements

At present reliability and validity of the best thermodynamic data selection for chemical systems do not correspond to modern experimental and theoretical studies of chemical thermodynamics. This is mainly due both to a wealth of those data and to labor consuming consistency procedure (global and local as well) [1,2]. The use of the modern-day information technologies developed in Internet could considerably improve the efficiency in this work.

The website "Thermodynamics of natural processes"(*www.tnpdata.ru*) being developed since 2004 by the "DiaNIK" team of Ecological-analytical Center of "Dubna"University, could be a prototype of that, which could permit in future to join forces of highly skilled experts on chemical thermodynamics from different organizations on development of a unified thermodynamic database. These experts should be presented with following possibilities:

- To perform convenient and quick search for various thermodynamic information on chemical system of expert interest;
- To have access to constantly updated bibliography information on as greater numbers of experimentally studied chemical systems as possible;
- To compare thermodynamic values recommended by basic thermodynamic reference books for individual substances and aqueous species;
- To become informed on the results of earlier critical evaluation of reliability and consistency of thermodynamic data in the framework of international and national projects;
- To perform independent data compilation, analysis and the best values selection for individual substances, aqueous species, as well as for chemical reactions. The values should be consistent with different types of the chemical systems phase diagrams in a large temperature and pressure range;
- To make the consistency procedure for various thermodynamic information on "local" and "global" levels. In this case a possibility of changing reference substances should be realized: simple substances, aqueous ions, atomic gases and so on [3];
- To calculate the phase and chemical compositions of homogeneous and heterogeneous chemical systems of arbitrary complexity with the purpose of specifying the interpretation of the experimental studies results;
- To reveal the priorities in determination of new experimental data required to make thermodynamic information more accurate and comprehensive;
- To secure their copyright in a straightforward and clear form when developing files of thermodynamic information, as well as of texts, tables and results of the literature data analysis.

It is expedient to use the developed algorithms and formats of the literature data presentation for the systematization of other physical-chemical information (kinetics, structure of the substance, sorption, etc.).

Some of the above-mentioned tasks were solved on the website (*www.tnpdata.ru*) for chemical systems containing radionuclides and toxic elements: Me_pO_q-H_2O and Me–F–Cl–S–C–N–P–H_2O as well (where Me = U, Th, Pu, Np, Am, Sr, Cs, Ce, Zr, Se, As, Pb, Zn, Cd, Hg, Cu, Be).

Compilation of the bibliography sources incorporating the results of experimental study of chemical systems is the first and very laborious step in systematization of physico-chemical information. For the purpose of initiating participation in the project of the maximum possible numbers of experts, the "DIAnik" team will begin since autumn 2006 to transfer the bibliography files (in "doc" format) from the web-publication of "Handbook of Thermodynamic Values" without compensation to users (not transferable).

Information files for inorganic substances (mainly for minerals), thermodynamic properties of which have not been measured will be transferred as well.

Those files could help to determine the priorities in experimental studies of chemical systems.

The main part of basic reference books published within the limits of national and international projects (USA NBS, USSR AS, IAEA, CODATA, IUPAC, etc.) is now difficult of access. On the other hand, the results of analysis of reliability of experimental data and substantiation of the best values selection incorporated in those books are valid for many chemical systems. The files containing such information (with corresponding references) could be transferred to users and experts according to their inquiries.

It is obvious, that the success of the proposed project depends entirely on participation of experts from different groups, post-graduates and students in it. Their work should be regulated by the rules developed by specially established Editorial Council incorporated the experts in different fields of chemical thermodynamics.

In annual update of the web-publication of the "Handbook of Thermodynamic Values" could participate any one of experts interested in specification and increasing of published materials for definite chemical systems.

The materials available to the members of the Editorial Council (reprints, information files, etc.) could be given to them.

This study was supported by Russian Foundation of Basic Research (project N 04-05-64829)

References

1. *Shapkin A.I., Khodakovsky I.L., Garanin A.V., Dorofeeva V.A., Semenov Yu.V.* Dialogue scientific-information complex of solution of the chemical thermodynamics tasks // Feed-back tasks of chemical thermodynamics. 1987. Novosibirsk: Nauka. PP. 80-88. (In Russian).
2. *Khodakovsky I.L., Westrum E.F., Hemingway B.S.* CODATA International Geothermodynamic Tables // Guidelines and set of prototype tables. 1995. 276p. (Beta version is available from Edgar Westrum. Michigan University. Chem. Dep.).
3. *Khodakovsky I.L.* Feedback of algorithms of thermodynamic data consistency and computer simulation of geological systems // Proc. Int. CODATA Conf. Volume Date 1986; 10th Comput. Handl. Dissemination Data. 1987. PP. 270-274.

Electronic Scientific Information Journal "Herald of the Department of Earth Sciences RAS" № 1(24)'2006
ISSN 1819 – 6586
Informational Bulletin of the Annual Seminar of Experimental Mineralogy, Petrology and Geochemistry – 2006
URL: http://www.scgis.ru/russian/cp1251/h_dgggms/1-2006/informbul-1_2006/mineral-9e.pdf

Published on July, 1, 2006