A NEW CODE FOR JOINT APPROXIMATION OF ENTHALPY INCREMENTS AND HEAT CAPACITY DATA

Sineva M.A.,[*1] ***Aristova N.M.,***[1] ***Belov G. V.,***[1,2] ***Morozov I. V.***[1]

[1] *JIHT RAS, Moscow, Russia,* [2] *MSU, Moscow, Russia*

[*] *maria.a.sineva@gmail.com*

Original experimental data on thermodynamic properties of substances in the condensed phase are often presented as tables and need to be approximated with functions that reproduce them with an acceptable accuracy. These functions can be used then for thermodynamic modeling and other theoretical studies. There are various codes for processing thermodynamic data. Some of them are meant for low-temperature heat capacity [1], others for high temperature data measured by, for example, laser flash method. Moreover, there is a significant amount of methods for processing data on enthalpy increment obtained by classic calorimetry. Filling databases (IVTANTHERMO, NASA etc.) with new information on substances requires fitting data with preset polynomials [2].

A new computer program based on a combination of fitting algorithms is proposed for analyzing experimentally obtained enthalpy and heat capacity of substances in the condensed state. The program is supposed to unite all processing steps (low- and high- temperature heat capacity data, enthalpy increment data etc) to combine and analyze available data of several types simultaneously. The program has a friendly user interface. It comes in the forms of a standalone application and web application with limited functionality. The enthalpy increment data can be fitted by a polynomial of a chosen degree which can be used at the next step to process heat capacity dependence on temperature. Provided the user has high temperature heat capacity experimental data, it can be fitted by a polynomial combined of elementary functions picked manually or by preset combinations. The results can be exported in various database formats.

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1. I. Roslyakova, B. Sundman, H. Dette, et al // Calphad 55 (2016) 165
2. G.V. Belov, N.M. Aristova, I.V. Morozov, M.A. Sineva. // J. Math. Chem. 55 (2017) 1683