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ON APPROXIMATING THERMODYNAMIC PROPETIES OF INDIVIDUAL SUBSTANCES

单一物质的热力学性能近似计算

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【ABSTRACT】 A method for complex approximation of the thermodynamic functions, such as enthalpy, entropy and heat capacity, with regard for the fixed points is presented, which has been successfully used in approximating about 1500 tables within temperature range from 100 to 20000K. The results of the thermodynamic calculations of mixture parameters on the basis of TDsoft system which includes the program approximation Package show high reliability of the polynomials in solving iteration problems for computing multicomponent systems.

【摘要】 本文介绍针对固定温度点的热力学函数 (如焓、熵、比热) 综合近似计算法。该方法已成功地用来近似计算温度范围为 100～20000K 的 1500 个热力学函数表。用内含近似计算程序包的 TD 软件系统对混合物参数进行热力计算的结果证明, 该多项式在求解多组元系统计算中迭代问题时具有很高的可靠性。

Key Words: thermodynamic properties, approximation, polynomials

1 Introduction

The thermodynamic properties of the individual substances are utilized as the information basis for simulating and computing thermal processes in various technical devices. Traditionally, these properties are presented in a tabular form. A number of papers (including those with reference data tables) substantiate the necessity of special polynomials and methods of approximation, and the corresponding studies are being curried out. As approximation criteria, accuracy and shortness are mostly considered. However, along with ever more extensive and deepgoing understanding in the field of the thermal power-plant processes, as well as due to intensive ecology investigations and enormous capability of modern computers to provide a proper data base and storage, on the order of the day has been put a pressing task to develop a new complex approach to solution of the optimization problems to evaluate interconnection and interdependence of parameters on the datum level gains actuality. To such kind of this complex approach we can refer the paper [1] in which the investigation adopted NASA polynomials.

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2 A New Complex Approach

We carried out a number of investigations on approximating the thermodynamic properties of the individual substances but with polynomials[2] as follows

$$P_I(x) = a_I + a_1 x + a_2 x^2 + \cdots + a_n x^n \tag{1}$$

$$P_S(x) = a_S + 0.001[a_1 \ln x + 2a_2 x + \cdots + (n/n-1) a_n x^{n-1}] \tag{2}$$

$$P_{C_p}(x) = 0.001(a_1 + 2a_2 x + \cdots + n a_n x^{n-1}) \tag{3}$$

where I —enthalpy, S —entropy, C_p —heat capacity, $x = 0.001T$ and T is temperature.

In the meantime, we take accuracy and shortness as the approximation criteria. As a result of the approximation investigation, we come to the conclusion that the complex approach is the most reliable and precise tool for approximating the thermodynamic properties of the individual substances. It is the complex approach based on using all the function values that makes it possible to smooth a certain inconsistency of the assumed function values and to diminish errors caused by the reference method due to only one function used in the direct approximation. In addition, the approach provides the possibility of introducing fixed point (or points) and enables not only to eliminate any discrepances in function values but also to fix a point (e. g. temperature 298, 15K) as error reference point.

So, the approximation of the enthalpy $I(T)$, entropy $S(T)$ and thermal capacity $C_p(T)$ within the temperature range $T \in [T_0, T_N]$ can be carried out with the aid of polynomials (1) – (3) for the fixed points T_1 where

$$P_I(x_1) = I(x_1), \quad P_S(x_1) = S(T_1), \quad P_{C_p}(x_1) = C_p(T_1), \quad x_1 = 0.001T_1 \tag{4}$$

and for T_2

$$P_I(x_2) = I(T_2), \quad P_S(x_2) = S(T_2), \quad P_{C_p}(x_2) = C_p(T_2), \quad x_2 = 0.001T_2 \tag{5}$$

then the approximation becomes a problem of finding the polynomial coefficients ξ_0^S, ξ_0^I, ξ_1, $\cdots$, ξ_n

$$P_I(x) = \xi_0^I P_0(x) + \xi_1 P_1(x) + \cdots + \xi_n P_n(x) \tag{6}$$

$$P_S(x) = \xi_0^S P_0(x) + 0.001[\xi_1 P_1^S(x) + \cdots + \xi_n P_n^S(x)] \tag{7}$$

$$P_{C_p} = 0.001[\xi_1 P_1^{C_p}(x) + \cdots + \xi_n P_n^{C_p}(x)] \tag{8}$$

where $P_0(x), P_1(x), \cdots, P_n(x)$ are the Chebyshov's polynomials which satisfy the conditions

$$P_0(x) = 1$$

$$P_1(x) = x + \gamma_1^{(1)}$$

$$P_2(x) = x^2 + \gamma_1^{(2)} x + \gamma_2^{(2)}$$

$$P_3(x) = x^3 + \gamma_1^{(3)} x^2 + \gamma_2^{(3)} x + \gamma_3^{(3)}$$

$$\vdots$$

$$P_n(x) = x^n + \gamma_1^{(n)} x^{n-1} + r_2^{(n)} x^{n-2} + \cdots + \gamma_n^{(n)}$$

for

$$\sum_{j=0}^{N} g_j P_K(x_j) P_m(x_j) = \begin{cases} 0, & k \neq m \\ \neq 0, & k = m \end{cases}$$

g_j are the weight fractions of points x_j.

Polynomial $P^{C_p}(x)$ are defined as follows:

$$P^{C_p}(x) = dP(x)/dx$$

Polynomials $P^S(x)$ are represented in the form:

$$P^S(x) = \int P^{C_p}(x)\, d\ln x$$

The connection between equations (1) – (3) and (6) – (8) is given in the form of relations

$$a_I = \xi_0^I + \sum_{i=0}^{n} \xi_i \gamma_i^{(i)} \quad , \quad a_S = \xi_0^S \quad , \quad a_1 = \xi_1 + \sum_{i=2}^{n} \xi_i \gamma_{i-1}^{(i)} \quad , \cdots, \quad a_n = \xi_n$$

As the basis for this method the function minimization is taken

$$F = \sum_{j=0}^{N} g_j \{ [I(x_j) - P_I(x_j)]^2 + [S(x_j) - P_S(x_j)]^2 + [C_p(x_j) - P_{C_p}(x_j)]^2 \}$$

The set of equations of function approximation without fixed point is as follows:

$$\left(\frac{\partial F}{\partial \xi_0^I}\right) = 0 \quad , \quad \left(\frac{\partial F}{\partial \xi_0^S}\right) = 0 \quad , \quad \left(\frac{\partial F}{\partial \xi_1}\right) = 0 \quad , \cdots, \quad \left(\frac{\partial F}{\partial \xi_n}\right) = 0$$

—with fixed point x_1

$$P_I(x_1) = I_{x_1} \quad , \quad P_S(x_1) = S(x_1) \quad , \quad P_{C_p}(x_1) = C_p(x_1)$$

$$\left(\frac{\partial F}{\partial \xi_2}\right) = 0 \quad , \cdots, \quad \left(\frac{\partial F}{\partial \xi_n}\right) = 0$$

—with fixed points x_1 and x_2

$$P_I(x_1) = I_{x_1}(x_1) \quad , \quad P_S(x_1) = S(x_1) \quad , \quad P_{C_p}(x_1) = C_p(x_1)$$

$$P_I(x_2) = I_{x_2}(x_2) \quad , \quad P_S(x_2) = S(x_2) \quad , \quad P_{C_p}(x_2) = C_p(x_2)$$

$$\left(\frac{\partial F}{\partial \xi_5}\right) = 0 \quad , \cdots, \quad \left(\frac{\partial F}{\partial \xi_n}\right) = 0$$

3 Conclnsions

We have also carried out a series of investigations to solve the problem for qualitative and quantitative evaluation of errors.

The method developed was successfully used in approximating about 1500 tables within temperature range from 100 to 20000K. The results of the thermodynamic calculations of mixture parameters on the basis of TDsoft system which includes the program approximation Package show high reliability of the polynomials in solving iteration problems for computing multicomponent systems.

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