ORT
Publishing

6th International Scientific Conference

Science progress in European countries:

new concepts and modern solutions

Hosted by the ORT Publishing and

The Center for Scientific Research "Solution"

Conference papers

April 19, 2019

Stuttgart, Germany

6th International Scientific Conference

"Science progress in European countries: new concepts and modern solutions": Papers of the 6th International Scientific Conference. April 19, 2019, Stuttgart, Germany. 427 p.

Edited by **Ludwig Siebenberg**

Technical **Editor: Peter Meyer**

Published and printed in Germany by ORT Publishing (Germany) in association with the Center For Scientific Research "Solution" (Ukraine) April 19, 2019.

ORT Publishing

Schwieberdinger Str. 59

70435 Stuttgart, Germany

APPLICATION OF LOG-LOGISTIC DISTRIBUTION FOR CALCULATIONS OF THERMODYNAMIC PARAMETERS

P.A.KOZUB,

Candidate of Technical Science, Associate Professor,

Associate Professor of Department of Natural Science

Kharkiv National University of Radio Electronics

Kharkiv, Ukraine

V.L.MIGUNOV

Deputy Director

Art School of Kharkiv City Council

Харків, Україна

S.N.KOZUB,

Candidate of Technical Science,

Associate Professor of Department of Medical and Bioorganic Chemistry

Kharkiv National Medical University

Kharkiv, Ukraine

As was shown earlier [1], the dependence of the heat capacity of solids is very well described by the probability distribution function (CDF) of the lognormal distribution. Depending on the value of only two parameters, this function can approximate both the heat capacity of crystalline bodies and polymeric materials, with one of the parameters having a unique connection with the Debye temperature, and the other is closely related to the structure of the substance.

But the main problem of using of this function in practice is the computational complexity of its derivative functions. For example, in order to calculate specific heat, it is necessary to know the value of error function, which can not be expressed

through elementary functions. And for other derivatives of thermodynamic functions - enthalpy and entropy, integrals of this function are required.

Theoretically, calculation of these functions is possible either by using approximation dependencies or using numerical methods with any accuracy. But in practice, this is not very convenient for most reseachers.

Using function of another distribution (log-logistic distribution [2]) with similar characteristics but with a simpler mathematical dependence instead of the function of the lognormal distribution is mach more effective approache.

Its parameters are similar to lognormal distribution, so log-logistic distribution is used to description of various physical, economic, social processes, along with the traditional lognormal distribution [3-4].

So if the function of the isochoric heat capacity of solids for any temperature can be defined as

$$C_v(T) = 3 \cdot R \cdot Q(T)$$

where R – universal gas constant, J·mol^{-1}·K^{-1},

the temperature dependence through the probability function of the lognormal distribution will have the form

$$Q(T) = \frac{1}{2} + \frac{1}{2} \cdot Erf\left(\frac{v}{2 \cdot \sqrt[4]{2}} \ln\left(\frac{T}{\zeta}\right) \right)$$

and through the log-logistic distribution function it will be much simpler

$$Q(T) \approx \frac{1}{1 + \left(\dfrac{T}{\zeta}\right)^{-v}}$$

where

T – temperature, K;

ζ – scale factor (characteristic temperature), K;

v – rate of state changes.

As a result, functional dependencies for the calculation of entropy (S) and temperature variation of enthalpy (ΔH) are considerably simplified.

$$S(T) = -3 \cdot R \cdot \frac{1}{v} \ln\left[1 - Q(T)\right]$$

$$\Delta H(T) = 3 \cdot R \cdot \left[T - \zeta \cdot Q(T)^{\frac{1}{v}} \frac{1 + k}{1 + k \cdot \{1 - Q(T)\}^{\frac{1}{2}}} \right],$$

$$k = \frac{1.138}{8 \cdot (v - 1) + v^3},$$

In the absence of experimental data, the values v and ζ can be taken for inorganic glassy, amorphous and crystalline (3D) structure - – $v=2.5\div2.8$ and $\zeta=0.35 \cdot \theta$, for graphite-shaped (2D) structure - $v=1.7\div2.0$ and $\zeta=0.26 \cdot \theta$, for polymer materials (1D, linear) structure - $v=1.1\div1.3$ and $\zeta=0.14 \cdot \theta$. Where θ is Debye temperature.

Thus, the application of probability function of the log-logistic distributiont as universal approximation function of isochoric heat capacity allows not only to solve the problem of convenience of computing thermodynamic parameters, but also to use it for interpolation and prediction of missing thermodynamic data.

Referenses

1. Kozub P.A. Lognormal distribution as universal function of temperature dependence of heat capacity / P.A.Kozub, S.N. Kozub // Science and society. Proceedings of the 5th International conference. Accent Graphics Communications & Publishing. Hamilton, Canada. 2018, p. 682-692.

2. A. K. Dey and D. Kundu. Discriminating between the log-normal and log-logistic distributions.Communications in Statistics-Theory and Methods, 39, 280-292, (2010).

3. R. C. Gupta, O. Akman, and S. Lvin. A study of log-logistic model in survival analysis. Biometrical Journal, 4(41), 431-443, (1999).

4. R. R. Kantam, K. Rosaiah, and G. Srinivasa Rao. Acceptance sampling based on life tests: log-logistic model . Journal of Applied Statistics, 28(1), 121-128, (2001).