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DYNAMICS OF THE DEVELOPMENT OF WORLD SCIENCE

ABSTRACTS OF XIII INTERNATIONAL SCIENTIFIC AND PRACTICAL CONFERENCE SEPTEMBER 2-4, 2020

VANCOUVER 2020

DYNAMICS OF THE DEVELOPMENT OF WORLD SCIENCE

Abstracts of XIII International Scientific and Practical Conference

Vancouver, Canada

2-4 September 2020

Vancouver, Canada

2020

UDC 001.1

The 13th International scientific and practical conference "Dynamics of the development of world science" (September 2-4, 2020) Perfect Publishing, Vancouver, Canada. 2020. 399 p.

ISBN 978-1-4879-3791-1

The recommended citation for this publication is:
Ivanov I. Analysis of the phaunistic composition of Ukraine // Dynamics of the development of world science. Abstracts of the 13th International scientific and practical conference. Perfect Publishing. Vancouver, Canada. 2020. Pp. 21-27. URL: https://sci-conf.com.ua/xiii-mezhdunarodnaya-nauchno-prakticheskaya-konferentsiya-dynamics-of-the-development-of-world-science-2-4-sentyabrya-2020-goda-vankuver-kanada-arhiv/.

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УДК 536.632

SET OF FUNCTIONS FOR CALCULATION OF HEAT CAPACITY OF LIQUIDS

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Annotation: A mathematical dependence for the temperature function of the heat capacity of liquids is proposed. Its compliance with such requirements as continuity for the whole temperature scale, simplicity in calculation, absence of results inconsistent with the theory in calculations are shown. An example of calculation for heat capacity of water is given.

Key words: heat capacity, liquids, thermodynamic calculations, temperature dependence.

The temperature dependence of the heat capacity of liquids is the least studied compared to solids and gases. The main reasons for this are the relatively small temperature range of the existence of liquids, too small or large melting points. Therefore, for most substances, the heat capacity for the liquid state is given as invariant values or in the form of a polynomial dependence.

Given the relatively small temperature range of the liquid state, the error of thermodynamic calculations can sometimes be considered uncritical, but when thermodynamic calculations are required in the widest possible temperature range or in the presence of all three phases of matter, the use of such empirical dependences becomes a real problem.

The experience of thermodynamic calculations has allowed us to offer a more convenient dependence, which must meet several criteria. Firstly, it should not lead to knowingly false results of calculations (in terms of theory) on the entire numerical axis. Secondly, it should take into account the already known theoretical provisions (which will fulfill the first requirement), and thirdly, it should be as simple as possible in the calculations.

It is known that at low temperatures the heat capacity of a liquid is changed like the heat capacity of solids (glassy state), but with increasing temperature it becomes greater than the heat capacity of the crystalline substance. Further increase of temperature can lead to a decrease in heat capacity, but at higher temperatures the increase in heat capacity becomes similar to the dependence for solids. Near the critical point, the heat capacity can become infinitely large, but at higher pressures has a smooth maximum [1].

Since a substance in a liquid state can exist both up to the melting point (supercooled liquid, glass) and above the boiling point (superheated liquid), such a dependence must formally give correct results at any temperature value.

To ensure these features, a temperature dependence similar to the heat capacity for solids and gases has been proposed [2-4]

$$C_{A\pm} = \frac{C \cdot \dfrac{T-\zeta}{|T-\zeta|}}{\left(\dfrac{\nu+1}{\nu}\right)\cdot\left(\dfrac{T}{\zeta}\right)^{\frac{T-\zeta}{|T-\zeta|}}-1} + C\cdot\nu\cdot\left(1-\frac{T-\zeta}{|T-\zeta|}\right),$$

$$C_v = \frac{C}{\left(\dfrac{T}{\zeta}\right)^{\nu}+1},$$

$$C_p = C_V + C_{m+} - C_{m-} + C_{b+} - C_{b-}$$

where

T – temperature, K;

C_V – part of solid isochoric heat capacity, kJ/(mole□K);

C_{m+}, C_{m-}, C_{b+}, C_{b-}, – member of isochoric heat capacity for transition regions, , kJ/(mole□K);

ζ – characteristic temperature for each member, K;

 – rate of specific heat change for each member.

Thus, the example of water (Fig. 1) clearly shows that the first term of the dependence is similar to the temperature dependence of the isochoric heat capacity of solids (ice) [5].

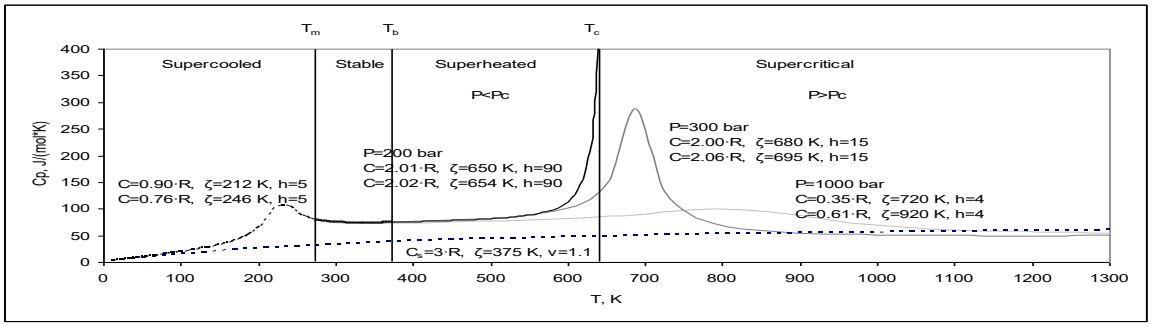

Fig.1 Example of using of proposed dependence to approximation of isobaric heat capacity of water

Increasing the temperature to the melting point leads to an increase in heat capacity, which is reflected in the form of two members of the dependence, similar to the dependence for the additional member of the heat capacity of solids. But in contrast to the lambda transition of solids, the maximum heat capacity is smoother, and its value for a liquid in a stable state becomes greater than for a solid.

A further increase in temperature again leads to an increase in heat capacity, which at the critical point takes an infinite value. The increase of pressure greater than the critical point, the value of heat capacity is decreased again and the temperature function of heat capacity becomes smoothly extreme. In the supercritical region, with increasing pressure the amplitude of the extremum is decreased and its maximum shifts toward higher temperatures.

A study of the literature showed that the proposed dependence allows us to approximate the heat capacity of both inorganic and organic liquids for any temperature. And if necessary, to perform semi-empirical calculations of the coefficients using experimental data of similar substances [6].

But the most important is that the proposed dependence can be used for thermodynamic calculations without the need to divide it into segments and for

approximation of behavior heat capacity outside the experimental data (in the supercooled and superheated state).

Thus, the use of the proposed dependence simplifies and unifies the calculations of thermodynamic parameters of liquid substances for any temperature, makes it impossible to obtain obviously absurd results and allows to move away from the practice of interval calculations.

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