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SET OF FUNCTIONS FOR CALCULATION OF SPECIFIC HEAT OF GASES

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By analogy of the heat capacity of solids, to describe the temperature dependence of the heat capacity of gases scientists have suggested approaches that are based on the foundations of statistical physics. But in most cases, they are used to explain the existing experimental data, but not to carry out practical calculations.

So the heat capacity of real gases can be explained like the sum of energy state of various degrees of freedom, which can be theoretically grounded on the basis of the structure of the molecule. But in practice, the parameters for these degrees of freedom for real gases depend on many parameters that now can only be obtained from experimental data.

That is why for calculating the heat capacity of gases polynomial

dependencies are used most often. Their main advantage is the ease of calculating the coefficients by experimental data, but their biggest drawback is the complete neglect of the theoretical basis. As a result, calculations with their use outside the experimental data interval can lead to absurd results from the point of view of theory.

Using log-logistic dependencies can solve this problem. Thus, the processing of experimental data showed that for most gases, heat capacity can be represented as a sum of log-logistic distribution functions

$$C_p = \sum \frac{C_i}{1 + \left(\dfrac{\zeta_i}{T}\right)^{\nu_i}}$$
(1)

где C_i – heat capacity of corresponding freedom degrees;

ζ_i – frozen out temperature of corresponding freedom degrees;

ν_i – degree index of corresponding freedom degrees.

The processing of a large array of experimental data showed that for most technically important gases, the heat capacity can be approximated with an error not exceeding the error of polynomial dependencies when using only 4 members. Moreover, for temperatures up to 400 K, it is enough just 2 members, and for temperatures less than 2000 K, it is enough 3 members of the dependence.

It should be noted that the comparison of the "frozen out" temperatures of the degrees of freedom and their energies allows recording the specified dependence in the form in which the values of the coefficients have some physical meaning

$$C_p = \frac{C_{tr}}{1 + \left(\dfrac{\zeta_{tr}}{T}\right)^{\nu_{tr}}} + \frac{C_{rot}}{1 + \left(\dfrac{\zeta_{rot}}{T}\right)^{\nu_{trot}}} + \frac{C_{vibr}}{1 + \left(\dfrac{\zeta_{vibr}}{T}\right)^{\nu_{vibrr}}} - \frac{C_{diss}}{1 + \left(\dfrac{\zeta_{diss}}{T}\right)^{\nu_{tdiss}}}$$
(2)

The value of ζ_{tr} is within the range of 0.01-1.2 K. The C_{tr} is about 3.5R for linear molecules and 4R for nonlinear molecules. The value of the degree can be

taken as 2.

For the second member of the dependence, C_{rot} is about one, and ζ_{tr} is within the range of 200-1500 K, the degree value is in the range of 2.5 to 3.7. Thus, this member begins to noticeably affect on the heat capacity at temperatures above 400 K.

The value of the third member (C_{vibr}) is within 1-5, and ζ_{tr} is within 2000-6000 K, the degree value varies from 3 to 6. Thus, this member begins to noticeably affect on the heat capacity at temperatures above 2000 K.

The fourth member of the dependence is responsible for the reduction of the heat capacity which may be explained by the dissociation of the molecule or the weakening of the bonds between the parts of the molecules. Often ζ_{diss} has a value greater than 5000 K, but for some molecules (for example, Na_2, Li_2) they can be 1500-2000 K. The values of C_{diss} vary within 1-4 R, and the value of the degree index is within the range of 4-9.

$$C_p = A + B \cdot T + \frac{C}{T^2} + D \cdot T^2$$

$$C_p = \frac{3.5 \cdot R}{1 + \left(\frac{0.411}{T}\right)^2} + \frac{R}{1 + \left(\frac{1170}{T}\right)^3} + \frac{5 \cdot R}{1 + \left(\frac{12410}{T}\right)^{5.5}} - \frac{4.5 \cdot R}{1 + \left(\frac{20810}{T}\right)^8}$$
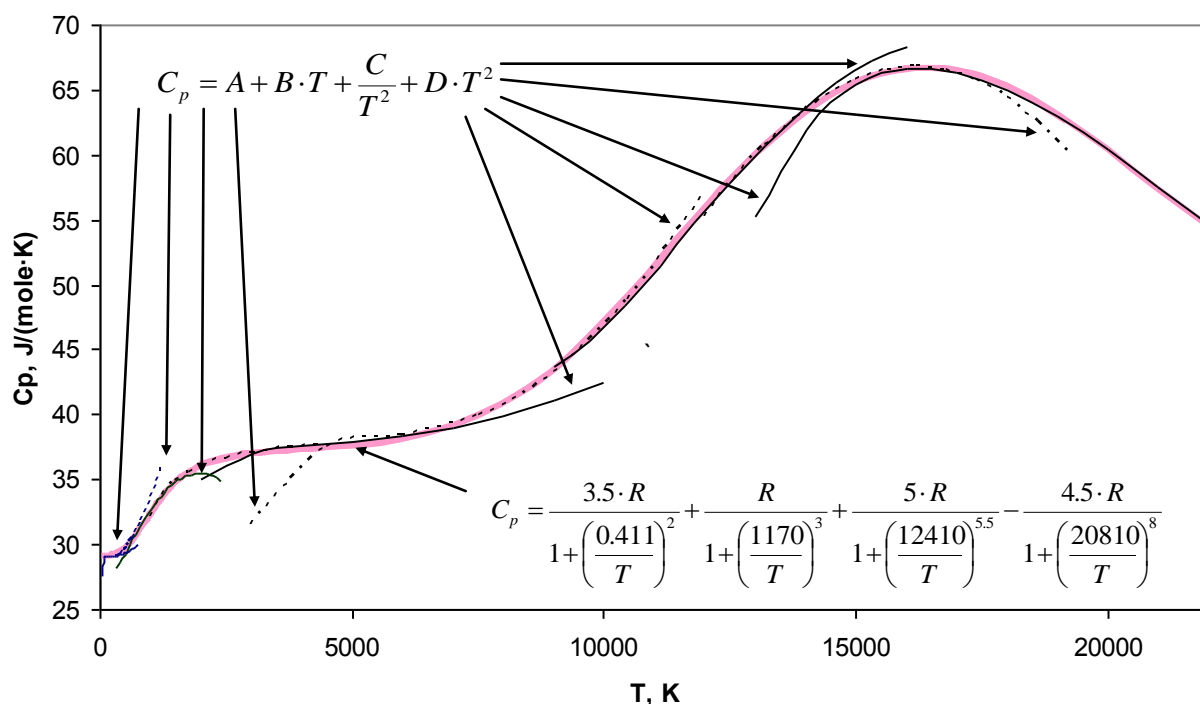
Fig. Approximation of experimental data of heat capacity N_2

As can be seen from the figure the use of the proposed dependence allows approximating the heat capacity of nitrogen by only four members to a temperature of 22000 K instead of the 9 polynomial dependencies used in the thermodynamic

calculations program «HSC Chemistry® for Windows». Furthermore for temperatures less than 6000 K just the first two terms are sufficient, which simplifies the calculations even more.

Thus, the use of log-logistic dependence simplifies and unifies the calculations of thermodynamic parameters of gas substances at any temperature with full consistency with the theoretical principles.

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