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Gase's thermal Conductivity Calculation by low Pressures

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Abstract*: Data on the thermal conductivity of industrial gases (vapors) are used in chemical technology, in the processing of oil and gas for analysis, calculation, and design of thermal processes and apparatus (heat exchangers, furnaces). It is believed that information requests for this property can be satisfied due to the data and recommendations for calculation available in the reference literature. Thus, it is of interest to develop a more convenient (modified) approach to the calculation of the thermal conductivity of gases at a "reference" temperature and low pressures, bypassing the aforementioned problems of the Roy – Todos method. Reliable reference materials were used as an information database of the thermal conductivity of hydrocarbons in the gas (vapor) phase. About 40 hydrocarbons representing various classes with molecular weights of 26 ... 254.5 were selected. Physico-chemical characteristics of the substances taken according to the data. The article considers the calculation of the thermal conductivity of gases at the "reference" temperature value. The proposed formulas make it possible to determine the temperature dependence of thermal conductivity at low pressures.

***Keywords*: Industrial Gases, Thermal Conductivity, Low Pressure, Calculation.**

I. INTRODUCTION

Data on the thermal conductivity of industrial gases (vapors) are used in chemical technology, in the processing of oil and gas for analysis, calculation and design of thermal processes and apparatus (heat exchangers, furnaces). It is believed that information requests for this property can be satisfied due to the data available in the reference literature and recommendations for calculation [1,2].

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II. MATERIALS AND METHODS

In this paper, the object of consideration is the thermal conductivity of hydrocarbon gases at low pressures.

If there is data on the thermal conductivity λ at a certain "reference" value of temperature T_1, then they can be used for calculations at other temperatures, for example T_2, according to the dependence [2].

$$\frac{\lambda_{T_2}}{\lambda_{T_1}} = \left(\frac{T_2}{T_1}\right)^n \quad (1)$$

where T_1, T_2 are the temperatures corresponding to the values of thermal conductivity, K;

n = 1,786.

A sufficiently detailed analysis of the most well-known methods for calculating the thermal conductivity of gases is given in [2]; these methods are based on the conclusions of the molecular kinetic theory. Approximate methods of calculation using nomograms are also proposed [1,2]. It is noted that "the expected range of error is quite wide, but usually they are less than 10%." In this case, the Roy – Todos calculation method gives the most accurate results.

The basic equation for the thermal conductivity of gases at low pressures (~ 0.1 MPa) in the Roy - Todos method can be written as

$$\lambda\Gamma = (\lambda\Gamma)_n + (\lambda\Gamma)_{vn} \quad (2)$$

where λ is the coefficient of thermal conductivity of the gas at low pressure; $G = T_{kp}^{1/6} M^{1/2} P_{kp}^{2/3}$; T_{cr} critical temperature, K; M molecular weight; R_{kr} critical pressure, atm.

The heat equation contains two parts. The first of these is (λ_n), the data obtained by the curve, and the data obtained for rarefied gases. This part only changes with temperature. The second part (λ_{vn}), taking into account the mutual exchange of energy, vibrations, etc., was associated with the reduced temperature and a special constant determined by the group components.

The components of the heat equation have the form (λ by calories/(cm·s·K)

$$(\lambda\Gamma)_n = 99{,}6 \cdot 10^{-6} \cdot (e^{0{,}0464 \cdot \tau} - e^{-0{,}2412 \cdot \tau}) \quad (3)$$

$$(\lambda\Gamma)_{vn} = b \cdot f(\tau) \quad (4)$$

where is $\tau = T/T_{kp}$– reduced temperature, K;

T – current temperature, K.

The ratios for f(τ) were presented [2] in the form of polynomials describing individual classes of substances (saturated hydrocarbons, olefins, acetylene, naphthenes and aromatic, etc.). The constant b is specific for each substance and is determined by the method of group components based on the structure of the molecule. For a representative group of hydrocarbons (paraffins, isoparaffins, olefins and diolefins, naphthenes, aromatic hydrocarbons) studied by Roy and Todos, they proposed a "rough" (according to the authors), but often satisfying the accuracy of calculations graphic correlation of the constant b. The error of the calculation method of the thermal conductivity of Roy – Todos gases was estimated ± 10% [2].

III. RESULT AND DISCUSSION

An analysis of the calculation procedure shows that f(τ) depends not only on the reduced temperature, since separate equations are used for different classes of substances, but also on the characteristics of the substance, which are usually taken into account in generalized methods for predicting thermophysical properties by the determining similarity criterion [3,4]. In addition, the calculation of f(τ) for mixtures of uncertain composition (such as vapors of petroleum products) is difficult to implement. It should also be noted that the part of the Roy – Todos method related to the determination of the constant b is very laborious and requires preliminary "manual" calculation.

Thus, it is of interest to develop a more convenient (modified) approach to the calculation of the thermal conductivity of gases at a "reference" temperature and low pressures, bypassing the aforementioned problems of the Roy – Todos method.

Credible reference materials were used as an information database of the thermal conductivity of hydrocarbons in the gas (vapor) phase [3]. About 40 hydrocarbons representing various classes with molecular weights of 26 ... 254.5 were selected. Physico-chemical characteristics of the substances are taken according to [2].

The dependence of b on molecular weight [2], presented in "Fig. 1", was digitized by us and described as an equation.

$$b \cdot 10^5 = 0{,}0161 \cdot M + 0{,}0034 \cdot M^2 - 9 \cdot 10^{-6} \cdot M^3 \quad (5)$$

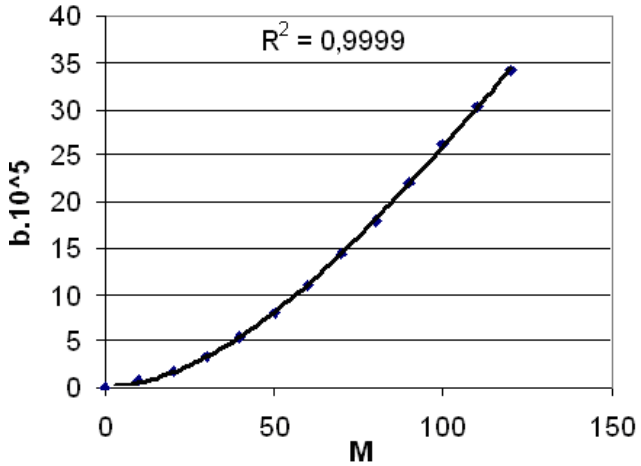

Fig. 1. Correlation for constant b hydrocarbons in the Roy - Todos method (R^2 - approximation reliability)

The individual ratios f(τ) of individual classes of substances [2] were considered by us in the application to hydrocarbons in the range of reduced temperatures of 0.3 ... 0.81 in the form of a single graph shown in "Fig. 2", on which some stratification of points between groups of substances is noticeable.

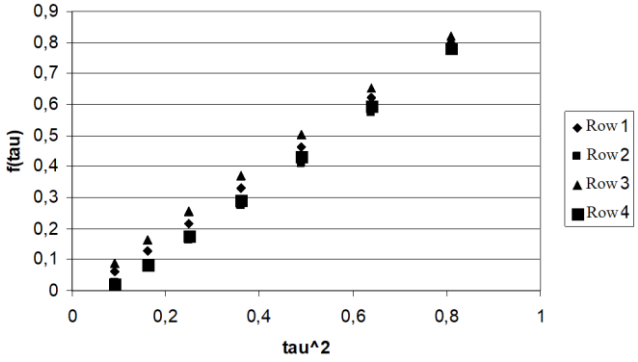

Fig. 2. Correlation of the ratio f(τ) τ^2 for hydrocarbons in the Roy − Todos method: row 1 - saturated (paraffinic and isoparaffinic); row 2 olefinic; row 3 - naphthenic and aromatic; row 4 - acetylene hydrocarbons

The correlation f(τ) τ^2 can be described by a single equation with a sufficiently high approximation confidence value.

The obtained equations for the constants b and f(τ) made it possible to verify the adequacy of these approximations for the Roy - Todos method.

Control calculations of the thermal conductivity of gases (vapors) were performed for the "reference" value at the boiling point, i.e. at $\tau_k = T_k / T_{kp}$, where T_k is the normal boiling point of hydrocarbon, K. This temperature is sometimes used as the base temperature when developing generalized methods for calculating the properties of substances [3,4].

The error in calculating the thermal conductivity coefficient λ_{ras} was estimated in relation to the reference data λ_{op} by the formula.

$$\delta\lambda = 100 \cdot (\lambda_{ras} - \lambda_{op})/\lambda_{op}, \%.$$

The calculation results showed that about 24% of hydrocarbons have an error in calculating thermal conductivity of more than 10%, among them: light hydrocarbons C2, heavy paraffinic and aromatic. The average calculation error for the data set is $\delta\lambda = \pm 8.4\%$. Thus, the considered approximations for the Roy - Todos method need improvement.

Using the data of the compiled hydrocarbon information base, at $\tau_к$ the "experimental" values of the thermal conductivity coefficient were selected for the second part of the equation in the Roy Todos method ($\lambda_{vn\ op}$), W / (m×K)

$$\lambda_{vnop} = \lambda_к - \lambda_n,$$

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where $\lambda_к$ - thermal conductivity coefficient at normal boiling point temperature to, W / (m×K);

$\lambda_п$ - the value of the translational part of the coefficient of thermal conductivity at $\tau_к$, calculated by the formula (2), W / (m×K).

The values of f $(\tau_к)_{op}$ were determined by the formula

$$f(\tau_к)_{on} = 10^5 \cdot \Gamma \cdot \lambda_{vnop}/(418{,}6 \cdot b),$$

where b is the constant value found by formula (5).

The calculated values of f $(\tau_к)_{op}$ were presented as a correlation from the reduced boiling point $\tau_к$ on the graph in "Fig. 3".

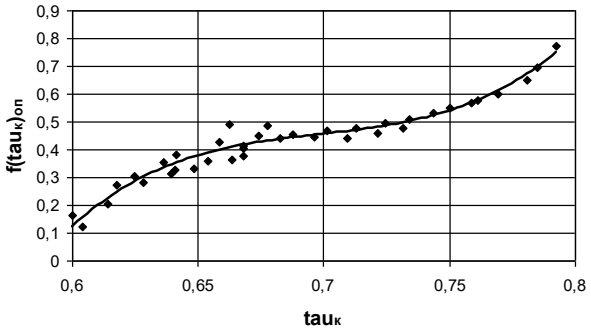

Fig. 3. Correlation of the ratio $f(\tau_к)_{op}$ in the Roy - Todos method for hydrocarbons

The nature of the correlation is quite complex, however, there is no noticeable stratification of points relative to the trend line. The correlation f $(\tau_к)$ - $\tau_к$ was described by a single equation with a fairly high level of reliability of the approximation (R2 = 0.96) in the form

$$f(\tau_к) = -82{,}774 + 355{,}46 \cdot \tau_к - 507{,}46 \cdot \tau_к^2 + 242{,}17 \cdot \tau_к^3.$$

The results of calculating the error $\delta\lambda_k$ of the thermal conductivity coefficient at the "reference" temperature $\tau_к$ using formulas (5.6) and elements of the Roy Todos method are presented in "Fig. 5".

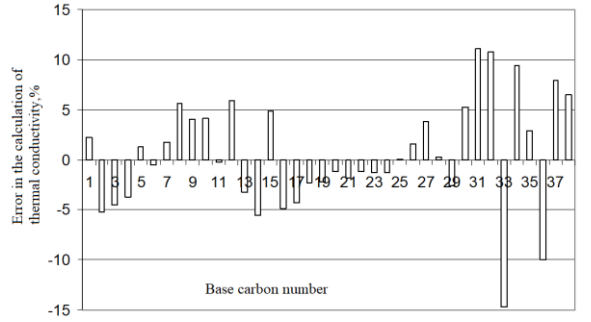

Fig. 5. Errors in the calculation of the thermal conductivity of hydrocarbon gases $\delta\lambda_к$ by the modified Roy - Todos method

IV. CONCLUSION

An analysis of the data shows that 12 hydrocarbons from the used array have a calculation error $\delta\lambda_k$ of more than 5%, and only 3 of them (benzene derivatives) are more than 10%. The average calculation error for the data array is $\delta\lambda_к$ = ± 4.2%, which is comparable with the Roy – Todos method [2].

Further calculations of the temperature dependence of the thermal conductivity coefficient can be carried out according to formula (1).

If necessary, take into account the effect of pressure on the thermal conductivity of gases, you should use the recommendations [2].

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