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Mathematical description of the diffusion in a temperature field and measuring the heat of transport

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Abstract

A critical review of the existing analytical solutions of the thermodiffusion equation and methods for measuring heat of transport was performed. Particular emphasis is placed upon the fact that of the reported solutions yielding reasonable accuracy, there is no one solution that describes the diffusion profile behavior while making possible to measure the diffusion substance's heat of transport. Simple thermodiffusion equation solutions were obtained by taking into account the coordinate dependence of the diffusion coefficient and thermodiffusion factor in a temperature field. Such an approach has allowed the proposal of a new method for measuring the heat of transport similar to the conventional method for measuring a diffusing impurity's activation energy. © 2001 Elsevier Science Ltd. All rights reserved.

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1. Introduction

Thermodiffusion in the solid is one of a transport process that has great practical importance. Most of the research associated with the presence of concentration and temperature gradients has been made with metals and alloys. The first critical review of such research was published in the work of Oriani [1]. With the advance of a nuclear energetics the interest in thermodiffusion has returned to metallic oxides that often heats up in inhomogeneous temperature fields [2] in connection with technological conditions. Further expansion of investigations in this field associated with the advent of semiconductor devices and the advancement of microelectronics [3]. The presence of temperature gradient that is inherent to some technological processes have led to the necessity of an investigation of thermodiffusion in semiconductor materials, and a refinement of "isothermal" technologies. Under conditions of inhomogeneity of the concentration and temperature distribution an impurity behavior is defined by a series of parameters, of which the more important are the temperature gradient ∇T and the heat of transport Q^*. The latter defines the value and direction of the substance flux that are caused by the temperature gradient. Whereas ∇T is given by experimental conditions, the heat of transport needs to be defined. At the moment few methods for its measuring exist. The best method uses the velocity of the mass profile center [4]. In principle, knowing the Q^* and ∇T we can define the concentration of impurity $C(x,t)$ for the time moment t and the point x using a computer simulation or an analytical expression for $C(x,t)$. Unfortunately, until the present time an exact solution of the thermodiffusion equation has not been derived and the familiar ones is carried out with some degree of approximation. Most consistently this problem is solved in the works [5–7] where the x-dependence of the diffusion coefficient $D[T(x)]$ and thermodiffusion factor $Q^*/[kT(x)]$ in linear approximation of expanding of the function $1/T(x)$ into Macloren's series is taken into account.

Thus, with the method of measuring for the Q^* [4] and the solutions [5–7] we can find an analytical description of the thermodiffusion process to an acceptable approximation. However, the solutions [5–7] have cumbersome form and they are inconvenient for an analysis of the thermodiffusion process, and the method [4] does not use an explicit form of the solution $C(x,t)$; a uniform approach to process analysis is lost.

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Nomenclature

$C(x,t) = C$	solvent substance concentration ($\mathrm{m^{-3}}$)
$C_\mathrm{M}(x,t)$	solvent substance concentration defined in Eq. (9) ($\mathrm{m^{-3}}$)
$D(T(x)) = D$	diffusion coefficient ($\mathrm{m^2\ s^{-1}}$)
$D(0)$	diffusion coefficient at the coordinate $x = 0$ ($\mathrm{m^2\ s^{-1}}$)
D_1	diffusion coefficient defined in Eq. (22) ($\mathrm{m^2\ s^{-1}}$)
D^*	diffusion coefficient defined in Eq. (26) ($\mathrm{m^2\ s^{-1}}$)
D_0^*	diffusion coefficient defined in Eq. (30) ($\mathrm{m^2\ s^{-1}}$)
E	activation energy (J)
$\vec{J}$	diffusing substance flux ($\mathrm{m^{-2}\ s^{-1}}$)
$\vec{J}_0$	diffusing substance flux at the point r_m ($\mathrm{m^{-2}\ s^{-1}}$)
k	Boltzmann's constant ($\mathrm{J\ K^{-1}}$)
ΔL	thickness of the layer where diffusion takes place (m)
m_0	mass of a single atom (kg)
M	total substance amount referred to by unit of area of the layer ($\mathrm{kg\ m^{-2}}$)
N	number of the diffusing substance atoms
$\vec{r}$	position vector continuum's point (m)
r_m	absolute value of position vector of the $C(r,t)$ function maximum (m)
Q^*	heat of transport (J)
t	time (s)
$T(x) = T$	temperature (K)
$T_\mathrm{m} = T(r_\mathrm{m})$	temperature at the point r_m (K)
$T_0 = T(x=0)$	temperature at the coordinate $x = 0$
ΔT	temperature difference in the layer where diffusion takes place (K)
∇T	temperature gradient ($\mathrm{K\ m^{-1}}$)
$U = U(x,t)$	concentration defined in Eq. (20) ($\mathrm{m^{-3}}$)
$\vec{v}^*$	velocity of continuum's particle (diffusing substance atoms) ($\mathrm{m\ s^{-1}}$)
$\vec{v}_0^*$	velocity of continuum's particle (diffusing substance atoms) at the point r_m ($\mathrm{m\ s^{-1}}$)
$\vec{v}$	velocity of $C(\vec{r},t)$ profile maximum ($\mathrm{m\ s^{-1}}$)
v	absolute value of $\vec{v}$ ($\mathrm{m\ s^{-1}}$)
v_M	absolute value of $C(x,t)$ profile maximum defined in Eq. (10) ($\mathrm{m\ s^{-1}}$)
$\bar{v}^*$	mean velocity of diffusing atoms ($\mathrm{m\ s^{-1}}$)
v'^*	velocity of $C(\xi,t)$ profile maximum defined in Eq. (87) ($\mathrm{m\ s^{-1}}$)
v'	velocity of $C(\xi,t)$ profile maximum defined in Eq. (89) ($\mathrm{m\ s^{-1}}$)
x	current coordinate (m)
x_max	abscissa of $C(x,t)$ profile maximum (m)
$\bar{x}$	abscissa mass center of profile (m)
Greek symbols	
α_0	parameter defined in Eq. (31) ($\mathrm{m^{-1}}$)
β	dimensionless parameter, $(\nabla T/T)x$
γ	dimensionless parameter, $\alpha_0\sqrt{D_0^* t}$
ρ	density of continuum's mass ($\mathrm{kg\ m^{-3}}$)
ξ	coordinate defined in Eq. (24) (m)

At the same time, however, for the coordinate-independent approximation of the diffusion coefficient and thermodiffusion factor, a simple analytical solution of the thermodiffusion equation [8] is obtained. This solution simultaneously allows definition of Q^* from the profile peak position of the diffusing substance. The approximation assumes that peak velocity is constant. But as shown, the peak velocity is strongly dependent on thermodiffusion time, and so, this assumption causes a substantial error in the measurement the Q^* [4].

In our work a unified approach is proposed for an analytical description of the thermodiffusion process and the heat of transport's measurement on the basis of a simple solution of form presented by Mock in the work [8]. However in the solution we take into account the temperature dependence of the diffusion coefficient $D[T(x)]$ and thermodiffusion factor $Q^*/[kT(x)]$.

2. Methods of solving the thermodiffusion equation and measuring heat of transport

Let us make an overview of the principal methods of thermodiffusion equation decisions and measuring heat of transport. Note the advantages and disadvantages and justify necessity of searching simple solutions convenient for the process's practical analysis, while also taking into account the temperature dependence of $D[T(x)]$ and $Q^*/[kT(x)]$.

2.1. Measuring heat of transport from atomic velocity in peak concentration

Let us first write an equation of balance expressing the condition of continuum's mass conservation [9]

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \vec{v}^* = 0, \tag{1}$$

here ρ is the density of continuum's mass, $\vec{v}^{*}$ is the velocity of continuum's particles.

Represent ρ by the formula

$$\rho = \frac{M}{V} = \frac{Nm_0}{V} = m_0 C, \tag{2}$$

where $C = N/V$ is the concentration of a diffusing substance, N is the number of the diffusing substance atoms contained in the volume V, and m_0 is the mass of a single atom.

Thus, formula (1) is rewritten as

$$\frac{\partial C}{\partial t} + \nabla\ C\vec{v}^{*} = 0, \tag{3}$$

where $C\vec{v}^{*}$ is formulated for thermodiffusion process as

$$C\vec{v}^{*} = \vec{J} = -D\left(\nabla C + C\frac{Q^{*}}{kT}\frac{\nabla T}{T}\right). \tag{4}$$

Here (4) is representative of the diffusing substance flux, $D = D_0 \exp[E/(kT)]$ is the diffusion coefficient, E is the activation energy, T is absolute temperature, k is Boltzmann's constant, and Q^{*} is the heat of transport.

If $\nabla C = 0$ at the point r_{m} of the maximum of the $C(\vec{r})$ function, then $(T = T(r_{\mathrm{m}}) = T_{\mathrm{m}})$, the Eq. (4) may be written

$$\vec{J}_0 = C\vec{v}_0^{*} = -DC\frac{Q^{*}}{kT_{\mathrm{m}}}\frac{\nabla T}{T_{\mathrm{m}}}. \tag{5}$$

From this equation one can find the velocity of diffusing substance atoms at the profile maximum point of impurity distribution [10]

$$v_0^{*} = -D\frac{Q^{*}}{kT_{\mathrm{m}}}\frac{\nabla T}{T_{\mathrm{m}}}. \tag{6}$$

Gerl [10] identifies the velocity (6) with the velocity $\vec{v}$ of $C(\vec{r}, t)$ profile maximum. Then, knowing the experimental value of maximum position change in the time Δt and values $D, T, \nabla T$, we can define Q^{*}.

In Section 2.2 it will be shown that the aforementioned assumption holds true for such diffusion processes in an external force field where directional substance velocity, received in response to a field, is not dependent on diffusing atom coordinates; for example, as occurs in an uniform electrical field. As seen from formula (6), for thermodiffusion process the independence of substance velocity from diffusing atom coordinates is possible only when the condition $\nabla T/T = \mathrm{const}$ is fulfilled. At this point, exponential temperature distribution must be set in a sample. The approximation, as we shall see later, appears to be overly rough for the constant temperature gradient.

2.2. Decision of the thermodiffusion equation in an external force field approximation and measurement of heat transport from velocity of the concentration profile maximum

First, the uniform thermodiffusion Eq. (3) must be written ($\nabla T = \mathrm{const}$) in which a substance flux is defined by formula (4)

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left[D\left(\frac{\partial C}{\partial x} + \frac{Q^{*}}{kT}\frac{\nabla T}{T}C\right)\right]. \tag{7}$$

Differentiating the right-hand side of (7) leads to the expanded equation

$$\frac{\partial C}{\partial t} = D\left[\frac{\partial^2 C}{\partial x^2} + \frac{Q^{*}+E}{kT}\frac{\nabla T}{T}\frac{\partial C}{\partial x} + \frac{Q^{*}}{kT}\left(\frac{\nabla T}{T}\right)^2 \times \left(\frac{E}{kT} - 2\right)C\right]. \tag{8}$$

In his work, it should be noted, Mock [8] neglects the third term in brackets of formula (8). From this action, besides equating $T = T_0$, $D = D(0) = D_0 \exp[E/(kT_0)]$, one gets the solution characterizing diffusion in the field of external force for diffusion from an instantaneous plane source in a semiinfinite media

$$C(x,t) = \frac{M}{\sqrt{\pi D t}} \exp\left[-\frac{(x - vt)^2}{4Dt}\right], \tag{9}$$

where

$$v = -D(Q^{*} + E)\frac{\nabla T}{kT^2}, \tag{10}$$

where M is the total substance amount referred to by unit of area of the layer. In what follows solution (9) and velocity (10) will be specified by $C_{\mathrm{M}}(x,t)$ and v_{M}, respectively.

The velocity of the maximum profile $C(x,t)$ may be estimated from the condition

$$\frac{\partial C}{\partial x} = 0.$$

Taking into account that

$$\frac{\partial C}{\partial x} = C\left[-\frac{2(x - vt)}{4Dt}\right],$$

we find

$$x_{\max} = vt.$$

The maximum velocity of distribution $C(x,t)$ is defined by Eq. (10) and, in Mock's approximation, is not coincident to Gerl's approximation where the velocity is v_0^{*}.

In the general case from the formula representing flux it follows that the atomic velocity of a diffusing substance should be defined as:

$$v^* = -D\frac{\nabla C}{C} + v_0^*. \tag{11}$$

Assuming that C is defined by the (9), we find

$$\frac{\nabla C}{C} = -\frac{x - vt}{2Dt}$$

and

$$v^* = \frac{x}{2t} - \frac{v}{2} + v_0^*.$$

Considering time as a parameter, and taking into account that $\bar{x} = x_{\max} = vt$ as a consequence of profile symmetry, we find the mean velocity of diffusing atoms

$$\bar{v}^* = \overline{\frac{x}{2t} - \frac{v}{2} + v_0^*} = \frac{\bar{x}}{2t} + v_0^* - \frac{v}{2} = v_0^*. \tag{12}$$

Thus, in Mock's approximation the atomic velocity v_0^* of a diffusing substance in the profile's maximum is equal to the mean velocity $\bar{v}^*$ of all atoms and is not coincident with the peak velocity v of profile $C(x,t)$.

Similarly, as in Gerl's approximation, heat of transport is easily defined when diffusion time and maximum position $x_{\max}$ are known.

If in Eq. (7) the factor located in front of the concentration C is set equal to a constant when differentiation of the right-hand side is performed, then the thermodiffusion equation takes the form that is characteristic of diffusion in a uniform field. For this case

$$v = -D\frac{Q^*}{kT}\frac{\nabla T}{T},$$

that is, coincides with the velocity v_0^* (formula (6), where $T_m = T_0$) of diffusing atoms in peak concentration. Thus, Gerl's method provides a rougher estimate of Q^* than Mock's [8].

2.3. The profile's peak and center of mass velocities and measuring heat of transport

As is shown in [4], a profile asymmetry arising from its spreading in a temperature field leads to a strong dependence of maximum velocity from the time. The expression obtained for the profile maximum velocity is

$$v = -D[Q^*(1 - A) + 2E + B]\frac{\nabla T}{kT^2}, \tag{13}$$

where

$$A = -\left(\frac{\partial^2 \ln C}{\partial x^2}\right)^{-1}_{\partial C/\partial x = 0}\left(\frac{\nabla T}{T}\right)^2\left[\left(\frac{E}{kT}\right)^2 - \frac{6E}{kT} + 6\right] \tag{14}$$

and

$$B = \frac{kT^2}{\nabla T}\left(\frac{\partial^3 C}{\partial x^3}\Big/\frac{\partial^2 C}{\partial x^2}\right)_{\partial C/\partial x = 0}. \tag{15}$$

The summand B in brackets of formula (13) has large time dependence, because as the profile asymmetry is increased in the point of its extremum, the function $\partial^3 C/\partial x^3$ is increased and $\partial^2 C/\partial x^2$ is decreased [4]. As we can see, the profile form is not changed if the point of its extremum is transformed to the origin of coordinates. Then, expanding the function $C(x,t)$ into a Macloren's series, and taking into account $\partial C/\partial x = 0$ in the extremum point, we have

$$C(x,t) = C(0) + \frac{1}{2!}\frac{\partial^2 C(0)}{\partial x^2}x^2 + \frac{1}{3!}\frac{\partial^3 C(0)}{\partial x^3}x^3 + \cdots \tag{16}$$

If function (16) is illustrated graphically, then the first and second terms draw a symmetric parabola about the C axis; and the third, gives an antisymmetric cubic parabola. The ratio of the coefficients (is located in front of x^3 and x^2) characterizes the degree of the total graphic asymmetry. The summand B, defined by formula (15), is proportionate to this ratio; and, as the degree of asymmetry increases it also rises very quickly and monotonically. Thus, averaging the maximum profile velocity v over time can result in essential error when heat of transport Q^* is measured. This drawback can be practically eliminated if, when measuring heat of transport, the value of the profile's mass center velocity is used. The value of the velocity in a linear approximation about the abscissa $x_{\max}$ of the $C(x,t)$ peak is defined by the following formula [4]:

$$v_c = -D(x_{\max})(Q^* - E)(1 - C)\frac{\nabla T}{kT^2(x_{\max})}, \tag{17}$$

where

$$C = (\bar{x} - x_{\max})\frac{\nabla T}{T(x_{\max})}\left[\frac{E}{kT(x_{\max})} - 2\right] \tag{18}$$

and $\bar{x}$ is the coordinate mass center of the profile.

The value of C is almost always much less than unity. As we can see, if ΔL is the thickness of the layer where diffusion takes place and ΔT is the temperature difference in this layer; then, $\nabla T = \Delta T/\Delta L$ and

$$C = \frac{(\bar{x} - x_{\max})}{\Delta L}\frac{\Delta T}{T(x_{\max})}\left[\frac{E}{kT(x_{\max})} - 2\right]. \tag{19}$$

Because

$$\frac{E}{kT(x_{\max})} - 2 \sim 1, \quad \frac{(\bar{x} - x_{\max})}{\Delta L} \ll 1,$$

and almost without exception $\Delta T/T(x) \ll 1$, then the value of C (formula (19)) can be neglected.

The time dependence of the mass center velocity will be defined by factor $D(x_{\max})/kT^2(x_{\max})$. The relative error in the process of defining mass center velocity is equal to

$$\left(\frac{E}{kT_0} - 2\right)\frac{T(x_{\max}) - T_0}{T_0}$$

and for small values of the difference $\Delta T(x_{\max}) = T(x_{\max}) - T_0$ mass center velocity can be considered as a constant. Emphasis must be placed on formula (17) derivation, which occurred without the deduction of an explicit dependence $C(x,t)$.

Thus, this method provides a highly accurate way of measuring heat of transport without employing the thermodiffusion equation.

2.4. The thermodiffusion equation's solution within a linear approximation by expansion of the $1/T(x)$ function in a Macloren series

The diffusion substance flux is shown in the works [5–7] by substitution

$$U(x,t) = C(x,t)\exp\left(-\frac{Q^*}{kT(x)}\right) \tag{20}$$

in the one-dimensional case, can be reduced to

$$J = D_1\frac{\partial U}{\partial x}, \tag{21}$$

where

$$D_1 = D_0\exp\left(-\frac{E - Q*}{kT}\right). \tag{22}$$

Then, the thermodiffusion Eq. (8) may be written as follows:

$$\exp\left(\frac{Q^*}{kT}\right)\frac{\partial U}{\partial t} = -\mathrm{div}\vec{J} = \frac{\partial}{\partial x}\left(D_1\frac{\partial U}{\partial x}\right). \tag{23}$$

Introducing the new variable ξ, defined by

$$\frac{\partial}{\partial \xi} = \exp\left(-\frac{Q^*}{kT}\right)\frac{\partial}{\partial x} \tag{24}$$

Eq. (23) can be reduced to the second Fick equation

$$\frac{\partial U}{\partial t} = \frac{\partial}{\partial \xi}\left(D^*\frac{\partial U}{\partial \xi}\right) \tag{25}$$

for the U function at the diffusion coefficient

$$D^* = D_0\exp\left(-\frac{E - 2Q^*}{kT}\right). \tag{26}$$

By expressing $1/T[\xi(x)]$ as the Macloren series in ξ in a linear case, we have

$$\frac{1}{T(\xi)} = \frac{1}{T_0} - \frac{T'(0)}{T^2(0)}\left.\frac{\mathrm{d}x}{\mathrm{d}\xi}\right|_{\xi=0}\xi + \cdots \tag{27}$$

Then,

$$\xi(x) = \int_0^x \exp\left(\frac{Q^*}{kT(\upsilon)}\right)\mathrm{d}\upsilon \approx -\frac{kT_0^2\exp\left(Q^*/kT_0\right)}{Q^*T'(0)}\left[\exp\left(-\frac{Q^*T'(0)}{kT_0^2}\right)x - 1\right], \tag{28}$$

$$D^* = D_0^*\exp\left(\alpha_0\xi\right), \tag{29}$$

$$D_0^* = D_0\exp\left(-\frac{E - 2Q^*}{kT_0}\right), \tag{30}$$

$$\alpha_0 = \frac{E - 2Q^*}{kT_0^2}\nabla T\exp\left(-\frac{Q^*}{kT_0}\right). \tag{31}$$

The solution of Eq. (25) at $\alpha_0\xi \ll 1$ for diffusion from an instantaneous plane source in semi-infinite media, was found in the work of Rudakov and Ovcharov [7] as an asymptotic series. Introducing variables $K(\xi), W(\xi,t), A(\xi,t), B(\xi,t)$, we present this solution in a more compact form

$$C(\xi,t) = K(\xi)\times\left\{A(\xi,t)\frac{\exp\left[-W^2(\xi,t)\right]}{\sqrt{\pi D(0)t}} + B(\xi,t)\frac{\alpha_0\exp\left(Q^*/kT_0\right)}{2^8}\mathrm{erfc}[W(\xi,t)]\right\}, \tag{32}$$

where

$$K(\xi) = M\exp\left\{\frac{Q^*}{k}\left[\frac{1}{T(\xi)} - \frac{1}{T_0}\right] - \alpha_0\xi/4\right\}, \tag{33}$$

$$W(\xi,t) = \frac{1 - \exp\left(-\alpha_0\xi/2\right)}{\alpha_0\sqrt{D_0^*t}}, \tag{34}$$

$$A(\xi,t) = 1 - \frac{\alpha_0^2D_0^*t}{2^{12}}\left[85\exp(\alpha_0\xi) - 90\exp(\alpha_0\xi/2) + 16\exp(-\alpha_0\xi/2) - 27\right] + \cdots, \tag{35}$$

$$B(\xi,t) = 5\exp(\alpha_0\xi) - 59\exp(\alpha_0\xi/2) - 7\exp(-\alpha_0\xi/2) + 32\left\{\alpha_0^2D_0^*t + 2\left[1 - \exp(-\alpha_0\xi/2)\right]^2\right\} - 3 + \cdots \tag{36}$$

In this paper the accuracy of calculation of the functions $A(\xi,t)$ and $B(\xi,t)$ is better than in the work [7].

The chief drawback of solution (32) is its unwieldy form. This fact strongly reduces its practical implementation to analysis of the actual processes.

3. An investigation of the thermodiffusion equation solution obtained in a linear approximation and establishment of a form suitable for its use in applied problems

A characteristic feature of diffusion in a temperature field is the availability of a diffusing substance's asymmetric profile [4,8]. The feature is observed experimentally [8] and substantiated theoretically in the work of Crolet and Lasarus [4]. Quantitative consideration of asymmetry on diffusion from an extended source of infinite extent and on diffusion from an instantaneous plane source in semi-infinite media is also made by contemporary authors in works [5–7]. The formula descriptive of the last case is presented in the previous section: formula (32). It takes the form typical of diffusion in a uniform external field (formula (9)) and descriptive of a symmetric profile when the following conditions are fulfilled:

$$A(\xi,t)=1, \tag{37}$$

$$B(\xi,t)=0, \tag{38}$$

$$K(\xi)\exp[-W^2(\xi,t)]=f(t)\exp(x-vt)^2, \tag{39}$$

where $f(t)$ is a function of time.

For small values of the parameter $\gamma=\alpha_0\sqrt{D_0^*t}$ and value $\xi\sim\sqrt{D_0^*t}$ we can consider the condition (37) as fulfilled. Then,

$$W(\xi,t)=\lim_{\gamma\to 0}\frac{1-\exp(-\alpha_0\xi/2)}{\alpha_0\sqrt{D_0^*t}}=\frac{\xi}{2\sqrt{D_0^*t}} \tag{40}$$

hence, an profile asymmetry results from the $K(\xi)$ factor; the $B(\xi,t)\mathrm{erfc}W(\xi,t)$ summand in a bracket of formula (32); and, an asymmetrical form of the $\xi(x)$ dependence. This raises the next series of questions: first, how do each of the approve-listed factors affect profile asymmetry; and second, how can the dependence $C(x,t)$ be approximated in its simplest form while still describing the diffusion processes most characterizing features in a temperature field?

Analysis of the solution derivation (32) allows us to separate out three principal stages. This is the transition from the function $C(x,t)$ to the function $U(x,t)$ (substitution of formula (20)), the change of the variable $\xi\to x$ (formula (24)), and an expansion of the function $1/T[\xi(x)]$ into the series up to a linear term (by formula (27)). To realize their influence on the solution's form let us separate the each of the stages. To start with, we will investigate the role of substitution of formula (20) by changing the $C(x,t)$ function to new functions with no change of variables $\xi\to x$. As it turns out, this approach enables us to take into account the x-dependence occurring in a temperature field from basic diffusion process parameters; namely, a diffusion coefficient and a thermodiffusion factor attained by restricting only the zeroth term of $1/T(x)$'s the function expansion in Macloren series

$$\frac{1}{T(x)}\approx\frac{1}{T_0}. \tag{41}$$

This kind of co-ordinate dependence on the diffusion parameters in a temperature field shall be said to be the temperature dependence for shortening and expanding formula (41), and shall also be the zeroth approximation of the $1/T(x)$ function. Comparing these solutions with the Mock solution $C_{\mathrm{M}}(x,t)$, one finds similarly for small values for the x variable.

At the next stage, within the framework of the $1/T(x)$ function's zeroth approximation, accuracy is improved by changing to the new variable ξ. Finally, these solutions for small values of x may be compared to solution of (32) obtained in linear approximation.

Operating in such a manner (that is, gradually improving the solution's accuracy) one discovers the fundamental factor responsible for profile asymmetry.

3.1. Solutions taking into account temperature dependence of thermodiffusion coefficients in the zeroth approximation

3.1.1. Considering the diffusion coefficient's temperature dependence

The diffusion substance flux can be written

$$J=-D\frac{\partial C}{\partial x}-D\frac{Q^*}{kT}\frac{\nabla T}{T}C. \tag{42}$$

The new function can be introduced

$$F(x,t)=D(x)C(x,t). \tag{43}$$

Its partial derivative with respect to x is

$$\frac{\partial F}{\partial x}=\frac{\partial D}{\partial x}C+D\frac{\partial C}{\partial x}. \tag{44}$$

Then, taking into account

$$\frac{\partial D}{\partial x}=\frac{E}{kT}\frac{\nabla T}{T}D, \tag{45}$$

we can formulate

$$D\frac{\partial C}{\partial x}=\frac{\partial F}{\partial x}-\frac{E}{kT}\frac{\nabla T}{T}F. \tag{46}$$

Hence,

$$J=-\frac{\partial F}{\partial x}+SF, \tag{47}$$

where

$$S=\frac{E-Q^*}{kT(x)}\frac{\nabla T}{T(x)}. \tag{48}$$

The divergence of the J flux can be found

$$\mathrm{div}\vec{J}=\frac{\partial J}{\partial x}==-\frac{\partial^2 F}{\partial^2 x}+S\frac{\partial F}{\partial x}-2\frac{\nabla T}{T}SF \tag{49}$$

since,

$$\frac{\partial S}{\partial x}=-2\frac{\nabla T}{T}S. \tag{50}$$

For the value F that is small when compared to its first and second derivative (that is, on the concentration profile's tail regions) we can disregard the third term on the right-hand side of formula (49). Naturally, this approximation introduces a very large error as Q^* is defined from the distribution profile maximum's position. It has a more illustrative character, allowing it to be compared with Mock's solution [8], that is got noteworthy for similar assumptions. Thus, the thermodiffusion equation becomes

$$\frac{1}{D}\frac{\partial F}{\partial t}=\frac{\partial^2 F}{\partial t^2}-S\frac{\partial F}{\partial x}. \tag{51}$$

Setting $T=T(0)=T_0$ (that is $D=D(0), S=S(0)$) we immediately can write a solution similar to Mock's solution (9)

$$F(x,t) = \frac{MD(0)}{\sqrt{\pi D(0)t}} \exp\left[-\frac{(x-vt)^2}{4D(0)t}\right], \tag{52}$$

where

$$v = -D(0)S(0) = -D(0)\frac{Q^* - E}{kT_0}\frac{\nabla T}{T_0}. \tag{53}$$

The factor $D(0)$ on the right-hand side of formula (52) originates from a conservation condition of the diffusing substance: because, $C(x,0) = F(x,0)/D(0)$. In addition, since we know $F = DC$, the expression for C taking into account the dependence $D(T)$ for zeroth approximation becomes

$$\begin{aligned} C(x,t) &= \frac{MD(0)}{D\sqrt{\pi D(0)t}} \exp\left[-\frac{(x-vt)^2}{4D(0)t}\right] \\ &= \frac{M\exp\left[\frac{E}{k}\left(\frac{1}{T}-\frac{1}{T_0}\right)\right]}{\sqrt{\pi D(0)t}} \exp\left[-\frac{(x-vt)^2}{4D(0)t}\right]. \end{aligned} \tag{54}$$

The characteristic factor

$$\exp\left[\frac{E}{k}\left(\frac{1}{T}-\frac{1}{T_0}\right)\right]$$

takes into account the temperature dependence of a diffusion coefficient and is responsible for the asymmetric evolution of the diffusing profile during the thermodiffusion process.

Solution (54) for small x or, more precisely, for the values of non-dimensional parameter

$$\beta = (\nabla T/T)x \ll 1$$

may be found by taking into account

$$\frac{1}{T} - \frac{1}{T_0} = \frac{1}{T_0 + \nabla Tx} - \frac{1}{T_0} \approx -\frac{\nabla T}{T_0^2}x.$$

After a number of rearrangements, we find

$$C(x,t) = H(t)C_{\mathrm{M}}(x,t), \tag{55}$$

where

$$H(t) = \exp\left[\frac{EQ^*}{(kT_0)^2}\left(\frac{\nabla T}{T_0}\right)^2 D(0)t\right]. \tag{56}$$

It follows that in this approximation the profile maximum velocity of the distribution $C(x,t)$ coincides with the velocity in Mock's; whereas, its value grows in agreement with the $H(t)$ law in time.

3.1.2. Considering the temperature dependence of the thermodiffusion factor

As in other notable works [5–7], we introduce the function

$$U(x,t) = C(x,t)\exp\left(-\frac{Q^*}{kT(x)}\right). \tag{57}$$

Thermodiffusion equation then takes the form

$$\frac{\partial U}{\partial t} = \exp\left(-\frac{Q^*}{kT}\right)\frac{\partial}{\partial x}\left[D\exp\left(\frac{Q^*}{kT}\right)\frac{\partial U}{\partial x}\right]. \tag{58}$$

In the zeroth approximation of an expanding Macloren series we set the function

$$\frac{1}{T(x)} = \frac{1}{T_0 + \nabla Tx} \approx \frac{1}{T_0}.$$

Thus,

$$\frac{\partial U}{\partial t} = D(0)\frac{\partial^2 U}{\partial x^2}. \tag{59}$$

The solution of the equation for diffusion from an instantaneous plane source in semi-infinite media is

$$U(x,t) = \frac{M\exp\left(-\frac{Q^*}{kT_0}\right)}{\sqrt{\pi D(0)t}}\exp\left(-\frac{x^2}{4D(0)t}\right). \tag{60}$$

Then it follows that:

$$C(x,t) = \frac{M\exp\left[\frac{Q^*}{k}\left(\frac{1}{T}-\frac{1}{T_0}\right)\right]}{\sqrt{\pi D(0)t}}\exp\left(-\frac{x^2}{4D(0)t}\right). \tag{61}$$

For this solution as well as in the previous case the appearance of an exponential factor as

$$\exp\left[\frac{P}{k}\left(\frac{1}{T}-\frac{1}{T_0}\right)\right]$$

characterizes the asymmetric evolution of the profile.

The form of the solution for small values of the $\beta = (\nabla T/T)x$ parameter is written as

$$C(x,t) = \frac{MH_1(t)}{\sqrt{\pi D(0)t}}\exp\left[-\frac{(x-vt)^2}{4D(0)t}\right], \tag{62}$$

where

$$v = -D(0)\frac{2Q^*}{kT_0}\frac{\nabla T}{T_0}, \tag{63}$$

$$H_1(t) = D(0)t\left(\frac{Q^*}{kT_0}\right)^2\left(\frac{\nabla T}{T_0}\right)^2. \tag{64}$$

Hence, the velocity v of the maximum of distribution $C(x,t)$ is distinguished from velocity v_{M} in Mock's approximation.

Falling back upon a higher approximation, the modified diffusion coefficient

$$D_1 = D_0\exp\left(-\frac{E-Q^*}{kT}\right)$$

is introduced. Then, Eq. (58) takes the form

$$\frac{\partial U}{\partial t} = \exp\left(-\frac{Q^*}{kT}\right)\left[\frac{\partial D_1}{\partial x}\frac{\partial U}{\partial x} + D_1\frac{\partial^2 U}{\partial x^2}\right]. \tag{65}$$

Taking into account,

$$\frac{\partial D_1}{\partial x} = -D_1 \frac{Q^* - E}{kT} \frac{\nabla T}{T} \tag{66}$$

we get

$$\frac{\partial U}{\partial t} = D\left[\frac{\partial^2 U}{\partial x^2} - \frac{Q^* - E}{kT} \frac{\nabla T}{T} \frac{\partial U}{\partial x}\right]. \tag{67}$$

Once again, assuming that $1/T(x) \approx 1/T_0$, we find a solution in the form

$$U = \frac{M \exp\left(-\frac{Q^*}{kT_0}\right)}{\sqrt{\pi D(0) t}} \exp\left[-\frac{(x - vt)^2}{4D(0)t}\right], \tag{68}$$

where

$$v = -D(0) \frac{E - Q^*}{kT_0} \frac{\nabla T}{T_0}. \tag{69}$$

Thus,

$$C(x,t) = \frac{M \exp\left[\frac{Q^*}{k}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right]}{\sqrt{\pi D(0) t}} \exp\left[-\frac{(x - vt)^2}{4D(0)t}\right]. \tag{70}$$

For small values of the $\beta = (\nabla T/T)x$ parameter it may be written

$$C(x,t) = H(t) C_{\mathrm{M}}(x,t), \tag{71}$$

that is, for small β this solution coincides with solution (55) – taking into account the temperature dependence $D[T(x)]$. In case condition $\beta \ll 1$ is not fulfilled, we can expect discordance. It is reasonable a solution will be tried to find that conserves both of these temperature dependences:

$$\exp\left[\frac{E}{kT(x)}\right] \text{ and } \exp\left[\frac{Q^*}{kT(x)}\right].$$

3.1.3. Combined consideration of the temperature dependence of the diffusion coefficient and thermodiffusion factor

Introduce the function Z such that

$$C = Z \exp\left[\frac{Q^* + E}{kT}\right]. \tag{72}$$

Substituting C from formula (72) and re-inserting it in Eq. (42), we obtain the expression for the diffusing substance flux

$$J = -D_0 \exp\left(\frac{Q^*}{kT}\right)\left(\frac{\partial Z}{\partial x} - \frac{E}{kT} \frac{\nabla T}{T} Z\right). \tag{73}$$

Then,

$$\operatorname{div} J = \frac{\partial J}{\partial x} = -D_0 \exp\left(\frac{Q^*}{kT}\right)\left[\frac{\partial^2 Z}{\partial x^2} - \frac{Q^* + E}{kT} \frac{\nabla T}{T} \frac{\partial Z}{\partial x} + \frac{E}{kT}\left(\frac{\nabla T}{T}\right)^2\left(\frac{Q^*}{kT} + 2\right) Z\right]. \tag{74}$$

In exactly the same manner as for the function F, disregarding the third term in brackets on the right-hand side of formula (74), we transform the thermodiffusion equation

$$\frac{\partial Z}{\partial t} = D\left[\frac{\partial^2 Z}{\partial x^2} - \frac{Q^* + E}{kT} \frac{\partial Z}{\partial x}\right]. \tag{75}$$

Its solution for the zeroth approximation ($D = D(0)$, $T = T_0$) is given by formula

$$Z(x,t) = \frac{M \exp\left(-\frac{Q^* + E}{kT_0}\right)}{\sqrt{\pi D(0) t}} \exp\left[-\frac{(x - vt)^2}{4D(0)t}\right], \tag{76}$$

where

$$v = D(0) \frac{Q^* + E}{kT_0} \frac{\nabla T}{T_0}. \tag{77}$$

Thus,

$$C(x,t) = \frac{M \exp\left[\frac{Q^* + E}{k}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right]}{\sqrt{\pi D(0) t}} \exp\left[-\frac{(x - vt)^2}{4D(0)t}\right]. \tag{78}$$

For small values of the parameter $\beta = (\nabla T/T)x$,

$$C(x,t) = C_{\mathrm{M}}(x,t). \tag{79}$$

This solution is identical to Mock's solution [8] (9). Thus, we may consider solution (78) as a generalization of Mock's solution for any value of the parameter β. Unfortunately, as in Mock's solution, it is a not very appropriate for measure of Q^* (for the same reasoning previously noted).

3.2. The influence of the change of variable $\xi \to x$ on the solution's form derived in the zeroth approximation

Now let us consider the manner in which the change of variable $\xi \to x$ affects the solution derived in the zeroth approximation for the $U(x,t)$ function (formula (20)). Taking into account that

$$\frac{\partial D^*}{\partial \xi} = D^* \exp\left(-\frac{Q^*}{kT}\right) \frac{E - 2Q^*}{kT} \frac{\nabla T}{T} \tag{80}$$

we transform Eq. (25) to the form

$$\frac{\partial U}{\partial t} = D^* \frac{\partial^2 U}{\partial \xi^2} + D^* \exp\left(-\frac{Q^*}{kT}\right) \frac{E - 2Q^*}{kT} \frac{\nabla T}{T} \frac{\partial U}{\partial \xi}. \tag{81}$$

Setting

$$D^* = D^*(0) = D_0 \exp\left(-\frac{E-2Q^*}{kT_0}\right), \tag{82}$$

$$v = -D^*(0)\exp\left(-\frac{Q^*}{kT_0}\right)\frac{E-2Q^*}{kT_0}\frac{\nabla T}{T_0} \tag{83}$$

we immediately obtain the solution for U:

$$U(\xi,t) = \frac{M}{\sqrt{\pi D^*(0)t}}\exp\left(-\frac{(\xi - vt)^2}{4D^*(0)t}\right). \tag{84}$$

Thus,

$$C(\xi,t) = \frac{M\exp\left[\frac{Q^*}{k}\left(\frac{1}{T(\xi)}-\frac{1}{T_0}\right)\right]}{\sqrt{\pi D(0)t}}\exp\left(-\frac{(\xi - vt)^2}{4D^*(0)t}\right). \tag{85}$$

For small values of the parameter

$$\beta^* = \frac{\nabla T}{T_0}\xi\exp\left(-\frac{Q^*}{kT_0}\right)$$

$$C(\xi,t) = \frac{MH^*(t)}{\sqrt{\pi D(0)t}}\exp\left[-\frac{(\xi - v'^*t)^2}{4D^*(0)t}\right], \tag{86}$$

where

$$v'^* = -D^*(0)\frac{E}{kT_0}\frac{\nabla T}{T_0}\exp\left(-\frac{Q^*}{kT_0}\right), \tag{87}$$

$$H^*(t) = \exp\left[\frac{(Q^*-E)Q^*}{(kT_0)^2}\left(\frac{\nabla T}{T_0}\right)^2 D(0)t\right]. \tag{88}$$

Going into the variable x for small $\beta = (\nabla T/T)x$, we find

$$v'^* \approx v' = -D(0)\frac{E}{kT_0}\frac{\nabla T}{T_0} \tag{89}$$

and,

$$C(x,t) = \frac{MH^*(t)}{\sqrt{\pi D(0)t}}\exp\left[-\frac{(x - v't)^2}{4D(0)t}\right]. \tag{90}$$

Thus, using the example of solution (86), we see that the change $\xi \to x$ leaves the general structure, obtained in the zeroth approximation, unchanged. In the general case, an asymmetric character of dependence $\xi(x)$ leads to the increase of the asymmetric graph $C[\xi(x),t]$ in comparison with the graph $C(x,t)$. Comparing solution (90) (obtained from solution (86) for small β) with solution (55), shows that a consideration of the relation $\xi(x)$ leads to a change of both peak value (the function $H(t) \neq H^*(t)$) and its velocity ($v_M \neq v'$).

This result may be explained in the following manner. The relation $\xi(x)$, as well as the function $U(x,t)$, contains the exponential factor $\exp[-P/kT(x)]$ type ($P = \pm Q^*$). During the process of solving the equation, up to realizing the final result: (the function $U(\xi(x),t)$), an explicit form of the relation is not discovered; thus, the complete information contained in the equation is still not visible. Revealing and approximating the relations is carried out in the final step of solving the transformations $U \to C$ and $\xi \to x$. The method of attack improves the accuracy of the diffusion process descriptions. Because of this, of the two solutions (70) and (90), the second is decidedly the more exact.

3.3. Analysis of the solution obtained in a linear approximation and its transformation for small values of the β parameter

The influence of

$$C(x,t)\exp\left[\frac{P}{kT(x)}\right]\ (P = \text{const})$$

substitutions and the change of the variable $\xi \to x$ on the structure of the diffusion equation solution in a temperature field has already been established in the preceding sections. Summarizing the results, we can, therefore, make the following conclusions.

The influence of temperature on thermodiffusion coefficients – $D[T(x)]$ and $Q^*/kT(x)$ – should be taking into account in the linear approximation for each steps founding the solution independently of one another (solution (32)). In the solution the $K(\xi)$ factor arises primarily because of the

$$U(x,t) = C(x,t)\exp\left(-\frac{Q^*}{kT(x)}\right)$$

substitution. The addendum in brackets of solution (32) arises from taking into account the linear term for expansion into the Macloren series of the function $1/T(\xi)$. Since the substitution of the variable $\xi \to x$ does not change the structure of solution obtained in the zeroth approximation, one might expect it would not have a profound impact on the structure of solution obtained in the linear approximation. Thus, eliminating the addendum in brackets of solution (32) we conserve information about thermodiffusion coefficients' (the diffusion coefficient and thermodiffusion factor) temperature dependence, but drastically simplify the final solution's form. Assuming $\xi \sim \sqrt{D_0^* t}$ and the value of $\alpha_0\sqrt{D_0^* t} \ll 1$ in formulae (32)–(35), the following are obtained:

$$K(\xi) = M\exp\left\{-\frac{2Q^*+E}{4kT_0}\frac{\nabla T}{T_0}\xi\exp\left(-\frac{Q^*}{kT_0}\right)\right\}, \tag{91}$$

$$W(\xi,t) = \frac{\xi}{2\sqrt{D_0^* t}}, \tag{92}$$

$$A(\xi,t) \approx 1. \tag{93}$$

Referring to the variable x for small $\beta = (\nabla T/T)x$ we find

$$\xi(x) = x\exp\left(\frac{Q^*}{kT_0}\right),$$

$$\frac{1}{T(x)} = \frac{1}{T_0 + \nabla T x} \approx \frac{1}{T_0}\left(1 - \frac{\nabla T}{T_0}x\right),$$

$$C(x,t) = \frac{MH_2(t)}{\sqrt{\pi D(0)t}}\exp\left[-\frac{(x - vt)^2}{4D(0)t}\right], \tag{94}$$

where

$$H_2(t) = \exp\left[-\left(\frac{E + 2Q^*}{4kT_0}\frac{\nabla T}{T_0}\right)^2 D(0)t\right], \tag{95}$$

$$v = -\frac{E + 2Q^*}{2kT_0}\frac{\nabla T}{T_0}D(0). \tag{96}$$

Solution (94) has a structure identical to the structure of the solution obtained in the zeroth approximation. Estimate the margin of error involved when the $\operatorname{erfc}W(\xi,t)$ function addendum for the small values of $\alpha_0\sqrt{D_0^* t}$ and $\xi \sim \sqrt{D_0^* t}$ is eliminated. For small values of $\alpha_0\sqrt{D_0^* t}$ and $\xi \sim \sqrt{D_0^* t}$, the value of $A(\xi,t) \approx 1$, then first compare the value of (97)

$$\frac{\alpha_0\exp\left(\frac{Q^*}{kT_0}\right)B(\xi,t)\sqrt{\pi D(0)t}}{2^6} \tag{97}$$

with unity.

Assuming $Q^* \sim E \sim E - 2Q^* \sim 1$ eV, $T \sim 10^3$ K, $\nabla T \sim 10^5$ K/m, $D(0) \sim 10^{-14}$ m^2/s (for self-diffusion of Au [8]), $t \sim 10^4$ s, we find, that the value (97) is equal $\sim 5 \times 10^{-3}$. Consequently, over peak concentration $C(\xi,t)$ we can disregard the summand influence. For small values $\alpha_0\xi$ the function $W(\xi,t)$ is not too different from the function $x/2\sqrt{D(0)t}$. A relative decrease velocity defined as ratio between decrease velocity of exponential function and decrease velocity of error–function complement, which are in brace of relation (32)

$$\frac{(\exp[-W^2(\xi,t)])'}{(\operatorname{erfc}W(\xi,t))'} \sim W(\xi,t) \sim \frac{x}{2\sqrt{D(0)t}}$$

increases proportionally to x. That is the addendum where $\operatorname{erfc}W(\xi,t)$ (for small $\alpha_0\sqrt{D_0^* t}$) emerges only in the distant portions ($\sim 10^2\sqrt{D(0)t}$) of profile tails.

Thus, for small values of the parameters $\alpha_0\sqrt{D_0^* t}$ and β, formula (94) highly accurately describes the diffusion process in a temperature field over a sufficiently wide range of a concentration peak.

As is seen from solution (94) (for small values of the parameter $\beta = (\nabla T/T)x$) the profile is symmetric. A profile asymmetry shows up as the value of β is increased, and can be described in the more general solution

$$C[\xi(x),t] = \frac{K(\xi)}{\sqrt{\pi D(0)t}}\exp\left[-W^2(\xi,t)\right], \tag{98}$$

where $K(\xi)$ and $W(\xi,t)$ is defined by formulae (91) and (92).

3.4. A new method for measuring heat of transport, taking into account the diffusion coefficient and a thermodiffusion factor's temperature dependence

Let the general prerequisites that open the way to formulating new methods for measuring heat of transport be stated.

Consideration of the temperature dependency of the factor $\exp(-P/kT(x))$ in the thermodiffusion equation, leads to an appearance of the factors

$$\exp\left[\frac{P}{k}\left(\frac{1}{T(x)} - \frac{1}{T_0}\right)\right]$$

in its solutions. It has a pronounced effect on the dependence $C(x,t)$, expressed in a profile asymmetry. The result is in agreement with qualitative conclusions regarding the profound influence that profile asymmetry has on the maximum distribution velocity of a diffusing substance [4].

For small values of the parameter $\beta = (\nabla T/T)x$ the factor is written

$$\exp\left[\frac{P}{k}\left(\frac{1}{T(x)} - \frac{1}{T_0}\right)\right] \approx \exp\left[-\frac{P}{kT_0}\frac{\nabla T}{T_0}x\right]$$

and, an index of an exponent is set linear with respect to x. In this case the information on profile asymmetry is lost, however, its velocity and value do differ greatly from the corresponding dependence derived without consideration of this factor.

Different form of the solutions $C(x,t)$ that the temperature dependence of $\exp(-P/kT(x))$ is taken into account against the value of P and the way of solving of the thermodiffusion equation shows that even with a small value of β, the zeroth approximation of $\exp(-P/kT(x))$ (for reasonable description of the process) is lacking. To make an estimate of heat of transport the linear approximation formula (32) is required. For small values of β solution (32) can be put in form (94) whose simplicity provides a new method for measuring heat of transport.

Denote

$$C_0 = \frac{M}{\sqrt{\pi D(0)t}}. \tag{99}$$

Then, taking the logarithm of formula (94) we find

$$\ln C - \ln C_0 = y = -\frac{E + 2Q^*}{4kT_0}\frac{\nabla T}{T_0}x - \frac{1}{4D(0)t}x^2. \tag{100}$$

Further, taking a derivative of this function, we can write

$$\frac{\mathrm{d}\ln C}{\mathrm{d}x} = y' = -\frac{E + 2Q^*}{4kT_0}\frac{\nabla T}{T_0} - \frac{1}{2D(0)t}x. \tag{101}$$

The dependence $y'(x)$ is a linear function. Giving the function $\ln C$ in the tabulated manner at equally small intervals Δx, we can approximately formulate

$$y' = \frac{\Delta \ln C}{\Delta x}. \tag{102}$$

The graphic $\Delta \ln C/\Delta x(x)$ will illustrate a straight line. Then, from the condition $x = 0$ we find

$$Q^* = -\left[2kT_0 \frac{T_0}{\nabla T} y'(0) + \frac{E}{2}\right]. \tag{103}$$

4. Conclusion

The thermodiffusion equation's analysis has been completed, taking into account the diffusion coefficient and thermodiffusion factor's temperature dependence (which, is involved in the exponential factors such as $\exp(-P/kT(x))$ $(P = \text{const})$) in a linear approximation of expanding the function $1/T(x)$ into Macloren's series. Three principal stages of its derivation are recognized: namely, the substitution $U(x,t) \to C(x,t)$, the changing $\xi \to x$, and the expansion of the function $1/T[\xi(x)]$ into Macloren's series up to the linear term. The affect of each on the equation's finite form is examined. It is shown that even within the limits of the zeroth approximation, expansion of the function $1/T(x)$ into Macloren's series, brings to light the principal factors having a substantial effect on the dependence $C(x,t)$, and which cause profile asymmetry namely, the factor

$$\exp\left[\frac{P}{k}\left(\frac{1}{T(x)} - \frac{1}{T_0}\right)\right].$$

A number of the approximations in which P takes the values $E, Q^*, Q^* + E$ are examined. A comparison of these solutions with the solutions in the linear approximation allows a conclusion to be made regarding the zeroth approximation if temperature dependence of $D[T(x)]$ and $Q^*/[kT(x)]$ is taken into account: a reasonable degree of accuracy is not yielded for the diffusion process descriptions in the temperature field; and, for measuring its central parameters (namely, the heat of transport – Q^*). Using the thermodiffusion equation's solution for an instantaneous plane source in semi-infinite media [7] at the value of the parameters $\alpha_0\xi$ and $\beta \ll 1$, the new method of measuring of heat of transport Q^* has been proposed.

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