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COMPUTATION OF THE DIFFUSION COEFFICIENT FOR A NONMETAL MATERIAL IMMERSED IN LIQUID

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Abstract

In this paper we consider a mathematical model of the diffusion process for nonmetal materials immersed into liquids. A method for determination of the diffusion coefficient characterizing the evolution process of liquid penetration into the non metal body is established. A practical example illustrating the method is considered.

Keywords: *diffusion; evolution process; parabolic differential equation; Bessel functions; Dirichlet boundary condition*

1 Introduction.

In this paper the authors investigate the diffusion problem connected with the penetration of any fluid in nonmetal cylindrical body Ω, a vulkanizat, with a boundary $\partial\Omega$, whose length *L* exceeds many times its diameter *d*. Similar problems are considered in the illustrious monograph of Krank, [7]. We consider the initial and boundary value problem (IBVP for short) with Dirichlet boundary condition,

$$\frac{\partial C}{\partial t} = D\Delta C\,,\ (t,x,y,z)\in(0,T]\times\Omega\,,\ \Omega\subset\mathbb{R}^3 \qquad (1)$$

$$C(0,x,y,z) = C_0(x,y,z)\,,\ (x,y,z)\in\Omega\,, \qquad (I)$$

$$C(t,x,y,z)\big|_{\partial\Omega} = C_1(t,x,y,z)\ \ (t,x,y,z)\in[0,T]\times\partial\Omega\,, \qquad (B)$$

where (I) and (B) are initial and boundary data, respectively, and *C* is the concentration of the penetrating liquid in the cylindrical body; $J=(0,T]\subset\mathbb{R}_+$; Δ is the Laplace operator. Here accept the notations $C_t\equiv\dfrac{\partial C}{\partial t}\equiv\partial_t$, $\Delta\equiv\partial^2_{xx}+\partial^2_{yy}+\partial^2_{zz}$; note that is possible $T=+\infty$. The diffusion equation (1) as it is known is a parabolic PDE. We prefer to represent it further in cylindrical variables under very simple initial and boundary data. As we mentioned above the cylindrical body, that is a rod, is made of nonmetal material, which is actually immersed into an aggressive liquid. This diffusion problem may encounter everywhere in the practice, [1], [8-11]. Also it is known that the molecules of the liquid penetrate into the cylinder as the evolution process starts at the initial moment *t* = 0, and continue to the final point of the fixed interval *J* = [0; *T*] (*T* > 0). The IBVP is well learned, [5,6], but the calculation of diffusion coefficient *D* used in the diffusion equation turns out a difficult task which motivate us to offer a practical approach of computation of *D*. We establish a practical method to assessment of the diffusion coefficient *D* as for this purpose use the solution of the IBVP that is a function expressed by Bessel functions, [2-7]. Thus the solution is the map $\tilde{u}=\tilde{u}(\tau,\rho)$, where the variable τ and ρ are linear functions of time *t* and radial variable *r*, respectively, and $\tilde{u}$ is a linear function of the real concentration *C*. Therefore we have three variables which do not depend on their physical measures, moreover, the triple $(\tau,\rho,\tilde{u})$ sweeps the set $[0,1]\times[0,1]\times[0,1]$. Taking into account the graph $\Gamma_{\tilde{u}}\equiv\{(\tau,\rho,\tilde{u}):0\le\tau,\rho,\tilde{u}\le 1;\tilde{u}=\tilde{u}(\tau,\rho)\}$ of the function $\tilde{u}=\tilde{u}(\tau,\rho)$, that is the solution of the considered IBVP, and measuring the distribution of liquid's concentration in radial direction of the considered rod, then after simple computing obtain the coefficient of diffusion *D*. The advantage of this method is that one may assess the diffusion coefficient *D* to any unknown diffusion process concerning nonmetal materials immersed in any liquid independently of the interior structure of the material. The problem (1) is well learned, [6,7], but the calculation of *D* turns out that is a difficult task which motivate us to offer a practical approach of computation of *D*. More intricate mathematical models describing the diffusion processes with nonlinear reaction functions can be found in [8-11]. Finally, conclude that almost the same method can be used for nonlinear diffusion problems.

2 Preliminaries and assessment of diffusion coefficient.

Consider the classical IBVP (1) with initial and boundary data (I) and (B), respectively. Here *C* is the concentration of the penetrating liquid in the cylindrical body, which is an unknown function, $\Omega\subset\mathbb{R}^3$ is a bounded domain with sufficiently smooth boundary $\partial\Omega$, and the initial and boundary functions C_0 and C_1, respectively, are sufficiently smooth as well. The main object under consideration is a set having cylindrical shape (rod) denoted by Ω immersed into a liquid. It is known that the molecules of the liquid penetrate into the cylinder as the evolution process starts at the initial moment *t* = 0 and continue to the end of a fixed interval *J* = [0; *T*].

Assume that the cylinder has radius *r = a* and length *L* > > *a*. Taking into account that Ω is a cylinder therefore we introduce in (1) cylindrical coordinates as for this purpose introduce the radial variables *r*, θ (polar angle), and *z*-coordinte, that is, from *(t; x; y; z)* get to *(t;r)* due to the axial symmetry of the cylindrical domain Ω. Thus from IBVP (1) obtain the following one-dimensional IBVP with proper initial and boundary conditions:

$$\begin{aligned} &C_t = D\left(\frac{1}{r}C_r + C_{rr}\right),\ 0 < r < a,\ 0 < t < T, \\ &C = 0,\ r = 0,\ r = a,\ 0 < t < T, \\ &C = \varphi(r),\ 0 < r < a,\ t = 0. \end{aligned} \tag{2}$$

Here we are interested in the analytical solution of (2). It is known that it can be represented by a functional series containing the known Bessel functions:

$$C = \frac{2}{a^2}\sum_{k=1}^{\infty} e^{-D\alpha_k^2 t}\,\frac{J_0(\alpha_k r)}{J_1^2(\alpha_k a)}\int_0^a r\varphi(r)J_0(\alpha_k r)dr\ . \tag{3}$$

Here $J_0(x),\ J_1(x)$ are the Bessel functions of the first kind, and of the zero and first order, respectively; the numbers $\alpha_k a$ are roots of J_0, i.e. $J_0(\alpha_k a) = 0\ (k = 1, 2, \ldots)$ (see e.g., [2], [3], [5-7]). Obviously the unknown function *C(t,r)* is differentiable infinitely many times. Furthermore, consider the inhomogeneous Dirichlet problem (2) under the boundary condition $C\,|_{\partial\Omega} = C_1$, for $r = 0$ and $r = a\ (t > 0)$, and the initial condition $C = C_0$ for $0 < r < 0,\ t = 0,$ where C_0, C_1 are some real constants. Next in order to make the problem independent of the physical measurement we introduce in (2) certain dimensionless variables instead *C, r,* and *t* as for this purpose set

$$C = (C_1 - C_0)u + C_0\ ,\ \tau = \frac{D}{a^2}t\ ,\ \rho = \frac{1}{a}r\ ,$$

whence obtain the transformation formulae for the differential operators

$$\partial_t = \frac{D}{a^2}\partial_\tau,\ \partial_\tau = \frac{D}{a^2}\partial_\rho,\ \partial_{rr}^2 = \frac{D}{a^2}\partial_{\rho\rho}^2\ .$$

The new IBVP in the new variables τ, ρ, u has the form

$$\begin{aligned}&\partial_t u = \frac{1}{\rho}\partial_\rho u + \partial^2_{\rho\rho} u,\ \ 0<\tau\le 1,\ \ 0<\rho\le 1,\\&u=1,\quad \text{for}\quad \rho=0,\ \ \rho=1,\ \ 0<\tau\le 1,\\&u=0,\quad \text{for}\quad 0<\rho<1,\ \ \tau=0.\end{aligned} \tag{4}$$

Therefore the solution of (4) takes the form:

$$u \equiv \frac{C-C_0}{C_1-C_0} = 1-\frac{2}{a}\sum_{k=1}^{\infty} e^{-\alpha_k^2 a^2 \tau}\,\frac{J_0(\rho a\alpha_k)}{\alpha_k J_1(a\alpha_k)}\ . \tag{5}$$

We observe that the quantity $u \equiv \dfrac{C-C_0}{C_1-C_0}$ $(C_1 > C_0)$ is dimensionless, and taking into account the known fact that only the first four summands in the series (5) have essential contribution to the quantity $u(\tau,\rho)$, i.e. one has that

$$u(\tau,\rho) \approx \tilde{u}(\tau,\rho) = 1-\frac{2}{a}\sum_{k=1}^{4} e^{-\alpha_k^2 a^2 \tau}\,\frac{J_0(\rho a\alpha_k)}{\alpha_k J_1(a\alpha_k)}, \tag{6}$$

where the roots α_k $(k=1,2,3,4)$ of Bessel functions are known (see e.g., [1], [5], [6]),

$$\alpha_1 = \frac{2,405}{a},\ \ \alpha_2 = \frac{5,52}{a},\ \ \alpha_3 = \frac{8,654}{a},\ \ \alpha_4 = \frac{11,7915}{a}\ .$$

The latter means that $J_0(2.405) = J_0(5.52) = J_0(8.654) = J_0(11.7915) = 0.$ It is convenient the approximate solution (6) of the considered problem (4) to be written in the form

$$\begin{aligned}\tilde{u}(\tau,\rho) = 1 &- 2e^{-2,405^2\tau}\,\frac{J_0(2,405\rho)}{2,405 J_1(2,405)} - 2e^{-5,52^2\tau}\,\frac{J_0(5,52\rho)}{5,52 J_1(5,52)} -\\ &-2e^{-8,654^2\tau}\,\frac{J_0(8,654\rho)}{8,654 J_1(8,654)} - 2e^{-11,7915^2\tau}\,\frac{J_0(11,7915\rho)}{11,7915 J_1(11,7915)}.\end{aligned} \tag{7}$$

This function has the following 3-D graph as for this purpose Matlab was used:

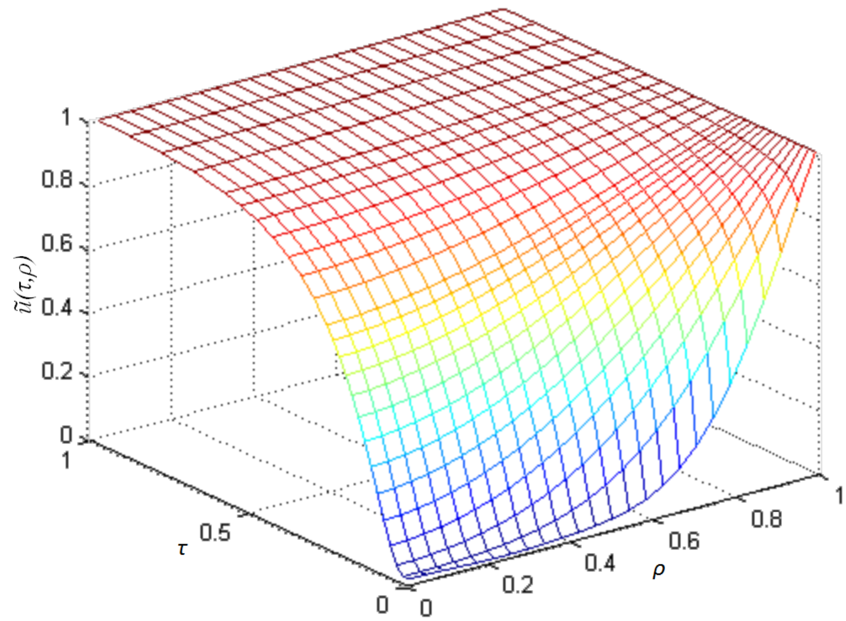

Fig. 1

An example for assessment of diffusion's coefficient. The method that we consider here is built on two basic facts:

(i) Experimental data of the radial distribution to the concentration *C* of the penetrating liquid

substance into the cylindrical surface provided that the initial and boundary data are known preliminarily.

(ii) Theoretical distribution received as an approximate solution $\tilde{u}(\tau,\rho)$ of the IBVP (4) to the diffusion equation under the same initial and boundary data, which can be seen on Fig. 1.

Assume that the liquid is water which does not provoke any chemical reaction with the matter of the surface layer of the cylindrical body, and the period of time $T = 7 \times 10^5$ [s]. Therefore, the liquid penetrates in the cylinder through the radial direction without changing the chemical structure. Assume that the radius of the cylinder is $a = 0.005$ [m], and its length is many times greater than *2a*. In order to calculate *D* we measure experimentally the concentration $\tilde{C}$ at a finite number of points on the radius of the circular section of the immersed rod, and at many fixed times $t_0=0, t_1, t_2, \ldots, T$. Next using the transformation formulae $\tilde{u}(\tau,\rho) \equiv \dfrac{\tilde{C}-C_0}{C_1-C_0}$, $\tau = \dfrac{D}{a^2} t$,

$\rho = \frac{1}{a} r$, as well the measured data for *t* and *r*, obtain the following numerical results written in the following table:

$\tilde{u}(\tau, \rho_i)$	0.15	0.25	0.35	0.45	0.55	0.65	0.75	0.85	0.95
D	34.72 $\times 10^{-12}$	34.72 $\times 10^{-12}$	34.72 $\times 10^{-12}$	34.72 $\times 10^{-12}$	34.72 $\times 10^{-12}$	34.72 $\times 10^{-12}$	34.72 $\times 10^{-12}$	34.72 $\times 10^{-12}$	34.72 $\times 10^{-12}$
τ_i	0.005	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08
t_i [s]	3.6 $\times 10^3$	5 $\times 10^3$	1 $\times 10^4$	5 $\times 10^4$	1 $\times 10^5$	5 $\times 10^5$	7 $\times 10^5$	8 $\times 10^5$	9 $\times 10^5$

Table. 1

Thus for instance the concentration $\tilde{u}$ = 0.15 measured at the moment $t_1 = 3.6 \times 10^3$ (first vertical column) concerns the points located nearby the surface of the cylinder at the distance defined by $\rho_1 = 0.825$. Notice that the quantity ρ = *r/a* give us an information for the distance measured from the center of the circle through radial direction. The already measured quantity $\tilde{u}$ = 0.15 corresponds to the function $\tilde{u} = \tilde{u}(0.005; \rho)$ along with the corresponding graph made at the fixed parameter τ_1 = 0.005, that is shown on the following graph:

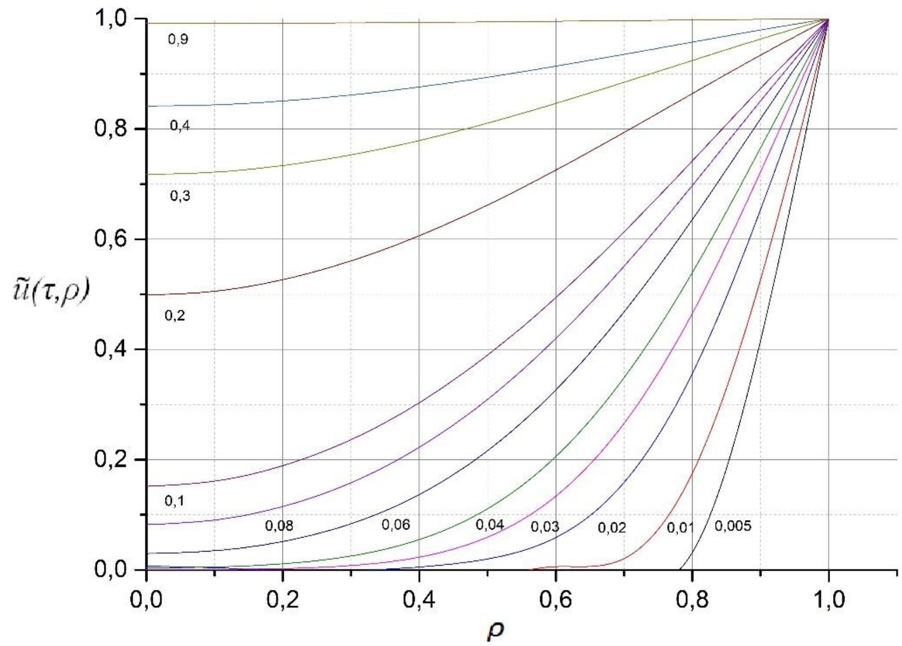

Fig. 2

We note that the family of graphs of Fig. 2 are the orthogonal projections of the parallel to the coordinate plane $\rho O\tilde{u}$ (on Fig. 1) sections cutting the graph of the solution $\tilde{u} = \tilde{u}(\tau;\rho)$.

The problem for assessment of *D* can be seen also after drawing a parallel to $O\rho$ line crossing the graph of the function $\tilde{u} = \tilde{u}(0.005;\rho)$ at the point $(0.825; 0.005)$. Next we draw a vertical line at the point $\rho = 0.825$ and consider the crossing points located on the graphs corresponding to the quantities ρ_i (Table. 1). Finally, calculate the diffusion coefficient by the formula $D = \frac{a^2}{t_i}\tau_i = const \quad (i = 1, 2, ..., 9)$, thus conclude that $D = 34.72\ 10^{-12}[m^2 / s]$ is a constant. Furthermore, we demonstrate the constant value of *D* by computing with aid of the same method for $\tau_2 = 0.01$, $\tau_3 = 0.02$, . . . , $\tau_9 = 0.08$ which can be seen in Tabl.1.

As a conclusion we suggest that one may apply the above stated method to calculate the diffusion coefficient for nonlinear diffusion models.

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