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A DIRECT VARIATIONAL METHOD FOR THE DETERMINATION OF THE EQUIVALENT TIME CONSTANT OF DIFFUSION PROCESSES

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Abstract—The Ritz variational method is suggested for use in the determination of the equivalent time constant of diffusion processes. General formulas are obtained and illustrated with examples.

NOMENCLATURE

A, **C**,	symmetric matrixes of elements a_{ij}, c_{ij};
B, **Θ**, **Ψ**,	column matrixes of elements b_i, ϑ_i, $\psi_i(t)$;
D,	coefficient of diffusion;
$\mathscr{F}\langle T\rangle$,	function;
T_0,	input progress;
T,	output progress;
$W(s)$, $W_i(s)$,	polynomials;
a, R,	linear dimensions;
t,	time;
s,	parameter of Laplace transform.

Greek symbols

α_i,	coefficients;
τ_0, τ,	equivalent time constants;
τ_i,	time constants;
$\varphi_i(P)$,	coordinate functions;
$\psi_i(t)$,	functions of variable t;
$L^2(\Omega)$,	space of functions which are integrable with a square.

1. INTRODUCTION

THE DIFFUSION processes, such as thermal conduction, osmosis in solutions, and the diffusion of an electromagnetic field, are described by the equation [6, 8]

$$\Delta T = D\frac{\partial T}{\partial t}. \tag{1}$$

A solution of equation (1) under certain boundary conditions is the sum of the elementary exponential functions [6]

$$T(P,t) = \sum_{i=1}^{\infty} T_i(P,0)\exp(-t/\tau_i). \tag{2}$$

The estimation of the duration of an unsteady process using equation (2) is very difficult. To avoid such difficulties one can introduce an equivalent time constant [5]

$$\tau(P) = \int_0^\infty \frac{T(P,t)-T(P,\infty)}{T(P,0)-T(P,\infty)}\,\mathrm{d}t \tag{3}$$

which is a characteristic parameter of the duration of an unsteady process at a certain point P.

It is only possible to obtain the exact solution, equation (2), of equation (1) in a few cases. The problem is more complicated when the coefficient D in equation (1) is not a constant, but a function $D(P)$. A variational method which allows one to determine an approximate solution of equation (1) in an analytic form has been suggested [2, 3, 7]. After using the Ritz variational method for the boundary problem of equation (1), a general equation for the determination of the equivalent time constant of diffusion processes can be obtained. Some examples are presented.

2. GENERAL CASE

Let us consider equation (1) bounded by a smooth curve Γ, area Ω, with the boundary

$$T(P,t)|_{P\in\Gamma} = T_0(t) \tag{4}$$

and the initial conditions

$$T(P,0) = T^* \equiv 0. \tag{5}$$

The calculation of the solution of equation (1) is equivalent to the variational problem of the determination of the minimum of the energy function [3, 7]

$$\mathscr{F}\langle T\rangle \equiv \int_\Omega\int\left[(\nabla T)^2 + 2DT\frac{\partial T}{\partial t}\right]\mathrm{d}\Omega = \text{minimum}. \tag{6}$$

One can carry out a minimalisation of equation (6) by means of the Ritz method [4]. According to this method the approximate solution is of the form

$$\tilde{T}(P,t) = T_0(t) + \sum_{i=1}^{n}\psi_i(t)\varphi_i(P) \tag{7}$$

where the functions $\varphi_i(P)$ vanish on the boundary Γ and form a complete, linearly independent set in Hilbert space $L^2(\Omega)$. The functions $\psi_i(t)$ can be determined from the system of linear differential equations

$$\mathbf{A}\Psi(t) + \mathbf{C}\frac{\mathrm{d}\mathbf{\Psi}(t)}{\mathrm{d}t} = -\frac{\mathrm{d}T_0(t)}{\mathrm{d}t}\,\mathbf{B}. \tag{8}$$

Applying the criterion of least square deviation,

$$\int_{\Omega}\int [\tilde{T}(P,0)-T^{*}]^{2}\,\mathrm{d}\Omega = \text{minimum}, \qquad (9)$$

one can show that

$$\mathbf{\Psi}(0) = \mathbf{0}. \qquad (10)$$

The system of equations (8) arose from the condition of the existence of the variational integral (6). The elements of matrices **A**, **B** and **C** can be calculated from

$$\begin{aligned} a_{ij} &= \int_{\Omega}\int \nabla\varphi_i \nabla\varphi_j\,\mathrm{d}\Omega, \\ b_i &= \int_{\Omega}\int D\varphi_i\,\mathrm{d}\Omega, \\ c_{ij} &= \int_{\Omega}\int D\varphi_i\varphi_j\,\mathrm{d}\Omega. \end{aligned} \qquad (11)$$

Thus the boundary problem, equations (4) and (5), for equation (1) has been resolved into a system of linear differential equations.

3. EQUIVALENT TIME CONSTANT

Let $T(P,s)$ be the image of the Laplace transform of the function $T(P,t)$. Then equation (3) is equivalent to [5]

$$\tau(P) = \frac{\lim_{s\to 0}[sT(P,s)]'}{T(P,0)-T(P,\infty)}. \qquad (12)$$

Transforming the system, equation (8), one can obtain

$$(\mathbf{A}+s\mathbf{C})\mathbf{\Psi}(s) = -sT_0(s)\mathbf{B} \qquad (13)$$

from which it is easy to calculate the functions

$$\psi_i(s) = -sT_0(s)\frac{W_i(s)}{W(s)} \qquad (14)$$

where $W(s)$ and $W_i(s)$ are appropriate determinants obtained from Cramer formulas.

If τ_0 is the equivalent time constant for $T_0(t)$ then from equations (7) and (12) one can finally derive the equivalent time constant for the process $T(P,t)$

$$\tau = \tau_0 + \sum_{i=1}^{n}\frac{W_i(0)}{W(0)}\varphi_i(P) \qquad (15)$$

where as it is easily seen that the quotients $\vartheta_i = [W_i(0)/W(0)]$ form the solution of the following system of linear algebraic equations

$$\mathbf{A}\cdot\mathbf{\Theta} = \mathbf{B}. \qquad (16)$$

Equations (15) and (16) allow one to determine the equivalent time constant for $T(P,t)$ a simple and convenient numerical method. The accuracy of the calculation depends directly on the number of functions φ_i taken.

4. EXAMPLES OF APPLICATION

4.1. *Equivalent time constant for an infinite sheet*

The system under consideration is shown in Fig. 1. Obtaining a solution of equation (1) for an arbitrary function $D = D(\rho)$, where $\rho = x/a$ is not easy, even in that simple system.

Representing the function $D(\rho)$ as the sum of a power series, one can approximate it by the polynomial

$$D(\rho) = \sum_{p=0}^{k}\alpha_p\rho^{p}. \qquad (17)$$

It is assumed that the functions φ_i have the form

$$\varphi_i(\rho) = (1-\rho^2)\rho^{i-1} \qquad (18)$$

These functions fulfil all the conditions mentioned above. Using equation (11) one can obtain

$$a_{ij} = \frac{1}{a}\int_{-1}^{1}\varphi_i'\varphi_j'\,\mathrm{d}\rho = \begin{cases} 0 & \text{for } i+j \text{ odd}, \\ \dfrac{8(2ij-i-j-1)}{a[(i+j)^2-1](i+j-3)} & \text{for } i+j \text{ even}, \end{cases}$$

$$b_i = a\int_{-1}^{1}D(\rho)\varphi_i\,\mathrm{d}\rho = \begin{cases} 0 & \text{for } i+p \text{ even}, \\ \displaystyle\sum_{p=0}^{k}\frac{4a\alpha_p}{(i+p+1)^2-1} & \text{for } i+p \text{ odd}. \end{cases} \qquad (19)$$

Numerical calculations have been based on equations (18), (19), (15) and (16). Figure 2 shows the distribution of the function $f = (\tau-\tau_0)/a^2$ for various forms of $D(\rho)$. In the particular case when D = const. one can obtain by that means the equation, well-known in the literature [5],

$$\tau = \tau_0 + 0.5D(a^2-x^2)$$

4.2 *Infinitely long cylinder*

Assuming $D(\rho)$ in the form of equation (17), and that the φ_is have the form

$$\varphi_i(\rho) = (1-\rho)\rho^{i-1}; \quad \rho = \frac{r}{R}, \qquad (20)$$

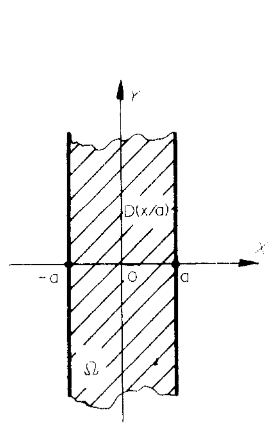

FIG. 1. Sheet of infinite dimensions in Cartesian coordinate system.

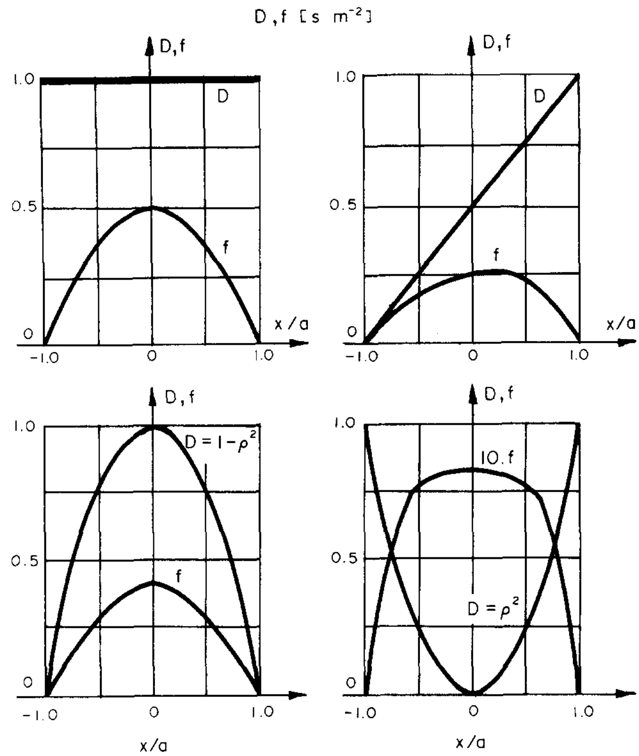

FIG. 2. Function $f = (\tau-\tau_0)/a^2$ vs x.

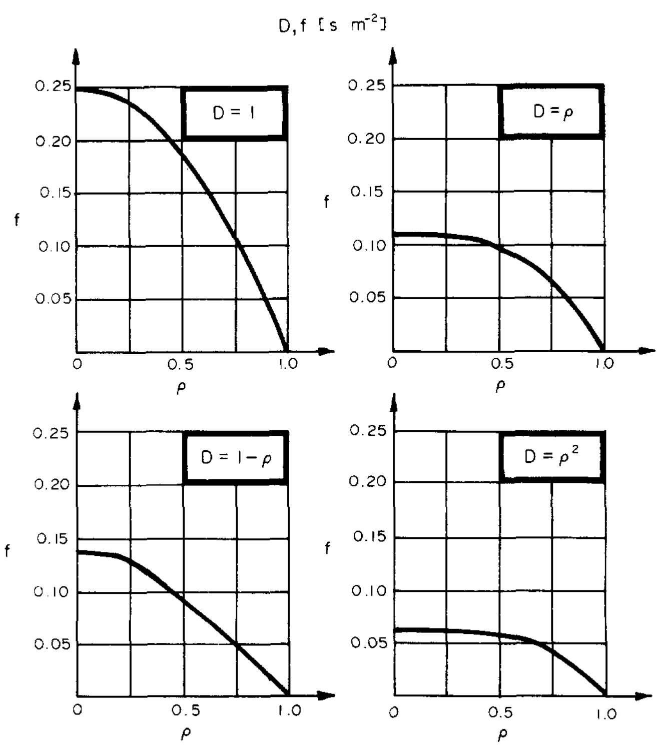

FIG. 3. Function $f = (\tau-\tau_0)/R^2$ vs r for various types of function $D(\rho)$.

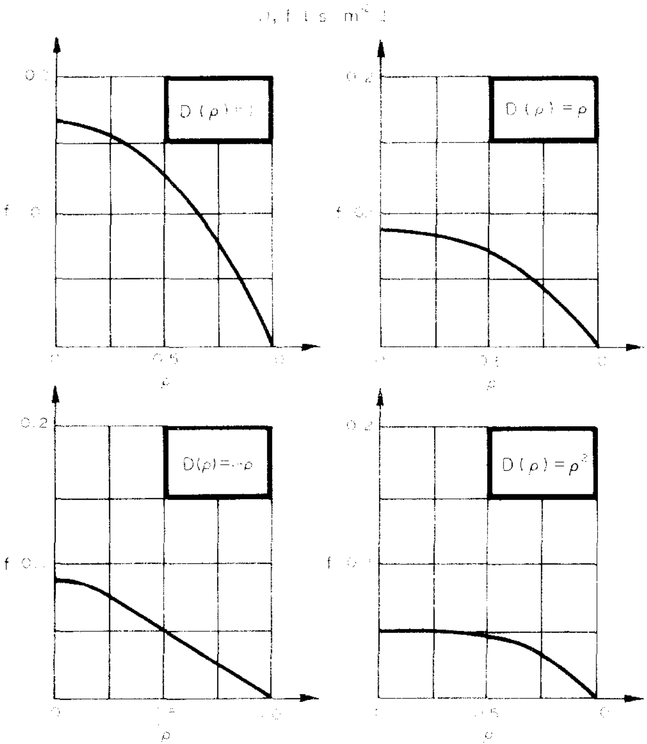

FIG. 4. Function $f = (\tau - \tau_0)/R^2$ vs r for various types of function $D(\rho)$.

Consequently from equation (11), one can obtain

$$a_{11} = \frac{1}{2},$$

$$a_{ij} = \int_0^1 \varphi_i'\varphi_j'\rho \, d\rho = \frac{2ij - i - j}{(i+j)(i+j-1)(i+j-2)}$$

$$\text{for } i+j > 2$$

$$b_i = R^2 \int_0^1 D(\rho)\varphi_i\rho \, d\rho = R^2 \sum_{p=0}^{k} \frac{\alpha_p}{(p+i+1)(p+i+2)}. \tag{21}$$

The results of the numerical calculation of the function $f = (\tau - \tau_0)/a^2$ for various forms of $D(\rho)$ are presented in Fig. 3. The case where D = const. has been investigated in ref. [5]. The equivalent time constant was expressed there by means of a Bessel function. The results were the same as obtained here.

4.3. *Ball*

Taking for a ball of radius R, the functions φ_i and $D(\rho)$ in the same form as equations (20) and (17), respectively, one can calculate the elements of the matrices **A** and **B**

$$a_{ij} = R \int_0^1 \varphi_i'\varphi_j'\rho^2 \, d\rho = \frac{2ijR}{(i+j-1)(i+j)(i+j+1)}$$

$$b_i = R^3 \int_0^1 D(\rho)\varphi_i\rho^2 \, d\rho = R^3 \sum_{p=0}^{k} \frac{\alpha_p}{(p+i+2)(p+i+3)}. \tag{22}$$

The function $f = (\tau - \tau_0)/R^2$ for various forms of $D(\rho)$ is plotted in Fig. 4. The results for D = const. do not differ from these obtained in ref. [5] by means of Legendre functions.

5. CONCLUSIONS

In this paper, the Ritz variational method has been applied to determine the equivalent time constant of diffusion processes. General formulas have been obtained which allow one to calculate the duration of an unsteady diffusion process in a simple and convenient numerical method. The method has been illustrated by cases which are generalisations of those in ref. [5]. Taking appropriately large values of the number n, one can perform the calculations with any required accuracy.

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METHODE VARIATIONNELLE DIRECTE POUR LA DETERMINATION DE LA CONSTANTE DE TEMPS EQUIVALENTE DU PROCESSUS DE DIFFUSION

Résumé—La méthode variationnelle de Ritz est suggérée pour la détermination de la constante de temps équivalente du processus de diffusion. Des formules générales ont été obtenues et elles sont illustrées par quelques exemples.

EIN DIREKTES VARIATIONSVERFAHREN ZUR BESTIMMUNG DER MITTLEREN ZEITKONSTANTE DER DIFFUSIONSPROZESSE

Zusammenfassung—In der vorliegenden Arbeit wurde ein direktes Variationsverfahren angegeben, welches die Bestimmung der mittleren Zeitkonstante der Diffusionsprozesse gestattet. Es werden die allgemeine Formeln vorausgesetzt und die Anwendungsbeispiele dargestellt.

НЕПОСРЕДСТВЕННЫЙ ВАРИАЦИОННЫЙ МЕТОД ОПРЕДЕЛЕНИЯ ЭКВИВАЛЕНТНОЙ ПОСТОЯННОЙ ВРЕМЕНИ ДИФУЗИОННЫХ ПРОЦЕССОВ

Аннотация—В настаящем труде представлен непосредственный метод, который разрешяет определить эквивалентную постоянную времени. Выведено общие формулы и представлено пимеры применений.