SOLUTION OF A BOUNDARY-VALUE PROBLEM FOR THE GENERALIZED DIFFUSION EQUATION

V. N. Chigarev and I. M. Fedotkin

UDC 532.52; 532.72

The boundary-value problem is solved for the complete diffusion equation and then for the same equation with a chemical reaction taken into account, for the case of a liquid flow for which the width and length are much larger than the thickness.

The problem of diffusion in a thin liquid layer in laminar flow around a plate with a length and width much larger than the layer thickness was solved in [1-4], but under various assumptions, used to simplify the basic diffusion equation

$$\frac{\partial C}{\partial t}+v_x\frac{\partial C}{\partial x}+v_y\frac{\partial C}{\partial y}=D\left(\frac{\partial^2 C}{\partial x^2}+\frac{\partial^2 C}{\partial y^2}\right). \tag{1}$$

These solutions were found for the particular cases in which this equation does not contain the terms corresponding to local, convective, or molecular diffusion. As a consequence, the solutions of the boundary-value problems for Eq. (1) for various initial and boundary conditions suffered from a loss of completeness. It is therefore a matter of practical interest to seek an effective method for solving such problems for Eq. (1) in its complete form. Below we take up one of these problems, which is solved by the method of a complex two-dimensional Fourier transformation with infinite integration limits [5-7]. The problem involves seeking the function C (t, x, y) which determines the concentration of particles of the material diffusing in a liquid flow of thickness δ and of width and length much larger than δ. The initial condition is $C(t,x,y)|_{t=0} = C(x, y)$ and the boundary conditions are

$$C|_{x=\infty}=\left.\frac{\partial C}{\partial x}\right|_{x=\infty}=0,\quad C|_{y=\infty}=\left.\frac{\partial C}{\partial y}\right|_{y=\infty}=0.$$

The flow velocity is assumed known, the velocity components v_x and v_y are given and are independent of the coordinates, and the diffusion is assumed plane-parallel, i.e., independent of the coordinate z (Fig. 1).

In this solution method, Eq. (1) is subjected to a Fourier transformation with respect to two variables, in our case, the coordinates x and y; in this manner the partial differential equation can be reduced to an ordinary differential equation for the transforms. It is a simpler matter to solve the latter type of equation [5-7]. Under the assumption that the unknown function C (t, x, y) satisfies Dirichlet conditions on the intervals (−∞, ∞) along the x and y axes, we can write the two-dimensional transform of this function as

$$\bar{C}(t,\ \zeta,\ \eta)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}C(t,\ x,\ y)\exp i(\zeta x+\eta y)\,dxdy, \tag{2}$$

We can write the function itself in terms of the transform:

$$C(t,\ x,\ y)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\bar{C}(t,\ \zeta,\ \eta)\exp[-i(\zeta x+\eta y)]\,d\zeta dy. \tag{3}$$

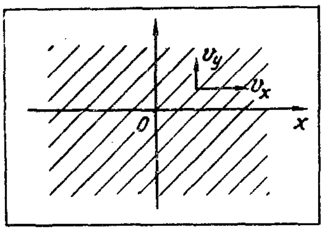

Fig. 1. Flow diagram.

Kiev Technological Institute of the Food Industry. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 27, No. 4, pp. 714-719, October, 1974. Original article submitted February 25, 1974.

Accordingly, we find, for example,

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\partial C}{\partial t}\exp i(\zeta x+\eta y)\,dxdy$$

$$=\frac{1}{2\pi}\int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty}\frac{\partial C}{\partial t}\exp i\zeta x dx\right)\exp i\eta y dy$$

$$=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\partial\bar{C}(t,\ \zeta,\ y)}{dt}\exp i\eta y dy=\frac{d\bar{C}(t,\ \zeta,\ \eta)}{dt}; \tag{4}$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\partial C}{\partial x}\exp i(\zeta x+\eta y)\,dxdy=-i\zeta\bar{C}(t,\ \zeta,\ \eta); \tag{5}$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\partial^2 C}{\partial x^2}\exp i(\zeta x+\eta y)\,dxdy=-\zeta^2\bar{C}(t,\ \zeta,\ \eta)\quad(6)\ \text{etc.} \tag{6}$$

Multiplying (1) term by term by $1/2\pi \exp i(\zeta x+\eta y)$ and evaluating the double integrals of all terms in (1), as in the preceding examples, we find

$$\frac{\partial\bar{C}}{\partial t}+[D(\zeta^2+\eta^2)-i(v_x\zeta+v_y\eta)]\,\bar{C}=0. \tag{7}$$

In evaluating the integrals like those in (4)-(6) we used the boundary conditions specified in the formulation of the problem.

Separating variables in Eq. (7), we find

$$\frac{d\bar{C}}{\bar{C}}=-[D(\zeta^2+\eta^2)-i(v_x\zeta+v_y\eta)]\,dt,$$

and thus

$$\ln\bar{C}=-[D(\zeta^2+\eta^2)-i(v_x\zeta+v_y\eta)]\,t+C_1$$

or

$$\bar{C}=C_0\exp\{-[D(\zeta^2+\eta^2)-i(v_x\zeta+v_y\eta)]\,t\}, \tag{8}$$

where C_1 and C_0 are arbitrary constants. To determine the constant C_0 we use the initial condition. Since $C(t,\ x,\ y)|_{t=0}=C(x,\ y)$, then the Fourier transform of the initial condition becomes, according to (2),

$$\bar{C}(\zeta,\ \eta)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}C(x,\ y)\exp i(\zeta x+\eta y)\,dxdy. \tag{9}$$

Substituting this latter equation into (8) we find, at $t=0$, $\bar{C}(\zeta,\ \eta)=C_0$; then the final expression for the solution of differential equation (7) is

$$\bar{C}(t,\ \zeta,\ \eta)=\bar{C}(\zeta,\ \eta)\exp\{-[D(\zeta^2+\eta^2)-i(v_x\zeta+v_y\eta)]\,t\}. \tag{10}$$

We find the solution of the boundary-value problem with which we are concerned here, according to (3), on the basis of this result for $\bar{C}(t,\ \zeta,\ \eta)$:

$$C(t,\ x,\ y)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\bar{C}(t,\ \zeta,\ \eta)\exp[-i(\zeta x+\eta y)]\,dxdy. \tag{11}$$

Let us apply these results to a concrete example. We assume $C(t,\ x,\ y)|_{t=0}=\exp[-|x|+|y|)]$ to be a function which satisfies both the Dirichlet conditions and the boundary conditions at infinity. Then from (9) we find

$$\bar{C}(\zeta,\ \eta)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp[-(|x|+|y|)]\exp i(\zeta x+\eta y)\,dxdy. \tag{12}$$

where

$$\int_{-\infty}^{\infty} \exp(-x) \exp\, i\zeta x dx = \int_{-\infty}^{\infty} \exp[-|x|] (\cos \zeta x + i \sin \zeta x)\, dx$$

$$= 2\int_{0}^{\infty} \exp(-|x|) \cos \zeta x dx + i \int_{-\infty}^{\infty} \exp(-|x|) \sin \zeta x dx$$

$$= 2\int_{0}^{\infty} \exp(-x) \cos \zeta x dx,$$

since the second integral of the odd function with respect to the symmetric interval vanishes. For the rest of the integral we find

$$2\int_{0}^{\infty} \exp(-x) \cos \zeta x dx = \frac{2\exp(-x)(\zeta \sin \zeta x - \cos \zeta x)}{1+\zeta^2}\Bigg|_0^{\infty} = \frac{2}{1+\zeta^2}. \tag{13}$$

Evaluating the outer integral in (12) we find

$$\int_{-\infty}^{-\infty} \exp(-|y|) \cos \eta y dy + i \int_{-\infty}^{\infty} \exp(-|y|) \sin \eta y dy = 2\int_{0}^{\infty} \exp(-y) \cos \eta y dy.$$

The last integral is [8]

$$2\int_{0}^{\infty} \exp(-y) \cos \eta y dy = \frac{2}{1+\eta^2}. \tag{14}$$

Then the expression for $C(t, \zeta, \eta)$ becomes, according to (10), (12)-(14),

$$\bar{C}(t, \zeta, \eta) = \frac{2}{\pi(1+\zeta^2)(1+\eta^2)} \exp\{-[D(\zeta^2+\eta^2) - i(v_x\zeta + v_y\eta)]\, t\}. \tag{15}$$

Using the transform and Eq. (11) we find the solution of the boundary-value problem to be

$$C(t, x, y) = \frac{1}{\pi^2} \int_{-\infty}^{-\infty}\int_{-\infty}^{\infty} \frac{\exp\{-[D(\zeta^2+\eta^2) - i(v_x\zeta + v_y\eta)]\, t\}}{(1+\zeta^2)(1+\eta^2)} \times \exp[-i(\zeta x + \eta y)]\, d\zeta d\eta. \tag{16}$$

This solution can be written in a form more convenient for calculations:

$$C(t, x, y) = \frac{1}{\pi^2} \int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty} \frac{\exp[-D\zeta^2 t + i\zeta(v_x t - x)]}{1+\zeta^2}\, d\zeta\right) \times \frac{\exp[-D\eta^2 t + i\eta(v_y t - y)]}{1+\eta^2}\, d\eta. \tag{17}$$

Using properties of the integrals of even and odd functions, we can convert the inner integral in (17) (which we denote by I) to

$$I = 2\int_{-\infty}^{\infty} \frac{e^{-D\zeta^2 t}}{1+\zeta^2} \cos(x - v_x t)\, \zeta d\zeta.$$

To evaluate this integral approximately we replace the exponential expression by the first terms in the corresponding power-series expansion, finding

$$I \approx 2\int_{0}^{\infty} \frac{\cos(x - v_x t)\, \zeta d\zeta}{(1+Dt\zeta^2)(1+\zeta^2)} = \frac{\pi}{1-Dt}\left[\exp(v_x t - x) - \sqrt{Dt}\, \exp\frac{v_x t - x}{\sqrt{Dt}}\right].$$

For the outer integral, I_1, we find, analogously,

$$I_1 \approx \frac{\pi}{1-Dt}\left[\exp(v_y t - y) - \sqrt{Dt}\, \exp\frac{(v_y t - y)}{\sqrt{Dt}}\right].$$

Taking into account the "symmetry" of the unknown solution, we write

$$C(t,\ x,\ y) \approx \frac{1}{(1-Dt)^2}\Big\{\exp\,[(v_x+v_y)\,t-(|x|+|y|)]$$

$$+\,Dt\,\exp\frac{1}{\sqrt{Dt}}\,[(v_x+v_y)\,t-(|x|+|y|)]-\sqrt{Dt}\,\Big\{\exp\Big[\Big(v_x+\frac{v_y}{\sqrt{Dt}}\Big)\,t\cdot$$

$$-\Big(|x|+\frac{|y|}{\sqrt{Dt}}\Big)\Big]+\exp\Big[\Big(v_y+\frac{v_x}{\sqrt{Dt}}\Big)\,t-\Big(|y|+\frac{|x|}{\sqrt{Dt}}\Big)\Big]\Big\}\Big\} \tag{18}$$

We now consider the case in which some chemical reaction causes an addition or loss of diffusing particles; this process is occurring simultaneously with the molecular diffusion and the convective mass transfer. As was shown in [3], if we take this addition or loss of particles into account on the basis of the mass balance, we find a complication of Eq. (1):

$$\frac{\partial C}{\partial t}+v_x\frac{\partial C}{\partial x}+v_y\frac{\partial C}{\partial y}+kC^n=D\left(\frac{\partial^2 C}{\partial x^2}+\frac{\partial^2 C}{\partial y^2}\right), \tag{19}$$

where k is some constant which is a measure of the reaction rate and n is a natural number.

To show that in this case this problem, with the same initial and boundary conditions, can be solved effectively by means of a double exponential Fourier transformation, we set $n = 1$ to simplify the calculations. Multiplying (19) term by term by $1/2\pi\,\exp i\,(\zeta x+\eta y)$ and integrating over x and y, over the interval $(-\infty,\ \infty)$, and using

$$\bar{C}=\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}C\exp i\,(\zeta x+\eta y)\,dxdy,$$

as above, we find

$$\frac{d\bar{C}}{dt}+[D\,(\zeta^2+\eta^2)+k-i\,(v_x\zeta+v_y\eta)]\,\bar{C}=0. \tag{20}$$

The general solution of this latter equation is

$$\bar{C}\,(t,\ \zeta,\ \eta)=C_0\exp\{-[D\,(\zeta^2+\eta^2)+k-i\,(v_x\zeta+v_y\eta)]\,t\}. \tag{21}$$

Since, according to one of our conditions, the initial distribution of material in the flow is a function of the coordinates, $C\,(t,\ x,\ y)|_{t=0} = C\,(x,\ y)$, we have $\bar{C}_0 = C\,(\zeta,\ \eta)$, and the solution of Eq. (20) can be written finally as

$$\bar{C}\,(t,\ \zeta,\ \eta)=\bar{C}\,(\zeta,\ \eta)\exp\{-[D\,(\zeta^2+\eta^2)+k-i\,(v_x\zeta+v_y\eta)]\,t\}. \tag{22}$$

We find the solution of Eq. (19), on the other hand, which satisfies the initial and boundary conditions to be

$$C\,(t,\ x,\ y)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\bar{C}\,(t,\ \zeta,\ \eta)\exp\,[-i\,(\zeta x+\eta y)]\,d\zeta d\eta. \tag{23}$$

If we consider a particular boundary-value problem for Eq. (19), with the initial condition $C\,(t,\ x,\ y)|_{t=0} = C\,(x,\ y)$ and the boundary conditions

$$C|_{x=\infty}=\frac{\partial C}{\partial x}\Big|_{x=\infty}=0;\quad C|_{y=\infty}=\frac{\partial C}{\partial y}\Big|_{y=\infty}=0$$

and if we set $C\,(x,\ y) = \exp\,[-(|x|+|y|)]$, as in the example above, then Eqs. (12)-(14) remain valid, as is easily shown. However, the equation for $\bar{C}\,(t,\ \zeta,\ \eta)$ becomes

$$\bar{C}\,(t,\ \zeta,\ \eta)=\frac{2}{\pi\,(1+\zeta^2)\,(1+\eta^2)}\exp\{-[D\,(\zeta^2+\eta^2)+k-i\,(v_x\zeta+v_y\eta)]\,t\}. \tag{24}$$

Accordingly, we find an equation like (17) for the desired function:

$$C\,(t,\ x,\ y)=\frac{1}{\pi^2 e^{kt}}\int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty}\frac{e^{[-D\zeta^2t+i\zeta(v_xt-x)]}\,d\zeta}{1+\zeta^2}\right)\cdot\frac{e^{[-D\eta^2t+i\eta(v_yt-y)]}\,d\eta}{1+\eta^2}. \tag{25}$$

Using the same approximate values for the integrals I_1 and I, we find

$$C(t,\ x,\ y) \approx \frac{\exp(-kt)}{(1-Dt)^2}\left\{\exp\left[(v_x+v_y)t-(|x|+|y|)\right]\right.$$
$$+Dt\exp\frac{1}{\sqrt{Dt}}\left[(v_x+v_y)t-(|x|+|y|)\right]-\sqrt{Dt}\left\{\exp\left[\left(v_x+\frac{v_y}{\sqrt{Dt}}\right)t\right.\right.$$
$$\left.\left.\left.-\left(|x|+\frac{|y|}{\sqrt{Dt}}\right)\right]+\exp\left[\left(v_y+\frac{v_x}{\sqrt{Dt}}\right)t-\left(|y|+\frac{|x|}{\sqrt{Dt}}\right)\right]\right\}\right\}. \tag{26}$$

We see from this equation that when a chemical reaction, proceeding at a rate characterized by the constant k and associated with the absorption of diffusing material, occurs in the flow, the amount of material in the flow is smaller by a factor of exp kt than in a flow in which no reaction occurs.

LITERATURE CITED

1. V. G. Levich, Physicochemical Hydrodynamics, Prentice-Hall, Englewood Cliffs, N. J. (1962).
2. V. G. Levich, Zh. Fiz. Khim., 22, 721 (1948).
3. D. A. Frank-Kamenetskii, Diffusion and Heat Transfer in Chemical Kinetics [in Russian], Izd. Akad. Nauk SSSR (1947).
4. R. M. Barrer, Diffusion In and Through Solids, Macmillan, Cambridge (1941).
5. I. A. Sneddon, Fourier Transforms, McGraw-Hill, New York (1951).
6. B. Noble, Methods Based on the Wiener—Hopf Technique for the Solution of Partial Differential Equations, Pergamon, New York (1958).
7. V. N. Chigarev, Certain Mappings of a Multivalued Function and Their Application [in Russian], Naukova Dumka, Kiev (1971).
8. I. S. Gradshtein and I. M. Ryzhik, Tables of Integrals, Sums, Series, and Products [in Russian], Nauka, Moscow (1971).