THE PROBLEM OF TURBULENT DIFFUSION IN ACTIVE IMPURITIES

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We examine the problem of turbulent diffusion in dynamically active gases in an air stream. We found the relationship between the diffusion factor and the Richardson number, as well as the relationship between the gas concentration of the gas-release wall from the decisive parameters. A method is presented for the numerical solution of the resulting system of relationships for the diffusion of an active gas, and the results of the calculation are also presented.

The diffusion of an active impurity (i.e., an impurity whose presence in an air stream will alter the diffusion properties of the latter) is a phenomenon particularly widespread in nature. It assumes particular importance in mine shafts. Because of the release of methane, hydrogen, and several other gases into the ventilation air streams of shafts, regions of degenerated turbulence may develop and substantial amounts of explosive and harmful gases may accumulate in these.

Despite the great significance of the processes of active-impurity diffusion (gases, heat, moisture) with respect to the various branches of engineering, the theory of these processes has not been adequately developed. The present paper represents a study of the diffusion of a light gas in an air stream moving through a rectangular channel; the gas is liberated throughout the entire surface of the upper wall.

Observations show that under the specified conditions we can neglect the diffusion in the direction toward the side walls. The diffusion equation in this case will be

$$\overline{U}\,\frac{\partial c}{\partial x_1}=\frac{\partial}{\partial x_2}\left[(\varepsilon+D)\,\frac{\partial c}{\partial x_2}\right], \tag{1}$$

where the Ox_1-axis is directed along the stream, while the Ox_2-axis is directed from the gas-release wall toward the stream, in a direction perpendicular to that of the main flow.

The unique feature of Eq. (1) in the case under consideration is the fact that $\overline{U}$ and ε are functions of the gas concentration c in the flow.

The function $\overline{U}(c)$ is valid only for stratified inclined flows for which it can be determined, in approximate terms, from the expression

$$\overline{U}=\overline{U}'-\mathrm{sign}\,(\beta)\,\overline{U}_c. \tag{2}$$

For a plane-parallel flow the Reynolds equation assumes the form

$$\frac{d\tau}{dx_2}=h'+F, \tag{3}$$

where

$$h'=\frac{dp}{dx_1}.$$

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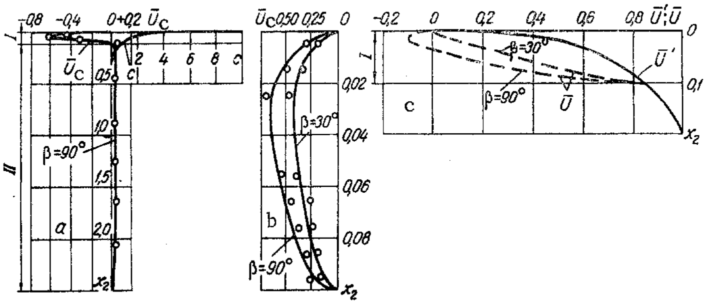

Fig. 1. Graphs showing the velocities $\overline{U}_c$, $\overline{U}'$, and $\overline{U}$ (m/sec) for the case of methane liberation from the roof: I and II) zones; c, %; x_2, m.

Bearing in mind that F = 0 in a homogeneous flow and that

$$\tau = (\mu + \rho\varepsilon_I)\frac{d\overline{U}'}{dx_2}, \quad h' = \alpha_0 U_{av}^2 \frac{P}{S},$$

after double integration for the boundary conditions $x_2 = 0$, $\tau = \tau_w = \alpha_w U_{av}^2$, $U' = 0$ from (3) we obtain

$$\overline{U} = v^* \frac{H_0}{H}\left(\varkappa_1 \frac{\alpha_w}{\alpha_0}\theta_1 - \varkappa_2 \frac{PH_0}{S}\theta_2\right), \tag{4}$$

where

$$v^* = U_{av}\sqrt{\frac{\alpha_0}{\rho}}.$$

The velocity $\overline{U}_c$ can be derived by integration of (3) for $F = g(\rho_{av} - \rho)\sin\beta$

$$\overline{U}_\kappa = v^{*'}\frac{H_0'}{H}\left[\varkappa_1\frac{\alpha_w}{\alpha_0}\int\frac{dx_2^*}{\rho^*\varepsilon_I^*} - \varkappa_2\frac{P'H_0'}{S'}\int\frac{x_2^*\,dx_2^*}{\rho^*\varepsilon_I^*} + \sin\beta\frac{gH_0'}{v^{*'2}}\int\frac{1}{\rho^*\varepsilon_I^*}\int(1-\rho^*)\,dx_2^*\,dx_2^*\right]. \tag{5}$$

In (5) the primes denote that the corresponding quantities refer to those regions [zones] of the flow in which the motion is proceeding in a single direction (with the free convection of the gas–air mixture in the air duct and with the release of a light gas from the upper wall we find two zones in which the air is moving in the same direction: at the upper wall the motion is upward and at the lower wall the motion is downward

$$\rho^* = \frac{\rho}{\rho_{av}}; \quad \varepsilon_I^* = \frac{\varepsilon_I}{v^{*'}H'}.$$

Expression (2), in conjunction with (4) and (5), determines the values of $\overline{U}$ in the diffusion equation (1). Calculation of the velocity from these expressions for a given concentration profile and $U_{av} = 1$ m/sec and for $\alpha_0 = 20\cdot10^{-4}$ kg·sec²/m⁴ is given in Fig. 1.

The turbulent diffusion of an active gas in an air stream alters the diffusion properties of the latter.

Let us examine the volume element Ω of the gas–air mixture (Fig. 2) which, as a result of pulsating motion, is mixed from layer 1 of density ρ_1 to layer 2 with density $\rho_2 (\rho_1 > \rho_2)$. The volume Ω is affected by the specific ejection force F_e whose work over the length l – equal to the mixing length – is given by

$$a = \frac{gl^2}{2}\left|\frac{\partial\rho}{\partial x_2}\right|\cos\beta. \tag{6}$$

A flow of a liquid moving at some velocity s may exert a resistance to the volume Ω that is identical to the action of the ejection force. In this case

$$a = \frac{\rho s^2}{2},$$

whence with consideration of (6), and if we also bear in mind that

$$l = u_1 \Big/ \frac{\partial\overline{U}}{\partial x_2}.$$

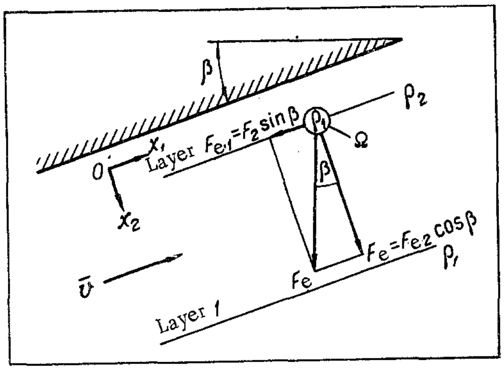

Fig. 2. Diagram for the calculation of the ejection force.

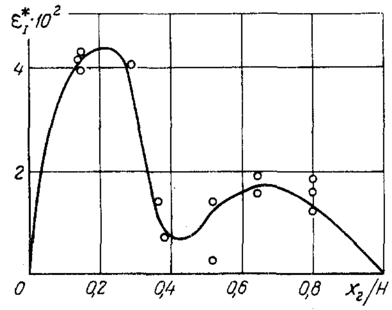

Fig. 3. Universal function $\varepsilon_I^*(x_2)$ for a meandering shaft.

we find

$$s = u_1 \mathrm{Ri}^{1/2}, \tag{7}$$

where

$$\mathrm{Ri} = \frac{\frac{g}{\rho}\left|\frac{\partial\rho}{\partial x_2}\right|}{\left(\frac{\partial \bar{U}}{\partial x_2}\right)^2} \cos\beta \tag{8}$$

is the Richardson number.

As a result of the diffusion in the direction of the Ox_2-axis we will develop a certain "diffusion velocity"

$$v = u_2 \pm s. \tag{9}$$

As is well known, the coefficient of turbulent diffusion is equal to

$$\varepsilon = -\overline{l_c v}. \tag{10}$$

With the diffusion of passive impurities we have $v = u_2$ and $l_c = l$. We then have

$$\varepsilon = \varepsilon_I = -\overline{l u_2}. \tag{11}$$

The mixing length l_c must be a function of the ejection force F_e, vanishing at some critical value of $F_{e.cr}$. Assuming a linear relationship, we can write

$$l_c = l + bF_e. \tag{12}$$

For gas liberation from the roof with $F_e = F_{e.cr} = 0$ and from (12) we have

$$\frac{l_c}{l} = 1 - \frac{F_e}{F_{cr}}. \tag{13}$$

Assuming F_e to be proportional to Ri and bearing in mind that in the case of gas liberation from the lower wall the second term in (13) will be positive, we have

$$\frac{l_c}{l} = 1 \pm \mathrm{Ri}^*, \tag{14}$$

where $\mathrm{Ri}^* = \mathrm{Ri}/\mathrm{Ri}_{cr}$.

Since ε_I is the limit value for ε in the event of diffusion of a passive impurity, it is natural to seek the ratio

$$\frac{\varepsilon}{\varepsilon_I} = \omega \tag{15}$$

as a function of the Ri number.

Expressing $\overline{l_c v}$ and $\overline{l u_2}$ in (10) and (11) in terms of the corresponding correlation coefficients r_c and r, and bearing in mind expressions (7), (9), and (14), from (15) we find that

$$\omega = \frac{r_c}{r} \mathrm{Ri}_{cr}^{1/2} (\mathrm{Ri}^{*3/2} \pm \mathrm{Ri}^* \pm \mathrm{Ri}^{*1/2} + 1).$$

When Ri = 0, $\omega = 1$ and, consequently, $r_c/r = \mathrm{Ri}_{cr}^{-1/2}$.

Assuming $r_c/r = \mathrm{Ri}_{cr}^{-1/2} = \text{const}$, we find

$$\varepsilon = \varepsilon_I (\mathrm{Ri}^{*3/2} \pm \mathrm{Ri}^* \pm \mathrm{Ri}^{*1/2} + 1). \tag{16}$$

The quantity ε_I is determined in terms of the relative coefficient of turbulent exchange, i.e., $\varepsilon_I^* = \varepsilon_I / v^* H$, which for the given type of air conduit is a universal function of the coordinates. The graph of the function $\varepsilon_I^*(x_2)$, obtained experimentally for the conditions of a meandering shaft, is shown in Fig. 3.

Expression (16) closes the system of relations needed for the solution of the problem of active-gas diffusion in a ventilation stream:

$$\begin{gathered} \bar{U} \frac{\partial c}{\partial x_1} = \frac{\partial}{\partial x_2} \left[(\varepsilon + D) \frac{\partial c}{\partial x_2} \right], \\ \bar{U} = \bar{U}' - \operatorname{sign}(\beta) \bar{U}_\kappa, \\ \varepsilon = \omega \varepsilon_I . \end{gathered} \tag{17}$$

We have the following boundary conditions: $x_2 = 0$, $c = c_w$, $x_2 = H$ $\partial c / \partial x_2 = 0$.

The concentration c_w can be determined from the following considerations.

The quantity of gas q emitted per unit of the gas-release surface per unit time moves only in the direction of the Ox_2-axis in the form of the convection flow $c_w \bar{U}_w$ (a Stefan flow) and in a molecular diffusion flow $D(\partial c / \partial x_2)_w$, where $\bar{U}_w$ is the velocity with which the mixture moves in the direction of the Ox_2-axis, and the subscript w refers to the gas-release wall. Consequently, bearing in mind that $q = \bar{U}_w$, we have

$$\bar{U}_w = c \bar{U}_w - D \left(\frac{\partial c}{\partial x_2} \right)_w . \tag{18}$$

Using the Crocco integral [1, 2]

$$c = n\bar{U} + m,$$

using the wall boundary conditions $\partial \bar{U} / \partial x_2 = (\partial \bar{U} / \partial x_2)_w$ and $\partial \tau / \partial x_2 = (\partial \tau / \partial x_2)_w$ when $x_2 = 0$, $\bar{U} = 0$, and $\rho = \rho_w$ and using the conditions at the axis when $x_2 = H_0$, $\bar{U} = \bar{U}_0$, and $c = c_0$, we obtain

$$\begin{gathered} c = \frac{c_0 - c_w}{\bar{U}_0} \bar{U} + c_w, \\ \left(\frac{\partial c}{\partial x_2} \right)_w = \frac{c_0 - c_w}{\bar{U}_0} \left(\frac{\partial \bar{U}}{\partial x_2} \right)_w . \end{gathered} \tag{19}$$

Bearing in mind the following relationships:

$$\rho_w D = \frac{\mu}{\mathrm{Sc}}; \ \mu \left(\frac{\partial \bar{U}}{\partial x_2} \right)_w = \tau_w = \alpha_w U_{av}^2; \ \rho_w = \rho_a - (\rho_a - \rho_g) c_w,$$

from (18) and (19) we obtain

$$c_w = \frac{1}{2} (1 + \rho_a^* + \Pi) - \sqrt{\frac{1}{4} (1 + \rho_a^* + \Pi) - (\rho_a^* + c_0 \Pi)}, \tag{20}$$

where

$$\Pi = \frac{\alpha_w U_{av}^2}{\mathrm{Sc}\, \bar{U}_0 q (\rho_a - \rho_g)}; \quad \rho_a^* = \frac{\rho_a}{\rho_a - \rho_g} .$$

Mathematically the solution of system (17) is formulated as follows.

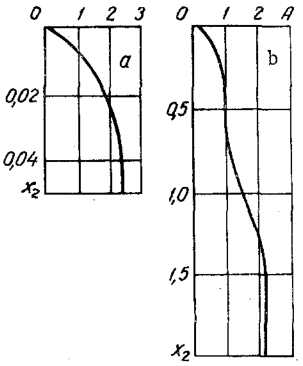

Fig. 4

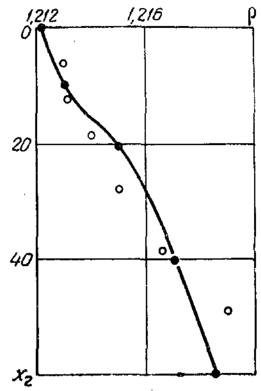

Fig. 5

Fig. 4. Graphs showing the solutions of the diffusion equations ($A = (\rho - \rho_W) \cdot 10^4$ kg $\cdot$ sec^2/m^4, and x_2, m): a) $x_1 = 45$ m; b) $x_1 = 300$ m.

Fig. 5. Comparison of the theoretical solution with the experimental data (the solid line denotes theory; ρ, N $\cdot$ sec^2/m^4, and x_2, mm).

We have to find the solution of equation

$$\frac{\partial \rho}{\partial x_1} = \frac{\partial}{\partial x_2} D'(\rho) \frac{\partial \rho}{\partial x_2}, \tag{21}$$

so as to satisfy the earlier-cited boundary conditions.

In this equation the value of the diffusion coefficient $D'(\rho)$ at a given point is the function of the behavior of the ρ function over the entire interval of variation in x_2.

If we replace the derivatives in Eq. (21) by differences, we obtain a different equation which relates the values at the three points with the numbers $k-1$, k, and $k+1$ for a fixed value of x_1 which numerically is solved by the pivot method in conjunction with iteration over ρ. The pivot method is effective for equations such as (21) when the diffusion coefficient is a known function of x_1 and x_2. The unique feature of this problem lies in the fact that $D'(\rho)$ is a function of the unknown function ρ over the entire region of definition, i.e., $D'(\rho)$ is the operator applied to the function ρ.

In our case, to use the pivot method we must resort to iterations.

We will replace the derivative in the left-hand member of Eq. (21) by a difference. We obtain

$$\frac{\rho^{\nu+1} - \rho^n}{\tau} = \frac{\partial}{\partial x_2} D'(\rho^\nu) \frac{\partial \rho^{\nu+1}}{\partial x_2}. \tag{22}$$

Here ρ^n is the value of the function ρ at the n-th layer at x_1, while ρ^ν and $\rho^{\nu+1}$ are the values of ρ obtained from the ν-th and $(\nu + 1)$-th iterations at the $(n + 1)$-th layer over x_1.

Let ρ^ν be unknown. Then $D'(\rho^\nu)$ is a known function and, having solved Eq. (3) by the pivot method, we find $\rho^{\nu+1}$. Assuming the value of ρ at the zeroth iteration to be equal to ρ^n, we can thus find all of the values of ρ^ν.

We will prove the convergence of the iterations, i.e., the existence of $\lim\limits_{\nu\to\infty} \rho^\nu = \rho^{n+1}$ in the assuming that D' is a continuous operator satisfying the condition

$$D'(\rho)\, a > 0. \tag{23}$$

The continuity condition can be written in the form

$$\| D'(\rho') - D'(\rho'')\| \leqslant M_0 \|\rho' - \rho''\| \tag{24}$$

for any ρ' and ρ''.

As proof we will write an equation such as (22) for the ν-th iteration:

$$\frac{\rho^{\nu} - \rho^{n}}{\tau} = \frac{\partial}{\partial x_2} D'(\rho^{\nu-1}) \frac{\partial \rho^{\nu}}{\partial x_2}, \qquad (22')$$

and from this we will subtract Eq. (22) for the $(\nu + 1)$-th iteration. If we denote the difference $\rho^{\nu+1} - \rho^{\nu}$ by $\delta\rho^{\nu+1}$, the resulting equation is written as follows:

$$\frac{\delta\rho^{\nu+1}}{\tau} = \frac{\partial}{\partial x_2} D'(\rho^{\nu}) \frac{\partial \delta\rho^{\nu+1}}{\partial x_2} + \frac{\partial}{\partial x_2} [D'(\rho^{\nu}) - D'(\rho^{\nu-1})] \frac{\partial \rho^{\nu}}{\partial x_2}. \qquad (25)$$

Let us now replace the derivatives in the right-hand member by differences and we will write the resulting system of equations in matrix form. We obtain the following equation:

$$\frac{\delta\rho^{\nu+1}}{\tau} = -L\delta\rho^{\nu+1} + Q[D'(\rho^{\nu}) - D'(\rho^{\nu-1})]. \qquad (26)$$

Here L and Q are matrices, while $\delta\rho^{\nu+1}$, $D'(\rho^{\nu})$, and $D'(\rho^{\nu-1})$ are vectors.

The coefficients of the matrix Q are functions of ρ^{ν}, but because of the maximum principle which ρ^{ν} satisfies, the following inequality is valid:

$$\|Q\| \leqslant M, \qquad (27)$$

where M is independent of ρ^{ν}.

The matrix Q is positive-definite. We can assume that $\delta\rho^{\nu+1}$ for all ν satisfies the zero boundary conditions. It then follows from condition (23) that

$$\|L\delta\rho^{\nu+1}\| \geqslant \varepsilon \|\delta\rho^{\nu+1}\|. \qquad (28)$$

Let us now find $\delta\rho^{\nu+1}$ from Eq. (26):

$$\delta\rho^{\nu+1} = (E + \tau L)^{-1} \tau Q [D'(\rho^{\nu}) - D'(\rho^{\nu-1})].$$

Here E is a unit matrix.

From the positive definiteness of matrix L and from condition (28) we have the inequality

$$\|(E + \tau L)^{-1}\| \leqslant \frac{1}{1 + \tau\varepsilon}.$$

From inequality (27) and from condition (24) we obtain

$$\|Q[D'(\rho^{\nu}) - D'(\rho^{\nu-1})]\| \leqslant M_0 M \|\delta\rho^{\nu}\|.$$

Hence for $\|\delta\rho^{\nu+1}\|$ we have

$$\|\delta\rho^{\nu+1}\| \leqslant \frac{\tau M_0 M}{1 + \tau\varepsilon} \|\delta\rho^{\nu}\|.$$

As is well known, the interations will converge if

$$\frac{\tau M_0 M}{1 + \tau\varepsilon} < 1,$$

which can always be achieved through proper selection of τ.

The problem was solved on a Ural-2 digital computer.

Figure 4 shows the graphs for the resulting solutions under natural conditions for $U_{av} = 0.15$ m/sec, $\bar{U}_0 = 0.2$ m/sec, $\alpha_0 = 17 \cdot 10^{-4}$ kg $\cdot$ sec^2/m^4, $q = 1.6 \cdot 10^{-4}$ m^3/sec $\cdot$ m^2, while Fig. 5 shows the comparison of this solution and the data from a laboratory experiment for the downward motion of the air ($\beta = 30°$), $U_{av} = 1.31$ m/sec, $\bar{U}_0 = 2.5$ m/sec, $q_{gas} = 1.21 \cdot 10^{-4}$ m^3/sec $\cdot$ m^2, and $\alpha_0 = 29 \cdot 10^{-4}$ kg $\cdot$ sec^2/m^4.

NOTATION

α_0 is the perimeter averaged friction factor;
α_w is the friction factor of the wall;
β is the angle of inclination to the horizontal for the air duct;

c is the concentration;
c_w is the concentration at the wall;
D is the coefficient of molecular diffusion;
ε is the coefficient of turbulent diffusion;
ε_I is the coefficient of turbulent transfer for momentum;
F is the body force;
g is the acceleration of the force of gravity;
H is the height of the air duct;
H_0 is the distance between the wall of the air duct and the axis of the flow;
θ_1, θ_2 are functions of ε_I which are universal for the specified lateral cross section and the given roughness of the channel;
$\varkappa_1, \varkappa_2$ are the coefficients by means of which we take into consideration the effect of the side walls;
l_c is the mixing length for concentration;
m, n are constants;
μ is the absolute viscosity;
P is the perimeter of the lateral cross section of the air duct;
p is the pressure;
ρ is the density;
ρ_{av} is the average density of the flow at a given cross section;
ρ_a is the air density;
ρ_g is the density of the liberated gas;
S is the cross-sectional area of the air duct;
Sc is the Schmidt number;
τ is the total shear stress in the flow;
τ_w is the shear stress at the wall;
$\bar{U}$ is the averaged velocity in the direction of the main flow;
$\bar{U}'$ is the averaged velocity for a flow of uniform density;
$\bar{U}_c$ is the averaged velocity of flow with free convection;
U_{av} is the averaged flow velocity;
u_1, u_2 are the mean square pulsating velocities in the directions of the Ox_1- and Ox_2-axes;
v is the "diffusion velocity."

LITERATURE CITED

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