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## **MATHEMATICAL MODELING OF MIXING MICROJETS OF GAS APPLIED TO THE FLAW DETECTION PROBLEMS**

A mathematical model for the process of a gas jet outflow with account of diffusion in space filled with another gas is considered. A calculation algorithm is suggested for the concentration of the initial gas in the jet and the velocity of the mixed jet. The region of sharp change in the concentration of the initial gas is determined. The problem under consideration relates to the study of the processes of technical constructions tightness control and increasing sustainability of technological processes.

**Key words:** *mathematical modeling, gas jets mixing, outflow of gas jets, microchannels.*

**Introduction.** Sustainable development of modern energy and transport technologies is determined by an increase in requirements for the production and maintenance of appropriate technical means. The quality of the energy and transport equipment is provided, in particular, by the constant improvement of the control means. One of the problems of increasing the efficiency of the above objects' tightness control is conducting research and mathematical modeling of the processes of gas outflow through the technical constructions' microcogaps/microchannels.

**Mathematical model of gas jets outflow through microchannels.** Questions related to the study of the problem of mathematical modeling and calculation of laminar and turbulent gas jets are treated in many theoretical, experimental, and applied publications. However, the problem of outflow of gas jets from microchannels that plays an important role in various kinds of instrument depressurization (in flaw detection / defectoscopy problems) has not practically been studied. In the present paper the problem of outflow of a gas jet is considered in the statement of Bai Shiet al. [1–8]. The physical essence of the problem consists in the following. Let there be an outflow from a volume filled with gas *A* under a definite pressure through a microchannel into a chamber filled with gas *B*. Proceeding from the given initial velocity, physical properties of gas, and microchannel radius, it is required to determine the distribution of the concentration of gas *A* under the gas mixing in the jet and to find the velocity at an arbitrary point in the jet.

It should be noted that by a jet is meant (according to the definition of Zucker, Vincenti et al. [9–10]) the part of the medium bounded by a

surface of trajectories of points forming the flow lines. This definition is not exactly applicable to the process of jet outflow with account of diffusion of one gas in the other. In this case the presence of a sharply outlined boundary distorts the real pattern. In problems on jets propagating in an immovable medium, particularly in a region directly adjoining the microchannel exit section, there actually occurs a sharp transition of the velocity from the initial value at the channel exit to zero. Nevertheless, if the flow in the initial region is assumed to be laminar, axisymmetric, and isothermal, then, using the laws of conservation of mass and moment and the diffusion equation in the moving medium, the process of gas outflow through microchannel can be described by the system of equations [11]:

$$\begin{aligned} \frac{\partial(\rho u)}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r}(\rho v r) &= 0, \\ \rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial r} &= \frac{1}{r} \frac{\partial}{\partial r} \left( \mu r \frac{\partial u}{\partial r} \right), \\ \frac{\partial(cu)}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r}(c v r) &= \frac{\partial}{\partial r} \left( D \frac{\partial c}{\partial r} \right) + \frac{1}{r} D \frac{\partial c}{\partial r}. \end{aligned} \quad (1)$$

Here  $D$  — const is the molecular diffusion coefficient;  $u$  and  $v$  are the components of the mixture velocity;  $c$  is the concentration of one gas in the other; and  $\mu$  is the dynamic viscosity coefficient of the mixture.

In the statement of the problem the kinetic theory of gas mixtures is used, according to which we have:

$$\mu = \frac{\mu_1}{1 + \frac{(1-c)}{c} A_x} + \frac{\mu_2}{1 + \frac{c}{1-c} A_2}.$$

Under the assumption that the Dalton law  $N = N_x + N_2$  holds, where  $N$  is the total number of molecules per unit volume;  $N_x$  and  $N_2$  are the numbers of molecules of gases  $A$  and  $B$ , respectively; and  $A_x$  and  $A_2$  are constants depending on the properties of gas. It is assumed that the mixture satisfies the criterion of continuity, i. e., the linear dimensions of the jet substantially exceed the molecule free path length. Then the mass density of the mixture is determined by the expression  $\rho = m_x N_x + m_2 N_2$ ,  $N = \text{const}$  for  $T = \text{const}$ , where  $m_x$  and  $m_2$  are the masses of molecules of gasses  $A$  and  $B$ , respectively.

The dependence of mixture density on concentration is determined by the linear relation  $\rho = Z / (3c + 1)$ .

System (1) is derived under the assumption that the concentration gradient in the direction of the flow is less than in the perpendicular direction.

The boundary conditions for system (1) are determined by the values of velocity and concentration at the channel exit:

$$\begin{aligned} c = c_0 = 1, u = 0, v = 0 & \text{ if } x = 0, 0 \leq r \leq r_k; \\ c = 0, u = 0, v = 0 & \text{ if } r > r_k. \end{aligned}$$

It can be shown that in this statement of the problem the jet momentum is an integral of system (1).

After some simple transformations system (1) is reduced to the form:

$$\begin{aligned} \frac{\partial(su)}{\partial x} + \frac{1}{r} \frac{\partial(svr)}{\partial r} &= 0, \\ su \frac{\partial u}{\partial x} + sv \frac{\partial u}{\partial r} &= \frac{1}{r} \frac{\partial}{\partial r} \left( \frac{\mu r}{l} \frac{\partial u}{\partial r} \right), \\ \frac{\partial u}{\partial x} + \frac{1}{r} \frac{\partial}{\partial r} (vr) &= -D \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial s}{\partial r} \right), \end{aligned} \quad (2)$$

where  $s = p / l$  is a dimensionless parameter.

Multiplying the first equation of system (2) by  $u$  and adding it to the second equation we obtain:

$$\frac{\partial(su^2r)}{\partial x} + \frac{\partial}{\partial r} (svur) = \frac{\partial}{\partial r} \left( \frac{\mu r}{l} \frac{\partial u}{\partial r} \right).$$

The integration with respect to  $r$  results in an expression for the variation of jet momentum in the direction of the axis  $x$ :

$$\frac{d}{dx} \int_0^r su^2 r dr = -svur + \frac{\mu r}{l} \frac{du}{dr}, \quad I = \int_0^r su^2 r dr. \quad (3)$$

It is clear that the value of  $I$  is retained at  $r \rightarrow \infty$ , where  $u$  and  $\partial u / \partial r$  vanish.

Passing to the Mises coordinates  $\chi, \psi$  (where  $\psi$  is the stream function) and applying the transformation formulas

$$rsu = \frac{\partial \psi}{\partial r}; \quad rsu = -\frac{\partial \psi}{\partial x} \quad (4)$$

we obtain a system of equations in the new coordinates:

$$\begin{aligned} \frac{1}{2} \frac{\partial \left( \frac{1}{s} \right)}{\partial x} &= D \frac{\partial}{\partial \psi} \left( s^2 \left( R / \frac{\partial R}{\partial \psi} \right) \frac{\partial}{\partial \psi} \left( \frac{1}{s} \right) \right), \\ \frac{1}{2} \frac{\partial}{\partial x} \left( 1/s \frac{\partial R}{\partial \psi} \right) &= \frac{\partial}{\partial \psi} \left( \frac{\mu}{l} \left( R / \frac{\partial R}{\partial \psi} \right) \frac{\partial}{\partial \psi} \left( 1/s \frac{\partial R}{\partial \psi} \right) \right), \end{aligned} \quad (5)$$

where the velocity components  $u$  and  $v$  are expressed in terms of the unknowns  $s$  and  $R$ :

$$v = \frac{\frac{\partial R}{\partial x}}{\frac{\partial R}{\partial \psi}} \cdot \frac{1}{s} \cdot \frac{1}{\sqrt{R}}, \quad u = 2/s \frac{\partial R}{\partial \psi}, \quad R = r^2. \quad (6)$$

The boundary conditions for the new unknowns and  $R$  have the form:

$$\left. \frac{\partial R}{\partial \psi} \right|_{x=0} = 2/s_0 u_0, \quad \left. \frac{\partial R}{\partial x} \right|_{x=0} = 0, \quad s|_{x=0} = s_0. \quad (7)$$

Using notation (4) we find:

$$\frac{1}{u} \frac{\partial \psi}{\partial r} = -\frac{1}{v} \frac{\partial \psi}{\partial x} \text{ or } v \frac{\partial \psi}{\partial r} + u \frac{\partial \psi}{\partial x} = 0. \quad (8)$$

Expression (8) is a scalar product of two vectors, and the fact that it is equal to zero means orthogonality, i. e., the velocity vector  $\{u, v\}$  is orthogonal to the vector  $\{\partial \psi / \partial r, \partial \psi / \partial x\}$  and hence is in fact directed along the flow lines  $\psi = \text{const}$ . On introducing the scale factors implied by the initial data of the problem, i. e., on dividing all linear dimensions and velocity terms by the channel radius and the initial velocity, respectively, we obtain:

$$\bar{x} = \frac{x}{r_k}; \quad \bar{R} = \frac{r^2}{r_k^2}; \quad \bar{D} = \frac{D r_k}{\psi};$$

$$\bar{\mu} = \frac{\mu r_k}{\psi}. \quad (9)$$

In this case the boundary conditions are:

$$\left. \frac{\partial \bar{R}}{\partial \bar{\psi}} \right|_{x=0} = 2\psi / r_k^2 s u_0; \quad \left. \frac{\partial \bar{R}}{\partial x} \right|_{x=0} = 0, \quad s|_{x=0} = \beta + 1. \quad (10)$$

The scale factor  $\psi$  is chosen from the condition  $\psi|_{x=0, r=r_k} = 1$ , i. e., by integrating the expression  $\partial \bar{R} / \partial \bar{\psi} = 2\psi / r_k^2 s u_0$  we find  $1 = 2\psi \psi_k / r_k^2 s u_0$ , whence  $\psi = 0.5 r_k^2 s u_0$ .

We shall carry out an analytical investigation of system (5). Writing in full the derivatives on the right-hand sides of the system we obtain:

$$1/2 \cdot \frac{\partial}{\partial x} (1/s) = D s^2 \frac{\partial}{\partial \psi} (1/s) + R D \cdot \frac{\partial}{\partial \psi} \left( \frac{\partial}{\partial \psi} (1/s) s^2 / \frac{\partial R}{\partial \psi} \right),$$

$$1/2 \cdot \frac{\partial}{\partial x} \left( 1/s \frac{\partial R}{\partial \psi} \right) = \frac{\mu}{l} \frac{\partial}{\partial \psi} \left( 1/s \frac{\partial R}{\partial \psi} \right) +$$

$$+ R \frac{\partial}{\partial \psi} \left( \frac{\partial}{\partial \psi} \left( 1/s \frac{\partial R}{\partial \psi} \right) \cdot \left( \frac{\mu}{l} \right) \left( 1/s \frac{\partial R}{\partial \psi} \right) \right). \quad (11)$$

It follows that for  $R = 0$  (or, which is the same, for  $\psi = 0$ ) we have the conditions:

$$1/2 \cdot \frac{\partial(1/s)}{\partial x} \Big|_{\psi=0} = Ds^2 \frac{\partial}{\partial \psi} (1/s) \Big|_{\psi=0},$$

$$1/2 \cdot \frac{\partial}{\partial x} \left( 1/s \frac{\partial R}{\partial \psi} \right) \Big|_{\psi=0} = \frac{\mu}{l} \frac{\partial}{\partial \psi} \left( 1/s \frac{\partial R}{\partial \psi} \right) \Big|_{\psi=0}. \quad (12)$$

In the case when the discarded terms are small as compared to the remaining ones, condition (12) can be regarded as an equation describing the behavior of the solution for small  $R$ .

Integrating the two equations (5) with respect to the variable  $\psi$  we obtain the following relations important for the organization of the computational process:

$$1/2 \frac{\partial}{\partial x} \left( \int_0^{\psi} 1/s d\psi \right) = Ds^2 \left( R / \frac{\partial R}{\partial \psi} \right) \frac{\partial}{\partial \psi} (1/s) = Ds^2 \frac{R}{2} u \frac{\partial}{\partial \psi} (1/s),$$

$$1/2 \frac{\partial}{\partial x} \left( \int_0^{\psi} 1/s \frac{\partial R}{\partial \psi} \right) = \frac{\mu R}{l2} u \frac{\partial}{\partial \psi} \left( 1/s \frac{\partial R}{\partial \psi} \right). \quad (13)$$

The resulting expressions testify to the existence of two conserved integrals under the condition  $u = 0$ , which corresponds to the above-mentioned conservation laws. The first integral determines the volume flow rate of the mixture depending on  $x$ , and for  $\psi \rightarrow \infty$  its value is retained. The momentum of the jet is determined by the second integral. The right-hand sides of equations (13) tend to zero for  $\psi \rightarrow \infty$ . However, in the first equation this follows from the speculative idea that  $u$  tends to zero faster than  $R$  tends to  $\infty$ . In the

second equation the rate at which the integral  $\int_0^{\psi} \left( 1/s \frac{\partial R}{\partial \psi} \right) d\psi$  tends to  $I_0$  is determined by the rate at which  $u$  tends to zero because for  $\psi \rightarrow \infty$  we have  $1/s \rightarrow 1/s_{\infty}$ , where  $s_{\infty}$  is the (dimensionless) density of the environmental medium; note that we have  $R \cdot \frac{\partial^2 R}{\partial \psi^2} / \left( \frac{\partial R}{\partial \psi} \right)^2 \rightarrow 1$  because the numerator and

the denominator are of the same order of magnitude relative to the variable  $\psi$ . Therefore the parameter  $l$  is the main control characteristic in the organization of the computational process. The available literature data point to the now popular tendency to consider the region where the velocity makes up 1-3% of the velocity at the jet axis as the boundary of the jet.

What has been said clarifies a degree of idealization in the model in question because, by definition, we have  $u = \left(\frac{1}{s}\right)\left(\frac{dr}{d\psi}\right)$ , and the value of  $u$  can vanish only for  $\frac{\partial R}{\partial \psi} \rightarrow \infty$ . By virtue of this fact, it is impossible to

obtain a complete conservation of the jet momentum, and it is only possible to speak of the attainment of an acceptable accuracy.

We shall show that the curves on which the values of the integrals  $\int_0^\psi 1/s d\psi$  and  $\int_0^\psi \left(1/s \frac{\partial R}{\partial \psi}\right) d\psi$  retain are characteristics of system (5). Introduce the following notation:

$$\frac{\partial \Phi}{\partial \psi} = \frac{1}{2} \cdot \frac{1}{s}; \frac{\partial \Phi}{\partial x} = Ds^2 \left( R / \frac{\partial R}{\partial \psi} \right) \cdot \frac{\partial}{\partial \psi} (1/s). \quad (14)$$

Then we have  $d\Phi = (\partial\Phi / \partial\psi) d\psi + (\partial\Phi / \partial x) dx$ . For  $d\Phi = 0$ , i. e., for  $\Phi = const$ , the first equation implies:

$$\frac{\partial \psi}{\partial x} = - \frac{\partial \Phi / \partial x}{\partial \Phi / \partial \psi} = \frac{2Ds \partial s / \partial \psi}{\partial \ln R / \partial \psi} = D \frac{\partial s^2 / \partial \psi}{\partial \ln R / \partial \psi}. \quad (15)$$

However, we have  $\Phi = 1/2 \int_0^\psi 1/s d\psi$ . Hence, the integral  $\Phi$  assumes the same values on the lines (15). Similarly, the integral  $\int_0^\psi \left(\frac{1}{s}\right) (\partial R / \partial \psi) d \ln R / \partial \psi$  is constant on the curves determined by the equation:

$$\frac{\partial \psi}{\partial x} = 2\mu / l \cdot Rs \frac{\partial}{\partial \psi} \left( 1/s \frac{\partial R}{\partial \psi} \right). \quad (16)$$

It appears impossible to obtain an explicit analytical expression for the characteristics of system (5).

To determine a numerical solution to the system, the classical factorization method is used. The application of this method requires the presence of a fixed region and the setting of conditions on the boundary of the region. Here the advantage of the employment of Mises coordinates is evident because in the original coordinates  $x, r$  the network cannot be uniform, whereas the coordinates  $x, \psi$  make it possible to use a uniform network.

A finite-difference analog of the system of differential equations under study is:

$$\begin{aligned} Ha_{i+1} y_{i+1}^{n+1} - (Ha_{i+1}^n + Ha_i^n + 1) y_i^{n+1} + Ha_i^n y_{i-1}^{n+1} &= -y_i^n, \\ Hb_{i+1}^n z_{i+1}^{n+1} - (Hb_{i+1}^n + Hb_i^n + 1) z_i^{n+1} + Hb_i^n z_{i-1}^{n+1} &= -z_i^n, \end{aligned} \quad (17)$$

where

$$\begin{aligned} a_i^n &= 0,5 \left( \mu_{i-1}^n / l s_{i-1}^n R_{i-1}^n y_{i-1}^n + \mu_i^n / l \cdot s_i^n R_i^n y_i^n \right), \\ b_i^n &= 0,5 \left( (s^3)_{i-1}^n R_{i-1}^n y_{i-1}^n + (s^3)_i^n R_i^n y_i^n \right), \\ y &= 1 / s \frac{\partial R}{\partial \psi}; z = 1 / s; H = 2H_x / H_\psi^2. \end{aligned}$$

The superscript  $n$  and the subscript  $i$  in the terms  $a_i^n$  indicate the index of the section along the axis  $x$  and the index of the stream function along the axis  $\psi$ , respectively. Because the original system is nonlinear, at each step along the axis  $x$  the matrix elements are linearized. In this case the related error is often eliminated by introducing iterations as stated by Strikwerda [12].

The boundary conditions at  $x = 0$  (in dimensionless form) are determined by the expression:

$$z_i^1 = 1 / (\beta + 1); \left( 1 / s \frac{\partial R}{\partial \psi} \right)_i = \frac{0,5 u_0 r_k^2}{\psi}. \quad (18)$$

Passing to the finite-difference analog in expression (12) we obtain the boundary conditions at  $\psi = 0$ :

$$\begin{aligned} z_2^{n+1} HD (s^2)_i^n - (HD (s^2)_i^n + 1) z_1^{n+1} &= -z_1^n, \\ y_2^{n+1} H \mu_1^n / l - (H \mu_1^n / l + 1) y_1^{n+1} &= -y_1^n. \end{aligned} \quad (19)$$

The linearization is also introduced for finite-difference approximation of conditions (12), which are then refined in the course of the computational process. The conditions on the jet boundary are written as:

$$u = 0, s = s_b, \quad (20)$$

where  $s_b$  is the dimensionless density of the environmental medium. This applies in the presence of an ideal boundary in the form of flow lines. However, in the suggested model the process of formation of the jet boundary depends on the relation between the processes of diffusion and convective motion, which is expressed by the ratio of the Peclet (diffusion) number  $Pe_d = VL / D$  to the Reynolds number  $Re = VL / \nu$ . Here  $V$ ,  $L$ , and  $\nu$  are the characteristic velocity, length scale, and dynamic viscosity, respectively.

For a large diffusion coefficient and a comparatively small outflow velocity there occurs a fast «smearing» of the jet, and, since the assumption of conservation of the total number of molecules per unit volume has been made, the flow region involves some gas from the environmental medium,

i. e., there appear new flow lines, and the jet expansion takes place. Therefore the flow region is no longer bounded by flow lines issuing from the outlet, and the only means for controlling the computational process is the initial value of the jet momentum. To check the adequacy of the calculated values of velocity and concentration we use expression (13).

The calculations are carried out according to the following scheme.

For  $x = 0$  the value of the integral  $\int_0^{\psi_k} \left( 1/s \frac{\partial R}{\partial \psi} \right) d\psi$  is calculated (the value

of the stream function  $\psi_k$  corresponds to the magnitude of the channel radius). At the next step along the axis  $\chi$  the concentration  $c = (s+1)/\beta$ , the jet velocity and radius, and the value of the integral within the same limits (i. e., the value of the momentum) are calculated. If the new value of the momentum differs from the one calculated at the foregoing step, then the step along the axis  $\chi$  is reduced, and all calculations are repeated; if this does not provide the desired result, then the value of the upperagain, etc.

The solution of the finite-difference equations (17) with boundary conditions (18)–(20) is carried out using the factorization method. An *a priori* choice of the step along the axis  $\chi$  is performed proceeding from the idea that the coefficients of the finite-difference equation must not strongly differ from unity. The calculation step is then further refined automatically with account of the requirements of the method. Because the concrete calculations were performed for microchannels of very small radius, the region of existence of the jet is also very small. However, as is shown by practical calculations, an acceptable accuracy can be attained by using a large number of jet sections.

According to the calculations in the cases when  $Pe_d \ll Re$ , there is a narrow region of sharp change in the concentration, and the order of magnitude of the value of  $x$  in whose neighborhood these changes occur can be estimated by analyzing conditions (12). If these conditions are regarded as equations for small values of  $R$ , then it is possible to find their exact solutions with account of the given boundary conditions at  $x=0$ . After the change of variable  $s^2 = f$  the first equation in system (12) is written in the form:

$$\frac{\partial f}{\partial x} = 2Df \frac{\partial f}{\partial \psi}. \quad (21)$$

This equation with boundary conditions (10) has a self-similar solution:

$$f = 1 - (1 - f_0) \theta(-\psi + 1 - 2fxD). \quad (22)$$

Expression (21) implies that  $f = f_0$  for  $-\psi + 1 - 2fxD > 0$ , i. e.,  $x < (1 - \psi) / 2f_0D$ , and, consequently, the value of  $s$  is retained on the axis  $\psi = 0$  up to



$$x = \frac{0,5u_0s_0r_k}{2s_0^2D} = \frac{u_0r_k}{4s_0D}$$

and becomes equal to unity for  $x > u_0r_k / 4s_0D$ .

Thus, for approximated equation (21) the value of  $D$  is the main characteristic of the region of change of the concentration of gas  $A$  in the mixture. However, the value of  $x_c$  is an analog of the well-known Peclet number and serves as an important characteristic of gas dynamics processes related to mass transfer.

The numerical experiments show that in the case  $x_c \ll \text{Re}$  the velocity at the jet axis is retained at some distance from the microchannel under a sharp drop of the concentration of the original gas, i. e., system (5) splits into two equations that can be solved independently, namely, first the equation with respect to the concentration is solved for a constant velocity, and then the other equation is solved for a slowly varying velocity.

In contrast to ordinary jets where the velocity at the axis is retained at a distance of several diameters, the jets out flowing from a microchannel exist at very short distances from the microchannel exit, and the velocity at the axis is retained for  $x_c \ll \text{Re}$  at distances substantially less than the diameter. If the orders of magnitude of  $x_c$  and  $\text{Re}$  are approximately the same, then the processes of velocity and concentration variation take course simultaneously.

**Conclusions.** As a result of numerical experiment based on the proposed mathematical model for the process of a gas jet outflow with account of diffusion in space filled with another gas and the calculation algorithm for the concentration of the initial gas in the jet and the velocity of the mixed jet we managed to establish that the jet expansion depends on the ratio of the molecular weights of gases entering the mixture. The numerical calculations were carried out for three sorts of gas  $A$ , namely heavier than air (gas  $B$ ), lighter than air, and close to air in the molecular weight.

Thus, the Peclet and Reynolds numbers and also their ratio completely characterize the stationary process of propagation of a mixed laminar gas jet.

The proposed mathematical model can be used to reduce energy losses and increase efficiency of technological processes in order to make them more sustainable.

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Розглянуто математичну модель процесу відтоку газового струменя з урахуванням дифузії в просторі, що заповнений іншим газом. Запропоновано алгоритм розрахунку концентрації початкового газу в струмені і швидкості змішаного струменя. Визначено область різкої зміни концентрації початкового газу. Розглянута задача відноситься до проблем дослідження процесів контролю герметичності технічних конструкцій та підвищення сталості технологічного процесу.

**Ключові слова:** математичне моделювання, змішування газових струменів, відтік газових струменів, мікроканали.

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