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Modeling the spread of harmful substances in the atmosphere at a variable velocity profile

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Abstract: This study developed a mathematical model for the dispersion and transportation of pollutants in the atmosphere. The problem associated with the spread of monodisperse passive tracer from an instantaneous point source in the atmosphere assuming a partial absorption of surface impurities is solved. One version of the computational algorithm and a theoretical justification, is that, the applicability of numerical methods for computational experiment is developed. These results are consistent with the physical laws of the section under consideration.

Keywords: A mathematical model; distribution of pollutants in the atmosphere; monitoring; transfer equation; splitting method; harmful substances; numerical method

Nomenclature

$\alpha > 0$	coefficient of impurity interaction with the underlying surface;
$\mu > 0$, $\nu > 0$	horizontal and vertical viscosity coefficients;
$\sigma = const > 0$	interaction rates of substance environment;
φ	the intensity of the impurities, migrating from the air flow;
$f(x, y, z, t)$	function characterizing the source of the contaminant;
h	indicates that we are working in grid spaces.
Q	capacity;
t_0	on time source;
u, v, w	velocity components along the axes OX, OY, OZ, respectively;
$x_0,\ y_0,\ z_0$	coordinates of the source;

1 Introduction

Atmospheric processes are developing under the joint influence of natural and anthropogenic factors of different spatial and temporal scales. Therefore, there is a nontrivial question of how to build a mathematical model in order to take account of the circumstances of the two competing simultaneously. On the other hand, a variety of physical processes and the necessity to consider a wide range of disturbances require that the models were rich in their physical content, and their discrete approximations should provide high spatial and temporal resolution. At the same time, it is necessary that these patterns can be effectively implemented on computers. Taking into account the existing experience in solving problems of atmospheric physics and considering the processes of moisture exchange and interaction of the atmosphere with a thermally inhomogeneous ground, it is better to take the model described by equations of hydrodynamics systems full of atmosphere in the non-adiabatic approximation as the basis. Among the active factors, first of all, there is the impact of air masses in a limited area on the background processes and the impact of anthropogenic sources - heat, moisture, various impurities and changes the dynamic, hydro and thermal characteristics of the earth's surface [1–6].

Environmental issues are now becoming a priority, in a view of the growing environmental degradation in many regions due to the presence and distribution of contaminants in the atmosphere. One of the sources of pollution is industrial facilities. This raises the problem of limiting emissions of existing enterprises while maintaining their full capacity. Also it raises the question about the optimal placement of industrial facilities, taking into account the environmental situation in a particular region. To solve these problems we need to develop a mathematical model of impurity propagation from the source of pollution, con-

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sidering the factors affecting the process and the corresponding sustainable computing process.

The actual process takes place at a variable speed profiles. Therefore, an attempt to create a mathematical model of impurity propagation with variable speed profile is becoming interesting. In this formulation, the problem is much more complicated because, firstly, there is a problem: what happens to the law change in velocity, secondly, there now the complicated form of the most stable computing algorithm for solving the problem, and there are also difficulties in the direct implementation of the algorithm on the computer.

Presume that the boundaries of the area and the XY plane of the values of the impurity assumed to be zero. This means that the size of the area is so large that the impurity concentration becomes lower than the maximum permissible.

On the surface of the earth interacts with the underlying surface. At the boundary of the surface layer of the impurity value also becomes small. Now we are going to investigate the general case of variable velocity field.

2 Research methods

The mathematical model of the problem involves the transport equation with the source term. Coefficients of viscosity and turbulence in the first approximation is assumed constant. Thus, we consider the differential equation in partial derivatives of the form:

$$\frac{\partial\varphi}{\partial t}+\frac{\partial u\varphi}{\partial x}+\frac{\partial v\varphi}{\partial y}+\frac{\partial w\varphi}{\partial z}+\sigma\varphi- \\ -\mu\frac{\partial^2\varphi}{\partial x^2}-\mu\frac{\partial^2\varphi}{\partial y^2}-\nu\frac{\partial^2\varphi}{\partial z^2}=f(x,y,z,t) \tag{1}$$

under initial and boundary conditions:

$$\varphi=\varphi_0(x,y,z)\ \text{ when }\ t=0; \\ \varphi=0\quad \text{in}\quad \Omega=\{x=0,y=0,x=a,y=b\}; \tag{2}$$

$$\frac{\partial\varphi}{\partial t}=\alpha\varphi\quad\text{when}\quad z=0 \\ \text{and}\quad \varphi=0\quad\text{when}\quad Z=H; \tag{3}$$

Here φ – the intensity of the impurities, migrating from the air flow; u, v, w – velocity components along the axes OX, OY, OZ, respectively; $\mu > 0$, $\nu > 0$ – horizontal and vertical viscosity coefficients; $\sigma = const > 0$ – interaction rates of substance environment; $\alpha > 0$ – coefficient of impurity interaction with the underlying surface; $f(x, y, z, t)$ – function characterizing the source of the contaminant. In addressing this task, the source function given as:

$$f=Q\delta(x-x_0)\delta(y-y_0)\delta(z-z_0)\delta(t-t_0),$$

where, x_0, y_0, z_0 – coordinates of the source; t_0 – on time source; Q – its capacity.

A solution is sought in $\Omega\times\Omega_t$, where $\Omega = \{x\in[0,a],\ \ y\in[0,b],\ \ z\in[o,H]\}$, $\Omega_t=\{o\le t\le T\}$.

It is assumed that the parameters of the area [a,b] are large enough to satisfy the condition $\varphi = 0$ on the boundary. The variable rate field imposes certain features in the solution of the task. There is a problem in the approximation of the differential task (1)-(3) corresponding difference tasks. We considered the approximation of the corresponding operators in (1) in the case of variable velocity profile. First, we considered the transport equation that contains only the convective terms, *i.e.* a two-dimensional task. We write the original equation in the form:

$$\frac{\partial\varphi}{\partial t}+u\frac{\partial\varphi}{\partial x}+v\frac{\partial\varphi}{\partial y}=f\ \text{ in }\ \Omega\times\Omega_t \tag{4}$$

where, $\Omega=\{x\in[0,a],y\in[0,b]\}$, $\Omega_t=\{o\le t\le T\}$.

The velocity components generally are functions of x, y and z. In this case, the continuity equation must be satisfied:

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0 \tag{5}$$

at each instant of time t. The equation (4) can be rewritten in the form of:

$$\frac{\partial\varphi}{\partial t}+A\varphi=0 \tag{6}$$

where, $A\varphi=u\frac{\partial\varphi}{\partial x}+v\frac{\partial\varphi}{\partial y}$

By introducing the scalar product in a conventional manner, then:

$$(A\varphi,\varphi)=\int_0^a dx\int_0^b\left(u\frac{\partial\varphi}{\partial x}+v\frac{\partial\varphi}{\partial y}\right)\varphi dy \tag{7}$$

Taking into account (2) the expression (4) can be transformed to:

$$(A\varphi,\varphi)=\int_0^a dx\int_0^b\frac{1}{2}\left(\frac{\partial u\varphi^2}{\partial x}+\frac{\partial v\varphi^2}{\partial y}\right)dy \tag{8}$$

Next presume that $A=A_1+A_2$. Then for each A_α ($\alpha = 1, 2$) alone we have:

$$\left.\begin{aligned}(A_1\varphi,\varphi)&=\frac{1}{2}\int_0^a dx\int_0^b\varphi^2\frac{\partial u}{\partial x}dy\\(A_2\varphi,\varphi)&=\frac{1}{2}\int_0^a dx\int_0^b\varphi^2\frac{\partial v}{\partial y}dy\end{aligned}\right\} \tag{9}$$

In [1] as the operators A_1 and A_2 it is recommended to choose the following form

$$\left.\begin{aligned} A_1\varphi &= u\frac{\partial\varphi}{\partial x} + \frac{\varphi}{2}\frac{\partial u}{\partial x} \\ A_2\varphi &= v\frac{\partial\varphi}{\partial y} + \frac{\varphi}{2}\frac{\partial v}{\partial y} \end{aligned}\right\} \tag{10}$$

It is recognized that the relation $A = A_1 + A_2$ is satisfied. Really,

$$\begin{aligned}(A_1 + A_2)\varphi &= u\frac{\partial\varphi}{\partial x} + v\frac{\partial\varphi}{\partial y} + \frac{\varphi}{2}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) = \\ &= u\frac{\partial\varphi}{\partial x} + v\frac{\partial\varphi}{\partial y} = A\varphi\end{aligned}$$

by condition of continuity (5).

Let us now consider the real three-dimensional problem, described by the equation of type (1), but written in the operator form:

$$\frac{\partial\varphi}{\partial t} + \sum_{\alpha=1}^{3} A_\alpha\varphi = f \quad \text{in} \quad \Omega\times\Omega_t \tag{11}$$

where, according to the following notation given reasons:

$$\begin{aligned} A_1\varphi &= \frac{\partial u\varphi}{\partial x} - \mu\frac{\partial^2\varphi}{\partial x^2} - \frac{\varphi}{2}\frac{\partial u}{\partial x}; \\ A_2\varphi &= \frac{\partial v\varphi}{\partial y} - \mu\frac{\partial^2\varphi}{\partial y^2} - \frac{\varphi}{2}\frac{\partial v}{\partial y}; \\ A_3\varphi &= \frac{\partial w\varphi}{\partial z} - \nu\frac{\partial^2\varphi}{\partial z^2} - \frac{\varphi}{2}\frac{\partial w}{\partial z} + \sigma\varphi. \end{aligned}$$

This notation is more convenient when using conventional splitting scheme for the numerical solution of the problem. The solution of equation (11) is sought in

$$\Omega = \{x \in [0, a], y \in [0, b], z \in [o, H]\}, \quad \Omega_t = \{o \le t \le T\}.$$

with the following initial and boundary conditions:

$$\begin{aligned} &\varphi = \varphi_0(x, y, z) \ \text{ when } \ t = 0; \\ &\varphi = 0 \ \text{ when } \ \{x = 0, x = a, y = 0, y = b\}; \\ &\frac{\partial\varphi}{\partial z} = \alpha\varphi \ \text{ when } \ z = 0; \ \ \varphi = 0 \ \text{ when } \ z = H. \end{aligned} \tag{12}$$

For the numerical solution of the problem this study will be using finite difference schemes based on splitting method [2]. There are various approaches and methods of splitting [1, 2, 7], for example, splitting into physical processes and splitting the space variables. This study used the splitting method which in the first stage includes a horizontal transfer and diffusion of impurities, and the second stage includes the convection and diffusion in the direction OZ axis. However, before using the splitting scheme, it is necessary to ensure the applicability of the method, *i.e.*, check the sign-definiteness of the operators of the original differential problem. In other words, we checked the execution of relations:

$$(A_\alpha\varphi, \varphi) > 0, \quad \alpha = 1, 2, 3. \tag{13}$$

Let us consider the following case: $u = u(z)$, $v = const$, $w = const$.

$$\begin{aligned}(A_1\varphi, \varphi) &= \int_0^a\int_0^b\int_0^H \left(\frac{\partial u\varphi}{\partial x} - \mu\frac{\partial^2\varphi}{\partial x^2} - \frac{\varphi}{2}\frac{\partial u}{\partial x}\right)\varphi dxdydz = \\ &= \int_0^b dy\int_0^H dz\int_0^a \left[\frac{u}{2}\frac{\partial\varphi^2}{\partial x} - \mu\frac{\partial^2\varphi}{\partial x^2}\varphi\right]dx = \\ &= \int_0^b dy\int_0^H \left[\frac{u}{2}\varphi^2\Big|_0^H - \mu\left(\frac{\partial\varphi}{\partial x}\right)\varphi\Big|_0^a\right]xdz + \\ &+ \int_0^b dy\int_0^H \left[\mu\left(\frac{\partial\varphi}{\partial x}\right)^2\right]dz = \\ &= \mu\int_0^b\int_0^H\int_0^a \left(\frac{\partial\varphi(x, y, z, t)}{\partial x}\right)^2 dxdydz > 0\end{aligned}$$

According to the boundary conditions (12), as well as of the conditions $u = (z)$, $v = const$ and $w = const$ we obtain positive definiteness of the operator A_1. Similarly, we can show a positive definite operator A_2. It remains to show positive definite operator A_3. To this end, we consider the scalar product $(A_3\varphi, \varphi)$, and the positive-definiteness takes place when $va - \frac{w}{2} > 0$. Really:

$$\begin{aligned}&\iiint_\Omega \left[\frac{\partial w\varphi}{\partial z} - \nu\frac{\partial^2 w\varphi}{\partial z^2} - \frac{\varphi}{2}\frac{\partial w}{\partial z} + \sigma\varphi\right]\varphi d\Omega = \\ &= \int_0^a dx\int_0^b dy\int_0^H \left[\frac{w}{2}\frac{\partial\varphi}{\partial z} - \nu\frac{\partial^2 w\varphi}{\partial z^2} + \sigma\varphi^2\right]dz = \\ &= \frac{w}{2}\int_0^a\int_0^b \varphi^2\Big|_0^H dxdy - \int_0^a\int_0^b\int_0^H \nu\frac{\partial^2\varphi}{\partial z^2}\varphi dxdydz + \\ &+ \int_0^a\int_0^b\int_0^H \sigma\varphi^2 d\Omega = J_1 + J_2 + J_3\end{aligned}$$

Let us consider separately J_α $(\alpha = 1, 2, 3)$:

$$\begin{aligned}J_1 &= \frac{w}{2}\int_0^a\int_0^b \left[\varphi^2(x, y, H, t) - \varphi^2(x, y, 0, t)\right]dxdy = \\ &= -\frac{w}{2}\int_0^a\int_0^b \varphi^2(x, y, 0, t)dxdy;\end{aligned}$$

$$J_2 = -\int_0^a dx \int_0^b dy \int_0^H \nu \frac{\partial^2 \varphi}{\partial z^2} \varphi dz =$$

$$= \left| \begin{array}{ll} \frac{\partial^2 \varphi}{\partial z^2} dz = dz & \varphi = q \\ z = \frac{d\varphi}{dz} & dq = \frac{\partial \varphi}{\partial z} dz \end{array} \right| =$$

$$= -\int_0^a \int_0^b dxdy\nu \left[\frac{\partial \varphi}{\partial z} \varphi \Big|_0^H - \int_0^H \left(\frac{\partial \varphi}{\partial z} \right)^2 dz \right] =$$

$$= -\int_0^a \int_0^b \nu \left[-\alpha \varphi^2(x,y,0,t) - \int_0^H \left(\frac{\partial \varphi}{\partial z} \right)^2 dz \right] dxdz =$$

$$= \int_0^a \int_0^b \left[\nu\alpha\varphi^2(x,y,0,t)dxdy + \int_0^H \nu \left(\frac{\partial \varphi}{\partial z} \right)^2 dxdydz \right]$$

$$J_1 + J_2 = \int_0^a \int_0^b \left[\nu\alpha - \frac{w}{2} \right] \varphi^2(x,y,0,t)dxdy +$$

$$+ \iiint_\Omega \nu \left(\frac{\partial \varphi}{\partial z} \right)^2 d\Omega;$$

$$J_3 = \iiint_\Omega \sigma \varphi^2 d\Omega.$$

Due to a positive value w, σ, α, as well as the conditions $\nu\alpha - \frac{w}{2} > 0$, the operator A_3 is positive definite. Thus, the requirements of positive semidefinite operators A_α $(\alpha = 1, 2, 3)$ are satisfied. But we must assume that the operators A_1, A_2, A_2 have no common zeros.

Differential problem (11) – (12) we approximate the corresponding difference problem. For this, as usual, built net difference in Ω. Accordingly, the mesh moves along the axes is denoted by Δx, Δy and Δz. The coordinates of grid points are (x_i, y_j, z_k), where $i = \overline{0, M}$; $j = \overline{0, N}$; $k = \overline{0, K}$.

Differential operators A_α $(\alpha = 1, 2, 3)$ we approximate following difference ratios, respectively, denoted by Λ_α :

$$\begin{aligned} \Lambda_1 \varphi &= u_k \frac{\varphi_{i+1,j,k} - \varphi_{i-1,j,k}}{2\Delta x} - \\ &- \frac{\mu}{\Delta x^2} \left[\varphi_{i+1,j,k} - 2\varphi_{i,j,k} + \varphi_{i-1,j,k} \right]; \\ \Lambda_2 \varphi &= \nu \frac{\varphi_{i,j+1,k} - \varphi_{i,j-1,k}}{2\Delta y} - \\ &- \frac{\mu}{\Delta y^2} \left[\varphi_{1,j+1,k} - 2\varphi_{i,j,k} + \varphi_{i,j-1,k} \right]; \\ \Lambda_3 \varphi &= w \frac{\varphi_{i,j,k+1} - \varphi_{i,j,k-1}}{2\Delta z} - \\ &- \frac{\mu}{\Delta z^2} \left[\varphi_{i,j,k+1} - 2\varphi_{i,j,k} + \varphi_{i,j,k-1} \right]; \\ i &= \overline{0, M-1};\ j = \overline{0, N-1};\ k = \overline{0, K-1}. \end{aligned} \tag{14}$$

where, M, N, K – respectively, are the number of grid points in the direction of the axes OX, OY, OZ. The boundary conditions are approximated by first order accuracy. (Later we will raise the order of approximation of the boundary conditions at $H = 0$). So,

$$\begin{aligned} \varphi_{i,j,k} &= 0 \ \text{ when } \ i = 0, \ \ i = M; \\ \varphi_{i,j,k} &= 0 \ \text{ when } \ j = 0, \ j = N; \\ \left(\varphi_{i,j,k} - \varphi_{i,j,k-1} \right) / \Delta z &= \alpha \varphi_{i,j,k} \ \text{ when } \ k = 1; \\ \varphi_{i,j,k} &= 0 \ \text{ when } \ k = K. \end{aligned}$$

For simplicity we will refer to the following grid functions:

$$\begin{aligned} &\varphi(t) = \left\{ \varphi_{i,j,k}(t) \right\};\ f = \left\{ f_{i,j,k} \right\};\ g = \left\{ g_{i,j,k} \right\}, \\ &\quad (i = \overline{0, M-1};\ j = \overline{0, N-1};\ k = \overline{0, K-1}); \\ &\varphi(t) \in \Phi_h;\ f \in F_h;\ g \in G_h, \end{aligned} \tag{15}$$

where, h – indicates that we are working in grid spaces. Taking into account (14), (15), we write the difference analog of the original problem (11) – (12) in the following form:

$$\frac{\varphi^{n+1} - \varphi^n}{\tau} + \sum_{i=1}^{3} \Lambda_\alpha \varphi^n = f^n \ \text{ in } \ \Omega_h \times \Omega_\tau, \tag{16}$$

where, $\Omega_h = \{t_n, n = \overline{0, L}, t_n = n \times \tau\}$; $l\varphi = g$.

Let us note that the difference problem (14) is recorded by means of the explicit scheme. Therefore, it is conditionally stable. It will replace the equivalent of an implicit scheme of the order of approximation. This scheme is a scheme of two-cycle component splitting. When recording (14) will assume the boundary conditions accounted for in the structure of the operator Λ_α. In fact, they are necessary in the immediate implementation of the scheme when preparing for the programming algorithm. Thus, the scheme is implemented in the form:

$$\begin{aligned} \left(E + \frac{\tau}{2} \Lambda_1^j \right) \varphi^{j+2/3} &= \left(E - \frac{\tau}{2} \Lambda_1^j \right) \varphi^{j-1} \\ \left(E + \frac{\tau}{2} \Lambda_2^j \right) \varphi^{j-1/3} &= \left(E - \frac{\tau}{2} \Lambda_1^j \right) \varphi^{j+2/3} \\ \left(E + \frac{\tau}{2} \Lambda_3^j \right) \left(\varphi^j - \tau f^j \right) &= \left(E - \frac{\tau}{2} \Lambda_3^j \right) \varphi^{j-1/3} \\ \left(E + \frac{\tau}{2} \Lambda_3^j \right) \varphi^{j+1/3} &= \left(E - \frac{\tau}{2} \Lambda_3^j \right) \left(\varphi^j + \tau f^j \right); \\ \left(E + \frac{\tau}{2} \Lambda_2^j \right) \varphi^{j+2/3} &= \left(E - \frac{\tau}{2} \Lambda_2^j \right) \varphi^{j+1/3}; \\ \left(E + \frac{\tau}{2} \Lambda_1^j \right) \varphi^{j+1} &= \left(E - \frac{\tau}{2} \Lambda_1^j \right) \varphi^{j+2/3}; \\ J &= 1, 2, \ldots, \varphi^0 = g, \end{aligned} \tag{17}$$

where, $\Lambda_\alpha^j = \Lambda_\alpha(t_j)$; $f^j = f(t_j)$.

On smooth solutions, having a second order of approximation on τ, b is absolutely stable if Λ_1, Λ_2, Λ_3 are positive definite operators. Here τ – time step, n – number of time-layer $(\tau L = T)$. Each equation of the system is implemented using the sweep method. Here, the principal point

Table 1: Table of regime parameters.

No	Name of parameter	Meaning of parameter		
1	Size of field $a \times b \times H, m$	$10^4 \times 10^4 \times 10^2$	$10^3 \times 10^3 \times 50$	$10^4 \times 10^4 \times 10^2$
2	Reynolds criterion	5	67	15
3	Power source, from unit	1	1	1
4	Coefficient of the absorption of the impurity, $1/s$	1	0	1
5	Coefficient of impurity interaction with the surface, $1/m$	1	1	1
6	The source position in m	$2000 \times 1500 \times 100$	$200 \times 500 \times 100$	a) $2000 \times 1500 \times 100$ b) $7000 \times 4500 \times 100$
7	Original wind velocity, m/s	5	10	15

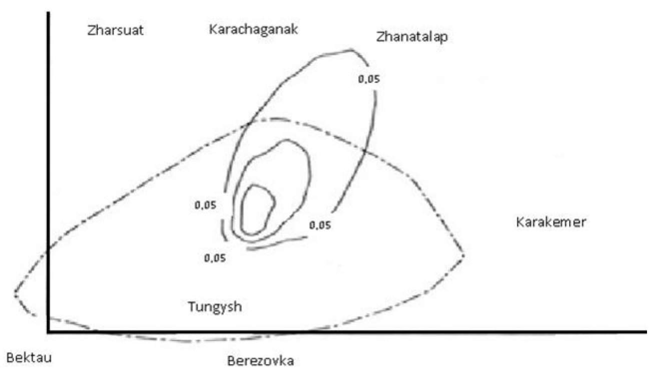

Figure 1: Isolines of the CO_2 concentration in the maximum permissible concentration shares at a height of $650m$. Max CO_2 – 0, 22.

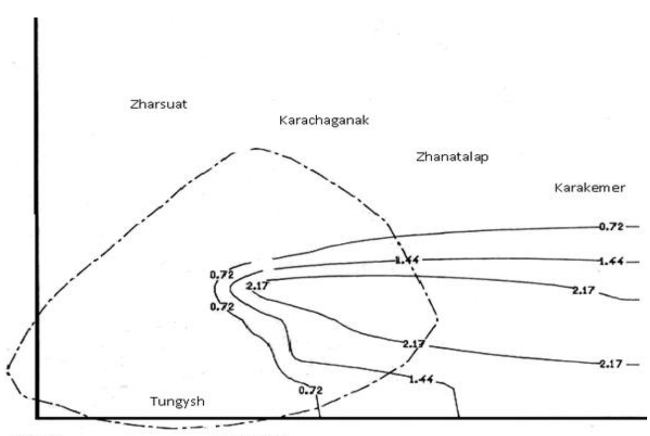

Figure 2: Isolines of the CO_2 concentration in the maximum permissible concentration shares at a height of $10m$. Max CO_2 – 2, 89.

is the definition of the boundary conditions at the intermediate steps. However, the structure of the boundary conditions is to determine the necessary parameters for the easy sweep. Generally, for three dimensional problems, circumstance is one of the most difficult problems in terms of algorithmic plan [8].

3 Analysis of the results

Currently, the first version prepared by a computational algorithm is implemented, *i.e.* debugging the corresponding program.

In conclusion, we need to note that we are going to test other options of computational algorithm to identify effective option.

The problem of the spread of monodisperse passive tracer from an instantaneous point source in the atmosphere assuming a partial absorption of surface impurities is solved. The mathematical model described by equations (11) – (12) is the longitudinal component of velocity u – function of the coordinate z. As outlined above, the algorithm is based on the method of splitting, compiled and plotted numerical calculation program. We got impurity distribution for the various regime parameters (Table 1).

Types of the initial profile of the longitudinal velocity $u = f(z)$, the Reynolds number values, have changed. Calculations are performed in the presence of two instantaneous sources.

Here are some of the results of computer simulations in the form of contour lines on the example of the Karachaganak oil and gas field.

These results are comparable with results of other authors, such as [8].

4 Conclusions

Solution of the problem of passive distribution monodisperse impurities was carried out by numerical methods. Previously developed method for calculating the spread of impurities afforded solution of the problem at a constant speed. At this stage, the algorithm for the case of variable velocity profile was developed. These results are consistent with the physical laws of the flow.

A single version of the computational algorithm and a theoretical justification, that is, the applicability of numerical methods for computational experiment was also developed.

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