

# Random walk with finite speed as a model of pollution transport in turbulent atmosphere

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IN THE PAPER we apply the model of random walk with finite speed to the description of the pollution transport in the atmosphere. We consider one, two and three-dimensional models. We obtain the systems of equations for the conditional probability distribution functions of particle's locations in space and time. They are convenient to describe the evolution of the probability distribution of the range of the pollutant emitted from the source, its distribution over the earth surface and its spatial distribution. The sedimentation (absorption of the particles on earth's surface) is taken into account in the models.

## 1. Introduction

THE PROBLEM of the pollution transport and its modeling is, at present, one of the most important tasks of the physics of atmosphere. This phenomenon is a very complicated physical process, depending on a number of factors, not always completely identified [8]. These factors can be of very different nature. First of all, the final distribution of the pollutant depends of the kind of its source (temporal or permanent, concentrated or distributed, more or less intensive). Secondly, the properties of the motion of air transporting the pollutant particles (both large-scale, laminar and local, turbulent) have a strong effect on their concentration in space and time. Also physical and chemical properties of the pollutant particles, such as their possible coagulation, absorption by vapors or rains, sedimentation facility or chemical reactions, can affect the transport process. Finally, the properties of the earth surface have an influence on the sedimentation of the particles and should be taken into account. Studying the transport process in turbulent atmosphere we must realize all these facts, in spite of our limited abilities of including them into the mathematical models.

Considering the process of the pollution transport in the atmosphere, we are interested in obtaining some equations describing the mass transfer on a large scale. However, to obtain such global equations we must start the considerations from the small-scale behavior of the particles. Unfortunately, we are not able to take into account all really existing physical phenomena that take place in interparticle influences. Therefore we must treat the problem in a statistical way, assuming certain reactions of particles with some probability and, eventually, identifying particular probabilities in the model and comparing the resulting equations of the mass transfer with experimental results.

The description of the neutral particle flowing through and interacting with some environmental materials needs, at any time  $t$ , the knowledge of six variables: three position variables and three momentum variables. In the statistical model we should know the probability distributions of these variables (see [7]). Sometimes it is more convenient to replace the momentum variable with three equivalent variables: kinetic energy of the particle and two angular variables specifying the velocity direction vector. Such a description implicitly permits the particles to have different masses and velocities and freely change the travel direction.

One of the possible small-scale methods of description of particle motion is a random-walk concept (see [9]). In the literature many different random-walk models have been proposed to describe the dispersion of particles in inhomogeneous or unsteady turbulence. In most of them it is assumed that the flowing particles have equal masses. Moreover, some restrictive conditions on their possible velocities and the movement directions are assumed. For such simplified models the position variables are sufficient to describe the transport process.

Among the proposed random walk models there are more or less suitable ones to describe the process of transport of the pollutant particles. Selecting one of them we need some a priori criteria to distinguish good models from the bad ones.

Several authors apply such criteria to verify their models of random walk. These quality measures are often very intuitive and sound quite different, but in mathematical formulation they give the same results (cf. [10]). Choosing the random walk model we postulate its good large-scale and small-scale behavior. In the large scale we require the well-mixing condition; that is, if the particles are initially well mixed, they will remain well-mixed during the diffusion process. In small scale, we postulate that random walk should reduce to a diffusion-equation model as the Lagrangian time scale tends to zero.

In many problems the diffusion equation is sufficient to describe the pollution transport process (e.g. the global mass transport or large-scale changes of the pollutant concentration — see e.g. [5, 6]). However, in some problems we must know the instant of time at which the pollutant reaches a certain area; in such a case the widely used diffusion equation is not sufficient — one needs models where the velocity of particles is taken into account. The random walk processes make it possible to consider also this parameter in the global transport equation.

Let us remark that, in modeling of the real physical phenomena, the final correctness criterion is the compliance of the results deduced from the mathematical model with experimental observations.

Modeling the process of pollution transport we know that it takes place in a three-dimensional physical space. Nevertheless, we often use one- or two-dimensional models to describe such a phenomenon. Applied to real transport process, such simplified models need some interpretation: the one-dimensional model can describe a distance of the pollutant particle from the source, and the two-dimensional model — the distribution of the particles around the source. Only three-dimensional models can give real traces of the particles and their actual location in space.

In this paper we consider all these models: one, two and three-dimensional. All of them are based on the model of random walk process proposed by G. I. Taylor and S. Goldstein where the possibility of sedimentation of the particle (its death) has been included. Identifying the probabilities of jumps in any direction or imprisoning the particle at a given point, we can describe the transport process by means of the models proposed.

## 2. The model of one-dimensional random walk with finite speed

Our considerations are a generalization of the one-dimensional model of random walk proposed by G. I. Taylor and S. Goldstein and presented in a transparent way in KAC'S lecture notes [2]. In this section we introduce the problem following their reasoning.

Assume that we have one particle moving to the left and to the right along a straight line. It starts at time  $t = 0$  and goes from point  $x = 0$  in a fixed direction. In time  $\Delta t$  it covers the distance  $\Delta x$ ,

$$(2.1) \quad \Delta x = v\Delta t,$$

where parameter  $v$  plays the role of finite velocity of the particle. After the jump, the particle changes its direction to the opposite one with probability  $a\Delta t$  or continues its motion in the same direction with probability  $1 - a\Delta t$ . The location on the line, of the particle starting from 0, after  $n$  steps (that is after the time  $n\Delta t$ ), is  $S_n$ .

To describe this model mathematically we must introduce a specific notation. Let  $\varphi(x)$  be an arbitrary function. We are interested in the evolution of the function  $\langle \varphi(x + S_n) \rangle$  in time (symbol  $\langle \cdot \rangle$  denotes the mathematical expectation of a random variable).

Define the random variable  $\varepsilon$  in the following way:

$$(2.2) \quad \varepsilon = \begin{cases} 1 & \text{with probability } 1 - a\Delta t, \\ -1 & \text{with probability } a\Delta t. \end{cases}$$

Consider the following sequence of independent random variables with identical distributions, defined above:

$$(2.3) \quad \varepsilon_1, \varepsilon_2, \varepsilon_3, \dots, \varepsilon_{n-1}.$$

Assume that the particle starts from point  $x$  in the positive direction. Then the change of location of the particle after  $n$  steps is

$$(2.4) \quad S_n^+ = v\Delta t(1 + \varepsilon_1 + \varepsilon_2\varepsilon_1 + \dots + \varepsilon_{n-1}\varepsilon_{n-2} \dots \varepsilon_2\varepsilon_1).$$

If the particle starts in negative direction, the analogous variable is

$$(2.5) \quad S_n^- = -v\Delta t(1 + \varepsilon_1 + \varepsilon_2\varepsilon_1 + \dots + \varepsilon_{n-1}\varepsilon_{n-2} \dots \varepsilon_2\varepsilon_1) = -S_n^+.$$

We investigate two following functions:

$$(2.6) \quad F_n^+(x) = \langle \varphi(x + S_n^+) \rangle$$

and

$$(2.7) \quad F_n^-(x) = \langle \varphi(x - S_n^+) \rangle.$$

Writing explicitly,  $F_n^+(x)$  is

$$(2.8) \quad F_n^+(x) = \langle \varphi(x + v\Delta t(1 + \varepsilon_1 + \varepsilon_2\varepsilon_1 + \dots + \varepsilon_{n-1}\varepsilon_{n-2}, \dots, \varepsilon_2\varepsilon_1)) \rangle$$

or

$$(2.9) \quad F_n^+(x) = \langle \varphi(x + v\Delta t + v\Delta t(1 + \varepsilon_2 + \dots + \varepsilon_{n-1}\varepsilon_{n-2}, \dots, \varepsilon_2))\varepsilon_1 \rangle.$$

We calculate the conditional expectation of the formula (2.9) with respect to  $\varepsilon_1$ :

$$(2.10) \quad F_n^+(x) = a\Delta t \langle \varphi(x + v\Delta t - v\Delta t(1 + \varepsilon_2 + \dots + \varepsilon_{n-1}\varepsilon_{n-2}, \dots, \varepsilon_2)) \rangle + (1 - a\Delta t) \langle \varphi(x + v\Delta t + v\Delta t(1 + \varepsilon_2 + \dots + \varepsilon_{n-1}\varepsilon_{n-2}, \dots, \varepsilon_2)) \rangle,$$

or, in a recurrent way,

$$(2.11) \quad F_n^+(x) = a\Delta t F_{n-1}^-(x + v\Delta t) + (1 - a\Delta t) F_{n-1}^+(x + v\Delta t).$$

Making the analogous operation for the particle starting in the negative direction we obtain:

$$(2.12) \quad F_n^-(x) = a\Delta t F_{n-1}^+(x - v\Delta t) + (1 - a\Delta t) F_{n-1}^-(x - v\Delta t),$$

what, together with the relationship (2.11), gives the system of difference equations for  $F_n^+(x)$  and  $F_n^-(x)$ .

From Eq. (2.11) we obtain

$$(2.13) \quad \frac{F_n^+(x) - F_{n-1}^+(x)}{\Delta t} = \frac{v(F_{n-1}^+(x + v\Delta t) - F_{n-1}^+(x))}{v\Delta t} + aF_{n-1}^-(x + v\Delta t) - aF_{n-1}^+(x + v\Delta t)$$

and, going to the limit for  $n \rightarrow \infty$ ,  $\Delta t \rightarrow 0$ ,  $t = n\Delta t = \text{const}$ , the following differential equation:

$$(2.14) \quad \frac{\partial F^+}{\partial t} = v \frac{\partial F^+}{\partial x} + aF^- - aF^+.$$

Analogously, for  $F^-$  we have from Eq. (2.12)

$$(2.15) \quad \frac{F_n^-(x) - F_{n-1}^-(x)}{\Delta t} = \frac{-v(F_{n-1}^-(x + v\Delta t) - F_{n-1}^-(x))}{-v\Delta t} + aF_{n-1}^+(x - v\Delta t) - aF_{n-1}^-(x - v\Delta t)$$

and

$$(2.16) \quad \frac{\partial F^-}{\partial t} = -v \frac{\partial F^-}{\partial x} + aF^+ - aF^-.$$

We introduce new functions  $F$  and  $G$ , defined by

$$(2.17) \quad F = \frac{1}{2}(F^+ + F^-), \quad G = \frac{1}{2}(F^+ - F^-).$$

Function  $F$  can represent the probability density function that particle at time  $t$  is located at point  $x$  provided that it started from point  $x = 0$  in the positive or the negative directions with the same probability equal to  $1/2$ .

Adding Eqs. (2.14) and (2.16) results in the following equation:

$$(2.18) \quad \frac{\partial F}{\partial t} = v \frac{\partial G}{\partial x};$$

analogously, subtraction of Eq. (2.14) from Eq. (2.16) gives a supplementary partial differential equation

$$(2.19) \quad \frac{\partial G}{\partial t} = v \frac{\partial F}{\partial x} - 2aG.$$

By eliminating  $G$  from Eqs. (2.18) and (2.19) we obtain

$$(2.20) \quad \frac{1}{v} \frac{\partial^2 F}{\partial t^2} = v \frac{\partial^2 F}{\partial x^2} - \frac{2a}{v} \frac{\partial F}{\partial t}$$

– the telegrapher's equation (or, the string equation with damping); this is the equation for the probability density function which describes the distribution of the particles starting from point  $x = 0$  at time  $t = 0$  in a symmetric way and travelling along the line with the finite speed  $v$  changing the direction in the manner defined in Eq. (2.2).

To solve the problem of particles diffusion on the line, we must complete equation (2.20) with the initial conditions

$$(2.21) \quad F(x, 0) = \varphi(x), \quad \left[ \frac{\partial F}{\partial t} \right]_{t=0} = 0,$$

describing the initial location of diffusing particles.

To consider the limiting case in Eq. (2.20), we assume:  $a \rightarrow \infty$ ,  $v \rightarrow \infty$ , but  $2a/v^2$  remains constant (the particle makes more and more small, quick jumps):

$$(2.22) \quad \frac{2a}{v^2} = \frac{1}{D}.$$

In the limit we obtain the well-known parabolic diffusion equation:

$$(2.23) \quad \frac{1}{D} \frac{\partial F}{\partial t} = \frac{\partial^2 F}{\partial x^2}.$$

This means that the random walk with finite speed defined in this section satisfies one of the required correctness conditions, and the present random walk process can be regarded as a good model of the transport process of pollutant particles.

### 3. The one-dimensional model of the transport with sedimentation

To make the description of the particles diffusion more realistic, let us assume that after some travel time the particle is absorbed by the environment and stops the diffusion. In the model of random walk this fact can also be taken into account. Let us assume that the particle starts from point  $x = 0$ , as in the previous section, goes in a fixed direction (to the right or to the left) or remains at that point never leaving it. At time  $\Delta t$  it has covered the distance  $\Delta x$ , where

$$(3.1) \quad \Delta x = v\Delta t.$$

After the jump the particle changes its direction to the opposite one with probability  $a \Delta t$ , sediments at its new location with probability  $b \Delta t$  or continues the motion in the previous direction with probability  $1 - (a + b) \Delta t$ .

Similarly to the previous section, to describe this model mathematically we introduce the following notation. Let  $S_n$  be the location of the particle after  $n$  steps (that is after the time  $n\Delta t$ ). Let  $\varphi(x)$  be an arbitrary function. We are interested in the evolution of the averaged function  $\varphi$ ,  $\langle \varphi(x + S_n) \rangle$ . If  $\varphi(x)$  is the Dirac delta function, then  $\langle \varphi(x + S_n) \rangle$  represents the probability density function of location of the diffusing particle.

Define the random variable  $\varepsilon$  in the following way:

$$(3.2) \quad \varepsilon = \begin{cases} 1 & \text{with probability } 1 - (a + b)\Delta t, \\ -1 & \text{with probability } a\Delta t, \\ 0 & \text{with probability } b\Delta t. \end{cases}$$

To describe the walk of the particle let us consider the sequence of independent, identically distributed random variables with the distribution defined in Eq. (3.2),

$$(3.3) \quad \varepsilon_1, \varepsilon_2, \varepsilon_3, \dots, \varepsilon_{n-1}.$$

Assume that the particle starts from point  $x$  in the positive direction. Then the change of location of the particle after  $n$  steps is

$$(3.4) \quad S_n^+ = v\Delta t(1 + \varepsilon_1 + \varepsilon_2\varepsilon_1 + \dots + \varepsilon_{n-1}\varepsilon_{n-2}, \dots, \varepsilon_2\varepsilon_1).$$

When the particle starts into the negative direction, the analogous variable is

$$(3.5) \quad S_n^- = -v\Delta t(1 + \varepsilon_1 + \varepsilon_2\varepsilon_1 + \dots + \varepsilon_{n-1}\varepsilon_{n-2}, \dots, \varepsilon_2\varepsilon_1) = -S_n^+.$$

The last possible solution, the particle remains in the starting point, gives the variable describing its location in the following form:

$$(3.6) \quad S_n^0 = 0.$$

Substituting the three expressions for the location of the particle, we obtain the following versions of  $\langle \varphi(x + S_n) \rangle$ :

$$(3.7) \quad F_n^+(x) = \langle \varphi(x + S_n^+) \rangle,$$

$$(3.8) \quad F_n^-(x) = \langle \varphi(x + S_n^-) \rangle = \langle \varphi(x - S_n^+) \rangle,$$

$$(3.9) \quad F_n^0(x) = \langle \varphi(x + S_n^0) \rangle = \langle \varphi(x) \rangle.$$

Explicitly,  $F_n^+(x)$  is

$$(3.10) \quad F_n^+(x) = \langle \varphi(x + v\Delta t(1 + \varepsilon_1 + \varepsilon_2\varepsilon_1 + \dots + \varepsilon_{n-1}\varepsilon_{n-2} + \dots + \varepsilon_2\varepsilon_1)) \rangle,$$

or

$$(3.11) \quad F_n^+(x) = \langle \varphi(x + v\Delta t + v\Delta t(1 + \varepsilon_2 + \dots + \varepsilon_{n-1}\varepsilon_{n-2} + \dots + \varepsilon_2)\varepsilon_1) \rangle.$$

Calculating the conditional expectation of the formula (3.11) for  $F_n^+(x)$  with respect to  $\varepsilon_1$ , we obtain

$$(3.12) \quad F_n^+(x) = a\Delta t \langle \varphi(x + v\Delta t - v\Delta t(1 + \varepsilon_2 + \dots + \varepsilon_{n-1}\varepsilon_{n-2} + \dots + \varepsilon_2)) \rangle \\ + (1 - (a+b)\Delta t) \langle \varphi(x + v\Delta t + v\Delta t(1 + \varepsilon_2 + \dots + \varepsilon_{n-1}\varepsilon_{n-2} + \dots + \varepsilon_2)) \rangle \\ + b\Delta t \langle \varphi(x + v\Delta t) \rangle,$$

or, in a recurrent way,

$$(3.13) \quad F_n^+(x) = a\Delta t F_{n-1}^-(x + v\Delta t) + (1 - (a+b)\Delta t) F_{n-1}^+(x + v\Delta t) \\ + b\Delta t F_n^0(x + v\Delta t).$$

Performing this operation for the particle starting in the negative direction we obtain the recurrent equation for  $F_n^-(x)$ ,

$$(3.14) \quad F_n^-(x) = a\Delta t F_{n-1}^+(x - v\Delta t) + (1 - (a+b)\Delta t) F_{n-1}^-(x - v\Delta t) \\ + b\Delta t F_n^0(x - v\Delta t).$$

Analogously, the recurrent equation for the function  $F_n^0(x)$  describing the behavior of the sedimented particle is

$$(3.15) \quad F_n^0(x) = F_{n-1}^0(x).$$

These three formulae constitute the system of difference equations and give a complete characteristics of the diffusion process (random walk).

Analogously to the considerations of the previous section, we can consider the continuous version of the equations for  $F_n^+(x)$ ,  $F_n^-(x)$  and  $F_n^0(x)$  (the conditional probability density functions). From Eq. (3.13) we obtain

$$(3.16) \quad \frac{F_n^+(x) - F_{n-1}^+(x)}{\Delta t} = \frac{v(F_{n-1}^+(x + v\Delta t) - F_{n-1}^+(x))}{v\Delta t} + aF_{n-1}^-(x + v\Delta t) \\ - (a+b)F_{n-1}^+(x + v\Delta t) + bF_n^0(x + v\Delta t).$$

Going to the limit for  $n \rightarrow \infty$ ,  $\Delta t \rightarrow 0$ ,  $t = n\Delta t = \text{const}$ , we obtain the following differential equation:

$$(3.17) \quad \frac{\partial F^+}{\partial t} = v \frac{\partial F^+}{\partial x} + aF^- - (a+b)F^+ + bF^0.$$

Repeating the procedure for  $F^-$  we obtain from Eq. (3.14)

$$(3.18) \quad \frac{F_n^-(x) - F_{n-1}^-(x)}{\Delta t} = \frac{-v(F_{n-1}^-(x - v\Delta t) - F_{n-1}^-(x))}{-v\Delta t} + aF_{n-1}^+(x - v\Delta t) - (a+b)F_{n-1}^-(x - v\Delta t) + bF_n^0(x - v\Delta t)$$

and, in the limit,

$$(3.19) \quad \frac{\partial F^-}{\partial t} = -v \frac{\partial F^-}{\partial x} + aF^+ - (a+b)F^- + bF^0.$$

The supplementary equation for  $F^0$  obtained from the difference equation (3.15) takes the following form:

$$(3.20) \quad \frac{\partial F^0}{\partial t} = 0.$$

To obtain the equation for probability density function  $F$  of the location of the particle (under the condition that it left the point  $x = 0$  equiprobably in both directions), we introduce new variables:

$$(3.21) \quad F = \frac{1}{2}(F^+ + F^-), \quad G = \frac{1}{2}(F^+ - F^-).$$

Adding Eqs. (3.17) and (3.19) we obtain

$$(3.22) \quad \frac{\partial F}{\partial t} = v \frac{\partial G}{\partial x} - bF + bF^0;$$

subtraction of Eq. (3.19) from Eq. (3.17) gives

$$(3.23) \quad \frac{\partial G}{\partial t} = v \frac{\partial F}{\partial x} - (2a+b)G.$$

Eliminating  $G$  from Eqs. (3.22) and (3.23) we obtain the equation for the probability density function  $F$ ,

$$(3.24) \quad \frac{1}{v} \frac{\partial^2 F}{\partial t^2} = v \frac{\partial^2 F}{\partial x^2} - \frac{2(a+b)}{v} \frac{\partial F}{\partial t} + \frac{(2a+b)b}{v} F - \frac{(2a+b)b}{v} F^0,$$

where Eq. (3.20) has been also taken into account.

To consider the limit (diffusion) case let us transform Eq. (3.24) to a more convenient form:



$$(3.25) \quad \frac{1}{v^2} \frac{\partial^2 F}{\partial t^2} = \frac{\partial^2 F}{\partial x^2} - \left[ \frac{2a}{v^2} + \frac{2b}{v^2} \right] \frac{\partial F}{\partial t} + \left[ \frac{2ab}{v^2} + \frac{2b^2}{v^2} \right] [F - F^0].$$

Similarly to Sec. 2, consider such a limiting case of Eq. (3.25), where  $a \rightarrow \infty$ ,  $v \rightarrow \infty$  but  $2a/v^2$  remains constant:

$$(3.26) \quad \frac{2a}{v^2} = \frac{1}{D};$$

moreover, the constant  $b$  is assumed to be a finite number. Then Eq. (3.25) takes the form

$$(3.27) \quad \frac{1}{D} \frac{\partial F}{\partial t} = \frac{\partial^2 F}{\partial x^2} + \frac{b}{D} [F - F^0].$$

It is seen that the resulting equation is the diffusion equation with annihilation terms. Also in this case the limiting equation is of a diffusive character, so the preliminary condition of correctness of the random walk model as a description of the transport process is satisfied.

#### 4. The case of two-dimensional models

The one-dimensional model makes it possible to describe the pollution transport phenomenon only in a limited way. To take into account the spatial distribution of the particles around the source, we should consider a two-dimensional model. For this purpose we can apply the models of random walk being a certain generalization of the random walk defined in Sec. 2 and the random walk with absorption defined in Sec.3.

##### 4.1. The random walk without sedimentation

Consider the motion of a particle in the plane, analogous to the one presented in Sec.2. The particle staying at an instant of time  $t_0$  at point  $x = (x_1, x_2)$  covers during the time period  $\Delta t$  the distance  $\Delta x = v\Delta t$ , possibly changing its direction. The trajectories of the particle lie piecewise on the straight lines parallel to the axes of the coordinate system  $x_1, x_2$ . Moving, the particle can choose one of the four possible directions (follow the previous one, turn to the left or right or go back). This process can be written mathematically similarly to the previous case with application of the matrix-vector notation.

Assume that the particle goes to the left with probability  $a\Delta t$ , goes back with probability  $b\Delta t$ , goes to the right with probability  $c\Delta t$  and continues its way in the previous direction with probability  $1 - (a + b + c)\Delta t$ . This means that the particle moves from the initial point along one of the vectors:

$$(4.1) \quad \mathbf{a} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} -1 \\ 0 \end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, \quad \mathbf{d} = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

with some probability, dependent on the previous direction of particle's motion.

We can introduce the matrix of rotation of the particle's velocity vector, which is random and takes the values according to our assumptions concerning the model. The matrix of rotation  $\mathbf{E}(\omega)$  takes the following values:

$$(4.2) \quad \mathbf{E}(\omega) = \mathbf{A} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \quad \text{with probability } a\Delta t,$$

$$(4.3) \quad \mathbf{E}(\omega) = \mathbf{B} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \quad \text{with probability } b\Delta t,$$

$$(4.4) \quad \mathbf{E}(\omega) = \mathbf{C} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \quad \text{with probability } c\Delta t,$$

$$(4.5) \quad \mathbf{E}(\omega) = \mathbf{D} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{with probability } 1 - (a + b + c)\Delta t.$$

The rotation matrices act on the direction vectors on the following way:

$$(4.6) \quad \mathbf{A}\mathbf{d} = \mathbf{a}, \quad \mathbf{B}\mathbf{d} = \mathbf{b}, \quad \mathbf{C}\mathbf{d} = \mathbf{c}, \quad \mathbf{D}\mathbf{d} = \mathbf{d},$$

$$(4.7) \quad \mathbf{A}\mathbf{a} = \mathbf{b}, \quad \mathbf{B}\mathbf{a} = \mathbf{c}, \quad \mathbf{C}\mathbf{a} = \mathbf{d}, \quad \mathbf{D}\mathbf{a} = \mathbf{a},$$

$$(4.8) \quad \mathbf{A}\mathbf{b} = \mathbf{c}, \quad \mathbf{B}\mathbf{b} = \mathbf{d}, \quad \mathbf{C}\mathbf{b} = \mathbf{a}, \quad \mathbf{D}\mathbf{b} = \mathbf{b},$$

$$(4.9) \quad \mathbf{A}\mathbf{c} = \mathbf{d}, \quad \mathbf{B}\mathbf{c} = \mathbf{a}, \quad \mathbf{C}\mathbf{c} = \mathbf{b}, \quad \mathbf{D}\mathbf{c} = \mathbf{c}.$$

The change of location of the particle in  $n$  steps is

$$(4.10) \quad \mathbf{S}_n^r = v\Delta t(\mathbf{I}\mathbf{d} + \mathbf{E}_1 + \mathbf{E}_2\mathbf{E}_1 + \dots + \mathbf{E}_{n-1}\mathbf{E}_{n-2}, \dots, \mathbf{E}_2\mathbf{E}_1)\mathbf{r},$$

where  $\mathbf{r}$  is the initial direction of particle's motion and takes one of four values:  $\mathbf{r} = \mathbf{a}$ ,  $\mathbf{r} = \mathbf{b}$ ,  $\mathbf{r} = \mathbf{c}$ , or  $\mathbf{r} = \mathbf{d}$ .

Consider an arbitrary real-valued function on  $\mathbb{R}^2$ ,  $\varphi(\mathbf{x})$ , and the function being its average value:

$$(4.11) \quad F_n^r(\mathbf{x}) = \langle \varphi(\mathbf{x} + \mathbf{S}_n^r) \rangle.$$

Written down in an explicit form, function  $F_n^r(\mathbf{x})$  is

$$(4.12) \quad F_n^r(\mathbf{x}) = \langle \varphi(\mathbf{x} + v\Delta t \mathbf{r} + v\Delta t(\mathbf{E}_1 + \mathbf{E}_2\mathbf{E}_1 + \dots + \mathbf{E}_{n-1}\mathbf{E}_{n-2}, \dots, \mathbf{E}_2\mathbf{E}_1)\mathbf{r}) \rangle.$$

Like in the one-dimensional model, we can calculate the conditional mean value of this expression with respect to the random transition matrix  $\mathbf{E}_1$ . We obtain

$$(4.13) \quad F_n^r(\mathbf{x}) = a\Delta t F_{n-1}^{\mathbf{Ar}}(\mathbf{x} + v\Delta t \mathbf{r}) + b\Delta t F_{n-1}^{\mathbf{Br}}(\mathbf{x} + v\Delta t \mathbf{r}) \\ + c\Delta t F_{n-1}^{\mathbf{Cr}}(\mathbf{x} + v\Delta t \mathbf{r}) + (1 - (a + b + c)\Delta t) F_{n-1}^{\mathbf{Dr}}(\mathbf{x} + v\Delta t \mathbf{r}),$$

or, since  $\mathbf{D}\mathbf{r} = \mathbf{r}$ ,

$$(4.14) \quad F_n^r(\mathbf{x}) = a\Delta t F_{n-1}^{Ar}(\mathbf{x} + v\Delta t \mathbf{r}) + b\Delta t F_{n-1}^{Br}(\mathbf{x} + v\Delta t \mathbf{r}) \\ + c\Delta t F_{n-1}^{Cr}(\mathbf{x} + v\Delta t \mathbf{r}) + (1 - (a + b + c)\Delta t)F_{n-1}^r(\mathbf{x} + v\Delta t \mathbf{r}).$$

The difference equations (4.14) for  $\mathbf{r} = \mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$  can be written in the following form:

$$(4.15) \quad \frac{F_n^r(\mathbf{x}) - F_{n-1}^r(\mathbf{x})}{\Delta t} = \frac{v(F_{n-1}^r(\mathbf{x} + v\Delta t \mathbf{r}) - F_{n-1}^r(\mathbf{x}))}{v\Delta t} \\ + aF_{n-1}^{Ar}(\mathbf{x} + v\Delta t \mathbf{r}) + bF_{n-1}^{Br}(\mathbf{x} + v\Delta t \mathbf{r}) \\ + cF_{n-1}^{Cr}(\mathbf{x} + v\Delta t \mathbf{r}) + (a + b + c)F_{n-1}^r(\mathbf{x} + v\Delta t \mathbf{r}).$$

Passing to the limit ( $\Delta t \rightarrow 0$ ) we obtain the system of partial differential equations for the conditional probability density functions  $F^r$ ,  $\mathbf{r} = \mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$ :

$$(4.16) \quad \frac{\partial F^r}{\partial t} = v\mathbf{r} \nabla F^r(\mathbf{x}) + aF^{Ar}(\mathbf{x}) + bF^{Br}(\mathbf{x}) + cF^{Cr}(\mathbf{x}) - (a + b + c)F^r(\mathbf{x}).$$

Taking successively  $\mathbf{r} = \mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$ , we obtain the system of equations in an explicit form:

$$(4.17) \quad \frac{\partial}{\partial t} \begin{bmatrix} F^a \\ F^b \\ F^c \\ F^d \end{bmatrix} - v \begin{bmatrix} \frac{\partial}{\partial x_2} & 0 & 0 & 0 \\ 0 & -\frac{\partial}{\partial x_1} & 0 & 0 \\ 0 & 0 & -\frac{\partial}{\partial x_2} & 0 \\ 0 & 0 & 0 & \frac{\partial}{\partial x_1} \end{bmatrix} \begin{bmatrix} F^a \\ F^b \\ F^c \\ F^d \end{bmatrix} \\ = \begin{bmatrix} -(a + b + c) & a & b & c \\ c & -(a + b + c) & a & b \\ b & c & -(a + b + c) & a \\ a & b & c & -(a + b + c) \end{bmatrix} \begin{bmatrix} F^a \\ F^b \\ F^c \\ F^d \end{bmatrix}.$$

Introducing new unknown functions  $P, R, Q, T$ , defined by

$$(4.18) \quad P = F^a + F^c, \quad Q = F^a - F^c,$$

$$(4.19) \quad R = F^b + F^d, \quad T = F^b - F^d,$$

we obtain the new system of equations

$$(4.20) \quad \frac{\partial}{\partial t} P - v \frac{\partial}{\partial x_2} Q = -(a+c)P + (a+c)R,$$

$$(4.21) \quad \frac{\partial}{\partial t} Q - v \frac{\partial}{\partial x_2} P = -(a+2b+c)Q + (a-c)T,$$

$$(4.22) \quad \frac{\partial}{\partial t} R + v \frac{\partial}{\partial x_1} T = -(a+c)R + (a+c)P,$$

$$(4.23) \quad \frac{\partial}{\partial t} T + v \frac{\partial}{\partial x_1} R = -(a+2b+c)T - (a-c)Q.$$

To obtain the equation for the unconditional probability density function, let us introduce two new functions:

$$(4.24) \quad U = P + R = F^a + F^c + F^b + F^d,$$

$$(4.25) \quad S = P - R = F^a + F^c - F^b - F^d.$$

Now, the function  $F$ , defined as

$$(4.26) \quad F = \frac{1}{4} U,$$

represents the probability density function of the event that the pollutant particle reaches a certain area, independently of its initial direction. The above substitution and differentiation with respect to spatial variables transforms the equations to the following form:

$$(4.27) \quad \frac{\partial}{\partial t} P - v \frac{\partial}{\partial x_2} Q = -(a+c)S,$$

$$(4.28) \quad \frac{\partial}{\partial x_1} \frac{\partial}{\partial t} Q - v \frac{\partial}{\partial x_1} \frac{\partial}{\partial x_2} P = -(a+2b+c) \frac{\partial}{\partial x_1} Q + (a-c) \frac{\partial}{\partial x_1} T,$$

$$(4.29) \quad \frac{\partial}{\partial t} R + v \frac{\partial}{\partial x_1} T = (a+c)S,$$

$$(4.30) \quad \frac{\partial}{\partial x_2} \frac{\partial}{\partial t} T + v \frac{\partial}{\partial x_2} \frac{\partial}{\partial x_1} R = -(a+2b+c) \frac{\partial}{\partial x_2} T - (a-c) \frac{\partial}{\partial x_2} Q.$$

Addition and subtraction of the pairs of the equations gives the following system of partial differential equations for four functions  $U$ ,  $S$ ,  $T$ ,  $Q$ :

$$(4.31) \quad \frac{\partial}{\partial t} U - v \frac{\partial}{\partial x_2} Q + v \frac{\partial}{\partial x_1} T = 0,$$

$$(4.32) \quad \frac{\partial^2}{\partial t \partial x_1} Q + \frac{\partial^2}{\partial t \partial x_2} T - v \frac{\partial^2}{\partial x_1 \partial x_2} U \\ = -(a + 2b + c) \left[ \frac{\partial}{\partial x_1} Q + \frac{\partial}{\partial x_2} T \right] + (a - c) \left[ \frac{\partial}{\partial x_1} T - \frac{\partial}{\partial x_2} Q \right],$$

$$(4.33) \quad \frac{\partial}{\partial t} S - v \frac{\partial}{\partial x_2} Q - v \frac{\partial}{\partial x_1} T = -2(a + c)S,$$

$$(4.34) \quad \frac{\partial^2}{\partial t \partial x_1} Q - \frac{\partial^2}{\partial t \partial x_2} T - v \frac{\partial^2}{\partial x_1 \partial x_2} S \\ = -(a + 2b + c) \left[ \frac{\partial}{\partial x_1} Q + \frac{\partial}{\partial x_2} T \right] + (a - c) \left[ \frac{\partial}{\partial x_1} T + \frac{\partial}{\partial x_2} Q \right].$$

The system of equations obtained can be used for the calculation of the probability density  $U$  describing the unconditional location of the particle. Elimination of the functions  $S$ ,  $T$ ,  $Q$  from Eqs. (4.31) – (4.34) is too complicated and, moreover, it would change the class of the function sought; therefore, we leave this system of equations in its present form.

#### 4.2. Random walk with sedimentation

Modeling the two-dimensional diffusion process we can also take into account the possibility of the sedimentation of the particles in the environment. Then, analogously to Sec. 3, the particle can either move in one of the four possible directions:

$$(4.35) \quad \mathbf{a} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} -1 \\ 0 \end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}, \quad \mathbf{d} = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

with probability dependent on the previous direction of the particle's motion, or remain at the point of its present location, what can be represented by a zero vector of motion

$$(4.36) \quad \mathbf{g} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

We can also introduce the matrix of rotation (or annihilation) of the particle's velocity vector, which is random and takes the values according to our assumptions concerning the model. The matrix of rotation  $\mathbf{E}(\omega)$  takes the following values:

$$(4.37) \quad \mathbf{E}(\omega) = \mathbf{A} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \quad \text{with probability } a\Delta t,$$

$$(4.38) \quad \mathbf{E}(\omega) = \mathbf{B} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \quad \text{with probability } b\Delta t,$$

$$(4.39) \quad \mathbf{E}(\omega) = \mathbf{C} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \quad \text{with probability } c\Delta t,$$

$$(4.40) \quad \mathbf{E}(\omega) = \mathbf{G} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \quad \text{with probability } g\Delta t,$$

$$(4.41) \quad \mathbf{E}(\omega) = \mathbf{D} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{with probability } 1 - (a + b + c + g)\Delta t.$$

The rotation matrices defined above act on the velocity direction vectors in the following way:

$$(4.42) \quad \mathbf{A}\mathbf{d} = \mathbf{a}, \quad \mathbf{B}\mathbf{d} = \mathbf{b}, \quad \mathbf{C}\mathbf{d} = \mathbf{d}, \quad \mathbf{D}\mathbf{d} = \mathbf{d}, \quad \mathbf{G}\mathbf{d} = \mathbf{g},$$

$$(4.43) \quad \mathbf{A}\mathbf{a} = \mathbf{b}, \quad \mathbf{B}\mathbf{a} = \mathbf{c}, \quad \mathbf{C}\mathbf{a} = \mathbf{a}, \quad \mathbf{D}\mathbf{a} = \mathbf{a}, \quad \mathbf{G}\mathbf{a} = \mathbf{g},$$

$$(4.44) \quad \mathbf{A}\mathbf{b} = \mathbf{c}, \quad \mathbf{B}\mathbf{b} = \mathbf{d}, \quad \mathbf{C}\mathbf{b} = \mathbf{a}, \quad \mathbf{D}\mathbf{b} = \mathbf{b}, \quad \mathbf{G}\mathbf{b} = \mathbf{g},$$

$$(4.45) \quad \mathbf{A}\mathbf{c} = \mathbf{d}, \quad \mathbf{B}\mathbf{c} = \mathbf{a}, \quad \mathbf{C}\mathbf{c} = \mathbf{b}, \quad \mathbf{D}\mathbf{c} = \mathbf{c}, \quad \mathbf{G}\mathbf{c} = \mathbf{g},$$

$$(4.46) \quad \mathbf{A}\mathbf{g} = \mathbf{g}, \quad \mathbf{B}\mathbf{g} = \mathbf{g}, \quad \mathbf{C}\mathbf{g} = \mathbf{g}, \quad \mathbf{D}\mathbf{g} = \mathbf{g}, \quad \mathbf{G}\mathbf{g} = \mathbf{g}.$$

The change of location of the particle in  $n$  steps (under the condition that the particle has really left the starting point) is

$$(4.47) \quad \mathbf{S}_n^{\mathbf{r}} = v\Delta t(\mathbf{I}\mathbf{d} + \mathbf{E}_1 + \mathbf{E}_2\mathbf{E}_1 + \dots + \mathbf{E}_{n-1}\mathbf{E}_{n-2}, \dots, \mathbf{E}_2\mathbf{E}_1) \mathbf{r},$$

where  $\mathbf{r}$  is the initial direction of particle's motion, that is  $\mathbf{r} = \mathbf{a}$ ,  $\mathbf{r} = \mathbf{b}$ ,  $\mathbf{r} = \mathbf{c}$ , or  $\mathbf{r} = \mathbf{d}$ ; in the case of not leaving the point, the motion vector can be written as

$$(4.48) \quad \mathbf{S}_n^{\mathbf{g}} = \mathbf{g}.$$

Consider an arbitrary real-valued function  $\varphi(\mathbf{x})$  defined on  $\mathbb{R}^2$ , and its conditional average values (under the conditions of all possible initial directions of the walking particle)  $\langle \varphi(\mathbf{x} + \mathbf{S}_n^{\mathbf{r}}) \rangle$ ,  $\mathbf{r} = \mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}, \mathbf{g}$ . Performing the reasoning analogous to the one made in the non-sedimentation case, we obtain the system of equations for the conditional probability density functions  $F^{\mathbf{r}}$ ,  $\mathbf{r} = \mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}, \mathbf{g}$ :

$$(4.49) \quad \frac{\partial F^{\mathbf{r}}}{\partial t} = v\mathbf{r} \cdot \nabla F^{\mathbf{r}}(\mathbf{x}) + aF^{\mathbf{A}\mathbf{r}}(\mathbf{x}) + bF^{\mathbf{B}\mathbf{r}}(\mathbf{x}) + cF^{\mathbf{C}\mathbf{r}}(\mathbf{x}) \\ - (a + b + c + g)F^{\mathbf{r}}(\mathbf{x}) + gF^{\mathbf{g}}(\mathbf{x}),$$

for  $r = a, b, c, d$  and

$$(4.50) \quad \frac{\partial F^g}{\partial t} = 0.$$

The system of equations (4.49) can be written in the vector form

$$(4.51) \quad \frac{\partial}{\partial t} \begin{bmatrix} F^a \\ F^b \\ F^c \\ F^d \\ F^g \end{bmatrix} - v \begin{bmatrix} \frac{\partial}{\partial x_2} & 0 & 0 & 0 & 0 \\ 0 & -\frac{\partial}{\partial x_1} & 0 & 0 & 0 \\ 0 & 0 & -\frac{\partial}{\partial x_2} & 0 & 0 \\ 0 & 0 & 0 & \frac{\partial}{\partial x_1} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} F^a \\ F^b \\ F^c \\ F^d \\ F^g \end{bmatrix} = \begin{bmatrix} -(a+b+c+g) & a & b & c & g \\ c & -(a+b+c+g) & a & b & g \\ b & c & -(a+b+c+g) & a & g \\ a & b & c & -(a+b+c+g) & g \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} F^a \\ F^b \\ F^c \\ F^d \\ F^g \end{bmatrix}.$$

Similarly to the model without sedimentation, assuming that the probabilities of the initial directions of the pollutant particles are equal, we can obtain the system of equations where the probability density function of the actual location of the particle is one of the functions sought for. Repeating the calculations in the way analogous to the previous case of non-sedimenting particles, we can obtain the system of equations for the following sets of functions

$$(4.52) \quad P = F^a + F^c, \quad Q = F^a - F^c,$$

$$(4.53) \quad R = F^b + F^d, \quad T = F^b - F^d \quad \text{and } F^g,$$

or alternatively,

$$(4.54) \quad U = F^a + F^c + F^b + F^d, \quad Q = F^a - F^c,$$

$$(4.55) \quad S = F^a + F^c - F^b - F^d, \quad T = F^b - F^d \quad \text{and} \quad F^g.$$

In the first case the system of equations is

$$(4.56) \quad \frac{\partial}{\partial t} P - v \frac{\partial}{\partial x_2} Q = -(a + c + g)P + (a + c)R + 2gF^g,$$

$$(4.57) \quad \frac{\partial}{\partial t} Q - v \frac{\partial}{\partial x_2} P = -(a + 2b + c + g)Q + (a - c)T,$$

$$(4.58) \quad \frac{\partial}{\partial t} R + v \frac{\partial}{\partial x_1} T = -(a + c + g)R + (a + c)P + 2gF^g,$$

$$(4.59) \quad \frac{\partial}{\partial t} T + v \frac{\partial}{\partial x_1} R = -(a + 2b + c + g)T - (a - c)Q,$$

$$(4.60) \quad \frac{\partial F^g}{\partial t} = 0,$$

while in the second case we obtain

$$(4.61) \quad \frac{\partial}{\partial t} U - v \frac{\partial}{\partial x_2} Q + v \frac{\partial}{\partial x_1} T = -gU + 4gF^g,$$

$$(4.62) \quad \frac{\partial^2}{\partial t \partial x_1} Q + \frac{\partial^2}{\partial t \partial x_2} T - v \frac{\partial^2}{\partial x_1 \partial x_2} U \\ = -(a + 2b + c + g) \left[ \frac{\partial}{\partial x_1} Q + \frac{\partial}{\partial x_2} T \right] + (a - c) \left[ \frac{\partial}{\partial x_1} T - \frac{\partial}{\partial x_2} Q \right],$$

$$(4.63) \quad \frac{\partial}{\partial t} S - v \frac{\partial}{\partial x_2} Q - v \frac{\partial}{\partial x_1} T = -2(a + c)S - gS,$$

$$(4.64) \quad \frac{\partial^2}{\partial t \partial x_1} Q - \frac{\partial^2}{\partial t \partial x_2} T - v \frac{\partial^2}{\partial x_1 \partial x_2} S \\ = -(a + 2b + c + g) \left[ \frac{\partial}{\partial x_1} Q - \frac{\partial}{\partial x_2} T \right] + (a - c) \left[ \frac{\partial}{\partial x_1} T + \frac{\partial}{\partial x_2} Q \right],$$

$$(4.65) \quad \frac{\partial F^g}{\partial t} = 0.$$



## 5. The model of pollution transport with sedimentation in three-dimensional space

Modeling the pollution transport in three-dimensional space, we can also use the random walk process. In such a case we can describe the flow of particles in a much more realistic way than in the one- or two-dimensional cases. At present the phenomenon of sedimentation of the particles doesn't require to introduce the probability of annihilation of the particle. In order to describe it, we can simply assume that the particle reaches a certain surface (ground surface) which is an absorbing boundary, characterized by an appropriate boundary condition for the probability density function (see [11]). We can alternatively assume that the boundary reflects the particle, what is expressed mathematically by vanishing of the particles flux on the surface (expressed in terms of the probability density function), see [11]. Obviously, the boundary can also partially reflect and partially absorb the particles. In such a situation the boundary condition is a certain combination of the conditions for the reflecting and absorbing boundary.

Let us consider a random walk in a three-dimensional space. We define the source point  $\mathbf{x}_0$  and the sedimentation plane  $\mathcal{Z}(x - y)$ , described in the three-dimensional Euclidean space coordinates in such a way that

$$(5.1) \quad \mathbf{x}_0 = \begin{bmatrix} 0 \\ 0 \\ z_0 \end{bmatrix} \quad \text{and} \quad \mathcal{Z}(x - y) = \left[ \mathbf{x} = \begin{bmatrix} x \\ y \\ 0 \end{bmatrix}, \quad x \in \mathbf{R}, y \in \mathbf{R} \right].$$

The particle starting from the source point can walk in one of the six possible directions, parallel to the coordinate axes of the space; staying at any point at a given instant of time, it also can continue its walk in one of six possible directions with probability dependent on the direction of its previous step. The direction vectors of possible particle's steps in a three-dimensional space are:

$$(5.2) \quad \mathbf{a} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} 0 \\ -1 \\ 0 \end{bmatrix}, \quad \mathbf{d} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{e} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} 0 \\ 0 \\ -1 \end{bmatrix},$$

where  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ ,  $\mathbf{d}$ , represent the possible directions of transport,  $\mathbf{e}$  – the direction of convection and  $\mathbf{f}$  – the direction of sedimentation. Reaching the sedimentation plane  $\{\mathbf{x} = (x, y, 0)^T, \quad x, y \in \mathbb{R}\}$  the particle stops and is excluded from the balance of mass of the travelling particles.

Change of direction is governed by some rotation matrix  $\mathbf{A}$ , depending on the initial direction (direction of the previous step). To define the random walk we assume the probabilities of changes of the direction of particle's motion and, consequently, the probability that the rotation matrix  $\mathbf{A}$  takes a given value.

To model the transport process we assume that the rotation matrix takes its value depending not only on the rotation angle but also on the initial and final direction of particle's velocity.

In the transport plane  $x - y$  transformations of the velocity vector are the rotations around the axis  $\mathbf{e}$ , and they are described by the following matrices:

- turning to the left ( $\mathbf{a} \Rightarrow \mathbf{b}$ ,  $\mathbf{b} \Rightarrow \mathbf{c}$ ,  $\mathbf{c} \Rightarrow \mathbf{d}$ ,  $\mathbf{d} \Rightarrow \mathbf{a}$ )

$$(5.3) \quad \mathbf{A} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{with probability } \alpha_1 \Delta t;$$

- reflecting ( $\mathbf{a} \Rightarrow \mathbf{c}$ ,  $\mathbf{b} \Rightarrow \mathbf{d}$ ,  $\mathbf{c} \Rightarrow \mathbf{a}$ ,  $\mathbf{d} \Rightarrow \mathbf{b}$ )

$$(5.4) \quad \mathbf{A} = \begin{bmatrix} -1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{with probability } \beta \Delta t;$$

- turning to the right ( $\mathbf{a} \Rightarrow \mathbf{d}$ ,  $\mathbf{b} \Rightarrow \mathbf{a}$ ,  $\mathbf{c} \Rightarrow \mathbf{b}$ ,  $\mathbf{d} \Rightarrow \mathbf{c}$ )

$$(5.5) \quad \mathbf{A} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{with probability } \alpha_2 \Delta t.$$

The matrices describing changes from the transport process in plane  $x - y$  to the convection (that is the walk with the velocity vector  $\mathbf{e}$ ) have the following form:

for the transformation  $\mathbf{a} \Rightarrow \mathbf{e}$

$$(5.6) \quad \mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix};$$

for the transformation  $\mathbf{b} \Rightarrow \mathbf{e}$

$$(5.7) \quad \mathbf{A} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix};$$

for the transformation  $\mathbf{c} \Rightarrow \mathbf{e}$

$$(5.8) \quad \mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix};$$

for the transformation  $\mathbf{d} \Rightarrow \mathbf{e}$

$$(5.9) \quad \mathbf{A} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix};$$

all with the probability  $\kappa \Delta t$ , and

for the transformation  $\mathbf{f} \Rightarrow \mathbf{e}$

$$(5.10) \quad \mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad \text{with probability } \psi \Delta t.$$

Similarly, the change from the transport to sedimentation (the walk with velocity  $\mathbf{f}$ ) is described by the following matrices:

for the transformation  $\mathbf{a} \Rightarrow \mathbf{f}$

$$(5.11) \quad \mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix};$$

for the transformation  $\mathbf{b} \Rightarrow \mathbf{f}$

$$(5.12) \quad \mathbf{A} = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix};$$

for the transformation  $\mathbf{c} \Rightarrow \mathbf{f}$

$$(5.13) \quad \mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 1 & 0 \end{bmatrix};$$

for the transformation  $\mathbf{d} \Rightarrow \mathbf{f}$

$$(5.14) \quad \mathbf{A} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix};$$

all with probability  $\gamma\Delta t$ , and

for the transformation  $\mathbf{e} \Rightarrow \mathbf{f}$

$$(5.15) \quad \mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad \text{with probability } \varepsilon\Delta t.$$

The last possible changes of the direction of the particle velocity are the changes from convection to transport:

for the transformation  $\mathbf{e} \Rightarrow \mathbf{a}$

$$(5.16) \quad \mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix};$$

for the transformation  $\mathbf{e} \Rightarrow \mathbf{b}$

$$(5.17) \quad \mathbf{A} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix};$$

for the transformation  $\mathbf{e} \Rightarrow \mathbf{c}$

$$(5.18) \quad \mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix};$$

for the transformation  $\mathbf{e} \Rightarrow \mathbf{d}$

$$(5.19) \quad \mathbf{A} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix};$$

all with probability  $\delta\Delta t$ , and from sedimentation to transport:

for the transformation  $\mathbf{f} \Rightarrow \mathbf{a}$

$$(5.20) \quad \mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix};$$

for the transformation  $\mathbf{f} \Rightarrow \mathbf{b}$

$$(5.21) \quad \mathbf{A} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix};$$

for the transformation  $\mathbf{f} \Rightarrow \mathbf{c}$

$$(5.22) \quad \mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix};$$

for the transformation  $\mathbf{f} \Rightarrow \mathbf{d}$

$$(5.23) \quad \mathbf{A} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix},$$

with probability  $\varphi \Delta t$ .

To derive the equations for the probability of the location of the walking particle we repeat the procedure applied in the two-dimensional model. Let us assume that  $\mathbf{w}$  is the initial velocity vector of the particle (taking the value  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ ,  $\mathbf{d}$ ,  $\mathbf{e}$  or  $\mathbf{f}$ ), while  $\mathbf{x} = (x_1, x_2, x_3)$  is the starting point (at initial time  $t = 0$ ). Then the change of location of the particle after  $n$  time steps is

$$(5.24) \quad S_n^{\mathbf{w}} = v \Delta t [\mathbf{w} + \mathbf{A}_1 \mathbf{w} + \mathbf{A}_2 \mathbf{A}_1 \mathbf{w} + \dots + \mathbf{A}_{n-1} \mathbf{A}_{n-2} \dots \mathbf{A}_1 \mathbf{w}].$$

We consider the function of the actual location of the particle defined as

$$(5.25) \quad F_n^{\mathbf{w}}(\mathbf{x}) = \langle \Phi[\mathbf{x} + S_n^{\mathbf{w}}] \rangle.$$

Writing  $S_n^{\mathbf{w}}$  explicitly we obtain

$$(5.26) \quad F_n^{\mathbf{w}}(\mathbf{x}) = \langle \Phi \left[ \mathbf{x} + v \Delta t [\mathbf{w} + \mathbf{A}_1 \mathbf{w} + \mathbf{A}_2 \mathbf{A}_1 \mathbf{w} + \dots + \mathbf{A}_{n-1} \mathbf{A}_{n-2} \dots \mathbf{A}_1 \mathbf{w}] \right] \rangle.$$

The conditional expectation of the function  $F_n^{\mathbf{w}}(\mathbf{x})$  with respect to matrix  $\mathbf{A}_1$  (under the condition that  $\mathbf{w}$  is equal, respectively, to  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$ ,  $\mathbf{d}$ ,  $\mathbf{e}$ , and  $\mathbf{f}$ ) is the following:

$$(5.27) \quad F_n^{\mathbf{a}}(\mathbf{x}) = \alpha_1 \Delta t F_{n-1}^{\mathbf{b}}(\mathbf{x} + v \Delta t \mathbf{a}) + \alpha_2 \Delta t F_{n-1}^{\mathbf{d}}(\mathbf{x} + v \Delta t \mathbf{a}) \\ + \beta \Delta t F_{n-1}^{\mathbf{c}}(\mathbf{x} + v \Delta t \mathbf{a}) + \kappa \Delta t F_{n-1}^{\mathbf{e}}(\mathbf{x} + v \Delta t \mathbf{a}) + \gamma \Delta t F_{n-1}^{\mathbf{f}}(\mathbf{x} + v \Delta t \mathbf{a}) \\ + (1 - (\alpha_1 + \alpha_2 + \beta + \kappa + \gamma) \Delta t) F_{n-1}^{\mathbf{a}}(\mathbf{x} + v \Delta t \mathbf{a}),$$

$$(5.28) \quad F_n^b(\mathbf{x}) = \alpha_1 \Delta t F_{n-1}^c(\mathbf{x} + v \Delta t \mathbf{b}) + \alpha_2 \Delta t F_{n-1}^a(\mathbf{x} + v \Delta t \mathbf{b}) \\ + \beta \Delta t F_{n-1}^d(\mathbf{x} + v \Delta t \mathbf{b}) + \kappa \Delta t F_{n-1}^e(\mathbf{x} + v \Delta t \mathbf{b}) + \gamma \Delta t F_{n-1}^f(\mathbf{x} + v \Delta t \mathbf{b}) \\ + (1 - (\alpha_1 + \alpha_2 + \beta + \kappa + \gamma) \Delta t) F_{n-1}^b(\mathbf{x} + v \Delta t \mathbf{b}),$$

$$(5.29) \quad F_n^c(\mathbf{x}) = \alpha_1 \Delta t F_{n-1}^d(\mathbf{x} + v \Delta t \mathbf{c}) + \alpha_2 \Delta t F_{n-1}^b(\mathbf{x} + v \Delta t \mathbf{c}) \\ + \beta \Delta t F_{n-1}^a(\mathbf{x} + v \Delta t \mathbf{c}) + \kappa \Delta t F_{n-1}^e(\mathbf{x} + v \Delta t \mathbf{c}) + \gamma \Delta t F_{n-1}^f(\mathbf{x} + v \Delta t \mathbf{c}) \\ + (1 - (\alpha_1 + \alpha_2 + \beta + \kappa + \gamma) \Delta t) F_{n-1}^c(\mathbf{x} + v \Delta t \mathbf{c}),$$

$$(5.30) \quad F_n^d(\mathbf{x}) = \alpha_1 \Delta t F_{n-1}^a(\mathbf{x} + v \Delta t \mathbf{d}) + \alpha_2 \Delta t F_{n-1}^c(\mathbf{x} + v \Delta t \mathbf{d}) \\ + \beta \Delta t F_{n-1}^b(\mathbf{x} + v \Delta t \mathbf{d}) + \kappa \Delta t F_{n-1}^e(\mathbf{x} + v \Delta t \mathbf{d}) + \gamma \Delta t F_{n-1}^f(\mathbf{x} + v \Delta t \mathbf{d}) \\ + (1 - (\alpha_1 + \alpha_2 + \beta + \kappa + \gamma) \Delta t) F_{n-1}^d(\mathbf{x} + v \Delta t \mathbf{d}),$$

$$(5.31) \quad F_n^e(\mathbf{x}) = \delta \Delta t [F_{n-1}^a(\mathbf{x} + v \Delta t \mathbf{e}) + F_{n-1}^b(\mathbf{x} + v \Delta t \mathbf{e}) \\ + F_{n-1}^c(\mathbf{x} + v \Delta t \mathbf{e}) + F_{n-1}^d(\mathbf{x} + v \Delta t \mathbf{e})] \\ + \varepsilon \Delta t F_{n-1}^f(\mathbf{x} + v \Delta t \mathbf{e}) + (1 - (4\delta + \varepsilon) \Delta t) F_{n-1}^e(\mathbf{x} + v \Delta t \mathbf{e}),$$

$$(5.32) \quad F_n^f(\mathbf{x}) = \varphi \Delta t [F_{n-1}^a(\mathbf{x} + v \Delta t \mathbf{f}) + F_{n-1}^b(\mathbf{x} + v \Delta t \mathbf{f}) \\ + F_{n-1}^c(\mathbf{x} + v \Delta t \mathbf{f}) + F_{n-1}^d(\mathbf{x} + v \Delta t \mathbf{f})] \\ + \psi \Delta t F_{n-1}^e(\mathbf{x} + v \Delta t \mathbf{f}) + (1 - (4\varphi + \psi) \Delta t) F_{n-1}^f(\mathbf{x} + v \Delta t \mathbf{f}).$$

Passing to the limit in the difference equations (5.27)–(5.32), as in the previous cases, we obtain the following system of partial differential equations for the conditional probability density functions:

$$(5.33) \quad \frac{\partial F^a(t, \mathbf{x})}{\partial t} = \alpha_1 F^b(t, \mathbf{x}) + \alpha_2 F^d(t, \mathbf{x}) + \beta F^c(t, \mathbf{x}) + \kappa F^e(t, \mathbf{x}) + \gamma F^f(t, \mathbf{x}) \\ - (\alpha_1 + \alpha_2 + \beta + \kappa + \gamma) F^a(t, \mathbf{x}) + v \mathbf{a} \cdot \nabla F^a(t, \mathbf{x}),$$

$$(5.34) \quad \frac{\partial F^b(t, \mathbf{x})}{\partial t} = \alpha_1 F^c(t, \mathbf{x}) + \alpha_2 F^a(t, \mathbf{x}) + \beta F^d(t, \mathbf{x}) + \kappa F^e(t, \mathbf{x}) + \gamma F^f(t, \mathbf{x}) \\ - (\alpha_1 + \alpha_2 + \beta + \kappa + \gamma) F^b(t, \mathbf{x}) + v \mathbf{b} \cdot \nabla F^b(t, \mathbf{x}),$$

$$(5.35) \quad \frac{\partial F^c(t, \mathbf{x})}{\partial t} = \alpha_1 F^d(t, \mathbf{x}) + \alpha_2 F^b(t, \mathbf{x}) + \beta F^a(t, \mathbf{x}) + \kappa F^e(t, \mathbf{x}) + \gamma F^f(t, \mathbf{x}) \\ - (\alpha_1 + \alpha_2 + \beta + \kappa + \gamma) F^c(t, \mathbf{x}) + v \mathbf{c} \cdot \nabla F^c(t, \mathbf{x}),$$

$$(5.36) \quad \frac{\partial F^d(t, \mathbf{x})}{\partial t} = \alpha_1 F^a(t, \mathbf{x}) + \alpha_2 F^c(t, \mathbf{x}) + \beta F^b(t, \mathbf{x}) + \kappa F^e(t, \mathbf{x}) + \gamma F^f(t, \mathbf{x}) \\ - (\alpha_1 + \alpha_2 + \beta + \kappa + \gamma) F^d(t, \mathbf{x}) + v \mathbf{d} \cdot \nabla F^d(t, \mathbf{x}),$$

$$(5.37) \quad \frac{\partial F^e(t, \mathbf{x})}{\partial t} = \delta [F^a(t, \mathbf{x}) + F^b(t, \mathbf{x}) + F^c(t, \mathbf{x}) + F^d(t, \mathbf{x})] + \varepsilon F^f(t, \mathbf{x}) \\ - (4\delta + \varepsilon) F^e(t, \mathbf{x}) + v \mathbf{e} \cdot \nabla F^e(t, \mathbf{x}),$$

$$(5.38) \quad \frac{\partial F^f(t, \mathbf{x})}{\partial t} = \psi [F^a(t, \mathbf{x}) + F^b(t, \mathbf{x}) + F^c(t, \mathbf{x}) + F^d(t, \mathbf{x})] + \psi F^e(t, \mathbf{x}) \\ - (4\varphi + \psi) F^f(t, \mathbf{x}) + v \mathbf{f} \cdot \nabla F^f(t, \mathbf{x}),$$

where symbol “ $\cdot$ ” denotes the inner product of vectors and  $\nabla$  is the symbol of gradient.

In the matrix form the system of equations takes the form

$$(5.39) \quad \frac{\partial}{\partial t} \begin{bmatrix} F^a \\ F^b \\ F^c \\ F^d \\ F^e \\ F^f \end{bmatrix} = \begin{bmatrix} -\Omega & \alpha_1 & \beta & \alpha_2 & \kappa & \gamma \\ \alpha_2 & -\Omega & \alpha_1 & \beta & \kappa & \gamma \\ \beta & \alpha_2 & -\Omega & \alpha_1 & \kappa & \gamma \\ \alpha_1 & \beta & \alpha_2 & -\Omega & \kappa & \gamma \\ \delta & \delta & \delta & \delta & -(4\delta + \varepsilon) & \varepsilon \\ \varphi & \varphi & \varphi & \varphi & \psi & -(4\varphi + \psi) \end{bmatrix} \begin{bmatrix} F^a \\ F^b \\ F^c \\ F^d \\ F^e \\ F^f \end{bmatrix} \\ + v \begin{bmatrix} \frac{\partial}{\partial x_2} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{\partial}{\partial x_1} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\partial}{\partial x_2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{\partial}{\partial x_1} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\partial}{\partial x_3} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\partial}{\partial x_3} \end{bmatrix} \begin{bmatrix} F^a \\ F^b \\ F^c \\ F^d \\ F^e \\ F^f \end{bmatrix},$$

where  $\Omega = (\alpha_1 + \alpha_2 + \beta + \kappa + \gamma)$ .

To complete the mathematical description of the transport phenomenon we must assume the initial and boundary conditions for the probability density (or in another interpretation: the pollutant concentration density) functions sought for. As we have assumed, the plane  $\{\mathbf{x} = (x, y, 0)^T, x, y \in \mathbb{R}\}$  is the absorbing boundary. This causes the vanishing of all the conditional probability density functions (see [11]):

$$(5.40) \quad F^{\mathbf{a}}(t, x, y, 0) = F^{\mathbf{b}}(t, x, y, 0) = F^{\mathbf{c}}(t, x, y, 0) = F^{\mathbf{d}}(t, x, y, 0) \\ = F^{\mathbf{e}}(t, x, y, 0) = F^{\mathbf{f}}(t, x, y, 0) = 0.$$

In our interpretation of the functions  $F^{\mathbf{w}}$ ,  $\mathbf{w} = \mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}, \mathbf{e}, \mathbf{f}$ , the initial condition represents the initial location of the fractions of the pollutant particles initiating their walk in a given direction. Since we have assumed the point source of the particles, the initial functions are three-dimensional Dirac delta-functions concentrated at point  $(0, 0, z_0)^T$ ,

$$(5.41) \quad F^{\mathbf{a}}(0, x, y, z) = a_0 \delta(x) \delta(y) \delta(z - z_0),$$

$$(5.42) \quad F^{\mathbf{b}}(0, x, y, z) = b_0 \delta(x) \delta(y) \delta(z - z_0),$$

$$(5.43) \quad F^{\mathbf{c}}(0, x, y, z) = c_0 \delta(x) \delta(y) \delta(z - z_0),$$

$$(5.44) \quad F^{\mathbf{d}}(0, x, y, z) = d_0 \delta(x) \delta(y) \delta(z - z_0),$$

$$(5.45) \quad F^{\mathbf{e}}(0, x, y, z) = e_0 \delta(x) \delta(y) \delta(z - z_0),$$

$$(5.46) \quad F^{\mathbf{f}}(0, x, y, z) = f_0 \delta(x) \delta(y) \delta(z - z_0),$$

where the sum of all intensities equals one,

$$(5.47) \quad a_0 + b_0 + c_0 + d_0 + e_0 + f_0 = 1.$$

Certainly, one can consider some more general problem in which the boundary absorbing condition is given on a more complicated surface, or the initial condition is distributed over the space in a different manner.

## 6. Concluding remarks

In this paper we have proposed several models of the random walk process occurring with a finite speed, useful for the description of transport of the particles. The models are not very restrictive. They can be easily adopted to describe the transport process in many physical environments: turbulent atmosphere, soil or water, depending on the selection of the parameters.

In our considerations, starting from the law of motion of the particle, we have derived the global transport equations for the probability density functions of particle location (or the equations for the pollutant concentration). The obtained equations constitute the system of linear partial differential equations with constant coefficients. The problem of existence and uniqueness of the solutions to such equations has been



already solved. Since we assume that the solutions of the equations are probability density functions, we are looking for the solutions in the class of functions integrable with some polynomial weights (functions with finite moments). It is proved (see [1]) that if the initial conditions and possible excitations (sources) have this property, then the solution will exist, will be unique and also (locally) integrable with a polynomial weight.

The equations obtained can be used for a quantitative analysis of the modeled transport processes. The simplest way of doing this is based on their numerical solution. This is quite natural since they are obtained as the limit of the difference equations, directly applicable for computational analysis. Some conclusions concerning the transport process can be also drawn analytically. Since the transport equations are hyperbolic, we can estimate the effective velocity of the pollutant front from the source.

The proposed random walk process can be studied not only globally, by the analysis of the transport equation. Another possible approach is the investigation of the trajectory equation (2.4) and its multi-dimensional generalizations. It necessitates the application of the random matrix methods (see [4]); in such a manner we can obtain another kind of information concerning the diffusion particles – the areas of concentration, eventual attraction curves, etc.

Application of the proposed models for the description of real transport problems requires identification of the parameters characterizing the probability intensities of the velocity direction jumps, as well as the absolute values of the velocity.

Studying the pollutant particles structure we can try to estimate the probability intensities (e.g. large particle rather sediments than convects, etc.), but complete identification of the model needs some well-prepared experimental data to estimate the parameters of the model. The measurements in the experiment must be performed in a specific way to make them useful for the identification of our model (see [3]). Design of such an experiment and estimation of the parameters is a very important task to solve in modeling of the pollution transport in turbulent atmosphere with the use of random walk process.

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