Modeling of the atmosphere pollution from coal trains

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Abstract. Coal trains have an intensive impact on environment pollution. It is very important to predict adequately this impact during coal transportation. In Ukraine to predict atmosphere pollution from coal trains the regulatory model «OND-86» is used. This model does not take into account some important factors and coal train movement. We present numerical models to solve two problems:1) prediction of atmosphere pollution in the case of moving coal train; 2) prediction of atmosphere pollution in the case of additional special boards installation on the coal wagon. To solve these problems equation of coal duct convective- diffusive dispersion (Lagrange model of admixture dispersion) and equation of potential flow were used. Governing equations were numerically integrated using implicit difference schemes. For coding difference equations we used FORTRAN language. We present results of numerical experiments and laboratory experiments which illustrate the efficiency of the special additional boards installation on the coal wagon. These boards have «internal wing» and «external wing». The obtained results illustrate that installation of additional boards allows to minimize the atmosphere pollution near transport corridor.

1. Introduction

A problem of fugitive dust release from coal trains is of great importance in the problem of environmental protection and attracts scientist's attention in different countries [1-4].

For decreasing of the air pollution during coal transportation different measures are used. For example, one of the ways is wetting of a cargo with water or special solutions. Other way is to give special shape for cargo or to compact it. One of the most effective measures is using covers. Covers are placed on the wagon for full (Figure 1) or partial (Figure 2) covering of a cargo.

Fig. 1. Coal wagon with full covers (Australia) [5]

A literature search made by authors showed that research work in the field of dust release during coal transportation in wagons has not been conducted in Ukraine.
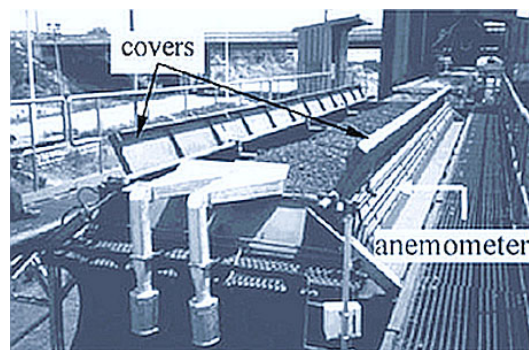

Fig. 2. Coal wagon with covers (Portugal) [1]

In addition, in Ukraine, to estimate the atmosphere pollution during coal transportation in open wagons the empirical model OND-86 is used. This model does not take into account some very important factors, for example: coal train movement, atmosphere turbulent diffusion, etc. Therefore, the prognostic results obtained with this model are not reliable. In addition, the problem of coal dust reduction from coal trains, practically, was not studied in Uktraine. Authors present some 'research directions" which are developed in Dnipro National University of Railway Transport named after academician V. Lazaryan (Ukraine, Project 0115U007227 "Environment protection at the elements of transport infrastructure").

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2. Experimental section

For the experimental simulation, a 1:100 scale model of the open wagon 12-1592 type was used. This type of the open wagon is often used in Ukraine. The model of the open wagon is shown in Figure 3. We studied the case of "poor" loaded wagon.
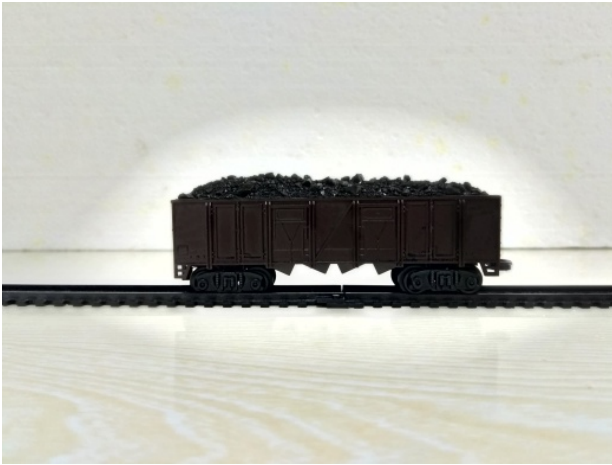

Fig. 3. Model of the open wagon (poorly loaded).

Also a model of this open wagon with additional boards was used in the experiments. Additional board had an "internal" wing which was like a "shelf" on the board and an "external" wing (Figure 4). To show the form of these additional boards we present in Figure 4 the model of the wagon without front side additional board. It is supposed that additional boards can be made of wood or any other cheap material. Installation of these boards on the wagon does not imply special equipment.

Fig. 4. Model of the open wagon with additional boards (model without front side additional board): 1 - "internal wing"; 2 – "external" board

Because of the problems with the wind tunnel equipment which is situated in Dnipro City, an industrial fan was used in the experiments to produce wind flow over the wagon. The Reynolds number in the experiments was Re=10^5. Coal from Mezhdurechenskaya Central Enriching Factory (Donetsk Region, Ukraine) was used in the experiments. Before each experimental run coal has been put into the drying stove for 3 hours. The temperature in the drying stove was +40^0C. After each experimental run coal dust which

had been fallen on the surface of laboratory table was weighted. To weight coal dust we used balance KL168.

The small scale experiments showed that application of additional boards with "internal" and "external" wings reduces the amount of dust released approximately 22% of the quantity emitted from the open wagon without additional boards. The position of the "wings" on the additional board and their length influence the amount of dust released.

3. Mathematical model

Mathematical modeling of the atmosphere pollution during coal transportation was conducted in two scales: microscale and local scale.

To study atmosphere pollution near the wagon (microscale) we used fluid dynamics model of potential flow and equation of convective-diffuse dust dispersion. Model of potential flow allows to create a fast-calculating computer model. In this case the basic equation has the following form:

$$\frac{\partial^2 P}{\partial^2 x} + \frac{\partial^2 P}{\partial^2 y} = 0 \qquad (1)$$

where P is velocity potential.

When applying this equation, it is assumed that the Y axis is directed vertically upwards.

Components of wind velocity are determined as

$$u = \frac{\partial P}{\partial x}, \quad v = \frac{\partial P}{\partial y}.$$

To solve (1) the following boundary conditions were used:

1) at the solid surfaces, upper boundary, the boundary condition was: $\partial P/\partial \mathbf{n} = 0$, where $\mathbf{n}$ is unit vector of external normal to the boundary;

2) at the inlet boundary we set: $\partial P/\partial \mathbf{n} = V_n$, where V_n is known airflow velocity;

3) at the outlet boundary we set: $P = P_0$ +const, P_0 is an arbitrary number (Dirichlet condition).

To simulate the coal dust dispersion from the wagon the mass transfer equation was used [6]:

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial (v - w_s)C}{\partial y} =$$
$$= \frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial C}{\partial y}\right) + \qquad (2)$$
$$+ \sum q_i \delta(x - x_i)\delta(y - y_i)$$

where C is dust concentration in the atmosphere; u, v are wind flow velocity components; w_s is dust fallout speed; $\mu=(\mu_x, \mu_y)$ are turbulent diffusion coefficients. q_i is pollutant emission rate at the point (x_i, y_i); $\delta(x - x_i)\delta(y - y_i)$ are Dirac's delta function, t is time.

Coal surface in the wagon is represented as a number of points (x_i, y_i). Pollutant emission rate q_i at any point (x_i, y_i) depends on the local wind speed. Local wind

speed near the coal surface is computed using (1) and dependencies (2). To compute q_i we used empirical formulae [7] which include the local speed near the coal surface.

Initial and boundary conditions for (2) are discussed in [6].

For prediction of the atmosphere pollution in the transport corridor and in adjacent territory (local scale) in the case of coal train movement, we used the following equation of convective-diffusive dust dispersion [6]:

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} + \frac{\partial (w - w_S)C}{\partial z} =$$
$$= \frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu_z \frac{\partial C}{\partial z}\right) + \quad (3)$$
$$+ \sum Q_i(t)\delta(x - x_i(t))\delta(y - y_i(t))\delta(z - z_i),$$

where C is dust concentration in the atmosphere; (x_i, y_i, z_i) are coordinates of dust emission point source on the surface of the cargo; $\delta(x - x_i(t))\delta(y - y_i(t))\delta(z - z_i)$ is Dirac's delta-function; $Q_i(t)$ is coal dust emission rate (intensity of dust emission from the wagon); t is time; μ_x, μ_y, μ_z are turbulent diffusion coefficients (computed using empirical formulae [8]); w_s is coal dust fallout speed; *u, v, w* are wind flow velocity components.

In the developed model each wagon is represented as a point source having emission rate $Q_i(t)$.This emission rate is calculated using empirical formula [7].

Worthy of note that coordinates *x, y* of each wagon depends on time *t*. These coordinates are changed in time and this change depends on the known train speed. This approach allows to simulate the movement of coal train with the speed we want to represent in the numerical experiment.

4. Numerical integration

Numerical integration of governing equations (1)-(3), was carried out using a rectangular difference grid. To create the form of the wagon, coal surface, geometrical form of the additional boards in 2D simulation (microscale level) we used "markers method" (porosity technique). In the case of 3D simulation "markers" show coal train route.

To solve (1) we wrote it in evolutionary form [7]:

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial^2 x} + \frac{\partial^2 P}{\partial^2 y}, \quad (4)$$

where *t* – fictitious time.

It is known, that when *t*→∞ the solution of this equation will approach to the solution of Laplace equation (1). To solve (4), it is necessary to set "initial' field of velocity potential in computational region at *t*=0. For example, before starting the calculation, we may set *P*=0 in the entire computational domain for *t*=0. Samarsky method [9] was used for numerical integration

of (4). In this case difference equations of splitting are written as following:

1) first step of splitting:

$$\frac{P_{ij}^{n+\frac{1}{2}} - P_{ij}^n}{0.5\Delta t} = \frac{P_{i+1,j}^n - P_{i,j}^n}{\Delta x^2} +$$
$$+ \frac{-P_{ij}^{n+\frac{1}{2}} + P_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{P_{i,j+1}^n - P_{i,j}^n}{\Delta y^2} + \frac{-P_{ij}^{n+\frac{1}{2}} + P_{i,j-1}^{n+\frac{1}{2}}}{\Delta y^2}; \quad (5)$$

2) second step of splitting:

$$\frac{P_{ij}^{n+1} - P_{ij}^{n+\frac{1}{2}}}{0.5\Delta t} = \frac{P_{i+1,j}^{n+1} - P_{ij}^{n+1}}{\Delta x^2} +$$
$$+ \frac{-P_{ij}^{n+\frac{1}{2}} - P_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{P_{i,j+1}^{n+1} - P_{ij}^{n+1}}{\Delta y^2} + \frac{-P_{ij}^{n+\frac{1}{2}} - P_{i,j-1}^{n+\frac{1}{2}}}{\Delta y^2}. \quad (6)$$

At each splitting step, the unknown value of the velocity potential *P* is determined by the explicit formula of "running calculation" [6, 9]. The calculation is finished when the following condition is fulfilled:

$$\left|P_{ij}^{n+1} - P_{ij}^n\right| \leq \varepsilon,$$

where ε is a small number (e.g., ε =0.001); n is an iteration number.

After determining the velocity potential field, the components of the air velocity vector are calculated at the sides of computational cell using dependencies:

$$u_{ij} = \frac{P_{ij} - P_{i-1,j}}{\Delta x}, v_{ij} = \frac{P_{ij} - P_{i,j-1}}{\Delta y}. \quad (7)$$

For the numerical integration of Eq. (2) we used the change – triangle difference scheme.

To integrate numerically equation (2) we represent the convective derivatives as following:

$$\frac{\partial uC}{\partial x} = \frac{\partial u^+ C}{\partial x} + \frac{\partial u^- C}{\partial x},$$
$$\frac{\partial vC}{\partial y} = \frac{\partial v^+ C}{\partial y} + \frac{\partial v^- C}{\partial y},$$

where

$$u^+ = (u + |u|)/2, u^- = (u - |u|)/2,$$
$$v^+ = (v + |v|)/2, v^- = (v - |v|)/2$$

For approximation of the derivatives we used the following expressions:

$$\frac{\partial u^+ C}{\partial x} \approx \frac{u_{i+1,j}^+ C_{ij}^{n+1} - u_{ij}^+ C_{i-1,j}^{n+1}}{\Delta x} = L_x^+ C^{n+1},$$

$$\frac{\partial u^- C}{\partial x} \approx \frac{u_{i+1,j}^- C_{i+1,j}^{n+1} - u_{ij}^- C_{ij}^{n+1}}{\Delta x} = L_x^- C^{n+1},$$

$$\frac{\partial v^+ C}{\partial y} \approx \frac{v_{i,j+1}^+ C_{ij}^{n+1} - v_{ij}^+ C_{i,j-1}^{n+1}}{\Delta y} = L_y^+ C^{n+1} \;,$$

$$\frac{\partial v^- C}{\partial y} \approx \frac{v_{i,j+1}^- C_{i,j+1}^{n+1} - v_{ij}^- C_{ij}^{n+1}}{\Delta y} = L_y^- C^{n+1} \;.$$

Time – depended derivative was approximated as following:

$$\frac{\partial C}{\partial t} = \frac{C_{ij}^{n+1} - C_{ij}^n}{\Delta t} \;.$$

For approximation of the second derivatives the following formulas were used:

$$\frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x}\right) \approx \tilde{\mu}_x \frac{C_{i+1,j}^{n+1} - C_{ij}^{n+1}}{\Delta x^2} - \tilde{\mu}_x \frac{C_{ij}^{n+1} - C_{i-1,j}^{n+1}}{\Delta x^2} =$$
$$= M_{xx}^- C^{n+1} + M_{xx}^+ C^{n+1},$$

$$\frac{\partial}{\partial y}\left(\mu_y \frac{\partial C}{\partial y}\right) \approx \tilde{\mu}_y \frac{C_{i,j+1}^{n+1} - C_{ij}^{n+1}}{\Delta y^2} - \tilde{\mu}_y \frac{C_{ij}^{n+1} - C_{i,j-1}^{n+1}}{\Delta x^2} =$$
$$= M_{yy}^- C^{n+1} + M_{yy}^+ C^{n+1}.$$

2D equation of the dust transfer can be written in the following difference form [6]:

$$\frac{C_{ij}^{n+1} - C_{ij}^n}{\Delta t} + L_x^+ C^{n+1} + L_x^- C^{n+1} +$$
$$+ L_y^+ C^{n+1} + L_y^- C^{n+1} + \sigma C_{ij}^{n+1} = \qquad (8)$$
$$= (M_{xx}^+ C^{n+1} + M_{xx}^- C^{n+1} +$$
$$+ M_{yy}^+ C^{n+1} + M_{yy}^- C^{n+1}) + Q_{ij}\delta_{ij} \;.$$

In this equation symbol δ_{ij} can be equal either "1" or "0", depending whether the source of dust emission is located in cell "ij" or not. Emission Q_{ij} *was* calculated as following:

$$Q_{ij} = Q_k / \Delta x / \Delta y \;,$$

where Q_k is point source intensity in k-th point which is located in the difference cell "ij"

To solve the equation (8) we use the following 4 steps scheme of splitting [6]:

1) at the first step k=1/4 the difference equation is:

$$\frac{C_{ij}^{n+k} - C_{ij}^n}{\Delta t} + \frac{1}{2}(L_x^+ C^k + L_y^+ C^k) + \frac{\sigma}{4} C_{ij}^k =$$
$$= \frac{1}{4}(M_{xx}^+ C^k + M_{xx}^- C^k + \qquad (9)$$
$$+ M_{yy}^+ C^n + M_{yy}^- C^n) + \sum_{l=1}^{N} \frac{Q_l}{4}\delta_l \;;$$

2) at the second step k=n+1/2; c=n+1/4 the difference equation is:

$$\frac{C_{ij}^k - C_{ij}^c}{\Delta t} + \frac{1}{2}(L_x^- C^k + L_y^- C^k) + \frac{\sigma}{4} C_{ij}^k =$$
$$= \frac{1}{4}(M_{xx}^- C^k + M_{xx}^+ C^c + \qquad (10)$$
$$+ M_{yy}^- C^k + M_{yy}^+ C^c) + \sum_{l=1}^{N} \frac{Q_l}{4}\delta_l \;;$$

3) at the third step k=n+3/4; c=n+1/2 the difference equation is:

$$\frac{C_{ij}^k - C_{ij}^c}{\Delta t} + \frac{1}{2}(L_x^+ C^k + L_y^- C^k) + \frac{\sigma}{4} C_{ij}^k =$$
$$= \frac{1}{4}(M_{xx}^- C^c + M_{xx}^+ C^k + \qquad (11)$$
$$+ M_{yy}^- C^k + M_{yy}^+ C^c) + \sum_{l=1}^{N} \frac{Q_l}{4}\delta_l \;;$$

4) at the fourth step k=n+1; c=n+3/4 the difference equation is:

$$\frac{C_{ij}^k - C_{ij}^c}{\Delta t} + \frac{1}{2}(L_x^- C^k + L_y^+ C^k) + \frac{\sigma}{4} C_{ij}^k =$$
$$= \frac{1}{4}(M_{xx}^- C^k + M_{xx}^+ C^c + \qquad (12)$$
$$+ M_{yy}^- C^c + M_{yy}^+ C^k) + \sum_{l=1}^{N} \frac{Q}{4}\delta_l \;.$$

The unknown value of the dust concentration from equations (9)-(12) on the new time layer is calculated with explicit formula of "running calculation". Initial condition for these equations is written as following:

$$C^1\Big| = C(x,y,t^n), \; C^k\Big| = C^{k-1}\Big|.$$

For realizing of the boundary condition ∂C/∂n=0 on the solid walls, fictitious cells were used.

Main features of the difference scheme for integrating equation of dust convective-diffusive dispersion (3). Before numerical integration of this equation we split it as follows [6]:

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} + \frac{\partial (w - w_s)C}{\partial z} = 0,$$

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu_z \frac{\partial C}{\partial z}\right), \quad (13)$$

$$\frac{\partial C}{\partial t} = \sum Q_i(t)\delta(x - x_i(t))\delta(y - y_i(t))\delta(z - z_i).$$

For numerical integration of the first equation from (13) we used the following formulae:

$$\frac{\partial uC}{\partial x} = \frac{\partial u^+ C}{\partial x} + \frac{\partial u^- C}{\partial x},$$

$$\frac{\partial vC}{\partial y} = \frac{\partial v^+ C}{\partial y} + \frac{\partial v^- C}{\partial y},$$

$$\frac{\partial wC}{\partial z} = \frac{\partial w^+C}{\partial z} + \frac{\partial w^-C}{\partial z},$$

$$\frac{\partial u^+C}{\partial x} \approx \frac{u^+_{i+1,jk}C^{n+1}_{ijk} - u^+_{ijk}C^{n+1}_{i-1,jk}}{\Delta x} = L^+_x C^{n+1},$$

$$\frac{\partial u^-C}{\partial x} \approx \frac{u^-_{i+1,jk}C^{n+1}_{i+1,jk} - u^-_{ijk}C^{n+1}_{ijk}}{\Delta x} = L^-_x C^{n+1},$$

$$\frac{\partial v^+C}{\partial y} \approx \frac{v^+_{i,j+1,k}C^{n+1}_{ijk} - v^+_{ijk}C^{n+1}_{i,j-1,k}}{\Delta y} = L^+_y C^{n+1},$$

$$\frac{\partial v^-C}{\partial y} \approx \frac{v^-_{i,j+1,k}C^{n+1}_{i,j+1,k} - v^-_{ijk}C^{n+1}_{ijk}}{\Delta y} = L^-_y C^{n+1},$$

$$\frac{\partial w^+C}{\partial y} \approx \frac{w^+_{ij,k+1}C^{n+1}_{ijk} - w^+_{ijk}C^{n+1}_{i,j,k-1}}{\Delta z} = L^+_z C^{n+1},$$

$$\frac{\partial w^-C}{\partial y} \approx \frac{w^-_{ij,k+1}C^{n+1}_{ij,k+1} - w^-_{ijk}C^{n+1}_{ijk}}{\Delta z} = L^-_z C^{n+1}.$$

where

$$u^+ = (u+|u|)/2, u^- = (u-|u|)/2,$$
$$v^+ = (v+|v|)/2, v^- = (v-|v|)/2 \quad , \text{ etc.}$$

Here we use designation $w=w-w_s$.

To solve the first equation from (13) we use the following 4 steps scheme of splitting:

1) at the first step the difference equation is:

$$\frac{C^k_{ijk} - C^n_{ijk}}{\Delta t} + \frac{1}{2}(L^+_x C^k + L^+_y C^k + L^+_z C^k) = 0 \qquad (14)$$

2) at the second step the difference equation is:

$$\frac{C^k_{ijk} - C^c_{ijk}}{\Delta t} + \frac{1}{2}(L^-_x C^k + L^-_y C^k + L^-_z C^k) = 0 \qquad (15)$$

3) at the third step we use difference expression (15);

4) at the fourth step we use difference expression (14).

The unknown value of dust concentration C is calculated from (14)-(15) using explicit formula of "running calculations". The second equation from (7) is similar to (4) that is why we can use Samarsky method [9] to solve it. To solve the third equation from (13) we used Eurler's method [9]. For coding difference equations we used FORTRAN language.

5. Results

Figure 5 shows coal dust concentration field over the open wagon (upper part of the wagon) with additional boards and in the case of cross wind.

From Figure 5 one can see that "internal" wings play role of a small "cover" which partially localize zone of dust emission in the wagon. But it is clear that for this case these "wings" are short. The "external" wings play the role of "flaps" and guide the wind flow with coal dust upward to the atmosphere layers with more high
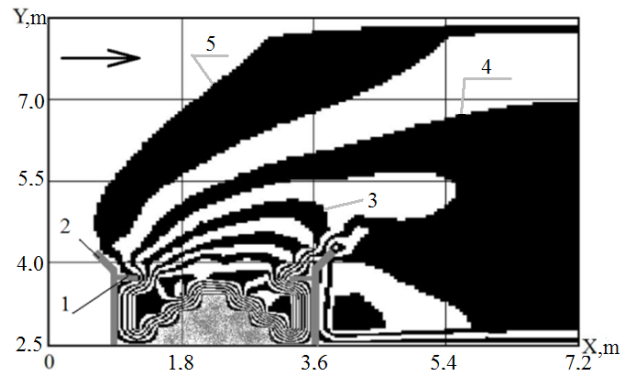
wind speed. Computing time to solve this problem was 5 s.

Fig. 5. Dust concentration field near the wagon with additional boards: 1 – "internal" wing, 2 – "external" wing, 3 – concentration C=0.36 mg/m³, 4 – concentration C =0.22 mg/m³, 5 – concentration C=0.04 mg/m³

Figure 6 (scale 1:1000) shows predicted coal dust concentration at level z=5 m for coal train moving with speed 30 km/h and in the case of cross wind. In Figure 6 arrow indicates the direction of coal train movement. Numerical simulation has been carried out for site near Sinelnikovo Railway Station, Ukraine.
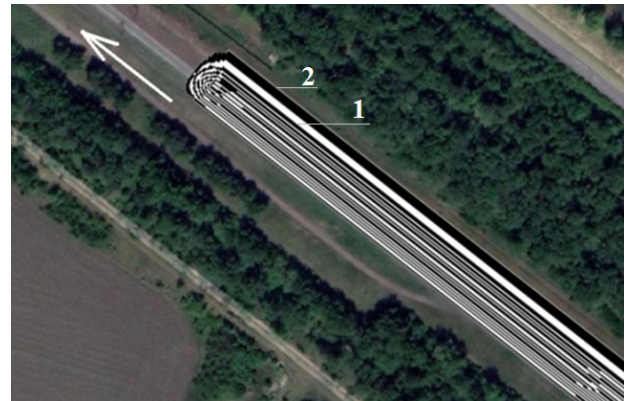

Fig. 6. Predicted coal dust concentration (level z=5 m, t=15 sec): 1 – C=0.31 mg/m³; 2 – C=0.20 mg/m³

Computing time to solve 3D problem was 3 sec.

6. Conclusions

In short, numerical models were developed to predict atmosphere pollution in case of fugitive dust emission from coal train. These models allow to take into account physical factors which influence pollutant dispersion in the atmosphere and which the Regulatory method OND-86 does not take into account. Small scale experiments showed that additional boards on the wagon can reduce coal dust emission.

Future research will focus on development quick computing 3D CFD model which allows to take into account the geometrical form of the wagon. This CFD model will be used do estimate effectiveness of additional boards installation on the wagon.

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