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# Numerical simulation of pollutant dispersion from road with barrier

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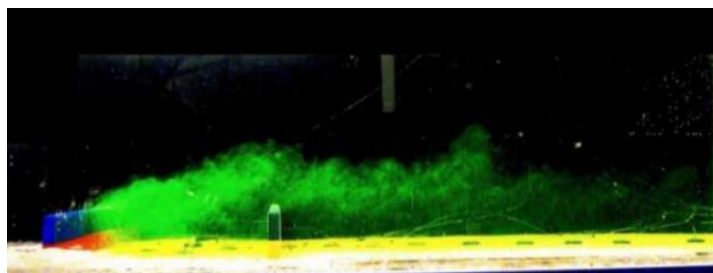
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**Abstract.** The impact of protective barriers on air pollution dispersion near the road was examined using developed numerical model. To simulate wind flow over barrier model of potential flow was used. To simulate pollutant dispersion from road convective-diffusive equation was used. Difference schemes of splitting were used for numerical integration of governing equations. Dispersion of pollutant was modeled for scenarios with no barrier near the road, vertical solid barrier, vertical barriers with additional elements, combination “vertical barrier and plate on the pavilion”. To estimate the efficiency of each scenario potential hazard risk indicator was used. Results of numerical experiment are presented.

## 1. Introduction

It is known that intensive air pollution occurs near highways. Car emissions contain a significant number of harmful substances that are hazardous to health. Trade pavilions are often located near highways. This location of people during the working day near the highway creates a risk of illness for workers. Therefore, it is important to reduce the intensity of air pollution. The simplest and most effective way to protect against air pollution near highways is the use of barriers [1-5, 8-12]. Experimental methods are widely used to evaluate the effectiveness of barriers (Figures 1-2). But the use of such research methods is time consuming and expensive.



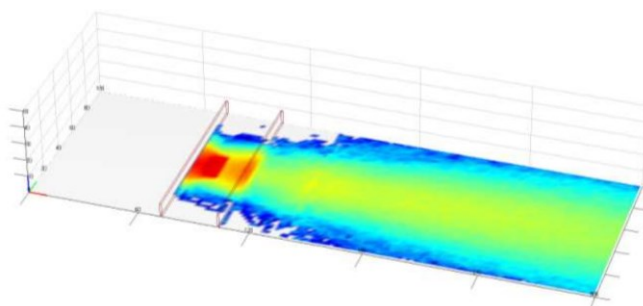
**Figure 1.** Experimental study of contamination zones using a rectangular barrier [2].





**Figure 2.** Experimental study of contamination zones using barrier with inclined element: 1–emission source; 2–contamination zone in front of the barrier; 3–contamination zone above the inclined element [7].

It is important to have computational methods that can determine contaminated zones near highways for specific conditions. Such methods include, among others, the Gaussian model [2], various CFD models [2, 4].



**Figure 3.** CFD modeling pollution zone near barrier [2].

For practice it is also important to have quick computing models to evaluate the effectiveness of barriers for specific conditions. Below we consider such CFD model to analyze the intensity of pollution zones near the highway and to evaluate the effectiveness of using different shaped barriers to reduce the intensity of air pollution near pavilions.

## 2. Methods

### 2.1 Modeling pollutant dispersion near road with barrier

In this paper CO pollution near the road with barrier was considered. To compute contamination zones (combustion product emissions), mass transfer equation was used [3, 5, 6]:

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} = \frac{\partial}{\partial x} \left( \mu_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu_y \frac{\partial C}{\partial y} \right) + Q_i \delta(x - x_i) \delta(y - y_i), \quad (1)$$

where  $C$  is CO concentration in air,  $u$ ,  $v$  are components of the wind speed vector,  $x_i$ ,  $y_i$  are Cartesian coordinates of emission source,  $t$  is time,  $\mu_x$ ,  $\mu_y$  are atmospheric turbulent diffusion coefficients,  $\delta(x_i, y_i)$  is Dirac delta function,  $Q$  is CO emission rate.

The atmospheric turbulent diffusion coefficients were defined as follows:

$$\mu_x = 0.1 \cdot u, \mu_y = 0.1 \cdot v.$$

Boundary conditions for (1) were as follows:

1. At the inflow boundary:  $C=0$ .
2. At the outflow boundary:  $\partial C/\partial n=0$ .
3. On the solid boundaries and on the surfaces  $y=0, y=L_y$  ( $L_y$  is the upper boundary of the region):  $\partial C/\partial n=0$ , where  $n$  is the unit vector of the external normal to the surface.

For time  $t=0$  the initial condition was  $C=0$ .

Numerical integration of the mass transfer equation (1) was carried out using finite-difference schemes and rectangular grid. To form the geometrical view of the computational region (form of barrier, its position, pavilion position etc.) markers were used [6].

First, (1) was split as follows:

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} = 0, \quad (2)$$

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left( \mu_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu_y \frac{\partial C}{\partial y} \right). \quad (3)$$

The convective flow of pollutant was described by (2) and pollutant dispersion due to turbulent diffusion was described by (3).

For numerical solving of (2), a two-step splitting scheme was used:

– step 1:

$$\frac{C_{ij}^k - C_{ij}^n}{\Delta t} + L_x^+ C^k + L_y^+ C^k = 0;$$

– step 2:

$$\frac{C_{ij}^{n+1} - C_{ij}^k}{\Delta t} + L_x^- C^{n+1} + L_y^- C^{n+1} = 0.$$

Here the following designations were used:

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

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

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

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

For the numerical solution of (3) numerical scheme of conditional approximation was used. At the first step the approximation formulae was as follows:

$$\frac{C_{i,j}^{n+\frac{1}{2}} - C_{i,j}^n}{\Delta t} = \left[ \mu_x \frac{-C_{i,j}^{n+\frac{1}{2}} + C_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} \right] + \left[ \mu_y \frac{-C_{i,j}^{n+\frac{1}{2}} + C_{i,j-1}^{n+\frac{1}{2}}}{\Delta y^2} \right].$$

At the second step the approximation formulae was as follows:

$$\frac{C_{i,j}^{n+1} - C_{i,j}^{n+\frac{1}{2}}}{\Delta t} = \left[ \mu_x \frac{C_{i+1,j}^{n+1} - C_{i,j}^{n+1}}{\Delta x^2} \right] + \left[ \mu_y \frac{C_{i,j+1}^{n+1} - C_{i,j}^{n+1}}{\Delta y^2} \right].$$

Unknown meaning of pollutant concentration C was found using explicit formulae from above finite difference equations.

## 2.2 Modelling of wind flow over barrier and building

Body of automobile, barrier and pavilion (building) influence wind flow pattern near the road. To compute velocity field model of potential flow was used. In this case the governing equation was:

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} = 0 \quad (4)$$

where  $P$  is velocity potential.

Boundary conditions for (4) were considered in [3]. At the inflow boundary following wind speed profile was used:

$$u(y) = u_1 \cdot (y/y_1)^{n_1},$$

where  $u_1$  is wind speed at height  $y_1=1$  m.

Wind speed components were determined as follows:

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

For numerical integration of (4), it was written in the form:

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2}, \quad (5)$$

where  $t$  is fictitious time. For  $t \rightarrow \infty$  the solution of (5) will tend to "steady" solution, i.e. to the solution of (4).

Two-steps change-triangle method was used for numerical integration of (5). These steps of splitting were as follows:

– step 1:

$$\frac{P_{i,j}^{n+1/2} - P_{i,j}^n}{0.5\Delta t} = \frac{P_{i+1,j}^n - P_{i,j}^n}{\Delta x^2} + \frac{-P_{i,j}^{n+\frac{1}{2}} + P_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{P_{i,j+1}^n - P_{i,j}^n}{\Delta y^2} + \frac{-P_{i,j}^{n+\frac{1}{2}} + P_{i,j-1}^{n+\frac{1}{2}}}{\Delta y^2};$$

– step 2:

$$\frac{P_{i,j}^{n+1} - P_{i,j}^{n+1/2}}{0.5\Delta t} = \frac{P_{i+1,j}^{n+1} - P_{i,j}^{n+1}}{\Delta x^2} + \frac{-P_{i,j}^{n+\frac{1}{2}} + P_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{P_{i,j+1}^{n+1} - P_{i,j}^{n+1}}{\Delta y^2} + \frac{-P_{i,j}^{n+\frac{1}{2}} + P_{i,j-1}^{n+\frac{1}{2}}}{\Delta y^2}.$$

At each step, the velocity potential was calculated at the centers of the difference cells using an explicit formula. The calculation was over when the following condition was fulfilled:

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

where  $\varepsilon$  is a small number ( $\varepsilon=0.001$ ),  $n$  is iteration number.

After calculation of the velocity potential field, the components of the air flow velocity vector were calculated according to the dependencies:

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

To estimate the barrier efficiency the follows parameter was used:

$$HQ = \frac{C_R}{RfC},$$

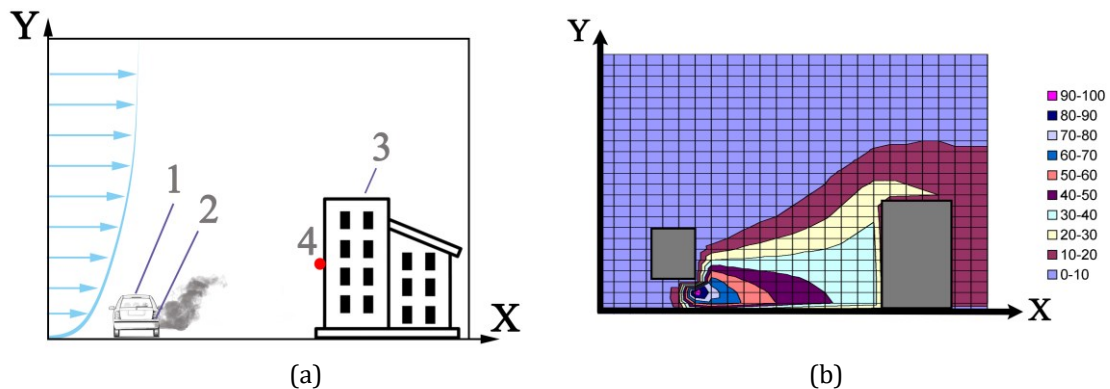
where  $HQ$  is potential hazard risk indicator (Hazard quotient);  $C_R$  is CO concentration at receptor;  $RfC$  is reference concentration ( $RfC = 3 \text{ mg/m}^3$ ). If  $HQ < 1$ , it means that risk for health hazard is minimum.

FORTTRAN was used to code the developed numerical model.

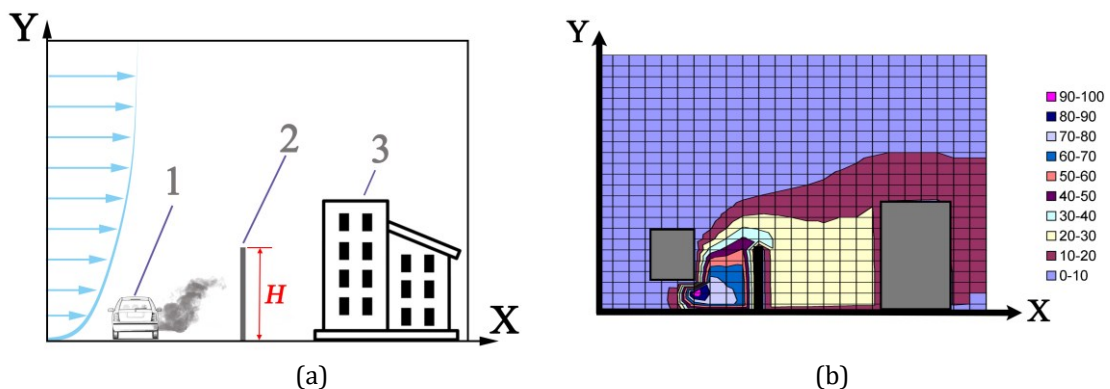
### 3. Results

Developed numerical model was used to compute contamination zones in case of CO emission from road with protective barrier. Five scenarios were considered: scenario #1 – no protective barrier (Figure 4, a); scenario #2 – vertical barrier,  $H=3$  m (Figure 5, a); scenario #3 –  $\Gamma$ -shaped barrier, length of horizontal element was 1 m (Figure 6, a); scenario #4 – barrier with additional inclined element, length of the element was 2 m (Figure 6, a); scenario #5 – vertical barrier +

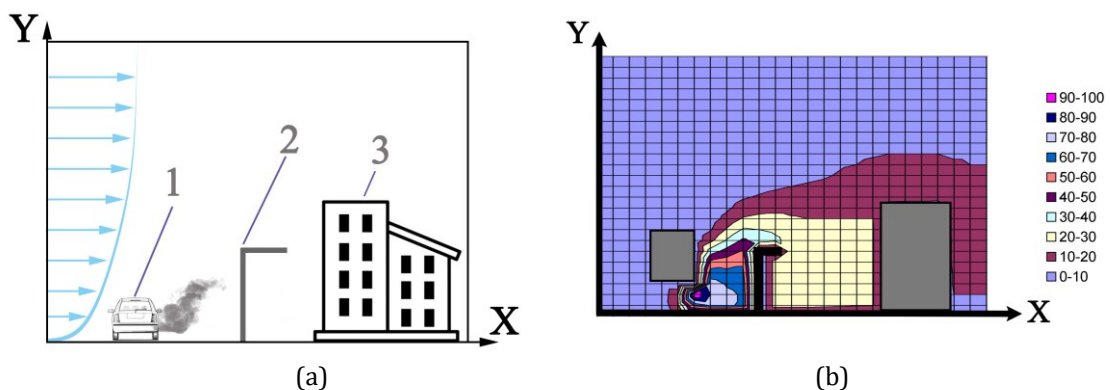
plate on the roof of pavilion, length of the plate was 3 m (Figure 7, a). The initial data were as follows:  $u_1=5$  m/s; pavilion height was 5 m; barrier was situated 7 m from pavilion; dimensions of computational region were 25 m $\times$ 12.5 m; CO emission rate was 33 mg/sec. Point of “interest” (receptor) was at the pavilion wall at height 1.7 m (Fig.4, a). Results of numerical experiment (contamination zones) are shown in Figures 4, b-8, b below. Every number in these Figures shows pollutant concentration as the percentage of maximum concentration  $C_{max}$ .



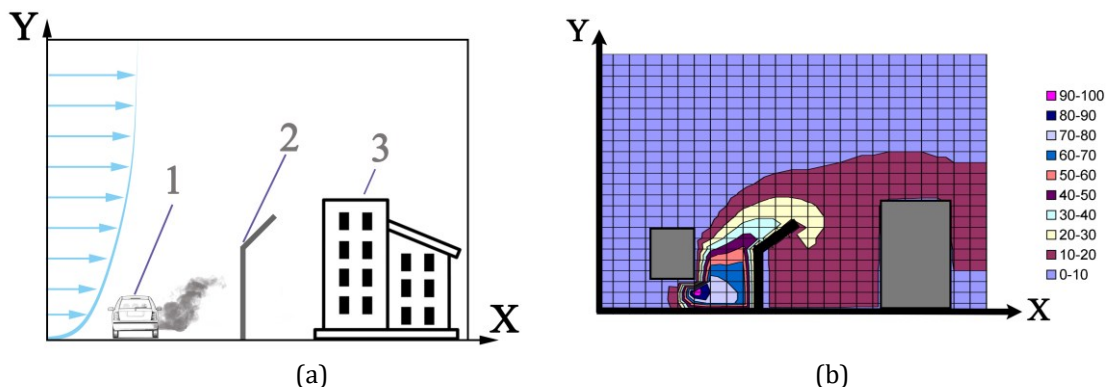
**Figure 4.** (a) Sketch view of computational region and (b) Concentration field of CO (Scenario #1, no barrier),  $C_{max}=5.39$  mg/m $^3$ : 1–automobile; 2–pollutant emission; 3–trade pavilion; 4–receptor.



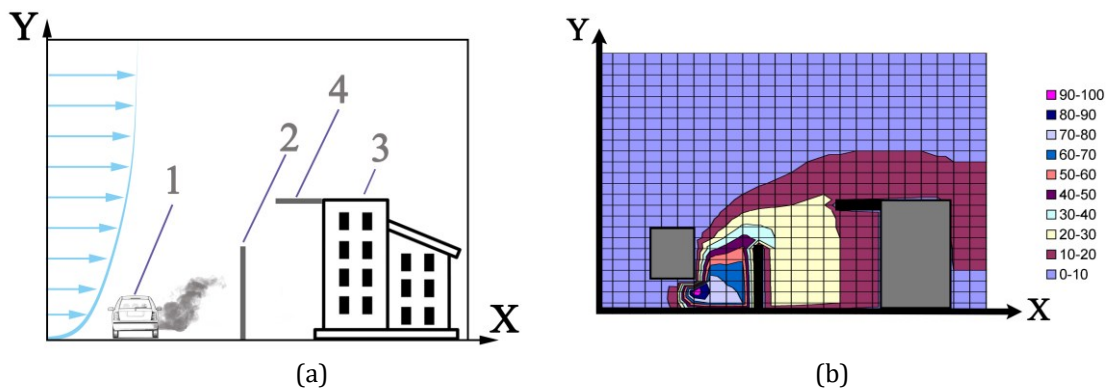
**Figure 5.** (a) Sketch view of computational region and (b) Concentration field of CO (Scenario #2, barrier, H=3 m),  $C_{max}=6.23$  mg/m $^3$ : 1–automobile; 2–barrier; 3– trade pavilion.



**Figure 6.** (a) Sketch view of computational region and (b) Concentration field of CO (Scenario #3,  $\Gamma$ -shaped barrier, H=3 m),  $C_{max}=6.26$  mg/m $^3$ : 1–automobile; 2–barrier; 3– trade pavilion.



**Figure 7.** (a) Sketch view of computational region and (b) Concentration field of CO (Scenario #4, barrier with additional element, H=3 m),  $C_{max}=6.43 \text{ mg/m}^3$ : 1–automobile; 2–barrier; 3–trade pavilion.



**Figure 8.** (a) Sketch view of computational region and (b) Concentration field of CO (Scenario #5, barrier and additional element on the roof of trade pavilion, H=3 m),  $C_{max}=6.33 \text{ mg/m}^3$ : 1–automobile; 2–barrier; 3–trade pavilion; 4–plate on the roof

Figures 4, b-8, b show that barrier causes deformation of contamination zone near the road. The most contaminated zone was formed between automobile (source of emission) and barrier because of wind flow braking in this region.

In Table 1 potential hazard risk indicator is presented.

**Table 1.** Potential hazard risk indicator  $HQ$  (Hazard quotient)

Scenario	$HQ$
Scenario #1	0.65
Scenario #2	0.48
Scenario #3	0.45
Scenario #4	0.35
Scenario #5	0.36

Data from Table 1 shows that the most effective scenario is the 4<sup>th</sup> one, that is when barrier with additional inclined element was used. It can be seen from Figure 2 that inclined element on

barrier guides the pollutant flow upward to the region where the wind speed is more. That allows to decrease contamination level near pavilion wall. Also, one can see that if combination “vertical barrier + plate on the pavilion roof” is used, it makes possible to achieve also not bad result.

Worthy of note that computational time was 2 sec for each scenario.

#### 4. Conclusions

The impact of barriers on the air pollution near road was modeled. To do this, CFD model was developed. Developed CFD model consumes not much computational time due to application of potential flow model to simulate wind flow pattern in the region which had comprehensive geometrical form.

Results of numerical experiment show that vertical barrier with additional inclined element may better improve environment conditions than just a vertical barrier or  $\Gamma$ -shaped barrier. Also, combination “vertical barrier + plate on the pavilion roof” allows to decrease pollutant concentration near pavilion which has been installed near the road.

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