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# Simulation of environmental pollution from diesel locomotive

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**Abstract.** Diesel locomotives are widely used at Ukrainian railway stations as maneuvering locomotives. Emissions from these diesel locomotives contain different toxic chemicals. It is important to understand air contamination patterns which are formed at railway stations. Understanding of these contamination patterns allows to evaluate the negative impact of diesel locomotive emissions on environment. To solve this problem it is necessary to use mathematical models which take into account the most important factors influencing formation of contamination zones. This paper introduces numerical model which allows to simulate pollutants dispersion from moving diesel locomotive. Developed numerical model is based on three dimensional equation of potential flow and three dimensional equation of pollutant dispersion. The model takes into account pollutants ( $NO$ ,  $NO_2$ ) chemical transformation. To solve three dimensional equation of potential flow the implicit difference scheme of splitting was used. To solve three dimensional equation of pollutant dispersion the implicit difference scheme of splitting was used. Euler method was used to solve numerically equations of pollutant chemical transformation. Developed numerical model allows to take into account influence of buildings at the railway station on the contamination zones formation. Developed model consumes not much computer time. Results of performed numerical experiment are presented.

## 1. Introduction

Various types of transport have an intense impact on the environment. Environment protection is a problem of great interest for exploitation of different types of transport [1, 2]. Noise pollution and chemical pollution of the environment are typical for cars and rail transport and this set a problem of their reducing [2-4]. High pollution levels are observed near roads, railways where diesel engines work. Accurate prediction of air pollution near traffic routes requires mathematical models which take into account most important factors which influence the pollutants dispersion. In assessing the negative impact of transport on the environment, two classes of problems are considered. The first class of problems is the assessment of the intensity of noise or chemical pollution from specific sources (car, locomotive, etc.). The second class of problems is predicting zones of noise and chemical



pollution of environment both in the transport corridor and beyond its borders [5-7]. This paper discusses a numerical model for assessing the level of air pollution during the operation of a diesel locomotive.

During diesel locomotive work the intensive air pollution takes place (Figure 1). The main diesel engine pollutants are  $NO_x$ ,  $CO$ . Air quality near the railway track, where diesel locomotives work, depends on a few factors. Among these factors the most important are speed of locomotive, chemical transformations of pollutants and presence of different buildings near railway track. Unfortunately, the existing predictive models in Ukraine, such as OND-86 model, do not take into account these factors. The purpose of this work is development of physically based, quick computing predictive model to evaluate air pollution near railway track where diesel locomotives work. The main feature of the model is taking into account diesel locomotive movement, chemical transformation of pollutants and influence of buildings near transport corridor on contamination zone formation.



**Figure 1.** Emissions from diesel locomotive.

## 2. Mathematical model

From the modern point of view, air quality predictive models must take into account pollutants chemical transformations. Emissions from diesel locomotives include, in particular,  $NO$ ,  $NO_2$ . In this work the following transformations of these pollutants are taken into account [7, 8]:



Process of these pollutants dispersion from the moving diesel locomotive can be described by the following equations of conservation [9, 10]:

$$\frac{\partial[NO]}{\partial t} + \frac{\partial u[NO]}{\partial x} + \frac{\partial v[NO]}{\partial y} + \frac{\partial w[NO]}{\partial z} = \frac{\partial}{\partial x} \left( \mu_x \frac{\partial[NO]}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu_y \frac{\partial[NO]}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu_z \frac{\partial[NO]}{\partial z} \right) + Q_{NO} \delta(x - x_0(t)) \delta(y - y_0(t)) \delta(z - z_0) \quad (4)$$

$$\frac{\partial[NO_2]}{\partial t} + \frac{\partial u[NO_2]}{\partial x} + \frac{\partial v[NO_2]}{\partial y} + \frac{\partial w[NO_2]}{\partial z} = \frac{\partial}{\partial x} \left( \mu_x \frac{\partial[NO_2]}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu_y \frac{\partial[NO_2]}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu_z \frac{\partial[NO_2]}{\partial z} \right) + Q_{NO_2} \delta(x - x_0(t)) (\delta(y - y_0(t))) (\delta(z - z_0)) \quad (5)$$

$$\frac{\partial[O_3]}{\partial t} + \frac{\partial u[O_3]}{\partial x} + \frac{\partial v[O_3]}{\partial y} + \frac{\partial w[O_3]}{\partial z} = \frac{\partial}{\partial x} \left( \mu_x \frac{\partial[O_3]}{\partial x} \right) + \frac{\partial}{\partial y} \left( \mu_y \frac{\partial[O_3]}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu_z \frac{\partial[O_3]}{\partial z} \right), \quad (6)$$

where  $Q_{NO}$  is emission rate of  $NO$  from diesel locomotive,  $Q_{NO_2}$  is emission rate of  $NO_2$  from diesel locomotive;  $u, v, w$  are wind speed components;  $\mu_x, \mu_y, \mu_z$  are coefficients of turbulent diffusion;  $x_0(t), y_0(t), z_0$  are coordinates of emission source;  $\delta(x - x_0(t))\delta(y - y_0(t))\delta(z - z_0)$  are Dirac delta-function.

Equations (4), (5) describe dispersion of  $NO, NO_2$  from moving diesel locomotive. Speed of locomotive is set by dependencies  $x_0(t), y_0(t)$  which describe position of locomotive for each time step. Equation (6) describes change of  $O_3$  concentration in computational region due to wind speed and turbulent diffusion.

Process of chemical transformation of pollutants (1), (2), (3) is described as following [7, 8]:

$$\frac{d[NO]}{dt} = -k_1[NO][O_3] + J[NO_2], \quad (7)$$

$$\frac{d[NO_2]}{dt} = k_1[NO][O_3] - J[NO_2], \quad (8)$$

$$\frac{d[O_3]}{dt} = -k_1[NO][O_3] + J[NO_2], \quad (9)$$

where  $J, k_1$  are empirical constants [7, 8].

To simulate wind pattern over buildings the model of potential flow was used [9]:

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + \frac{\partial^2 P}{\partial z^2} = 0, \quad (10)$$

where  $P$  is velocity potential.

The components of wind velocity are determined as:

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

Boundary conditions for modeling equations are discussed in [9].

### 3. Numerical model

To compute wind pattern it is necessary to integrate equation (10). For the numerical integration this equation was written in a «time dependent» form:

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + \frac{\partial^2 P}{\partial z^2}, \quad (11)$$

where  $t$  is fictitious time.

For the numerical integration equation (11) the difference scheme of «conditional» approximation was used [11]. In this case the procedure of numerical integration of equation (11) is split in two steps. At the first step the following approximation was used [11]:

$$\frac{P_{i,j,k}^{n+\frac{1}{2}} - P_{i,j,k}^n}{\Delta t} = \left[ \frac{-P_{i,j,k}^{n+\frac{1}{2}} + P_{i-1,j,k}^{n+\frac{1}{2}}}{\Delta x^2} \right] + \left[ \frac{-P_{i,j,k}^{n+\frac{1}{2}} + P_{i,j-1,k}^{n+\frac{1}{2}}}{\Delta y^2} \right] + \left[ \frac{-P_{i,j,k}^{n+\frac{1}{2}} + P_{i,j,k-1}^{n+\frac{1}{2}}}{\Delta z^2} \right]. \quad (12)$$

At the second step the following approximation was used:

$$\frac{P_{i,j,k}^{n+1} - P_{i,j,k}^{n+\frac{1}{2}}}{\Delta t} = \left[ \frac{P_{i+1,j,k}^{n+1} - P_{i,j,k}^{n+1}}{\Delta x^2} \right] + \left[ \frac{P_{i,j+1,k}^{n+1} - P_{i,j,k}^{n+1}}{\Delta y^2} \right] + \left[ \frac{P_{i,j,k+1}^{n+1} - P_{i,j,k}^{n+1}}{\Delta z^2} \right]. \quad (13)$$

Unknown  $P_{ijk}$  in (12), (13) is computed using explicit formulae at each step. To begin computation procedure it is necessary to set field of potential at fictitious time  $t=0$ , for example:  $P=0$  at  $t=0$ . The computation procedure is finished if:

$$|P_{i,j,k}^{n+1} - P_{i,j,k}^n| \leq \varepsilon,$$

where  $\varepsilon$  is a small number;  $n$  is number of iterations.

Velocity components are computed as follows:

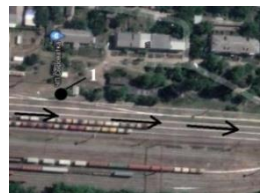
$$u_{ijk} = \frac{P_{i,j,k} - P_{i-1,j,k}}{\Delta x}, v_{ijk} = \frac{P_{i,j,k} - P_{i,j-1,k}}{\Delta y}, w_{ijk} = \frac{P_{i,j,k} - P_{i,j,k-1}}{\Delta z}.$$

For the numerical integration of equations (4)–(6) the implicit difference scheme of splitting was used [9, 10]. For the numerical integration equations (7)–(9) Euler method was used [11]. FORTRAN language was used to develop code.

#### 4. Results

The developed numerical model was used to compute contamination zone formation at *Gruzovoy* Railway Station (Pridneprovsk railway, Ukraine) during the work of diesel locomotive *ChME3* (Figure 2). Arrows in Figure 2 indicate direction of the diesel locomotive movement.

Numerical experiment was performed for the following data: west wind direction; wind speed at the height 10m was 6m/s;  $NO$  emission rate was 0.32 g/s;  $NO_2$  emission rate was 1.98 g/s; diesel locomotive speed was 10.5 km/h;  $O_3$  background concentration was  $0.15 \mu\text{g}/\text{m}^3$ , it was set that wind with this  $O_3$  concentration entered the computational region through the inlet boundary.



**Figure 2.** Sketch of computational region (*Gruzovoy* Railway Station, Google Image, 2020): 1 – receptor position.



**Figure 3.** Predicted  $NO_2$  concentration contours, level  $z = 3\text{m}$ ,  $t = 8\text{s}$ .



**Figure 4.** Predicted  $NO_2$  concentration contours, level  $z = 3\text{m}$ ,  $t = 15\text{s}$ .



**Figure 5.** Predicted  $NO_2$  concentration contours, level  $z = 3\text{m}$ ,  $t = 22\text{s}$ .

As one can see from Figures (3)–(5), large contamination zone is formed near the railway track during diesel locomotive movement at the railway station. Station buildings deformed the

contamination zone. One can see that pollutant can penetrate through windows inside the buildings near the railway tracks.

In Table 1 predicted  $NO_2$  concentrations at receptor position (Figure 2) are presented.

**Table 1.**  $NO_2$  concentration at receptor (level  $z = 2m$ ).

time, s	12	18	29
$NO_2$ concentration ( $\mu\text{g}\cdot\text{m}^{-3}$ )	0,18	0,41	0,11

As one can see from Table 1,  $NO_2$  concentration at receptor position is higher than the Admitted Level. So, diesel locomotive work has negative effect on environment. Worthy of note, that computational time was 10 s.

## 5. Conclusions

During diesel locomotives work intensive air pollution occurs. The computer model has been developed to assess the zones of chemical pollution. The model allows calculating the dynamics of the formation of pollution zones taking into account diesel locomotive movement and various obstacles (station buildings, etc.) that are located near the railways. The model is based on the numerical integration of 3D equation of potential flow and 3D equation of pollutant dispersion. Chemical transformations of  $NO$ ,  $NO_2$  are taken into account. The model can be used to understand the process of air pollution at railway stations where diesel locomotives are widely used. The developed numerical model consumes not much computational time and does not require much computational memory. This is very important in case when many numerical experiments must be performed. Developed numerical model can be used at the laboratories of environment protection at railways.

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