MATHEMATICAL MODELING OF CONTAMINATION ZONES OF HIGHWAY ROADSIDES BY HEAVY METALS

Irina I. Kosinova\textsuperscript{1}, Svetlana I. Fonova\textsuperscript{2}, Gennadii V. Zibrov\textsuperscript{3}, Vadim P. Zakusilov\textsuperscript{4}

\textsuperscript{1,2}Voronezh State University, Voronezh, Russia

\textsuperscript{3,4}Federal state military educational institution of higher professional education "Military educational scientific center air force "air force Academy named after Professor N. E. Zhukovsky and Y. A. Gagarin"

kosinova777@yandex.ru, sveta.27@mail.ru, zakusilov04@yandex.ru

Corresponding Author: Irina I. Kosinova

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Abstract

The urgency of the problem under consideration in modern conditions is determined by the leading influence of road transport in polluting the components of the surrounding environment. Previous scientific developments focus mainly on the assessment of the effect of gaseous emissions; an estimate of the intensity of heavy metal contamination in the form of aerosols is practically absent. The article is aimed at developing a method for assessing the contamination of roadside areas with heavy metals contained in emissions and waste from moving vehicles. The leading method in the study of this problem was the mathematical model and methodology for estimating the aerosol contamination of the atmosphere by heavy metals on the basis of experimental studies of atmospheric pollution and pollution of soils at 240 locations along the profiles on the M-4 autoroute. The total number of samples analyzed was 840 units. The mathematical model took into account the meteorological indicators and the integral indicator of soil contamination at the depth of 1m. It was revealed that the main pollution is observed at a distance of up to 10 m from the roadway edge, which confirms the developed model and methodology. Copper, lead, zinc, and cadmium were singled out as the main pollutants. The scale of the index of environmental risk categories based on the specified total contamination index of the roadside area was developed. Based on the research results it was recommended to locate economic activities at distances more than 25 m from the roadway edge. The materials of the article can be useful for scientists in the field of environmental protection, as well as for environmental organizations that make decisions on the feasibility of practical and economic development of first-order highway roadside areas.

Keywords: Heavy metals (HM), aerosol pollution, roadside area.
I. Introduction

The problems of the environmental impact of man on the environment are exacerbated every year, while at the first stage of technological development they were mainly associated with environmental pollution by industrial enterprises [I]. This pollution is mostly local in nature, and to date, in connection with the transition to a new technological structure, the main scientific and technical problems of combating industrial pollution are being solved [VI, XIX, X].

The data on the behavior of aerosol particles in the fields of pollution is scarce. Despite the noted high ecological danger of this pollution, it should be taken into account that the processes describing the geo-ecological phenomenon of contamination with aerosol particles have not been well-covered [X].

Only the processes of contamination by gaseous products of emissions, both industrial enterprises and vehicles, have been sufficiently studied – there are well-developed models and techniques for describing spatial pollution from high emission sources of industrial enterprises (the methods of the Supervisory Activity Department-86), and low automobile and aviation (at aerodromes) emissions [XXI, XXIII, V, VII, IX, XVI].

II. Research Methodology

The method for assessing environmental pollution by gaseous emissions is based on the Marchuk equation of turbulent diffusion in its various modifications and simplifications, which makes it possible to use it for specific ecological problems [XVII, XVIII]. In this case, the molar mass and the sizes of the gaseous pollutants are comparable with the molar mass and the size of the contamination environment molecules (air in this case), which allows using the laws of the physical kinetics of gases.

The situation is different in the case of aerosol atmospheric contamination by heavy metals [XIV, XV, VIII]. The size of air molecules is estimated at about $10^{-10}$ m, while that of off-shell nuclear aerosols is twice as large, and the radius of cased aerosols is 3-5 times as large. Air density at normal conditions is 1.2 kg/m$^3$, while that of aerosols is 3 times greater. The shape of coarse cased aerosols is close to spherical, i.e., the motion of an aerosol particle in the atmosphere should be described not by the laws of the physical kinetics of gases, but by the laws of aerodynamics.

The physics of dispersion of HM aerosol particles in the atmosphere is based on the principle of vertical deposition of particles and their horizontal displacement under the impact of wind in a viscous medium.

Mathematical Model of Aerosol Particles Dispersion in the Atmosphere

The rate of vertical deposition of aerosol particles follows from the well-known differential equation. Particles with radii of less than 10 μm are evenly deposited at a velocity of $v_0 = \frac{2\rho R^2 g}{9\eta}$, where $\rho$ is particle density, $R$ is particle...
radius, \( g \) is acceleration of gravity, \( \eta \) is coefficient of dynamic viscosity of air. The deposition time from height \( H_0 \) equals \( t_0 = \frac{9\eta H_0}{2\rho R^2 g} \).

Since the radii and densities of HM aerosols are much larger than those of air molecules, the motion of aerosols cannot be considered as displacement at windspeed.

The horizontal motion of particles in a viscous medium occurs due to numerous elastic impacts of air molecules; hence the differential equation of the horizontal motion of the particle has the following form:

\[
\frac{du}{dt} + au = c, \quad (1)
\]

\[
a = \frac{mv_f}{M\lambda} + \frac{9\eta}{2\rho R^2}, \quad c = \frac{mv_f^2}{M\lambda}, \quad (2)
\]

where \( m \) is average mass of air molecules, \( v_f \) is horizontal component of wind speed, \( \lambda \) is mean-free path of air molecules, \( M \) is aerosol particle mass.

The solution of this equation for the velocity of horizontal motion of an aerosol particle will be:

\[
u = \frac{mv_f^2}{M\lambda} \left[ 1 - e^{-\left(\frac{mv_f}{M\lambda} + \theta\right)t} \right] = \frac{v_f^2}{v_f + \frac{M\lambda}{m}} \left[ 1 - e^{-\left(\frac{mv_f}{M\lambda} + \theta\right)t} \right] \quad (3)
\]

where \( B = \frac{6\pi\eta R}{m} = \frac{g\eta}{2\rho R^2} \) is the characteristic parameter of the particle motion, \( t \) is the time of particle motion.

The distance to which HM aerosol particles are dispersed is determined by the following formula:

\[ S = ut_0 \quad (4) \]

For on-shell particles of sizes \( R \leq 10 \) \( \mu \)m and densities of 2000 kg/m\(^3\) - 6000 kg/m\(^3\) the exponent in Equation (3) can be neglected, and the range of particles dispersion is determined by the following equation:
\[ S_i = \frac{v_i^2}{v_r} + \frac{6\eta}{\rho_s R_i} H_o \eta \frac{H_o}{2\rho_s R_i^2}, \tag{5} \]

where \( \rho_s \) is air density.

The general procedure for using the model includes the following steps:
- the average wind speed is measured at the height of 1.5 m;
- samples of air are taken at the height of 1.5 m;
- the granulometric composition of HM solid particles is determined by their size;
- for each granulometric difference, the density of particles and their mass repetition are calculated
  \[ \sum_{i=1}^{n} m_i = \sum_{i=1}^{n} m_i \]
  where \( m_i \) is aerosol mass in i-gradation, \( \sum_{i=1}^{n} m_i \) is gross release of solid aerosols, \( n \) is the number of gradations, \( \rho_i = \frac{3m_i}{4\pi R_i^2} \) is particle density in i-gradation;
- according to Formula (5), the dispersion distances of the particles of each gradation from the source are calculated taking into account the meteorological parameters of the atmosphere, on the temperature and pressure of which the air density and the coefficient of its dynamic viscosity depend;
- the influence zone of aerosols source is determined from the maximum spread range of solid on-shell particles.

Figure 1 shows the dispersion range of solid on-shell HM particles from the roadway edge at various radii and densities.

Fig. 1: Dependence of the HM shell particles dispersion range on the particle size: 1 - \( \rho=2000 \text{ kg/m}^3 \); 2 - \( \rho=3000 \text{ kg/m}^3 \); 3 - \( \rho=6000 \text{ kg/m}^3 \)
It can be seen that on-shell particles having a radius of more than 0.1 μm are dispersed at distances not exceeding 300 m from the roadway edge, while nuclear particles are dispersed at distances larger than 300 m from the roadway edge; coarse soot-coated particles are dispersed at distances up to 25 m from the roadway edge. The speed of car engine aerosol emissions does not affect the dispersion distance, since the highway is a linear source on which a lot of cars are moving. In general, all the emissions amalgamate, forming a turbulent cloud of pollutants, including HM. It is assumed in the model (Formulas (1) - (3)) that the volume distribution of HM in the turbulent cloud is constant. The main contamination of the roadside area is observed at distances up to 10 m from the edge by particles with radii of 3-5 μm. Particles with radii greater than 5 μm fall directly onto the road or next to it. As roads are built with a slope of the curb, these particles are later washed off into the ditch. All the calculations were made for the perpendicular component at each point of the road.

The concentration of TM aerosols deposited at large distances is insignificant due to their large dispersion area; it does not drastically exceed the average values and does not represent a significant ecological hazard.

The developed model and methodology [I, IV] for assessing the impact zone of the road required a field test. For this purpose, samples of near-surface sediments (0-20 cm) at distances of 5 m, 10 m and 25 m from the roadway edge were collected on the M-4 federal highway in 2007, starting at 464 km and ending at 789 km (every 25 km). In a certified laboratory, concentrations of mobile forms of the following heavy metals were measured: lead, zinc, copper and cadmium.

Table 1 shows the dimensionless concentration coefficients of HM mobile forms (sampling points at the distances of 5 m and 10 m from the roadway edge) calculated by the formula $K = C/MPC$, where $C$ is the concentration of HM and MPC is the maximum permissible concentration of its mobile form. The maximum permissible concentrations of mobile forms of the studied HM are also given.

| HM          | Lead | Zinc | Copper | Cadmium | Nickel | Chromium |
|-------------|------|------|--------|---------|--------|----------|
| MPCmobile form, mg/m$^3$ | 6    | 23   | 3      | 1       | 4      | 6        |

The graphs of the HM concentration coefficients dependencies which determine the excess of MPC in roadside areas are shown in Fig. 2.
The integral level of pollution of the entire roadside area was determined by the adjusted total pollution index:

\[ z_y = \sum_{i=1}^{n} K_i - \log_2 n, \]  

(6)

where \( n \) is the number of pollutants. This indicator takes into account all possible concentration coefficients \( K_i \) both more and less than one, the lower level being the value of minus three. The values of the indicator \( z_y \) at various points of the highway are shown in Figure 3. The scale of the environmental risk categories index is given in Table 2.

### Table 2: Environmental risk categories index

| \( Z_y \) | Category            |
|---------|---------------------|
| - 3 ≤ * < -1 | Natural background  |
| - 1 ≤ * < 0  | Technogenic background |
| 0 ≤ * ≤ 2   | Environmental standard |
| 2 ≤ * ≤ 4   | Environmental risk   |
| 4 ≤ * ≤ 8   | Compensated crisis   |
| 8 ≤ * < 16  | Uncompensated crisis |
| * ≥ 16      | Disaster             |

**Fig. 2:** Concentration coefficients of HM mobile forms in the roadside area of the first category highway M4 ‘Don’ (2007)
Fig. 3: Adjusted total pollution index of near-surface deposits by heavy metals in the roadside area of the first category highway M4 ‘Don’ (2007)

Average values of the indicator $Z_y$ along the highway are as follows: 1.17 (the norm) at the distance of 5 m from the roadway; -0.8 (technogenic background bordering at the norm) at the distance of 10 m; -1.41 (the natural background) at the distance of 25 m.

There is quite close connection between the $Z_y$ exponent at the distances of 5 and 10 m from the roadway edge. Along the highway the correlation coefficient is 0.72, and starting from 589 km and further, the connection is extremely close, the correlation coefficient being 0.95. Correlations between the $Z_y$ index and distances from the roadway edge (5, 10 and 25 m) are not observed, which confirms the main aerosol deposition within 10 m from the roadway edge. The technogenic background does not correlate with the main profiles, because the lifetime of the particles at a distance of 25 m is sufficiently large, and the deposition is subject to a lot of random factors [XIII, VIII].

The obtained results of contamination of the roadside area with HM aerosols (Pb, Cu, Cd, Ni) confirm the reliability of the developed model and the method for calculating the impact zone of the road. Model calculations and experimental results make it possible to define the size of the sanitary protection zone for the soils of the roadside area as 25 m from the roadway edge.

In 2013 to study the pollution dynamics of the roadside area of the M-4 and the migration of HM near Voronezh (from 464 km to 564 km) the roadside area was again surveyed at the sites where in 2007 the most polluted samples were collected, and the soil represented the greatest environmental hazard, and two more components, nickel and chromium, were also added. The measurements results of near-surface sediments in the form of concentration coefficients are shown in Figures 4 and 5.
Fig. 4: Concentration coefficients of HM mobile forms in the roadside area of the first category highway M-4 ‘Don’ in 2013 (5m from the roadway edge)

Graphs analysis reveals that the pollution peak shifted from 514 km to 539 km, where intensive construction of residential houses is under way and Saratov junction led to a sharp increase in traffic. Note the minimum concentration (at 514 km) of nickel and chromium and a sharp increase in nickel, chromium and copper by 539 km. Copper concentrations increased drastically along the whole distance of 100 km (Table 3);

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concentration of lead increased slightly, the concentration of zinc remained practically unchanged and at some points even decreased. The concentration of cadmium did not change, remaining at the level of the natural background.

Table 3. Change (increase or decrease) in HM concentration in 2013 compared to 2007

| HM      | Distance from the roadway edge (m) | Km of the road |
|---------|-----------------------------------|----------------|
|         | 464 | 489 | 514 | 539 | 564 |
| Lead    | 5   | >1,8 | >1,7 | >1,6 | >1,8 | >1,6 |
|         | 10  | >2   | >1,7 | >1,5 | >2,75 | >1,5 |
| Zinc    | 5   | >1,15 | >1,06 | <1,16 | >1,15 | >1,58 |
|         | 10  | 1    | <1,8 | <2  | 1    | >1,43 |
| Copper  | 5   | >4,33 | >1,27 | >1,29 | >3,46 | >2,73 |
|         | 10  | >5,25 | >2,4 | >1,7 | >3,33 | >4 |
| Cadmium | 5   | 1    | <2  | 1   | >2  | 1 |
|         | 10  | 1    | 1   | 1   | 1   | 1 |

It should be noted that the concentrations of lead, zinc, copper and nickel at almost all points at the distance of 5 m exceed the MPC except for nickel and chromium at 514 km. Apparently, the near-surface deposits here were destroyed during construction for the modernization of the ring road. At the distance of 10 m lead and zinc are at the boundaries of MPC, copper is above the MPC, and nickel and chromium stay at the same levels as at the distance of 5 m.

Figure 7 shows the dynamics of the Zy index at the distances of 5 and 10 m from the roadway edge. The graph shows that at the distance of 5 m the state of the roadside area is within the levels of the environmental risk/crisis, and only the point at 514 km remains within the norm. At the distance of 25 m the Zy index falls into the rank of technogenic background.
Fig. 6: Adjusted total pollution index of HM mobile forms in the roadside area of the federal highway M-4 ‘Don’ in 2013

The average value of the Zy index on the analyzed 100 km of the most overloaded part of the highway in the Voronezh Region in 2007 was 2.02 at the distance of 5 m and -0.4 at the distance of 10 m. This means that at the distance of 5 m the boundaries of the norm and ecological risk are observed, while at the distance of 10 m the boundaries of the technogenic background and the norm are observed. Consequently, the condition of this roadside section in 2007 was satisfactory. At the same site in 2013 at the distance of 5 m Zy was 8.15, which means a four-time increase, and at the distance of 10 m the index was 5.29 – a 5.5-time increase; evidently, such growth cannot be explained by an increase in the traffic only.

The value of Zy in 2013 at the distance of 25 m from the roadway edge is given in Table 4.

Table 4: The value of Zy in 2013 at the distance of 25 m from the roadway edge

| km | 464 | 489 | 514 | 539 | 564 | average |
|----|-----|-----|-----|-----|-----|---------|
| Zy | -0.07 | -0.05 | -0.15 | -0.12 | -0.1 | -0.12 |

The data above means that the ecological state of the roadside area at the distance of 25 m is in the boundaries of the technogenic background.

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III. Conclusions

1. The transport impact on the components of the natural environment is currently one of the leading negative factors that lead to the degradation of the plant and animal life in the zone of influence, which affects people’s health. These reactions are observed both within the residential and industrial zones, and in the areas of interurban highways.

2. The mathematical modeling of aerosol particles dispersion takes into account the main parameters of both the particles themselves and the conditions of their migration in the atmosphere, related to the density and viscosity of the air.

3. Negative effects are manifested in the form of thermal and chemical transformations of the adjacent territories. Basic elements of pollution are lead, copper and zinc. Formation of complex anomalies of sophisticated composition under the influence of photochemical and thermal effects is noted.

4. The developed universal mathematical model is useful in carrying out engineering and environmental surveys in areas where industrial enterprises are located related to enrichment and processing of HM, as well as near highways with heavy traffic. Modeling the dispersion of aerosols will allow both analyzing the existing ecological and geological situation and fulfilling the forecast of its development.

5. The border of the sanitary protection zone of the roadside area in conditions of intensive traffic is defined at 25 m from the roadway edge, which confirms the reliability of the theoretical model and the developed methodology.

IV. Discussion

The ecology of motor transport is studied to a lesser extent than the industrial one. Most studies have been conducted for harmful gaseous emissions [XX, XXI], since in percentage terms they make up the bulk of the exhaust gases.

However, despite their significant environmental hazards, harmful exhaust gases are rapidly dispersed in the atmosphere, and in general their influence near the roads is insignificant [XII, XIX, XXI]. An exception is the combination of meteorological characteristics of the atmosphere, combining low levels of air movements in the absence of wind and surface temperature inversion [VIII, III].

Much less attention in previous studies was paid to aerosol pollution of the environment by heavy metals (HM), which is due to their low percentage in the exhaust gases. However, their ecological hazard is rather serious for the following reasons:

- most of the HM contained in the exhaust gases of cars are pollutants of the first and second hazard classes;

- unlike gaseous pollutants, they are not diluted in pure atmospheric air, but deposited on the road or near it;
- the soils of the roadside territory are a depositing medium that accumulates HM [II]. Due to strong gusts of wind, HM and dust rise into the atmosphere, getting into the lungs of drivers and people on the roadside area. During the flushing process, HM accumulate in low relief areas and migrate to groundwater, infecting aquifers used for drinking purposes.

Basically, gaseous cars emissions of pollutants are investigated; this is justified by the fact they directly enter the human body through respiratory organs. It is believed they represent the main environmental hazard [X]; however, gaseous pollutants are effectively dissipated by wind, and their concentration is rapidly reduced by dilution in uncontaminated air. Therefore, high environmental hazard occurs only under certain weather conditions: low wind speeds, low temperature inversions, smog. Of great importance is also the presence of green roadside zones which correct the migration processes of aerosols [VI].

High environmental hazard from solid particles containing HM is that their concentration cannot be reduced by the dilution process. At the same time, they have low mobility in the atmosphere and accumulate in the soil of roadside areas, which is a depositing medium [XXIV].

The research carried out answers the designated questions and allows complexly solving the problems of pollution estimation concerning roadside areas contaminated by emissions and motor transport waste.

Recommendations

The results of the presented studies will be useful for scientist in the field of environmental protection, students of higher education institutions following the programs ‘industrial ecology’, ‘environmental protection’, ‘ecology’, ‘ecological geology’, etc. Justification of alienation of roadside areas is of high importance for representatives of state environmental authorities issuing permits for the practical development of such sites.

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