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SEMI-EMPIRICAL MODEL OF THE SIMULATION OF TRAFFIC POLLUTION DISPERSION NEAR ROADWAYS

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Abstract. A semi-empirical statistical model based on physical processes intended for simulation of traffic pollution dispersion near roadways is applied. The pollution source is a road and transport, which in this model is simulated as an undeviating cut-off cylinder, formed along the roadway and filled with aerosol particles. The dispersion of the cloud of these aerosol particles into the environment by the crosswind directed perpendicularly to the road is investigated, including the gravitation, particle buoyancy and diffusion of atmosphere effects. The main attention is focused on the concentration change of the particles size range of 0.05–0.22 μm when receded further from the road in the direction of the wind. Parameters of the model are adjusted to the data of the experiment above the ground surface in horizontal locality. Good agreement between the model and experimental results is obtained.

Keywords: modelling, traffic pollution, aerosol particles, roadside.

1. Introduction

Traffic pollution depending from various reasons has a large impact on ecological processes and various components of ecosystems and causes serious health effects. It forms about 70% of the whole air pollution in the biggest cities of Europe and Lithuania (Vaiškūnaitė *et al.* 2009).

While there is a lack of some essential parameters specifying the level of noxiousness of some materials, the effect of air pollution on human health is often evaluated statistically by epidemiological studies. It is determined that traffic pollution effect on human health depends directly on total aerosol particles concentration, without distinguishing concrete particles, moreover, the effect increases due to ultrafine particles (diameter < 0.1 μm), which are produced in the engines of vehicles. The concentration of ultrafine particles near the road with the downwind is approximately 25–30 times higher than with the upwind, these particles often cause respiratory diseases (Zhu, Hinds 2005). Whole view of the dispersion of pollutants is presented in the exceptional work (Zhu *et al.* 2002), where the data of CO, black carbon (BC), total particle number and mass concentration at 30, 60, 90, 150 and 300 m downwind and 300 m upwind in freeway 405 near Los Angeles is presented. The place chosen for measurements is characterized intense traffic flow – average traffic flow during the sampling periods 230 vehicles per min, of them 93% vehicles gasoline – powered cars or light trucks. Besides, the breeze that blows from the ocean keeps the stable speed perpendicular to the road for a long time. This makes average concentration of the measured sizes not inconsiderable, for example 30 m distance from the road it was 1.7–2.2 ppm, 3.4–10 μg/m^3, (1.3–2.0) × 10^5 1/cm^3 and 30.2–64.6 μg/m^3, respectively. Moreover, it is well known that the roadside soil contains a lot of accumulated metals, most of which are transferred by aerosol particles size range of 0.32–1.0 μm. It is determined that Pb, Zn, Mb, As are distributed mainly in fine aerosols, and the noxiousness of heavy metals for human health is well known.

Traffic pollution extends even up to 300 m wide zone from both sides of the road, so a lot of inhabitants can feel its effect. The great many of experiments referred to aerosol particles dispersion show that the problem is topical. The search of theoretical models of the road pollution are carried out permanently and for the last years the attention of scientists is focused on applying Gaussian model, which is used to determine the dispersion of exhausted aerosol particles from chimneys that is from the point sources (Seinfield, Pandis 1998). As the type of traffic pollution source is not the point one, it is attempted to solve this problem by finding the pollution source, e.g. by replacing the road with a line of points imitating emission (Chock 1978) or with a system of planes, formed of such points (Karim, Matsui 1998; Rao *et al.* 2002). In all cases the results obtained were only satisfactory, although complex computer programme packages were used. One of the main reasons of the misfortune is mathematical dif-

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ficulties occurring while simulating the dispersion of aerosol particles concentration above the road. These difficulties arise due to high air convection.

Short-term meteorology has big impact on the dispersion of the pollution without the wind (Chock 1978; Laurinavičius *et al.* 2007). Therefore the analysis of the pollution becomes a problem that is difficult to solve. Semi-empirical model of the dispersion of pollution which is made by us on the base of the physical processes will be used to express the tendencies of the long-term pollution dispersion.

The aim of the work is the research of the influence of the dust cloud expansion on the aerosol concentration distribution near roadways; the main attention is paid to the dispersion of aerosol particles in the size range of 0.05–0.22 μm (Zhu *et al.* 2002), which the Gaussian plume model cannot explain.

2. Theoretical base of the model

The process of traffic pollution dispersion is very complex due to complicated, trickily explained physical and chemical phenomena in the process. Due to the fact that in atmosphere aerosols have hard, liquid and air stages with high temperature and a rapid cooling, the processes of steaming, condensation and coagulation occur (Jacobson, Seinfeld 2004), though the experimental and theoretical evaluations show that the greatest impact on decrease of particles dispersion has atmospheric dispersion – dilution process near the source (Zhu, Hinds 2005). Thus, a conclusion can be drawn that the sum of particles in the cloud, formed above the road, settled particles and particles remaining in the air do not change a lot. This enables from the view of the long term pollution, to interpretate the cloud, formed above the road when the traffic is intensive, as a generator of pollution particles with constant power, e.g. as the source of environmental pollution.

As the crosswind, directed perpendicularly to the road blows, the formed cloud shifts downwards spreads in the direction of the wind and expands causing the decrease of particle concentration in it. To evaluate the velocity of cloud's expansion usually the line source emission model is used (Chock 1978; Zhu, Hinds 2005), which is applied in the work as well. In line source emission modelling the road is replaced by emission generating line and the best results are obtained when the line is at 4.5 m height (Chock 1978), but in the work (Zhu, Hinds 2005) the road is elevated ~4.5 m above the surrounding terrain.

To evaluate the expansion of the cloud a simplified atmospheric diffusion Eq is applied:

$$U\frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\left(K_{zz}\frac{\partial C}{\partial z}\right), \tag{1}$$

where U – the mean ambient wind speed at source height, m/s; C – mean concentration of a pollutant, g/m^3; K_{zz} – the vertical addy diffusivity, m^2/s.

And the solution for the line source per unit length, considering it to be a dotted line without the gravitation effect (Zhu, Hinds 2005), is given by

$$K_{zz} = \gamma U x, \tag{2}$$

where γ – turbulence parameter. The solution for Eq (1) is

$$C(x,y) = \frac{q}{Ux\sqrt{2\pi\gamma}}\left\{\exp\left(-\frac{(z-h)^2}{2\gamma x^2}\right) + \exp\left(-\frac{(z+h)^2}{2\gamma x^2}\right)\right\}, \tag{3}$$

where q – line source strength (particle/ms); h – the height of line source, m.

From solution (3) it follows that the parameter of vertical dispersion coefficient σ_z usually used in Gaussian method alters according to the line law

$$\sigma_z = \sqrt{\gamma}x, \tag{4}$$

which determines the expansion of the γ emission cloud.

3. Construction of the model

Having constructed the model it is assumed that, when there is no wind, the cloud, formed above the road, is the pollution source with permanent power in a shape of a cut-off cylinder, which afterwards is transferred to the roadside by the wind directed perpendicularly to the road. The aerosol particle dispersion in the cloud, formed by vehicle- and gravitation-intended turbulent air streams, when the wind blows, conditions the law of the changes of aerosol particles concentration near roadside above the ground surface. Such model describes well the dispersion of carbon oxide, black carbon (soot) and general concentration of particles (Grigaliūnaitė–Vonsevičienė *et al.* 2008). Having incounted the particle buoyancy and thermal pollutant plume rise effects, it is obtained the dispersion of concentration typical for particles size range of 0.050–0.300 μm, which has some peculiarities typical only for this fraction (Martinėnas, Špakauskas 2010). The concentration of aerosol particles of such size range receding from the road is decreasing slower than the concentration of smaller particles, what is more, at the certain distance the decrease vanishes otherwise the increase is observed, its place depending on the wind speed (Zhu *et al.* 2002). The concentration of heavy metals in the air, soil and plants near the roadside alters according to analogical consistent patterns (Carsignol, Calovi 2005), because aerosol particles of this size range are related to the transfer of heavy metals (Martuzevičius *et al.* 2004). This fact is also confirmed by the investigations of heavy metals concentration carried out in Lithuania (Juknevičius *et al.* 2007).

The work continues the modification of the model, when the cut-off cylinder shaped emission cloud recedes from the road in the horizontal direction of the wind and the expansion of the cloud is taken into consideration.

Mathematical model of the traffic pollution expansion is constructed to determine the unitary length cloud expansion, formed above the road. Let us assume that vehicle-intended mechanical and thermal turbulence in the volume of cut-off cylinder's radius r_0 and unitary length V_0 create permanent aerosol particles concentration ρ_0 in the cloud, which is $\rho_0 = \frac{n}{V_0}$, where n – the number of aerosol particles in the volume V_0 (Fig. 1), and with its expansion to the roadside at a permanent velocity v_x due to the gravitation, buoyancy and thermal effects plume rises and aerosol particles concentration ρ alters and with a distance from the road x and a height above the ground surface Δh is expressed by function, i.e. $\rho = \rho(x, \Delta h)$.

The expansion of the cloud in the vertical direction is evaluated according to vertical dispersion coefficient σ_z and the alteration laws in Gaussian point source model, when under neutral atmospheric conditions at the beginning of coordinates $\sigma_{z0} = a$, where a is an empirical parameter. Then vertical dispersion coefficient σ_z at distance x from the source is (Chock 1978)

$$\sigma_{zx} = (a + bx). \tag{5}$$

Having used Eq (5) in the model (Fig. 1) and having equated a with r_0, the alteration law of cylinder radius r is obtained when it is transferred further from the road by the wind:

$$r_x = r_0 + \beta x, \tag{6}$$

where r_0 = 15 m and is a radius of cylinder, which is selected for the flat width of the road, m; β – expansivity of radius of cloud. Cylindrical plume, which moves in the direction of wind at the velocity v_x, settles slowly falling at a constant velocity v_z. Having assumed that the cloud carried by the wind at the distance Δx shifts downwards at Δh, and the whole aerosol particle cloud settles at the distance $x_{\max}$from the road, we get:

$$\Delta h = \frac{h_0}{x_{\max}} \Delta x \text{ (m)}. \tag{7}$$

The horizontal velocity of plume movement, that is along the z axis, consists of falling velocity $\vec{v}(z)$ and plume rise velocity $\vec{\omega}(z)$. To evaluate the plume rise we use the tendency of velocity change typical for plume centerline rise above the source (Linden 2010):

$$\omega(z) = C_1 B^{\frac{1}{3}} z^{-\frac{1}{3}}, \tag{8}$$

where C_1 – the dimensionless constant; B – the buoyancy flux constant. Therefore, for plume rise velocity is

$$\vec{v}(z) = \vec{v}_0(z) + \vec{\omega}(z). \tag{9}$$

Moreover, due to the heated air flow rising from the roadside and the buoyancy effect, the concentration of aerosol particles is increasing when shifting upwards (Imhol *et al.* 2005; Zhu, Hinds 2005).

The volume $V(\alpha)$ of the cloud is equal to the area, which is the cut-off circle (further we will use this consideration) multiplied by the length l of the aerosol particle cloud located along the roadway:

$$V(\alpha) = \frac{l r_x^2}{2}(\alpha - \sin\alpha). \tag{10}$$

The initial angle α_0 corresponds to the initial volume $V_0 = V(\alpha_0)$ in m/s.

The probability density function $f(\alpha)$ obtained according to definition is given by

$$f(\alpha) = \frac{dn}{n d\alpha} = \frac{\rho dV}{n d\alpha} = \frac{1}{V_0}\frac{dV(\alpha)}{d\alpha} = \frac{1 - \cos\alpha}{\alpha_0 - \sin\alpha_0}, \tag{11}$$

where $\alpha_0 \geq \alpha \geq 0$, α_0 – an angle of the cylinder segment at the initial time moment, and the angle α when the cylinder settles by Δh (Fig. 1).

As Fig. 1 shows:

$$h_x = h_{0x} - \Delta h = h_{0x} - \frac{v_z}{v_x}\Delta x, \tag{12}$$

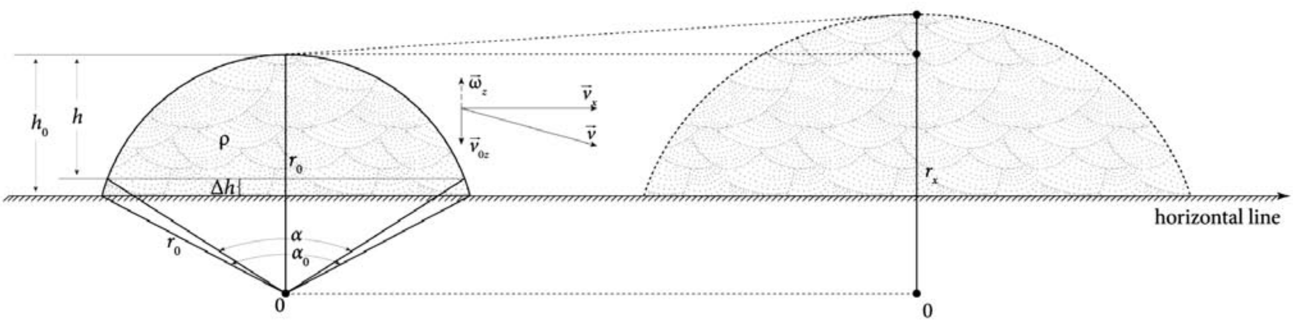

Fig. 1. Development of the whirl of aerosol particles on the ground surface

$$h_x = r_x\left(1-\cos\frac{\alpha}{2}\right). \quad (13)$$

We include the mentioned gravitation, buoyancy and thermal effects as the probability density function factor $g(\Delta h)$:

$$g(\Delta h) = \frac{1}{N}(e^{-a\Delta h} + ce^{b\Delta h}), \quad (14)$$

where a and b express the gravitation and buoyancy coefficients, c – the relative weight of buoyancy contribution, $\Delta h_{\max}$ is the initial height of a dust cloud, N is the normalizing coefficient:

$$N = \frac{1}{a}(1-e^{-a\Delta h_{\max}}) - \frac{c}{b}(1-e^{b\Delta h_{\max}}). \quad (15)$$

Therefore, we multiply the probability density function $f(\alpha)$ by the coefficient $g(\Delta h)$ and obtain the probability density function $\gamma(\alpha,\Delta h)$:

$$\gamma(\alpha,\Delta h) = f(\alpha)g(\Delta h). \quad (16)$$

Passing from the probability density function to the quantitative concentration evaluation, the probability density function $\gamma(\alpha,\Delta h)$ should be multiplied by the emission rate per unit length Q (kg/ms).

4. Results and discussions

For the validation of the model developed in our study the experimental data obtained in (Zhu *et al.* 2002) were used. Substantial changes in the investigations of the traffic pollution dispersion near roadways were obtained during the experiment in the vicinity of roadways in the Los Angeles area using the *CPC 3022A* aerosol particle counter for measuring the aerosol particle number concentration and the *SMPS 3936* aerosol particle seizer for the aerosol particle size distribution with expected error ±10%. The aerosol particle number concentration and the size distribution in the size range from 0.006 to 0.22 μm were measured. Measurements were carried out at a distance of 30, 60, 90, 150 and 300 m downwind from the central line of the highway, which is 30 m wide, when the average crosswind velocity was 1 m/s and 2.5 m/s. A general concentration decrease of all aerosol particles receding from the highway and the dependence of their fraction dispersion on the particle size were obtained.

It has been determined that the number concentration for all size aerosol particles dropped to approx half its original value at the distance somewhere between 90 and 150 m. The decrease of the normalized total particle number and volume concentration in the size range of 0.006–0.22 μm is close by the exponential law, but in the size range of 0.05–0.1 μm and 0.1–0.22 μm a decrease has some peculiarities. For these size ranges, when the wind speed is 1 m/s at the 60 m distance from the roadway in the concentration diagram a small hole is observed, while at the 90 m distance from the roadway the concentration increase is observed. When the wind speed is 2.5 m/s, the min of the particle size range of 0.05–0.1 μm shifts towards 90 m, and the max – towards 150 m. For the size range of 0.1–0.22 μm, the concentration extremums of these aerosol particles disappear completely.

The probable ω_0 value over the road at the 1 m height was evaluated in (Chock 1978) by improving the common Gaussian line source model, where Eqs evaluating the plume rise speed were obtained. From these equations it follows that under neutral atmospheric conditions, when the wind speed is 1 m/s and 2.5 m/s, the plume rising velocity is 0.062 m/s and 0.042 m/s, respectively.

In the model the optimal probability density function for aerosol particles in the size range of 0.05–0.1 μm was obtained when α_0 = 4.8 rad (it corresponds to the max plume height equal 4.8 m over the road), with the road half width r = 15 m. When the wind speed v_x = 1 m/s and 2.5 m/s, then v_z = 0.1 m/s, and ω_0 = 0.045 and 0.04 m/s, respectively. In the probability density function the gravitation and buoyancy effect conditioned statistical weights at the initial time moment $\frac{1}{N}$ = 0.39 and $\frac{c}{N}$ = 0.18 when the wind speed v_x = 1 m/s, and $\frac{1}{N}$ = 0.45 and $\frac{c}{N}$ = 0.03 when the wind speed v_x = 2.5 m/s and N is function of x. Gravitation and buoyancy coefficients a and b, expansivity of cloud β when the wind speed v_x = 1 m/s, are a = 0.9; b = 0.7; β = 0.15, and when v_x = 2.5 m/s – a = 1.4; b = 0.7; β = 0.04.

The normalized (equated to one in point of concentration values at the distance of 90 m) model and experimental (Zhu *et al.* 2002) curves, when the wind speeds are v_x = 1 m/s and v_x = 2.5 m/s, are shown in Figs 2 and 3. The pollutants concentration of CO, BC, NC only at a distance of 300 m downwind and upwind from the roadside becomes equal, the pollutant concentration at a 300 m distance from the roadside can be considered as background. Thus the values of the probability density and experimental concentrations are with the background concentration illegibly, and the concentration value at the x_{max} = 300 m distance should be equal to 0. True, these particles form small part of the total mass of the particles of pollutants. The bigger particles do not reach this distance (Figs 1, 2).

A better congruity with the experiment was obtained when the wind speed was 1.0 m/s because selected parameters of the model not always correspond precisely to the aerosol particles in the size ranges of 0.05–0.1 μm, as at the same distance there are also particles in the size ranges of 0.1–0.22 μm, dispersion of which is similar. When the wind speed is 2.5 m/s, the dispersion consistent pattern of aerosol particles in the size ranges of 0.05–0.1 μm is the same as of aerosol particles in the size ranges of 0.1–0.22 μm, although the latter concentration in both velocities is a lot less.

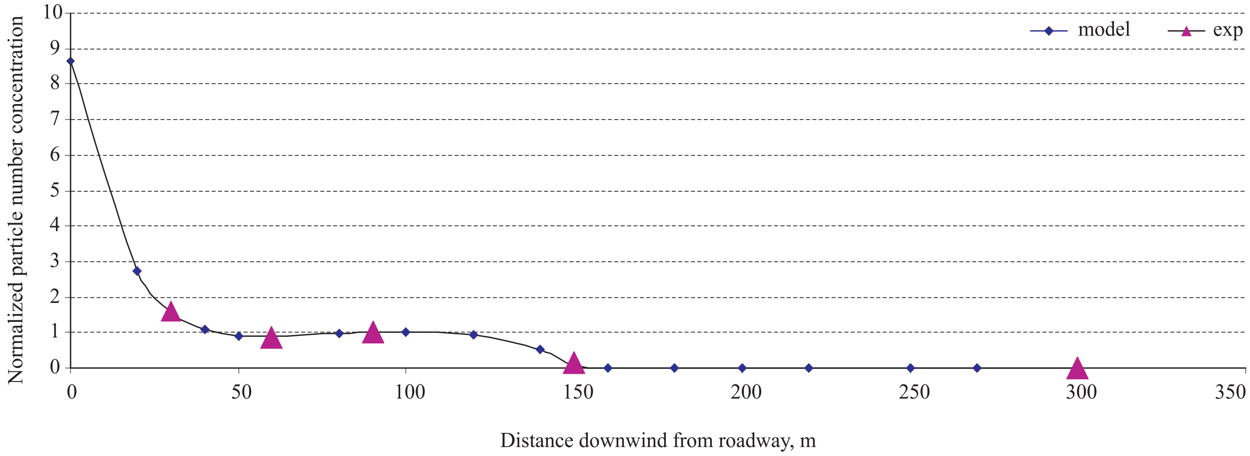

Fig. 2. Dependence of normalized experimental aerosol particle concentrations (Zhu *et al.* 2002) and probability density function γ (a, Δh) from the distance of the roadway when the wind speed is 1 m/s

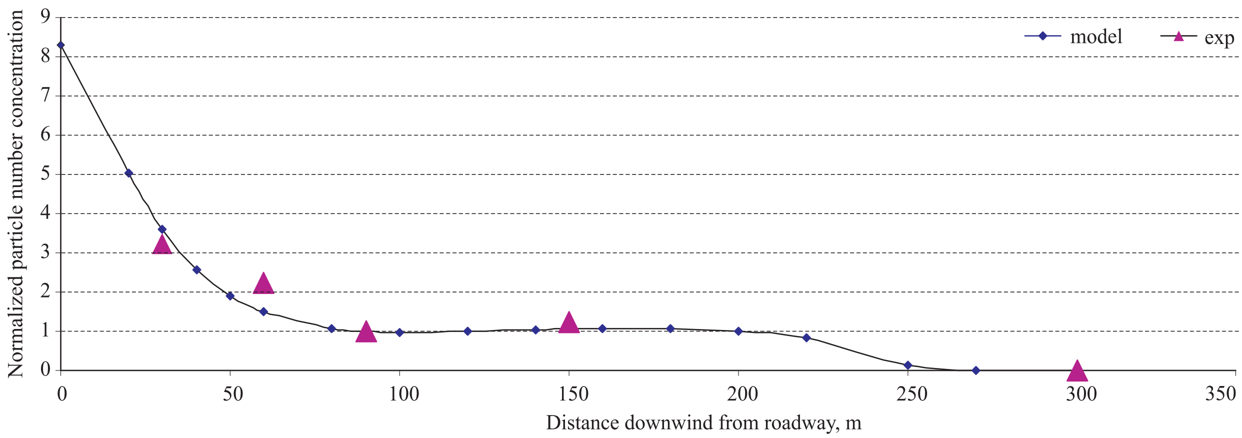

Fig. 3. Dependence of normalized experimental aerosol particle concentrations (Zhu *et al.* 2002) and probability density function γ (a, Δh) from the distance of the roadway when the wind speed is 2.5 m/s

It is noticed that aerosol particles dispersion peculiarities depend on their settle velocity $\vec{v}_z$, which depends on buoyancy effect, determined by the size of the particles.

5. Conclusions

A semi-empirical model intended for simulation of dispersion of particles with the diameter larger than 0.05 μm near roadways has been proposed in the work. Mathematically described dispersion of aerosol particles (>0.05 μm) in a pollution source allows simulation of the pollutant concentration change near roadways which well coincides with the experimental measurements. Experimental data shows that the dispersion of aerosol particles in the size ranges of 0.05–0.1 μm and 0.1–0.22 μm depends on the wind speed. When the wind speed is 1 m/s, the concentration of aerosol particles of both size ranges at the beginning decreases at the distance of up to 60 m from the road, and increases at the distance of 90 m, but further it decreases again. When the wind speed is 2.5 m/s, the concentration decay of aerosol particles of the first size range (0.05–0.1 μm) is observed at the distance of up to 90 m, and an increase – at up to 150 m, but further it again decreases. The concentration of aerosol particles of the second size range (0.1–0.22 μm), when the wind speed is 2.5 m/s, decreases uniformly receding from the road.

By simulating the pollution source as a cut-off cylinder, which is formed on the roadway at the initial time moment due to traffic pollution and is uniformly filled with aerosol particles, and with the wind transfer further from the road aerosol particles settle influenced by the gravitation, particle buoyancy and thermal pollutant plume rise effects.

According to the model it was obtained that the semi-empirical parameters of the model, including the dispersion of the dust cloud transferred by the wind further from the road, depend on the size of the aerosol particles. It was determined that the second important factor after the wind speed that causes the dispersion of the particles is the particle settle velocity $\vec{v}_z$, which changes depend on buoyancy effect, that in its turn depends on the size of the particles. This fact was not taken into account while counting the dispersion of the particles in Gaussian model and only one parameter γ was applied for all particles which allowed to obtain only approximate particle dispersion.

The obtained aerosol particle concentration change near roadways better coincides with the experimental data and explains why the heavy metals pollution near the roadside practically doesn't vary in a wide range from 50 to 150 m away from the road.

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