

SIMULATION OF TRAFFIC-RELATED AEROSOL DISPERSION

V. Špakauskas and D. Melichov

Vilnius Gediminas Technical University, Saulėtekio 11, LT-10223 Vilnius, Lithuania

E-mail: valdas.spakauskas@vgtu.lt

Received 27 October 2011; revised 28 February 2012; accepted 1 March 2012

This paper presents a quasi-empirical model of the distribution of pollutant particles along the roadway. By modelling the source of the pollutant as a cut-off cylinder we assume that aerosol particles (of 0.3–15 μm in diameter) are distributed according to the Gaussian law both along the vertical and horizontal axes. A cross wind translates the pollutant cloud away from the road and the particles are being influenced by gravity, particle buoyancy and thermal plume rise effects. The obtained pollutant concentration function coincides well with the experimental data obtained by Zhu et al. (2011), Grigalavičienė and Rutkoviėnė (2006), and Zechmeister et al. (2005).

Keywords: aerosol particles, Gaussian distribution, modelling, road dust, dispersion, roadside

PACS: 92.60.Sz, 91.62.Rt, 92.60.Mt, 91.67.gp

1. Introduction

The sources of heavy metal pollution are various, for example Pb from leaded gasoline, Cu, Zn and Cd from car components, tire abrasion, lubricants, industrial and incinerator emissions, etc. [1, 2]. The source of Ni and Cr in street dust is believed to be the corrosion of cars [3, 4], and Cr and Pt of some motor vehicle parts [5]. Moreover, some sorts of gasoline contain 30–120 ng g^{-1} of As [6] and 0.2–3.3 ng g^{-1} of Hg [7]. Traffic and roads are one of the largest sources of metal pollution, because the number of vehicles in developing countries has been progressively increasing in recent years.

The trace metals near the roadways are transported as particulate matter (PM) ($r > 0.1 \mu\text{m}$ in diameter). The mean mass median aerodynamic diameter (MMAD) of PM was found to be $0.85 \pm 0.71 \mu\text{m}$. The MMADs of Pb ($0.96 \pm 0.71 \mu\text{m}$), Cd ($1.14 \pm 0.82 \mu\text{m}$), V ($1.38 \pm 0.63 \mu\text{m}$), Fe ($3.82 \pm 0.88 \mu\text{m}$) [8] can be used to evaluate the concentration of various metal aerosol particles near the roadway. Pollution by heavy metal exists in all countries and is characterised by different ranges of concentration ($\mu\text{g g}^{-1}$) in street dust [9].

Atmospheric dispersion modelling employs statistical tools such as artificial networks (ANN) [10], fuzzy logic theory (FLT) [11], deterministic Lagrangian and Eulerian models [11–14] and so on. But Gaussian type models based on a Gaussian distribution of the plume are most widely used, despite the difficulties in determining the variance [15, 16].

Computational fluid dynamics (CFD) models are used as a tool to assess urban air quality [17, 18]. They are based on solving the Navier–Stokes equation, which is completed by finite difference and finite volume methods. Rao et al. [19] showed a significant role of turbulent kinetic energy in dispersion of aerosols.

In the studies of the dispersion of aerosol particles from a road, there were proposed various modifications of the Gaussian models in which the road was considered to be either a linear source, a set of point sources, or a planar source with a specified height. By modelling the dispersion of fine aerosol particles near a road it must be taken into account that these particles are affected by gravitation, particle buoyancy and thermal pollutant plume rise effects and are not uniformly distributed. A good agreement between the model and

experimental results, taking into account the aforementioned effects, was obtained by Martinėnas and Špakauskas [20].

The results of studies of the vertical aerosol particles dispersion near the ground level [21–23] emphasise the increasing concentrations of PM_{10} , $PM_{2.5}$ and CO. Weber et al. [24] evaluated the vertical distribution of particle fractions PM_1 and $PM_{2.5}$ under different meteorological conditions and found that for up to 3.9 metres the concentration of aerosol particles was increasing. The dispersion measurements of ultrafine, fine and coarse aerosol particles ($PM_{0.03-0.3}$, PM_1 and $PM_{2.5}$) in an urban street canyon [25] show that their concentration increases up to 2.25 metres.

A number of experiments show that the wake of vehicles has a certain structure and this may have a significant effect on the dispersion of vehicle pollutants. The wind-tunnel studies of exhaust gas dispersion behind a single vehicle [26] and a queue of vehicles [27] show that concentration contours in cross-section are the optimal fit of the Gaussian distribution. The characterisations of aerosol particles in a dust whirl near the road with accurate measurements have been a key interest in aerosol research for the last several decades. Therefore, in this paper we will investigate the characteristics of heavy metal aerosol particles distribution from roads using a physical model of volume source of pollution in which the pollutants above the road are distributed according to the Gaussian law in both vertical and horizontal directions.

The observed profiles of concentrations of aerosol particles on the road in idle conditions [28] or near the road [29] could be simulated using Gaussian models. Nowadays more and more experiments investigate the vertical concentration profiles near the road. Zhu and Hinds [30] measured the vertical profiles of aerosol particle concentrations 50 metres downwind from the roadway and found that the maximum concentration of the pollutant was observed at a height of 5 metres above the ground. Gillies et al. [31] measured that the size of a wake created by a vehicle depends on the size of that vehicle, i. e. the turbulent wake height h_0 equals 1.7 multiplied by vehicle height. Based on the results of these measurements the authors obtained the vertical turbulence parameters.

The aim of this work is to develop a model in which aerosol particles over the road would have

a Gaussian distribution in the horizontal direction and a truncated Gaussian distribution in the vertical direction and to examine the concentration function of the settled aerosol particles.

2. Modelling

We are proposing a quasi-empirical model of settling aerosol particles which are mainly larger than 0.3μ on the ground surface. The scheme of the model is shown in Fig. 1. When there is no wind, the cylindrical whirl of aerosol particles formed by the vehicle-induced mechanical and thermal turbulence gets a cut-off elliptic cylindrical shape. The width R of the cut-off cylinder equals half of the roadway width, and the height of this cylinder is h_0 (Fig. 1). A cross wind translates the wake away from the road with the speed v_x and is directed perpendicularly to the roadway, concurrently the cloud of aerosol particles settles at a constant velocity v_z .

The particles are not uniformly distributed within the cloud. We assume that the distribution along the x axis, where x is perpendicular to the roadway and coincides with the direction of the wind, is

$$f(x, x_0 - R, \sigma_x) = \frac{1}{\sqrt{2\pi}\sigma_x} e^{-\frac{(x-(x_0-R))^2}{2\sigma_x^2}}, \quad (1)$$

where $f(x, x_0 - R, \sigma_x)$ is the probability density, σ_x is the horizontal Gaussian dispersion parameter, x_0 is the point at which the concentration of aerosols is evaluated, $2R$ is the diameter of the cut-off cylinder (which is greater than the width of the roadway due to the wake expansion effect).

Consequently, in this paper the truncated Gaussian distribution is suggested to model the distribution of the particles along the z axis, where z is the height above the ground:

$$f(z, z_0, \sigma_z) = \frac{1}{\sqrt{2\pi}\sigma_z \Phi(z_0/\sigma_z)} e^{-\frac{(z-z_0)^2}{2\sigma_z^2}}, \quad (2)$$

where $f(z, z_0, \sigma_z)$ is the probability density function, $\Phi(z_0/\sigma_z)$ is the cumulative distribution function of the standard Gaussian random variable, z_0 is the maximum of the probability distribution density function of the particles, σ_z is the vertical Gaussian dispersion parameter.

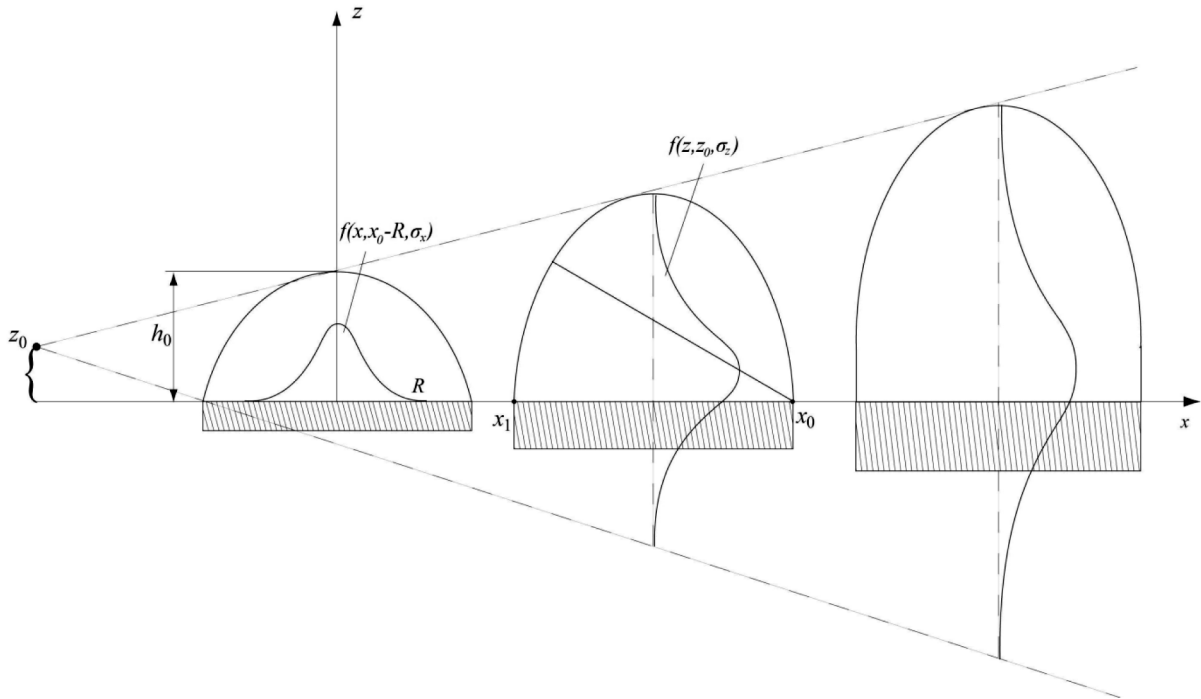


Fig. 1. Settling of the pollutant cloud on the ground surface.

The settling of aerosols carried by the wind is modelled by a moving cut-off cylinder of unitary length $l = 1$ (m). Suppose that when the centre of this cylinder is at the point $x_0 - R$, the average density of the particles is

$$n(x_0) = \frac{N}{V(x_0)} = \frac{N}{\frac{1}{2}\pi R l (h_0 + mx_0 + \beta x_0)}, \quad (3)$$

where h_0 is the height of the line source (m), $V(x_0)$ is the volume of the cloud when the centre of the cylinder is at $x_0 - R$, N is the total number of aerosols in the cloud, $m = v_z/v_x$, β is the parameter describing the expansion of turbulent flow.

The cloud carried by the wind at the distance x_0 shifts downwards at Δh :

$$\Delta h = v_z \frac{\Delta x_0}{v_x} = m \Delta x_0. \quad (4)$$

The movement of particles is influenced by two main factors, namely the settlement and the chaotic movement due to the turbulence effects. In this paper it is assumed that the regular settlement factor is dominant, and on the average the amount of particles settled at the point x_0 is proportional to the

length of the line $z = m(x - x_0)$ which intersects with the x axis at the point x_0 and has the slope m . In this case, the concentration of particles at the point x_0 is

$$c(x_0) = \int_{x_1}^{x_0} n(x_0) f(x, x_0 - R, \sigma_x) f(z, z_0, \sigma_z) dx, \quad (5)$$

where x_1 and x_0 are the points where the line z and the cut-off cylinder intersect. Further,

$$f(x, x_0 - R, \sigma_x) f(z, z_0, \sigma_z) = \frac{1}{2\pi\sigma_x\sigma_z\Phi(z_0/\sigma_z)} e^{-\frac{(x-(x_0-R))^2}{2\sigma_x^2}} e^{-\frac{(z-z_0)^2}{2\sigma_z^2}}. \quad (6)$$

If we define $c_0 = mx_0 - z_0$ and $d_0 = x_0 - R$, then denoting

$$a = \frac{\sigma_z^2 + m^2\sigma_x^2}{2\sigma_x^2\sigma_z^2}, \quad b = -\frac{d_0\sigma_z^2 + c_0m\sigma_x^2}{2\sigma_x^2\sigma_z^2}$$

$$\text{and } c = \frac{d_0^2\sigma_z^2 + c_0^2\sigma_x^2}{2\sigma_x^2\sigma_z^2}, \quad (7)$$

we get

$$c(x_0) = \frac{1}{2\pi\sigma_x\sigma_z} \frac{N}{\Phi(z_0/\sigma_z)} \frac{1}{2} \pi R l (h_0 + mx_0 + \beta x_0) \times e^{-\frac{(z_0 - mR)^2}{2(m^2\sigma_x^2 + \sigma_z^2)}} \int_{x_1}^{x_0} e^{-a(x - \frac{b}{a})^2} dx. \quad (8)$$

The Gaussian distribution is always connected with turbulent transport and hence continuous growing of the plume, because of the assumptions that $\sigma_z = h_0 + \beta x_0$ [30] and $\sigma_x = R$. Therefore, the concentration function can be written as

$$c(x_0) = \frac{N}{\sqrt{2\pi^3} R l \sigma_z \Phi(z_0/\sigma_z) (\sigma_z + mx_0)} \times e^{-\frac{(z_0 - mR)^2}{2(m^2 R^2 + \sigma_z^2)}} \zeta(x_0, x_1, a, b), \quad (9)$$

where

$$\zeta(x_0, x_1, a, b) = \operatorname{erf}\left(x_0 \sqrt{a} - \frac{b}{\sqrt{a}}\right) - \operatorname{erf}\left(x_1 \sqrt{a} - \frac{b}{\sqrt{a}}\right). \quad (10)$$

Further, since the value of $m\sigma_x$ is much smaller than the value of $\sigma_z = h_0 + \beta x_0$ and x_1 can be approximated as $x_1 = x_0 - 2R$, the function $\zeta(x_0, x_1, a, b)$ can be approximately computed as

$$\zeta(x_0) = \operatorname{erf}\left(\frac{2x_0 - R}{\sqrt{2R}}\right) - \operatorname{erf}\left(\frac{2x_0 - 3R}{\sqrt{2R}}\right). \quad (11)$$

The method and formulas presented above allow evaluating the concentration of aerosol particles near the roadway.

3. Results and discussion

For the validation of the model developed in our study we use the experimental data obtained by Zhu et al. [32]. In their experiment an optical particle counter with an expected error $\pm 10\%$ was employed to evaluate the distributions of concentrations of differently sized aerosol particles at certain distances from the roadway. Aerosol particle concentrations and size distributions in the ranges of 0.3–0.5, 0.5–0.7, 0.7–1, 1–2.5, 2.5–5, 5–10, 10–15, >15 μm were measured at the distances of 5, 30 and 100 m downwind from the central line of a 30 metre wide roadway, when the crosswind velocity varied from 0.5 to 2.3 m/s [32].

The model and experimental [32] curves for the size range 10–15 μm were normalised at the distance of 30 metres. When wind speed is $v_x = 2$ m/s they are comparable with one another (Fig. 2). The study found that the shape of the functional dependence of the concentration of aerosol particles on the distance from the roadway is mainly

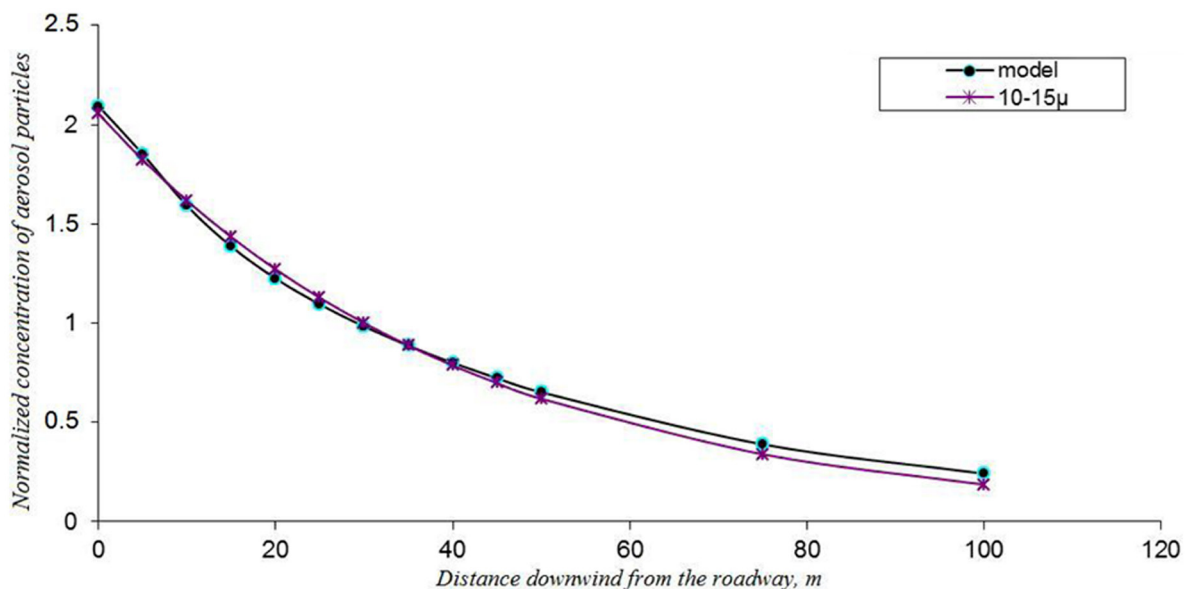


Fig. 2. Comparison of the normalised experimental (Zhu et al. 2011 [32]) and current work model dependence of aerosol particle concentrations on the distance from the roadway when wind speed is 2 m/s.

determined by the parameters m and β . The dependence on m can be explained by the fact that for up to 50 m from the road the turbulence effects are dominating; therefore, all the particles are uniformly mixed. The parameter β describes the expansion of the turbulent wake of the vehicle flow, and $\beta = 0.044 + 0.004d$, where d is the diameter of aerosol particles. When wind speed is different from that considered by Zhu et al. [32] the expression of β should also change, but this requires additional measurements.

4. Conclusions

The distribution of traffic-related aerosol particles on the roadside has been investigated using the developed model of volume source above the road. The pollution source is treated as a cut-off elliptic cylinder which is formed on the roadway at the initial time moment due to the traffic pollution and filled with aerosol particles which are distributed according to the Gaussian law in both vertical and horizontal directions. A semi-empirical model has been proposed for the simulation of dispersion of particles with the diameter larger than $0.3 \mu\text{m}$ near roadways. The modelled data agree with the experimentally measured dispersions of aerosol particles. The determined dispersion curves depend on the parameters m , describing sedimentation, and on β , which characterises the expansion of the turbulent wake of vehicle flow. Since the obtained concentration of the aerosol particles coincides well with the experimental data provided by Zhu et al. [32] and the shape of its functional dependence on the distance from the roadway agrees with the results of [33, 34] we assume that the proposed model can be successfully used to model the dispersion of aerosol particles near roadways.

References

- [1] J.A. Markus and A.B. McBratney, An urban soil study: heavy metals in Glebe, Australia, *Aust. J. Soil Res.* **34**, 453–465 (1996).
- [2] W. Wilcke, S. Muller, N. Kanchanakool, and W. Zech, Urban soil contamination in Bangkok: heavy metal and aluminium partitioning in topsoils, *Geoderma* **86**, 211–228 (1998).
- [3] J.E. Ferguson and N. Kim, Trace elements in street and house dusts source and speciation, *Sci. Total Environ.* **100**, 125–150 (1991).
- [4] M.S. Akhter and I.M. Madany, Heavy metal in street and house dust in Bahrain, *Water Air Soil Pollut.* **66**, 111–119 (1993).
- [5] S.M. Al-Shayeb and M.R.D. Seaward, Heavy metal content of roadside soils along ring road in Riyadh (Saudi Arabia), *Asian J. Chem.* **13**, 407–423 (2001).
- [6] Y. Nakamoto, Rapid determination of arsenic in thermally cracked gasoline by graphite-furnace AAS, *Bunseki Kagaku* **49**, 43–47 (2000) [in Japanese].
- [7] L. Liang, M. Horvat, and P. Danilchik, A novel analytical method for determination of picogram levels of total mercury in gasoline and other petroleum products, *Sci. Total Environ.* **187**, 57–64 (1996).
- [8] C. Samara and D. Vousta, Size distribution of airborne particulate matter and associated heavy metals in the roadside environment, *Chemosphere* **59**(8), 1197–1206 (2005).
- [9] A. Christoforidis and N. Stamatis, Heavy metal contamination in street dust and roadside soil along the major national road in Kavalas region, Greece, *Geoderma* **151**, 257–263 (2009).
- [10] D. Podnar, D. Koračin, and A. Panorska, Application of artificial neural networks to modeling the transport and dispersijon of tracers in complex terrain, *Atmos. Environ.* **36**(3), 561–570 (2002).
- [11] B. Fisher, Fuzzy environmental decision-making: application to air pollution, *Atmos. Environ.* **37**(14), 1865–1877 (2003).
- [12] D. Oettl, J. Kukkonen, R.A. Almbauer, P.J. Sturm, M. Pohjola, and J. Härkönen, Evaluation of a Gaussian and Lagrangian model against a roadside data set, with emphasis on low wind speed conditions, *Atmos. Environ.* **35**(12), 2123–2132 (2001).
- [13] S.S. Rasa, R. Avila, and J. Cervantes, A 3-D Lagrangian stochastic model for the meso-scale atmospheric dispersion applications. *Nucl. Eng. Des.* **208**(1), 15–28, (2001).
- [14] A.G. Clarke, L.A. Robertson, R.S. Hamilton, and B. Gorbunov, A Lagrangian model of the evolution of the particulate size distribution of vehicular emissions, *Sci. Total Environ.* **334–335**, 197–206 (2004).
- [15] F. Pasquill, The estimation of the dispersion of windborne material, *Meteorol. Mag.* **90**, 33–49 (1961).
- [16] Jr.F.A. Gifford, Consequences of effluent releases, *Nucl. Safety* **17**(1), 68–86 (1976).
- [17] P. Neofytou, A.G. Venetsanos, S. Rafailidis, and J.G. Bartzis, Numerical investigation of the pollution dispersion in an urban street canyon, *Environ. Model. Software* **21**, 525–532 (2006).
- [18] D.R. Parsons, G.F.S. Wiggs, I.J. Walker, R.I. Ferguson, and B.G. Garvey, Numerical modelling of airflow over an idealised transverse dune, *Environ. Model. Software* **19**, 153–162 (2004).

- [19] K.S. Rao, R.L. Gunter, J.R. White, and R.P. Hosker, Turbulence and dispersion modeling near highways, *Atmos. Environ.* **36**, 4337–4346 (2002).
- [20] B. Martinėnas and V. Špakauskas, Simulation of traffic pollution dispersion near roadways, *Lith. J. Phys.* **50**(2), 255–260 (2010).
- [21] A. Micallef and J.J. Colls, Variation in airborne particulate matter concentration over the first three metres from ground in an urban street canyon: implication for human exposure, *Atmos. Environ.* **32**(21), 3795–3799 (1998).
- [22] J.J. Colls and A. Micallef, Measured and modelled concentrations and vertical profiles of airborne particulate matter within the boundary layer of a street canyon, *Sci. Total Environ.* **234**, 221–233 (1999).
- [23] S.-K. Park, S.-D. Kim, and H. Lee, Dispersion characteristics of vehicle emission in urban street canyon, *Sci. Total Environ.* **233**, 263–271 (2004).
- [24] S. Weber, W. Kuttler, and K. Weber, Flow characteristics and particle mass and number concentration variability within a busy urban street canyon, *Atmos. Environ.* **40**, 7565–7578 (2006).
- [25] P. Kumar, P. Fennell, D. Langley, and R. Britter, Pseudo-simultaneous measurements for the vertical variation of coarse, fine and ultrafine particles in an urban street canyon, *Atmos. Environ.* **42**, 4304–4319 (2008).
- [26] I. Kanda, K. Uehara, Y. Yamao, Y. Yoshikawa, and T. Morikawa, A wind-tunnel study on exhaust gas dispersion from road vehicles–Part I: Velocity and concentration fields behind single vehicles, *J. Wind Eng. Ind. Aerodyn.* **94**, 639–658 (2006).
- [27] I. Kanda, K. Uehara, Y. Yamao, Y. Yoshikawa, and T. Morikawa, A wind-tunnel study on exhaust-gas dispersion from road vehicles–Part II: Effect of vehicle queues, *J. Wind Eng. Ind. Aerodyn.* **94**, 659–673 (2006).
- [28] Z. Ning, C.S. Cheung, Y. Lu, M.A. Liu, and W.T. Hung, Experimental and numerical study of the dispersion of motor vehicle pollutants under idle condition, *Atmos. Environ.* **39**(40), 7880–7893 (2005).
- [29] P.E. Benson, Modifications to the Gaussian vertical dispersion parameter σ_z near roadways, *Atmos. Environ.* **16**(6), 1399–1405 (1982).
- [30] Y. Zhu and W.C. Hinds, Predicting particle number concentrations near a highway based on vertical concentration profile, *Atmos. Environ.* **39**, 1557–1566 (2005).
- [31] J.A. Gillies, V. Etyemezian, H. Kuhns, D. Nikolic, and D.A. Gillette, Effect of vehicle characteristics on unpaved road dust emissions, *Atmos. Environ.* **39**(13), 2341–2347 (2005).
- [32] D. Zhu, H.D. Kuhns, J.A. Gillies, V. Etyemezian, A.W. Gertler, and S. Brown, Inferring deposition velocities from changes in aerosol size distributions downwind of a roadway, *Atmos. Environ.* **45**, 957–966 (2011).
- [33] I. Grigalavičienė and V. Rutkoviėnė, Heavy metals accumulation in the forest soils and mosses along highway Vilnius–Kaunas, *Miškininkystė* **2**(60), 12–19 (2006).
- [34] H.G. Zechmeister, D. Hohenwallner, A. Riss, and A. Hanus-Illnar, Estimation of element deposition derived from road traffic sources by using mosses, *Environ. Poll.* **138**, 238–249 (2005).

TRANSPORTO SUKELTŲ AEROZOLIŲ DALELIŲ SKLAIDOS MODELIAVIMAS

V. Špakauskas, D. Melichov

Vilniaus Gedimino technikos universitetas, Vilnius, Lietuva

Santrauka

Darbe pasiūlytas kvaziempirinis modelis, skirtas didesnio kaip $0,3 \mu\text{m}$ skersmens dalelių sklaidai pakelėse modeliuoti. Modeliuojant taršos šaltinį kaip nupjautinį cilindrą laikome, kad aerzolių dalelės ($0,3\text{--}15 \mu\text{m}$ diametro) taršos šaltinyje vertikalia ir horizontalia kryptimis pasiskirsto pagal Gauso dėsnį. Pučiant vėjui, kurio

kryptis statmena keliui, dulkių debesis yra nešamas tolyn nuo kelio, o aerzolio dalelės yra veikiamos gravitacijos, dalelių plūdrumo ir terminio teršalų fakelo kilimo efektų. Gauta teršalų koncentracijos kaita transporto magistralės šalikelėse sutampa su eksperimentiniais matavimais (Zhu ir kt., 2011; Grigalavičienė ir Rutkoviėnė, 2006; Zechmeister ir kt., 2005).