

Dispersion modelling of solid particles from vehicle exhaust into the atmosphere

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The research carried out in major towns has revealed that the highest level of pollution is registered during the morning and afternoon rush hours when traffic intensity is the greatest. Traffic pollutant emissions are very concentrated in streets of high traffic intensity, but at a distance of 1–2 meters and especially 4–6 meters from the carriageway their amount is sharply reduced. The concentration of aerosol particles is directly dependent on the intensity of the traffic flow. Their concentration is evenly reduces with the distance from the carriageway, and at a distance of 300 m particles tend to deposit on the ground surface.

The research was carried out at 14 selected points of Vilnius, Žirmūnai neighbourhood streets, where the number of vehicles passing by (light, medium, heavy traffic) has been counted. The obtained results have been applied to determine the mean concentrations of solid particles (SP) in the morning and afternoon rush hours. The data were used for the mathematical modelling of solid particle dispersion in Žirmūnai neighbourhood. In some cases, the maximum allowable concentration (MAC) of solid particles was exceeded.

Key words: environment, atmosphere, air pollution, mobile recourses of pollution, solid particles, transport, modelling of pollution dispersion

INTRODUCTION

Particle matter (PM) is generally designated as a mixture of solid and liquid particles in the air. The diameter of a particle in the air ranges from 0.005 to 100 microns (μm). Fine particles fired in the air have a diameter of 2, 5 μm and even less (Zhu et al., 2002; Shi et al., 1999; Hitchins et al., 2000). Fine particles are produced by firing coal, petrol, diesel fuel or any other fossil fuel and wood (Baltrėnas, Masilevičius, 2004). The ultrafine particle resources come from motor cars equipped with petrol and diesel motors, power plants firing coal or burning biomass (Martuzevičius et al., 2004; Makela, Salo, 1994; Petraitis, Vasarevičius, 2001).

Particles with a diameter less than 0.1 μm and produced in the car engine during the fuel combustion process are considered to be most hazardous for human health. They are discharged into the environment as a waste after the combustion process. Even though they comprise only a small part (1–8%) of the mass of the finest PM discharged into the environment from the engines, there have been written a lot of scientific articles to analyse their concentration and dispersion in the environment and production areas, and only a small part of articles analyse the distribution of such particles along the highways (Zhu et al., 2002; Shi et al., 1999; Hitchins et al., 2000).

Many pollutants in the form of solid particles are produced by motor car discharges. Therefore, it is very important to investigate emissions of pollutants caused by vehicles (Petraitis, Vasarevičius,

2001; Baltrėnas et al., 1997; Hjertager et al., 1998; Mathiesen, Solberg, 1999; Baltrėnas et al., 2004; Baltrėnas et al., 1998). To investigate the dispersion of SP theoretical (Petraitis, Vasarevičius, 2001; Baltrėnas et al., 1997; Hjertager et al., 1998; Mathiesen, Solberg, 1999; Baltrėnas et al., 2004) and experimental (Baltrėnas et al., 2004; Baltrėnas et al., 1998) methods have been used.

In the exhaust gas from the combustion engines of motor cars and in SP there are found more than 200 various chemical compounds the majority of which are hazardous for human health and for the development of all organisms (Ptašekas et al., 2004).

The atmosphere is mostly polluted at the moment of starting a car, using brakes and driving slowly. At the very start of a car and at the very beginning of driving from the standstill, air pollution is 50 times higher than the general average, therefore the largest sources of pollutant emissions are considered to appear in the vicinity of crossroads. At the sections between crossroads, the air is polluted most when vehicles move at a speed no higher than 30 km/h; on increasing the speed up to 90 km/h, vehicles consume less fuel, and pollutant emissions into atmosphere are twice lower (Makela, Salo, 1994).

In the territorial planning, in selecting new sites for residential areas, identifying the troublesome points as well as in designing the relocation of the existing traffic flows, the values of pollutant emissions become the most significant factors in the decision-making. The existing background of contamination determines the number of development alternatives, possibilities, etc.

The number of toxic matters from internal combustion engines exhausted into the atmosphere depends on fuel and air mixture formation, the air surplus coefficient λ , which means the ratio of the amount of air practically used to fire fuel to the theoretically determined and required one (Baltrėnas et al., 2004).

For air pollution modelling, there are the most widely used models based on the Gaussian dispersion, such as CALINE, ISC3, PRIME, SCREEN3, SLAB (United..., 2002; ISCST, 2002), the program VARSA (Petraitis, Vasarevičius, 2001). The other group of models such as PHOENICS (PHOENICS 3.5, 2002), FLUENT (FLUENT, 2004) are based on the numerical solution of equations of transfer processes. These models have not been compiled for one and the same purpose – some of them are applied for modelling the dispersion of dense gas, others are more suitable for modelling traffic exhaust gas emissions, yet others for production premises, etc. The PHOENICS program is applied for modelling the transfer of gaseous and liquid pollutants in the air, water and soil, and of solid particle transfer (ASM, GENTRA, IPSA, SEM).

The objective of the current research was the mathematical simulation of SP transfer processes from the street into the environment in order to determine the mean SP concentrations in Žirmūnai neighbourhood in the Vilnius City. SP emissions on the streets are calculated using the COPERT program.

DESCRIPTION OF MATHEMATICAL MODEL (PROGRAM)

In the general case, to describe the recirculation flows with transfer of mass, the system of three-dimensional continuity and the Navier–Stokes equations could be used. Their summarised expression for a stationary process is the following (PHOENICS 3.5, 2002; Pavitsky et al., 1993):

$$\operatorname{div}(\rho \bar{V} \phi - \Gamma_{\phi} \operatorname{grad} \phi) = S_{\phi}, \quad (1)$$

where ρ is density, kg/m³; ϕ is dependant variable: $\phi = 1$ is the equation of continuity, U, V, W are the components of impulse towards the direction of coordinates x, y and z , m/s; \bar{V} is the vector of velocity, m/s; Γ_{ϕ} is the effective coefficient of diffusion of a variable ϕ ; S_{ϕ} is the source term of variable ϕ . The (1) system of equations is compiled from Navier–Stokes equations and the continuity equation solved by the finite volume method (Baltrėnas et al., 1998; PHOENICS 3.5, 2002). The turbulence of the atmospheric border layer has been simulated according to the hypothesis of turbulent viscosity (Baltrėnas et al., 1998; Pavitsky et al., 1993).

The software of calculated fluid dynamics (CFD) such as PHOENICS applies various models for calculating the processes of two-phase flows of transfer. One of such models used is the algebraic slip model (ASM) applied together with the equations of motion (1).

ASM. For description of the task to be solved, the Algebraic Slip Model (ASM) is applied. The model postulates that there exists one continuous medium in which there are dispersed various phase components. These may be droplets, bubbles or solid particles. The mixture of the continuous and dispersed phases behaves as a single fluid,

with fluid properties that may or may not depend on the dispersed phases. This is referred to as the mixture, and correspondingly its properties are referred to as the mixture density and the mixture viscosity (Idzelis et al., 2005).

Each dispersed phase is represented by a species concentration equation. The transport equation for each dispersed phase allows for relative movement between the dispersed phase and the continuous phase. This extra migration or drift of the dispersed phase is known as the phase slip. It is assumed that the slip velocity can be calculated from algebraic equations involving only local variables, rather than from the full partial differential equations.

The equations to be solved for the phase-concentration distributions are therefore the partial differential equations (PDEs) of continuity and momentum of the mixture, the PDEs of conservation of the particle groups, with additional slip–velocity–transport terms, the algebraic equations which allow the latter terms to be evaluated.

Calculation of slip velocity. The frictional drag on the particle is given by

$$F_d = C_d \cdot A_p \cdot 0.5 \cdot \rho \cdot (v_s)^2, \quad (2)$$

where A_p is the projected area of the particle, ρ is the fluid density and v_s is the slip velocity (eq. 4). The slip force is given by

$$F_s = B \cdot V_p \cdot \Delta \rho, \quad (3)$$

where V_p is the volume of the particle, $\Delta \rho$ is the density difference, and B is the body force per unit mass. Hence,

$$(v_s)^2 = K \cdot \Delta \rho \cdot d_i \cdot B / \rho, \quad (4)$$

where d_i is the particle diameter, and the coefficient $K = 4/(3 \cdot C_d)$ may be a function of the slip Reynolds number Re via C_d . The slip Reynolds number $Re = d \cdot V/v$, where v is the kinematic viscosity. The body force includes gravitational acceleration. The slip velocity is added to the mixture velocity to construct the dispersed-phase convection fluxes.

Built-in drag coefficient. The built-in drag coefficient is a simplified model which breaks the drag curve into three parts. At a low slip Reynolds number the relationship is:

$$C_d = 24/Re; \quad 0.02 < Re < 100, \quad (5)$$

$$C_d = \frac{24}{Re} + \frac{4}{\sqrt[3]{Re}}, \quad 100 < Re < 400. \quad (6)$$

At a higher slip Reynolds number, $Re > 400$,

$$C_d = 0.42. \quad (7)$$

Auxiliary formulae for the ASM. The mixture density

$$\rho_m = (1 - \sum(P_i)) \cdot \rho_c + \sum(P_i \cdot \rho_i). \quad (8)$$

The mixture viscosity

$$v_m = (1 - \sum(P_i)) \cdot v_c + \sum(P_i \cdot v_i). \quad (9)$$

In both cases, m refers to the mixture, c to the continuous phase (air flow), and i to the i th dispersed phase. P_i is the volume fraction of the i th phase.

Discretisation of the space. The map of Žirmūnai neighbourhood (Fig. 1, scale 1 cm = 135 m), the area includes $3675 \times 1536 \text{ m}^2$ area, is discretised by the differential network $x \cdot y \cdot z = 92 \cdot 13 \cdot 220$. In accordance with the map (Fig. 1), in the discretion area there are marked streets where the concentrations of pollutants had to be measured. Buildings, fences and trees located near the streets are measured by means of blocked cells or groups of cells, etc.

The following solid particles have been analysed: diameter $1.0 \cdot 10^{-4} \text{ m}$ up to $1.0 \cdot 10^{-6} \text{ m}$, density 1700 to 7800 kg/m^3 .

Initial conditions: according to the data of Table, concentration at 14 points is set in the area of the streets. For the remaining streets, the values of concentration have to be based on the results of these 14 points and the assessment of traffic flows of the corresponding streets.

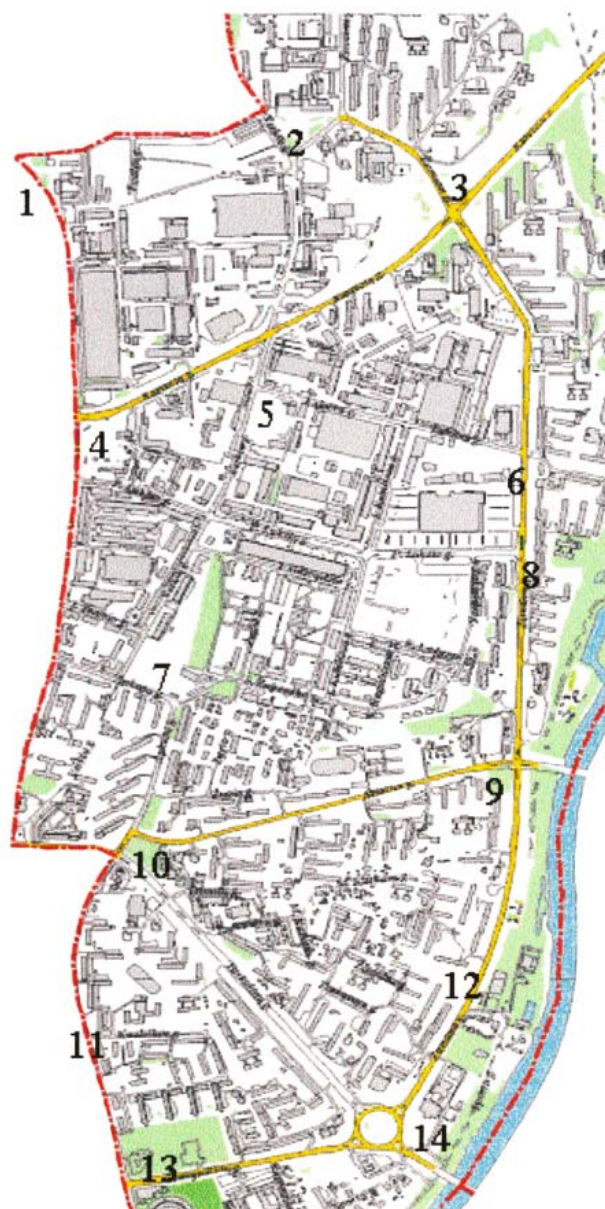


Fig. 1. Žirmūnai neighbourhood map with the marked 14 points of traffic flow measurements

Table. Total number of vehicles per hour and SP emissions ($\mu\text{g}/\text{m}^3$) in Žirmūnai neighbourhood streets, Nos. 1–14 (in Fig. 1)

Measurement points	Total number of vehicles per hour	SP, $\mu\text{g}/\text{m}^3$
1	463	40.0
2	186	160.0
3	533	40.0
4	387	40.0
5	191	10.0
6	315	30.0
7	203	20.0
8	308	20.0
9	97	10.0
10	216	20.0
11	135	10.0
12	312	20.0
13	250	20.0
14	543	40.0
MAC	–	50.0
Background concentration	–	0.5

Wind direction and strength, air density and background concentration are chosen at the inflow along the whole way of a volume area or along two ways when the wind direction is south-east, south-west, north-east and north-west.

RESULTS AND ANALYSIS

The research was done to model SP dispersion in the Vilnius City, Žirmūnai neighbourhood (Fig. 1). On the map, there are marked 14 places on the streets where three times a day (at 8–9, 12–13 and 17–18 o'clock) calculations were made investigating traffic flows of various vehicles including light weight, medium weight, heavy weight ones. The results of measurements of traffic flows during the rush hours are presented in Fig. 2. They were received by means of COPERT program, the obtained SP emissions are in $\mu\text{g}/\text{m}^3$. The total number of vehicles and 14 sites for measuring SP emission are presented in Table.

The results of modelling were obtained by modelling SP transfer from linear sources of pollutants taking into account the background number of SP in the air, buildings located near the streets. In the Žirmūnai area, the dispersion of these pollutants from the maximum at point 2 and from all other streets with the set initial number of pollutants, varied from the medium up to background. The maximum allowable concentration (MAC) is $50 \mu\text{g}/\text{m}^3$. The type of dispersion depends on the strength and direction of wind and on the buildings located close to the streets.

In Fig. 3 are presented contours of SP concentration modeling results, southeastern wind (field of velocity vectors and SP concentration at 1.5 m high from the earth) in the whole area. On the streets, as boundary conditions are indicated linear SP concentration values up to 4 m high from the street and its downwind transfer. There are presented the results of modelling of SP concentration ($\mu\text{g}/\text{m}^3$) when the south-east wind is blowing at a speed of 5 m/s. The background SP concentration is $0.5 \mu\text{g}/\text{m}^3$. The maximum SP concentration is in the street with

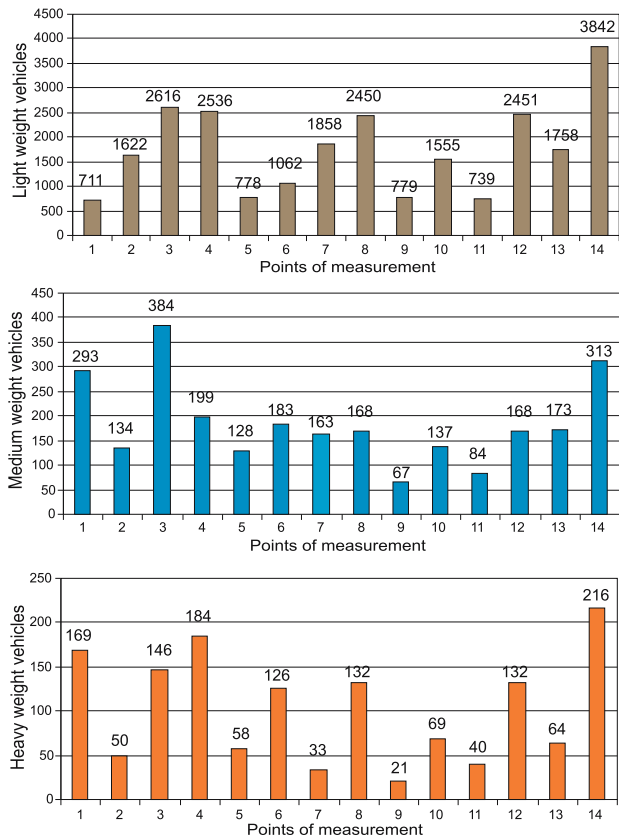


Fig. 2. Light weight, medium weight and heavy weight vehicle number per hour at 14 measurement sites

measurement points Nos. 5 up to 2, somewhat down the street with No. 4 and No. 1, namely in the streets where measurement points Nos. 1, 3, 4, 14 are located ($40 \mu\text{g}/\text{m}^3$). We have to single out a significant territory embracing the dispersion of SP concentration to the northwest from the streets with points Nos. 4 and 14, as well as from the roundabout circle in the south of the area. When the wind is blowing along the street with Nos. 10 and 14, the increased concentration of SP is formed in it, and lateral transfer develops by diffusion.

Figure 4 shows the contours of SP concentration modeling results with the southwestern wind (field of velocity vectors and SP concentration 1.5 m high above the ground) in the whole area. Dispersion of SP concentration at the height of 1.5 m in Žirmūnai when the southwest wind is blowing at the speed of 5 m/s is presented (buildings were accounted for). The maximum concentration is at point No. 2 ($160 \mu\text{g}/\text{m}^3$). The highest concentration of SP is formed in the street with measuring points Nos. 3 and 4 (because the wind is blowing along the street) and in the street segment from No. 2 to No. 3. In the south part of the area, near the roundabout, the concentration of SP is also high. In this case, there are formed larger areas with an increased concentration downwind; the concentration withdrawing from the streets downwind is rapidly reduced by depositing in the form of particles on the ground. In the streets in which there are measuring points Nos. 1, 3, 4, 14 ($40 \mu\text{g}/\text{m}^3$), also increased concentrations were transferred by convection and downwind.

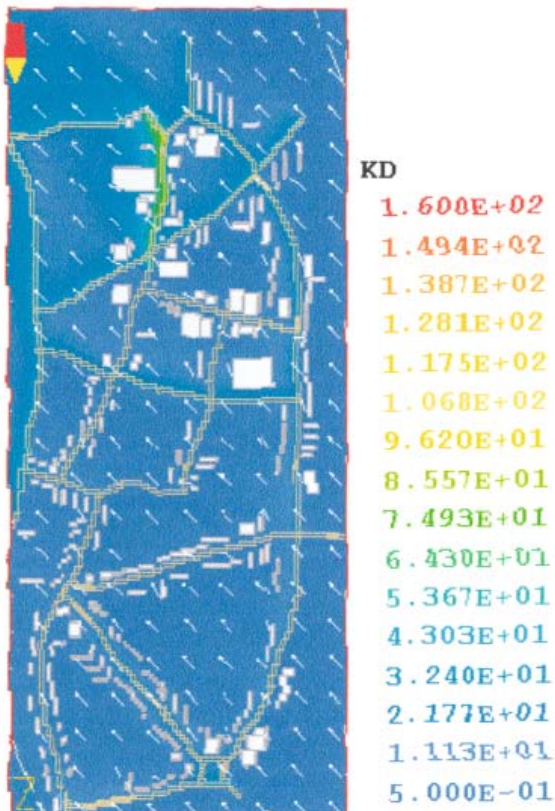


Fig. 3. SP (KD) concentrations $\mu\text{g}/\text{m}^3$, dispersion modelling contours and vectors of speed 1.5 m above the ground surface in Žirmūnai when south-eastern wind is blowing at 5 m/s

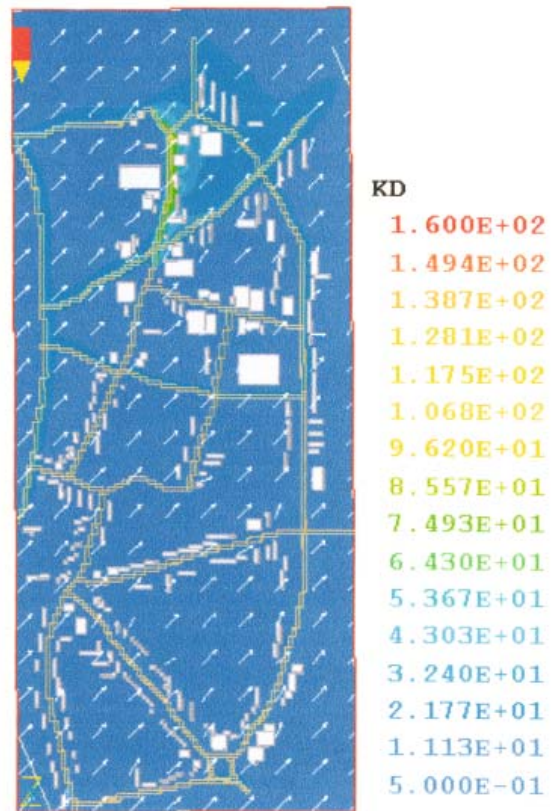


Fig. 4. SP (KD) concentration, $\mu\text{g}/\text{m}^3$ as the contours of dispersion modelling and vectors of velocity 1.5 m above the ground surface in Žirmūnai when the south-west wind is blowing at 5 m/s

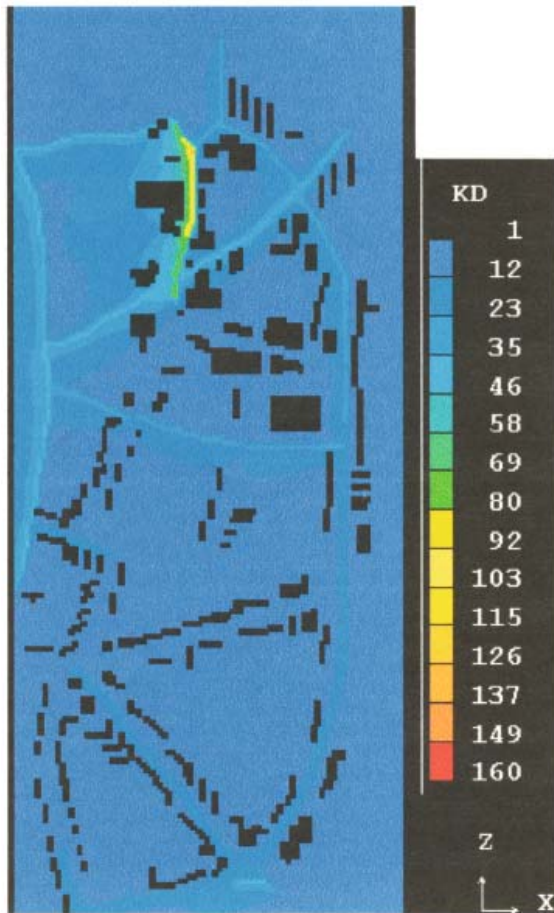


Fig. 5. SP (KD) concentrations, $\mu\text{g}/\text{m}^3$ as the contours of dispersion modelling 1.5 m above the ground surface in Žirmūnai when the north-eastern wind is blowing at 3 m/s

In Fig. 5 are presented contours of SP concentration modelling results with the north-eastern wind (SP concentration 1.5 m above the ground) in the whole area. SP dispersion in the area is presented 1.5 m above the ground when the speed of the north-eastern wind is 3 m/s. The buildings located near-by change the type of the dispersion of SP concentration. Areas with a increased SP concentration were observed downwind from the street with points Nos. 4, 5, 3, 8 and 6 and at the roundabout located in the south part of the area from the street segment with points Nos. 14 to 13.

In Figs. 3–5 we present the results of transfer of SP concentrations from vehicle emissions, which indicate a rather generalized situation concerning the SP dispersion map under the influence of wind and buildings. A detailed view of pollutant dispersion is possible to obtain when investigating an area several times smaller than that presented in Fig. 6. There is presented a fragment of the map (Fig. 1) with measuring points Nos. 7, 8, 9 and 10. The scale of the map with zone discretisation is $1\text{ cm} = 55.5\text{ m}$. The area of the zone is $x \cdot z = 1304.25 \cdot 666.0\text{ m}^2$, the discretised territory has $x \cdot y \cdot z = 94 \cdot 13 \cdot 48$ cells.

Figure 7 shows SP concentration isolines ($\mu\text{g}/\text{m}^3$) 1.5 m above the ground surface, when the east wind is blowing at a speed of 2 m/s. The increased SP concentration was registered going west from the street (Nos. 3, 6, 8, 12 and 14), and it decreased downwind. The increased SP concentration was registered going west from the street (Nos. 7, 8 and 9), it was three times lower in the street (No. 9) from which the dispersion spreads at a distance of 50 to 250 m downwind. Buildings serve as obstacles to SP convective transfer. In Fig. 7, in the left bottom part, SP dispersion behind the buildings is of a background level: the zone is limited by the 10th isoline.

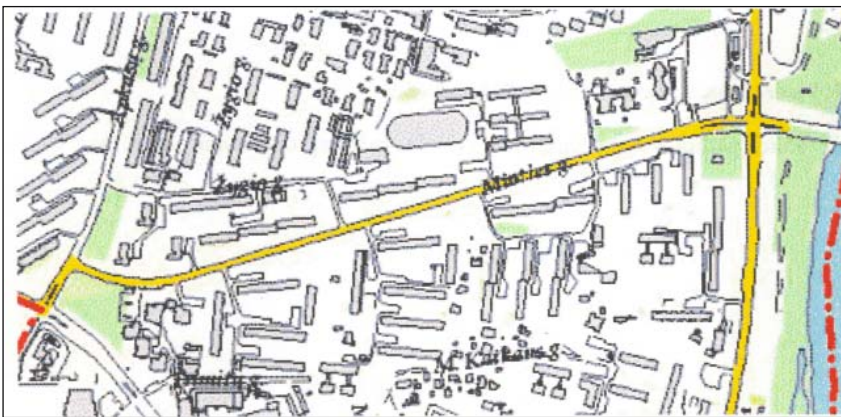


Fig. 6. A fragment of Žirmūnai Municipality map: Minties–Apkasių streets, part of Tuskulėnų street

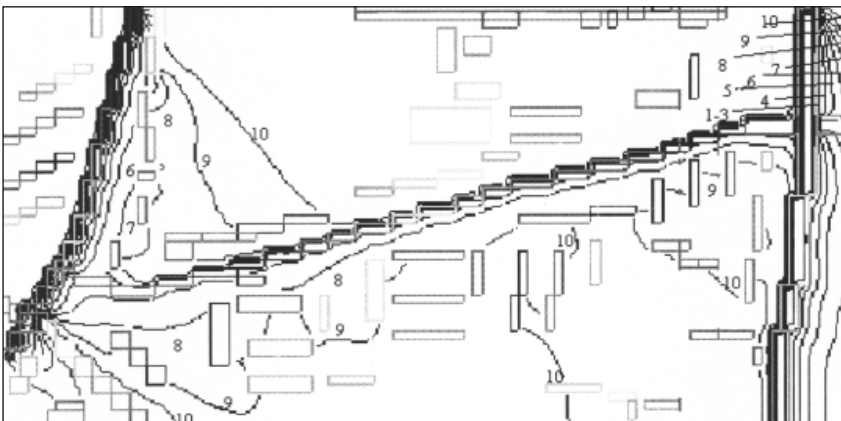


Fig. 7. SP dispersion from Žirmūnai streets (see Fig. 6) when the north-west wind is blowing at 2 m/s. The values of concentration isolines: 1 – 20, 2 – 17, 3 – 14, 4 – 12, 5 – 10, 6 – 8, 7 – 6, 9 – 4, 10 – $2\text{ }\mu\text{g}/\text{m}^3$

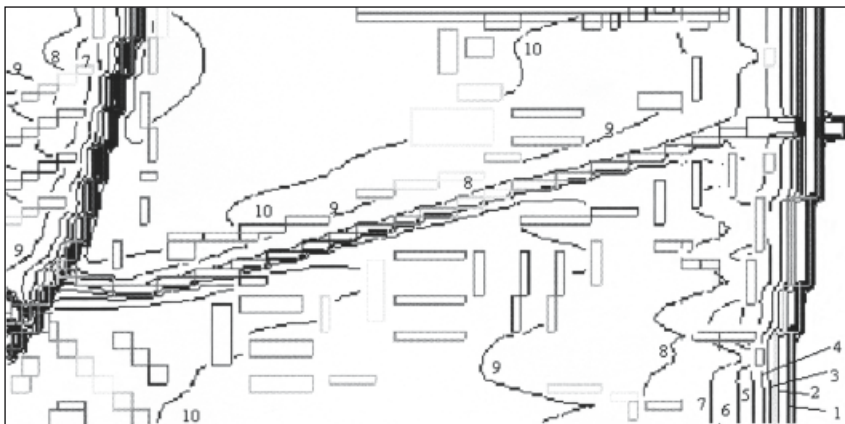


Fig. 8. SP dispersion from Žirmūnai streets (see Fig. 6) when the eastern wind is blowing at 2 m/s. The values of concentration isolines: 1 – 20, 2 – 17, 3 – 14, 4 – 12, 5 – 10, 6 – 8, 7 – 6, 9 – 4, 10 – 2 $\mu\text{g}/\text{m}^3$

In Fig. 8 we present SP concentration isolines (Fig. 1). Behind the 10th isoline the concentration is low and close to the background one. In Figs. 7 and 8, isolines show SP concentration transfer and its differences when north-west and east winds are blowing.

When the north-west wind is blowing (2 m/s), the concentration is decreasing downwind. An increased SP concentration is observed to the southeast from the street (Nos. 8, 7), and it is three times lower than in the street (No. 9) from which dispersion takes the distance of 50 to 200 m downwind. It can be noted that the street with point No. 7 was not covered by the modelling process, and the northern part of the figure shows an unreal view of the concentration. For analysis, it is necessary to give the modelled results with analogous boundary conditions in the whole area.

The deposit of particles with the diameter $d = 10 \mu\text{m}$ was modelled in the following way (in the presence of a 3 m/s wind): when $\rho_p = 2000 \text{ kg}/\text{m}^3$, the end of transfer is approximately 290 m; when $\rho_p = 4000 \text{ kg}/\text{m}^3$, it is 250 m, and when $\rho_p = 7880 \text{ kg}/\text{m}^3$, it is 200 m.

Particles with a density $\rho = 7880 \text{ kg}/\text{m}^3$, when $d_i = 1.0 \mu\text{m}$, had the non-dimensional concentration of $c/c(90 \text{ m}) = 0.028$; when $d_i = 5.0 \mu\text{m}$, their $c/c(90 \text{ m}) = 0.0015$, where $c(90 \text{ m})$ is SP concentration within the distance of 90 m. Ultrafine particles ($d_i = 0.1 \mu\text{m}$) by means of the presented model are simulated in the following way: when the value of $\rho_p = 2000 \text{ kg}/\text{m}^3$, the non-dimensional concentration within the distance of 300 m from the road is $c/c(90 \text{ m}) = 0.52$, and when $\rho_p = 7880 \text{ kg}/\text{m}^3$ it is $c/c(90 \text{ m}) = 0.28$. Thus, it is possible to state that by means of the proposed method it is possible to model the transfer of particles when their density is from $2000 \text{ kg}/\text{m}^3$ to $7880 \text{ kg}/\text{m}^3$ and diameter from $0.3 \mu\text{m}$ to $10.0 \mu\text{m}$. The results of modelling have been compared with the experimental ones (Shi et al., 1999; Baltrėnas et al., 1998), which coincided within the error limit of $\pm 10\%$.

In the air, SP of the size of $0.4 \mu\text{m}$ prevailed. The most significant influence was exerted by the prevailing flow of light-weight vehicles (Baltrėnas, Masilevičius, 2004; Martuzevičius et al., 2004; Ptašek et al., 2004).

CONCLUSIONS

1. The concentration it is possible to state that contamination caused by SP depends on the intensity of the flow of vehicles and on the time the measurements have been carried out (the maximum contamination was registered during the rush hours from 8–10 and from 16–18 o'clock).

2. During the study, in the air SP $0.4 \mu\text{m}$ in size prevailed. The prevailing flow of light-weight vehicles was registered.

3. SP concentration directly depends on traffic intensity. SP concentration evenly reduces with increasing the distance from the carriageway of the motorway. At the measuring point No. 2, the maximum allowable concentration was exceeded three times. Points Nos. 1, 4 and 14 noted the concentration of SP close to the maximum allowable one, comprising 80% of standard maximum allowable concentration.

4. The results of modelling have been compared with the experimental ones and theoretical results obtained by various authors, and coincided within the error boundaries of $\pm 10\%$.

Received 26 March 2007

Accepted 14 March 2008

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AUTOTRANSPORTO Į ATMOSFERĄ IŠSKIRIAMŲ KIETŪJŲ DALELIŲ SKLAIDOS MODELIAVIMAS

Santrauka

Miestuose atlikti tyrimai rodo, kad daugiausiai teršalų yra išskiriama rytinio ir vakarinio eismo piko valandomis, kai autotransporto eismas yra intensyviausias. Autotransporto tarša ypač didelė miesto intensyvaus eismo gatvėse ir 1–2 metrų atstumu nuo važiuojamosios kelio dalies, o esant 4–6 metrų atstumui jų kiekiai staigiai sumažėja. Nustatyta, kad aerozolių dalelių koncentracijos tiesiogiai priklauso nuo autotransporto eismo intensyvumo. Koncentracija tolygiai mažėja didėjant atstumui nuo kelio važiuojamosios dalies, apie 300 m atstumu dalelės nusėda ant žemės paviršiaus.

Tyrimai atlikti 14 Vilniaus m. Žirmūnų gatvių vietų, kuriose pagal pravažiuojančio autotransporto (lengvųjų, vidutinių, sunkiųjų) skaičių nustatytos vidutinės kietųjų dalelių (KD) koncentracijos rytinio ir vakarinio eismo piko valandomis. Naudojantis jomis atliktas kietųjų dalelių sklaidos Žirmūnuose matematinis modeliavimas. Keliose vietose KD koncentracija buvo didesnė už didžiausią leistiną koncentraciją.

Raktažodžiai: aplinka, atmosferos oro tarša, mobilieji taršos šaltiniai, kietosios dalelės, autotransportas, taršos sklaidos modeliavimas