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MATHEMATICAL SIMULATION OF SOLID PARTICLE DISPERSION IN THE AIR OF VILNIUS CITY

Pranas Baltrėnas¹, Jurgita Morkūnienė², Petras Vaitiekūnas³

Vilnius Gediminas Technical University, Saulėtekio al. 11, LT-10223 Vilnius, Lithuania E-mail: ¹pbalt@ap.vgtu.lt; ²aak@ap.vgtu.lt; ³vaitiek@ap.vgtu.lt Submitted 6 June 2007; accepted 20 June 2007

Abstract. One of the main methods for the air quality assessment and forecast is mathematical simulation of pollutants. In order to simulate the dispersion of solid particles (SP) in the air, there may be applied the package of "Phoenics" software in which the proximity methods of equation solution are used, because an accurate analytic solution of movement equations is not possible to be applied. The software was used in Žvėrynas district of Vilnius city in which the exact values of SP were selected.

The paper presents the technique of mathematical simulation of SP dispersion in the air, the Algebraic Slip Model is described which is used for the solution of the problem; the model uses calculation-based formulas. Based on the results of the experiment (the values of SP concentration) and the obtained results by applying "Phoenics" mathematical simulation program, the feasibility of the simulation program for modeling the SP concentration dispersion is determined. The results of simulation are submitted in figures and tables, and conclusions have been derived.

Keywords: mathematical simulation, Scalar Equation Method, Algebraic Slip Model, dispersion of solid particles (SP).

1. Introduction

To assess the air quality (pollution by SP is also considered as a detector of air quality) there may be applied any method allowing to measure (Baltrenas, Morkūnienė 2006; Baltrenas, Kvasauskas 2005; Baltrenas, Masilevičius 2004), calculate (Mathiesen, Solberg 1999; Baltrenas *et al.* 1998; Petraitis, Vasarevičius 2001) or forecast (Hjertager *et al.* 1998) the level of air pollution.

The measurement made concerning air pollution as well as inventory of pollutant sources are considered to be reliable methods and are widely applied in Lithuania, but the pollutant dispersion in the surrounding air from stationary and mobile sources of pollutants depends on many factors, so in order to determine the typical regularities of the dispersion for specific conditions, the method of numerical simulation is considered to be more suitable as it could evaluate the input of sources of various pollutants; it also increases the possibility to depict the spatial distribution of pollutants on the map as well as reduces the number of sites to be measured, and there arises possibility to evaluate correspondence/non-correspondence to the limited values (environmental air quality measurement by means of models).

At present to assess air pollution various numerical models are applied. One of the programs that is applied in our country for numerical simulation of SP dispersion in the atmosphere is "Phoenics" mathematical simulation program. Multiphase flows are of great practical importance in many common engineering and environmental applications. Multiphase flows are characterized by two or more fluids in motion relative to each other. The fluids will also usually have different physical properties – temperature, density, conductivity. For solid particle transfer simulation in a continuous medium with dispersed various-phase components, some numerical methods may be used: Interphase Slip Algorithm – IPSA, Scalar Equation Method – SEM, and Algebraic Slip Model – ASM.

By means of the package of "Phoenics" software it is possible to simulate the processes of the transfer of pollutants in the atmosphere, hydrosphere and geosphere (Vaitiekūnas 2004). The method of discreteness of the equations of pollutant transfer applied in the software is the method of finite volumes, because it is impossible to solve analytically precisely the equations of movement (Petraitis, Vasarevičius 2001).

2. Description of mathematical simulation model (program)

The program of "Phoenics" as a mathematical simulation program is based on the proximity methods of equation solution. It may be used for solving numerical simulation problems in a SP dispersion environment, taking into consideration the peculiarities of the process operating within a real environment (Mathiesen, Solberg 1999; Baltrenas *et al.* 1998; Petraitis, Vasarevičius 2001). To solve a numerical simulation problem with the help of which the dispersion of SP in the environment is determined, the Algebraic Slip Model is used. The Model is based on the existence of pollutant transfer media in which the phases of various particles are spread. The droplets, air bubbles or solid particles may constitute these particles (the Algebraic Slip Model).

The mixture of a productive phase and particle phase has a tendency to function as one fluid, possessing the characteristics of a fluid that may depend or not on the phases of dispersed particles. The mentioned above mixture is signified by all the characteristics typical for the mixture itself, such as the density of the mixture and viscosity. By applying the Algebraic Slip Method an assumption is derived that the phase of particles is of a halfset state, preconditioned by local conditions. It is required that the relaxation time of the phase of particles is sufficiently low if compared to the changes of flow, i.e. the number of Stokes is <<1. The number of Stokes is described as the ratio of the particle relaxation time and flow time of a pollutant carrier.

Precise conditions depend on resistance. In general this could be achieved only in cases when the particles are small, and the viscosity of the fluid is high. Only such a model is suitable for simulation of particles influenced by the gravitation force, centrifugal force or any other force separation.

The friction force F_d which affects the particle in the Algebraic Slip Model is calculated according to formula (1) (The Algebraic Slip Model):

$$F_d = C_d \cdot A_p \cdot 0.5 \cdot \rho \cdot (v_s)^2, \tag{1}$$

where C_d – coefficient of resistance; A_p – area of the particle, m²; ρ – fluid density, kg/m³; v_s – slip velocity, m/s.

The slip force F_s is calculated using formula (2) (the Algebraic Slip Model):

$$F_s = B \cdot V_p \cdot \Delta \rho, \qquad (2)$$

where *B* –force to the amount of material; V_p –particle volume; $\Delta \rho$ – density difference.

Then the velocity of the slip v_s is calculated:

$$(v_s)^2 = K \cdot \Delta \rho \cdot d \cdot B/\rho, \qquad (3)$$

where K – coefficient ($K = 4/(3 \cdot C_d)$) which is considered to be the slip Reynolds number Re function from the coefficient of resistance C_d .

The density of the mixture ρ_m in the Algebraic Slip Model is calculated according to formula (4):

$$\rho_m = (1 - \Sigma(P_i)) \cdot \rho_c + \Sigma(P_i \cdot \rho_i), \qquad (4)$$

where P_i – part of *i*-particle phase volume; ρ_i – *i*-particle phase density, kg/m³; ρ_c – density of the transfer medium (air flow), kg/m³.

Viscosity of the mixture v_m in the Model is calculated according to formula (5):

$$v_m = (1 - \Sigma(P_i) \cdot v_c + \Sigma(P_i \cdot v_i), \qquad (5)$$

where v_c –viscosity of the transfer medium; v_i – *i*-particle phase viscosity; v_c –viscosity of the carrier media.

In a general case, to describe recirculation flows with the mass carrier, the equation system of Navje-Stokes as well as a diffusion equation system for a single phase theoretical model are solved. Their generalized expression for the stationary process is the following (The Algebraic Slip Model):

$$\operatorname{div}(\rho \,\overrightarrow{V_{\phi}} - \Gamma_{\phi} \operatorname{grad} \phi) = S_{\phi} \,, \tag{6}$$

where ρ – density, kg/m³; ϕ – dependant variable: $\phi = 1$ – equation of continuity ; \vec{V} – velocity vector; Γ_{ϕ} – variable ϕ diffusion coefficient (for the equations of movement it is the coefficient of cinematic viscosity); S_{ϕ} – source term of variable ϕ .

The generalized system of equations (6) is comprised of the Navje-Stokes and continuity equations solved by the method of finite volumes.

The instability of the atmosphere under a slight velocity of the wind (1–5 m/s) is assessed by the formula of the turbulent viscosity v_t (The Algebraic Slip Model):

$$\mathbf{v}_t = C \cdot U_0,\tag{7}$$

where $1.1 \le C \le 1.4$ – atmospheric stability constant; U_0 – velocity of the wind.

Then the coefficient of diffusion Γ_{ϕ} consists of two

components – molecular and turbulent. The coefficient of diffusion for the equations of movement is the following:

$$\Gamma_{\phi} = \nu + \nu_{\rm t},\tag{8}$$

where v – molecular viscosity; v_t – turbulent viscosity.

3. Calculation technique

Žvėrynas district municipality (the map scale is 1 cm = 100 m) area occupies $1500 \times 1900 \text{ m}^2$ territory. This area is digitized by the following differential network: $x \cdot y \cdot z = 150 \times 13 \times 190$. The following streets are included into the simulation: Kraševskis, Liubartas, Traidenis, Treniota, Poška, Latviai, Bebrai, Lenktoji, Žalioji, Latgaliai, Narbutas, Pieninė, Paribis, Saltoniškės, Vytautas, Birutė, Liepynas, Stumbrai, Elniai, Stirnos, Sakalai (Vaitiekūnas *et al.* 1998). Following the map, in the digitized areas streets with prescribed concentrations of pollutants are marked (Fig. 1).

Initial conditions: at selected 32 points (out of 40 points where the concentration of the investigated solid particles was measured) SP concentration in the area of the streets was prescribed (Baltrénas, Morkūnienė 2006).

At the remaining 8 points the values of SP concentration, based on the results of 32 points, had to be determined theoretically by means of the mathematical simulation "Phoenics" program. The results obtained theoretically were compared with the results of the experiment.

40 points were chosen for measuring particulate matter concentration in Žvėrynas district (Fig. 1).

As shown in Fig. 1, the investigated area of Žvėrynas district was divided into 11 cross-sections. Each section had from 3 to 5 measuring points.

The direction of the wind, its strength, air density and phonic concentration were prescribed at the inflow along the whole side of the area volume when the wind direction was northeastern (on April 26), eastern (on July 11) and northwestern (on January 30) (the data used were borrowed from the State Air Monitoring the "Phoenics" program solved by means of the finite volume method. A three-dimensional problem was solved, i.e. the coordinates x, y, z were used. In each unit of the net the concentration of SP was calculated (Table 1). Differential equations were integrated in the volume of each cell or area.

Table 1. Calculation of initial conditions

	Prescribed concentration, mg/m ³										
Point No.	April 26, 2005. ("rush" hours), north-eastern wind, speed 1.8 m/s	July 11, 2005 ("out-of- rush" hours), eastern wind, speed 1.8 m/s	January 30, 2006 ("rush" hours), north- western wind, speed 2.3 m/s	January 30, 2006 ("out-of –rush" hours), north-western wind, speed 2.5 m/s							
1	2 0.540 0.555	3	4	5							
1	0.540	0.380	0.132	0.128							
2	0.555	0.390	0.154	0.150							
4	0.590	0.430	0.398	0.385							
5	0.560	0.430 0.396	0.145	0.135							
6	0.600	0.420	0.145 0.152	0.141							
	0.650 0.588	0.420	0.143	0.135 0.185							
7 8	0.588	0.410	0.188	0.185							
10	0.600	0.420	0.185	0.185							
12	0.600	0.415	0.156	0.185							
12 13	0.601	0.423	0.320	0.248							
14	0.660	0.420	0.612	0.600							
15	0.592	0.410	0.283	0.279							
16 17	0.600	0.400	0.814	0.810							
17	0.570	0.400 0.425	0.136 0.725	0.129 0.719							
19	0 608	0.425	0.725	0.719							
20 21	0.508 0.573 0.574 0.575 0.575 0.575 0.576 0.587	0.403	0.140	0.135							
21	0.574	0.405	0.168	0.160							
22	0.575	0.401	0.800	0.645							
23	0.575	0.403	0.169	0.152							
24	0.576	0.404	0.165	0.152							
25	0.587	0.410	0.172	0.164							
26	0.375	0.402	0.133	0.130							
27	0.570 0.595 0.572	0.400	0.174	0.165							
28	0.595	0.412	0.182	0.182							
29	0.572	0.401	0.134	0.133							
31	0.590	0.412	0.176	0.168							
33	0.613	0.421 0.415	0.185	0.171							
34	0.594	0.415	0.190	0.175							
36	0.602	0.423	0.203 0.215	0.176							
37	0.601	0.421	0.215	0.192							
39	0.561	0.392	0.138	0.134							
40	0.572	0.402	0.138	0.135							

4. Analysis of simulation results

The results of simulation were received by simulating the process of transfer of the pollutants from linear pollutant sources, evaluating the background value of SP in the air. In Žvėrynas district the dispersion of this pollutant from maximum concentrations up to the entire initially prescribed amount of the pollutants in all the streets have a tendency to spread in the surrounding environment reaching the background concentration. The type of dispersion depends on the strength of the wind and direction.

Fig. 2 shows the results of SP concentration (mg/m³) simulation when the northeastern wind was blowing, and



Fig. 1. Žvėrynas map: a - map with 40 measuring points in the streets; b - streets marked within the digitized area

the speed wss 1.8 m/s measured using the "Phoenics " post-processor PHOTON.

It is accepted that SP background concentration is 0.05 mg/m^3 . The maximum prescribed concentration is at point 14 (at the exit from Hanner Business Center) (Municipality of Žvėrynas). It is equal to 0.660 mg/m^3 .

As it is seen from Fig. 2, SP concentration in the entire area of simulation varies from 0.05 mg/m^3 to 0.66 mg/m^3 . Higher levels of pollutant concentration (an intensive red colour) are observed in Narbutas st, Séliai st, at the roundabout near Hanner Business Center. In the remaining area SP concentration is nearly equal.

SP concentration of the streets gets lower in the direction of the northeastern wind. Within a distance of 150 m from the street the initial prescribed or calculated SP concentration is half-reduced. The end boundary of the transfer of the pollutant is about 300 m. Within such a distance from the street the prescribed SP concentration is dispersed in the surrounding area reaching the phonic one.

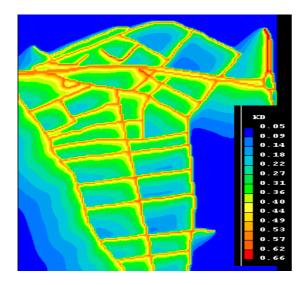


Fig. 2. Results of SP concentration dispersion on April 26, 2005 (during "rush" hours) in Žvėrynas district area

Taking into consideration the file of the results when solving the problem by means of "Phoenics" program, the values of SP concentrations are found. The results calculated theoretically as well as their comparison with the results of the experiment are presented in Table 2.

As the table shows, the results obtained both after theoretical investigation (using the mathematical simulation program "Phoenics") and experimental measuring differ by 1.8 % to 3.4 %.

Fig 3 presents the results of the simulation of dispersion of SP concentration (mg/m^3) , when the wind was blowing from the east within the speed of 1.8 m/s, by means of PHOTON post-processor. The prescribed SP background concentration is the same (0.05 mg/m³). The maximum prescribed concentration is at point 19 (Narbutas – Saltoniškės st crossroad). It is equal to 0.425 mg/m³.

As it is clearly seen from Table 3, the results theoretically calculated (applying the mathematical simulation program "Phoenics") and experimentally measured on July 11, 2005 ("out-of rush" hours) differ by 1.5 % to 4.3 %.

Fig. 4 shows SP dispersion concentration (mg/m³) simulation results at the north-western wind with a speed of 2.3 m/s, obtained with the help of PHOTON post-processor. It is accepted that SP background concentration at that time is lower because even the average SP concentration there is lower than in the cases mentioned above. The prescribed SP background concentration is equal to 0.01 mg/m³. The maximum prescribed concentration (0.814 mg/m³) is at point 16 (Kęstutis – Sėliai st crossroad).

From Fig. 4 it is possible to conclude that SP concentration within the whole area of simulation varies from the background value (0.01 mg/m^3) up to the maximum prescribed one (0.81 mg/m^3) . The dispersion of the investigated pollutant concentration decreases from the street in the direction of the northwestern wind movement (change of colour from red to blue is observed). SP concentration from the initial prescribed is reduced by half at about 120 m distance from the street and reaches the background value within 310 m distance from the street.

In this case it is possible to exclude clearly the location places of higher SP concentrations, namely, at the beginning of Narbutas st, Saltoniškės st section behind the crossing with Narbutas st, Sėliai st section up to the crossing with Kęstutis st and the section of Kęstutis st up to the crossing with Bebrai st as well as near the traffic route roundabout where there is a constant heavy traffic. A little lower SP concentrations are registered in Pieninė and Žalioji sts. In the remaining territory SP concentrations are very similar.

As it is seen from Table 4, the results, theoretically calculated (applying the mathematical simulation program "Phoenics") and experimentally measured on January 30, 2006 ("rush" hours), differ by 2.7 % to 5.8 %.

Fig. 5 shows the results of SP concentration dispersion (mg/m³), when the north-western wind was blowing with a speed of 2.5 m/s, after using PHOTON postprocessor. In this case the prescribed background concentration is also equal to 0.01mg/m³. The maximum prescribed SP concentration, as previously, is at point 16 (Kęstutis–Sėliai crossroad). It is equal to 0.810 mg/m³.

In Fig. 5 a very similar situation to that in Fig. 4 is seen. SP concentrations vary from an intensive red (0.81 mg/m^3) to intensive blue colour (the background is 0.01 mg/m^3). The dispersion of the concentration of the investigated pollutant is getting lower from the street in the direction of northwestern wind, SP pollutants decrease within 310 m distance from the initially prescribed value, namely, the concentration of SP is reduced up to the background value.

SP concentrations in the same zones were observed higher than in the remaining part of the simulation area (but lower than during "rush" hours), namely, at the beginning of Narbutas st, Saltoniškės st section behind the crossroad with Narbutas st, Sėliai st section up to the crossroad with Kęstutis st and in Kęstutis st section up to the crossroad with Bebrai st, near the traffic route roundabout.

The theoretically calculated results and their comparison with the experimental results are given in Table 5.

As it is seen from Table 5, the theoretically calculated results (applying the mathematical simulation program "Phoenics") and those obtained experimentally on January 30, 2006 ("out-of-rush" hours) vary by 2.7 % to 5.8 %.

Table 2. Comparison of the results obtained experimentally (on April 26, 2005) and theoretically

Points	3	9	12	18	30	32	35	38
Measured value, mg/m ³	0.560	0.600	0.600	0.602	0.583	0.570	0.562	0.559
Calculated value, mg/m ³	0.575	0.612	0.590	0.580	0.595	0.560	0.550	0.540
Error, %	2.7	2.0	3.3	2.0	2.1	1.8	2.1	3.4

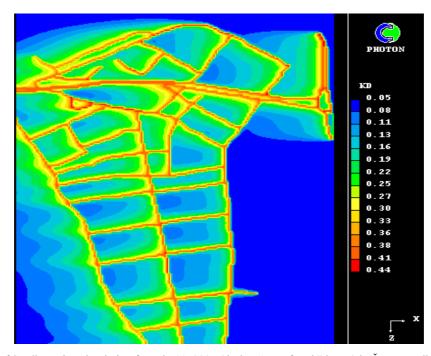


Fig. 3. Results of SP dispersion simulation for July 11, 2005 (during "out-of-rush" hours) in Žvėrynas district area

Table 3. Comparison of experimental results	(of July 11, 2005) and theoretical ones
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Points	3	9	12	18	30	32	35	38
Measured value, mg/m ³	0.410	0.422	0.415	0.424	0.410	0.400	0.393	0.390
Calculated value, mg/m ³	0.420	0.440	0.405	0.410	0.416	0.390	0.380	0.382
Error, %	2.4	4.3	2.4	3.3	1.5	2.5	3.3	2.1

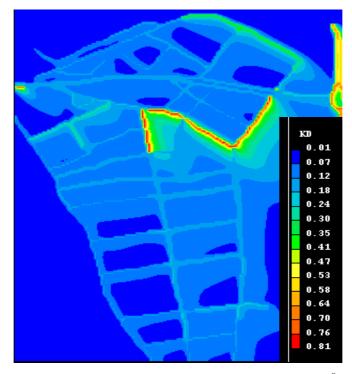


Fig. 4. Results of SP concentration dispersion on January 30, 2006 ("rush" hours) in Žvėrynas district area

Table 4. Comparison of experimental results (of January 30, 2006 during "rush" hours) and theoretically calculated ones

Points	3	9	12	18	30	32	35
Measured value, mg/m ³	0.159	0.314	0.156	0.223	0.185	0.140	0.139
Calculated value, mg/m ³	0.150	0.325	0.163	0.235	0.180	0.133	0.132
Error, %	5.7	3.5	4.5	5.4	2.7	5.0	5.0

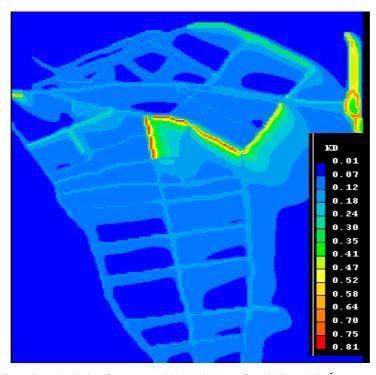


Fig. 5. Results of SP dispersion simulation for January 30, 2006 ("out-of rush" hours) in Žvėrynas district area

Table 5. Comparison of experimental results (of January 30, 2006 during "out-of -rush" hours) and theoretically calculated ones

Points	3	9	12	18	30	32	35
Measured value mg/m ³	0.143	0.214	0.185	0.221	0.185	0.140	0.135
Calculated value, mg/m ³	0.138	0.225	0.190	0.233	0.175	0.136	0.138
Error, %	3.5	5.1	2.7	5.4	5.4	2.9	2.2

Further using the previously described Algebraic Slip Model (ASM), the type of dispersion was evaluated at the randomly selected crossroad of Kęstutis–Latviai st, depending on the wind direction and strength as well as at the buildings located near the streets.

For simulation, the areas of Kęstutis–Latviai st, were digitized on different nets: $x \cdot y \cdot z = 40 \times 13 \times 36$, and enclosed 200 × 180 m² territory. According to the Žvėrynas map, on the digitized area there are marked parts of Kęstutis and Latviai st where it was required to prescribe SP concentrations (according to the results of experimental measurements of April 26, 2005). The buildings situated nearby are marked using blocked strips or groups of strips (Municipality of Žverynas), Fig. 6.

The direction and strength of the wind, air density and SP background concentration (0.05 mg/m^3) is prescribed at the entrance along the whole side of the area when the wind direction is northeastern.

The results of simulation were obtained by simulating SP pollutants from linear resources of pollutants, taking into consideration the background SP amount in the air. Dependence of dispersion type on the strength and direction of the wind as well as on the buildings, located near the streets, is presented in Fig. 6.

From the presented figure, one can see that the maximum SP concentration is observed at the roadway of the analysed Kestutis and Latviai streets. The pollutant concentration on the streets is getting lower in the direction of the northeastern wind moving up to the backg-

round one. The maximum SP concentration in this simulated area is equal to 0.58 mg/m^3 , the minimum is 0.05 mg/m^3 .

From Fig. 6 we can draw a conclusion that the buildings, located very close to the streets, comprise certain barriers against pollutant dispersion.

It is possible to draw a conclusion from Fig. 6 stating that the average SP concentration in the analysed Kęstutis–Latviai st area is equal to 0.212 mg/m³ (average value). The red-colour probe position exhibits SP concentration in that location (probe value) which is very close to the background and is equal to 0.055 mg/m³.

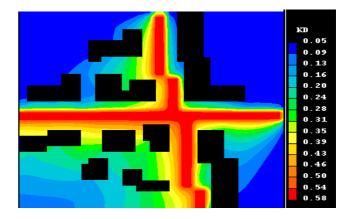


Fig. 6. Results of SP concentration simulation in Kęstutis–Latviai st sections

As it is seen from Fig. 6, SP concentration in the direction of pollutant dispersion (the northeastern wind direction) doesn't get lower than the background but is only 0.109 mg/m³ (at 116 m distance from the street). At the crossroad SP concentration is equal to 0.565 mg/m³. Within the distance of 30 m from the crossroad SP concentration decreases up to 0.238 mg/m³, but within the distance of 50 m it is reduced up to 0.156 mg/m³.

Due to the fact that during the experiment SP concentration was measured at Kęstutis–Latviai st crossroad, it is possible to compare the registered pollutant amount with the theoretically calculated one.

That is why the measured SP concentration at the crossroad of Kęstutis–Latviai st is 0.576 mg/m^3 , the theoretically calculated one is 0.565 mg/m^3 , the error is of 1.9 %. As the given data indicate, the error of 1.9 % is not great.

During the investigation (Baltrenas, Morkūnienė 2006) it was established that particles of 0.4 μ m size (0.1–1.0 μ m) are predominant in the air. The main influence for such a distribution is caused by motor vehicle flow which is predominant in comparison with other means of communication. Summarizing the modeling results, it can be said that the method used is the most suitable when the density of particles is from 2000 kg/m³ to 7880 kg/m³, and the diameter is from 0.3 μ m to 10.0 μ m.

5. Conclusions

1. The end of SP pollutants is at a distance of 300– 310 m in the direction of the prevailing wind, namely, within a distance the concentration of SP decreases up to the background.

2. In a warm season and during "rush" hours, the measured SP concentration distribution range fluctuated from 0.540 mg/m³ to 0.660 mg/m³, during the experiment, there were registered and theoretically simulated results varying from 1,8 % to 3.4 %. During "out-of-rush" hours, the measured SP concentration distribution range fluctuated from 0.380 mg/m³ up to 0.425 mg/m³, during the experiment, there were registered and theoretically simulated results correspondingly varying from 1.5 % to 4.3 %. The errors are not great, so the "Phoenics" Algebraic Slip Model satisfies and fits simulating a narrow dispersion of SP concentration.

3. In a cold season during "rush" hours, the range of measured SP concentration distribution fluctuated from 0.132 mg/m^3 to 0.814 mg/m^3 , during the experiment, there were registered and theoretically simulated results varying from 2.7 % to 5.8 %. During "out-of-rush" hours, the measured SP concentration distribution range fluctuated from 0.128 mg/m^3 to 0.810 mg/m^3 , during the experiment, there were registered and theoretically simulated results varying from 2.7 % to 5.8 %. The errors are not great, though a bit higher than those calcu-

lated, when simulating a narrower SP concentration dispersion.

4. When simulating SP dispersion at one of the selected crossroads, the experimentally measured and registered as well as theoretically simulated results varied by 1.9%. The simulation at the crossroad was carried out during a warm season the dispersion of measured SP, there was determined the error value similar to the errors, calculated by simulating the dispersion of SP in the entire area of Žvėrynas district.

References

- Baltrénas, P; Špakauskas, V.; Vaitiekūnas, P. 1998. An analysis of heavy aerosols dispersion, *The PHOENICS Journal of Computational Fluid Dynamics & Its Applications* 11(3): 284–292.
- Baltrénas, P; Masilevičius, R. 2004. Investigation of the properties of solid particle emissions into the environment in the wood-burning process, *Geochemistry International*, "Interperiodika". Moscow, 42(9): 887–891.
- Baltrénas, P.; Kvasauskas, M. 2005. Experimental investigation of particle concentration using mass and optical methods, *Journal of Environmental Engineering and Landscape Management* 12(2): 57–64.
- Baltrénas, P.; Morkūnienė, J. 2006. Investigation of particulate matter concentration in the air of Žvérynas district of Vilnius, *Journal of Environmental Engineering and Landscape Management* 14(1): 23–30.
- Hjertager, B. H.; Mathiesen, V.; Solberg, T. 1998. Computational analysis of some Fluidized Systems, in *Proceedings* of Advanced Technologies for Particle Processing, AIChE. II, 462–468.
- Interphase Slip Algorithm. Available from Internet: http://www.cham.co.uk/phoenicsd_polis/d_lecs/ipsa.htm>.
- Mathiesen, V.; Solberg, T. 1999. Gas/Particle two-phase flow modelling of a circulating fluidized bed using kinetic theory for granular flow, *The PHOENICS Journal Computatio-nal Fluid Dynamics & Its Applications* 12(2): 111– 157.
- Municipality of Žvėrynas. Available from Internet: http://www.vilnius.lt/new/vadovybe.php?open=637&mid={lt;3;82}>.
- Petraitis, E.; Vasarevičius, S. 2001. Numerical modeling of solid particle dispersion in the atmosphere using the programs "Varsa" and "Phoenics", *Aplinkos inžinerija* [Environmental Engineering] 9(1): 23–28.
- Scalar Equation Method. Available from Internet: http://www.simuserve.com/phoenics/d_polis/d_lecs/semlec.htm>.
- The Algebraic Slip Model. Available from Internet: http://www.simuserve.com/phoenics/d_polis/d_lecs/asml ec.htm>.
- Vaitiekūnas, P.; Petkevičienė, J.; Katinas, V. 1998. A numerical simulation of three-dimensional hydrothermal processes in a cooling pond, *The PHOENICS Journal of Computational Fluid Dynamics & Its Applications* 11(3): 348–354.
- Vilnius Buildings. Žvėrynas. Available from Internet: http://www.paveldas.vilnius.lt/gatves.php?ID=12>.

KIETŲJŲ DALELIŲ DISPERSIJOS ORE VILNIAUS MIESTE MATEMATINIS MODELIAVIMAS

P. Baltrėnas, J. Morkūnienė, P. Vaitiekūnas

Santrauka

Oro kokybei vertinti taikytas teršalų sklaidos ore matematinis modeliavimas. Kietųjų dalelių (KD) dispersijai ore modeliuoti taikytas PHOENICS programinės įrangos paketas, kuris duoda artutinius skaitinius pernašos lygčių sprendinius, nes tikslūs analiziniai sprendiniai yra negalimi. Programa naudota Vilniaus miesto Žvėryno rajone, kurio daugelyje vietų naudotos tikslios (eksperimentinės) KD koncentracijų reikšmės.

Pateikta kietujų dalelių dispersijos ore matematinio modeliavimo metodika taikant algebrinės šlyties metodą, naudotos bazinės pernašos procesų lygtys. Kaip KD pradinės sąlygos miesto gatvėse naudoti eksperimentiniai duomenys (KD koncentracijos reikšmės) ir, gautus duomenis panaudojant PHOENICS matematinio modeliavimo programoje, gauta KD koncentracijos dispersija aplinkoje. Rezultatai pateikti paveiksluose ir lentelėse, jie palyginti su eksperimentiniais rezultatais.

Reikšminiai žodžiai: matematinis modeliavimas, algebrinės šlyties metodas, skaliarinių lygčių metodas, kietųjų dalelių dispersija.

МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ РАСПРЕДЕЛЕНИЯ ФРАКЦИЙ ТВЕРДЫХ ЧАСТИЦ В ВОЗДУХЕ ГОРОДА ВИЛЬНЮСА

П. Балтренас, Ю. Моркунене, П. Вайтекунас

Резюме

Для оценки качества воздуха применено математическое моделирование распределения загрязнений в воздухе. Для моделирования распределения фракций твёрдых частиц применен пакет программного обеспечения PHOENICS, позволяющий решать артутивные числовые уравнения переносов, так как точные аналитические решения невозможны. Программа применена для района Жверинас города Вильнюса, в котором в ряде мест использованы точные (экспериментальные) значения концентраций твердых частиц.

Применена методика математического моделирования распределения фракций твердых частиц в воздухе с применением метода алгебраического сдвига (МАС). В модели применены уравнения процессов базовых переносов. Первоначальные условия распределения твердых частиц на улицах города получены из экспериментальных данных (значений концентраций твердых частиц). С помощью программы математического моделирования PHOENICS получено распределение фракций твердых частиц в воздухе. Результаты, представленные на рисунках и таблицах, сравнены с экспериментальными данными.

Ключевые слова: математическое моделирование, метод алгебраического сдвига, метод скалярных уравнений, фракции твердых частиц.

Pranas BALTRENAS. Dr Habil, Prof and head of Dept of Environmental Protection, Vilnius Gediminas Technical University (VGTU).

Doctor Habil of Science (air pollution), Leningrad Civil Engineering Institute (Russia), 1989. Doctor of Science (air pollution), Ivanov Textile Institute (Russia), 1975. Employment: Professor (1990), Associate Professor (1985), senior lecturer (1975), Vilnius Civil Enginering Institute (VISI, now VGTU). Publications: author of 13 monographs, 24 study - guides, over 320 research papers and 67 inventions. Honorary awards and membership: prize-winner of the Republic of Lithuania (1994) a corresponding Member of the Ukrainian Academy of Technological Cybernetics, a full Member of International Academy of Ecology and Life Protection. Probation in Germany and Finland. Research interests: air pollution, pollutant properties, pollution control equipment and methods.

Jurgita MORKŪNIENĖ. Master student (environmental protection engineering), Dept of Environmental Protection, Vilnius Gediminas Technical University (VGTU).

Bachelor of Science (environmental engineering), VGTU, 2004. Research interests: environmental protection, air pollution.

Petras VAITIEKŪNAS. Dr Habil, Prof, Dept of Environmental Protection, Vilnius Gediminas Technical University (VGTU).

Doctor Habil of Science (energy and thermal engineering), 1999. Doctor of Science, Lithuanian Energy Institute, 1972. Employment: Professor (2002); Associate Professor (1997). Publications: author of 2 monographs, over 190 scientific publications. Membership: a corresponding member of International Academy of Ecological and Life Protection Sciences. Research interests: hidrodynamics, convective heat transfer and thermophysics, computational fluid dynamics, modelling transfer processes in the environment. Research interests: air pollution, pollutant properties, pollution control equipment and methods.