

Simulating the Dynamics of Distribution of Hazardous Substances Emitted by Motor Engines in a Residential Quarter

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Abstract—This article is dedicated to development of mathematical models for determining the dynamics of concentration of hazardous substances in urban turbulent atmosphere. Development of the mathematical models implied taking into account the time-space variability of the fields of meteorological items and such turbulent atmosphere data as vortex nature, nonlinear nature, dissipativity and diffusivity. Knowing the turbulent airflow velocity is not assumed when developing the model. However, a simplified model implies that the turbulent and molecular diffusion ratio is a piecewise constant function that changes depending on vertical distance from the earth surface. Thereby an important assumption of vertical stratification of urban air due to atmospheric accumulation of hazardous substances emitted by motor vehicles is introduced into the mathematical model. The suggested simplified non-linear mathematical model of determining the sought exhaust concentration at a priori unknown turbulent flow velocity through non-degenerate transformation is reduced to the model which is subsequently solved analytically.

Keywords—Urban ecology, time-dependent mathematical model, exhaust concentration, turbulent and molecular diffusion, airflow velocity.

I. INTRODUCTION

ANTHROPOGENIC pollution of atmospheric and aquatic urban medium pertains to ecologic problems. Atmospheric air pollution is one of the most vexed ecological problems accompanied by a number of adverse effects. Among anthropogenic emissions into the atmosphere, the following substances are the most dangerous: carbon dioxide, sulfur and nitrogen oxides (nitrogen dioxide, sulfur dioxide), metal dust, carbon monoxide, ozone, aldehydes, lead, phenol etc. The motor transport is ranking first in the list of principal anthropogenic sources of pollution of urban atmospheric air in large cities of the world. A moving motor vehicle emits jet-shaped exhaust gases into the environment. At the expense of gas diffusion, the exhaust gases are mixed up and re-distributed in space. As to the urban atmosphere – it is a complex dynamic system featuring various inherent physico-chemical processes, the intensity of which depends on specific characteristics of the city concerned.

To describe these complex turbulent atmospheric processes, one needs to develop a complex symbolic model that would allow one to solve a broad spectrum of problems

in the field of environmental protection. Such a model should include:

- 1) The model of hydro-thermodynamics of urban and/or regional turbulent atmospheric processes;
- 2) Models taking into account kinetic processes, condensations, coagulations as well as mass exchange processes on the gas-particle phase;
- 3) Transfer and diffusion equations for gas-borne particles (and aerosols) in the atmosphere of a city and/or region, - taking into account photochemical and other transformation.

The investigation of ecological problems of such kind does not differ fundamentally from the solution of other tasks pertaining to natural sciences. A specific feature of ecological problems is, first, an extreme uncertainty of problem setting and – secondly – the complex character of the task implying the necessity of taking into account heterogeneous factors as it was shown above. According to engineering practice, the error in estimation and calculation of urban air contamination levels may come up to hundreds per cent.

II. THE PROBLEMS OF THE EXISTING SYMBOLIC MODELS

The majority of the modern systems of dynamics and kinetics of atmospheric disperse systems (see [1-9] and the corresponding literature therein) is described by multivariate nonlinear partial differential equations, - and the solution of problems of such class may be obtained only roughly - through approximation of initial differential problem by finite-dimensional model.

In general, the research methodology for urban ecological problems looks as follows:

- Formalization of concepts “environment”, “environmental quality” and other concepts of the specific subject;
- Formulation of environmental criteria;
- Detection, more precise definition, and investigation of the main factors rendering impact on the life of urban population from the ecological standpoint;
- Development of methods of monitoring and integral assessment of environmental quality;
- Development of a well-founded scientific concept of urban environmental quality control and a possibility of a short-term or a long-term prediction.

Currently, the most widely-used models are the ones based on the mathematical statistics apparatus. The usage of

the mathematical statistics apparatus as well as other mathematical apparatuses implying the model development based on results of single shots and integral measurements of environmental quality, - in particular, urban atmospheric air, - and determination of the dynamics of concentration of exhaust gases in urban atmospheric air is connected with the problem of measurement accuracy. Namely, single shots of pollutant concentration in urban atmospheric air have a low-accuracy level. If one improves accuracy by increasing measurement rate – the condition of urban atmospheric air can not be inferred after single shots – especially, under the dynamic circumstances of urban environment. Consequently, to estimate the quality of urban atmospheric air, one can not be content with the accuracy of integral criteria, indices, and indicators. Moreover, it seems impossible to place measurement instrumentation at each point of the city; therefore, one has to restore the general picture of atmospheric air contamination, taking as a basis the measurements made at single points, with the help of interpolation models. So far, such interpolation models have not been developed to the extent of a wide practical usage. Therefore, to apply the mathematical statistics apparatus for atmospheric air monitoring, one selects the method of construction of fixed automated control points exercising control over the quality of atmospheric air, -supplementing those by mobile inspection facilities.

III. FORMALIZATION OF THE PROBLEM OF DETERMINATION OF EXHAUST GASES DYNAMICS IN THE TURBULENT ATMOSPHERE OF URBAN AIR

Let the set vector $X(t) = \{x_1(t), x_2(t), \dots, x_n(t)\}$ characterize the air medium condition at a given point of three-dimensional space t , where $x_j(t)$; $j = \overline{1, N}$ determines the concentration of j -th substance. We assume that, at a certain moment of time t_e the air medium condition can be derived from the functional equation $X^*(t_e) = F[X(t_i), i = \overline{1, k}; Y^*(t_1, \dots, t_k; t_e); Z^*(t_1, \dots, t_k; t_e)]$, where F – is a composed function. $X(t_1), X(t_2), \dots, X(t_k)$ – characterizing vectors the condition of air medium at the investigated point at the time points t_1, t_2, \dots, t_k , preceding t_e , t.e. $t_e > t_i, i = 1, 2, \dots, k$. $Y^*(t_1, \dots, t_k; t_e)$ – vector of controlled parameters describing the characteristics of external medium affecting airborne pollutant concentration – primarily, the weather conditions (air temperature, wind direction and speed) etc. $Z^*(t_1, \dots, t_k; t_e)$ – vector of external medium parameters controlled fully or partially, the regulation of which also influences the airborne concentration of substances - like for instance, traffic intensity, vehicle types etc. Generally, the problem of operating management of transportation flows and planning of urban housing and laying new motorways – is set as follows: given the sets as follows: $Y^*(t_1, \dots, t_k; t_e)$ и $Z^*(t_1, \dots, t_k; t_e)$ it is required to estimate the airborne harmful substances concentration $X(t_e)$ in the investigated filed of the urban airspace, - and, given the concentration of i -th substance exceeds the admissible level x_i^{\max} - one has to change the controlled

parameters $Z^*(t_1, \dots, t_k; t_e)$ so that elements of the set $X^*(t_e)$ would be admissible, - i.e., the concentration levels $x_j(t_e)$ would be within tolerable limits: $x_j(t_e) \leq x_j^{\max}, j = 1, 2, \dots, n$.

One should note that calculation according to the above-stated functional relationship should be performed with respect to different alternatives of the external medium condition $Y^*(t_1, \dots, t_k; t_e)$; besides, the corresponding managerial solutions will be defined for each alternative. The totality of these solutions allows one to formulate the urban traffic system control strategy and to bring forward proposals concerning its development.

IV. STATEMENT OF NON-STATIONARY SYMBOLIC MODEL OF DETERMINATION OF EXHAUST GASES CONCENTRATION IN URBAN ATMOSPHERE

One has to determine concentrations $C^{(n)}(x_1, x_2, x_3, t)$ n -го ($n = \overline{1, N}$) of a harmful substance at any spatial point (x_1, x_2, x_3) of the field $[0, l_1] \times [0, l_2] \times [0, l_3]$ at any instant of time $t \in [0, T]$ from the following equation:

$$\frac{\partial C^{(n)}(x, t)}{\partial t} = \operatorname{div} \left(D(\bar{\vartheta}(x, t)) \cdot \overline{\operatorname{grad}} C^{(n)}(x, t) \right) - \bar{\vartheta}(x, t) \cdot \overline{\operatorname{grad}} C^{(n)}(x, t),$$

$$t \geq 0, x = (x_1, x_2, x_3): 0 < x_i < l_i \quad (i = \overline{1, 3});$$

from the initial condition

$$C^{(n)}(x, t) \Big|_{t=0} = C_0^{(n)}(x), \quad x = (x_1, x_2, x_3): 0 \leq x_i \leq l_i \quad (i = \overline{1, 3});$$

from boundary conditions (at each fixed $j = \overline{0, M-1}$)

$$\gamma_{i,1,j}^{(n)} \cdot \frac{\partial C^{(n)}(x, t)}{\partial x_i} \Big|_{x_i=a_{i,j}} - \gamma_{i,2,j}^{(n)} \cdot C^{(n)}(x, t) \Big|_{x_i=a_{i,j}} =$$

$$= C_{i,j}^{(n)}(x/\{x_i\}, t), \quad a_{i,j} \leq x_i \leq b_{i,j} \quad (i = \overline{1, 3}), \quad t \geq 0,$$

$$\gamma_{i,3,j}^{(n)} \cdot \frac{\partial C^{(n)}(x, t)}{\partial x_i} \Big|_{x_i=b_{i,j}} + \gamma_{i,4,j}^{(n)} \cdot C^{(n)}(x, t) \Big|_{x_i=b_{i,j}} =$$

$$= C_{i,j}^{(n)}(x/\{x_i\}, t), \quad a_{i,j} \leq x_i \leq b_{i,j} \quad (i = \overline{1, 3}), \quad t \geq 0,$$

from conjugating conditions

$$C^{(n)}(x, t) \Big|_{x_3=l_3^{(j)}-0} = C^{(n)}(x, t) \Big|_{x_3=l_3^{(j)}+0},$$

$$j = \overline{1, M-1}, \quad 0 \leq x_i \leq l_i \quad (i = 1, 2),$$

$$D(\bar{\vartheta}(x, t)) \cdot \frac{\partial C^{(n)}(x, t)}{\partial x_3} \Big|_{x_3=l_3^{(j)}-0} = D(\bar{\vartheta}(x, t)) \cdot \frac{\partial C^{(n)}(x, t)}{\partial x_3} \Big|_{x_3=l_3^{(j)}+0},$$

$$j = \overline{1, M-1}, \quad 0 \leq x_i \leq l_i \quad (i = 1, 2).$$

In the non-stationary initial boundary task (1)-(6), the expression $D(\bar{\vartheta}(x, t))$ is used to denote the turbulent and molecular diffusion ratio, which is supposed to be a piecewise constant function of the kind

fourth stratum) is equal to 24 meters which corresponds to the averaged height of buildings in Riga.

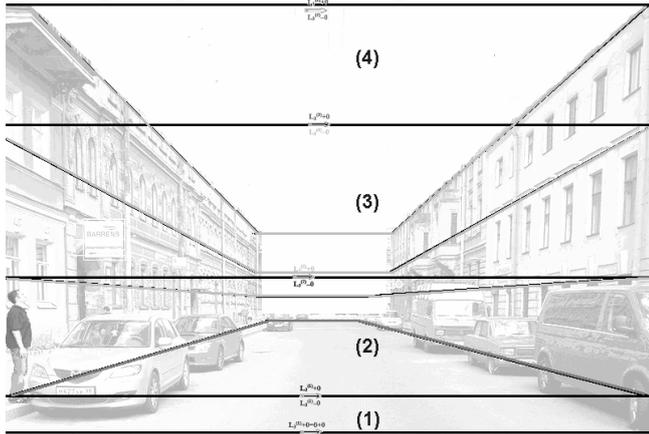


Fig.2 Stratified area of the simulated section of city road with motor traffic

Remark 2. In the formulated model (1)-(15) the boundary conditions (3)-(4) are mixed-type conditions, namely:

- For the first (low-earth) stratum:

$$0+0=l_3^{(0)}+0 \leq x_3 \leq l_3^{(1)}-0$$

- on the parallelepiped wall

$\{x_1=0+0, 0 \leq x_2 \leq l_2, 0 \leq x_3 \leq l_3^{(1)}\}$, perpendicular to the axis OX_1 at the point $x_1=0+0$ (that is, on the wall simulating the beginning of the section concerned), and

- on the wall $\{x_1=l_1-0, 0 \leq x_2 \leq l_2, 0 \leq x_3 \leq l_3^{(1)}\}$

perpendicular to the axis OX_1 at the point $x_1=l_1-0$ (i.e. on the wall simulating the end of the section concerned), - the boundary conditions are set as the third-kind conditions (that is to say, the Newton's conditions);

- On two other walls perpendicular the axis OX_2 at the points $x_2=0+0$ and $x_2=l_2-0$ (i.e., on the walls simulating buildings at the two waysides of the road concerned) - boundary conditions are set as the second-kind conditions (i.e., Neumann conditions);

- For all of the other strata $l_3^{(1)}+0 \leq x_3 \leq l_3-0$ on all the walls of the parallelepiped, the boundary conditions are set as the first-kind conditions (i.e., Dirichlet conditions).

Depending on what kind of instrumentation and technical facilities are owned by experimentalists (i.e., the experts measuring concentration of harmful substances) to fulfill the initial condition and the boundary conditions in the model suggested, - some other boundary conditions which may be more advantageous from the experimentalist's point of view can be examined instead of the boundary conditions (3) - (4). For example, if, instead of the formulas (7), (14) - (15), we write the following, respectively:

$$a_{i,j} = \begin{cases} 0 & \text{if } i=1,2; \\ l_3^{(j)} & \text{if } i=3; j \neq 0; \\ l_3^{(0)} = 0 & \text{if } i=3; j=0, \end{cases}$$

$$b_{i,j} = \begin{cases} l_i & \text{if } i=1,2; \\ l_3^{(j+1)} & \text{if } i=3, \end{cases} \quad (16)$$

$$\gamma_{i,k,j}^{(n)} = \begin{cases} \gamma_{i,k,j}^{(n)} > 0 & \text{if } j \neq 0, \forall i,k; \\ 0 & \text{if } j=0, k=1,3, \forall i; \\ -1 & \text{if } j=0, k=2, \forall i; \\ 1 & \text{if } j=0, k=4, \forall i, \end{cases} \quad (17)$$

$$C_{i,j}^{(n)}(\square t) = \begin{cases} C_{i,j}^{(n)}(\square t) \neq 0 & \text{if } j=0; \\ 0 & \text{if } j \neq 0, \forall i, \end{cases} \quad (18)$$

•for the first layer (the low-earth level) $0+0=l_3^{(0)}+0 \leq x_3 \leq l_3^{(1)}-0$ on all of the parallelepiped walls, the boundary conditions are set as the first-kind conditions (i.e. Dirichlet conditions);

•for all the rest of the layers $l_3^{(1)}+0 \leq x_3 \leq l_3-0$ on all of the parallelepiped walls the boundary conditions are set as third-kind conditions (i.e. Newton's conditions).

If, instead of the formulas (7), (14)-(15) we write, respectively,

$$a_{i,j} = \begin{cases} 0 & \text{if } i=1,2; \\ l_3^{(j)} & \text{if } i=3; j \neq 0; \\ l_3^{(0)} = 0 & \text{if } i=3; j=0, \end{cases}$$

$$b_{i,j} = \begin{cases} l_i & \text{if } i=1,2; \\ l_3^{(j+1)} & \text{if } i=3, \end{cases} \quad (19)$$

$$\gamma_{i,k,j}^{(n)} = \begin{cases} \gamma_{i,k,j}^{(n)} > 0 & \text{if } i \neq 1, \forall j,k; \\ 1 & \text{if } i=1, k=1,3, \forall j; \\ 0 & \text{if } i=1, k=2,4, \forall j, \end{cases} \quad (20)$$

$$C_{i,j}^{(n)}(\square t) = \begin{cases} C_{i,j}^{(n)}(\square t) \neq 0 & \text{if } \{j=0\} \wedge \{i=2,3,5,6\}; \\ 0 & \text{otherwise,} \end{cases} \quad (21)$$

Thereby we define the boundary conditions (3)-(4) of another character, namely -

• for all the strata $0=l_3^{(0)}+0 \leq x_3 \leq l_3$ on the walls, perpendicular to the axis OX_1 at points $x_1=0+0$ (i.e. at the walls simulating the beginning of the section concerned) и $x_1=l_1-0$ (i.e. on the walls simulating the end of the section concerned), the boundary conditions are set as second-kind conditions (i.e. by Neumann condition);

For all the strata $0=l_3^{(0)}+0 \leq x_3 \leq l_3$ on all the rest of the walls perpendicular to the axis OX_2 at the points $x_2=0+0$ и $x_2=l_2-0$ (i.e. on the walls simulating buildings at the sideways of the road concerned), - the boundary conditions are set as the third-kind conditions (i.e. the Newton conditions);

If, instead of the formulas (7), (14)-(15) we write accordingly:

$$a_{i,j} = \begin{cases} 0 & \text{if } j=0, i=\overline{1,3}; \\ 0 & \text{if } j \neq 0, i=1,2; \\ l_3^{(j)} & \text{if } j \neq 0, i=3, \end{cases}$$

$$b_{i,j} = \begin{cases} l_i & \text{if } i=1,2, \forall j; \\ l_3^{(j+1)} & \text{if } i=3, \forall j, \end{cases} \quad (22)$$

$$\gamma_{i,k,j}^{(n)} \in \square_+^1 \quad (i=\overline{1,2}; k=\overline{1,4}; j=\overline{0, M-1})$$

predetermined numbers; (23)

$$C_0^{(n)}(x), C_{i,j}^{(n)}(\square, t) \quad (i=\overline{1,6}; j=\overline{0, M-1})$$

predetermined functions. (24)

Thereby, we define the boundary conditions (3) – (4) of another character, - namely, with respect to all the strata on all the parallelepiped walls, - the boundary conditions are set only as third-kind conditions (i.e. by Newton conditions). It is obvious that, in this case, the boundary conditions are not mixed-type conditions, and some more complex and more accurate measurements are required to provide for their feasibility.

Some other types of boundary conditions are possible. In this work, the boundary conditions (3) – (4) are set by the formulas (7), (14) – (15); further, however, the obtained results may be quite easily distributed for symbolic models (1) – (6), (8) – (13) as well, - where the boundary conditions with respect to the sought concentration $C^{(n)}(x_1, x_2, x_3, t)$ are determined either by formulas (16)-(18) or formulas (19)-(21), or by formulas (22)-(24).

In conclusion of this remark, it is not out of place to remind that in the case where the boundary condition relative to concentration is set as Dirichlet condition, - it is required to measure the concentration proper at the corresponding boundary (on the surface, on the wall); when the boundary condition is set as Neumann condition – one has to measure not the concentration itself but rather “the flow” of concentration at the corresponding boundary of the area; if, however, the boundary condition is set as Neumann condition, it is required to measure concentration taking into account the molecular diffusion transfer to the environment, which is a more complicated measuring process requiring the appropriate engineering means and possibilities.

On finishing nontrivial calculations, the final formula was obtained for a 3D-symbolic model (1) – (15) of unambiguous definition of concentration $C^{(n)}(x_1, x_2, x_3, t)$ n -го ($n=\overline{1, N}$) of harmful substance in the urban atmospheric air.

V. EXAMPLE OF RESULTS

Let's consider the example of calculation of concentration change of harmful substance on a different height above the road area at the initiation fixed time moments 1, 2, 6 and 12 hours, respectively. We consider the road section with the width of 21 m and the length of 165 m (Fig.3). It is supposed that there are multistory buildings in both sides of considered road, at that the average height of buildings is 20 m. Besides, we assume that the number of cars driving through the road section per 12 hours is known

Vol:5, No:5, 2011 to 11000 units, i.e. the traffic flow rate in the considered road is accepted as equally distributed, namely, it equals to 917 cars/hour approximately. Other initial data are following: depending on the altitude wind velocity on layers changes from 4 m/s till 1 m/s; the coefficient of turbulent diffusion depends on altitude and it changes from 0.13 (highest) to 0.16 (lowest); average concentration of the investigated harmful substance (as investigated material is taken CO₂ particularly) is assumed as 179 g/km; exhaust speed near cars is 60-100 m/s.



Fig. 3 the city block of K. Valdemar Street of Riga (Latvia)

Computations will be performed for an "imaginary vertical column", the foundation of which is exactly in the middle of the considered road and it is determined for the point $(x_1 = 10.5 \text{ m}; x_2 = 82.5 \text{ m})$. Numerical implementation of considered mathematical model has been realized by the packaged MathCAD. The results of calculations for the different moments of time, passing after the beginning of turbulent diffusion process, are presented in Figure 4.

Figure 4a shows a change of concentration $C(x_1 = 10.5, x_2 = 82.5, x_3, t = 1)$ depending on the variable x_3 , i.e. the constructed curve reflects a change of harmful substance concentration depending on a height x_3 in 1 hour after the beginning of process of supervision of harmful substance turbulent diffusion in the fixed point of the road area $(x_1 = 10.5 \text{ m}; x_2 = 82.5 \text{ m})$.

Changes of concentration depending on a height in the same point at the moments 2, 6 and 12 hours after the beginning of turbulent diffusion process are presented in Figure 4b, 4c and 4d, respectively. Note that in Figure 4a scale of ordinates is compressed 10^2 times less, and in the other figures scales of ordinates are taken 10 times less, i.e. there is the graph of function $C(x_3) = 10^{-2} \cdot C(x_1, x_2, x_3, t) \Big|_{x_1=10.5; x_2=82.5; t=1}$ in Figure 1a, and there are the graphs of functions $10^{-1} \cdot C(x_1, x_2, x_3, t) \Big|_{x_1=10.5; x_2=82.5; t=2}$, $10^{-1} \cdot C(x_1, x_2, x_3, t) \Big|_{x_1=10.5; x_2=82.5; t=6}$ and

$10^{-1} \cdot C(x_1, x_2, x_3, t) \Big|_{x_1=10.5; x_2=82.5; t=12}$ in Figures 4b, 4c and 4d, respectively [10].

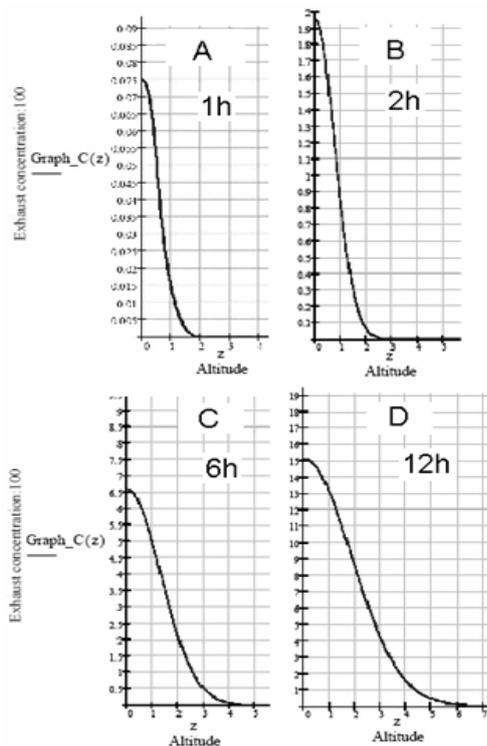


Fig.4 Change of the concentration of harmful matter on a different height above a road area

Let's note that this example considered by authors has illustrative character, because the solving of the offered mathematical model with respect to the considered example has been executed under some simplifying assumptions. For wide application of the offered mathematical model in practical questions it is necessary to develop more complex program using the high-level language.

VI. CONCLUSION

In this work, a scientific approach to monitoring the urban air pollution brought about by transportation vehicles.

A simplified 3D-symbolic model for determination of the dynamics of harmful substances concentration in stratified turbulent atmosphere of a city is proposed, with the basic requirement that the turbulent atmospheric air flow velocity is not preset a priori.

The results of the investigations performed in this work may be used when solving urgent issues of organizing road traffic within residential blocks in cities.

The models proposed and investigated in this work can be used in process of prospective planning of the city development when designing new blocks as well as constructing new motorways.

ACKNOWLEDGMENT

The article is written with the financial assistance of European Social Fund. Project Nr. 2009/0159/1DP/1.1.2.1.2/09/IPIA/VIAA/006 (The Support in Realisation of the Doctoral Programme "Telematics and

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