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Uhnenko Ye.B., Dr. Tech. Sci., **Uzhviieva O.M.,** Cand. Eng. Sci. (Ph.D.)

MATHEMATICAL MODELING OF POLLUTION PRODUCED BY MOTOR VEHICLES UNDER CONDITIONS OF HUMAN SETTLEMENTS

Abstact. The paper presents a mathematical model to describe the process of heat and mass transfer, and the calculation of velocity fields, temperature and concentrations of contaminants in the vicinity of roads, surrounded by buildings. Methods of predicting the distribution of contaminants released during the operation of vehicles can be used when planning the construction of roads and placing various buildings in their proximity.
Key words: forecasting methods, road transport, localities, differential equation.

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Угненко Є.Ю., д-р техн. наук, **Ужвієва О.М.,** канд. техн. наук

МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ ЗАБРУДНЕННЯ, СТВОРЮВАНОГО ВИКИДАМИ АВТОТРАНСПОРТНИХ ЗАСОБІВ В УМОВАХ НАСЕЛЕНИХ ПУНКТІВ

Анотація. У роботі наведена математична модель для опису процесу тепло- і масопереносу і розрахунку полів швидкості, температури і концентрацій забруднюючих речовин у придорожньому просторі населених пунктів. Методи прогнозу-вання розподілу забруднюючих речовин, що виділяються при роботі автотранспорту, можуть бути використані при плануванні будівництва автомобільних доріг і розміщенні поблизу них будівель та споруд.

Ключові слова: методи прогнозу, автомобільний транспорт, малі населені пункти, диференційне рівняння.

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Угненко Є.Ю., д-р техн. наук, **Ужвієва А.М.,** канд. техн. наук

МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ ЗАГРЯЗНЕНИЯ, СОЗДАВАЕМОГО ВЫБРОСАМИ АВТОТРАНСПОРТНЫХ СРЕДСТВ В УСЛОВИЯХ НАСЕЛЕННЫХ ПУНКТОВ

Аннотация. В работе представлена математическая модель для описания процесса тепло- и массопереноса и расчета полей скорости, температуры и концентраций загрязняющих веществ в придорожной полосе населенных пунктов. Методы прогнозирования распределения загрязняющих примесей, выделяющихся при работе автотранспорта, могут быть использованы при планировании строительства автомобильных дорог и размещении вблизи зданий и сооружений.

Ключевые слова: методы прогноза, автомобильный транспорт, малые населенные пункты, дифференциальное уравнение.

Formulation of the problem

As a result of motor vehicle operation gaseous and condensed products, such as carbon and nitrogen oxides, hydrocarbons, carbon black, lead, and others are emitted into the environment of human settlements. In addition, in the surface layer during the photochemical reaction there is formed ozone, nitrogen oxides and other hazardous to human health and the status of flora and fauna toxicants. Under certain weather conditions even minor traffic flows may create unfavorable environmental conditions in human settlements. For the design and construction of roads it is necessary to assess the environmental pollution, taking into account the above factors, as well as the topography, the nature of development, the presence of forests, traffic and the percentage composition of the traffic flow. We must also consider the resulting impact of environmental pollution from vehicles and other sources, such as industrial enterprises. As a result of analysis of existing models of pollution from motor vehicles in the framework of continuum mechanics there is given a mathematical model [1], based on the solution of equations for the turbulent diffusion of gaseous and condensed toxicants. This takes into account the wind direction and speed, the ambient temperature and the resulting movement of heated product emissions from motor vehicles over the roadway, as well as the terrain. With this approach it is possible to include additional factors to be taken into account in the calculation of environmental pollution. Using the laws of continuum mechanics [2] there is set the boundary value problem for the description of heat and mass transfer of pollutants in the vicinity of the highway.

Let us consider the plane problem of convective heat and mass transfer of pollutants from motor vehicles. The road is modeled by the surface source of weight of hot substances emitted by motor vehicles. It is believed that:

– the flow is developed turbulent;

– the density of the gas phase is not dependent on pressure as the flow velocity is significantly less than the speed of sound;

– to describe the convective transport under the influence of wind and gravity, two-dimensional Reynolds equations for a turbulent flow are used. The reference point $x_1 = 0$, $x_2 = 0$ is located in the center of the road, axis Ox_1 is facing right parallel to the Earth's surface perpendicular to the road in the direction of the wind, axis Ox_2 - upward. (Fig. 1).

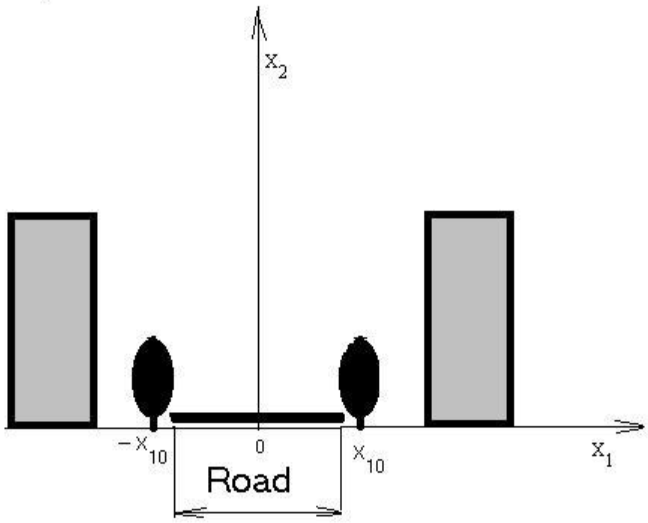


Figure 1 – Scheme of the pollution process from motor vehicles in the urban canyon

The formulated problem reduces to the solution of the following equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho v_j) = \dot{m}, \; j = 1,2, \; i = 1,2; \qquad (1)$$

$$\rho \frac{dv_i}{dt} = -\frac{\partial P}{\partial x_j} + \frac{\partial}{\partial x_j}(-\rho \overline{v_i' v_j'}) - \rho s c_d v_i |v| - \rho g_i - \dot{m} v_i, \quad (2)$$

$$\rho c_p \frac{dT}{dt} = \frac{\partial}{\partial x_j}(-\rho c_p v' \overline{v_i' T'}) + q_5 R_5 - \alpha_v (T - T_s) + c_p (T_s - T) Q + k(c U_R - 4\chi\sigma T^4), \quad (3)$$

$$\rho \frac{dc_\alpha}{dt} = \frac{\partial}{\partial x_j}(-\rho \overline{v_j' c_\alpha'}) + R_{5\alpha} - \dot{m} c_\alpha, \; \alpha = 1, 4, \quad (4)$$

$$\sum_{\alpha=1}^{5} c_\alpha = 1, \; P_e = \rho_5 R T \sum_{\alpha=1}^{5} \frac{c_\alpha}{M_\alpha}, \quad \vec{v} = (v_1, v_2), \quad \vec{g} = (0, g). \quad (5)$$

The initial and boundary conditions are as follows:

$$t = 0 : v_1 = 0, v_2 = 0, T = T_e, c_\alpha = c_{\alpha e}, \quad T_s = T_e, \varphi_1 = \varphi_{ie}, \quad (6)$$

$$x_1 = -x_{1e} : v_1 = V_e, v_2 = 0, T = T_e, \quad c_\alpha = c_{\alpha e}, -\frac{c}{3k}\frac{\partial U_R}{\partial x_1} + c U_R / 2 = 0, \quad (7)$$

$$x_1 = x_{1e} : \frac{\partial v_1}{\partial x_1} = 0, \frac{\partial v_2}{\partial x_1} = 0, \quad \frac{\partial c_\alpha}{\partial x_1} = 0, \frac{\partial T}{\partial x_1} = 0, \quad (8)$$

$$x_1 = -x_{1e} : v_1 = V_e, v_2 = 0, T = T_e, c_\alpha = c_{\alpha e}, -\frac{c}{3k}\frac{\partial U_R}{\partial x_1} + c U_R / 2 = 0, \quad (9)$$

$$x_1 = x_{1e} : \frac{\partial v_1}{\partial x_1} = 0, \frac{\partial v_2}{\partial x_1} = 0, \quad \frac{\partial c_\alpha}{\partial x_1} = 0, \frac{\partial T}{\partial x_1} = 0, \quad (10)$$

$\frac{d}{dt}$ – full derivative ($\frac{d}{dt} = \frac{\partial}{\partial t} + (v_j + w)\frac{\partial}{\partial x_j}$); C_p – specific heat capacity of the air at constant pressure; ρ – density of the air, T – ambient temperature; c_α – mass concentrations (α=1–CO, 2 – CH_x, 3 – NO_x, 4 – black soot, 5 – other components of the air); P – pressure; M_α - the molecular weight of individual; α – gas phase components, t – time. To close the system of equations (1)-(5), the components of the turbulent stress tensor, turbulent fluxes of heat and mass are defined in terms of the middle flow gradients [3-4]:

$$-\rho_5 \overline{u_i u_j} = \mu_T \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_i}{\partial x_i} \right) - \frac{2}{3} K \delta_{ij},$$

$$-\rho_5 \overline{u_j c_p T'} = \lambda_T \frac{\partial T}{\partial x_j}, \; -\rho_5 \overline{u_j c'_\alpha} = \rho_5 D_T \frac{\partial c_\alpha}{\partial x_i}, \tag{11}$$

$$\lambda_T = \mu_T c_p / Pr_T \;, \rho_5 D_T = \mu_T / Sc_T \,, \mu_T = c_\mu \rho_5 K^2 / \varepsilon,$$

where Pr_T. Sc_T – turbulent Prandtl and Schmidt numbers; μ_t, λ_t, D_t – coefficients of turbulent dynamic viscosity and thermal conductivity, K, ε – turbulent kinetic energy and its dissipation. Using the assumption that one can neglect unsteady, diffusion and convection terms in the transport equation for the turbulent kinetic energy, it is possible to obtain an algebraic expression for μ_t [5]:

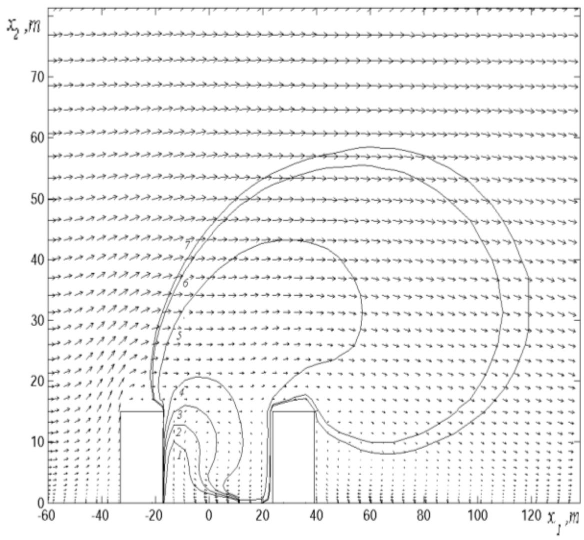
$$\mu_t = \rho l^2 \left\{ 2\left[\left(\frac{\partial v_1}{\partial x_1}\right)^2 + \left(\frac{\partial v_2}{\partial x_2}\right)^2\right] + \left(\frac{\partial v_1}{\partial x_2} + \frac{\partial v_2}{\partial x_1}\right)^2 - \frac{2}{3}\left[\frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2}\right]^2 - \frac{g}{T\,\mathrm{Pr}_t}\frac{\partial \theta}{\partial x_2} \right\}^{1/2}, \tag{12}$$

where the mean free path was determined by the formula $l = zk_T / (1 + 2{,}5z\sqrt{c_d s / h})$, taking into account that the drag coefficient of forest canopy c_d equals zero between the ground surface and the forest canopy. The constants are equal to: $k_T = 0{,}4$, $\theta = T - T_e$, $h = h_2 - h_1$ (h_2, h_1 – height of the trees and the distance to the base of crowns). This system of equations describes the processes within the region, which includes the urban canyon, buildings, roadside plantations and the surrounding area.

To calculate the field of the flow the algorithm Simple [5] is used. Construction of a discrete analogue for the set boundary problem was carried out based on the control volume approach. The resulting systems of finite-difference equations obtained in consequence of sampling were resolved by the method SIP [6]. The correctness of the program was tested using the method of introduction of analytical solutions. To account for the impact of the buildings there was used the method of fictitious domains, i.e. in control volumes of the computational region, where the buildings were located, there were set the initial values of functions, which were not changed in the process of calculation. In these calculations, the results were obtained with the following values T = 300K, V_e = 2 m/sec (at the hight of 1,5 m), the road width of 12 m, height of trees – 12 m, traffic (number of vehicles passing per unit of time) – 3000, the structure of traffic (passenger cars – 56%, trucks and buses – 19%, diesel cars – 25%). Information about the type of vehicle and traffic is used to determine the sources of contaminants.

As a result of numerical calculations there was obtained velocity distribution, temperature, component concentrations of contaminants at various time points. Fig. 2 shows the distribution of emitted CO_2 as a result of vehicle operation, and the velocity vector field, which is realized at a particular period of time. As a result of interaction of the external wind field with buildings the vector flow pattern is deformed.

It can be seen that within the Str. canyon there is generated a whirlwind due to the presence of an external field of speed, which promotes the redistribution of CO_2. As a result, the maximum concentration of contaminants will occur near the left wall of the canyon. In addition, on the right part of the illustration behind the building on the right there occurs a recalculating region of the flow. For other contaminants released into the atmosphere due to the operation of motor vehicles as a result of numerical calculations there are obtained similar concentration distributions.



1 – 5,0 mg/m^3, 2 – 2,0 mg/ m^3, 3 – 1,0 mg/m^3, 4 – 0,5 mg/m^3, 5 – 0,1 mg/m^3, 6 – 0,05 mg/m^3, 1 – 0,04 mg/m^3

Figure 2 – The vector velocity field and CO_2 concentration distribution

With an increase in wind speed there is implemented a somewhat different picture of the flow and distribution of contaminants. So with the increase of the wind speed to 5 m/s (Fig. 4) the contaminant is carried away by the wind more intensively and dissipates in the environment. As a result there is a concentration distribution and a velocity vector field shown in Fig. 3.

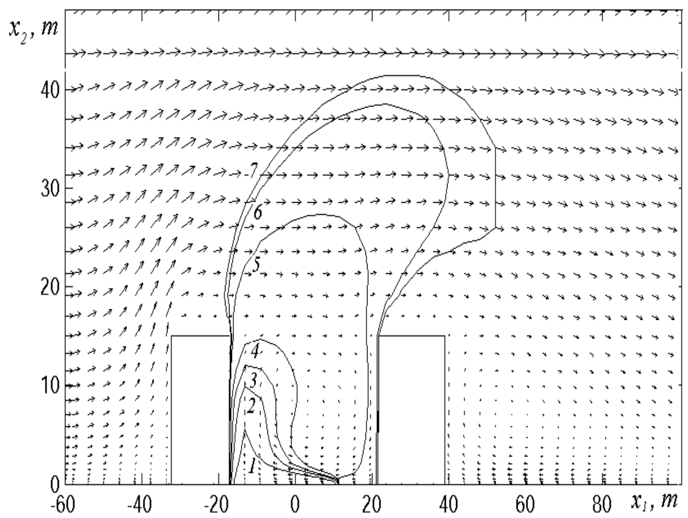


Figure 3 – The velocity vector field and distribution of CO_2 concentration (for the same values presented in Fig.2); V_e. = 5 m/s

The concentration level of the vertical direction (curve 7), which is achieved in the first case at a height of about 60 meters, in the second case, with increasing wind speed is realized at a height of just over 40 meters.

Fig. 4 shows the distribution of the velocity vector field and the concentration of the contaminant at the wind speed of 10 m/s.

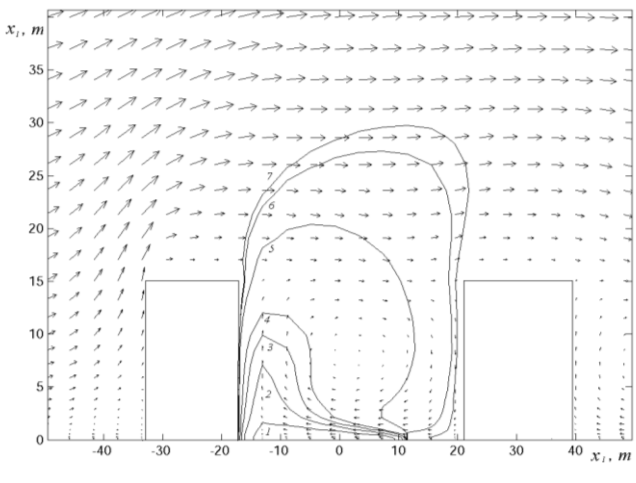


Figure 4 – The velocity vector field and distribution of CO_2 concentration (for the same values as in Fig.2); V_e. = 10 m/s

The results of the given numerical calculations are compared with the experimental results (Fig. 5). For comparison there were used the results of numerical calculations, which were obtained without taking into account the buildings under similar conditions as well as the data of experimental studies. The illustration shows that the experimentally measured values of CO_2 concentration at a height of 1,5 m fairly good agree with the results of numerical calculations.

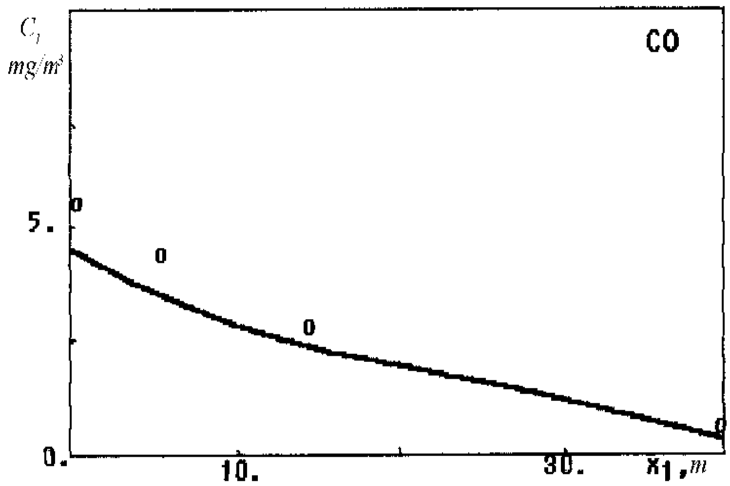


Figure 5 – Distribution of CO_2 concentration in the direction perpendicular to the road (o – the results of the experiment)

Conclusion

Using the mathematical model presented in this paper one can study the dynamics of pollution under the influence of various external conditions: the weather conditions (air temperature, wind speed, temperature stratification in the atmosphere, etc.), location and size of the buildings, as well as roadside plantations, transport flow options (such as cars and traffic density, etc.). Comparing the data obtained with the defined maximum - permissible concentration (MPC) one can analyze the pollution levels according to various components and to suggest the ways to reduce it. For example, to reduce the traffic density, to prohibit the movement of certain vehicles (trucks, with diesel or petrol engines, etc.).

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Рецензенти:
Славінська О.С., д-р техн. наук, Національний транспортний університет.
Хрутьба В.О., д-р техн. наук, Національний транспортний університет.

Reviewers:
Slavinska O.S., Dr. Tech. Sci., National Transport University.
Hrutba V.O., Dr. Tech. Sci., National Transport University.

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