27th International Scientific Conference
October 4-6, Palanga

TRANSPORT MEANS 2023

Proceedings
Part I

ktu
1922

ISSN 1822-296 X (print)
ISSN 2351-7034 (on-line)

KAUNAS UNIVERSITY OF TECHNOLOGY
KLAIPĖDA UNIVERSITY
IFToMM NATIONAL COMMITTEE OF LITHUANIA
LITHUANIAN SOCIETY OF AUTOMOTIVE ENGINEERS
THE DIVISION OF TECHNICAL SCIENCES
OF LITHUANIAN ACADEMY OF SCIENCES
VILNIUS GEDIMINAS TECHNICAL UNIVERSITY

TRANSPORT MEANS 2023

Sustainability: Research and Solutions

PROCEEDINGS OF THE 27th INTERNATIONAL SCIENTIFIC CONFERENCE

PART I

October 04-06 , 2023
Hybrid Conference - Palanga, Lithuania

CONFERENCE IS ORGANIZED BY
Kaunas University of Technology,
In cooperation with
Klaipeda University,
IFToMM National Committee of Lithuania,
Lithuanian Society of Automotive Engineers,
The Division of Technical Sciences of Lithuanian Academy of Sciences,
Vilnius Gediminas Technical University

The proceedings of the 27th International Scientific Conference Transport Means 2023 contain selected papers of 9 topics: Aviation, Automotive, Defence Technologies, Fuels and Combustion, Intelligent Transport Systems, Railway, Traffic, Transport Infrastructure and Logistics, Waterborne Transport.

All published papers are peer reviewed.

The style and language of authors were not corrected. Only minor editorial corrections may have been carried out by the publisher.

doi: 10.5755/e01.2351-7034.2023.P1

Proceedings of 27th International Scientific Conference. Transport Means 2023.

Modeling Influence of TiO_2 Barrier Coating on Pollutant Dispersion Near Road

M. Biliaiev[1], O. Berlov[2], V. Biliaieva[3], V. A. Kozachyna[4], V. V. Kozachyna[5], Z. Yakubovska[6]

[1]*Ukrainian State University of Science and Technologies, Lazaryan Str. 17, 49010, Dnipro, Ukraine,*
E-mail: biliaiev.m@gmail.com
[2]*Prydniprovska State Academy of Civil Engineering and Architecture, Petrov Str. 24a, 49005, Dnipro, Ukraine,*
E-mail: berlov.oleksandr@pdaba.edu.ua
[3]*Oles Honchar Dnipro National University, Haharin Ave. 72, 49010, Dnipro, Ukraine,*
E-mail: vikabelyaeva604@gmail.com
[4]*Ukrainian State University of Science and Technologies, Lazaryan Str. 17, 49010, Dnipro, Ukraine,*
E-mail: v.kozachyna@gmail.com
[5]*Ukrainian State University of Science and Technologies, Lazaryan Str. 17, 49010, Dnipro, Ukraine,*
E-mail: tsurkanvaleri1997@gmail.com
[6]*Ukrainian State University of Chemical Technology, Haharin Ave. 8, 49005, Dnipro, Ukraine,*
E-mail: zinaidaya25@gmail.com

Abstract

Mitigation strategies for near-road air pollution are of great interest nowadays. Sound barriers near the road are very effective to decrease pollutant concentration. The use of titanium dioxide (TiO_2) barrier coating provides an additional effect which allows to a decrease of pollutant concentration near roads. In this study quick- a computing CFD model was developed to access the influence of TiO_2 barrier coating on pollutant concentration. To simulate wind flow over the barrier with TiO_2 coating model of potential flow was used. The process of NO_x dispersion from the car was computed using a mass conservation equation. Finite-difference schemes were used for the numerical integration of governing equations. The computer code was developed on the basis of the proposed numerical model. Results of numerical simulations are presented.

KEY WORDS: *TiO_2 barrier coating, pollutant dispersion, CFD modeling*

1. Introduction

The design, construction and reconstruction of highways involves solving a set of problems to reduce the negative impact of cars on the environment. The solution to this problem is based on the implementation of special protective methods, very often – protective barriers [4, 7, 8, 12]. One of the methods to reduce the negative impact of car emissions is the use of a «photocatalytic» coating [6, 9-11, 13]. This coating allows to decompose NO into less hazardous substances. An important problem is to assess the effectiveness of this coating for specific operating conditions of different highways. Therefore, it is very important to have specialized calculation methods that allow for such assessments. A common method for solving this problem is the use of CFD models based on the application of the Navier-Stokes equations to solve the problem of determining the air velocity field near roads [5, 12, 13]. These models make it possible to determine in detail the parameters of the process being modeled and obtain important information for practice. However, the use of Navier-Stokes equations requires powerful computers and considerable time to perform a computational experiment. Therefore, it is important to have simplified calculation methods that allow to obtain quickly predictive information during serial calculations. In this paper, a numerical model for quick assessment of the impact of barriers with a TiO_2 surface on reducing air pollution near a highway is considered.

2. Mathematical Model of Impurity Dispersion Near a Highway

NO-absorbing surfaces («photocatalytic» surfaces, «TX Active» surfaces) are used not only to cover the roadway, but also to cover protective barriers. To solve the problem of determining the impact of barriers with a «photocatalytic» surface on the formation of air quality near the highway, a mathematical model was built.

The following mass transfer equation was used to model the process of NO transfer from cars [1]:

$$\frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}+\frac{\partial vC}{\partial y}=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C}{\partial y}\right)+\sum_{i=1}^{n}Q_i(t)\delta(x-x_i)\delta(y-y_i), \quad (1)$$

where C – NO concentration, mg/m^3; $Q_i(t)$ – NO emission rate; u, v – components of wind flow velocity vector, m/s; t – time, s; $\mu=(\mu_x, \mu_y)$ – turbulent diffusion coefficients, m^2/s; x_i, y_i – coordinates of emission source, m; $\delta(x-x_i)\delta(y-y_i)$ – Dirac delta-function, m^{-3}.

The location of NO emission sources is modeled using a delta-function.

The boundary conditions for the modeling Eq. 1 are as follows:

1. At the inlet boundary: $C = 0$.
2. At the outlet boundary: $\left.\frac{\partial C}{\partial n}\right|_{\Gamma_2} = 0$ (n – a unit vector of the external normal to the boundary).
3. On the surface $y = 0$, $y = L_y$ (L_y – upper boundary of the computational region): $\frac{\partial C}{\partial n} = 0$.

On the photocatalytic surface which is situated on the barrier, the following is accepted: $C_{surf} = 0$. This condition means that the surface completely absorbs the impurity. The initial condition was: $C = 0$.

The following dependencies were used to determine the turbulent diffusion coefficients:

$$\mu_x = k_0 \cdot u,\ \mu_y = k_0 \cdot v,$$

where $k_0 = 0.1$.

The presence of barriers significantly affects the formation of the flow pattern which changes the distribution of impurity concentration near the highway. The model of potential flow was used to calculate the air flow velocity in the presence of barriers. The modeling equation was as follows:

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} = 0, \tag{2}$$

where P is velocity potential.

The components of the air flow velocity vector are defined as follows:

$$u = \frac{\partial P}{\partial x};\ v = \frac{\partial P}{\partial y}. \tag{3}$$

The boundary conditions for the modeling Eq. 2 were as follows:

1. $\frac{\partial P}{\partial n} = 0$ – at the barriers surface and the low boundary of the computational region.
2. $\frac{\partial P}{\partial n} = 0$ – at the upper boundary.
3. $\frac{\partial P}{\partial n} = V_n$ – at the inlet boundary (V_n – air flow velocity).
4. $P = \text{const}$ – at the outlet boundary.

The following wind profile was assumed at the inlet boundary of the computational region:

$$u = u_1 \cdot \left(\frac{y}{y_1}\right)^{n_1},$$

where $n_1 = 0.15$, u_1 – wind velocity at the height 1 m.

Fick's law was used to determine the amount of pollutant absorbed by the «TX Active» surface during time period dt. According to this law, the mass flux of NO to the «TX Active» surface was determined as follows:

$$J = -\mu S \frac{\partial C}{\partial \delta} dt, \tag{4}$$

where J – mass flux of NO to the «TX Active» surface; μ – diffusion coefficient; S – TX surface area; $\frac{\partial C}{\partial \delta}$ – the pollutant concentration gradient to the TX surface. It should be noted that this transfer takes place in a turbulent boundary layer which is formed on the barrier surface. This layer has thickness δ.

For a vertical barrier within a two-dimensional model:

$$S = h_y \cdot 1\text{m},$$

where h_y – step of the difference grid in the vertical direction.

It should be noted that the value of this boundary layer varies along the barrier, i.e., $\delta = \delta(l)$, and depends on the specific hydrodynamic conditions [3]. The determination both the thickness of the turbulent boundary layer at the barrier and the value of the diffusion coefficient in this layer is a separate difficult problem. This problem requires numerical integration of Navier-Stokes equations using turbulence models. This is a difficult problem that requires much computer time. A simplified approach was used to calculate the diffusion flow of pollutant to barrier TX surface. The following relationship was used to determine the thickness of the turbulent boundary layer [3]:

$$\delta = 0.37l\left(\frac{Vl}{\mu}\right)^{-0.2}, \tag{5}$$

where l – barrier length; V – local air flow velocity near the barrier; μ – coefficient of kinematic viscosity.

In the developed model, the concentration gradient was represented as follows:

$$\frac{\partial C}{\partial \delta} = \frac{C_{i,j} - C_{surf}}{\delta},$$

where C_{surf} is concentration of the pollutant on the «photocatalytic» surface (as mentioned above, it was assumed $C_{surf} = 0.$); $C_{i,j}$ – concentration of the pollutant in the difference cell adjacent to the «photocatalytic» surface.

The algorithm for solving the problem is as follows.

1. Eq. 2 is numerically solved to find the velocity potential field.
2. The components of the air flow velocity vector in the computational domain are determined using Eq. 3.
3. Eq. 1 is solved and field of NO concentration is determined at time t.
4. The thickness of the boundary layer is determined using Eq. 5, $v = 14 \cdot 10^{-6}$ m^2/s.
5. On the basis of Eq. 4, the flow of NO mass from the cell adjacent to the TX surface is calculated.

3. Numerical Model

Finite difference schemes were used for numerical integration of the governing equations. The calculation was performed on a rectangular grid. The velocity potential is calculated at the centers of the difference cells. The velocity vector components are calculated on the sides of the difference cells. The pollutant concentration was calculated at the centers of the difference cells.

To solve Eq. 2, it was previously written as follows:

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2}, \tag{6}$$

where t – fictitious time.

Next, Eq. 6 was solved using Samarsky's finite difference scheme. The finite difference scheme was as follows [2]:

– in the first step of splitting:

$$\frac{P_{i,j}^{n+\frac{1}{2}} - P_{i,j}^{n}}{\Delta t} = \left[\frac{-P_{i,j}^{n+\frac{1}{2}} + P_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2}\right] + \left[\frac{-P_{i,j}^{n+\frac{1}{2}} + P_{i,j-1}^{n+\frac{1}{2}}}{\Delta y^2}\right];$$

– in the second step of splitting:

$$\frac{P_{i,j}^{n+1} - P_{i,j}^{n+\frac{1}{2}}}{\Delta t} = \left[\frac{P_{i+1,j}^{n+1} - P_{i,j}^{n+1}}{\Delta x^2}\right] + \left[\frac{P_{i,j+1}^{n+1} - P_{i,j}^{n+1}}{\Delta y^2}\right].$$

The calculation was finished when the following condition was fulfilled:

$$\left|P_{i,j}^{n+1} - P_{i,j}^{n}\right| \le \varepsilon,$$

where ε – a small number. To start of calculation, the following was accepted: $t = 0$, $P = 0$.

In discrete form, the components of the air flow velocity vector were calculated as follows:

$$u_{ij}=\frac{P_{i,j}-P_{i-1,j}}{\Delta x},\ v_{ij}=\frac{P_{i,j}-P_{i,j-1}}{\Delta y}$$

To solve Eq. 1, it was decomposed as follows:

$$\begin{cases} \frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}+\frac{\partial vC}{\partial y}=0; \\ \frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C}{\partial y}\right); \\ \frac{\partial C}{\partial t}=\sum_{i=1}^{n}Q_i(t)\delta(x-x_i)\delta(y-y_i). \end{cases} \tag{7}$$

To solve the first equation from system Eq. 7, the following approximations and transformations were made [1]:

$$\frac{\partial C}{\partial t}\approx\frac{C_{ij}^{n+1}-C_{ij}^{n}}{\Delta t};$$

$$\frac{\partial C}{\partial t}\approx\frac{C_{ij}^{n+1}-C_{ij}^{n}}{\Delta t};$$

$$\frac{\partial uC}{\partial x}=\frac{\partial u^{+}C}{\partial x}+\frac{\partial u^{-}C}{\partial x};$$

$$\frac{\partial vC}{\partial y}=\frac{\partial v^{+}C}{\partial y}+\frac{\partial v^{-}C}{\partial y};$$

$$\frac{\partial u^{-}C}{\partial x}\approx\frac{u_{i+1,j}^{-}C_{i+1,j}^{n+1}-u_{i,j}^{-}C_{i,j}^{n+1}}{\Delta x}=L_x^{-}C^{n+1};$$

$$\frac{\partial u^{+}C}{\partial x}\approx\frac{u_{i,j+1}^{+}C_{i,j}-u_{i,j}^{+}C_{i-1,}}{\Delta x}=L_x^{+}C^{n+1};$$

$$\frac{\partial v^{+}C}{\partial y}\approx\frac{v_{i,j+1}^{+}C_{i,j}-v_{i,j}^{+}C_{i,j-1}}{\Delta y}=L_y^{+}C^{n+1};$$

$$\frac{\partial v^{-}C}{\partial y}\approx\frac{v_{i,j+1}^{-}C_{i,j+1}-v_{i,j}^{-}C_{i,j}}{\Delta y}=L_y^{-}C^{n+1},$$

where $u^{+}=\frac{u+|u|}{2},\ u^{-}=\frac{u-|u|}{2},\ v^{+}=\frac{v+|v|}{2},\ v^{-}=\frac{v-|v|}{2}$.

Next, the following splitting was performed [1]:

– the first step, $k = 1/4$:

$$\frac{C_{ij}^{n+k}-C_{ij}^{n}}{\Delta t}+\frac{1}{2}\left(L_x^{+}C^{k}+L_y^{+}C^{k}\right)=0;$$

– the second step $k = 1/2$, $c = n + 1/4$:

$$\frac{C_{ij}^{k}-C_{ij}^{c}}{\Delta t}+\frac{1}{2}\left(L_x^{-}C^{k}+L_y^{-}C^{k}\right)=0;$$

– the third step $k = n + 3/4$, $c = n + 1/2$:

$$\frac{C_{ij}^{k}-C_{ij}^{c}}{\Delta t}+\frac{1}{2}\left(L_x^{-}C^{k}+L_y^{-}C^{k}\right)=0;$$

– the fourth step $k=n+1$, $c=n+3/4$:

$$\frac{C_{ij}^{k}-C_{ij}^{c}}{\Delta t}+\frac{1}{2}\left(L_{x}^{+}C^{k}+L_{y}^{+}C^{k}\right)=0.$$

An explicit formula was used to determine the unknown value of the concentration C at each step of the splitting.

To numerically solve the second equation from system Eq. 7, the following two-step splitting scheme was used [2]:

– at the first step of the splitting, the difference equation had the form:

$$\frac{C_{i,j}^{n+\frac{1}{2}}-C_{i,j}^{n}}{\Delta t}=\left[\mu_x\frac{-C_{i,j}^{n+\frac{1}{2}}+C_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2}\right]+\left[\mu_y\frac{-C_{i,j}^{n+\frac{1}{2}}+C_{i,j-1}^{n+\frac{1}{2}}}{\Delta y^2}\right]; \qquad (8)$$

– at the second step of the splitting, the difference equation had the form:

$$\frac{C_{i,j}^{n+1}-C_{i,j}^{n+\frac{1}{2}}}{\Delta t}=\left[\mu_x\frac{C_{i+1,j}^{n+1}-C_{i,j}^{n+1}}{\Delta x^2}\right]+\left[\mu_y\frac{C_{i,j+1}^{n+1}-C_{i,j}^{n+1}}{\Delta y^2}\right]. \qquad (9)$$

At each step of splitting, explicit formula was used to calculate concentration C.

The Euler method [2] was used to solve the third equation from system Eq. 7.

Computer code was developed on the basis of proposed mathematical model. FORTRAN was used for programming.

4. Results

Developed mathematical model was used to predict air pollution near the road with two barriers (Fig. 1). The first scenario was that there was no «TX» coating on the internal sides of each barrier. The second scenario was that A-B surface and C-D surface had «TX» coating (Fig. 1). The computational region had dimensions: length 33 m, height 21 m. Wind speed was $u_1 = 4$ m/s. Emission rate was 1 g/s. The height of the barriers was 5 m.

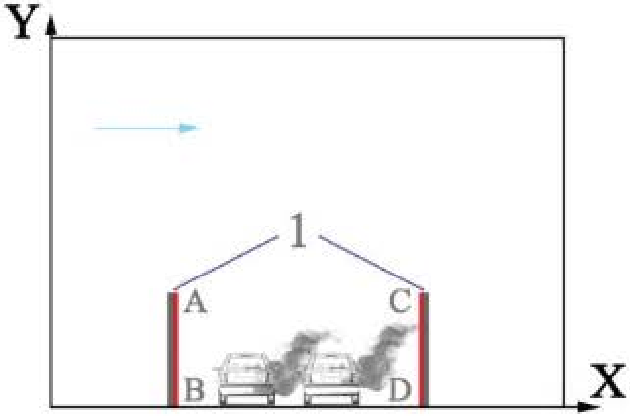


Fig. 1 Sketch of computational region: 1 – barriers with TX coating

In Fig. 2 predicted NO concentrations are presented for the first scenario (no TX coating on the barrier surface). NO concentrations in the computational region for the second scenario (TX coating on the barrier surface) are shown in Fig. 3. Every number in Fig. 1 and Fig. 2 shows concentration as the percentage of maximum concentration of pollutant in the computational region. The results in these figures were printed using «Integer» format. It means that only the integer part of the number was shown. This approach allows quickly analyze results of numerical experiment and quickly determine regions with high and low concentrations and find zone of influence of protection means.

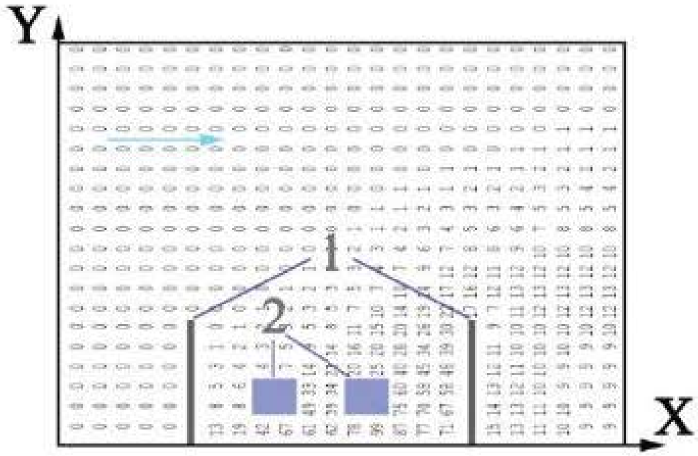


Fig. 2 Predicted NO concentration (scenario №1, no TX coating on barrier surface): *1* – barriers; *2* – vehicles

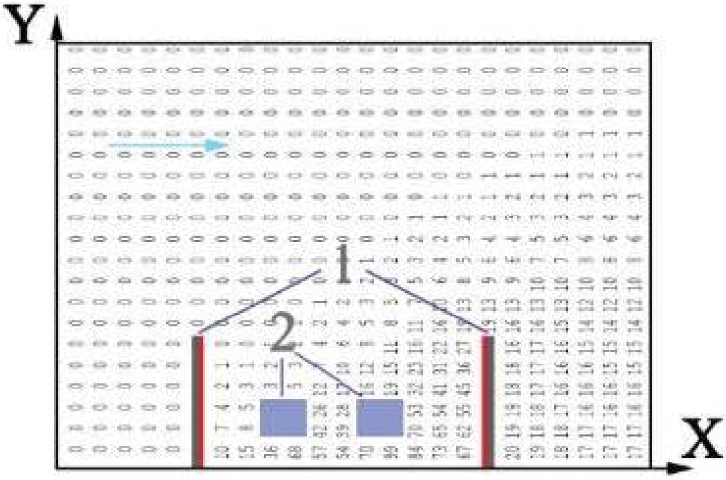
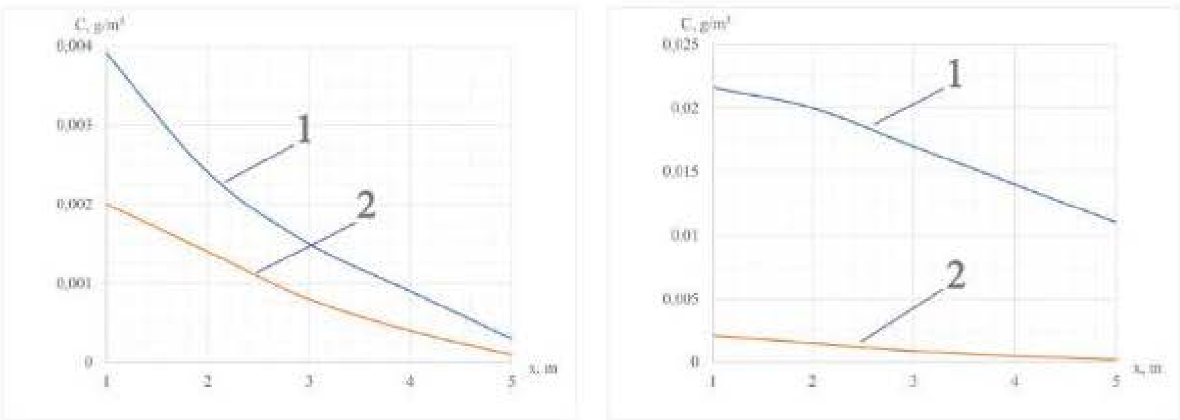


Fig. 3 Predicted NO concentration (scenario №2, TX coating on barrier surface): *1* – barriers; *2* – vehicles

The analysis of results presented in Fig. 2, Fig. 3 shows that TX coating allows to decrease pollutant concentration in vicinity of barrier. Concentration decrease is observed near the TX surface but this decrease is too local.

For a more detailed analysis of the results of numerical modeling, in Fig. 4, NO concentration change along both barriers is shown.



a b

Fig. 4 NO concentration: a – along the left barrier; b – along the right barrier; *1* – no TX coating on barrier surface; *2* – TX coating on barrier surface

It can be seen from Fig. 4 that NO concentration decreases more intensively along the right barrier. It can be explained by the fact that NO concentration and concentration gradient near the right barrier are greater than at the left barrier.

Worthy of note that computational time was 2 s.

5. Conclusions

A quick-computing numerical model was proposed for the prediction NO concentrations near roads with barriers that have TX coating. This numerical model takes into account: the height of barriers, their location near the road, pollutant emission rate from vehicles, the influence of barriers on the flow pattern, meteorological parameters. Computational calculations were carried out on the basis of the developed computer program.

The developed mathematical model can be used to establish the efficiency of TX coating on barriers depending on the specific operating conditions. This mathematical model is a necessary tool for justification measures aimed at improving the state of environment.

References

1. **Zgurovsky, M.Z.; Skopetsky, V.V.; Khrutch, V.K.; Biliaiev, M.M.** 1997. Numerical modeling of pollution dispersion in environment. Kyiv: Naukova dumka: 368 p.
2. **Samarsky, A.A.** 1983. Theory of difference schemes. Moskow: Nauka: 616 p.
3. **Schlichting, H.** 1969. Boundary-layer theory. M.: Nauka: 742 p.
4. **Biliaiev, M.; Pshinko, O.; Rusakova, T.; Biliaieva, V.; Sladkowski, A**. 2021. Computer Model for Simulation of Pollutant Dispersion Near the Road with Solid Barriers, Transport Problems 16(2) Part 1: 73-86.
5. **Madalozzo, D.M.S.; Braun, A.L.; Awruch, A.M.** 2012. A numerical model for pollutant dispersion simulation in canyons, Mecanica Computacional XXXI: 211-235.
6. **Guerrini, G.L.; Beeldens, A.; Crispino, M.; D'Ambrosio, G.; Vismara, S**. 2012. Environmental benefits of innovative photocatalytic cementitious road materials, 10th International Conference on Concrete Pavements, 912-923.
7. **Schulte, N.; Venkatram, A**. 2013. Effects of Sound Barriers on Dispersion from Roadways, Final Report**,** University of California: 100 p.
8. **Hagler, G.S.W.** 2011. Model evaluation of roadside barrier impact on near-road air pollution, Atmospheric Environment 45(15): 2522-2530.
9. **Horgnies, M.; Serre F.; Dubois-Brugger, I.; Gartner E.** 2014. NOx de-pollution Using Activated Charcoal Concrete – From Laboratory Experiments to Tests with Prototype Garages, Proceedings of the 4th International Conference on Environmental Pollution and Remediation, Prague, Czech Republic, XXX-1-XXX-8.
10. **Brolin, N.** 2010. Product Development of Curved Noise and NOx Barrier, Master of Science Thesis, Stockholm, Sweder: 51 p.
11. **Overman, H.T.** 2009. Simulation model for NO_x distribution in a street canyon with air purifying pavement, Master thesis, University Twente, Netherlands: 99 p.
12. **Sang Jin Jeong** 2015. A CFD Study of Road Barrier Impact on the Dispersion of Road Air Pollution, Asian Journal of Atmospheric Environment 9(1): 22-30.
13. **Xie, X, Hao, C, Huang, Y**. 2020. Influence of TiO2-based photocatalytic coating road on traffic-related NOx pollutants in urban street canyon by CFD modeling, Science of The Total Environment 724: 1-33.