UDC 504.056:656

Rostislav Sipakov[1]
Postgraduate at Occupational Safety and Environment Department

Volodimir Trofimovich[1]
Ph. D., Professor of Occupational Safety and Environment Department

Olena Voloshkina[1]
D. S., Professor, Head (BrE) of Occupational Safety and Environment Department

Julia Bereznitska[1]
Ph. D., Assistant professor of Occupational Safety and Environment Department

[1]Kyiv National University of construction and architecture, Kyiv Ukraine

ASSESSMENT AND FORECAST FOR THE CREATION OF PHOTOCHEMICAL SMOG OVER TRANSPORT OVERPASSES IN KYIV

Abstract. *This article deals with the analysis of existing models of smog situation formation over automobile overpasses and in places of substantial congestion of transport in large cities, for example, in Kyiv. A mathematical model consisting of two blocks – dynamic and kinetic, which allows determining the formation of the thermal dome of pollution and the concentration of hydrocarbon emissions in the air, depending on the number of working engines, is proposed. The kinetic block of the model allows determining the level of formaldehyde, as an indicator of the appearance of photochemical smog in conditions of atmospheric constancy. The concentration of emissions from motor vehicles in the air is calculated over the main transport overpasses of the city of Kyiv at their full load (peak hours).*
Key words: *bridge, smog, formaldehyde, indicator of pollution, formation of a dome of pollution, concentration of pollution, hydrocarbons, rate of conversion, mathematical model of atmospheric pollution.*

Introduction

The main factors and mechanism of formation of smog in large cities of Ukraine, including over the city of Kyiv, studied to date is not enough. Most works are devoted to a comprehensive assessment of the level of air pollution, where one of the leading contributing factors is formaldehyde. Formaldehyde proliferation in large cities is being addressed by such domestic and foreign scientists as Polischuk S.Z., Dotsenko L.V., Bezuglaya E.Y., Snizhko S.I., Shevchenko O.G., Kulbida M.I., Lezhenin A.O., Vorobyova I.A., H. Bridgman, H. John Seinfeld, L. Graham, and others. Recently, formaldehyde pollution of the urban environment and simulation at the local level of this phenomenon is widely studied on the example of cities of the post-Soviet Union countries (Sellegy T.S., Shlychkov V.A., Malbakhov V.M., Lenkovskaya T.N., Temirbekov and others), where there is a rather significant load on the atmosphere, in particular from point sources of pollution.

For the city of Kyiv average daily concentration of formaldehyde in summer can exceed twice the sanitary-and-hygienic standard, as evidenced by data from the Central Geophysical Laboratory of the Ukrainian Hydro Meteorological Center [5, 10, 18]. Many authors note that in large cities of Ukraine, and in Kiev, in the first place, the concentration of formaldehyde can serve as a sign of the appearance of photochemical smog in urban accumulations of motor vehicles under steady weather conditions of the atmosphere.

The dynamics of the formation of smog is studied for a long time on an example of its creation in Los Angeles, London, Sydney and other major metropolitan areas of the world. According to the World Health Organization in urban airspace under adverse weather conditions or with intensive motor transport, the concentration of formaldehyde may reach 0.1 mg / m^3 [13].

Although, the mechanism of the formation of smog, which was considered in the works of a number of foreign authors, is identical, the indicator of urban photochemical pollution of the atmosphere in each case is chosen different and depends on a number of factors of the area, primarily from the meteorological conditions of the terrain, the type of pollutants. For Kyiv, such an indicator can be the concentration of formaldehyde, as a product of oxidation of hydrocarbons from the emission of exhaust gases of various types of automobile engines and natural factors (hydrocarbons of vegetable origin). Taking into account the annual growth of motor transport on the roads of Kyiv and the correlation of the appearance of photochemical smog over automobile overpasses (especially on two or more levels) and on the traffic jams and the number of vehicles, the assessment of the formation of photochemical smog in these places is extremely important in order to provide a large city with sufficient level of environmental safety.

The aim of research. The work aims to reveal the peculiarities of the negative impact on the atmospheric air of motor transport in Kyiv, as a scientific basis for improving the environmental safety management system by estimating and predicting the formation of photochemical smog around overpasses and large intersections.

Presenting main material

Among the existing models of the formation of photochemical smog over a large city at present, the most common are statistical-hydrodynamic, which are adapted to the conditions of a large city. As a predicted value, the integral index of air pollution by formaldehyde in the city was calculated, which was calculated using regression analysis methods. The statistical component of the model gives the average prognostic concentration in the city; the spatial distribution details are based on the hydrodynamic block of the model [6, 7, 11, 14, 15, 16, etc.]. The modeling of the distribution of harmful impurities in the atmosphere from point sources and vehicles, taking into account photochemical transformation, was considered in a number of studies using the model of the boundary layer of the atmosphere to take into account the influence of anthropogenic heat sources and the heterogeneity of the underlying surface on the process of spreading pollution [1, 6, 13, 14, 16]. In the works [2, 13, 14] a mechanism for the formation of photochemical smog at maximum concentrations of formaldehyde, that fixed in weak winds and calm, and a model for the creation of formaldehyde from ethane (emissions from motor vehicles) by the balance method are presented [2].

In this article the model of the formation of photochemical smog in the places of a significant accumulation of vehicles in Kyiv is discussed, which consists of two blocks, namely:

The first block. It is based on the assumption that a "dome" of warm air, like a heat source, forms over a transport overpass. The convective heat that gives the heat source to the environment determines the nature and parameters of the convective air jet that develops over the heated surface. At the first stage, the equation of the amount of motion of polluted air is solved, which allows determining the main parameters of the contaminated jet and calculating the amount of heat coming from the warm source into the environment, as well as the nature and parameters of the convective jet. In this case, we have an assumption regarding the circular area of the transport node S diameter D.

We find the amount of heat in the area S.

$$Q_S = S \cdot \sum Qav,$$

$\sum Qav$ – the sum of direct and scattered radiation (for Kiev 645 + 194 = 893 MJ / m^2 respectively).

We find warmth from cars on the transport node.

By the number of lines, we determine the number of vehicles N. In times of maximum load (peak times), we assume the interval between cars L = 20 m and 1 km of road in these times, there are 40 cars.

$$N = n \cdot L' / (l_{car} + L),$$

where lcar – a length of the car, m; n – the number of automobile lanes on the overpass, L – the length of one lane, m.

The heat from cars is according to the dependence:

$$Q_{car} = q_{car} \cdot N \cdot 40000 \text{ J},$$

where q_{car} – fuel consumption for one car per 1 m way, l.

According to the found value $Q = Q_{car} + Q_8$, we calculate the average temperature and velocity in the transverse section of the convective jet.

The average of the area of the warm air, which is rising upward and the average temperature in the transitional section, respectively, are based on the following formulas:

$$V_y = 0{,}56\,(Q_{K\,/\,(y-y_o)})^{0.33},$$

$$\Delta t_{\text{уср}} = \frac{41 \cdot Q_K^{2/3}}{(y - y_0)^{5/3}}\ ,Degree$$

In the resulted formulas y-y_o – distance from the surface of the earth to the narrowest section of the thermal jet, m.

By source [17], the typical composition of exhaust gases (hydrocarbons $CH_{1,\,85}$) by type of engine:

Type of Engine		
CE	*Intermediate*	$7{,}5\ \frac{g}{kw \cdot h}$
DE	*Load*	$0{,}5\ \frac{g}{kw \cdot h}$

When calculating the average amount of emissions from vehicles, we accept the average power of one car of 100 kilowatts and the smooth arrival and departure from the transport unit of cars at a speed of ~ 60 km / h.

Table 1 shows data on some overpasses in Kyiv, calculated according to the given methodology.

Concentration of emissions from car transport of hydrocarbons on the largest transport overpasses in Kyiv.

Table 1

Overpass	Area of thermal surface, m^2	Heat from cars and warm surface at the transport node (per month), MJ / m^2	Consumption in the narrowest section of the convective jet, m^3 / s	Concentration of emissions from vehicles at a distance of 2D above the surface of the overpass, mg / m^3
1	2	3	4	5
Naddniprovske highway, st. Saperno-Slobidska (Vydubichi)	70650	63090450,28	70000	1,0
Avenue of the 40th anniversary of October, Nauky avenue (Central bus station)	96163	80680757	129513	0,4957
Mykoly Bazhana Ave, kil′tseva doroha	49086	41163857	73594,5	0,6200
Leningrad Square	61544	51635416	89222	0,5782
Industrial bridge, Borschagovska st.	96208	80718512	129574	0,4939
st. Saperno-Slobidska, street Kikvidze	70684	59303876	100165	0,5500
St. Akad. Zabolotnoho, Stolychne highway	125660	10548740	161944	0,4500
St. Bohatyrs′ka, st. Marshala Tymoshenko	61573	51635416	89222	0,5782

The second block provides for the consideration of kinetic models of converting the concentration of emissions of hydrocarbons from motor vehicles under certain weather conditions in formaldehyde.

Finding the concentration of ethane in a vertical convective stream at an altitude of up to 1 km above the surface of the overpass, we find the fraction of its transformation into formaldehyde under certain weather conditions.

The balance model of formation of formaldehyde from the inflow from mobile sources is presented in [2]:

$$C_2H_4 + OH\cdot + 2NO \rightarrow 2NO_2 + 1{,}44HCHO + 0{,}28\ HOCH_2CHO + OH\cdot$$

As a result of the attack of hydroxyl radicals on ethylene at a temperature of 298 K, there is the conversion of two NO molecules into NO_2, the formation of 1.44 formaldehyde molecules and 0.28 glycolic aldehyde molecules (HOCH2CHO) and regeneration of the hydroxyl radical. Comparing this mechanism with propane, we see the similarity of the conversion of NO to NO_2 and the formation of oxygen products.

The concentration of formaldehyde (secondary contamination) in the general form is written by the equation:

$$C_{CHOH} = K\cdot C_{CH},$$

where K is the coefficient that characterizes the reaction velocity or the conversion constant and depends on the temperature of the air, the time interval, the intensity of the sunlight, etc.

In works [1, 6, 14, 15] a method is presented for taking into account the transformation of harmful impurities in the atmosphere, taking into account photochemical transformations. For certain types of contaminants, the scheme of converting one substance to another under the action of temperature and humidity in the mixture is described by a system of differential equations, and each transformation has its rate constant, which is obtained by solving this system.

Another approach to determining the constant rate K is presented in [2, 4]. Gas molecules can react only when they are approaching each other for direct energy exchange, which can lead to the breakdown of connections. Since the collision of two molecules is a necessary condition for the reaction, there must be sufficient energy to break the chemical bond. This energy can be represented as exp (-E / RT), where R is a universal gas constant, T is temperature. The reaction rate is expressed in a form that defines both the collision frequency and the particle that exceeds the required energy for molecules of type i and j:

$$r = A(T)\cdot \exp(-E/RT)\cdot C^i\cdot C^j = K\cdot C^i\cdot C^j,$$

The finite-exponential factor A (T) depends on temperature since the transient kinetic energy and the internal degrees of freedom of the molecules influence the probability of the reaction.

The formula determines the rate constant in this case:

$$K = A(T)\cdot \exp(-E/RT),$$

But if A (T) does not depend on temperature, we have Arrhenius's dependence:

$$K = A\cdot \exp(-E/RT).$$

The coefficient of conversion rate K can also be found experimentally by measuring the concentration of formaldehyde at different times of day under different weather conditions.

The results of measurements and the analysis of literary sources regarding the determination of the coefficient of transformation K, give grounds to assert about its definition with sufficient accuracy for determining the degree of contamination by formaldehyde in places of high concentration of vehicles.

Conclusions

The approach proposed in this paper allows within the framework of a single model to take into account the complex interconnections between dynamic and physicochemical processes of photochemical smog formation from road transport and to assess the anthropogenic load on the environment, as well as its impact on public health. The model of the formation of formaldehyde as an indicator of the appearance of photochemical smog over transport overpasses in this paper allows to predict secondary photochemical pollution and to make optimal managerial decisions regarding the ecological condition of urbanized territories and to implement environmental measures taking into account the constancy of meteorological factors.

REFERENCES

1. Aloyan A.E. Modeling of dynamics and kinetics of gas impurities and aerosols in the atmosphere. / Institute of Numerical Mathematics RAS. – M.: Nauka, 2008. – 415 p. (in translation.)
2. John H. Seinfeld, Spiros N. Pandis / Atmospheric chemistry and physics/ A Wiley-Interscience Publication, Printed in the USA, QC879.6. S45 1997. – 1356 p.
3. Kenichi I., Toshiaki Y., Toshio T. Formaldehyde and acetaldehyde in exhaust gases emitted from an ethanol-fueled S.I. engine // Bull. ISNE. – 1984. – Vol. 27, No 227. – P. 945–951.
4. Rate constant for gas phase reactions of nitrate with a series of organics in the air at 298 _+ 1K / R. Atkinson, C.N. Plum, W.P.L. Carter, et al. // J. Phys. Chem. – 1984. – Yd88. – P. 1210–1215.
5. Pryschepov O.F., Levytska O.S. Peculiarities of the dispersion of harmful substances of airborne vehicle emissions in the city / Scientific works of the Petro Mohyla Black Sea State University. Sir Technogenic safety. – 2009. – 111, issue 98 – pp. 139–146.
6. Temirbekov A.N. Study of the development of atmospheric processes in an industrial city, taking into account photochemical transformations, // access mode: pps.kaznu.kz/kz/Main/FileShow2/37704/89/2/1/2014//
7. Antropov K.M. Mathematical models of pollution of atmospheric air of a megacity and the industrial center by emissions of motor transport and industrial enterprises. The abstract for the degree of Candidate of Sciences in Physics and Mathematics, specialty 05.13.18 – Mathematical modeling, numerical methods and program complexes. Ekaterinburg, 2012. – 24 p. (as a manuscript rights).
8. Misliuk O.O., Shaikin O.Y. Assessment of ecological safety of motor transport operation in the conditions of an industrial city / Bulletin of ZHDTU №3 (46), 2008. – P. 1–6.
9. Skubnevskaya G.I., Dultseva G.G. Pollution of the atmosphere with formaldehyde: Analytical review / RAS. Sib otd. GPNTB, IKHK&G. – Novosibirsk, 1994. – 70 p.
10. The level of atmospheric air pollution in Kyiv by formaldehyde / O.G. Shevchenko, M.I. Kulbida, S.I. Snizhko, L.S. Shcherbukha, N.O. Danilov // Ukrainian Hydrometeorological Journal, Odessa State Ecological University, 2014, # 14, – P. 2–22.
11. Polishchuk S.Z., Dotsenko L.V., Demidenko A.S. Estimation of the influence of meteorological factors on the state of atmospheric air pollution in the city of Dnipropetrovsk (on the example of formaldehyde) / Construction, materials science, machine building: Starodubsky Readings-2015, – P. 266–270.

12. Brigman, H. and Graham L., 2003 "Air pollution and meteorology in a small city: the case study of Newcastle,NSW, Australia", Fifth International Conference on Urban Climate, University of Lods, Poland, September, 2003.
13. Howard Brigman / Global air pollution, problems for the 1990s., CBS Publishers & Distributors – 1992. – P. 261.
14. Richard C. Flagan, John H. Seinfeld Fundamentals of air pollution engineering / California Institute of Technology, 1988 by Prentice-Hall, Inc. A Division of Simon & Schuster, Printed in the United States of America, 1988. – P. 542.
15. Aloyan A.E., Numerical modeling of the interaction of gas species and aerosol in the atmospheric dispersive system // Russ. J Num. Analysis Math. Modelling. – 2000. – Vol. 15, No 3-4. – P. 211–224.
16. Formaldehyde pollution of the urban atmosphere and its dependence on meteorological factors / T.S. Selegay, N.N. Filonenko, V.A. Shlychkov, A.A. Lezhenin, T.N. Lenkovskaya // Optics of the Atmosphere and the Ocean, # 25 (5), Novosibirsk. 2013, – P. 422–426.
17. Protection of the atmosphere from industrial pollution: Reference edition in 2 hours; Part 1: Trans. with eng. / edited by Kalverta S., Ingunda G. M.; M. Metallurgy, 1988, – 760 p.
18. Trofimovich V.V. Monitoring of atmospheric air. Problems of modeling and forecasting / V.V. Trofimovich, O.S. Voloshkina, M.M. Fandikova, I.V. Klimova, N.E. Zhuravska // Prob. Scientific works "Ecological safety and nature management", KNUBA, ITGIP NANU, K., 2012. – issue 10 – P. 102–120.
19. Lejenin A.A. Investigation of atmospheric pollution processes of Siberia territories on the basis of hydrodynamic models and observational data / The abstract for the degree of Candidate of Sciences in Physics and Mathematics, specialty 25.00.29 – Physics of the atmosphere and hydrophere, Novosibirsk, 2013. – 16 p. (as a manuscript rights).
20. Sheludenko L.S. Study of material balance "Fugitive emissions". Structure and volumes of harmful emissions, which are advanced by traffic flows // Collection of scientific works "Ecological safety and balanced resource-use", IFNTNUNG, – Ivano-Frankivsk, 2017. – issue 2 (16) – P. 133–139.
21. Methodology for calculation of pollutant emissions and carbon dioxide emissions from vehicles from the air / Approved by the State Statistics Committee of Ukraine on November 13, 2008, # 452, Electronic resource – access mode http: // ukrstat.org/.
22. Snizhko S.I. Urbometric aspects of atmospheric air pollution of a large city / S.I. Snizhko, O.G. Shevchenko, – K. – Publishing house geogr. litr. "Obriy", 2011 – 297 p.
23. Manual on the control of atmospheric pollution / M.E. Berlyand, G.I. Sidorenko. – L.: Gidrometeoizdat, 1979. – 448 p.

Text of the article was accepted by Editorial Team 16.01.2018

Сіпаков Р.В., Трофімович В.В., Волошкіна О.С., Березницька Ю.О.

ОЦІНКА ТА ПРОГНОЗ УТВОРЕННЯ ФОТОХІМІЧНОГО СМОГУ НАД ТРАНСПОРТНИМИ ШЛЯХОПРОВОДАМИ В М. КИЄВІ

Анотація. Дана стаття торкається аналізу існуючих моделей формування смогових ситуацій над автомобільними шляхопроводами та в місцях великого скупчення транспорту у великих містах на прикладі м. Києва. Запропоновано математичну модель, яка складається з двох блоків – динамічного та кінетичного, що дозволяє визначати формування теплового купола забруднення та концентрації викидів вуглеводнів в повітрі в залежності від кількості працюючих двигунів. Кінетичний блок моделі дозволяє визначати концентрацію формальдегіду, як індикатора появи фотохімічного смогу в умовах сталості атмосфери. Підраховано концентрацію викидів від автотранспорту в повітрі над основними розв'язками м. Києва при їх повному навантаженні (години пік).

Ключові слова: шляхопровід, смог, формальдегід, індикатор забруднення, формування куполу забруднення, концентрація забруднень, вуглеводні, швидкість перетворення, математична модель забруднення атмосфери.

УДК 504.056:656
Сіпаков Р.В., Трофімович В.В., Волошкіна О.С., Березницька Ю.О. **Оцінка та прогноз утворення фотохімічного смогу над транспортними шляхопроводами в м. Києві** // Екологічна безпека та природокористування. – 2018. – Вип. 1 (25). – С. 44–51.
Запропоновано математичну модель, що дозволяє визначати формування теплового купола забруднення та концентрації викидів вуглеводнів в повітрі в залежності від кількості працюючих двигунів. Підраховано концентрацію викидів від автотранспорту в повітрі над основними розв'язками м. Києва при їх повному навантаженні (години пік).

UDC 504.056:656
Sipakov R., Trofimovich V., Voloshkina O., Bereznitska J. **Assessment and forecast for the creation of photochemical smog over transport overpasses in Kyiv** // Environmental safety and natural resources. – 2018. – Issue 1 (25). – P. 44–51.
A mathematical model which allows determining the formation of the thermal dome of pollution and the concentration of hydrocarbon emissions in the air, depending on the number of working engines, is proposed. The concentration of emissions from motor vehicles in the air is calculated over the main transport overpasses of the city of Kyiv at their full load (peak hours).

Автори (науковий ступінь, вчене звання, посада):

Сіпаков Ростислав Васильович
аспірант кафедри охорони праці і навколишнього середовища
Київський національний університет будівництва і архітектури
Адреса робоча: 03037 Україна, м. Київ, проспект Повітрофлотський, 31
тел. (044) 241-54-91, 241-55-58
e-mail: kaflab241ecolog@gmail.com

Трофімович Володимир Володимирович
кандидат технічних наук, професор, професор кафедри охорони праці і навколишнього середовища
Київський національний університет будівництва та архітектури
Адреса робоча: 03037 Україна, м. Київ, проспект Повітрофлотський, 31
тел.: (044) 241-54-91, 241-55-58
e-mail: kaflab241ecolog@gmail.com
ORCID: 0000-0002-9706-6086

Волошкіна Олена Семенівна
доктор технічних наук, завідувач кафедри охорони праці та навколишнього середовища
Київський національний університет будівництва та архітектури
Адреса робоча: 03037 Україна, м. Київ, проспект Повітрофлотський, 31
тел.: +38(050) 384 06 40
e-mail: e.voloshki@gmail.com
ORCID: 0000-0002-3671-4449, Researcher ID: G-8607-2017.

Березницька Юлія Олегівна
кандидат технічних наук, доцент кафедри охорони праці і навколишнього середовища
Київський національний університет будівництва а архітектури
Адреса робоча: 03037 Україна, м. Київ, проспект Повітрофлотський, 31
тел.: (044) 241-54-91, 241-55-58
e-mail: juli_mmm@ukr.net
ORCID: 0000-0001-7953-3974