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Hazard modelling of accidental event in urban environment

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Abstract. This paper investigates the impact of accidental event at the gas station which is situated in Dnipro City. The processes of chemical and thermal air pollution were simulated on the basis of developed numerical models. To simulate chemical and thermal air pollution mass conversation equation and energy equation were used. For the numerical integration of governing equations finite difference schemes of splitting were used. Also, the process of fragments scattering which appears as the result of explosion at the gas station was modelled. To simulate fragments scattering Newton second Law was used. To solve the governing equation Euler's method was used. Results of numerical experiments are presented.

1. Introduction

Predicting the risk of human injury during extreme situations at energy facilities is of great importance, especially when such facilities are located in residential areas. Extreme situations can cause chemical, thermal and mechanical pollution of the environment and, as a result, toxic, thermal injury to humans, as well as injury from the throwing action of fragments.

Therefore, it is extremely important for each energy facility located in a residential area to identify the affected areas and create a map of danger zones in cities where many energy facilities are located.

Assessment of the affected areas in case of extreme situations is based on the use of mathematical models. The most common are the Gaussian model [5, 7–11], numerical models [1–3, 6], analytical models [4]. It should be noted that in Ukraine there is an extremely limited range of applied models for scientifically based assessment of the consequences of extreme situations at energy facilities. The paper considers the use of a set of numerical models developed for assessment of the risk of chemical, thermal and mechanical damage to a person in the event of a possible fire at a gas station

IOP Conf. Series: Earth and Environmental Science **1499** (2025) 012051 doi:10.1088/1755-1315/1499/1/012051

2. Methods

2.1 Modeling toxic substances dispersion in atmosphere

To assess chemical contamination zones during combustion product emissions in the event of a fire at a gas station, the mass transfer equation is used:

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

where C is concentration of a chemically hazardous substance (fuel combustion product), u, v, w are components of the wind speed vector in the projection on the x, y, z coordinate axes in accordance, x_i, y_i, z_i are Cartesian coordinates of the i^{th} source of emission of a chemically hazardous substance at the facility, t is time, μ_x, μ_y, μ_z are atmospheric turbulent diffusion coefficients, $\delta(x_i, y_i, z_i)$ is Dirac delta function, by which the location of the emergency emission is specified in the model, Q is emission intensity of a chemically hazardous substance.

The atmospheric turbulent diffusion coefficients are defined as follows:

$$\mu_x=0.1\cdot u,\mu_y=0.1\cdot v,\mu_z=k_1\left(\frac{z}{z_1}\right)^m,$$

where k_1=0.1 m^2/s, z_1=1 m, m=1.

Boundary conditions for (1):

1. At the flow input boundary: C=0.

2. At the edge of the flow exit: $\partial C/\partial n$=0.

3. On the surface z=0, $z=L_z$ (L_z is the upper boundary of the region): $\partial C/\partial n$=0,

where n is the unit vector of the external normal to the surface.

For t=0 the initial condition is C=0.

Numerical integration of the mass transfer equation (1) is carried out using finite-difference schemes. First, the geometric splitting of the mass transfer equation is performed as follows:

$$\begin{cases} \frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C}{\partial x}\right), \\ \frac{\partial C}{\partial t}+\frac{\partial vC}{\partial y}=\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C}{\partial y}\right), \\ \frac{\partial C}{\partial t}+\frac{\partial wC}{\partial z}=\frac{\partial}{\partial z}\left(\mu_z\frac{\partial C}{\partial z}\right), \\ \frac{\partial C}{\partial t}=\sum Q_i(t)\delta(x-x_i)\delta(y-y_i)\delta(z-z_i). \end{cases} \tag{2}$$

Then the following transformations are performed:

IOP Conf. Series: Earth and Environmental Science **1499** (2025) 012051 doi:10.1088/1755-1315/1499/1/012051

$$\frac{\partial uC}{\partial x} = \frac{\partial u^+ C}{\partial x} + \frac{\partial u^- C}{\partial x},$$
$$\frac{\partial vC}{\partial y} = \frac{\partial v^+ C}{\partial y} + \frac{\partial v^- C}{\partial y},$$
$$\frac{\partial wC}{\partial z} = \frac{\partial w^+ C}{\partial z} + \frac{\partial w^- C}{\partial z},$$

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

Approximation of the derivatives is as follows:

$$\frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x}\right) \approx \mu_x \frac{C^{n+1}_{i+1,j,k} - C^{n+1}_{i,j,k}}{\Delta x^2},$$
$$-\mu_x \frac{C^{n+1}_{i,j,k} - C^{n+1}_{i-1,j,k}}{\Delta x^2} = M^-_{xx} C^{n+1} + M^+_{xx} C^{n+1},$$
$$\frac{\partial}{\partial y}\left(\mu_y \frac{\partial C}{\partial y}\right) \approx \mu_y \frac{C^{n+1}_{i,j+1,k} - C^{n+1}_{i,j,k}}{\Delta y^2},$$
$$-\mu_y \frac{C^{n+1}_{i,j,k} - C^{n+1}_{i,j-1,k}}{\Delta y^2} = M^-_{yy} C^{n+1} + M^+_{yy} C^{n+1},$$
$$\frac{\partial}{\partial z}\left(\mu_z \frac{\partial C}{\partial z}\right) \approx \mu_z \frac{C^{n+1}_{i,j,k+1} - C^{n+1}_{i,j,k}}{\Delta z^2},$$
$$-\mu_z \frac{C^{n+1}_{i,j,k} - C^{n+1}_{i,j,k-1}}{\Delta z^2} = M^-_{zz} C^{n+1} + M^+_{zz} C^{n+1},$$
$$\frac{\partial u^- C}{\partial x} \approx \frac{u^-_{i+1,j,k} C^{n+1}_{i+1,j,k} - u^-_{i,j,k} C^{n+1}_{i,j,k}}{\Delta x} = L^-_x C^{n+1},$$
$$\frac{\partial v^+ C}{\partial y} \approx \frac{v^+_{i,j+1,k} C^{n+1}_{i,j,k} - v^+_{i,j,k} C^{n+1}_{i,j-1,k}}{\Delta y} = L^+_y C^{n+1},$$
$$\frac{\partial v^- C}{\partial y} \approx \frac{v^-_{i,j+1,k} C^{n+1}_{i,j+1,k} - v^-_{i,j,k} C^{n+1}_{i,j,k}}{\Delta y} = L^-_y C^{n+1},$$
$$\frac{\partial w^+ C}{\partial z} \approx \frac{w^+_{i,j,k+1} C^{n+1}_{i,j,k} - w^+_{i,j,k} C^{n+1}_{i,j,k-1}}{\Delta z} = L^+_z C^{n+1},$$
$$\frac{\partial w^- C}{\partial z} \approx \frac{w^-_{i,j,k+1} C^{n+1}_{i,j,k+1} - w^-_{i,j,k} C^{n+1}_{i,j,k}}{\Delta z} = L^-_z C^{n+1}.$$

For the first mass transfer equation from (2), the finite-difference scheme is written as follows:

IOP Conf. Series: Earth and Environmental Science **1499** (2025) 012051 doi:10.1088/1755-1315/1499/1/012051

– step 1:

$$\frac{C_{i,j,k}^{k}-C_{i,j,k}^{n}}{\Delta t}+L_{x}^{+}C^{k}=M_{xx}^{+}C^{k}+M_{xx}^{-}C^{n};$$

– step 2:

$$\frac{C_{i,j,k}^{n+1}-C_{i,j,k}^{k}}{\Delta t}+L_{x}^{-}C^{n+1}=M_{xx}^{+}C^{n}+M_{xx}^{-}C^{n+1}.$$

The finite-difference scheme for the second mass transfer equation is written as follows:
– step 1:

$$\frac{C_{i,j,k}^{k}-C_{i,j,k}^{n}}{\Delta t}+L_{y}^{+}C^{k}=M_{yy}^{+}C^{k}+M_{yy}^{-}C^{n};$$

– step 2:

$$\frac{C_{i,j,k}^{n+1}-C_{i,j,k}^{k}}{\Delta t}+L_{y}^{-}C^{n+1}=M_{yy}^{+}C^{n}+M_{yy}^{-}C^{n+1}.$$

The finite-difference scheme for the third mass transfer equation is written as follows:
– step 1:

$$\frac{C_{i,j,k}^{k}-C_{i,j,k}^{n}}{\Delta t}+L_{z}^{+}C^{k}=M_{zz}^{+}C^{k}+M_{zz}^{-}C^{n},$$

– step 2:

$$\frac{C_{i,j,k}^{n+1}-C_{i,j,k}^{k}}{\Delta t}+L_{z}^{-}C^{n+1}=M_{zz}^{+}C^{n}+M_{zz}^{-}C^{n+1}.$$

To integrate the last equation from (2), Euler's method is used.

2.2 Modeling of thermal pollution of atmospheric air

In the case of a fire at a gas station, zones of thermal pollution of the atmospheric air are formed. For an express forecast of the dynamics of the formation of zones of thermal pollution, the energy equation in the Boussinesq approximation is used:

$$\frac{\partial T}{\partial t}+\frac{\partial uT}{\partial x}+\frac{\partial vT}{\partial y}+\frac{\partial wT}{\partial z}=div\left(a\,grad\,T\right) \tag{3}$$

where T is atmospheric air temperature, a=(a_x, a_y, a_z) are thermal conductivity coefficients; x_i, y_i, z_i are Cartesian coordinates of the fire location, t is time.

The boundary conditions for equation (3) are as follows:

1. At the flow inlet boundary: $T=T_{atm}$, where T_{atm} is the temperature of the atmospheric air at the beginning of the fire.

2. At the boundary of the flow exit from the computational domain: $\partial T/\partial n=0$, where n is the unit vector external normal to the surface.

3. On the surface $z=0$, $z=L_z$ (L_z is the upper boundary of the region) $\partial T/\partial n=0$, where n is the unit vector of the external normal to the surface.

For $t=0$ the initial condition is $T=T_{atm}$.

To solve the energy equation, the following splitting is performed:

$$\frac{\partial T}{\partial t}+\frac{\partial uT}{\partial x}+\frac{\partial vT}{\partial y}+\frac{\partial wT}{\partial z}=0, \tag{4}$$

$$\frac{\partial T}{\partial t}=\frac{\partial}{\partial x}\left(a_x\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial y}\left(a_y\frac{\partial T}{\partial y}\right)+\frac{\partial}{\partial z}\left(a_z\frac{\partial T}{\partial z}\right). \tag{5}$$

For numerical integration of (4), the following transformations are used:

$$\frac{\partial uT}{\partial x}=\frac{\partial u^{+}T}{\partial x}+\frac{\partial u^{-}T}{\partial x},$$
$$\frac{\partial vT}{\partial y}=\frac{\partial v^{+}T}{\partial y}+\frac{\partial v^{-}T}{\partial y},$$
$$\frac{\partial u^{+}T}{\partial x}\approx\frac{u^{+}_{i+1,j}T^{n+1}_{i,j}-u^{+}_{i,j}T^{n+1}_{i-1,j}}{\Delta x}=L^{+}_{x}T^{n+1},$$
$$\frac{\partial u^{-}T}{\partial x}\approx\frac{u^{-}_{i+1,j}T^{n+1}_{i+1,j}-u^{-}_{i,j}T^{n+1}_{i,j}}{\Delta x}=L^{-}_{x}T^{n+1},$$
$$\frac{\partial \nu^{+}T}{\partial y}\approx\frac{\nu^{+}_{i,j+1}T_{i,j}-\nu^{+}_{i,j}T_{i,j-1}}{\Delta y}=L^{+}_{y}T^{n+1},$$
$$\frac{\partial \nu^{-}T}{\partial y}\approx\frac{\nu^{-}_{i,j+1}T_{i,j+1}-\nu^{-}_{i,j}T_{i,j}}{\Delta y}=L^{-}_{y}T^{n+1}.$$

The splitting scheme for equation (5) is written as follows:

– in the first step the difference equation has the form:

$$\frac{T^{k}_{i,j}-T^{n}_{i,j}}{\Delta t}+L^{+}{}_{x}T^{k}+L^{+}{}_{y}T^{k}=0;$$

– in the second step of splitting, the difference equation has the form:

$$\frac{T^{n+1}_{i,j}-T^{k}_{i,j}}{\Delta t}+L^{-}{}_{x}T^{n+1}+L^{-}{}_{y}T^{n+1}=0.$$

IOP Conf. Series: Earth and Environmental Science **1499** (2025) 012051 doi:10.1088/1755-1315/1499/1/012051

The unknown temperature value T in each equation is determined by the "running account" formula.

For numerical integration of (6) the difference scheme of conditional approximation is used. The calculated dependence has the form

– at the first stage:

$$\frac{T_{i,j,k}^{n+\frac{1}{2}}-T_{i,j,k}^{n}}{\Delta t}=a_x\left[\frac{-T_{i,j,k}^{n+\frac{1}{2}}+T_{i-1,j,k}^{n+\frac{1}{2}}}{\Delta x^2}\right]+a_y\left[\frac{-T_{i,j,k}^{n+\frac{1}{2}}+T_{i,j-1,k}^{n+\frac{1}{2}}}{\Delta y^2}\right]+a_z\left[\frac{-T_{i,j,k}^{n+\frac{1}{2}}+T_{i,j,k-1}^{n+\frac{1}{2}}}{\Delta z^2}\right];$$

– in the second stage:

$$\frac{T_{i,j,k}^{n+1}-T_{i,j,k}^{n+\frac{1}{2}}}{\Delta t}=a_x\left[\frac{T_{i+1,j,k}^{n+1}-T_{i,j,k}^{n+1}}{\Delta x^2}\right]+a_y\left[\frac{T_{i,j+1,k}^{n+1}-T_{i,j,k}^{n+1}}{\Delta y^2}\right]+a_z\left[\frac{T_{i,j,k+1}^{n+1}-T_{i,j,k}^{n+1}}{\Delta z^2}\right].$$

It should be noted the following aspect: when performing the calculations, it was assumed that the value of the thermal diffusivity coefficients is equal to the value of the atmospheric turbulent diffusion coefficients.

2.3 Determination of the fragments scattering zone

In an extreme situation at a gas station, an explosion is possible, in which various fragments are formed from damaged equipment. Since the fragments move at high speed, there is a risk of injury to a person at a certain distance from the gas station. Therefore, there is the task of determining the fragments scattering zone in order to determine the range from the explosion where a person can be injured arises.

Newton's second law was used to determine the dynamics of the movement of a fragment in atmospheric air:

$$m\frac{dV}{dt}=-F_R-F_g, \tag{6}$$

where m is mass of the fragment, $V(u, v)$ is vector of velocity of the fragment in the medium, $F_g=mg$ is force of gravity, $F_R=C_x\frac{\rho_в V^2}{2}S$ is force of resistance, C_x is coefficient of resistance, $\rho_в$ is density of the medium, S is area of the midsection of the fragment, t is time.

For practical use of equation (6), it's written in projection on the coordinate axis for each zone:

$$m\frac{du}{dt}=-C_x\frac{\rho_в u^2}{2}\mathrm{S}, \tag{7}$$

$$m\frac{dv}{dt}=-C_x\frac{\rho_в v^2}{2}S-mg, \tag{8}$$

where *u, v* are projections of the velocity vector of the fragment on the coordinate axis; S is the area of the midsection of the fragment.

Note that the Y axis has direction vertically upwards, and the X axis has direction of horizontal movement of the fragment.

Then, numerical integration of (2) and (3) is performed to determine the velocity of the fragment at different times. Numerical integration of (7) and (8) is performed using the Euler method.

The distance Δx of the fragment's flight per time step Δt is equal to:

$$\Delta x = \Delta t \cdot u(t).$$

Distance of fragment scattering from place explosion is defined as follows

$$x(t) = x_0 + \sum \Delta x,$$

where x_0 is the initial coordinate of the fragment location.

Since the mathematical model uses the value of the midsection S to calculate the resistance force, then the value of the parameter S is determined computationally. First, it is necessary to determine what shape of the fragment will be used in the model. For example, if the shape of the fragment is modeled as a "circle", then the volume of the fragment can be represented as follows:

$$W = \frac{4}{3}\pi R^3,$$

where W is volume of the fragment, R is radius.

The volume of the fragment W can be determined experimentally, for example, using Archimedes' principle, that is, by measuring the volume of water that was displaced from the container where the fragment was placed. Then, the radius of the "circle" is determined as:

$$R = \sqrt[3]{\frac{3W}{4\pi}}.$$

The value of the midsection area will be $S = 0.785(2R)^2$.

The developed numerical models were implemented in software. FORTRAN was used for programming.

3. Results

On the basis of the developed numerical models, calculations of chemical, thermal, and mechanical air pollution near the OKKO gas station in the event of a fire at the gas station due to an equipment explosion that leads to the dispersal of fragment were performed. It is assumed that at the time of the emergency at the gas station, the wind speed at a height of 10 m is 7 m/s; the air temperature at the fire site is 1100 °C; it is assumed that the intensity of CO (fuel combustion product) emission is 10000 g/s, the emission takes place at a height of 3 m; initial velocity of the fragment is 80 m/s; drag coefficient of the fragment is 0.47, it is assumed that the

IOP Conf. Series: Earth and Environmental Science **1499** (2025) 012051 doi:10.1088/1755-1315/1499/1/012051

fragment has the shape of a "ball", the reduced diameter of the fragment is 0.01 m, density of the fragment material is 7800 kg/m^3; height of the fragment ejection is 12 m, angle of departure of the fragment is α=15°. When the fragment was ejected, the impact zone was assumed to be the area where the fragment is at a height of about 1.5 m, which corresponds to the location of important human organs.

The modeling results are shown in Figures 1-3. Figure 1 shows the damage zone when the fragment is flying. The "circle" shown in Figure 1 shows the boundary where the fragment will be at a height of about 1.5 m. The diameter of this "circle" is about 370 m.

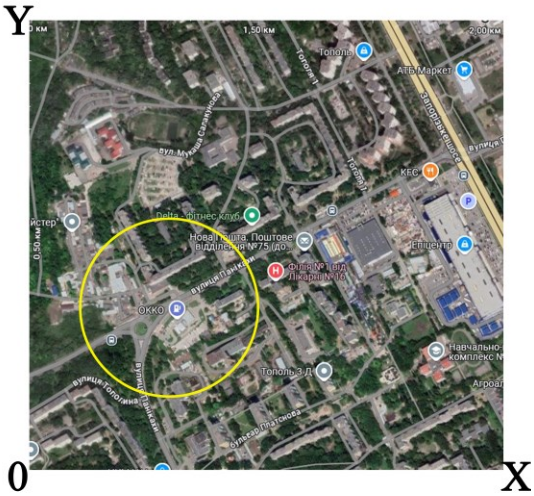

Figure 1. Impact zone in case of flying debris.

Further, the figures show the dynamics of the development of chemical air pollution zones in the event of a fire at a gas station. In the figures, the wind direction is shown by an arrow.

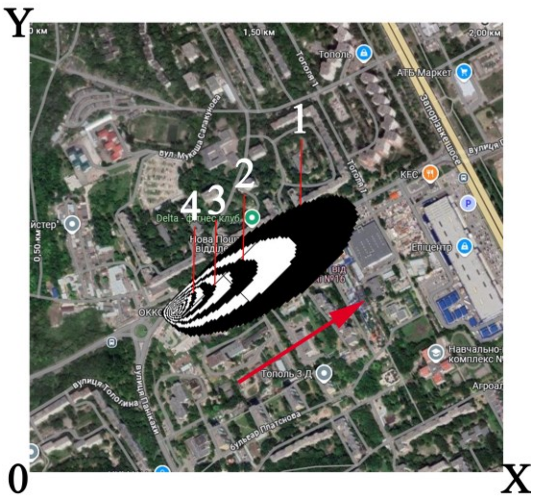

Figure 2. Chemical contamination zone (CO concentration, level z=3 m, t=1.2 min):
1–C=0.07 g/m^3; 2–C=0.12 g/m^3;3–C=0.26 g/m^3; 4–C=0.99 g/m^3.

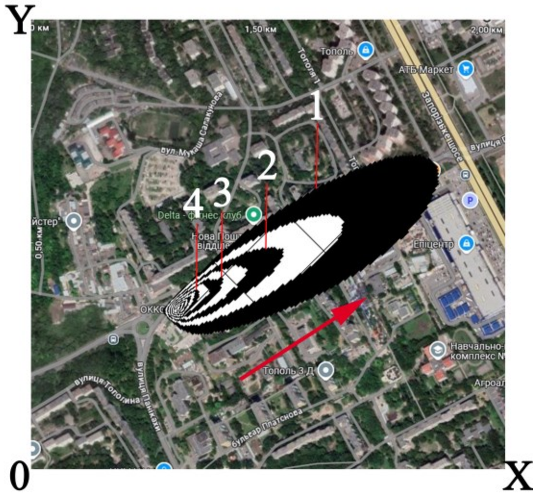

Figure 3. Chemical contamination zone (CO concentration, level z=3 m, t=1.5 min):
1–C=0.08 g/m^3; 2–C=0.14 g/m^3;3–C=0.27 g/m^3; 4–C=1.03 g/m^3.

If we take into account that the maximum single concentration for CO is 5 mg/m^3, we can see from the figures that very quickly a zone is created around the gas station where chemical poisoning is possible.

Further, Figure 4 shows the zone of thermal air pollution during a fire at a gas station for a time t=1.3 min after the start of the fire (z=3 m).

Figure 4. Thermal contamination zone (level z=3 m, t=1.3 min):
1–T=118 °C; 2–T=249 °C;3–T=379 °C; 4–T=447 °C.

If we take into account that at an air temperature of 100 °C and above, burns of the human respiratory tract occur, then, as can be seen from Fig. 4, people on the streets near gas stations will suffer severe thermal damage.

The results of the computational experiment show that the location of gas stations in rural areas creates a real risk of human injury. Thus, it is necessary to design systems to reduce the negative impact of an extreme situation on the environment near gas stations.

4. Conclusions.

A tool for comprehensive assessment of environmental pollution in case of an emergency at a gas station was created. The risk of damage is assessed using the developed tool on the basis of fundamental models, which allows to obtain scientifically sound forecast results. The modelling results show that the location of gas stations in rural areas poses a high risk of human exposure. To reduce risk of citizens hitting it is necessary to made protection screens near gas stations. It is also will be useful to have special water systems near the gas stations to create “water wall” near the spot of firing. This will allow to minimize the heat “load” on the environment if the accident takes place at the gas station.

References

[1] Biliaieva V V, Kalashnikov I V, Berlov O V, Kozachyna V A and Tymoshenko O A 2023 *Ukr. J. Civil Eng. Arch.* **6(018)** 22-18
[2] Biliaiev M M, Berlov O V, Biliaieva V V and Tymoshenko O A 2023 *Ukr. J. Civil Eng. Arch.* **4(016)** 34-39
[3] Biliaiev M M, Biliaieva V V, Berlov O V and Kozachyna V A 2022 *CFD modeling in analyzing the effectiveness of environmental and workplace protection systems* (Ukraine: Zhurfond) p 268
[4] Bruiatskyi Ye V 2000 Theory of atmospheric diffusion of radioactive releases (Kyiv, Ukraine: Institute of Hydromechanics of NAS of Ukraine) p 443
[5] Barret A M 2009 *Mathematical Modeling and Decision Analysis for Terrorism Defense: Assessing Chlorine Truck Attack Consequence and Countermeasure Cost Effectiveness* (Pittsburg, Pennsylvania, USA) p 123
[6] Biliaiev M M and Kharytonov M M 2012 *Air Pollut. Model. Appl.* **XXI** 87-91
[7] Ilic P, Ilic S and Stojanovic Bjelic L 2018 *Quality of Life* **9** 38-45
[8] Pourbabaki R, Karimi A and Yazdanirad S 2019 *J. Health. Field.* **6(3)** 24199-24199
[9] Ramli A, Ghani N A, Hamid N A and Desa M S Z M 2018 *Proceedings* **2(20)** 1-4
[10] Hui S and Guoning D 2012 *Procedia Engineering* **45** 352-359
[11] Tseng J M, Su T S and Kuo C Y 2012 *Procedia Engineering* **45** 384-389