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Numerical simulation of toxic chemical transport after accidental release at chemical plant

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Abstract. Toxic chemical release may occur at different plants and impact directly on the people in the working areas. It is very important to predict atmosphere pollution and make risk assessment for accidental releases. CFD modeling is a powerful tool to solve these problems. This work is concerning on development of quick computing numerical model to predict air pollution in case of accidental solid propellant burning at the chemical plant. The model is based on transport equation for the products of propellant burning. Air flow on the industrial site is computed on the basis of potential flow model. To solve governing equations implicit finite difference schemes of splitting have been used. The results of numerical experiments are presented.

Keywords: atmosphere pollution, accidental release, risk assessment, numerical model, missile solid propellant.

1. Introduction

Pavlograd Chemical Plant is one of the most powerful chemical plants in Ukraine. This is the main enterprise where solid propellants for missiles of different types are produced. It is very important to predict atmosphere pollution, assess risk of hitting in case of accidental emissions at this plant. These emissions appear in case of propellant firing because of the products of propellant burning are toxic chemicals. This atmosphere pollution may be very intensive especially at the territory of the plant. This information is especially important for emergency preparedness and response.

The most used mathematical models to predict atmosphere pollution in case of accidental emission may be divided into three groups. The first group consists of empirical models. Such models are used now in Ukraine, in The State Emergency Service. These empirical

models were developed more than 60 years ago and the models have been “updated” during the years. These models are based on some algebraic relations which are used to calculate area of contamination zone, but predictions are “correct” only for wind speed V=1m/s. The second group of models includes models which are based on Gaussian model or analytical solution of contaminant transport equation [1-3]. These models are implemented in different, widely used softwares, such as ALOHA, SLAB, PHAST, etc. These models allow to solve different problems in the field of air pollution and predict consequences of toxic chemical release. The models are widely used in practice because of their capability to obtain quick results which satisfy user. It is very important that these models take into account important physical factors which influence plume formation. The third group of models includes CFD models which allow to perform numerical experiment with account of complex configuration of different obstacles which distort airflow pattern and thus distort plume form and pollutant dispersion. CFD models are the most powerful tool to predict air contamination [4 -9]. The core of these models are Navier–Stokes equations (viscous flow model) which are coupled with different turbulence models [4-8]. CFD models are the basis of the world known codes, for example ANSYS. But, application of viscous flow model, for high Reynolds numbers, demands application of very refine grid in order to simulate correctly viscous effects, for example, near solid walls. Even, in case of laminar flow, we must choose small grid steps in order that the artificial viscosity which appears as a result of approximation, not exceed real viscosity. So, CFD models are not quick computing ones and this factor makes an obstacle for their everyday use.

In this paper we present numerical model which was developed for practical use in The State Emergency Service (SES) of Ukraine in Dnipropetrovsk region. According to the deal with SES we had to solve three problems: develop mathematical model to simulate pollutant dispersion in case of short-term pollutant emission during solid propellant accidental firing (1); develop numerical model of pollutant dispersion using finite difference schemes (2); develop Fluid Dynamic Computational program which is capable to compute air flow and pollutant dispersion at the industrial site using personal computers which are available in Ukraine (3). The main demand to the CFD model was quick computing and possibility to take into account buildings effect on plume formation.

2. Governing equations

We studied the problem of air pollution in case of accidental firing of solid propellant for missile Grim-2 (Fig. 1).

Fig. 1. Solid propellant engine for missile Grim-2
(https://www.kp.ru/online/news/2980501/)

In this case the process of pollutants emission is short – term and very intensive. Solid propellant for missile Grim-2 consists of: ammonium perchlorate (NH_4ClO_4), aluminium (Al) and astringent. During this propellant firing different pollutants are emitted into atmosphere. We studied atmosphere pollution as a result of an ammonium perchlorate transformation during firing. Chemical transformation of this component may be written as

follows:

$$2NH_4ClO_4 = Cl_2 + O_2 + 4H_2O + 2NO\,. \quad (1)$$

Dispersion of Cl_2 and NO in atmosphere is of main interest. To simulate process of their dispersion the following transport equation was used [10, 11]:

$$\begin{aligned} &\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} = \\ &= \frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial C}{\partial y}\right) + \\ &+ \sum Q_i(t)\delta(x - x_i(t))\delta(y - y_i(t)) \end{aligned} \quad (2)$$

where u, v denotes wind velocity components in x, y direction respectively; C denotes averaged concentration of chlorine or NO; μ_x, μ_y refer to the diffusion coefficients; $x_i(t)$, $y_i(t)$ are the coordinates of point source of emission; $Q_i(t)$ denotes pollutant emission rate;$\delta(x-x_i(t))\delta(y-y_i(t))$ denote Dirac delta-function; t is time.

Averaged concentration is determined as:

$$C(x,y) = \frac{1}{H}\int C(x,y,z)dz\,,$$

where H is height which is used to perform averaging.

In (2) coordinates of point source of emission depend on time and we can simulate, if we need, pollution from moving source of emission. To simulate this process we must set dependencies which indicate the law of motion: $x=f(t)$, $y=f(t)$ (speed and trajectory).

Worthy of note, that NO has chemical conversion in atmosphere. Chemical reactions may be written as follows [12, 13]:

$$NO + O_3 \xrightarrow{k_1} NO_2 + O_2\,, \quad (3)$$

$$NO_2 + h_v \xrightarrow{J} NO + O\,, \quad (4)$$

$$O + O_2 + M \longrightarrow O_3 + M\,. \quad (5)$$

To simulate NO, NO_2, O_3 decomposition, the following simplified equations may be used [12, 13]:

$$\frac{d[NO_2]}{dt} = -k_1[NO][O_3] - J_{NO_2}[NO_2]\,, \quad (6)$$

$$\frac{d[NO]}{dt} = -k_1[NO][O_3] + J_{NO_2}[NO_2]\,, \quad (7)$$

$$\frac{d[O_3]}{dt} = -k_1[NO][O_3] + J_{NO_2}[NO_2]\,, \quad (8)$$

where k_1, J_{NO_2} are constants [12].

In this work we simulate an atmosphere pollution during solid propellant firing with account of chemical reactions (3) – (5). To simulate NO_2, O_3 dispersion we also used transport equation (2).

To simulate an air flow at the industrial sites where different building are situated and these buildings “distort” wind pattern we used a model of potential flow (9), (10):

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} = 0 \quad (9)$$

$$u = \frac{\partial P}{\partial x}, v = \frac{\partial P}{\partial y} \tag{10}$$

where P denotes velocity potential.

Boundary conditions for governing equations are as follows [10, 11]:

1) at the inlet boundary: $\frac{\partial P}{\partial n} = V_n, C = C_{in}$, where V_n denotes known wind velocity; C_{in} is known concentration (we assume C_{in}=0 for Cl_2; for another pollutants this concentration was assumed to be the background concentration);

2) at the solid boundaries: $\frac{\partial P}{\partial n} = 0, \frac{\partial C}{\partial n} = 0$, where n denotes unit external normal to the solid boundary;

3) at the outlet boundary: $P=P_0$+const where P_0 is an arbitrary value and it is known. For concentration, we set $\frac{\partial C}{\partial n} = 0$, and it means that we neglect the diffusion process at the outlet boundary.

Initial condition, at t=0, is: C=0 (for Cl_2) and $C=C_0$ (C_0 is known background concentration of NO, NO_2, O_3).

3. Numerical model

In order to build a numerical model, we must transform differential equation into discrete form and use numerical technique of solving. For numerical integration of governing equations, we used implicit finite difference schemes of splitting which were traditionally used in School of Computational Fluid Dynamics in Dnipro City (former Dnipropetrovsk City, Ukraine).

Numerical integration was performed using rectangular grid. Concentration of pollutant and velocity potential P were determined in the centers of computational cells. Velocity components were determined at the sides of computational cells. This approach allowed to create conservative finite difference analog of transport differential equation (2).

To solve numerically (9) we used finite difference scheme of conditional approximation [14]. To perform integration this equation was written in evolutionary form:

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2}, \tag{11}$$

where t denotes fictitious time. For $t \to \infty$ solution of equation (11) tends to the solution of equation (9) [14].

Further, we approximated derivatives from equation (11) and split finite difference analog in two steps. Finite difference equation at the first step was as follows [14]:

$$\frac{P_{ij}^{n+\frac{1}{2}} - P_{ij}^{n}}{\Delta t} = \left[\frac{-P_{ij}^{n+\frac{1}{2}} + P_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} \right] + \left[\frac{-P_{ij}^{n+\frac{1}{2}} + P_{i,j-1}^{n+\frac{1}{2}}}{\Delta y^2} \right]. \tag{12}$$

Finite difference equation at the second step was as follows [14]:

$$\frac{P_{ij}^{n+1} - P_{ij}^{n+\frac{1}{2}}}{\Delta t} = \left[\frac{P_{i+1,j}^{n+1} - P_{ij}^{n+1}}{\Delta x^2} \right] + \left[\frac{P_{i,j+1}^{n+1} - P_{i,j}^{n+1}}{\Delta y^2} \right]. \tag{13}$$

Sum of equation (12) and equation (13) gives the full approximation of equation (11).

Finite difference equations (12), (13) are implicit ones, but unknown values $P_{ij}^{n+\frac{1}{2}}, P_{ij}^{n+1}$ are calculated using explicit formulae of "running calculation" at each step of splitting [14]. To begin calculations, we must set "initial" condition for fictitious time t=0. We set P=0 in the computational region for t=0.

Computational procedure is over if:

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

where ε is a small number.

After calculation velocity potential field *P* we can calculate velocity components as follows

$$u = \frac{P_{i+1,j} - P_{ij}}{\Delta x}, v = \frac{P_{i,j+1} - P_{ij}}{\Delta y}.$$

Computed velocity components *u*, *v* are used at the next step to simulate pollutant dispersion on the basis of equation (2).

To solve numerically (2) we used change–triangle finite difference scheme [11]. This is four steps scheme of splitting. The finite difference equations at each step are as follows:

At the first step of splitting (*k*=1/4):

$$\begin{aligned} &\frac{C_{ij}^{n+k} - C_{ij}^{n}}{\Delta t} + \frac{1}{2}(L_x^+ C^k + L_y^+ C^k) = \\ &= \frac{1}{4}(M_{xx}^+ C^k + M_{xx}^- C^n + M_{yy}^+ C^k + M_{yy}^- C^n) + \sum_{l=1}^{N} \frac{\overline{Q}_l}{4} \delta_l . \end{aligned} \tag{14}$$

At the second step of splitting (*k*=*n*+1/2; *c*=*n*+1/4):

$$\begin{aligned} &\frac{C_{ij}^{k} - C_{ij}^{c}}{\Delta t} + \frac{1}{2}(L_x^- C^k + L_y^- C^k) = \\ &= \frac{1}{4}(M_{xx}^- C^k + M_{xx}^+ C^c + M_{yy}^- C^k + M_{yy}^+ C^c) + \sum_{l=1}^{N} \frac{\overline{Q}_l}{4} \delta_l . \end{aligned} \tag{15}$$

At the third step of splitting (*k*=*n*+3/4; *c*=*n*+1/2):

$$\begin{aligned} &\frac{C_{ij}^{k} - C_{ij}^{c}}{\Delta t} + \frac{1}{2}(L_x^+ C^k + L_y^- C^k) = \\ &= \frac{1}{4}(M_{xx}^- C^c + M_{xx}^+ C^k + M_{yy}^- C^k + M_{yy}^+ C^c) + \sum_{l=1}^{N} \frac{\overline{Q}_l}{4} \delta_l . \end{aligned} \tag{16}$$

At the fourth step of splitting (*k*=*n*+1; *c*=*n*+3/4):

$$\begin{aligned} &\frac{C_{ij}^{k} - C_{ij}^{c}}{\Delta t} + \frac{1}{2}(L_x^- C^k + L_y^+ C^k) = \\ &= \frac{1}{4}(M_{xx}^- C^k + M_{xx}^+ C^c + M_{yy}^- C^c + M_{yy}^+ C^k) + \sum_{l=1}^{N} \frac{\overline{Q}_l}{4} \delta_l . \end{aligned} \tag{17}$$

In (14)-(17) we used the following designations [11]:

$$\overline{Q} = \frac{Q_{ij}}{\Delta x \Delta y}, u^+ = \frac{u + |u|}{2}, u^- = \frac{u - |u|}{2}, v^+ = \frac{v + |v|}{2}, v^- = \frac{v - |v|}{2},$$

$$\frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x}\right) \approx \mu_x \frac{C_{i+1.j}^{n+1} - C_{ij}^{n+1}}{\Delta x^2} - \mu_x \frac{C_{ij}^{n+1} - C_{i-1,j}^{n+1}}{\Delta x^2} = M_{xx}^- C^{n+1} + M_{xx}^+ C^{n+1}, \text{ etc.}$$

At each step of splitting the unknown value *C* is calculated using explicit formula of "running calculation" [11].

To solve (6)-(8) we used Euler method [14].

We programed all finite difference equations and developed computer program "Air2D". We used FORTAN PowerStation 4.0 to create tool for prediction accidental air pollution. Developed program consists of following subprograms:

- subprogram “Pot” serves to compute velocity potential field in the region;
- subprogram “Vel” serves to compute velocity components on the basis of velocity potential field;
- subprogram “Cont” serves to compute pollutant dispersion in the region;
- subprogram “Chem” serves to compute chemical transformation of pollutants;
- subprogram “Sou” serves to compute pollutants emission rate and change of source position in case if we study emission from moving source;
- subprogram “Ri” serves to compute potential risk on the basis of computed concentrations;
- subprogram “PRi” serves to print results of computer simulations.

Main Program coordinates work of all subprograms. Input of initial data (meteorological data, position of source, etc) is made using “Data” file. In this file user forms geometry of the computational region. To form position of the buildings we used “markers” (porosity technique) [11]. “Markers” separate computational cells where the air flow takes place from the cells where buildings are situated. Markers are also used to indicate computational cells where emission takes place. We also use markers to indicate the trajectory of source if we study emission from the moving source.

The main steps of the algorithm to solve the whole problem are as follows:
- we solve numerically equation (11) and obtain field of velocity potential P in the computational region where buildings are situated (step 1);
- on the basis of computed data for P we compute air velocity components in the computational region (step 2);
- we compute emission rate of pollutants (step 3)
- we solve numerically transport equation (2) to obtain concentration fields for different pollutants (step 4);
- we solve numerically equations of pollutants chemical transformations and , as a result, change of concentrations in the computational region (step 5);
- we repeat calculations from step (3).

Because of lack of experimental data, validation of numerical model was performed by comparing numerical results which were obtained on different grids with analytical solutions of (2) and (11).

For practice, it’s important not only to predict contamination zones after possible accidental release but to determine zones of potential risk at the enterprise. Change of wind velocity affects the dimensions and intensity of contamination zone and thus affects the length of hitting zone. Schematically it is shown in Fig. 2 [15].

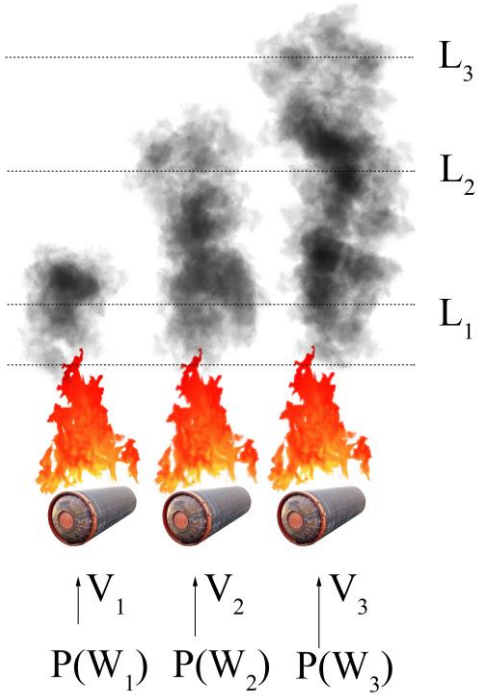

Fig. 2. Formation of hitting zone under different wind velocities [15]

For example, we have three typical meteorological situations, which have different wind velocities: V_1, V_2, V_3 (Fig .2). Assume, that for the region, where we study accidental

pollution, each meteorological situation has probability $P(W_i)$, (i=1, 2, 3). We can see from Fig. 2 that, for person, who is situated at distance "L_3" from the point of emission, threat of hitting exists only for the third meteorological situation. But, for person, who is situated at distance "L_1" from the point of emission, threat of hitting exists for all three meteorological situations. So, if person is situated at distance "l" from the point of emission then probability of toxic hitting (potential risk) can be determined as:

$$P(l) = \sum P(W_k) \geq l \,, \tag{18}$$

where $P(W_k)$ denotes probability of all typical meteorological situations for which the person falls into zone of hitting. In this zone concentration is higher than the level of concern.

For example, let us have: $P(W_1) = 60\%$, $P(W_2) = 30\%$, $P(W_3) = 10\%$. Then, potential risk, for person who is at distance L_1 (Fig. 2), is: $P(L_1)$ = 60%+30%+10%=100%. For person who is at distance L_2 (Fig. 2), potential risk of toxic hitting is: $P(L_2)$ = 30%+10%=40%. So, it means that it is very dangerous to be at the distance L_1 for all meteorological situations in the region.

So, if we have information about typical meteorological situations in the region, we can perform calculations for each meteorological situation and obtain concentrations in every point in domain of interest. On the basis of this information and using dependence (18) we can make "mapping" zones of potential risk. This "map" will be like a map of "minefield" and it shows points where toxic hitting will take place for each meteorological situation in the region or where the probability of toxic hitting is low.

4. Results

We used developed computer program to simulate air pollution at the industrial site of Pavlograd Chemical Plant. Fig. 3 shows computational region at the plant.

Fig. 3. Computational region (Google image 2019): 1 – emission place; 2 – working place; 3, 4, 5 – buildings

Numerical experiment was performed for the following data: duration of missile solid propellant firing was 4 minutes. Emission rate of Cl_2, NO was calculated using (1). Initial data (at t=0), background concentrations are: 0.06 mg/m^3 for NO, 0.04 mg/m^3 for NO_2; 0 mg/m^3 for Cl_2; 0.025 mg/m^3 for O_3. We assumed that probability of wind speed V=3 m/s was 86%; probability of wind speed V= 7 m/s was 14%. We used grid: 40x40 knots.

We assumed that if Cl_2 concentration was more than 3 mg/m3 and NO concentration was more than 0.6 mg/m^3, than a person, at this point, was in the risk zone.

Fig. 4 shows contaminated zone at the industrial site (modeling for wind velocity V=7 m/s).

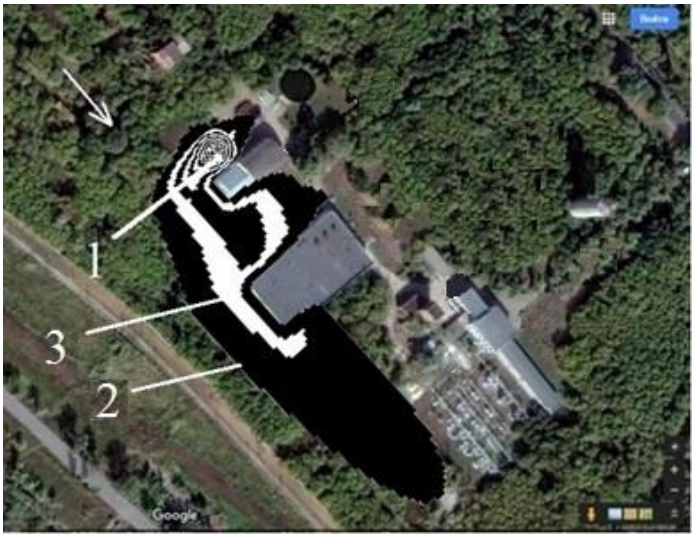

Fig. 4. Contamination zone (Cl_2), t=21s: 1 – emission place; 2 – concentration C= 250 mg/m^3; 3 – concentration C=1250 mg/m^3

We see from Fig. 4 that big contaminated zone was formed between two buildings (building #3 and #4, see Fig. 3). It means that pollutant can inflows these buildings and hit people there.

Fig. 5, 6 show map of potential risk in the computational region. In these figures number "99" means 100% probability of death hitting.

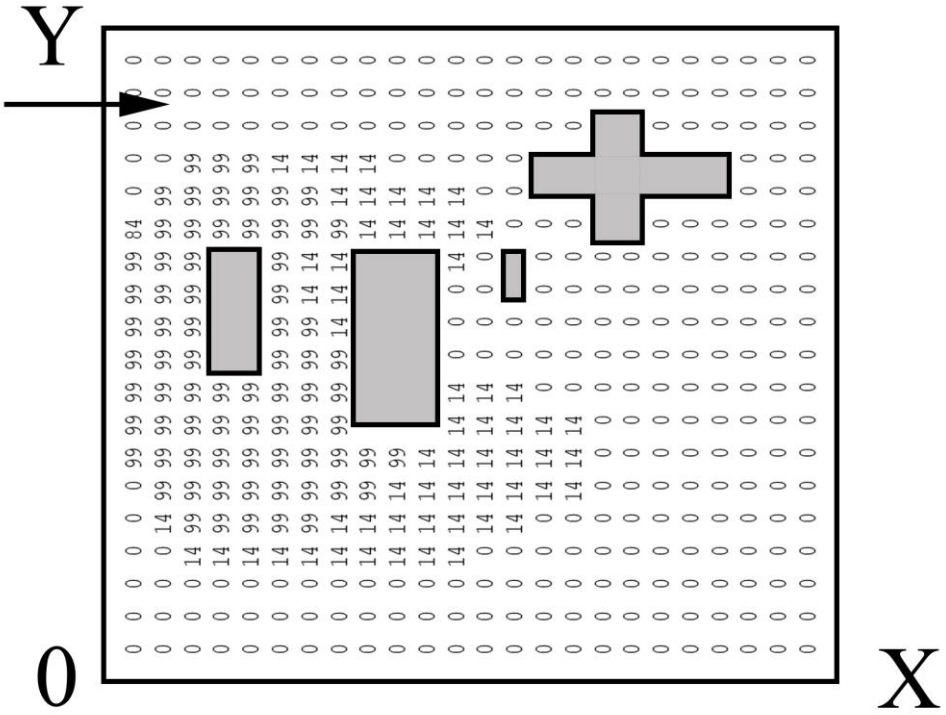

Fig. 5. Probability of toxic hitting, t= 8 s (for Cl_2 emission)

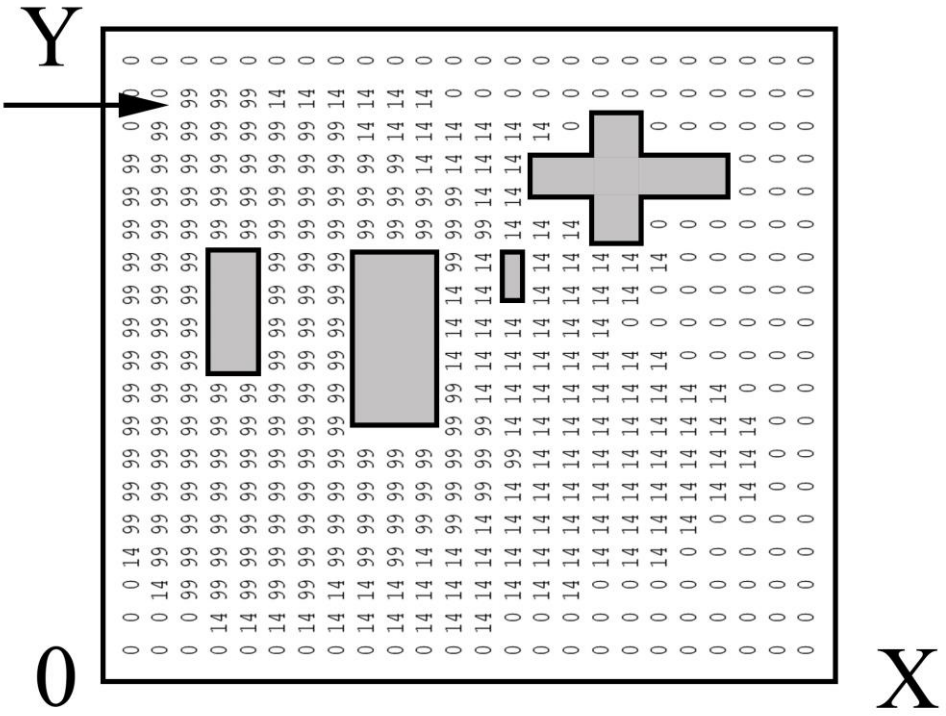

Fig. 6. Probability of toxic hitting, t= 8 s (for *NO* emission)

We can see from Fig. 5, 6 that for the meteorological situations which were considered the potential risk of toxic hitting is very high. Fig. 7 shows Cl_2 concentration at the working place (Fig. 3, position 2).

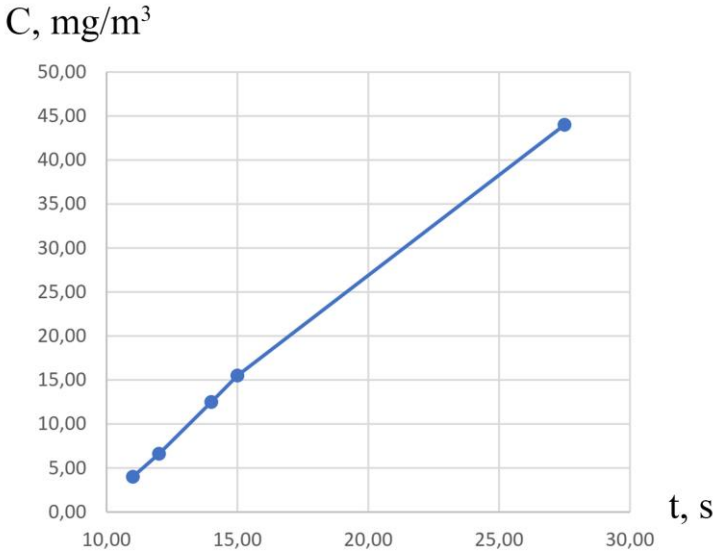

Fig. 7. Cl_2 concentration at working place

From Fig. 7 we see that toxic chemical concentration rapidly rises at the industrial site and its value is much more the level of concern. From practical point of view, it means that workers at this site are in zone of death hitting.

Worthy of note that computational time was 5 s. So, developed model can be used for everyday calculations to obtain "first order" information to determine zones of potential risk at the enterprise.

5. Conclusions

The paper presents the numerical model and computer program to perform risk analysis in

case of air pollution when the missile solid propellant is firing. The model allows to take into account buildings affect on contamination zone formation. Air flow pattern is computed using model of potential flow. That allows to solve quickly aerodynamic problem. Also, chemical transformations of pollutants are taken into account when the process of pollutants dispersion is under consideration. Results of numerical simulation show that developed model allows to obtain important information which is necessary to assess zones of potential risk at the territory of the chemical plant. Results of performed numerical experiment show that if accidental propellant firing at the industrial site takes place it will result in quick and very dangerous air contamination for lives.

Further, we will develop submodel to simulate pollutant intrusion into buildings for prediction the unsteady process of air pollution there.

6. Financial support

No.

7. Conflict of interest

The authors declare no conflicts of interest.

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Authors' contributions. Processed and analyzed primary data: OB, VK. Pollutant transport model development: MB, IK. Air flow model development: MB, IK. Risk assessment algorithm development: MB, IK. Programming finite difference equations: VB, VK, OB. Numerical experiments performing: VB, VK. Processed numerical experiments data: VK, OB. Wrote the paper: MB, VK.

References

[1]. HANNA S., CHANG J., MAZZOLA T., *An analytical urban puff dispersion model compared with tracer observations in JU2003*, 18th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, pp. 1-5, 2017.

[2]. ILIC P., ILIC S., STOJANOVIC BJELIC L., *Hazard modelling of accidental release chlorine gas using modern tool – ALOHA Software*, Quality of Life, **9**, pp. 38-45, 2018.

[3]. BHOSALE V.A., PATIL K.I., DEHANKAR P.B., *Study of accidental releases heavy gas dispersion comparing SLAB Model and SCREEN -3 Model*, International Journal of Engineering Sciences & Research Technology, **4(1)**, pp. 765 – 769, 2015.

[4]. BORIS J., PATNAIK G., OBENSCHAIN K., MOSES A., OBENSCHAIN M.-Y., THEODORE Y., DELANEY J., DONNELLY J., *Fast and accurate prediction of windborne contaminant plumes for civil defense in cities*, The Fifth International Symposium on Computational Wind Engineering (CWE2010), pp. 1-9, 2010

[5]. BIERINGER P.E., PIÑA A., SOHN M.D., JONKER H.J.J., BIEBERBACH G.JR., LORENZETTI D.M., FRY, R.N. JR., *Large-Eddy Simulation (LES) based system for producing coupled urban and indoor airborne contaminant transport and dispersion solutions*, 18th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, pp. 1-5, 2017.

[6]. SIDERIS G.M., CHRISTOLIS M.N., MARCATOS N.C., *Numerical simulation of pollutants dispersion around an electric-arc-furnace in case of an accidental release*, Biodiversity International Journal, **4(1)**, pp. 50-57, 2020.

[7]. LACOME J.-M., TRUCHOT D., DUPLANTIER S., *Application of an innovative risk dedicated procedure for both conventional and 3D atmospheric dispersion models evaluation*, 18th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, pp. 1-5, 2017.

[8]. NAKAYAMA H., TAKEMI T., *LES studies for predicting plume concentrations around nuclear facilities using an overlapping technique*, 18th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, pp. 1-5, 2017.

[9]. BILIAIEV M.M., *Numerical Simulation of Indoor Air Pollution and Atmosphere Pollution for Regions Having Complex Topography*, NATO Science for Peace and Security Series **C: Environmental Security**, pp. 87-91, 2012.

[10]. MARCHUK G.I., *Mathematical modeling in environmental problems*, Nauka, 1982.
[11]. ZGUROVSKIY M.Z., SKOPETSKIY V.V., KHRUTCH V.K., BILIAIEV M.M., *Numerical modeling of pollutant dispersion in environment*, Naukova dumka, 1997.
[12]. DÜRING I., BAECHLIN W., KETZEL M., BAUM A., FRIEDRICH U., WURZLER S, *A new simplified NO/NO_2 conversion model under consideration of direct NO2-emissions*, Meteorologische Zeitschrift, **20**, pp. 67-73, 2011.
[13] OVERMAN H.T.J., *Simulation model for NOx distributions in a street canyon with air purifying pavement: Master Thesis*, University of Twente, 2009.
[14]. SAMARSKII A.A., *The theory of difference schemes*, Nauka, 1977.
[15]. ALYMOV V.T., TARASOVA N.P., *Technogenic risk*, Akademkniga, 2004