Using mathematical modeling to assess the atmosphere of the industrial zone of Zhambyl region

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Abstract. There is no generally accepted method of evaluation of impact on the environment which allows characterization of an enterprise construction project as well as an enterprise activity in the period of operation. An unbiased evaluation of the system state rests on the group of indices, having a different physical nature and basing on different methods of measurements and control. Evaluation through mathematic modelling of the environmental pollution by aerosols caused by the manufacture of thermal phosphoric acid is given in the present article.

1. Introduction

The processes of impurity distribution in the atmosphere are of extreme interest for many types of human activity. Mathematical modeling of processes and phenomena is not an end in itself, but is intended to contribute to a deeper understanding of the nature of the phenomenon in order to ultimately obtain information about the real world. This information stimulates the development of new scientific problems and methods for their solution, and also serves as a basis for decision-making in the implementation of specific projects.

In recent years, the construction of mathematical models of environmental pollution, the forecast of pollution based on methods of mathematical modeling, the development based on mathematical models of pollution control and management systems, as well as the development of scientifically based methods of long-term planning of activities aimed at reducing emissions of harmful substances are of interest.

Currently, almost all industrialized countries are managing the environment state with regard to limiting emissions of harmful substances, including the atmosphere. The task of assessing the contamination of the atmosphere at present is thoroughly worked out at a theoretical and practical level both for point sources and for distributed sources of pollution [1-10].

2. Methods

With the aim of quantitative evaluation of atmosphere pollution by aerosols we have used Pasquille-Gifford empiric model based on the assumption of constant interference-free point source of a definite
capacity having homogenous characteristics of atmospheric dispersion. This model is based upon the conception of concentration of admixture emitted by a constant point source into atmosphere as a stream with vertical Gaussian distributions and transverse to wind:

\[ q(x, y, z) = \frac{Q}{2\pi \sigma_y(x) \sigma_z(x) u} \times f_F f_w \times \exp\left(-\frac{y^2}{2\sigma_y^2(x)}\right) \times \exp\left(-\frac{(z-h)^2}{2\sigma_z^2(x)}\right) + \exp\left(-\frac{(z-h)^2}{2\sigma_z^2(x)}\right) \]

where \( q \) is the impurity concentration at a given point in space, mg/m\(^3\); 
\( y, x, y, z \) are the Cartesian coordinates; 
\( Q \) - power source emission, g/s; 
\( \sigma_y(x) \) and \( \sigma_z(x) \) are the vertical and transverse variances of the impurity cloud; 
\( u \) is the wind speed averaged over the mixing layer m/s; 
\( f_F \) and \( f_w \) corrections for cloud depletion due to dry precipitation of the impurity and its washing out by sediments; 
\( h \) is the effective height of the source, m.

The sum of the exponents in this formula corresponds to the surface of the earth that does not absorb the impurity (with absolute absorption there will be a difference). The main contents of the model are generalizing numerous experimental data, specific functions \( \sigma_y(x) \) and \( \sigma_z(x) \) and expressions for \( h, f_F \) and \( f_w \).

To implement the Pascuille-Gifford model, it is necessary to find the approximate values of \( \sigma_y(x) \) and \( \sigma_z(x) \) from the actual experimental concentration data in the sanitary protection zone of the enterprise and then to determine the concentration fields in the adjacent region and to study the dependence of the concentration fields on the ejection power.

The main content of the model is presented by numerous summarizing experimental data, specific functions \( \sigma_y(x) \) and \( \sigma_z(x) \) and expressions for \( h, f_F \) and \( f_w \).

Actually sources of emission are not exactly point sources, but for the purposes of simplification of mathematical description it is possible to assume they are. The nature of specification of the chosen model allows taking into consideration the peculiarities of local meteorological conditions and calculate the distribution of the pollutants concentration in current meteorological conditions at various values of emission capacity [6, 7].

In this work we have used the data on technical characteristics of the emission sources and averaged value of aerosols in the conditions of its actual operation. Calculations were made by means of universal integrated suite MATLAB [8].

As the emissions contain simultaneously several substances having their own corresponding maximum concentration limits values (MCL) with concentration \( C_i \) \( (i=1,2,3,...n) \), it seems necessary to determine the distribution of the total concentration of aerosols of pollution agents emitted by the enterprise.

Total dimensionless spray concentration \( q \) is determined by the following formula:

\[ q = \frac{c_1}{MCL_1} + \frac{C_2}{MCL_2} + \frac{C_3}{MCL_3} + ... + \frac{C_n}{MCL_n}, \]

where \( C_1, C_2, ..., C_n \) are harmful substances concentrations in the atmospheric air in one and the same point of the area, mg/m\(^3\); \( MCL_1, MCL_2, ..., MCL_n \) are corresponding maximum concentration limits of harmful substances in the atmospheric air, mg/m\(^3\).

As the maximum environmental pollution takes place in the conditions of calm, we calculated the wind velocity of 0.1 m/s, i.e. in conditions close to calm.

3. Results and discussion

Fig.1 demonstrates spatial dispersion of polluting agents in the atmosphere. An emission source point corresponds to coordinates \( x = 0, y = 0 \). A wind direction is aligned with the direction of axis \( x \). It is
shown that the aerosol is distributed over the whole territory adjacent to the plant gradually decreasing at the distance from the source of emission down to 0.05-0.1 fractions of MCL at the range of 20 km.

The model allows prediction of the degree of atmospheric air pollution at different emission capacities and to obtain the data on the distribution of polluting aerosols and determine the zones of danger for human beings. Calculations for the emission capacity in the outlet of the conventional source equaling to 8.5 fractions of MCL demonstrated that in the situation close to calm, the aerosols concentration does not exceed MCL and in the residential area makes 0.16 fractions of MCL (fig.2).

Thus, the presented results of the calculation of the spray dispersion in the near-surface layer of the atmosphere using the empiric model of Pasquille- Gifford allows prediction of the toxic substances concentration distribution within the area, i.e. allows one to single out the most dangerous sites of the contaminated area. The feasibility of singling out the areas most harmful for human health is realized.

The analysis of the obtained data allows evaluation of the degree of the atmospheric pollution by emissions of aerosols caused by the manufacture of thermal phosphoric acid and gives the opportunity to predict the pollution of surface air at various degrees of intensity of polluting agents emissions.

![Figure 1. Spatial distribution of the aerosols in the near surface layer of the atmosphere. Axes x and y - distances, km; axis z – concentration, MCL fractions. Conventional point source of emission corresponds to coordinates x =0, y =0.](image-url)
Assessment of air pollution by substances is carried out using the effect of summation action. Since several substances possessing an action summation together with their maximum permissible concentrations and different concentration of each of them $C_i$ ($i = 1, 2, 3, \ldots n$) are jointly present in the NDFZ enterprise emissions. We performed a mathematical simulation of the distribution of the aerosol of pollutants, discarded by the enterprise.

When determining the dispersion of harmful substances that undergo completely or partially chemical transformations in the atmosphere into more toxic substances, the calculations were carried out taking into account the formation of new toxic substances. To this end, according to the recommendations of [11], the condition was fulfilled for calculating the emission of $M$ (g/s) of all harmful substances for each source to one of them. We calculated their dispersion in the atmosphere on the basis of the conditional reduction of the $M$ (g/s) emissions to the sulphurous gas by the formula:

$$M = M_1 + M_2 \frac{PDK_1}{PDK_2} + \ldots + M_n \frac{PDK_1}{PDK_n}.$$

Among harmful emissions of the enterprise NDFZ, groups of substances that have the effect of a combined harmful effect are formed. These include sulfur oxide (IV) - hydrogen fluoride; sulfur monoxide (IV) - nitrogen dioxide. The total emission power of pollutants, emitted by the enterprise and undergoing complete or partial chemical conversions in the atmosphere to more toxic substances, calculated by the above formula, for the SO$_2$-HF and SO$_2$ NO$_2$ groups, was 363.85 g/s and 123.01 g/s, respectively.

A clearer picture of the SO$_2$-HF aerosol spread is shown in the map diagram with a wind speed of 1 m/s (Figure 3) and 2.8 m/s (Figure 4), from which it can be seen that if the distance from the emission source is 15 km, the concentration of aerosol is reduced to 6.5 on the western boundary of the city, gradually decreasing in the southeast direction to 4.5 units.
Figure 3. Map-scheme of the zonal distribution of the SO$_2$ and HF concentration, having the summation of action in the surface layer of the atmosphere at a wind speed of 1 m/s.

Figure 4. Map-scheme of zonal distribution of the SO$_2$ and HF concentration, possessing the summation of action in the surface layer of the atmosphere at a wind speed of 1 m/s.

The increase in wind speed to 2.8 m / s contributes further to the dispersion of the aerosol concentration to 2.3 units at the western boundary of the city, reaching 1.5 units in the southeast (Figure 5).
Figure 5. Map-scheme of the zonal distribution of SO$_2$ and HF concentration, having the action summation in the surface layer of the atmosphere at a wind speed of 2.8 m/s

The image of the dispersion and the scattering map of a sulfur dioxide mixture and nitrogen dioxide (Figure 6), which have the effect of summation of action, clearly illustrates the state of the air basin of the city with an increase in wind speed of up to 2.8 m/s, which helps to reduce the aerosol concentration from 0.8 to 0.5 units in the direction of wind propagation.
Figure 6. Map-scheme of the zonal distribution of the SO$_2$ and NO$_2$ aerosol concentration in the surface layer of the atmosphere at a wind speed of 2.8 m/s

4. Conclusion
1. An estimation of environmental pollution of the Zhambyl region under the influence of the anthropogenic load method for predicting the contamination of the surface layer of the atmosphere using the Pascuilla-Gifford model was made.
2. Calculation of aerosol distribution of toxic substances released to the air basin by phosphate processing enterprises was carried out.

References
[1] Berlyand M E 1985 Forecast and regulation of atmospheric pollution. (L: Gidrometeoizdat)
[2] Turner D B, Bender L W, Paumier J O, Boone P F 1991 Evaluation of the TUPOS air quality dispersion model using data from EPRI KINCAID field study. Atmos.Env. 25A-10 2187-2201
[3] International Atomic Energy Agency 1987 Techniques and decision making in the assessment of off-site consequences of an accident in a nuclear facility. Vienna, Safety series 86
[4] Bykov A A, Neverova O A 2002 Simulation of atmospheric pollution and ecological zoning of the territory of the city of Kemerovo. Engineering ecology 6 25-32, 57-58
[5] Ku-Wel Zhen, Wang Wen-Jian 2005 Methodology of prediction of overpatching content of pollution at atmosphere Chemosphere 59-5 693-701
[6] Gidrometeoizdat 1991 Methodology for predicting the extent of contamination with potent poisonous substances in case of accidents (destruction) at chemically hazardous objects and transport. RD 52.04.253-90. (L.: Gidrometeoizdat)
[7] Berlyand M E, Sidorenko G I 1979 Manual on the control of atmospheric pollution. (L.: Gidrometeoizdat)
[8] Dyakonov V P 2001 MATLAB 6: Training course. (St. Petersburg: Ed. Peter)
[9] Raza S, Avila R, Cervantes J 2002 A 3D Lagrangian particle model for the atmospheric dispersion of toxic pollutants. *Int. J. Energy Res.* **26**, 93-104

[10] Mazur I I, Moldavanov O I 1999 *The course of engineering ecology*. (Moscow: Higher School)