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Solution to the Problem of Gas Impurities Distribution in the Surface Layer of the Atmosphere with Stationary Modeling Methods Applied

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Abstract: The greatest threat of the hazardous chemical release is posed by a cloud of contaminated air that spreads under the influence of wind near the soil surface. There is a problem of predicting the contaminated zone parameters in order to ensure safety. Normally, various methods are used to calculate the concentration of a hazardous impurity for this purpose. However, the obtained results correlate poorly often with each other and with the available experimental data. The *purpose* of this work is to assess the applicability of theoretical methods for calculating the parameters of the contamination zone formed as a result of the hazardous substance evaporation from the liquid strait surface. Several *methods* are used in this work: field tests, calculations using Gaussian distribution, solving a two-dimensional equation of turbulent diffusion with wind speed varying in height, and a computational experiment using the ANSYS software package. *Results*. The article presents the data of field tests with the spill of liquid chlorine, showing the distribution of impurities with the wind flow in the horizontal and vertical directions. It presents calculation results of the concentration of impurities entering the atmosphere from the surface of a liquid strait under conditions close to field tests. The applicability of the methods used to calculate the parameters of the contaminated zone are assessed taking into account the data of field tests. The correlation between the experimental and calculated data have been established to be observed in the range of specific concentrations only. The spectrum of high concentrations is better described by solving the two-dimensional equation of turbulent diffusion. The spectrum of average concentration values – by Gaussian distribution and computational experiment using the ANSYS software package. *Conclusion*. Understanding the specifics of computational methods application allows to predict the distribution of impurities in the surface air layer more accurately, taking into account the intensity of the emission, wind speed and surface roughness.

Keywords: Emergency, Chlorine, Spill, Dispersion of Impurities

1. Introduction

In cases of emergencies related to the emission of hazardous chemicals into the environment, the greatest threat is a cloud of contaminated air spreading near soil surface.

Actual contamination zone develops as a result of poisonous impurities coming from its source spreading under the influence of wind, buoyancy forces and turbulent diffusion [1]. The case where the spill of a low-boiling liquid is the emission source is the most complex and interesting from practical point of view. In this case contamination distributes directly on surface layer of the atmosphere and the turbulent diffusion coefficient depends on soil roughness [2].

Collection of experimental data on the distribution of toxic impurity, like Chlorine, in the surface layer of the atmosphere requires extensive efforts and involves significant technical difficulties [3]. Taking into account the results accumulated during field trials, it is still obvious that there is an urgent need of computational experiment to explain specific aspects of the experimental results obtained. Moreover, mathematical modeling is extremely important for predictive estimates [4].

In this paper, we assess the applicability of the Gaussian model of impurity dispersion in the surface layer of the atmosphere, the computational experiment, and the solution of the stationary two-dimensional turbulent diffusion equation by the method of lines to determine the parameters of the contamination zone formed as a result of dangerous impurity evaporation from the surface of liquid spill.

2. Experimental Data

Previously we have reported the results of full-scale tests to measure parameters of actual contamination zone forming as a result of hazardous chemical impurities distribution with wind flow from the emission source (spill). The available results allow making well-reasoned choice of prediction methods based on analysis of correlation between theoretical calculations and field experiment results [5, 6].

The tests enabled measuring the parameters of the actual contamination zone where chlorine evaporated from the spill surface with natural roughness and distributed freely. Liquid chlorine spill of 1 m^2 area was used as a model object. Liquid chlorine was poured into an open-topped 0,15 m high metal cylinder container designed for chlorine transportation. The weight of spilled chlorine was 25 kg.

The boundaries of the actual contamination zone on the terrain and the impurity area parameters were measured by chlorine concentration in the air at different heights: 0; 0,5; 1; 1,5 m (Figure 1a) [5]. Parameters of contamination concentration fields at different distances from the spill source provided large amount of data. Figure 1b illustrates the results of chlorine concentration measurements (volume fraction φ_{ch}) at different heights 100 m away from the spill boundary.

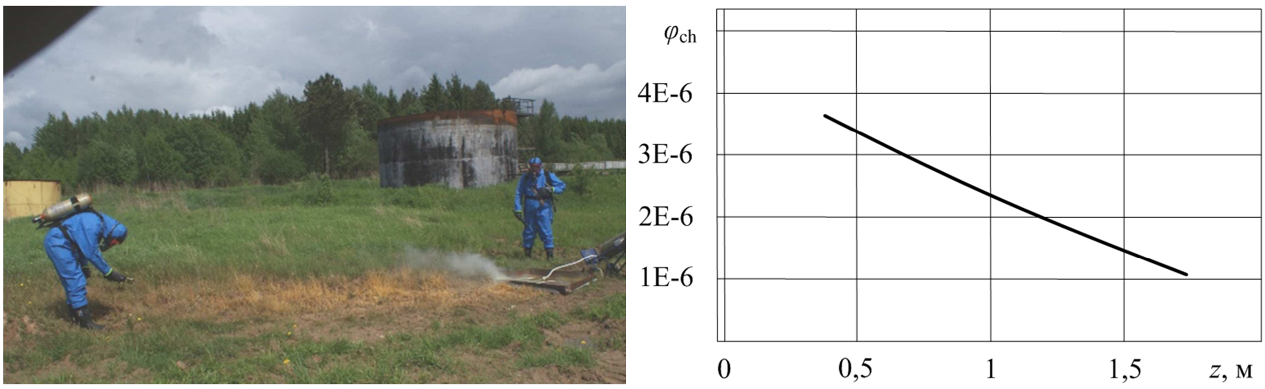


__Figure 1.__ Full-scale tests: a) measurements of the concentration near the emission source, b) height profile of chlorine concentration ≈100 m away from the source [5].

3. Calculation Results

3.1. The Gaussian Impurities Dispersion Model Application

The Gaussian impurities dispersion model is an effective tool for estimation of pollutants concentration in the surface layer of the atmosphere. The widespread usage of this model is explained by the following factors:

1) simple mathematical formulation of the model and, therefore, the ease of its transformation into program code;
2) relatively small number of input parameters of the model;
3) reliability of calculation results confirmed by many model verifications on the basis of special full-scale diffusion experiments and measurements of emission parameters from industrial enterprises.

However, its use beyond model applicability limits leads to a significant increase in the errors of the calculated values, up to incorrect calculation of the location and the size of the pollution area. Due to this we need to understand clearly the applicability limits of the Gaussian model and the margin of error within these limits and in a wider range of studies [7, 8].

The Gaussian model of the torch is the basis for the vast majority of all existing impurity dispersion models. The model is derived from the analytical solution of the dispersion equation that describes a continuous cloud of a pollutant in a turbulent flow and can be represented in the form [9]:

$$\frac{dC}{dt}+u\frac{dC}{dx}=\frac{d}{dy}\left(D_y\frac{dC}{dy}\right)+\frac{d}{dz}\left(D_z\frac{dC}{dz}\right)+S \quad (1)$$

where x is the coordinate directed along the wind velocity from the source; y – lateral (transverse) coordinate; z – vertical coordinate; $C\ (x, y, z)$ – average concentration of the diffusing substance at the point (x, y, z); D_y, D_z – diffusion coefficients in the direction of the y, z axes; u – mean wind velocity along x axis; S – source term (the combination of the production and dissipation terms).

Equation (1) is significantly simplified, since a number of assumptions was made to derive it, for example:

1) pollutant concentration does not affect the hydrodynamic characteristics of the incompressible carrier medium (passive admixture);
2) pollutant concentration can be presented as the sum of the mean and pulsating values (the mean value of the fluctuating component equals to zero) like components of the velocity field;
3) convective transport in the direction of airflow far exceeds impurity transport due to molecular and turbulent diffusion.

The Gaussian model is applicable to the simulation of long-term (continuous) constant power release, release of a finite time of action or a short-term (instantaneous) release.

The features of the analytical solution set the following limitations on the practical application of the Gaussian model: 1) the model can be used for distances of up to 10 km from the source (depending on the complexity of the terrain); 2) stationarity and horizontal homogeneity of meteorological conditions within the design area are assumed, as well as horizontal homogeneity of the underlying surface; 3) stationarity of emission source.

Taking into account the fact that under the experimental conditions [5] the impurity flow distributes from land-based source, formulation for impurity concentration measurement was obtained using the double distribution in the Gauss equation:

$$C(x,y,z)=\frac{2Q}{2\pi\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2}+\frac{z^2}{\sigma_z^2}\right)\right]=\frac{Q}{\pi\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma_y^2}+\frac{z^2}{\sigma_z^2}\right)\right], \quad (2)$$

where C is the impurity concentration, kg/m^3; Q – source power, kg/s; σ_y and σ_z – the dispersion coefficients along the y and z axes.

It is necessary to know σ_y and σ_z parameters in the Gaussian model to be able to determine the concentration value. Typically, σ_y and σ_z dispersion coefficients in the horizontal and vertical direction are calculated based on empirical correlations.

The nomograms by Pasquill-Gifford are the most well-known; they are compiled from the observations of concentrations in the flat terrain and, therefore, called "rural" [10].

Briggs conducted similar research and obtained empirical correlations for standard deviations for rural and urban areas separately [11]. The Briggs formulas in physical variables are applicable for distances in the range from 100 to 10,000 meters from the source. Concentrations time averaging during results processing of the experimental observations was 20 min. The roughness parameter for the countryside was 0,03 m, in urban areas – 1 m.

Calculated and experimental data were compared within the framework of the experiment determining the parameters of the actual contamination zone due to chlorine emission [5].

Figure 2 shows chlorine concentration at 0,5 m height along the trace axis: calculated results – curve 1, and the experimentally obtained data – points.

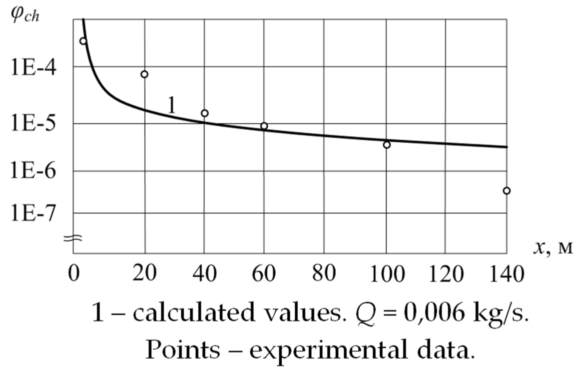


Figure 2. *Distribution of chlorine concentration values the trace axis. z = 0,5 m.*

The obtained results indicate the existence of only a qualitative correlation between calculated and experimental data. Quantitative correlation can be observed only in specific ranges of the emission intensity values and distances from the emission source.

Taking into account the fact that the spread of chlorine vapor from the emission source is a typical case of the so-called "heavy gas" spread, the use of Gaussian models is not entirely justified, since it leads to incorrect determination of concentrations near the source of pollution.

3.2. Use of Computational Experiment

In cases of accidents followed by hazardous chemicals spills prediction of the depth of the actual contamination zone and impurity concentration fields is complicated by the necessity to take into account number of factors. Among them: specific features of spilled substance, complex nature of air masses transfer in relatively small areas near the earth's surface, differences in physical mechanisms at certain stages of the accident process [11, 12]. It should be noted that the spill of a liquid with boiling point below ambient temperature is an impurity source of a complex type. There are recorded cases of such spills of significant sizes and depths, capable of prolonged existence.

At this moment preference in modeling the impurity distribution processes is given to the joint numerical solution (in two- and three-dimensional formulations) of the equations of medium motion and semi-empirical turbulence equations in Cartesian coordinates. Here, it is possible to take into account wide range of factors: impurity distribution in the direction of the flow, molecular and turbulent diffusion, convection, spatiotemporal inhomogeneity of the scattering parameters, interaction of the pollutant with the underlying surface and the upper boundary of the mixing layer, dry and wet subsidence on the underlying surface, pollutant transformation and other factors [13, 14].

ANSYS 14.0 software was used to solve the problem of impurity flow distribution.

The modeling area is a rectangle 20 m high and 110 m long in the direction of the wind. A fragment of the computational area is shown in Figure 3. There is an impurity source (1 m long liquid chlorine spill in the direction of the flow) on the surface, it is located 10 m away from the inflow boundary in the wind direction.

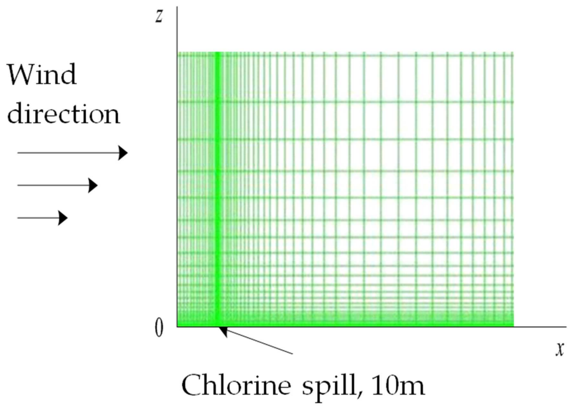
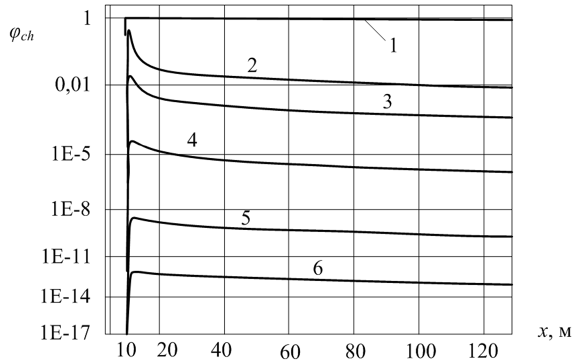


Figure 3. *Fragment of the computational grid.*



1 – z = 0,005 m; 2 – z = 0,1 m; 3 – z = 0,2 m;
4 – z = 0,5 m; 5 – z = 1 m; 6 – z = 1,5 m

Figure 4. *Chlorine concentration at different heights.*

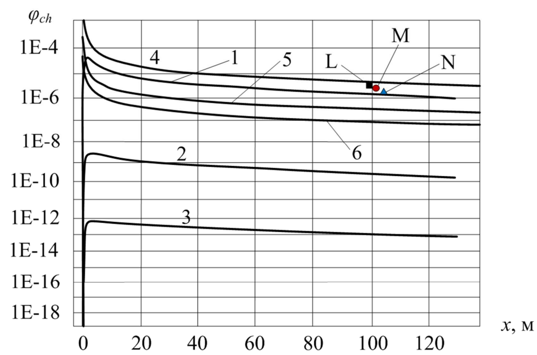
A two-dimensional setting is implemented; it takes into account the horizontal size of the liquid spill of 1 m in x-direction (linear source), the impurity inflow intensity, convective transport of air masses and turbulent mixing of impurities with the ambient air adjusted for the buoyancy forces. The system of equations was applied for process simulation of the impurity distribution in the surface layer of the atmosphere; it included continuity equation for the gas mixture; the Reynolds equation for the average velocity of the mixture turbulent motion; energy equation for the mixture; equations of motion for the volume concentration of secondary phases; algebraic ratio for the velocities of secondary phases relative to the carrier phase velocity (air). K-ε model of turbulence was applied to calculate the pulsation components of velocity with the influence of secondary phase (chlorine) concentration on production terms and dissipation of turbulent kinetic energy pulsation. The results of the computational experiment in this approximation can answer questions about the extent of the contamination zone, concentration distribution in elevation, and influence of temperature gradient, air flow velocity, surface roughness, etc. on these parameters.

Figure 4 illustrates the distribution of chlorine volume concentration in elevation above the ground surface (in the absence of obstacles in the transmission path).

The wind speed at 2 m height is 1,6 m/s. Soil temperature is 293 K; air temperature is 293 K (temperature gradient ΔT = 0 K). The power of chlorine source is Q = 0,006 kg/s.

Figure 5 compares chlorine volume concentrations calculated by means of the computational experiment and the Gaussian model.

The computational experiment that considers the influence of the heavy impurity on the velocity field shows that dangerous chlorine concentrations distribute from the impurity source over long distances near the earth's surface at heights of less than 1 m under weather conditions corresponding to the full-scale experiment. Calculation by the Gaussian models leads to variance of altitudes by 2 orders only, but the contamination zone extent is also very large. The theoretical results and their absolute values do not contradict to the results of the field tests.



z = 0,5 m (curves 1, 4, L); z = 1 m (curves 2, 5, M);
z = 1,5 m (curves 3, 6, N)

Figure 5. *Comparison of the results determining chlorine volume concentration by the means of: the computational experiment (curves 1, 2, 3); the Gaussian model for class C (curves 4, 5, 6); the full-scale experiment (points L, M, N).*

3.3. Solution of the Stationary Two-Dimensional Equation of Turbulent Diffusion by the Method of Lines

When the air moves over the strait, it mixes with the flow of the impurity rising from the surface. As a result, vapor cloud forms under the influence of two factors: the intake of impurities from the spill surface into the atmosphere and the movement of air masses. The resulting distribution of impurity concentration values is complex, both in horizontal and vertical directions [15].

Height above the spill surface is considered as one of the key characteristics of the process of contaminated cloud formation. The height of the impurity cloud above the spill surface h is maximal over the downwind boundary of the spill, which matches the area of the largest impurity concentrations. According to [16] h value can be estimated as

$$h \approx \sqrt{D_t L / u_0}, \quad (3)$$

where D_t is the coefficient of turbulent diffusion of the impurity in the surface layer; L is the downwind size of the spill; u_0 is the wind speed at 2 m height.

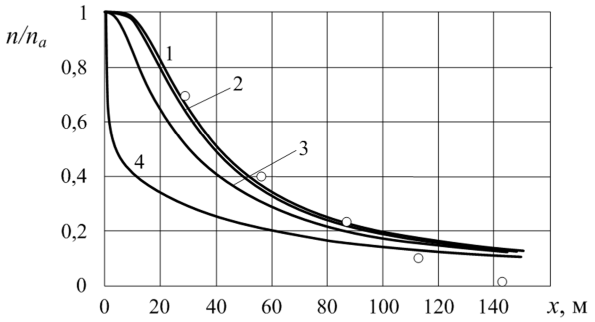
Two-dimensional stationary diffusion equation describing formation of impurity clouds over the spill surface has the form.

$$u(z)\frac{\partial n(x,z)}{\partial x} = D_t \frac{\partial^2 n(x,z)}{\partial z^2}, \quad (4)$$

where $u(z)$ – wind velocity profile in the surface layer; n is the numerical density of impurity molecules.

The solution of the two-dimensional equation (4) by the method of lines [17] establishes the values of heavy impurity concentrations in the near-surface layer. Normalized value of the impurity density is calculated considering averaged n_a value close to the conditions of full-scale tests [5]. The wind speed is 1,5 m/s (at 2 m height). The surface roughness size is 1 cm.

Figure 6 presents calculation results of the impurity numerical density outside the model spill in the wind direction. Curve 1 corresponds to 0,5 m height above the surface, curve 2 – 1 m height, curve 3 – 1,5 m height, curve 4 – 2 m height.



1 – z = 0,5 m; 2 – z = 1 m; 3 – z = 1,5 m; 4 – z = 2 m.
Points – experimental data

Figure 6. *Distribution of the normalized impurity density.*

Impurity concentration decreases with the growth of distance from the spill boundary at any value of the altitude above the soil surface. Only a small area (less than 10 m) is observed at 1 m altitude where the concentration of pollutant remains high.

The nonlinearity of the established relationships near the evaporation surface is explained by the fact that the coefficient of turbulent diffusion is unstable and increases with wind speed growth. The character of the impurity distribution here also confirms the exponential decrease of its content in the region of action of the dissipative factors.

Points in Figure 6 indicate values corresponding to the parameters of the actual contamination zone determined during the full-scale tests described in [5] (chlorine concentration was determined at 0,5 m height). Reasonably good correlation between the experimental and calculated data is observed here, except for low concentration area, which is explained by the contamination zone migration perpendicular to the wind direction.

4. Conclusion

The stationary two-dimensional modeling of impurity distribution in the ground layer of the atmosphere allows to calculate the impurity concentration above the spill surface and in the stream distributing above the soil surface. The outcomes of the stationary two-dimensional equation of turbulent diffusion by the method of lines and the Gaussian dispersion model of impurities are consistent with the results of full-scale tests. They allow to predict quantitatively the impurity distribution in the surface layer taking into account emission intensity, wind speed and surface roughness.

Determination of the impurity distribution pattern in the vertical and horizontal directions allows to make extrapolation and interpolation estimates, which is impossible to obtain empirically due to the complexity of the experimental studies. First of all, this is explained by the peculiarities of hazardous waste operations and demand in significant efforts and resources to support activities in contaminated area.

Particularly, the specification of the impurity distribution in the surface layer close to the emission source is the most interesting for the method of lines, and far from the emission source – for the Gaussian dispersion model.

The study identified the formation patterns of the actual contamination zone in the emergency situation related to the release (spill) of a hazardous chemical. These patterns point out possible existence of the contaminated areas with high impurity concentration that are not taken into account by existing regulatory documents. For example, there may be situations where impurity concentration can increase dangerously at a height of human respiratory system while moving away from the emission source.

From a practical standpoint, the calculation results based on the Gaussian model with a certain "safety margin" can be fully applied for quick quantification of the contamination zone size and the concentration of a heavy impurity, such as Chlorine, at the level of human height in course of free distribution of the impurity from the emission source.

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