Chapter 25
The Numeric Forecast of Air Pollution Caused by a Blasting Accident in the Enterprise Responsible for Rocket Fuel Utilization in Ukraine

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Abstract A mathematical model which can take into account all the scenarios of accidents has been developed. The code *AIR-SIM* was worked out on the basis of the described difference schemes. This code was used to simulate the atmospheric pollution for different accidents on the territory of the Pavlograd Chemical Plant. In particular, a numerical model was used to predict the atmospheric pollution in the case of *HCN* emission from the opening at the roof of the building. During the numerical experiment the dynamic of the toxic dose in each room was determined for each case study. It was established that the hitting zone will be about 6 km.

Keywords Air pollution • Numeric forecast • Blasting accident • Rocket fuel

25.1 Introduction

The State Enterprise Research-Industrial Complex "Pavlograd Chemical Plant" (SE RIC PCP) was established in 1929 as a plant for the production of explosive materials and charging of ammunition for various purposes (artillery, aviation, navy, engineering etc.). During the last decade the State Enterprise Research-Industrial Complex "Pavlograd Chemical Plant" has participated in international and state programs on elimination of strategic armaments, stage-by-stage reduction and elimination of ICBM SS-24, a program on the disposal of solid propellant of ICBM SS-24, a program on the disposal of conventional types of ammunition unsuitable for further application and storage, a regional comprehensive program

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I. Barnes and K.J. Rudziński (eds.), *Disposal of Dangerous Chemicals in Urban Areas and Mega Cities*, NATO Science for Peace and Security Series C: Environmental Security,
DOI 10.1007/978-94-007-5034-0_25,

on conversion of mining enterprises to use of environmentally safe and TNT-free explosives and the development of blasting science in Ukraine [1].

It is obvious that the Pavlograd Chemical Plant is the highest potential source of environment contamination in the case of an accident on its territory. The calculation of the hitting zone in the case of an accident at this plant was carried out using the empirical model at the Ministry of Emergency of Ukraine [2]. This model is used in Ukraine as the main tool to predict the pollution level caused by accidents at chemical plants, however, the results obtained were not satisfactory. The results could not be used to estimate the real scale of the danger of accidents at this plant. The model used could not predict the pollution dynamics in the merits of the plant territory, especially in the vicinity of the buildings. The model does not take into account different types of accidents, for example, the emission of the toxic gas from the partially destroyed building, the emission of the toxic gas through the roof of the building etc. The Representative of the Ministry of Emergency of Ukraine in Dnepropetrovsk Region set the problem to the authors of this paper to determine the level of pollution that would result from the different types of accidents which could take occur at the plant. Of special interest were pollution levels resulting from accidents with solid missile propellant. To solve the problem it was necessary to develop a mathematical model which could take into account all the possible accident scenarios which could occur at such a plant.

25.2 Materials and Methods

The Pavlograd Chemical Plant is situated 5 km to the west of Pavlograd City (Ukraine, Dnepropetrovsk Region). The nearest settlement (the so-called "workers village") is 2.5 km from this plant (Fig. 25.1).

Fig. 25.1 Location of the Pavlograd Chemical Plant near Pavlograd City

A distinct feature of this plant is the storage of a very large quantity of toxic substances at the site. The toxic substances at the plant can be divided on two classes: (a) "ordinary" chemical substances: HCl, HCN, etc. (b) solid missile propellant.

25.3 Mathematical Model of Pollutant Dispersion

To estimate the affected area, henceforth called "hitting zone", if an accident takes place at the chemical plant it is necessary to calculate the dispersion of toxic substances in the atmosphere. To simulate the dispersion process in the atmosphere the transport model is used

$$\frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}+\frac{\partial vC}{\partial y}+\frac{\partial (w-ws)C}{\partial z}+\sigma C=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu_z\frac{\partial C}{\partial z}\right)+\sum Q_i(t)\delta(x-x_i)\delta(y-y_i)\delta(z-z_i) \tag{25.1}$$

where C is the concentration of toxic gas; u, v, w are the wind velocity components; w_s is the rate of gravitional fallout; σ is a coefficient taking into account the process of pollutant decay or rain washout; $\mu = (\mu_x, \mu_y, \mu_z)$ are the diffusion coefficients; Q_i is the intensity of point source of ejection; $\delta(x-x_i)\delta(y-y_i)\delta(z-z_i)$ are Dirac's delta functions; $r_i = (x_i, y_i, z_i)$ are the coordinates of the ejection source.

In the numerical model developed the following approximations for the wind speed and diffusion coefficients are used [3]:

$$u = u_1\left(\frac{z}{z_1}\right)^n,$$

$$\mu_z = 0,11z \quad \mu_y = \kappa_0 u,$$

$$\mu_y = \mu_x$$

where u_1 is the wind speed at the height $z_1 = 10$ m; n = 0,15; k_0 is the empirical parameter [3].

25.4 Hydrodynamic Model

In the case of an accident the dispersion of pollutants will take place at first in the vicinity of buildings which are situated at the plant site. The simulation of the wind flow near buildings on the basis of *Navier – Stokes* equations and using different turbulent models needs a very refined mesh [4]. It would take days to obtain the results of the considered problem using computers which are currently in use in

Ukraine. To circumvent this problem the model of potential flow is used to simulate the *3D* wind flow at the chemical plant in the vicinity of buildings. In this case the governing equation is

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} + \frac{\partial^2 P}{\partial z^2} = 0, \tag{25.2}$$

where P is the potential of velocity. The velocity components are calculated as follows:

$$u = \frac{\partial P}{\partial x}, \quad v = \frac{\partial P}{\partial y}, \quad w = \frac{\partial P}{\partial z}.$$

25.5 Numerical Model

The numerical integration of the governing Eqs. (25.1) and (25.2) is carried out using a rectangular grid. The main features of the difference schemes which are used are considered below. The time dependence derivative in Eq. (25.1) is approximated as follows:

$$\frac{\partial C}{\partial t} \approx \frac{C_{ijk}^{n+1} - C_{ijk}^{n}}{\Delta t}.$$

In a first step the convective derivatives are represented in the following way:

$$\frac{\partial uC}{\partial x} = \frac{\partial u^+ C}{\partial x} + \frac{\partial u^- C}{\partial x};$$

$$\frac{\partial vC}{\partial y} = \frac{\partial v^+ C}{\partial y} + \frac{\partial v^- C}{\partial y};$$

$$\frac{\partial wC}{\partial z} = \frac{\partial w^+ C}{\partial z} + \frac{\partial w^- C}{\partial z},$$

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

In a second step the convective derivatives are approximated as follows:

$$\frac{\partial u^+ C}{\partial x} \approx \frac{u_{i+1,j,k}^{+} C_{ijk}^{n+1} - u_{ijk}^{+} C_{i-1,j,k}^{n+1}}{\Delta x} = L_x^+ C^{n+1},$$

$$\frac{\partial u^- C}{\partial x} \approx \frac{u_{i+1,j,k}^{-} C_{i+1,j,k}^{n+1} - u_{ijk}^{-} C_{ijk}^{n+1}}{\Delta x} = L_x^- C^{n+1},$$