Chapter 66
Numerical Simulation of the Atmosphere Pollution After Accident at the "Tolliaty – Odessa" Ammonia Pipe

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Abstract The results of numerical simulation of environment pollution after accident at the ammonia pipe are presented in this paper. The problem was solved for two different scenarios. Firstly only the ammonia ejection into the atmosphere was considered. 3D equation of pollutant dispersion (k – gradient model) and model of potential flow were used to simulate the process of air pollution. At the second step the problems of river Dnepr pollution and evaporation of ammonia from the water surface were considered. The developed numerical models and the code were used to calculate the scale of the air and water pollution. The code was used to calculate the toxic gas penetration into the dwellings of the settlements which are situated near the ammonia pipe. It allowed obtaining the information about the possibility of safety people evacuation.

Keywords Environment • Pollution • Numeric modeling • Ammonia pipe • Evacuation

66.1 Introduction

Transportation of liquid ammonia from Tolliaty City (the city where the ammonia is produced, Russia) to Odessa sea port (Ukraine) is carried out in ammonia pipe which is known as "*Tolliaty – Odessa*" pipe. This ammonia pipe was built in the former USSR according to the USA project. This pipe crosses 14 rivers on its 2,424 km route and only one river it crosses over the water surface. This is the river Dnepr which is the main water supply source of Ukraine.

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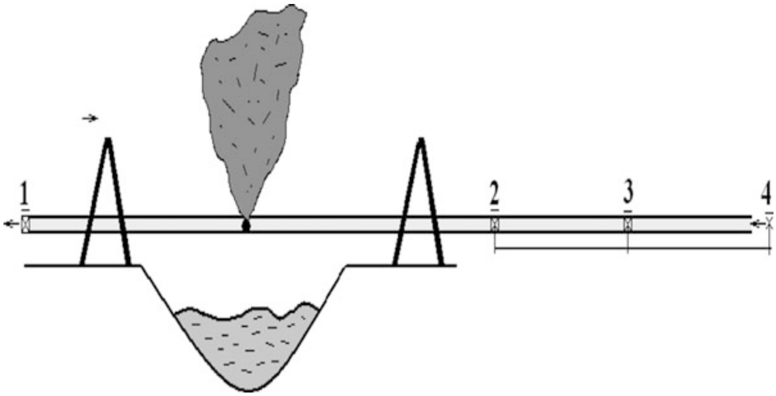

Fig. 66.1 Sketch of NH_3 emission from the opening at the ammonia pipe

The prediction of the possible air pollution level after accidents at this pipe was carried out in the seventies years of the past century on the basis of empirical models and later this prediction was carried out using the analytical models. Today the Ministry of Emergency of Ukraine needs more detailed and realistic information about the scale of environment pollution and risk assessment in the case of the different accidents or terror acts at this pipe.

In this paper two problems of the atmosphere pollution after accident at the ammonia pipe are considered.

1. *The first problem* is the scenario when the emission of NH_3 takes part at the ammonia pipe above the water surface (Fig. 66.1).

In this case to simulate the process of NH_3 dispersion in the atmosphere the equation of pollutant transport is used

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

where u, v, w – are the wind velocity components; C – is the concentration of NH_3; σ – is the parameter taking into account the process of NH_3 washout;

μ_x, μ_y, μ_z are the turbulent diffusion coefficients; x_i, y_i, z_i are the coordinates of the point source of NH_3 emission; $Q_i(t)$ – is the intensity of NH_3 emission; $\delta(x-x_i)\delta(y-y_i)\delta(z-z_i)$ – is Dirac's delta-function.

In the numerical model developed the following models to approximate the velocity component u and coefficients of diffusion are used:

$$u=u_1\left(\frac{z}{z_1}\right)^n,\quad \mu_z=k_1\left(\frac{z}{z_1}\right)^m,\quad \mu_y=\kappa_0\mathrm{u},\ \mu_y=\mu_x$$

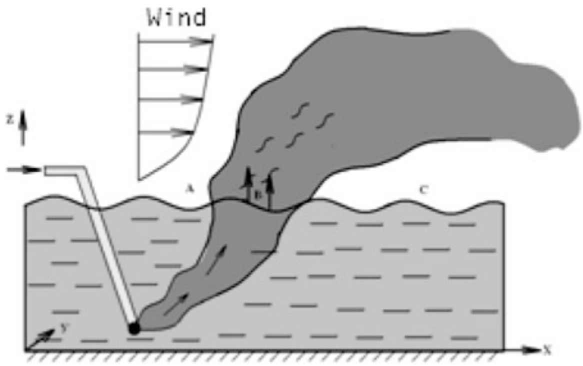

Fig. 66.2 Sketch of NH_3 emission from the ammonia pipe to the river

where u_1 is the wind speed at the height $z_1 = 10$ m; n = 0.15; k_0 is the empirical parameter; $k_1 = 0.2$; m ≈ 1.

In the case of the accident the NH_3 propagation will take place in the region with the complex terrain. To simulate the wind flow in the case of the complex terrain and among buildings of the settlement which is situated near the ammonia pipe the 3D model of potential flow is used

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

where P is the potential of velocity.

The wind velocity components are calculated as follows:

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

The process of the atmosphere pollution modeling in the case of the accident at the ammonia pipe consists of two steps. At the first step the wind velocity components are determined on the basis of the potential flow model and after that the NH_3 dispersion is studied using pollutant transport model.

2. *The second problem* is the scenario when the ammonia pipe has fallen into the river. In this case NH_3 discharges from the pipe contaminating the river and rising in the water to the water surface. This results in NH_3 plume formation over the river free surface (Fig. 66.2). This plume causes the atmosphere pollution.

In this scenario it is necessary to solve two problems. The first problem is the problem of the river pollution. To simulate the flow in the river Dnepr in this case the 2D Navier-Stokes equations which are written in the variables "vortex – flow function" are used:

$$\frac{\partial \omega}{\partial t} + \frac{\partial u\omega}{\partial x} + \frac{\partial v\omega}{\partial y} = \frac{1}{\text{Re}}\left(\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2}\right)$$

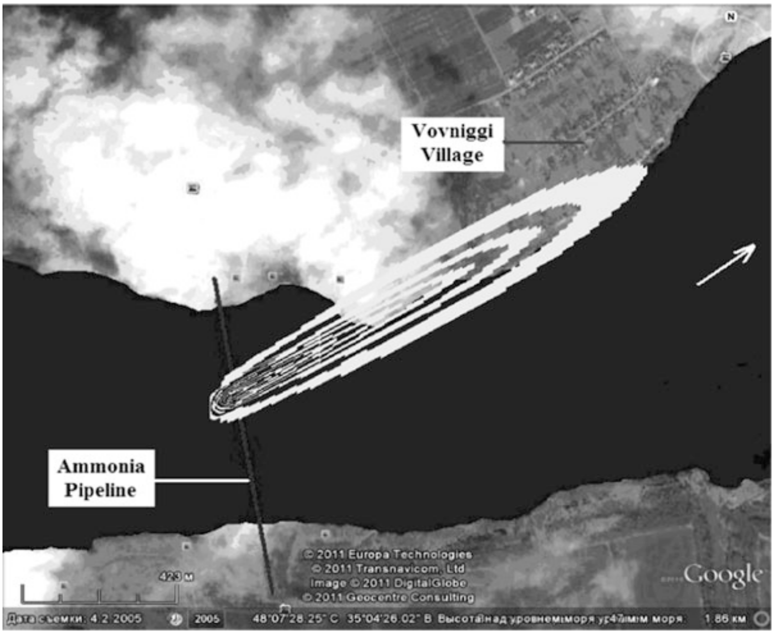

Fig. 66.3 Air pollution area after accident with NH_3 emission (t = 30s)

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\omega$$

where $\omega = \dfrac{\partial v}{\partial x} - \frac{\partial u}{\partial y}$ is the vortex; ψ is the flow function; Re is Reynolds number; $u = \dfrac{\partial \psi}{\partial y}; v = -\frac{\partial \psi}{\partial x}$ are the components of the velocity vector.

To simulate the NH_3 dispersion in the river the equation of pollutant transport is used.

For the '*pilot*' numerical simulation of the water flow the model of potential flow is also used.

The intensity of NH_3 emission from the pipe is calculated on the basis of the hydraulics formulae. The dimension of the NH_3 bubbles in the water and the speed of their rising in the water is calculated using empirical models.

The air pollution under the influence of the plume which is formed over the river surface is modeled on the basis of the equation of pollutant transport.

Numerical solution of the equations of the models is carried out using implicit difference schemes of splitting [1, 2]. On the basis of the numerical model the code '*Ammonia Release*' was developed.

Air pollution area after accident with NH_3 emission (t = 30 s) is shown in Fig. 66.3. The plume is forming over the water surface.

66.2 Conclusion

The developed code was used to simulate the intensity of the atmosphere pollution after the possible accidents at the ammonia pipe. This information allowed evaluating the risk of people hitting in their buildings and on the routes of evacuation.

References

1. Belayev NN, Kazakevitch MI, Khrutch VK (1999) Computer simulation of the pollutant dispersion among buildings. // Wind Engineering into 21st century. In: Proceedings of the tenth international conference on wind engineering. A. A. Balkema/Rotterdam/Brookfield, Copenhagen/Denmark, pp 1217–1220
2. Belayev NN, Khrutch VK (2000) An engineering approach to simulate the 3-d wind flows over buildings. In: Proceedings of the fourth international colloquium on bluff body aerodynamics & applications. Ruhr-Universitat, Bochum, Germany. Volume of Abstracts, 11–14 Sept 2000, pp 471–475