NUMERICAL MODELING OF THE EVAPORATION OF THE SPILL OF LIQUID TOXIC SUBSTANCE

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One of the most dangerous types of man-made accidents is the destruction of the storage tank of a toxic chemical (PCS) in a liquefied state with the formation of a strait spot, the evaporation of PCS with the formation of a toxic cloud. The mass concentration of PCS in the air is a dangerous parameter. The exposition of the facility’s personnel to certain concentrations of PCS is formed by a damaging factor — an inhalation toxoid dose, exceeding the threshold values of which leads to social consequences — poisoning of varying severity and human victims. Therefore, determining the risk of an enterprise for such an accident is an important and urgent engineering and practical task.

The assessment of the consequences of a technogenic accident includes the determination of the probability of damage to service personnel who may be exposed to PCS, based on mathematical modeling of the dispersion of toxic impurities in the atmosphere. The spatio-temporal fields of a dangerous parameter obtained as a result of modeling — the mass concentration of a toxic impurity — make it possible to determine the magnitude of the main damaging factor — the inhalation toxic dose and the conditional probability of damage to the personnel. The mathematical model is implemented as a subsystem of the Toxic Spill Safety research software complex.

Inhalation toxicosis D depends on the mass concentration of toxic impurities Q and exposure time $\tau_э$

$$D = \int_0^{\tau_э} Q^n d\tau, \qquad (1)$$

where n – tabular coefficient for each PCS.

The conditional probability of damage to a person under the influence of inhalation toxic doses of PCS depends on the probit function - the upper limit of a certain integral of the normal distribution law with a mean of 5 and variance 1.

$$P = \frac{1}{\sqrt{2\pi}} \int_0^{Pr} e^{-\frac{1}{2}(t-5)^2} dt. \qquad (2)$$

The probit function for toxic damage is generally determined by the formula 3.

$$P_r = a + b \cdot \ln(D), \qquad (3)$$

a and b – tabular semi-empirical coefficients.

For approbation of the developed information technology, the evaporation of 6925 kg of liquefied hydrogen cyanide (toxic explosive substance with a density of 689 kg / m3, molar mass of 0.027 kg / mol, boiling point of 298.6 K, evaporation heat of 933 kJ / kg) was simulated from a strait spot in the form of a circle with a radius of 8 m. The center of the spill spot circumference was located at a distance of 16 m from the origin of coordinates in the computational domain with dimensions of 85 Ч 10 Ч 85 m and the number of cells along the axes of 85 Ч 10 Ч 85. At a distance of 30 m along the OX axis and 28 m along the OZ axis from the origin, a building with dimensions of 15 Ч 5 Ч 25 m was located. The raid wind at a speed of 3 m / s at an angle of 45є to the OZ axis at a height of 0.5 m. Evaporation rate PCS was 0.00106 kg / s / m2.

Fields of conditional probability of death for a person during inhalation of hydrogen cyanide are presented in fig.1.

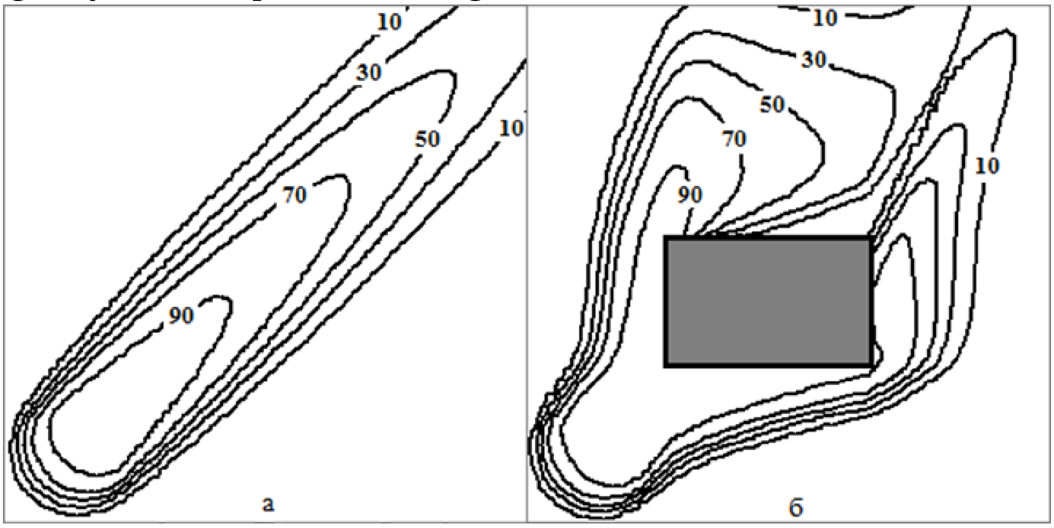

Fig. 1. Field of conditional probability of death of a person on the ground, %: a - without a building; b - with the building.

Conclusions. A computational safety assessment technology has been developed on the basis of probit analysis, which allows for automated analysis and forecasting in time and space of the relative mass concentration of a toxic gas as a dangerous parameter, inhalation tox dose, as a damaging factor, and the conditional probability of lethal damage to service personnel exposed to the poison chemical as an indicator of the degree of safety of a man-made object.