Accidents with the Release of Pollutants into the Atmosphere and the Issues of their Mathematical and Informational Modeling and Numerical Simulation

Allayarbek Aydosov[1], Nurgali Zaurbekov[2], Gulzat Zaurbekova[3], Galym Aydosov[4], Lyazzat Baibolova[5], Rakhatay Aitbayeva[6], Balzhan Talpakova[7]

Abstract

The primary material carriers of negative human impact on the natural environment are emissions. The authors researched the solid content of this concept which is fundamental when the sequel article materials. Some emissions are under human control and harmless. In emergency situations and accidents occur uncontrolled emissions of pollutants and toxic substances. They are often the objects of increased danger and risk and involve the professional interest of specialists. The authors developed a mathematical model of the processes determining the transport of pollutants into the atmosphere during accidental releases, classified atmospheric pollution sources in accidents and had a hierarchy of contaminants. It may regulate the process of environmental pollution, to take appropriate actions in time and improve the ecological situation in the world.

[1]PhD, Professor, Almaty Technological University, 50052, Republic of Kazakhstan, Almaty, Tole bi str., 100

[2]PhD, Professor, Almaty Technological University, 50052, Republic of Kazakhstan, Almaty, Tole bi str., 100, agu_nurgali@mail.ru

[3]Doctoral, Al-Farabi Kazakh National University, 050040, Republic of Kazakhstan, Almaty, 71 al-Farabi Ave., guzzzya_92@mail.ru

[4]PhD, Professor, Al-Farabi Kazakh National University, 050040, Republic of Kazakhstan, Almaty, 71 al-Farabi Ave., galym_a@mail.ru

[5]PhD, Professor, Almaty Technological University, 50052, Republic of Kazakhstan, Almaty, Tole bi str., 100, baybolova@mail.ru

[6]MS, Almaty Technological University, 50052, Republic of Kazakhstan, Almaty, Tole bi str., 100, rakhatay@mail.ru

[7]MS, Almaty Technological University, 50052, Republic of Kazakhstan, Almaty, Tole bi str., 100, balzhan_14@mail.ru

Keywords: pollutants, atmosphere, mathematical modeling, man-made disaster, environment, risk objects, numerical simulation.

Introduction

At present, efforts of scientists all over the world set up a single fund process of models occurring in animate and inanimate nature. These models are based on a few fundamental principles that bind together the various facts and views of the natural sciences. Each model in this fund has a definite place, set the limits of its applicability and relationship with other models. The presence of such a fund model gives researchers confidence in their use in practice. In fact, each of these models through linkages with other models based not so much on a particular test herself, but on the whole experience of humanity. For each object in this fund, there can be chosen the most appropriate model or modify it from close in character models.

With regard to the problems of environmental protection and development of the theory of origin and transformation of pollutants in natural environments, to prove itself in the presence of a grand fund of natural processes, on the one hand, defines the high efficiency of use of mathematical models and methods in engineering practice, and, on the contrary, gives researchers a single picture of the surrounding world.

In general, the basis of a constructive approach to the issue of human interaction with nature enables simulation (e.g., mathematical) in combination with targeted experimental studies. Environmental pollution is one of the most common manifestations of this interaction.

Some factors that should be taken into account in the models are at the crossroads of many research programs implemented within the framework of Earth Sciences. The complex nature of such programs and the availability of complex forward and backward linkages between the hydro-meteorological processes, pollution of the environment, the biosphere actively promote the development of the theoretical foundations of the system and the organization of mathematical models. At the higher level system organization operates with a "simple" models like the atomic objects.

Concerning the mathematical modeling of pollutants and toxic substances emergence and development process in an atmosphere of emergency emissions will come from the physical process models. These include the models of hydro-thermodynamics atmosphere with different spatial and temporal scales, as well as models of transport and transformation of pollutants, various ways of parameterization and so on. There are a lot of similar developments in the literature. Their physical meaning and the differences between them depend on the specific tasking. In any case, concerning the solution of the problem of numerical simulation methods are based on the concepts of state functions and parameters.

Computing models used the idea of expansion of parameters including not only the number of numerical values of some variables, and algorithms for their calculation. Then, the number of parameters includes schemes, algorithms, computation of radiation heat fluxes, turbulent exchange coefficients and coefficients in the models of the interaction of air masses from the underlying surface.

The development presented here is suitable for constructing discrete analogs of models, and computational algorithms are used variational principles, the use of which provides a qualitatively new information about the behavior of a mathematical model.

It is evident that the sense of numerical modeling should not get lost, inherent in the original formulation of the problem, and the results of calculations must correspond to actual running processes.

When solving practical problems, there is always an acute problem of the input parameters and initial data, the information on which, as a rule, is sketchy and incomplete. Therefore, the use of multi-dimensional and multi-component models, creating the illusion of a detailed review process, is not able to give results whose accuracy exceeds the precision of the initial staging parameters. Each mathematical model can only be considered useful when assessed the reliability of the results of its use.

Scenarios of Development of Emergencies and their Chronology

The emergence and development of emergencies in different industrial sites can occur in an infinite number of options, and complete their review, consideration, and discussion does not make sense (Shunxiang H., Feng L., Qingcun Z., Fei H., Jiang Zh., Zifa W., 2015). It is advisable to restrict a priori consideration of accidents the introduction of a criterion level or restrictions.

Currently, it is not decided whether an individual or a social risk is of that value when a decision on the admissibility of a security technology products should be made.

There is still no definite answer to the question, "Does a catastrophic accident is admissible if its probability is small, and can it be operated with the threat of industrial facility?" And though any moral position (positive or negative) answer to this question is debatable, for practical purposes the worst scenario analysis or the maximum possible accidents is justified, i.e. Results provide information to prepare for action in emergency situations. This analysis determines the potential costs of forces and means for protection of personnel, population, and the environment.

Besides, it is advisable to develop and investigate in detail the consequences of the most likely accident to the enterprise or an industrial facility (Pepea N., Pirovanoa G., Lonatib G., Balzarinia A., Toppettia A., Rivaa G.M., Bedognic M., 2016), based on an analysis of statistical data on accidents, the sequence (history) of their development, and expert opinion.

Sequences of possible accidents (Fig. 1) shows that in almost every major industrial accidents occur hearth deck, due to a large number of combustible materials available in the workplace.

It is known that the flame spreads representing a superposition of chemical reactions with the release of large amounts of heat in the ignition of combustible gas mixtures or gas thereon (Venkatram A., 2015). Upon detonation, these processes take place extremely rapidly, resulting in a blast wave; at relatively slow burning combustible mixtures of dust and gas most shock wave does not arise. Therefore, the explosion itself does not arise. Such an erroneous interpretation of combustion of gaseous and vaporous substances is apparently connected with the visible results of this phenomenon which leads to increased pressure on the premises and their partial or destruction. Therefore, if to not separate the combustion processes bearing on its external manifestations of an explosion, and the actual destruction of the membranes, and to consider all phenomena as a whole, such an emergency situation can be reviewed by the blast.

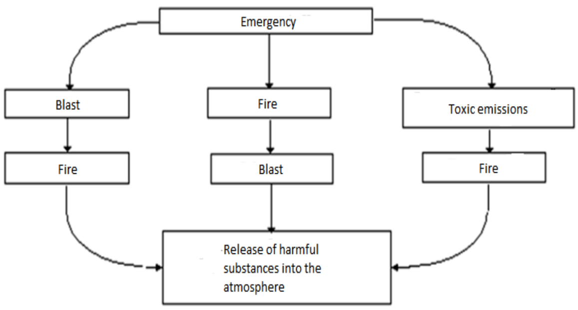

Fig. 1. Scheme of chronology of accidents development

Thus, calling combustible gaseous and vaporous substances, as well as dust and gas explosive mixture, and their burning – explosion (blast), should be aware of the conventions of these terms. In practice, it is often impossible to identify with certainty the combustion and explosion, as well as to establish the sequence of events. It should be noted that the probability of a fire after the blast is very high. Implementation of the explosion after a fire or a lamp after the release of toxic substances into the atmosphere to an appreciable extent by the thermodynamic characteristics of the moving bodies, their physical condition, and the presence of an oxidant access and so on.

Materials and Methods

The spread of pollutants in the atmosphere is described by the three-dimensional equations of conservation of mass:

$$\frac{\partial q}{\partial t}+\frac{\partial(uq)}{\partial x}+\frac{\partial(vq)}{\partial y}+\frac{\partial((w+v_g)q)}{\partial z}=K_S\left(\frac{\partial^2 q}{\partial x^2}+\frac{\partial^2 q}{\partial y^2}\right)+\partial$$

, (1)

where: q – volume concentration of impurities; u, v, w – components of wind speed, variables in space and time; v_g – the rate of gravitational deposition; K_S, K_z – coefficients of horizontal and vertical diffusion; IS – Field sources (instantaneous or continuous) emissions which are a function of space and time.

The horizontal components of the wind speed u, v – the input parameters of the model and determined from an objective analysis. The vertical component of the wind speed w determined from the continuity equation:

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0 \quad (2)$$

The speed of the gravitational settling is described by Stokes for particles with a radius r ≤ 10 μm was determined:

$$v_g = 1{,}26 * 10^{-5} * \rho * r^2, \quad (3)$$

where: ρ – density contaminants; r – particle radius.

Equation (1) was solved with the following initial and boundary conditions:

$$q(x, y, z, 0) = q_\Phi(x, y, z), \quad (4)$$

where: q_Φ(x, y, z) – background value bulk impurity concentration for the first day of the calculation:

$$q(x, y, z, 0) = q_0(x, y, z), \quad (5)$$

where: q_0(x, y, z) – volume concentration of impurities formed during the previous day.

The upper boundary of the area(H=5 км) set a zero concentration:

$$q(x, y, z, H) = 0 \quad (6)$$

At the lower boundary (the underlying surface) is given the full absorption conditions at the previous time step and the calculated full (turbulent and advective) impurities flow to the underlying surface in the current time step:

$$q(x, y, 0, t-\Delta t)=0;$$

$$\frac{\partial q(x,y,0,t)}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial q}{\partial z}\right) - (w + v_g)\frac{\partial q}{\partial z}. \quad (7)$$

Also, there is considered a setting of the boundary conditions of the third kind:

$$K_z \frac{\partial q}{\partial z} - \beta q = 0, \quad (8)$$

where: β – empirical constants, determining the absorption of the impurities of the underlying surface.

Condition (6) for the heavy impurities with a higher rate of gravitational settling; for the light impurities condition (7). Also, it takes into account the turbulent rise of pollutants which allows us to consider the underlying surface as the field of secondary sources and calculate the secondary transfer of the pollutant.

The lateral boundary conditions were as follows:

- in the area of inflow: q=0;

- in the area of outflow:

$$\frac{\partial q}{\partial t} = -\frac{\partial (uq)}{\partial x} - \frac{\partial (vq)}{\partial y} - \frac{\partial\left((w+v_g)q\right)}{\partial z}. \quad (9)$$

Distribution of impurities in difficult terrain and on a flat surface will vary significantly due to the deformation of the flow obstacles. In the presence of the relief system (1) - (9) should be addressed in a curvilinear boundary. The particular shape of the field, subject to rigid horizontal wall at a height H will be determined by the function that describes the shape of the relief Z_S(x, y). To avoid the difficulties associated with numerical integration in a curved area is usually transferred to the new coordinates in which the estimated area becomes straightforward. It was chosen the conversion, satisfying the following conditions: the transformation is reversible; identical when Z_S=0 и Z_S=H; It has continuous second derivatives; saves the mistake of approximation of the same order as in the Cartesian coordinate system which is achieved by its proximity to one of its determinant.

The boundary and initial conditions for the solution of this equation are selected the same as for the model of a uniform surface.

The model calculated convective movements caused by uneven heating of the underlying surface (the temperature of the cooling pond) and the non-uniformity of temperature in the surface layer (heat island over the pond-cooler):

$$w_{conv} = \left(\alpha \left| g\left(T_B - \overline{T_B}\right)/T_B \right| \Delta Z\right)^{1/2}, \quad T_B > \overline{T_B}, \quad \frac{\partial T_B}{\partial Z} > \gamma_{BA};$$

$$w_{conv} = 0, \quad T_B \le \overline{T_B}, \quad \frac{\partial T_B}{\partial Z} \le \gamma_{BA}, \quad (10)$$

where: α – empirical constant; T_B – virtual temperature; $\overline{T_B}$ – the average temperature of the virtual area; γ_{BA} – moist-adiabatic temperature gradient; ΔZ – layer thickness.

The proposed model for the numerical solution of equations (1) - (9) finite-difference method, well-established in many mathematical models of impurity transfer was selected. In this case, the differential equations describing the initial problem approximated by finite-difference scheme:

$$\prod_{S=1}^{p}\left(E-\frac{\Delta t}{2}L_S\right)\left(\varphi_i^{n+1}+\varphi_i^n\right)=\sum_{S=1}^{p}\Delta t L_S\left(\varphi_i\right)^n+\Delta t S_i^{n+1/2}, \quad (11)$$

where: $L_S(\varphi_i)=\frac{\partial(v_S\varphi)}{\partial x_S}+\frac{\partial}{\partial x_S}\left(K_S\frac{\partial\varphi}{\partial x_S}\right)$, (S=1, 2, 3), S_i – members of the equations describing the sources; Δt – the time step.

The circuit (11) is a two-layer difference scheme with a splitting operator, has second-order accuracy in time and is stable. When implementing the solution of the difference scheme, it was not for the function φ on g+1step, and for its transformation to the time step: $\varepsilon_{ø}^{ò+1}=\varphi_{ø}^{ò+1}-\varphi_{ø}^{ò}$. This implementation of the method allowed getting rid of the approximation of mixed derivatives. The implementation of the scheme for each spatial direction was carried out by the sweep method.

The main difficulties encountered in the formulation of the difference problem are the approximation of the advection operator of the transport equation (Ali A., Yousaf M.W., Awan M.M.S., 2015). The problem lies in the fact that the finite-difference scheme must satisfy the following basic requirements for solving the equation for positive definite functions:

- Have a low viscosity of the counting, that is, to have the order of approximation in time and space is not inferior to the second;

- Be monotonic, i.e., not generate non-physical, negative values;

- Be conservative, that is, it satisfies the equation of conservation of mass in a given volume;

- Have a small phase error, i.e. the maximum values of transfer functions and their gradients with given speed.

From File synoptic and upper-air observations were selected and then interpolated in a given grid nodes pressure, temperature, dew point, and wind speed components (U, V). The area of accounts was 30x30 km grid with step Δ x=Δ y=1 km horizontally and 5 km height variable pitch vertically. Then, from the continuity equation was calculated vertical component W. Speed ask five continuous source emitting pollutants. The coordinates correspond to the following sources of grid points:

- First source: i = 4, j = 4, k = 3;
- Second source: i = 8, j = 4, k = 2;
- Third source: i = 6, j = 16, k = 2;
- Fourth source: i = 16, j = 6, k = 2;
- Fifth source: i = 10, j = 10, k = 3.

Number of discharged impurities 0.5; 1.0; 1.0; 0.5; 1.0 g/s, respectively. Effective emission height was 100 m which corresponds to the third level of the model (k = 3). On the sixtieth time, step (in 6 hours) in fifth came anomalous emission source when one step at a time (360 s) thrown out 10^4 g of contaminants. The effective height of abnormal discharge was 190 m, which corresponds to the fourth level pattern (k = 4). Next, under the influence of the wind field, horizontal and vertical diffusion happened spread of pollutants and their loss on the underlying surface is mainly due to their gravitational sedimentation and turbulent.

Every day in the press were given field:

- Precipitated impurities on the surface of the basic (g);

- The remaining impurities in the air (g) at 40, 100, 190, 350 m respectively.

The field of precipitated impurities was issued in the form of contour lines for clarity and ease of analysis. Also released to control values: the amount of emitted pollutants (g); amounts precipitated impurities on the underlying surface (d); the remaining amount of substances in the atmosphere (i) and the ratio for the separated pollutant sources ejected as a percentage. In Figure 2 and Figure 3 are given the contour density (in mkg/m^2 * day) aerosol losses with a density ρ=1 г/см^3 and radius 1 mkm from five sources described above, after 1 day.

Results and Discussions

The results of numerical experiments on a computer model of pollutants transport on real data provide an opportunity to talk about quite realistic projections as impurities migration trajectories in given regions and on the values of the impurity concentration in the atmosphere. A software implementation of the model and the organization of the initial data allow modifying the configuration parameters of the model quickly; choose an arbitrary region in the Northern Hemisphere, the number of grid points of integration, the number of levels of emission sources and coordinates, etc.

The developed software can be used for predictive numerical experiments for modeling pollutant transport in the atmosphere from the field sources with varying intensity and density of contaminants.

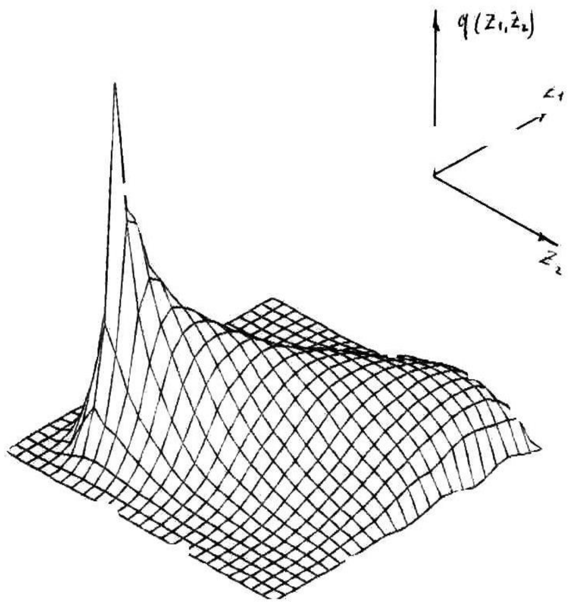

Fig. 2. The distribution of impurities from a single source

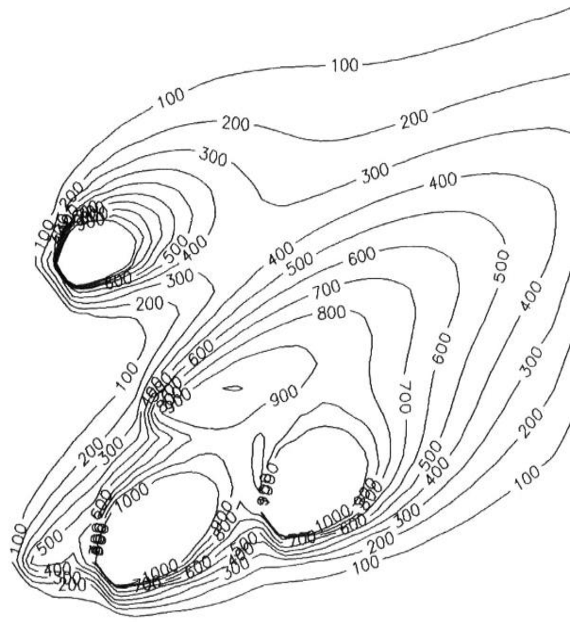

Fig. 3. Isolines density loss (in micrograms m^2/day)

Typing of pollutant emissions into the atmosphere

Emissions of pollutants and toxic substances in the atmosphere can be typed according to different parameters:

- By forming ejection time (instantaneous, short, long);

- In the spatial extent of release (local, compact and extended);

- According to the degree of turbulence in the substance (laminar and turbulent);

- By the presence of substances in different phases (plasma, gaseous or vaporous, liquid-phase or solid-phase, multi-phase);

- Chemical active substances (chemically active and passive).

In "pure" form when typing these toxicants emissions are relatively rare; usually of anthropogenic emissions is a combination of different kinds of species (Montero J.M., Fernández-Avilés G., 2015). For example, the jet stream (jet) include a combination of space-time typing emissions in addition to other typing, depending on the active and reactive materials, as well as the presence of one or more phase states of matter.

Thermals can be defined as compact vortex ejections varying degrees of reactivity, clouds of smoke - as turbulent small volumes, etc.

In terms of time typing, which is the most instrumental sound emissions can be roughly divided into instant, long and short. Consider the conditions of formation, and the specifics of such emissions.

Instant emissions occur at extremely rapid energy release and (or) of the substance into the environment. In this ejection it is formed as a torus with the circulating movement direction about the practical matter OBE. These emissions arise in the explosion of a nuclear warhead (Kallenborn R., 2016), containers with the hydrocarbon fuel in the gas phase or superheated steam, with the explosion of detonating chemical high explosive substance (ES), and so on. The distribution of physical properties in this release has a significantly heterogeneous nature, and which appeared after the explosion of the toroidal volume under the effect of buoyancy in the atmosphere begins to move.

Prolonged emissions are generated in the form of extended structures (jets) - the volume of non-uniform distribution along the course of the dynamic, thermal and concentration characteristics. Depending on the ratio of the density of the spray and substances ambient they are either float or sink. Calculation of features of the jet streams is a well-studied subject.

Partly emissions arise in the form of small clouds and thermals. Cloud is called a turbulent isolated volume chaotically moving vortices of various sizes and orientations (Dr Sambrani V.N., 2013). Stretch to the working fluid outlet time and a high level of turbulence leads to the fact that the release of pollutants into the atmosphere is formed by a limited amount of substantially uniform composition with relatively small differences in the sizes of different directions. Thermique is distinct from the presence of the club circular motion of matter about the direction of its movement (Sequeira R., Renil S., Yogesh B., Suryawanshi U., 2015).

It should be emphasized conditionality source separation for the duration of the working fluid outlet. It includes a clear time boundary separating the instantaneous emissions from short-term. In practice, it happens that the emissions are occurring a short period, generates a substantially uniform spatial distribution of mass, and the concentration of the thermodynamic characteristics. Such a case can be realized with a small density difference from the ambient density of the working fluid medium (the injection of gas at T = Const, "exploding wire," etc. The primary criterion for the short duration of release, in any case, should be considered after the termination of the existence of a source, but because of well-mixed material in a compact volume.

Concerning the issues of mathematical modeling of the main characteristic of the release, determines its consideration as a physical object, is its phase state. It can be used depending on the Euler or Lagrange approach. In turn, when typing gaseous and vaporous emissions, the spatiotemporal characteristics of the turbulence are necessary. It determines the nature of the continuum equations describing the origin and evolution of these formations (or this equation) (Chandrasekaran S.Sh., Muthukumar S., Rajendran S., 2013), characterizing laminar translational or rotational motion of a continuous medium, or the type of Stokes equations, describe the motion of turbulent compact or extended region.

Emissions of pollutants and toxic substances associated with human activities, the nature of the emerging power it is advisable to be divided into solid-phase (liquid phase) and gaseous (vaporous). And to describe the motion of the solid (liquid) impurities used ballistics equations for gas or steam – continuum equation. In the future, for brevity, it should be indicated only gaseous emissions and solid phase, bearing in mind that all the results obtained are suitable for steam and liquid phases, respectively (Cottrell M., 2014).

Note that the man-made solid-phase emissions are primarily of the explosive origin (Bowden R., 2015) unlike vaporous that arise from many causes: the explosion, evaporation, burning, etc. The most important practical applications of gas-vapor emissions are realized in the form of jets, thermals, and clubs (turbulent volume, thermodynamic), and concentration characteristics of which differ from the corresponding environmental characteristics.

The proposed emissions by typing phase nature of the sources of pollution created universal objects, i.e. it can be applied to radiation and chemical accidents (Fleming J.R., Johnson A., 2014). In any case, these accidents cause entry into the atmosphere of certain amounts of polluting substances mixed well in the gas-vapor phase or solid (liquid) particles. Ultimately, upon dilution in the environment of steam and gas emergency release or loss of solid phase, are formed and spatial field ground concentrations of toxicants.

Short solid-phase and gaseous emissions that occur in the atmosphere as a result of the rapid transformation of the working fluid internal energy into other forms of energy (to heat during combustion into kinetic energy of moving particles in the explosion, the energy of phase transition during evaporation) represent an important place in the problem of environmental pollution by anthropogenic sources. Solid-phase emissions are fluttering from the location of the accident (Walker C., 2014), and pieces are not chemically reacted portion crushed the working fluid (fuel, ground, exploding object). Gaseous (vaporous) emissions in the form of the volume of intensively turbulent detonation products (evaporation) are in a mixture with air occurring after termination of the source material and energy.

The expansion of the detonation shattered solid phase explosion occurs independently of the mechanical and physical characteristics of the blasted objects (Amano R.S., Sundén B., 2014). Any explosive energy release in the placed of the underlying surface or at a certain elevation will be the formation of explosive craters, shock air, and seismic waves, crushing the soil and explosives; fragmentation undermines product or object, as well as education of gaseous and vaporous (primary dust and gas) emissions.

With the explosion of explosives in the atmosphere or on the solid underlying surface, the expansion of the blast and its fallout on the surface, is determined by the fundamental relations of the macroscopic characteristics of the matter conservation and undermines involved in the process objects (soil, air, etc), as well as ballistic equations. These relations are the equations of conservation of mass and the mass of the substance in the release of impurities, the equation of conservation of momentum of the expanding matter, and energy conservation equation and the equation of state in the form of dynamic equilibrium of air and gaseous emissions formed part of the pressure.

Parameters of gas or vapor release can be obtained using relations conservation of macroscopic characteristics of the substance, averaged over the volume of emissions. These relationships express the laws of conservation of mass, energy and dynamic parameters of the turbulent volume of material in the process of forming a "fed" from the source of matter and energy in the presence of chemical reactions and phase transitions (Couling S., 2015). They are written as:

$M_2 = M_1 + Q_0\Delta t + ES\Delta t$,

$M_{2\,i} = M_{1\,i} + Q_0 C_{i0}\Delta t + ESC_{ie}\Delta t$,

$M_2 V_2 = M_1 V_1 + g(\rho_e - \rho)\nu\Delta t$,

$P = P_e$,

$M_2\Xi_2 = M_1\,\Xi_1 + Q_0 q_T\Delta t + ES\Xi_e\Delta t + \Delta Q_{\Phi\Pi} + W_j q_x\Delta t - H\Delta t$ where:

M, M_i – the mass of emissions and mass of ‘i' impurity in it,

Q_0 – expenditure function of forming emissions,

C_i – mass concentration of ‘i’impurity, $C_i = M_i/M$,

Ξ, Ξ_e – full of energy per unit mass of emissions and the environment,

p, v,V,S – ejection density, its volume, its velocity and engaging it in the area E of the environment,

g – acceleration due to gravity,

q_T – calorific fuel capacity,

P – the pressure of the gas or vapor,

W_i– formation rate of ‘i’ impurity by chemical reaction with the formation of heat q_x in the volume of emissions,

ΔQ_{PT} – heat of phase transitions (vaporization and condensation of liquid evaporating part ejection),

H – ejection energy loss (radiation, contact with the underlying surface, with precipitated impurities, etc.). Suffixes "1" and "2" refer to the respective points of time $t_2 = t_1 + \Delta t$, codes "0" and "e" refer to the parameters of expiration and environmental parameters.

When considering the finite difference equation of the jet stream is recorded on the characteristics of flow (the flow of substance and impurities, flows of momentum and energy).

The resulting finite-difference equation for aspiration time interval Δt to zero is converted to the differential. Their solution for the initial conditions, environmental conditions and characteristics of the object (geometric and thermodynamic) can solve the problem of finding the geometric, dynamic, and thermal characteristics of the turbulent volume concentration (ejection), moving in a casual environment.

Theoretical and Practical Implications

Examination of physical processes (Syngellakis S., 2014), describing the origin and evolution of polluting emissions and toxic substances in the atmosphere, are written many papers. The results obtained are at different stages of specific issues or problems in general summarized in monographs and books as well as periodicals. Most of the work on the subject solid-state emission (El-Hinnawi E., Hashmi M.H., 2015; Garrett H., 2014; Dr Kluin M., 2014; Steyn D., Mathur R., 2014) devoted to fractionation and formation of particles in the nuclear and chemical explosions, the physical characteristics of individual particles from the powerful blasts of air, precipitation of particles of explosive clouds. However, the explosive expansion of the solid phase explosion in the wind flow has not attracted the attention of researchers.

Details are scattering particle explosions and different substances in different vessels in a relaxed atmosphere were considered. Analyzing the data of works dealing with the origin and movement in the atmosphere of solid-phase (Godish Th., Davis W.T., Fu J.S., 2014; Mcevoy M., 2014; Klaassen C., Watkins J.B. III, 2015) particles can be concluded about the most important parameters of such problems: explosive energy properties and mechanical properties of the underlying surface. The conclusion can be made after the examined motion of particles and explosion in the wind flow in addition to the above parameters taking into account the meteorological parameters at the job site. Only under this condition can be expected to obtain the correct information about the calculation of dynamic and geometric characteristics of the solid phase of the explosion and the features of the density of its fallout on the ground surface.

Summarizing the data on the physical processes of occurrence and movement (Hemond H.F., Fechner E.J., 2014; Jacobs B.E.A., 2014; Jiménez E., Cabañas B., Lefebvre G., 2015) (particles in the atmosphere), it can be concluded that the determining parameters when creating the physical and mathematical models of solid-state short-term emissions are:

- Mass, energy and thermodynamic characteristics of explosives involved in the accident;
- Mass and geometric features of the emergency facility or part of it exploded;
- Strength and mass characteristics of the underlying surface (soil);
- Meteorological data;
- Temporary, geometric and structural features of the energy release and the working medium (scenario and emissions scheme, elevated above the ground, etc.)

Concerning the appearance and physical movement in an atmosphere of gaseous emissions, there are many researches on the current issue (McNeill J.R., Mauldin E.S., 2014; Kemmerer L., 2014; Ridley J.R., 2014). Most of them are carried out in the laboratory.

The authors consider emissions of combustion products energy-dense fuels, studied the detonation of explosives in the initial phase of development and the explosive release of heat during its ascent. It should be noted that the strict mathematical models for describing such processes to create extremely complicated. On the one hand, no clear physical picture of the course of development in the conditions of incomplete information about the site and the environment, on the contrary, the difficulties of numerical solutions of thermo-hydrodynamic equations provide primary and often insurmountable obstacles. Therefore, researchers are often limited to models that are used to describe the initial distribution of impurities in the space field observations.

Joint consideration of empirical data and mathematical modeling allows making quite an objective assessment of the geometric characteristics of the release, including the height of its rise and volume, as well as its dynamic features and the initial distribution of the contaminant in the atmosphere. These parameters are input data for the problem of propagation of the impurity in the air (Caradonna J.L., 2014).

Summarizing the results of the work mentioned above, it can be concluded that the initial data for the construction of such models must be dynamic and energy emission characteristics, as well as the original distribution of the contaminant in the space (Stern A.C., 2015) and the distribution of meteorological parameters (King A., 2015).

Defines the parameters when creating the physical and mathematical models of the gaseous emissions are:

- The nature of the ejection duration of the working fluid output (instantaneous, short, long);
- Mass, energy, and the dynamic characteristics of the formed release;
- Physical characteristics of the solid phase and aerosol emissions;
- Details of possible chemical reactions and phase transitions;
- Weather information, including information on the altitudinal gradient of meteorological parameters.

The principles of physical and mathematical models of the origin and movement of atmospheric pollutants and toxic emissions (Daniels J.A., 2015) are based on the allocation and the detailed analysis of the main defining characteristics of the research object. The most common main features of the study include:

- Accounting of emissions specifics on the nature of the phase (solid-state, gas);
- Depending on the type of account from the source of emission time of action and turbulence of emissions;
- Consideration of the total energy and its fractions, introduced source of emissions;
- Consideration of mass and energy characteristics of the working fluid;
- Records of meteorological data and high altitude distributions;
- Keeping data on possible chemical reactions and phase transitions.

Atmospheric Sources of Pollution in Case of Accidents

Anthropogenic accidents, usually accompanied by entering into the environment of pollutants in gaseous, liquid or solid form (Jingjing Y., 2014). Their physical and chemical characteristics correspond to the parameters of working bodies, of which the scene is created in fact the primary source of contamination. Its formation ends at the end of the atmosphere and lining material its pressure to a pressure value in the surrounding space.

The secondary atmospheric source appears as a natural extension of the primary source in space or in time. In real turbulent atmosphere rapidly occurring secondary source gas in the form of a compact volume has the almost uniform structure of macroscopic characteristics. Therefore, these sources are in the form of clubs are the well mixed (similar) matter with mass forces the application center at the geometric center of the volume.

With long-term receipt of the working fluid into the air stream there, and in the interim between the short-term and fixed in space can form a complex gas volume modeling of the physical characteristics of which is rather problematic. In this case, resorting to replacing the real object, it is modeling the regular geometric bodies such as a hemisphere, sphere, cylinder or combinations of such institutions. In particular, linear and point sources are idealizations of sources of finite size with the aspiration of their characteristic sizes to zero.

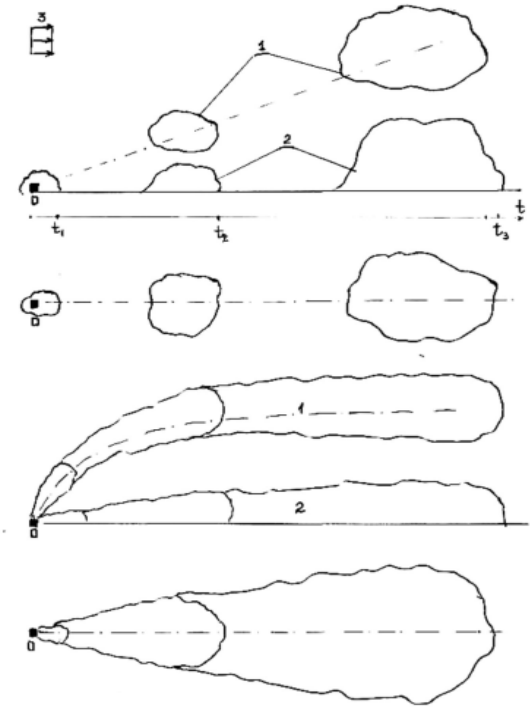

Fig. 4. The circuit of accidental release time of the atmosphere in the long- and short-time sources for light (1) and hard (2) gas: t_1, t_2, t_3 - moments of time after the gas outlet.

The formation and movement of the atmosphere in the gaseous emissions are also dependent on their density. If the working fluid is heavier than air, it tends to be the release of the earth's surface with a light gas - pops up in the atmosphere (Fig. 4).

Depending on the conditions of the working fluid entering (Constanda C., Kirsch A., 2015) the atmosphere and environmental performance at a single accident, there can be formed consistently various secondary sources and transformed into the three-dimensional areal, and areal into the bulk.

All the variety of sources of the atmospheric model, equivalent to real polluting entities, can be divided into several types or species. The simplest is the reference point source pollution which used in the calculation of environmental pollution as an idealization of the real emissions with a Gaussian distribution of impurities.

Other sources are the linear model sources in the form of a straight line of finite or infinite length, the emitting contaminant in the transverse direction. Elevated and high-altitude line sources used in the preparation of analytical solutions to the problems of a contaminant for the rocket trail, exhaust flying aircraft and other extended objects. The roads, highways, runways of airfields and many others are based on the linear model sources.

Ground area sources occur when burning vast areas of forest (Dincer I., Colpan C.O., Kizilkan O., 2015), spilled fuel oil, liquid evaporation, etc.

Another area sources in the form of a cross-section of the jet in place of the progressive loss of identity occurs when the flow of combustion in a relatively small zone. This source has raised character.

And finally, a raised surround source used to simulate emissions from explosions after equalization of pressure inside and outside the scope emerged. These sources also appear after the rapid combustion of the fuel, "one-shot" liquid evaporation, evaporation of cryogenic products and some other processes of rapid phase transition of substances from one state to another.

Sources complex form submitted emissions with "foot" floating jet emissions from fires of different types of objects, combined with accidents (explosion + fire, fire + strait, strait + explosion). They are modeled by a superposition of simple geometric volumes.

The liquid-vapor or aerosol (smoke) emissions are modeled geometric bodies with evenly distributed regarding impurity, solid-phase or liquid-drop - weightier particles are the geometrically correct shape.

Since the dispersion of pollution comes from emissions formed during the final stage of its dynamic individuality, for the settlement of environmental pollution in case of accidents becomes relevant knowledge of the information on secondary sources. This information is the input into the problems of calculation of dispersion admixtures and construction fields of spatial and land pollutant concentrations.

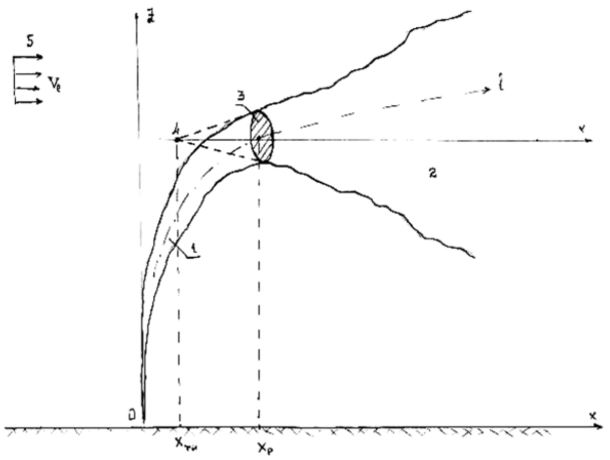

Fig. 5. Driving the upward flow in the fire and the formation of sources of pollution at weak-turbulent atmosphere: 0 - fireplace; 1 - the primary source of bulk (stream); 2 - impurity dissipated under the effect of atmospheric diffusion; 3 - secondary area sources (shaded); 4 - an imaginary point source; 5 - the wind.

As previously mentioned, the secondary sources of pollution occur when the dynamic and (or) the thermodynamic characteristics of emerging atmospheric emissions are markedly different from similar environmental characteristics. Such characteristics may be the density of matter, its temperature, the state of aggregation, as well as the rate of release of the movement as a whole, or the speed of its parts and fragments. In practice, any anthropogenic emissions can be represented consistently replaced by primary and secondary sources. Some typical situations are different types of accidents of environmental pollution sources are illustrated in the drawings Fig. 5 - Fig. 9.

Fig. 5 is a schematic diagram of the formation of atmospheric sources of fire relatively small area, where over the fireplace is formed by the convective stream of the mixture of combustion products and involves air. Under the effect of buoyancy force jet rises, bent wind flow, and after the destruction scattered by atmospheric diffusion.

It is assumed that the atmosphere is weak-turbulent and contaminant after the loss of a powerful personality jet on a background pulsating motion of atmospheric vortices moving in a continuous unbroken stream. These conditions correspond to a stable state of the atmosphere (Benítez M., Miramontes O., Valiente-Banuet A., 2014) when the vertical temperature gradient is close to zero or negative. Physically, this means an increase in height, and the pop-up volume of air is colder than the environment; its movement is slowed down and dies.

Persistent contrails or conditions characterized by a weak turbulent exchange and surface concentration of pollution are small. As the primary source in the figure, the spray 1 acts as the place of its degradation corresponding to X - in the point coordinate X_p. Further, there is an active flow dispersion of the effective cross section 3. This section of the jet and a secondary source of contamination.

If dispersion border continues upstream, in the case of isotropic scattering, they converge at a point 4 which is the place of effective point source scattered emissions.

The event of the formation of atmospheric sources of a fire in a highly unstable environment is considered in Fig. 6. Here, as in the previous situation, the primary source is the actual stream 1 to the place of its destruction 2. However, due to the nature of the vibrational motion of the jet stream (meandering) in the final stage of development of secondary sources of pollution will be quasi-clouds, recurring in 2. Quasi-clouds are split into fragments of separate portions of the jet material. They have a large-scale swirling movement of the "pocket track" occurring in the flow of the barrier. The valid point 4 of the source can be built as in the previous case, by reducing the envelopes clubs in some single center.

Note that this picture of the formation of atmospheric sources is characteristic of the states of the atmosphere with a vertical gradient of temperature greater than the adiabatic. The heated air portions are gaining momentum buoyancy forces, and cold air parts replaced them are omitted. As a result of the movement of air masses, the intensive vertical mixing impurity is increasing in Z layer.

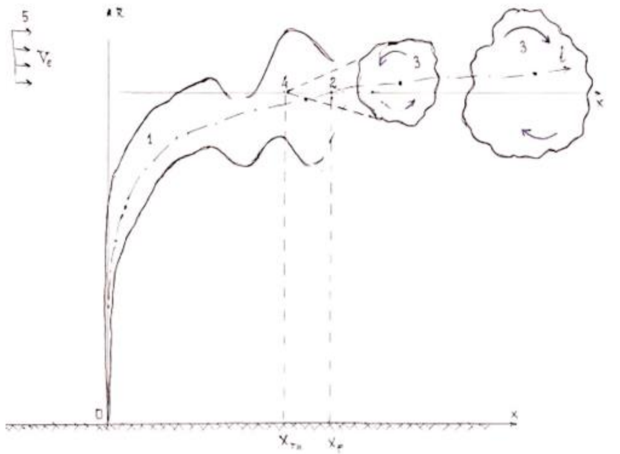

Fig. 6. Driving the upward flow in the fire, and the formation of sources of pollution with highly turbulent environment: 0 - fireplace; 1 - primary volume source (meandering stream); 2 - a place of destruction of the jet stream; 3 - secondary volume sources; 4 - an imaginary point source; 5 - the wind.

If the temperature outside is close to or equal to the gradient of the adiabatic (a decrease in temperature by about 1C every 100 meters high), then it implemented the so-called indifferent (or neutral) conditions. With a vertical gradient of temperature equal to (or below) the adiabatic rising gas, volume has the same temperature as the surrounding air mass. In this situation, there is no impetus to the ascent of forces, and the atmosphere does not have any impact on emissions in Z - direction.

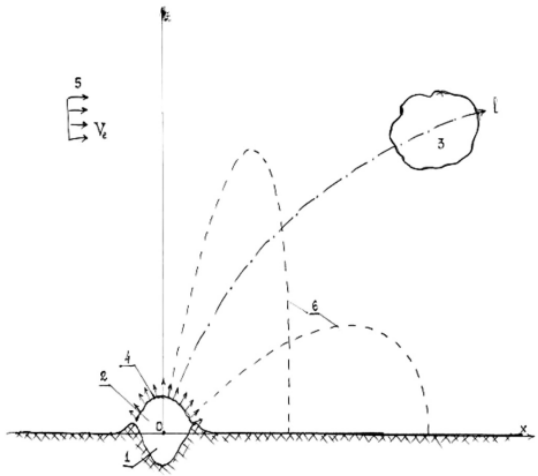

Fig. 7. Driving emissions movement in the explosion, and the formation of pollution sources: 0 - scene of the explosion; 1 - funnel; 2 - volume primary source; 3 - secondary volume source (explosive cloud); 4 - secondary surface source pollution solid and liquid phases of the explosion; 5 - the wind; 6 - particle trajectories.

Driving emissions movement in the blast and the formation of sources of air pollution and land are shown in Fig. 7. As can be seen from the figure, above the place of the explosion source 0 arises volume 2, consisting of explosive gasses particles and fragments of the crushed material of the underlying surface (soil), involved in the release of the cup 1; 2 in the air volume is available. During the time of ~ $10^{-2}c\Xi 10^{x}c$ gas pressure in the jet 2 is reduced to atmospheric pressure, and its hemispherical surface occupies a position in the space 4 which is a secondary surface source pollution robust and liquid phases of the explosion.

The gaseous products of the blast, the explosive momentum, and buoyancy forces leave the volume 2 and float in the atmosphere. So there is a secondary source of gas - the explosive cloud of 4. It is carried away wind flow and rises to a certain height, which loses its dynamic personality on the background of a turbulent environment. Then, under the action of atmospheric diffusion cloud substance is dispersed in the environment.

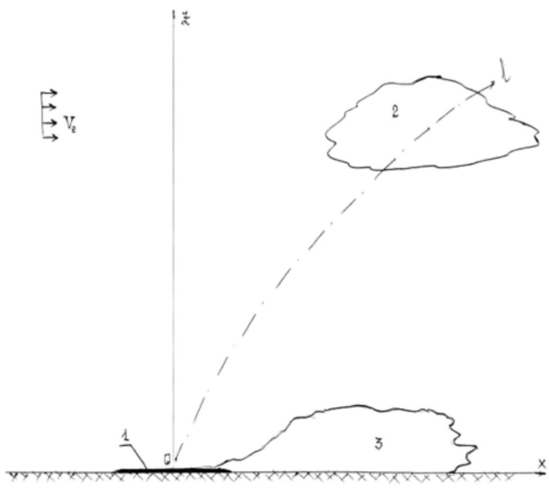

Fig. 8. The scheme of movement of toxic emissions from the strait and the formation of pollution sources: 0 - the place of the Strait; 1 - the primary source of the marketplace; 2 - secondary source volume (the evaporation of lighter gas); 3 - secondary source volume (the evaporation of the heavy gas); 4 - the wind.

Thus, in the case of explosion accident occur substantially simultaneously two secondary ejections. For solid-liquid separation is a secondary source of explosion hemispherical surface 4, and for the gaseous phase - the volume club 3.

Now, consider how to form the sources of environmental pollution from spills of toxic substances. As it follows from Fig. 8, the strait is the primary area sources 1 which depending on the density of the vaporized gas is formed or a secondary source of ground volume 3 (the evaporation of the dense gas), or high-altitude (upbeat) surround a secondary source 2 (the evaporation of lighter gas). Gas is considered difficult if the density is higher than that of air and light - if below.

Another practically important case of secondary sources is toxic explosion tank with toxicant, raised above the underlying surface to a certain height. This case corresponds to the blast of some types of chemical munitions.

As follows from the figure Fig. 9, in a place tank explosion toxic liquid volume, occurs vapor-liquid-droplet primary source 1 containing a toxic product in the vapor, the gas, and liquid phases. The explosive cloud 1 expands dangerous gasses until its pressure equals the atmospheric pressure. Then, from the volume 1 will depart liquid fraction and vaporized product leaves the scene of the explosion and a cloud of dense gasses begin to decline. Thus, there is a secondary volume source of 2 of toxicant.

The primary source 2 (explosive cloud) has a solid and liquid phase of the explosion and accelerates radially expanding gasses after beyond flying by the force of inertia and gravity on ballistic trajectories. Flying particles and fragments of destroyed in the explosion of an object end with the loss to the surface in some areas. The trajectories of particles emitted from the blast chamber at different angles are indicated in the figure by dashed lines.

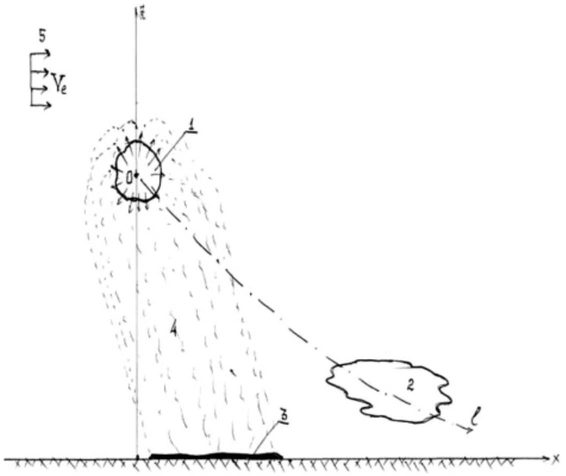

Fig. 9. Driving emissions movement and the formation of air pollution sources at the explosion of containers with toxic liquid: 0 - scene of the explosion; 1 - primary volumetric vapor-liquid-droplet source; 2 - secondary volume source (a cloud of heavy gas); 3 - secondary area sources (settled Strait); 4 - secondary source of bulk liquid-drop; 5 - the wind.

Two more toxic secondary sources may arise in the general case of the liquid explosion fractions: liquid-drop volume 4 and areal 3 from the liquid deposited on the underlying surface.

It should be noted that the examples of occurrence of the above sources of pollutants and toxic substances in the atmosphere do not exhaust the whole variety of possible situations in practice. In each case, an emergency should be considered a physically reasonable course of the incident, to analyze the most likely its development and identify emerging sources of pollution of the environment on this basis.

Conclusion

Incident or accident in the enterprise can be defined as a devastating release of its own stored energy industrial plant in which raw materials, intermediate products, company products and waste products, installed on-site processing equipment, engaging in the emergency process, create a striking factors for people, personnel, and human environment of the industrial enterprise (Layton A.T., Olson S.D., 2014).

In theory, any object can be represented by an infinite number of accident scenarios, but in reality, they can be implemented by no means all.

Some emergency situations are impossible for natural reasons, partly due to the violation of the causal conditions and connections. Such scenarios should be noted at the initial stage of its consideration of possible accidents at the facility; the other scenarios are theoretically feasible or hypothetical. Under this hypothetical, any accident generated by initiating events not prohibited by the laws of nature may be called

Currently, the scientific literature has a huge number of techniques (Xie L., Huang D., 2014), algorithms (Drake J.B., 2014), and formulas (Stech D.E., 2014) that enable allegedly authors to predict accidents, incidents and accidents of anthropogenic and natural origin. Detailed training materials, engineering studies, and mathematical models usually come from a consideration of some standard scenarios of occurrence and development of a dangerous phenomenon, which neglect the contribution of the environment in the course of the incident.

Usually, they ask some "average" importance of the environment (Drake J.B., 2014): air temperature and wind speed, very rarely - altitude temperature gradient, even rarer - atmospheric turbulence. Of course, this approach allows to evaluate the overall physical picture of the phenomenon, but can lead to significant errors in calculations, and sometimes mistakes in the forecast for some extreme or unusual natural phenomena.

To troubleshoot the error to an emergency should be added to the forecast meteorological forecast. It should be borne in mind that the meteorological prediction is not capable, in principle, provided all details of the future state of the atmosphere. It is necessary to proceed from the dialectical determination of the phenomena, the essence of which is in the fact that need manifests itself through accident. It follows that the events of future emergencies require credible approach taking into account the possible development of multi-variant processes.

Note that weather forecasts are categorized search estimates, based on a conditional extension of the future development trend of the process being studied in the past and present. The aim of these projections is the answer to the question, what will happen most likely while maintaining the current trends.

When forecasting emergency situations, it is advisable to use the classification adopted in the prognostication of accidents. According to the length of time for which the forecast is developed, all forecasts are divided into operating (current), short-term, medium-term, long-term and Superfund.

In integrated forecasting accidents taking into account the possible effects of the environment should be the following complementary sources of information about the future behavior of the object of research (fire, explosion, toxic release):

- Evaluation of the projected future state of the object by experience (often with the help of analogies with a rather well-known similar processes and phenomena);
- Extrapolation of the future trends, patterns of development which past and present are well known;
- A model of the future state of the research object, constructed by the anticipated changes in the number of conditions, laws, of which the past and present are well known.

In accordance with these three sources of information about the possible emergency facility, there are three complementary ways to develop forecasts: expert, extrapolation, and model.

Expert assessment is used when discussing predictions by some experts - qualified specialists in this area.

1. Shunxiang H., Feng L., Qingcun Z., Fei H., Jiang Zh., Zifa W., (2015). *Modeling and Optimal Control of Atmospheric Pollution Hazard in Nuclear and Chemical Disasters*

2. Pepea N., Pirovanoa G., Lonatib G., Balzarinia A., Toppettia A., Rivaa G.M., Bedognic M., (2016). *Atmospheric Environment, Development and application of a high resolution hybrid modeling system for the evaluation of urban air quality*

3. Venkatram A., (2015). *Lectures on air pollution modeling*

4. Ali A., Yousaf M.W., Awan M.M.S., (2015). *Environmental pollution: legislation and remedial measures* – J Environ Prot Sustain Dev

5. Montero J.M., Fernández-Avilés G., (2015). *Functional Kriging prediction of pollution series: The geostatistical alternative for spatially-fixed data* – Estudios Econ. Apl,

6. Kallenborn R., (2016). *Implications and Consequences of Anthropogenic Pollution in Polar Environments*

7. Sequeira R., Renil S., Yogesh B., Suryawanshi U., (2015). *Automated control system for air pollution detection in industries*

8. Dr Sambrani V.N., (2013). *Industrial emission – a case study‖* -- EXCEL International Journal of Multidisciplinary Management Studies, Volume 3(8), pp. 63-73

9. Chandrasekaran S.Sh., Muthukumar S., Rajendran S., (2013). *Automated Control System for Air Pollution Detection in Vehicles* -- 4th International Conference on Intelligent Systems, Modelling and Simulation

10. Cottrell M., (2014). *Guide to the LEED Green Associate* – V4 Exam, p. 109

11. Bowden R., (2015). *Impact of Science and Technology: Energy Sources* – p.34

12. Fleming J.R., Johnson A., (2014). *Toxic Airs: Body, Place, Planet in Historical Perspective*

13. Walker C., (2014). *Ecotoxicology: Effects of Pollutants on the Natural Environment*

14. Amano R.S., Sundén B., (2014). *Aerodynamics of Wind Turbines: Emerging Topics* – p. 161

15. Couling S., (2015). *Measurement of Airborne Pollutants* – p. 7

16. Syngellakis S., (2014). *Biomass to Biofuels* – p. 55

17. El-Hinnawi E., Hashmi M.H., (2015). *The State of the Environment* – p.5

18. Garrett H., (2014). *Organic Lawn Care: Growing Grass the Natural Way* – p.12

19. Dr Kluin M., (2014). *Environmental Crime and its Victims: Perspectives within Green Criminology*

20. Steyn D., Mathur R., (2014). *Air Pollution Modeling and its Application XXIII* – p .155

21. Godish Th., Davis W.T., Fu J.S., (2014). *Air Quality, Fifth Edition* – p. 461

22. Mcevoy M., (2014). *External Components*

23. Klaassen C., Watkins J.B. III, (2015). *Casarett & Doull's Essentials of Toxicology, Third Edition*

24. Hemond H.F., Fechner E.J., (2014). *Chemical Fate and Transport in the Environment* – p. 1

25. Jacobs B.E.A., (2014). *Fluidic Sensors and some Large Scale Devices: Course held at the Department of Hydro- and Gas-Dynamics*

26. Jiménez E., Cabañas B., Lefebvre G., (2015). *Environment, Energy and Climate Change* – I: Environmental Chemistry of Pollutants and Wastes

27. McNeill J.R., Mauldin E.S., (2014). A *Companion to Global Environmental History* – p. 222

28. Kemmerer L., (2014). *Eating Earth: Environmental Ethics and Dietary Choice*

29. Ridley J.R., (2014). *Safety at Work* – p. 462

30. Caradonna J.L., (2014). *Sustainability: A History*

31. Stern A.C., (2015). *Sources of Air Pollution and Their Control: Air Pollution*

32. King A., (2015). *The State of the Planet: A Report Prepared for the International Federation of Institutes for Advanced Study (IFIAS)* – Stockholm

33. Jingjing Y., (2014). *Comprehensive Evaluation of Effective Biomass Resource Utilization and Optimal Environmental Policies*

34. Constanda C., Kirsch A., (2015). *Integral Methods in Science and Engineering: Theoretical and Computational Advances*

35. Dincer I., Colpan C.O., Kizilkan O., (2015). *Progress in Clean Energy* – Volume 1: Analysis and Modeling

36. Benítez M., Miramontes O., Valiente-Banuet A., (2014). *Frontiers in Ecology, Evolution and Complexity* – p. 177

37. Layton A.T., Olson S.D., (2014). *Biological Fluid Dynamics: Modeling, Computations, and Applications, Contemporary Mathematics* – Vol. 628

38. Xie L., Huang D., (2014). *Advanced Engineering and Technology* – p. 557

39. Drake J.B., (2014). *Climate Modeling for Scientists and Engineers*

40. Stech D.E., (2014). *International Conference on Computational and Information Sciences (ICCIS)* – Publications, Inc.

41. Daniels J.A., (2015). *Advances in Environmental Research* – Vol. 41