
Models of radionuclides transport in atmosphere from integrated software package "NOSTRADAMUS"

Аннотация

Приведено описание моделей переноса радионуклидов, реализованных в интегрированной системе “NOSTRADAMUS” Института проблем безопасного развития атомной энергетики (ИБРАЭ). Модель мезомасштабного переноса базируется на разработанном в ИБРАЭ алгоритме случайно блуждающих гауссовых облаков. Стандартные методы блужданий частиц и PUFF-метод, т.е. регулярный транспорт гауссовых облаков в неоднородном ветровом поле являются частными случаями обобщенной модели. Предложенный алгоритм имеет существенные преимущества по вычислительным ресурсам без потери точности по сравнению с методом случайных блужданий частиц, используемым при моделировании мезомасштабного переноса. Тестовые примеры показывают убыстрение в десятки раз.

В пакете также используются разработанные быстрые коды моделирования начальной стадии выброса над источниками пожара или взрыва, основанные на интегрировании законов сохранения. В этих случаях облако может занимать несколько километров по высоте, и принимать во внимание сильный разброс скоростей ветра, аппроксимационные формулы типа Бригса оказываются слишком грубы.

В работе представлены верификационные и валидационные расчеты.

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Abstract

The characteristics of the radionuclides transport model imbedded into the NOSTRADAMUS integrated software package of the Nuclear Safety Institute are described. The mesoscale transport model based on the mixed techniques of randomly migrated gauss clouds which is designed in Institute. The model embraces as its particular cases: the standard method of point object random displacements; the PUFF-method, i.e. the regular transport of gauss clouds in a wind field. The mixed techniques of randomly migrated gauss clouds in nonuniform wind field designed in the Institute takes a great advantage in computation time over the point random displacement methods without appreciable loss of precision. Test runs of the model show its performance to be several tenth times better.

There are several models of a source of contamination. The package includes some local models of contamination transport over a fire or an explosion. For these processes the contamination distribution can embrace several km in height. Over this height interval the wind can be directed differently. In this case the approximation formulas of Brigs give only very rough assessment. Some verification and validation results are presented.

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1 Introduction

In the Nuclear Safety Institute the integrated software package NOSTRADAMUS is designed for the modeling of consequences of nuclear accidents and the support of decision making.

The software is able:

- to forecast the release propagation in atmosphere depending on meteorological situation,
- to estimate the atmospheric radioactive release consequences.

The software package includes both mesoscale model of radionuclides transport in real meteorological situation and a model of local atmospheric processes over the source of a fire or explosion.

**Mesoscale model type:** the stochastic random displacement model

**Meteorological data:** the information available from the Russian Meteorological Center for the standard isobaric surfaces in the nodes of 2.5°2.5 horizontal grid. The package carries out the interpolation and detalization of these data.

**The source:** the point polidisperse source; the volumetric polidisperse source including polluting distribution over the source of a fire or explosion.

**The processes are considered:** gravitational deposition, dry deposition at the surface, washing out by precipitation.

**Hardware:** IBM PC

**Program language:** C, PASCAL

In this paper the models of radionuclides transport in atmosphere from integrate software package NOSTRADAMUS are describe.

Stochastic models for impurity propagation in atmosphere may be divided on two classes.

- Track models with stochastic displacement of particles in turbulent atmosphere belong to the first class. Models with stochastic particles speeds disturbances that are defined from Langevin equations belong to the second class. Models of second class require much greater costs then models of first class.
- Models of first class, that are based on assumption of large diffusion scale, where most of details are averaged, are more economical.

In case of track models the requirement imposed for the period of averaging is connected with the fact that sequent shifts of diffusing particles are independent. The reduction of averaging time bring the necessity to consider second type models with dependent shifts where particles speeds undergo stochastic distribution.

The solution of track stochastic equations with general requirements comes to the solution of diffusion equation for average magnitudes (period of averaging is greater than Lagrangian time scale). Therefore track stochastic models for problems of impurity propagation have the same scope as equations of diffusion propagation.

Track models have gone through serious examination. These models are considered to be perspective numerical methods for calculation of impurity propagation in inhomogeneous field of wind velocity.

This examination figured out that formulation of track equations [1] in case when vertical diffusion coefficient is height dependent was incorrect. The vertical diffusion coefficient is growing fast with height for most of standard atmospheric conditions. In [1] the corrections which allow to take into consideration this dependence has been calculated.

For use as a base model we developed the stochastic particle displacement model taking into account the corrections for the vertical diffusion coefficients dependence on height. We have shown for several analytical solutions the great advantage of the new formulation over traditional one.

In particular if the diffusion coefficient changes with height realistically, the stochastic equations formulation in the model similar to that of the "TYPHOON" (Obninsk, Russia) [2] distorts the solution of semi-empirical diffusion equation significantly.

Along with this base model we are developing a couple of modified models. The first modification is supposed to be used for contamination transport simulation up to 50–100 km range with the wind varying with time and height. The second modification is intended for the transport modeling with arbitrary wind field. The first model considers the stochastic transport process of a plane Gauss clouds with their centers of mass subjected to random vertical displacements. Several test runs of the model show its performance to be several tenth times better then that the base type without any loss of results quality for appropriate tasks.
The second modification is the stochastic process of the transport of clouds with Gauss concentration distribution. The random process can be split into two independent processes. The sum of dispersions of these two processes must be equal to dispersion of former process. The dispersion of Gauss process is estimated considering the distance scale on which the wind speed variations are negligible. It gives a considerable advantage in computation time (up to ten times) without any loss of results quality.

In an emergency situation of great importance is the on-line exhaustion of the possible scenarios and their consequences. This requires high performance computational algorithms. Therefore the common stochastic methods mentioned above are used in on-line forecasts. This paper describes the mixed techniques, rising computational speed without noticeable loss of accuracy, that can be used for on line forecasts. Besides, the use of these techniques allows to consider many factors usually neglected in common Gauss models.

For example, Gauss models including Gauss–Puff models describe the concentration distribution mainly in terms of gauss low (RIPMUFF and other). The impurity transport in large-scale wind field does not obey gauss low. Strictly, the low is applicable for \( \gamma \) mesoscale (2–20 km) and in some cases for \( \beta \) mesoscale (20–200 km). In our opinion they are not applicable for \( \alpha \) mesoscale.

During the preliminary verification of stochastic model several parametrizations of diffusion coefficients have been tested. The most successful is the parametrization and typization of synoptical situation (the wind rotation with height) in terms of 7 stability types (Byzova, "TYPHOON", Obninsk, Russia) [3,4,7]. This typization is based on the data obtained at the Obninsk meteorological tower. We use these data to reconstruct the vertical wind profile if only poor data about synoptical situation are available.

Some verification and validation results are presented.

Mesoscale model for impurity propagation of Nuclear Safety Institute has been validated by five environmental experiments. The comparison of the results of the NSI model, two basic models of the Livermore Laboratory (USA) and nine European models have been made for all these five experiments. This intercomparison have shown the high competitivability degree of the stochastic model of the Nuclear Safety Institute.

2 Mesoscale model for impurity propagation in inhomogeneous velocity field

Equation of advection and diffusion, which describe impurity propagation in atmosphere is

\[
\frac{\partial c}{\partial t} + \frac{\partial uc}{\partial x} + \frac{\partial vc}{\partial y} + \frac{\partial wc}{\partial z} = \frac{\partial}{\partial x} (K_x \frac{\partial c}{\partial x}) + \frac{\partial}{\partial y} (K_y \frac{\partial c}{\partial y}) + \frac{\partial}{\partial z} (K_z \frac{\partial c}{\partial z}) + Q + S
\]

(1)

where \( c \) is volume concentration;
\( U, V \) — horizontal components of wind velocity;
\( W = W - W_p \);
\( W \) — vertical component of wind velocity;
\( W_p \) — speed of gravitational precipitation;
\( K_x, K_y \) — horizontal diffusion coefficients;
\( K_z \) — vertical diffusion coefficient;
\( Q \) — ejection source power;
\( S \) — term, which takes account of washout.

The following system of stochastic equations for particle coordinates is the base for analysis of impurity concentration propagation in inhomogeneous wind velocity field [1].

\[
\frac{dX}{dt} = U + U'; \quad \frac{dY}{dt} = V + V'; \quad \frac{dZ}{dt} = W + \frac{\partial K_z}{\partial z} + W'
\]

(2)

\( U', V', W' \) — component of wind velocity pulsation — stochastic quantities.

The system of stochastic equations (2) may be written in the following form

\[
dX = U dt + \sigma_x a_x; \quad dY = V dt + \sigma_y a_y; \quad dZ = (W + \frac{\partial K_z}{\partial z}) dt + \sigma_z a_z
\]

(3)
where $a_x, a_y, a_z$ are stochastic quantities with Gaussian probability distribution, unit dispersion and null mathematical expectation. The system of stochastic equations (3) is equal to the following equation (5):

$$
\frac{\partial c}{\partial t} + \frac{\partial U c}{\partial x} + \frac{\partial V c}{\partial y} + \frac{\partial W c}{\partial z} = \frac{\partial^2 (K_x c)}{\partial x^2} + \frac{\partial^2 (K_y c)}{\partial y^2} + \frac{\partial^2 (K_z c)}{\partial z^2}
$$

(4)

In case when $\sigma_x = \sqrt{2K_x dt}$, $\sigma_y = \sqrt{2K_y dt}$, $\sigma_z = \sqrt{2K_z dt}$.

Equation (4) may be rewritten as

$$
\frac{\partial c}{\partial t} + \frac{\partial (U - \frac{\partial K_x}{\partial x}) c}{\partial x} + \frac{\partial (V - \frac{\partial K_y}{\partial y}) c}{\partial y} + \frac{\partial W c}{\partial z} =
$$

$$
\frac{\partial}{\partial x} (K_x \frac{\partial c}{\partial x}) + \frac{\partial}{\partial y} (K_y \frac{\partial c}{\partial y}) + \frac{\partial}{\partial z} (K_z \frac{\partial c}{\partial z})
$$

(5)

As the rule derivative of coefficients of horizontal turbulent exchange may not be counted when compared with wind speed. In this case the system of stochastic equations (3) is equal to the equation (1). The term $(\partial K_x/\partial z)dt$ in the last equation of system (3) was not considered in many models of such type.

As shown in [1] this brings to non-realistic impurity disturbance with height, impurity accumulation near surface and overestimated magnitude of deposition. There is effective average (against a background of turbulent pulsations) vertical speed $\partial K_x/\partial z$ (pointed up) due to rapid growth with height of vertical diffusion coefficient in the low layers of atmosphere.

If source action $Q$ is represented as a set of great amount of discrete ejections and if their position in inhomogeneous speed field is defined by track equations (3) then cloud contour may be found in any moment and impurity concentration disturbance may be calculated

$$
c = \frac{mn}{V}
$$

(6)

where $m$ — mass of single particle, $n$ — number of particles in chosen volume $V$.

Wind velocity field and diffusion coefficients are the input information for calculating particles coordinates. Wind velocity in regular grid nodes is known from forecast of Russian Meteorological Center, which is based on synoptic information and routine forecasting model. The coefficients of vertical diffusion in grid nodes are defined from information about wind velocity and insolation class by the method described in [3]. Diffusion coefficients and its varyability with height depend upon: class of stability, season and surface friction. The value of wind velocity and diffusion coefficients components outside of discrete grid are linear interpolated from the neighboring nodes.

The coefficient of horizontal turbulent diffusion was defined from data obtained by “TYPHOON”, Obninsk

$$
\sigma_y = a_{i|1|} v^{a_{i|1|}}
$$

(7)

where $a_i$ and $b_i$ depend upon class of stability.

During the preliminary verification of model several parametrizations of diffusion coefficients have been tested. It is the parametrization which was found to be most successive.

The system of equations (3) may be rewritten in a form of finite difference equations. The position of particle in moment of time $(n+1)$ is defined as follows. First, particle is moved wind speed in a moment of time $n$:

$$
\dot{X}_t^{n+1} = X_t^n + U_t^n \Delta t;
$$

(8)

$$
\dot{Y}_t^{n+1} = Y_t^n + V_t^n \Delta t;
$$

(9)

$$
\dot{Z}_t^{n+1} = Z_t^n + (\dot{W}_t^n + \frac{\partial K_z^n}{\partial z}) \Delta t;
$$

(10)

Then the position of particle is corrected

$$
\tilde{X}_t^{n+1} = X_t^n + 0.5(U_t^n + \dot{U}_t^{n+1}) \Delta t;
$$

(11)

$$
\tilde{Y}_t^{n+1} = Y_t^n + 0.5(V_t^n + \dot{V}_t^{n+1}) \Delta t;
$$

(12)
\[
\tilde{z}^{n+1} = z^n + 0.5(\tilde{w}_i^n + \tilde{w}_i^{n+1}) \Delta t + \left( \frac{\partial \tilde{K}_{xi}^{n+1}}{\partial z} + \frac{\partial K_{yi}^n}{\partial z} \right) \Delta t;
\]

(13)

And finally, the particle undergoes the stochastic shift (the more diffusion coefficient the more the average amount of this shift).

\[
\begin{align*}
X^{n+1}_i &= \tilde{X}^n_i + \sqrt{2\tilde{K}_{xi}^{n+1}} \Delta t_x \\
Y^{n+1}_i &= \tilde{Y}^n_i + \sqrt{2\tilde{K}_{yi}^{n+1}} \Delta t_y \\
Z^{n+1}_i &= \tilde{Z}^n_i + \sqrt{2\tilde{K}_{zi}^{n+1}} \Delta t_z
\end{align*}
\]

Depending on the users' wishes, this particular realization of the stochastic model can work as:

a. Gauss model (single gaussian cloud)
b. Puff model (many gaussian clouds moving in the wind field)
c. Gaussian clouds moving in the wind field with their centers being subjected to random displacement.

In last case the random process is split by two independent processes. The sum of dispersions of this two processes is equal to dispersion of former process. The dispersion of Gauss process is estimated considering the distance scale on which the wind velocity variations are negligible. Diffusion coefficient for the center of Gaussian clouds is defined by relation \( K' = K - \frac{1}{2} \frac{d\sigma^2}{dt} \) (\( \sigma^2 \) — dispersion of Gauss clouds).

3 Verification of mesoscale Lagrangian transfer model

Results of calculation of impurity transfer with use of Lagrangian model and package "Voyage" (standard-technical document 38.220.56-84) have been compared. Parameters of dispersion of impurity cloud have been defined according to standard technical documentation of this package.

Results of this comparison are shown on Figure 1.

![Figure 1: Comparison with Gauss model. Impurity density distribution upon height at the distance: a) \( x = 20m \), b) \( x = 1000m \). Number of points \( N = 1000 \). Source height \( h = 50m \), wind velocity \( v = 5m/sec \), cross diffusion coefficient \( D = 0.5d(\sigma_0^2)/dt \), \( \sigma_0 = C_2(1 + 0.001x)^{-1/2} \), \( x = vt \).](image)

Gaussian profiles are the precise solutions of turbulent diffusion equation when turbulent parameters are independent of height and when wind speed is constant. Lagrangian model for impurity transfer gives the same results as package "Voyage" in this preside case.

The preside solution of diffusion equation for stationary impurity source with power profile of wind speed \( U = U_0z^m \) and power profiles of diffusion coefficients \( K = K_0z^m, K_z = K_1z \) has been used as the other test. The analytic solution is obtained in [5]. The comparison of theoretical and calculating profiles is shown on Figure 2.a. Here model gives the results that well agree with theory.
Figure 2: Comparison with analytic solution [5]. Density distribution upon cross wind horizontal coordinate on the heights: 1) $h = 0.2$, 2) $h = 0.9$. $U_1 = 4$; $m = 0.05$; $k_0 = 0.03$; $k_1 = 0.1$.
a) simple Monte Carlo method, points amount $N = 10000$.
b) modified method, 'clouds' amount $N = 200$.

Taking into consideration of correction terms in stochastic equation is demonstrated on two examples.

1. The first example is propagation from pulse ground point source in neutral stratified bounder layer of atmosphere. Logarithmic profile of wind speed is feature of such layer:

$$U(z) = \frac{U_*}{k} \ln \frac{z + z_0}{z_0}$$

(14)

where $k$ — Karman constant, $U_*$ — “friction velocity”, $z$ — height, $z_0$ — roughness parameter. Diffusion coefficient in directions $x, y, z$ ($x$ is direction of wind) are taken in form:

$$K_x = \alpha_x U_* z; \quad K_y = \alpha_y U_* z; \quad K_z = \alpha_z U_* z;$$

(15)

In this case analytical solutions of diffusion equations exist. They give the following expressions for statistical cloud characteristics.

Figure 3: The computation of point source evolution in neutrally stratified atmosphere.

$z_c$ — height of mass center, $\sigma$ — vertical dispersion of cloud; solid line — theory; stars — with correction $\frac{dK_z}{dt}$, crosses — without correction.
Figure 4: Experiment modeling [6]. 1 — Gauss model; 2 — ADPIC model; 3 — our solution; crosses — experiment.

Coordinations of center-of-mass:

\[ X(t) = \frac{U_0 t}{\kappa} \left( \ln \frac{\alpha x U_0 t}{z_0} - 1 - \gamma \right) \]  

\[ Z(t) = \alpha z U_0 t \]  

where \( \gamma = 0.58 \) — Euler constant, \( t \)-time. Horizontal and vertical dispersions:

\[ \sigma_x^2 = \left( \frac{\sigma_z^2}{6} - 1 \right) \frac{1}{K^2} + \alpha x \alpha z U_0^2 t^2 \]  

\[ \sigma_y^2 = \alpha y \alpha z U_0^2 t^2 \]  

\[ \sigma_z^2 = \alpha z^2 U_0^2 t^2 \]

According to the data of great number of laboratory measuring: \( \alpha z = 0.47, \alpha x = 5 \alpha z, \alpha y = 5.2 \).

The results of modeling with correction term and without it are shown on Figure 3. Calculating points, when corrections are not considered, are greatly different from theoretical; when corrections are considered solutions are close to theoretical.

2. The solution mentioned above for stationary source with power low profile of wind velocity is used as second example. Neglecting of correction term brings to overestimating of near-the ground concentrations more than twice when \( U_1 = 4, m = 0.15 K_0 = 0.03, K_1 = 4 \), source height \( h = 0.3 \).
Figure 5: Experiment E1: 1 — experiment, 2 — NSI model, 3,4,5 — other models

Figure 6: Experiment E2: 1 — experiment, 2 — NSI model, 3,4,5 — other models
Figure 7: Experiment E3: 1 — experiment, 2 — NSI model, 3,4,5 — other models

Figure 8: Experiment E4: 1 — experiment, 2 — NSI model, 3,4,5 — other models
4 Validation of mesoscale Lagrangian transfer model

The first experiment used for validation was made by Idaho National Engineering Laboratory (INEL) at september 22,1972 [6]. It's characteristics are: stability class of near the ground layer C(3); ground source in iodine isotope ($I^{131}$).

Time of source action 3 hours.
Source intensity — $0.379 \mu$Ci/sec.
Speed of gravitational deposition — $0.1 \text{m/sec}$.

The aim of this experiment was verification of Lagrangian particle advection-diffusion model of Livermore laboratory. Locality was smoothly heighten to the left of the source in direction of average wind (ridge). The height difference of between highest and lowest points was about 1000 meters. The distance between these points was about 35 km 17 stations gave the meteorological information. Wind field was corrected by means of the model for near the ground layer (MATHEW).

The only known information is value of near the ground wind (about $5 \text{m/sec}$ and stability class. Velocity and direction of wind in border layer of atmosphere depend upon height. This and velocity pulsation bring to scattering of impurity cloud. Beginning some moment of time contribution of this factor exceed contribution of normal diffusion. Method of restoration of wind profile and coefficient of vertical turbulence depending upon stability class, ground information and local latitude have been recommended basing on several years observations in [3,7]. It was supposed that ridge changes typical wind profile over plain locality and concentration disturbance which would be formed over plain locality only near the ridge because the ridge is quite plane. Results of our calculations confirmed this assumption.

Tracer time integrated concentration (TIC) at the distance $50 \text{km}$ from source calculated from stochastic advection model, Gaussian model and natural data are shown on Figure 4. Results calculated from model ADPIC-Livermore laboratory model for forecasting accident impurity propagation for 100 — $200 \text{ km}$ are shown on Figure 4 as well.

Gaussian model for such distances underestimates the latitude of cloud track. Stochastic model that considers typical wind turn with height gives better results. It underestimates concentration in wind direction on the left, where ridge was located because ridge existence has not been considered in calculations.

The next data used for validation was four natural atmospheric dispersion experiments described in KFK report [8].

This report has presented the results of the intercomparison of different mesoscale dispersion models and measured data of tracer experiments. These models are suited for the calculation of the atmospheric transport of radionuclides released from nuclear installation.

In the KFK the comparison between nine most prominent European mesoscale transport models have been made. The model results and the environmental data about four natural atmospheric dispersion experiments (E1,E2,E3,E4 experiments) have been compared. Among these nine models were the Gaussian, Eulerian and stochastical Lagrange models. The same experiments have been reproduced to verify the NSI model. The comparison of the experimental data and the model results are shown in the fig.5-8. For the sake of comparison the results of the best among these nine models — Gauss puff, Eulerian and Lagrangian models are presented in this figure also.

Shown on Fig.5-8 is normalized TIC angle distribution. 1 — experiment, 2 — NSI model, 3 — Lagrangian random walk model IABG (Schorling), 4 — Gauss-puff model Risø, Denmark (Mikkelsen), 5 — Eulerian model, Hamburg University (Dunat).

The comparison of the results of these models with that of NSI model shows the NSI model is at least not at disadvantage in relation to the models concerned. The advantages become more significant as a distance from a source increases. The fact should be noted that not all available meteorological data have been used when modeling E1—E4 experiments. In particular, the data about temporal and height variation of second moments of wind speed have not been used. This information is hardly rely able and usually unavailable. The imbedded in the package parameterizations of the intensity of vertical and horizontal turbulence have been used instead to check its performance. in our opinion, the advantages of the NSI model in E1—E3 experiments over the others that consider similar wide range of factors influencing impurity transport is mainly due to regard of the vertical diffusion coefficient variability with height. As our numerical experiments have shown, the choice of the vertical eddy transport model is critical (very important) for overall model performance. The most successive is the parameterization of vertical diffusion coefficients that of [3,4]. So the NSI model has been tested by five environmental experiments. The comparison of the results of the NSI model, two basic models of the Livermore Laboratory (USA)
and nine European models have been made for all these five experiments. This intercomparison have shown the high competitiveness degree of the stochastic model of the Nuclear Safety Institute.

5 The models of source of a contamination. The online models of emergency fire and explosion release

5.1 The online model of emergency fire release

Results of modeling convection, that is initiated by heat, show that injection height depends not only upon heat intensity, but also upon weather conditions [8-14]. The main factors among the factors that influence the height of convection penetration are temperature stratification of atmosphere and humidity level. That means that lift height of emergency release in atmosphere as result of fire occurrence will inevitably depend upon concrete state of atmosphere at time and place of fire occurrence.

The simple approximation formulas for smoke rise above the fire give crude approximations because they consider average state of atmosphere. The influence of atmospheric humidity on the strong convection parameters is not considered. The fact that the emergency release over the fire source can spread over several kilometers in height is not taken into account. Over this height interval the wind can have opposite directions.

There are a lot of one-dimensional models for estimating of distribution of emergency release with height above the fire source now. These models describe parameters of smoke column above the stationary source of heat. The main difference between them is the form of parametrisation of the velocity of ambient air entrainment into the plume.

Model of Morton–Teiler–Terner (MTT) [15,16,18,19] that doesn’t consider the phase change and model of Squers–Terner [17] that difference from MTT only by consideration of phase change are the most frequently used models. The influence of horizontal wind on parameters of smoke column are not considered in these models. The way of consideration of vertical profile of horizontal speed is developed in [20]. The characteristics property of this models is that they describe stationary parameters of convection for constantly active source. Thus the radius of convectual jet is tending to infinity when vertical speed is tending to zero near the upper bounder. The smoke or emergency release (that is accompanying the fire) is supposed to be distributed evenly between the level of null buoyancy and the top of convectual plume, but it seems to be quite crude approximation [13].

One-dimensional model for convectual flows above the source of fire will be described below. Using of this model allows to estimate the size of smoke column above the fire and distributions of emergency release with height (the source is continuous and quasi-stationary) depending on meteorological conditions at different moments of time. Factors that influence the character of impurity propagation for fire source are stratification of atmosphere, humidity of atmosphere, existence of wind and wind change with height.

Model has been verified for calculations of fires of different powers. The descriptions of these fires are described in literature sources [12, 19].

Results of calculations with use of operative one-dimensional model and results of calculation with use of three-dimensional hydrothermodinamical model of Livermore laboratory have been compared.

Model allows to estimate the presence of humidity that condensed in result of convectual movement and thus probability of rapid impurity washout.

There is additional reference information in programs package for user convenience.

The parameters of standard atmosphere for different seasons and latitudes may be used for methodological calculations.

If information about intensity of energy release from fire is absent then the special block in programs package for estimate may be used. This block consists of information above heat from 27 basic solid, liquid and gas combustibles. The tentative duration of fire depending on amount of combustibles on unit area is defined with the help of statistical diagrams from the same block [21].

If \( \alpha \) — parameter of ambient air entraining to the jet

\[
\alpha = \frac{1}{M_i} \frac{dM}{dz} \tag{21}
\]

Here \( M_i = r_i W_i R_i^2 \) — , \( r_i \) — density, \( W_i \) — speed, \( R_i \) — radius; index \( i \) is referred to parameters of convectual column. According to the Newton second low the equation of movement of convectual jet.
in vertical direction has the following view:

\[
\frac{dW_i}{dt} = -g - \frac{1}{\rho_i} \frac{\partial P}{\partial z} - \alpha W_i^2 = \frac{g(T_i - T)}{T} - \alpha W_i^2
\]  

(22)

It will be thought below that pressure in convectional jet is equal to the pressure of ambient air at the same level. Z-axis is directed up. Considering that \( Wdt = dz \), (22) may be rewritten as

\[
\frac{dW_i}{dt} = \frac{g(T_i - T)}{T} - \alpha W_i^2
\]  

(23)

According to

\[
C_p dT_i = \alpha C_p (T - T_i) + R_T T \frac{dP}{P} \]

(24)

where \( R \) — universal gas constant. Considering that for the ambient atmosphere \( \frac{dP}{P} = -\frac{d}{R_T T} dz \) the following may be obtained.

\[
\frac{dT_i}{dz} = \alpha (T_i - T) - \frac{g}{C_p} \frac{T_i}{T}
\]  

(25)

or

\[
\frac{dT_i}{dt} = \alpha W_i (T_i - T) - \frac{g}{C_p} \frac{T_i}{T}
\]  

(26)

For the movement in moist atmosphere all equations are correct, but \( T \) and \( T_i \) are changed to the virtual temperatures.

The equations (25),(26) should be corrected when saturation is reached due to appearance of new heat source that is bound up with condensation.

In this case equations (25) and (26) may be rewritten as

\[
\frac{d(T_i + \frac{L}{C_p} q_i)}{dz} = \alpha (T_i - T) + \alpha \frac{L}{C_p} (q - q_i) - \frac{g}{C_p} \frac{T_i}{T}
\]  

(27)

\[
\frac{d(T_i + \frac{L}{C_p} q_i)}{dt} = \alpha W_i (T_i - T) + \alpha W_i \frac{L}{C_p} (q - q_i) - W_i \frac{g}{C_p} \frac{T_i}{T}
\]  

(28)

where \( q, q_i \) — specific humidity. The change of specific humidity in the plume \( q_i \) up to condensational level is defined by the following correlation

\[
\frac{dq_i}{dz} = \alpha (q_i - q)
\]  

(29)

or

\[
\frac{dq_i}{dt} = \alpha W_i (q_i - q)
\]  

(30)

When saturation is reached moisture is condensed and temperature is risen. In this case optical energy \( T_i + q_i L/C_p \) stay the same. The condensed moisture is supposed to fallout.

The equations (21),(23) and (25) are the base for modeling the vertical convectional jets in many stationary model. The most full theory of plume movement in stratificational humid atmosphere that considers horizontal wind field is presented in [20]. The following expression for entraining speed has been obtained:

\[
\alpha W_i = \frac{2C T_i}{R_T T} \sqrt{W_i^2 + U_i^2}
\]  

(31)

or

\[
\frac{1}{M_i} \frac{dM_i}{dt} = \frac{2C T_i}{R_T T} \sqrt{W_i^2 + U_i^2}
\]  

(32)

where \( C \) — constant, \( U_i \) — horizontal speed of jet.

The calculations according to the model described in this section are taken using equations (22), (28), (30) and (32).
Figure 9: The view of smoke column and smoke propagation with height for Hamburg fire.

This set of equations is chosen because they allow to get the profile of convectional cloud at any moment of time. Parameters of convectional flow above the source is fast determined [8] when the fire is powerful and heat intensity may be considered as quasi-stationary. It is supposed that propagation of smoke column through any period of time beginning the time of fire occurrancy agree with contours of jet and smoke cloud that has been produced by established convectional flow for that period of time. In this case content of smoke or any other emergency release from continuously acting source in height interval [Z, Z+H] is defined by source release for the time when front of convectional flow has been in this interval.

If the release during the fire was shirt-termed then the movement track with height is defined by position of convectional flow front through the corresponding period of time.

The horizontal velocity of the plume is defined as follows:

$$\frac{dU_i}{dt} = \alpha W_i (U - U_i)$$ (33)

The basic variant of the model uses Bekryaev parametrization for entrainment [18]. The possibility to use any other known functional dependence for parametrizations of entrainment (models: MTT and Gostintsev [23]) is provided.

Using equations (21) and (22) the following correlations may be obtained:

$$\frac{1}{R_i} \frac{dR_i}{dz} = \frac{\alpha}{W_i} - \frac{T_i - T}{2T W_i^2} + \frac{g R_i}{2T} \left( \frac{1}{R_g} - \frac{1}{C_f} \right)$$ (34)

Thus

$$\frac{1}{R_i} \frac{dR_i}{dt} = \left( \frac{\alpha}{W_i} - \frac{T_i - T}{2T W_i^2} \right) W_i + \frac{g R_i}{2T} \left( \frac{1}{R_g} - \frac{1}{C_f} \right) W_i$$ (35)

According to the theory of Hauton and Kramer [22] $g T_i - T/2T W_i^2$ is proportional to $\frac{1}{M_i} \frac{d M_i}{dt}$. Coefficients of proportionality $\gamma$ and $C$ have been chosen from model verification. $\gamma = 0.66$, $C = 0.14$. $\alpha T_i/\alpha \approx \alpha$ for fires of even more intensity [8].

Figure 10: The view of smoke column and smoke propagation with height for fuel fire in Long Beach.

The third term in (34),(35) that characterize the increase of radius of convectional plume at a count of pressure change during vertical movement influences on the cloud contour only in case of fires of great areas.

The initial buoyancy produced by the fire source is defined as follows.
For the steady regime of convection the rise of convectional flow above the source in one second may be estimated by using

\[
\frac{d\pi \rho_1 R_1^2 W_i^2}{dz} = \frac{T_i - T}{T} \pi \rho_1 R_1^2
\]  

(36)

Thus

\[
\frac{d\pi \rho_1 R_1^2 W_i^2}{dt} = \frac{T_i - T}{T} \pi \rho_1 R_1^2 W_i \approx \frac{gQ}{C_p T}
\]  

(37)

where \(Q\) — source power.

Near the ground where vertical speed is fast increased it is considered that

\[
\frac{d\rho_0 R_0^2 W_i^2}{dz} = \rho_0 R_0^2 \frac{dW_i^2}{dt}
\]  

(38)

where \(\rho_0\) — near the ground density, \(R_0\) — radius of fire.

Then \(W = \sqrt{\frac{Q g}{T C_p \rho_0 R_0^2}}\) and rizing of convectional flow during one second above the source is

\[h = 0.66 \sqrt{\frac{Q g}{T C_p \rho_0 R_0^2}}\]  

Thus near the surface \(T_i - T = Q g / T C_p \rho_0 R_0^2\).

Explicit approximation in time is used while solving evolutionary equations of model. Temperature and humidity are defined by iterative Newton method when condencational level is reached.

![Figure 11: The view of smoke column and smoke distribution with height for Hamburg fire when horizontal wind was considered.](image1)

![Figure 12: The view of smoke column and smoke distribution with height for fire in Long Beach when horizontal wind was considered.](image2)

Verification of one-dimensional operative model has been conducted by means of comparison between calculations for some real fires (the information about them has been available) and results of calculations of Livermore laboratory using three-dimensional thermogydrodynamical model.

**Hamburg fire at the end of World War II.** The description of the fire is in [13]. The value of the fire power was 1700000 MW. The area was about 12 square kilometers. The wind at a moment of fire occurance was weak. Humidity in atmosphere was low. Temperature gradient in troposphere was about 6.4 degree per kilometer. Tropopause was at the level of about 11.5 km. Temperature in stratosphere was standard — 216°C. Temperature near the ground was 288.1°C. The height of smoke column was 12 km.

The information about the result of modeling of this fire using the three-dimensional thermogydrodynamical model of Livermore laboratory is available.

The variant of operative model that did not consider humidity and wind was used to model the smoke column above this fire.
The calculations showed that the height of fire column reached 12 km. The distribution of smoke with height and contours of cloud after 30 minutes from a moment of fire occurrence is shown on Figure 9. The maximum of horizontal spreading of cloud is 12.8 km. The three-dimensional model gave the same result.

Fuel fire in Long Beach (1958). The description of this fire is in [13]. Wind was practically absent. Temperature gradient was above 6.5 degrees per km of height. The fire was not accompanied by steam condensation and cloud development. Heat intensity was about 10000 MW. Radius of fire was 500 meters.

According to the description of smoke column its top reached 3300 meters. Smoke was distributed mainly between height of 1500 and 3300 meters. The information about results of modeling of this fire using three-dimensional thermodynamical model of Livermore laboratory was available.

The same variant as in the previous case was used for modeling of smoke column above this fire. The calculations showed that the height of smoke column reached 3.3 km and smoke was distributed in height interval that was observed.

The information about horizontal spreading of cloud with height at different moments of time is absent, but the results of calculations using the model of Livermore laboratory [13] showed that there is a agreement.

The smoke distribution with height and cloud in one hour after fire occurrence are shown on Figure 10. Maximum horizontal spreading of cloud is 3.6 km; the three-dimensional model gave the same results [13].

The calculations that take into consideration horizontal wind which is characteristic for middle latitudes (climatic data [24]) have been taken for Hamburg fire and fire in Long Beach. The smoke distribution with height and cloud contours for these fires are shown on Figure 11, 12.

The number of calculations for fires of different intensity have been taken aiming to verify the operative model for propagation of impurity from fire source in moist atmosphere when horizontal wind exists:

1) radius of fire 5 km, heat — 14000 W/m
2) radius of fire 5 km, heat — 2300 W/m
3) radius of fire 5 km, heat — 89000 W/m

Fires have been modeled for standard atmosphere with standard profiles of humidity and wind.

The comparison with results of three-dimensional thermodynamical model of Livermore laboratory has been taken. The agreement between height profiles of smoke distribution with height and results calculated with use of model of convectional flows above the fires (Livermore laboratory) was good in comparison with model MTT.

The model of Livermore laboratory for modeling of convectional flows above the fire source is the most full when factors that influence the convectional parameters are considered. In is widely used in practice. It was used by USA for prognosis the propagation of smoke if the fires in Kuwait would occur.

The graphical dialog interface for user has been worked out. The results of modeling are ocular demonstrated. Program package allows to get any reference information. Program package may be used for operative estimation of impurity rise for great fires and cloud contour depending on meteorological situation. Program package allows to determine the presence of steam condensation when convection occurs and the probability of release washout in the nearest zone.

5.2 An operative model of the size and rise for explosion

The code for operative estimation of rise of impurity release and dimensions of cloud for powerful explosion has been worked out basing on simple model for vortical ring. The factual meteorological situations are used for this estimation. The possibility of steam condensation inside of cloud is considered. The results: rise of release and dimensions of smoked zone may be used as input data for the problem of passive impurity advection by wind.

An online model of the size and height of the pollutant cloud over an explosive source of energy. This model is based on the fact that circulating flows inside of the clouds appear because of the surface friction when high heated cloud moves up after the explosion [26]. This cloud changes to toroidal vortical ring because of this flows. The presence of vortical movements in cloud is confirmed by observations of clouds of nuclear and ordinary explosions. The presence of the speed circulation brings to origin of Joukowsky lift force that stretch cloud in horizontal direction [27]. Therefore this model allows not only to estimate the rise of cloud but also to calculate its dimensions and to describe the effect of the horizontal spreading of the cloud that was observed in atomic explosions [27].
The scheme for calculation of buoyancy vorticial ring in gravitational field was suggested by S.C. Christianovich and worked out but A.T. Onufriev [27]. This scheme is used in this model as well as the results of the researches of vortex conduct that were published by M.A. Lavrentev in his book [28].

**Equations of vorticial ring movement.** In accordance with the work of Onufriev [27] and Lavrentev [28] the rising cloud may be visualized as the oblate ellipses which dimensions are shown on Figure 11. There is vorticial ring (vortex kernel) with radii \( R \) and \( r \) inside of ellipses \( 2R \simeq D - 2r \).

![Figure 13: The schematic representation of the vorticial cloud.](image)

The change of momentum of torus mass and ambient air that is entrained in movement is equal to the sum of forces that act on it (torus): Archimed force, Joukowsky lift force and resistant force. When vectorial equation is projected on vertical and horizontal directions the following equations of torus movement appears as:

in vertical direction

\[
\frac{d}{dt}((M + M_1)v) = g\Omega(\rho_0 - \rho) - 2\pi R \Gamma \rho_0 u \frac{C_d S_m}{2} \rho_0 v V \tag{39}
\]

in horizontal direction

\[
\frac{d}{dt}((M + M_1)u) = 2\pi R \Gamma \rho_0 v \frac{C_d S_m}{2} \rho_0 u V \tag{40}
\]

In formulas (39) and (40) \( \rho \) is an air density inside of torus, \( \rho_0 \) is an air density in atmosphere, \( M \) is air mass inside of torus, \( M_1 \) is an “associated” mass of torus (mass of ambient air that is entrained in movement when movement is not steady), \( v \) is a vertical speed of rising, \( u = 0.5dD/dt \) is horizontal speed of spreading, \( V = \sqrt{u^2 + v^2} \), \( g \) is an acceleration of gravity, \( \Gamma \) is a circulation of speed of vorticial ring, \( \Omega \) is volume of ellipse formed cloud with axis \( D = 2R + 2r \) and \( \Delta h = 2r \), \( R \) is a radius of axial ring of torus, \( r \) is a radius of cross-section of torus kernel, \( \Delta h \) is a vertical dimension of cloud, \( S_m \) is an area of center section of ellipsoid, \( C_d \) is a resistance coefficient.

There is a necessity to add an equation of torus movement when wind is present:

\[
\frac{d}{dt}((M + M_1)v_b) = v_{0b} \frac{dM}{dt} + C_d \rho_0 |v_{0b} - v_b| (v_{0b} - v_b) \frac{\pi}{4} D \Delta h \tag{41}
\]

where \( v_{0b} \) is a wind speed, \( v_b \) is speed of torus movement in direction of wind.

For the air mass that is entrained in a unit of time through the area \( S \) of the lateral surface the expression

\[
\frac{dM}{dt} = \alpha VS(\rho_0)^{1/2} \tag{42}
\]

may be used, where \( S \) is the area of the lateral surface of the cloud [26]. This expression appears as the result of turbulent mixture of heated air that is enclosed inside of torus, and cold ambient air.

The equation for determination of the circulation amount is derived from the following considerations. In nonstratification atmospheric, when Archimed force is constant \( (F_A = \text{const}) \) equations of vortex movement have selfsimilar solutions [28], \( x \sim t^{1/2}, v \sim t^{-1/2} \), where \( x \) is horizontal dimension of vortex and \( v \) is its speed. At the same time circulation \( \Gamma \sim vz = \text{const} \) does not change in time. From the other side when \( F_A = 0 \) (free movement of vortex without buoyancy) the other selfsimilar regime exist.

\[
x \sim t^{1/4}, v \sim t^{-3/4}, \Gamma \sim t^{-1/2}, \dot{\Gamma}/\Gamma = 2\dot{M}/3M \tag{43}
\]
Both regimes of vortex movement are confirmed by the experiment [28, 29, 27]. Here the interpolation equation for $\Gamma$, that combines these two limit regimes, is used. First, the order of magnitude of circulation, when the cloud is expended by the constant force $F_A$, will be defined. Velocity circulation in the vortex have an order of magnitude $\Gamma \sim zv$. The speed $v$ is defined by the balance of friction force $(S \sim z^2 \text{ -- cloud section}; C_d \text{ resistance coefficient})$ and force $F_A$ and is proportional to the $\sqrt{v} \sim \sqrt{F_A/S} \sim \sqrt{F_A/z}$. Thus

$$\Gamma \sim zv \sim \sqrt{F_A} \tag{44}$$

Then when $F_A$ is changing in time the circulation $\Gamma$ tends to new quantity (44) by the law (43). This gives an equation for $\Gamma$:

$$\frac{d\Gamma}{dt} = -\left(\frac{F_A}{F_{A0}} - \Gamma_0 - \Gamma\right) \frac{2}{3M} \frac{dM}{dt} \tag{45}$$

where $F_{A0}$ and $\Gamma_0$ are initial quantities for $F_A$ and $\Gamma$. When $F_A = F_{A0} = \text{const}$ the equation (45) gives $\Gamma = \text{const}$, and when $F_A = 0$ it gives limit regime (5). The circulation change that is described by the equations (45) in concrete variants appears to be close to the solution of equation $\Gamma = -1/M \dot{\rho} \beta \Gamma dM/dt$ with the empirical coefficient $\beta \sim 0.2$ that was used in work [27].

The initial circulation was chosen as $F_0 = \gamma_0 a_0 \sqrt{a_0 g}$ in accordance to [27], where $a_0$ is an initial radius of the fire sphere $\gamma_0$ dimensionless parameter. It’s magnitude is chosen in accordance of the calculated result with the experimental data.

The change of gas enthalpy in the cloud is happening because of the mixture with ambient air, change of ambient pressure and possible phase changes of the humidity in the cloud

$$\frac{dW}{dt} = C_p T_0 \frac{dM}{dt} + \frac{\gamma - 1}{\gamma} \frac{dp}{P} \frac{dM}{dt} + Q \frac{dM_s}{dt} \tag{46}$$

where $W = C_p M T$ is gas enthalpy in cloud, $C_p$ and $T_0$ are temperature and heat capacity of ambient air, $C_p$ and $T$ are temperature and heat capacity of cloud, $P$ is atmosphere pressure, $\gamma$ is adiabatic exponent for gas inside of cloud, $Q$ is heat of vaporization, $dM_s$ is mass of condensed vapor for time period $dt$.

The first term in (46) is concerned with the entraining of ambient air, the second term is corresponded to the adiabatic spreading of cloud that is due to the change of the atmosphere pressure with height during the rising and the third term is corresponded to the emission of heat when vapor is condensed.

The condensation of vapor inside of the cloud may occur when $\rho_c > \rho_s(T)$, where $\rho_c$ is vapor density inside of cloud, $T$ is cloud temperature, $\rho_s(T)$ is saturated density of vapor. The condensation is described by an equation $dM_c/dt = \Omega(\rho_c - \rho_s(T))/\tau$, where $\tau$ is characteristic time of the condensation. In the calculations this time was chosen much less than time scale of cloud movement and the magnitude of this time did not influence the result.

The heat capacity of dry air and vapor in atmosphere are not depend on temperature. The heat capacity of condensed water and the heat capacity of aerosol particles that are captured in cloud are considered too.

The gases in the cloud (dry air and vapor) are considered to be ideal and the equation of state has a form of:

$$P = T(n_a + n_s) = T\left(\frac{\rho_a}{m_a} + \frac{\rho_c}{m_c}\right) \tag{47}$$

where $n_a, n_s$ are concentrations of vapor and dry air; $m_a, m_s$ are their molecular masses.

The initial conditions for the problem of the cloud rise are specified immediately after the explosion, after departing of shock wave from fire sphere when air inside of fire sphere has a pressure that is equal to outside pressure and is stationary. The initial volume of the fire sphere is defined from

$$\Omega = \frac{ET}{\gamma/(\gamma - 1) P(T - T_0)} \tag{48}$$

where $E$ is the released energy to the air after the explosion; $T$ is temperature inside of the fire sphere; $T_0$ is temperature of ambient air. Temperature $T$ should be specified depending upon the type of explosive. Thus for the organic fuels it could be equal to 2500°K [33]. For the nuclear explosions the average temperature inside of the fire sphere is equal to 3000°K [31]. The calculations showed that the cloud movement slightly depends on $T$ when $T \gg 3000°K$. The energy $E$ is defined by caloricity and amount of matter. For the nuclear explosions $E$ is takes as 1/4 of full energy of charge [26] (other energy leaves sphere in terms of radiation and energy of shock wave).
Figure 14: Selfsimilar regime of thermic rising. \( \Pi_0 = (Q\beta_0/2\pi\rho_0 C_P)^{1/4} \). \( H \) is height, \( Q \) is charge energy, \( \beta \) is coefficient of thermal spreading. The points are the experiment by Gostintsev [5].

Model verification. The problem has three parameters that should be found out of experimental data: \( \alpha \) is entraining coefficient, \( C_d \) is resistance coefficient, \( \gamma_0 \) is magnitude of initial circulation. When \( \gamma = 0 \) the cloud has spherical form and the problem is equal to the problem of spherical thermic movement.

Coefficient \( C_d \) is taken \( \sim 0.4 \), that corresponds to the experimental data on flowing around the spheres for large Reinoolds numbers.

The coefficient \( \alpha \) is taken from the experiments with jets and is equal to 0.2.

The coefficient \( \gamma_0 \) defines the cloud spreading in horizontal direction and is found from the data on nuclear explosion clouds dimensions.

The first test consisted of the comparison of selfsimilar character of the thermic movement with the small scale explosion experiments (30 kg of powder), that were described by Gostintsev [28].

The results are shown on figure 14. The experimental points lies clear to calculated curve when \( \alpha = 0.13, C_d = 0.4, \gamma = 0.13 \). These magnitudes were used in the calculations that models the cloud rise after the nuclear explosion.

There is the data [25] on rise and dimensions of clouds for the explosions with charge energy from 0.5 to 50 \( kT \). The comparison of the calculated and experimental data is given in Table 1.

<table>
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<th>( Q/kt )</th>
<th>( H_s )</th>
<th>( \Delta h )</th>
<th>( D )</th>
<th>( D/\Delta h )</th>
<th>( \Delta h )</th>
<th>( D\Delta h )</th>
<th>( D/\Delta h )</th>
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<td>2.7</td>
<td>3.2</td>
<td>1.4</td>
</tr>
</tbody>
</table>

Table 1.
All calculations were taken for the standard atmosphere of middle latitudes (summer). The humidity condensation was considered. The calculated $D^*$ and $(D/\Delta h)^*$ are corresponded to the moment of time when maximum rise of cloud was reached, and $D \frac{D}{\Delta h}$ are taken for $t = 17$ min.

![Diagram 15](image15.png)

**Figure 15:** Change of rise of upper cloud level in time for energies $Q=20$ kT and $Q=1$ kT. Points represent the experimental data [31].

The change of cloud with time for energies $Q = 1$ kT and $Q = 20$ kT is shown on Figure 15, the amount of cloud spreading $(D/\Delta h)$ is shown on Figure 16. The experimental data [30] is shown by means of points. The clouds rise continuously for $6 - 8$ min (the same is for the experiments). Then movements inside of the clouds attenuate on the equilibrium height.

![Diagram 16](image16.png)

**Figure 16:** The amount of cloud spreading $(D/\Delta h)$ for energies $Q=20$ kT and $Q=1$ kT.

The accepted model describes the experimental data in the wide interval of explosion energies. The calculations have been done without consideration of ground ejection into the fire sphere and capturing of ground by rising cloud because of the lack of the experimental data. The experimental data [31] confirm that the tunnel volume for the contact explosion and the amount of ground in cloud increase slower than the explosion energy. That means that the influence of captured ground on buoyancy is greater when energies are small than when they are greater. Probably the consideration of the ground entraining will reduce rise (when the energies are small) and make it close to experimentally observed rise.
References


