Probabilistic models of pollution of the surface waters of large marine areas

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Abstract. Version of Monte-Carlo model for calculation of propagation of contamination in large marine areas with taking into account a coastline is presented. Based on long standing database of sea currents, bathimetry, and mixed layer depth, the probabilistic model of zoning marine areas by concentration of pollutant is offered. In accordance with modern IAEA recommendations general principles of estimation of radiation situation on radiation hazardous object in normal exploitation mode, conclusion of normal exploitation mode, or in accident mode exists. Practical methodology of safety case and tactics of monitoring of state of radiation hazardous object should rely not only on measuring, but also on model calculations and forecasts. Optimal tactics of monitoring includes definition of probabilistic picture of possible pollution different marine areas assuming hypothetical leak of pollutant with violation of defence barriers. One way of building such probabilistic pictures is execution of multi-variant calculations using long standing databases. Different calculations in multi-variant mode executes assuming different accident start time, in advance models multi-variant dynamic of marine area pollution. Not only maximum values of pollution to be interested, but and statistical estimations with different confidence levels (for filtration of rare big values) for hypothetical leak of pollutant. In the base of the numerical algorithm of proposed technique lies Monte-Carlo method using lagrangian particles with non-zero sizes.

1. Introduction
In the areas of Arctic (Arctic Ocean) and Far East (Pacific Ocean) radiation hazardous objects, containing spent nuclear fuel, liquid or solid radioactive waste, flooded in the time period from 1946 to 1993 years, is localized. So, Arctic and Far East should be considered as potentially dangerous regions with radiation risk factor. Accident situations has very low probability, but for analysis of radiation state and radiation safety, model calculations and forecasts of possible consequences of hypothetical accidents for terrestrial and marine environment, should be executed.

Last few years in NSI RAS develops the specialized computer code for calculation of propagation of radioactive pollution spot in marine area of Arctic or Pacific Ocean. Two version of model and computer code is developing. First version – is quasi three-dimensional model, intended for calculation consequences of accidents, occurring in upper layer of the ocean, higher than mixed layer depth. Second version – is fully three-dimensional model, intended for accident, occurring in arbitrary depth. In this paper both models is presented. Both computer codes allows define probabilistic characteristics of levels of possible radioactive contamination and location of most important marine areas for choose of places of monitoring and sampling points. Detection
of crucial marine areas, where expected the highest levels of contamination and measuring acts
aimed at definition of content of radionuclide in this areas, may serves as a signal (in case of
increasing levels of content) for carriage out further events for controlling radiation situ, and
about possible violation of defense barriers. Probabilistic approach to modeling consequences of
leak of radioactive pollution in coastal marine areas of Arctic and Pacific Oceans is needed owing
to seasoning variability of the ocean currents and mixed layer depth, uncertainty in accident
beginning time. Developed probabilistic approach lays in carriage out big amount of calculations,
each with different moment of the beginning of accident and using long standing, variable in
time, and heterogeneous in space, characteristics of the ocean flow (and mixed layer depth).
Ocean flow characteristics cannot be typify, in contrast of atmospheric conditions (wind velocity
and direction, stability, precipitation, ground type), which, in case of short-term atmospheric
releases, can be considered homogeneous in space and constant in time.

2. Available databases to provide input parameters for developed models
For big marine areas in Arctic and Pacific Oceans long standing databases with ocean flow
characteristics with acceptable spatial and time resolution come in sight relatively recently.
Four-dimensional databases of ocean flow may be received by reanalysis of common circulation
of ocean and atmosphere, with assimilation of measurement dataset. The problem is that
the measurements in ocean area carriage out much rarely, than in the atmosphere. However,
situation changed for the better last years.

Brief description of databases, used in the computer code, provides in this chapter. Source
database for building coastline in quasi three-dimensional version of model is ASTER GDEM [1].
This database contains high resolution data of height of the Earth relief (topography). Spatial
resolution of the data is 1/3600°. Missing values restores by the database with lower spatial
resolution (1/60°) – Smith and Sandwell surface relief [2]. Smith and Sandwell surface relief
database contains topography and bathimetry data, while ASTER GDEM – only topography.
Source database for mixed layer depth in quasi three-dimensional version of model is ORAS4
[3]. Mixed layer depth corrects by the depth of the ocean: it must be less or equal to deep in
current point. Spatial resolution of the data is 1°. Horizontal components of the velocity for
Arctic Ocean are taken form the database ORAS4, for Far East (Pacific ocean) - FRA-JCOPE
[4]. Spatial resolution of FRA-JCOPE is 1/12°.

Detailed description of these databases may be founded by specified above references.

3. Quasi three-dimensional model for accidents in upper mixed layer
In this section the quasi three-dimensional version of model is presented. This model is intended
for modeling propagation of pollutant in upper ocean layer. In this version of model is assumed,
that pollutant uniformly mixing in the upper ocean layer, until mixed layer depth. Mixed layer
depth is limited by seasonal thermocline, turbulent mixing through this boundary is negligible
small, but upper water layer is subject to intensive turbulent mixing. But there are exists
the vertical advection through this boundary due to horizontal macroscale divergent space-
heterogeneous ocean flows. In this version of the model it is assumed, that pollutant propagate
in soluble form or as fine aerosol. The model takes into account the following processes:

- horizontal advection with ocean flow in the upper layer;
- non-uniform horizontal turbulent diffusion (overgrid and subgrid);
- non-uniform and seasonaly variable 2D field of mixed layer depth field;
- horizontal macroscale ocean currents divergence, causing macroscale downvellings in the
  lower layers.

For modeling of horizontal subgrid turbulent diffusion the algebraic Ozmidov model is used [5].
In this model turbulent diffusion depends only from the linear scale of the pollutant spot. For
modeling of horizontal overgrid turbulent diffusion the algebraic Smagorinsky model is used. In this model turbulent diffusion calculates using shear flow deformations. The main differential equation in the model – is two-dimensional advection-diffusion equation in spherical coordinate system:

\[
\frac{\partial H C}{\partial t} + \frac{\partial (u H C)}{R \cos \theta \partial \phi} + \frac{\partial (v H C)}{R \partial \theta} = \frac{\partial}{R^2 \cos^2 \theta \partial \phi} \left( K \frac{\partial H C}{\partial \phi} \right) + \frac{\partial}{R^2 \partial \theta} \left( K \frac{\partial H C}{\partial \theta} \right) + Q(\phi, \theta, t) \tag{1}
\]

In the equation (1):
- \(\phi, \theta, t\) – longitude, latititide, and time (sec);
- \(R\) – Earth radius (m);
- \(H\) – mixed layer depth, depends from time, longitude and lattitude;
- \(C\) – volume concentration of the pollutant, depends from time, longitude, and lattitude (Bq/m^3);
- \(u, v\) – zonal and meridional velocities, depends from time, longitude, and lattitude (m/s);
- \(K\) – turbulent diffusion coefficient (m^2/s);
- \(Q\) – power of the pollutant source (Bq/s/m^2).

Reducing of \(H\) for time integration step do not lead to increasing the concentration of pollutant.

Equation (1) solves in lagrangian variables, using Monte-Carlo method. Pollution spot represents as a big amount of points. Each point moves in accordance with ocean flow, and subject to random (stochastic) displacement, which models turbulent diffusion. Volume concentration of points (count of points in a unit volume) associates with volume concentration of pollutant. Each point has a certain amount of pollutant \((A)\). If pollutant is radioactive contamination, then this amount of pollutant is radioactivity of a point. Regular and stochastic displacement of a point is described by a system of Ito differential equations (in Cartesian coordinate system): \(\dot{x} = u + u', \ \dot{y} = v + v'\). Omitting intermediate mathematical explanations, give the final (finite difference) formulas, which describes displacement of a point:

\[
\phi^{n+1} = \phi^n + \frac{u \tau}{R \cos \theta^n} + \xi \frac{\sqrt{2K\tau \beta}}{R \cos \theta^n}
\]

\[
\theta^{n+1} = \theta^n + \frac{v \tau}{R} + \eta \frac{\sqrt{2K\tau \beta}}{R}
\]

In equations (2) and (3) \(\tau\) – time integration step, \(\xi\) and \(\eta\) – random variables with normal distribution, \(\phi^n\) and \(\theta^n\) – longitude and lattitude of a point in \(n\)-th time step, \(\beta\) – is the model parameter form 0 to 1. Explain meaning of \(\beta\) below.

The lack of this way of definition volume concentration of pollutant is the need of using a large number of calculation points for a smooth result (without strong fluctuations). Thus, has been developed hybrid method of wondering clouds. In this method, a point is represented as a cloud, which has horizontal non-zero size \(\sigma\). Volume concentration near the center of a cloud obeys Gauss distribution:

\[
G(x, \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left( -\frac{(x - \mu)^2}{2\sigma^2} \right)
\]

\[
C(\phi, \theta) = \frac{A}{H} G((\phi - \phi^n) R \cos \theta^n, 0, \sigma) G((\theta - \theta^n) R, 0, \sigma)
\]

In equation (5) \(C(\phi, \theta)\) – is concentration in point \((\phi, \theta)\). In this version of model the size of a point enlarge in each time integration step: \((\sigma^2)^{n+1} = (\sigma^2)^n + 2(1 - \beta)K\tau\). Thus, \(\beta\) is
the tuning model parameter. If $\beta$ equal 1, then realized model with points. If 0 – model with clouds with non-zero size, turbulent diffusion only enlarge size of a cloud. In the presented model $\beta = 0.9$. If center of a cell is located farther then $3\sigma$, $C(\phi, \theta) = 0$. Concentrations is calculated on uniform longitude-latitude computational grid. Each computational cell is marine area, limited two values of longitude and two values of latitude.

Consider downvelling phenomena. This phenomena leads to decreasing of the pollutant in a cloud $A$ (radioactivity) in accordance with equation:

$$\dot{A} = -\frac{A \cdot W}{H}$$

In equation (6) $W$ – is vertical component of the flow, induced by its non-zero macro-scale horizontal divergent. Then, for the time integration step $\tau$ radioactivity of the cloud decrease in accordance with equation:

$$A^{n+1} = A^n \exp \left(-\frac{W \tau}{H}\right)$$

Further consider the turbulence models. The Ozmidov turbulence model is used to parametrize sub-grid turbulence:

$$K_O = 0.1 \cdot \epsilon^{1/3} \cdot L^{2/3}$$

In equation (8) $\epsilon$ – turbulent energy dissipation rate ($m^2/s^3$), $L$ – linear scale of pollutant spot. If $L < 10 \text{ km}$, then $\epsilon = 10^{-8} m^2/s^3$, else $\epsilon = 10^{-9} m^2/s^3$. The linear scale of pollutant spot calculates as standard deviation from the center of mass of all clouds, where mass of a cloud is its radioactivity ($A$).

The Smagorinsky model [6] is used to parametrize over-grid turbulence. Consider the flow deformation rate tensor:

$$S_{ij} = \frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right)$$

In equation (9) $v_1 = u$, $v_2 = v$. Turbulent diffusion coefficient is defined as below:

$$K_S = C_S^2 \Delta^2 \sqrt{2 S_{ij} S_{ij}} = C_S^2 \Delta^2 \left[ 2 \left( \frac{\partial u}{\partial x} \right)^2 + 2 \left( \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 \right]$$

In relation (10) $C_S$ – is the model dimensionless parameter from 0.6 to 0.28. In described model $C_S = 0.28$.

In described model for a cloud choosing maximum from $K_O$ and $K_S$.

Distinctive feature of the model is modeling of interaction of clouds with coastline. This interaction subdivided on two processes.

In first process a cloud considers as a point with zero size. Trajectory of a cloud on each time integration step – is a line segment, connecting initial and final position of a cloud. Final position calculates as summa of advection and turbulent diffusion. Coastline in the model considers as aggregate of segments – common sides of marine and terrestrial cells. Thus, model coastline – is broken line, whose segments oriented along longitude or latitude. If trajectory segment of a cloud intersects coastline, then segment specular reflects.

In second process clouds considers as a circle with radius of $3\sigma$. It is necessary to provide zero concentration in terrestrial cells, which located in a circle. For this it is necessary to correct the radius of a circle thus, that in a circle do not appears terrestrial cells. Let the distance from circle center to nearest terrestrial cell be equal to $r_t$. If $3\sigma \geq r_t$, then $\sigma$ becomes equal to $r_t/3$. 


4. Three-dimensional model for accidents in arbitrary deep

In three-dimensional model there is no assumption about instantaneous mixing in vertical up to mixed layer depth. Vertical turbulent diffusion models explicitly, using Munk-Anderson algebraic model. Besides, in this version of model ocean flow depends not only from longitude and latitude, but and from deep. Thus advection of the pollutant spot defines by three-dimensional field of horizontal flow velocities, vertical advection do not taking into account.

Consider Munk-Andersen vertical turbulence model [7]. Turbulent diffusion coefficient in this model depends on vertical gradient of horizontal flow and sea water density:

\[ R_i = \frac{g \rho}{\rho_0} \frac{\partial \rho}{\partial z} \left( \frac{\partial u}{\partial z} \right)^2 + \left( \frac{\partial v}{\partial z} \right)^2 \]  (11)

If \( R_i < 0 \), then \( K_{MA} = 0 \), else

\[ K_{MA} = \frac{\beta}{1 + \gamma R_i}^n \]  (12)

In formulas (11) and (12): \( R_i \) – Richardson number, \( g \) - acceleration of gravity (m\(^2\)/s), \( \rho \) – density of marine salinity water (kg/m\(^3\)), \( \rho_0 \) – density of pure water at 0\( ^\circ \)C, \( z \) - deep (m), \( \alpha = 5 \cdot 10^{-6} \text{m}^2/\text{s}, \beta = 5 \cdot 10^{-3} \text{m}^2/\text{s}, \gamma = 5, n = 3. \) Z axis directs down. Density \( \rho = \rho (T, S) \) – is the function of temperature \( T \) (\( ^\circ \)C) and salinity \( S \) (\( ^\circ/\circ \)):

\[ \rho(T, S) = \rho_p(T) \left( 1 + \frac{S}{1000} \right) \]  (13)

In relation (13) \( \rho_p(T) \) – is density of pure water at temperature \( T \). \( T = T(z), S = S(z) \). For calculation of \( K_{MA} \) three-dimensional fields of temperature and salinity should be available.

In this version of model clouds have not only horizontal, but vertical size too. As in the quasi three-dimensional model, here arises the problem of interaction of clouds and ocean floor. Floor of the ocean is the three-dimensional analog of coastline in quasi three-dimensional model. In general algorithm of interaction with ocean floor repeats algorithm of interaction with coastline in quasi three-dimensional version of model. First sub-problem is calculation of trajectory of a cloud under the assumption of specular reflection from faces of cells. Trajectory – is three-dimensional broken line. Second sub-problem is correction of sizes of a cloud thus, that no one cell under the floor of the ocean do not lay in cuboid with sides \( 3\sigma_{\text{lon}}, 3\sigma_{\text{lat}}, 3\sigma_z \), where \( 3\sigma_{\text{lon}} \) – is size of a cloud along longitude, \( 3\sigma_{\text{lat}} \) – along latitude, \( 3\sigma_z \) – along vertical. Unlike quasi three-dimensional model, here instead circle considering cuboid, and sizes of cuboid correcting independently. Both models have been parallelized and may run using arbitrary processor count.

5. Examples of application of the model

Give an example of a probabilistic picture of pollutant spot in coastal marine area of Japan Sea – in the bay Razboinik (Far East, Russia). Location of the source – 132, 36\( ^\circ \)E of east longitude, 42, 89\( ^\circ \)N of north latitude. Radioactivity of the source – 1, 87 \cdot 10^{15} \text{ Bq} of \(^{90}\text{Sr}, 6, 22 \cdot 10^{16} \text{ Bq of} \(^{137}\text{Cs. Release of radioactivity is instantaneous. Forecast time – 3 month. Multi-variant calculation has been carride out. Variable parameter – is accident start moment. It varied from 1-jan-2008 to 31-jan-2008 using step of 1 day (total number of calculation is 31). On the Fig. 1 presented time integrated concentration \( (TIC) \) field. TIC value in each point is equal maximum value over all calculations at the level of trust 95\%.}

Consider the example of application of three-dimensional version of model. Location of the source – 132, 69\( ^\circ \)E of east longitude, 41, 54\( ^\circ \)N of north latitude. Radioactivity of the source – 10^{11} \text{ Bq of} \(^{137}\text{Cs. Accident start moment – 12:00 1-jun-2007, source duration – 5 days, source deep – 19 m, forecast time – two month. Vertical size of the computational area is 300 m. TIC field calculated on the same deep as source – 19 m. This field is presented at Fig. 2.}
Figure 1. TIC – result of calculation using quasi three-dimensional model.

Figure 2. TIC – result of calculation using three-dimensional model.

References

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