Journal of the Georgian Geophysical Society,
Issue B. Physics of Atmosphere, Ocean and Space Plasma, v.19B, 2016, pp. 41-48

Modeling of Exhaust (Waste) Water in the Extraction of Hydrogen Sulfide Black Sea

[1]Marat S. Tsitskhishvili, [2]Alexander E. Shaptoshvili

[1]Georgian Academy of the Ecological Science, Georgia
[2]Israel Energy Initiatives

ABSTRACT

Numerical models, "basic control parameters", Simulation for the case of waste water discharge into the river, model parameters, MacCormack's predictor-corrector. Due to selection of more realistic parameter values in the numerical schemes, the use of Kolmogorov's approximation of turbulent diffusion obtained practically relevant values of pollution fields for the different placement of sources of pollution. The paper presents the results of calculations of pollution fields.

Key words: water pollution, hydrogen sulfide.

When implementing technical schemes energy use hydrogen sulfide from the deep layers of the Black Sea, there are problems of ecologically safe discharge "waste water." Offers numerical models allow calculating environmentally safe concentrations in the wastewaters at various depths of discharge into the sea and for different flow rates (reset) of wastewater.

Modern optimal management of the natural environment in order to achieve sustainable development must be based entirely on the processes of knowledge on detailed analysis, diagnosis and prognosis! Application of physic - mathematical modeling allows to predict the dynamics of the subsequent results of human impact on natural and social complex systems.

Extreme complexity of natural geo-environmental complex units (ecosystems) forces to build mathematical models only with a certain approximation. Purely empirical approach to the study of such complex systems is irrational; modeling allows identifying the main factors shaping, which is why the model, despite the proximity and limitations helps the cause - effect analysis system.

When modeling in natural environments (atmosphere, hydrosphere) must first of all:
- Clearly define the system;
- To evaluate the connection and exchange streams;
- Highlight the main features of the system;
- To assess the degree of accuracy required;
- To determine the dimensionality of the system;
- Evaluate a representative set of variables minimum defining the state of the system;
- Establish a system of basic equations describing the evolution of the system;
- Must be mentioned to define "basic control parameters", giving physically
a real sense of an abstract mathematical model.

As we move through the steps above to provide a consistent model increasingly filled with physical meaning, which allows us to call such a physical - mathematical modeling.
The most critical part of the so-called simulation the definition of "input - output", i.e. forming the boundary conditions. For natural ecosystems , with a spatial (geographic or geometric) isolating systems important to take these inputs and outputs, sources and sinks , namely the boundary conditions determine the impact of the environment on our " selection system" it is through these factors.

This is a first in a series of works devoted to the admixtures expansion in the high-speed stream. 2-dimensional model of admixture expansion in the high-speed stream is suggested. The model is based on the 3-dimensional model vertical averaging with taking into account ``shift'' and ``turbulent'' viscosity. Some numerical tests realized, with the stability of numerical scheme proving. 2-dimensional model gives us a possibility of approximation the concrete be high-speed stream cause we can take in account: depth, fluid speeds and a geographical configurations, depending on where the discharge takes place - in the coastal zone, estuary or far at sea.

1. Simulation for the case of waste water discharge into the river.

The 3-dimensional equation of passive admixtures expansion is:

$$\frac{\partial c}{\partial t}+\vec{\nabla}_h\cdot\left(c\vec{U}_h\right)+\frac{\partial}{\partial x_3}\left(cU_3\right)=S+\vec{\nabla}_h\cdot\left(k\vec{\nabla}_h c\right)+\frac{\partial}{\partial x_3}\left(\lambda\frac{\partial c}{\partial x_3}\right) \quad (1)$$

where [1]:

$$\vec{\nabla}_h\cdot\left(c\vec{U}_h\right)-\text{horizontal advection}$$

$$\frac{\partial}{\partial x_3}\left(cU_3\right)-\text{vertical advection}$$

$$\vec{\nabla}_h\cdot\left(k\vec{\nabla}_h c\right)-\text{horizontal diffusion}$$

$$\frac{\partial}{\partial x_3}\left(\lambda\frac{\partial c}{\partial x_3}\right)-\text{vertical diffusion}$$

$$S-\text{external sources}$$

Let us introduce a vertically averaged admixtures concentration:

$$\bar{c}=\frac{1}{H}\int_{-h}^{\xi}c\,dx_3$$

where $H(x,y)$ - full depth, ξ - surface of water,
and the deviation from the average concentration:

$$\hat{c}=c-\bar{c},\quad -\text{on the assumption of }\int_{-h}^{\xi}\hat{c}\,dx_3=0$$

Integrating (1) in the vertical direction, one obtains:

$$\frac{\partial\bar{c}}{\partial t}+\overline{\vec{U}_h}\cdot\vec{\nabla}_h\bar{c}=\Lambda+\Sigma+T \quad (2)$$

where:

$$T:\ \int_{-h}^{\xi}\vec{\nabla}_h\cdot\left(k\vec{\nabla}_h c\right)dx_3$$

$$\Sigma:\ \frac{1}{H}\vec{\nabla}_h\cdot\left(H\int_{-h}^{\xi}\hat{\vec{U}}_h\hat{c}\,dx_3\right)$$

$$\Lambda-\text{sum of external sources.}$$

Σ is the ``shift" effect contribution. It describes the following set of effects: there is two contributions appearing when we average in any direction - first is an advection by average moving and second is average of a product of deviations from the average, which gives us an addition in the form of ``turbulent" diffusion.

Let us estimate now the shift effect. Let us subtract (2) from (1) for obtaining the equation for $\hat{c}$:

$$\frac{\partial\hat{c}}{\partial t}+\overline{\vec{U}_h}\cdot\vec{\nabla}_h\hat{c}+\hat{\vec{U}}_h\cdot\vec{\nabla}_h\hat{c}+U_3\frac{\partial\hat{c}}{\partial x_3}+\Sigma-\vec{\nabla}_h\cdot\left(k\vec{\nabla}_h c\right)+T+\hat{\vec{U}}_h\cdot\vec{\nabla}_h\bar{c}=\frac{\partial}{\partial x_3}\left(\lambda\frac{\partial\hat{c}}{\partial x_3}\right)+S-\Lambda \quad (3)$$

Further $|\hat{c}| = |\bar{c}|$, but $\left|\hat{\vec{U}}_h\right|$ is not less than $\left|\overline{\vec{U}_h}\right|$ as function of x_3. It is possible to show that the main contribution from left side comes from horizontal advection $\hat{\vec{U}}_h \cdot \vec{\nabla}\bar{c}$.

Then:

$$\hat{\vec{U}}_h \cdot \vec{\nabla}\bar{c} \sim \frac{\partial}{\partial x_3}\left(\lambda \frac{\partial \hat{c}}{\partial x_3}\right) + S - \Lambda \tag{4}$$

It is possible in principle obtain $\hat{c}$ through $\vec{\nabla}\bar{c}$. Then multiplying by $\hat{\vec{U}}_h$ and integrating by vertical direction one obtains the expression for the shift effect. The expression of $\hat{c}$ by $\hat{\vec{U}}_h$ in a common case will contain double integral of $\hat{\vec{U}}_h \cdot \vec{\nabla}\bar{c}$ by vertical direction. We could avoid the integrals in the equation by making an assumption of a form of dependence of $\hat{\vec{U}}_h$ and Λ of time and coordinates. Bowden suggested [2]:

$$\hat{\vec{U}}_h = \overline{\vec{U}_h} \cdot \phi(\eta) \tag{5}$$

$$\lambda = \|\vec{U}_h\| \cdot H \cdot g(\eta) \tag{6}$$

where $\eta = \frac{1}{H}(x_3 + \xi)$

(5) is very strong and restrictive supposition. But from observational results follows that it is very realistic. Then:

$$\left(\overline{\vec{U}_h} \cdot \vec{\nabla}_h \bar{c}\right)\phi = \frac{\|\vec{U}_h\|}{H}\frac{\partial}{\partial \eta}\left(g\frac{\hat{c}}{\partial \eta}\right) + S - \Lambda \tag{7}$$

Integrating twice, multiplying by $\hat{\vec{U}}_h$ and averaging in the vertical dimension, one obtains:

$$\Sigma = \frac{1}{H}\vec{\nabla}_h \cdot \left[\frac{\gamma_1 H^2}{\|\vec{U}_h\|}\overline{\vec{U}_h}\left(\overline{\vec{U}_h} \cdot \vec{\nabla}_h \bar{c}\right)\right] \tag{8}$$

Combining (2) and (8) finally we will have:

$$\frac{\partial \bar{c}}{\partial t} + \overline{\vec{U}_h} \cdot \vec{\nabla}_h \bar{c} = \Lambda + \frac{1}{H}\vec{\nabla}_h \cdot \left[\frac{\gamma_1 H^2}{\|\vec{U}_h\|}\overline{\vec{U}_h}\left(\overline{\vec{U}_h} \cdot \vec{\nabla}_h \bar{c}\right)\right] + \vec{\nabla}_h \cdot k\vec{\nabla}_h \bar{c} \tag{9}$$

This is the model equation.

2. Model parameters

The motions could be considered as a hierarchy of turbulent vortexes with different scale of length and time. Suppose it could be described by Kolmogorov theory; then the energy is distributed by different scales of motions as:

$$E(l) \sim \varepsilon^{2/3} l^{5/3} \tag{10}$$

where l is a typical scale of length, ε - the speed of energy transport by descending cascade of vortexes. From this the typical speed and time are:

$$v_l \sim \varepsilon^{-1/3} l^{1/3} \tag{11}$$

$$\tau \sim \varepsilon^{1/3} l^{2/3} \tag{12}$$

This means that the model smoothing the motions with scales less of:

$$l : \ \varepsilon^{1/3}\tau^{5/3} \qquad (13)$$

By Kolmogorov their contribution in the evolution equation is the ``diffusion" term but with ``turbulent" diffusion coefficient:

$$\nu : \ \varepsilon^{1/4} l^{4/3} : \ \varepsilon\tau^{2} \qquad (14)$$

$\varepsilon : \ 10^{-6}$ for rivers [1], and from expression for the shift viscosity as function of average speed and depth we have:

$$\nu : \ \mathrm{P}\vec{U}_h \mathrm{P} \cdot H : \ 10^{1}$$

Then from length part of (14) we receive:

$$l^{4/3} : \ 316.23, \quad l : \ 74.08$$

i.e. the scale of length is $l : \ 100$ m.

From time part of (14) we receive:

$$\tau : \ 3162.28 \, \mathrm{sec}$$

and time scale is $\tau : \ 1$ hour.

Consider now the ``turbulent" viscosity. Let us take the grid step as 10 m. Than the the ``turbulent" viscosity will be:

$$\nu : \ 10^{-10/4} \cdot 10^{4/3} : \ 0.68$$

From time part of (14) we receive:

$$\tau^{2} : \ 10^{6}, \quad \tau : \ 10^{3} : \ 0.25 \, \mathrm{hour}$$

The ``turbulent" viscosity is about 10 times less than shift viscosity which describes the physics of model - it is acceptable. Next, the time scale is such that the numerical model allows us to obtain the time resolution more accurate than the physical model.

Further the scheme viscosity is $\mathrm{P}\vec{U}_h \mathrm{P}^2 \, \Delta t$ (this is for a MacCormack predictor-corrector type scheme[3]). If we will take a time step about 0.5 sec, the scheme viscosity will be negligible.

2. Deterministic models of waste water into the sea, at entering rivers. (East coast of the Black Sea)

The passive admixture's turbulence diffusion equation has form:

$$\frac{dc}{dt} + \frac{d}{dt}(cU) + \frac{d}{dy}(CV) = \frac{d}{dx}\left(K_x \frac{dc}{dx}\right) + \frac{d}{dy}\left(K_y \frac{dc}{dy}\right) + \frac{d}{dz}\left(K_z \frac{dc}{dz}\right)$$

where $k = 10$ sm^2/sec, $K_x, K_y = 5 * 10^{+6}$ sm/sec is the turbulent viscosities, c is concentration Grid's step is 26.88 km in horizontal direction and 20 m in vertical before depth 200 m. Number of grids knots is 4983 (Fig. A).

For numerical solving of the problem the MacCormack's predictor-corrector, second order in space and time desintegrated scheme was used. Let us introduce the operator

$$C^{*}_{i,j,k} = L_x(\Delta t_x) C^{n}_{i,j,k}$$

$$C^{*}_{i,j,k} = C^{n}_{i,j,k} - \Delta t_x \Delta_x + (C^{n}_{i,j,k} \cdot U_{i,j,k} - M^{n}_{i,j,k} \Delta_x \cdot C^{n}_{i,j,k})$$

$$C^{*}_{i,j,k} = 1/2(C^{*}_{i,j,k} + C^{n}_{i,j,k}) - 1/2 \Delta t_x \Delta_x - (C^{*}_{i,j,k} \cdot U_{i,j,k} - M^{n}_{i,j,k} \Delta_x \cdot C^{*}_{i,j,k})$$

$$M^{n}_{i,j,k} = 1/2(K_{x,i,j} + K_{x,i-1,j})$$

$$M_{i,j,k} = 1/2(K_{x,i+1,j} + K_{x,i,j})$$

Analogous operators $L_y(\Delta t_y)$, $L_z(\Delta t_z)$ were introduced. Then the scheme takes the form:

$$C_{i,j,k}^{n+1} = L_x(\Delta t/2)L_y(\Delta t/2)L_z(\Delta t/2)L_z(\Delta t/2)L_y(\Delta t/2)L_x(\Delta t/2)\cdot C_{i,j,k}^{n}$$

Such a scheme was searched because the turbulent viscosities is horizontal and vertical directions are very different and scheme allows us to do the independent steps in different directions (D. Anderson et al. 1990). The time step is determined as:

$$\Delta t/2 = \min(\Delta t_x, \Delta t_y, \Delta t_z)$$

$$\Delta t_x = \frac{(\Delta x)^2}{|U|\Delta x + 2K_x}, \quad \Delta t_y = \frac{(\Delta y)^2}{|V|\Delta y + 2K_y}, \quad \Delta t_z = \frac{(\Delta z)^2}{2K_z}$$

and can be big enough.

The results are showed at the pictures as follows:

Maximum of Remissible Consenttation (MPC) is 5.10^{-6} g/sm^3

0.01 MPC	<	=	C	<	0.5 MPC	–5
0.05 MPC	<	=	C	<	0.1 MPC	–4
0.1 MPC	<	=	C	<	0.2 MPC	–3
0.2 MPC	<	=	C	<	0.5 MPC	–2
0.5 MPC	<	=	C	<	1 MPC	–1
1 MPC	<	=	C	<	2 MPC	1
2 MPC	<	=	C	<	5 MPC	2
5 MPC	<	=	C	<	10 MPC	3
10 MPC	<	=	C	<	20 MPC	4
20 MPC	<	=	C	<	50 MPC	5

1. Source is in the Batumi area (Fig. B).
Source acts constantly on the depth 40 m.
The concentrations of admixture in sources is: $1.9*10^{-6}$ g/sm^3
Time step is 4 hour. 1 month of process has been calculated.
Picture is such as in Rioni case.

2. Source is in the Novorossisk area (Fig. C).
Source acts constantly on the depth 20-40 m.
The concentrations of admixture in sources is: $1.9*10^{-6}$ g/sm^3
Time step is 4 hour. 1 month of process has been calculated.
Admixture propagates at the East and North-East directions: in the cyclonic motion area and in the Kerch Strait.

3. Sources are in the rivers Rioni's, Inguri's, Bzib's mouths (Fig. D).
Sources act constantly on the depth 40 m.
The concentrations of admixture in sources is:
Rioni: $0.156*10^{-6}$ g/sm^3
Inguri: $0.007*10^{-6}$ g/sm^3
Bzib: $0.019*10^{-6}$ g/sm^3
Time step is 4 hour. 1 month of process has been calculated.
Admixture propagates at the South-West cyclonic motion area.

4. All sources work together (Fig. E).
Time step is 8 hour. 1 year of process has been calculated.
After 3 months the description of admixture reaches a ``quasi-stationar'' state and then does not change.
The tendency of growing the admixture in the cyclonic motion areas is clear.
Concentrations great than 1 MPC are seen at the 150 km radius around the Poti, Batumi, Novorosiisk and Kerch Strait.

Admixture propagates at the big depth, for example, at the sources's areas concentration is 5 MPC at the 120 m depth.

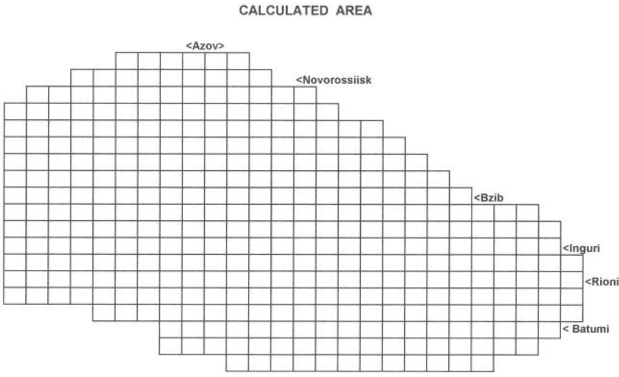


Fig. A

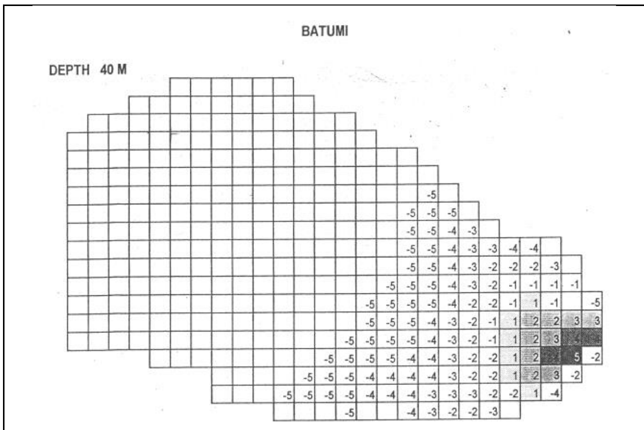


Fig. B

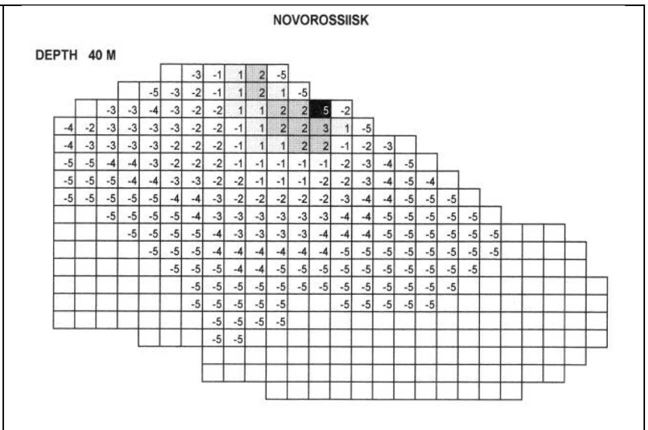


Fig. C

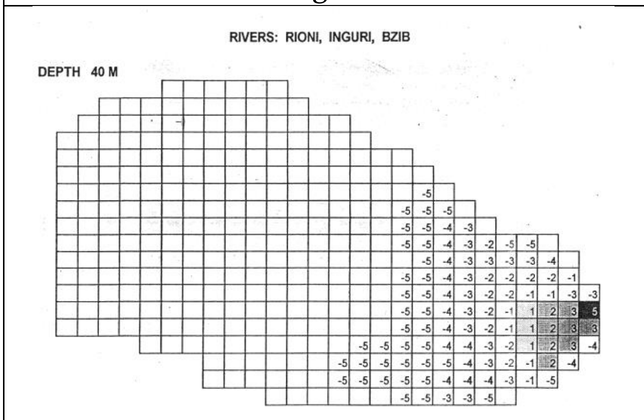


Fig. D

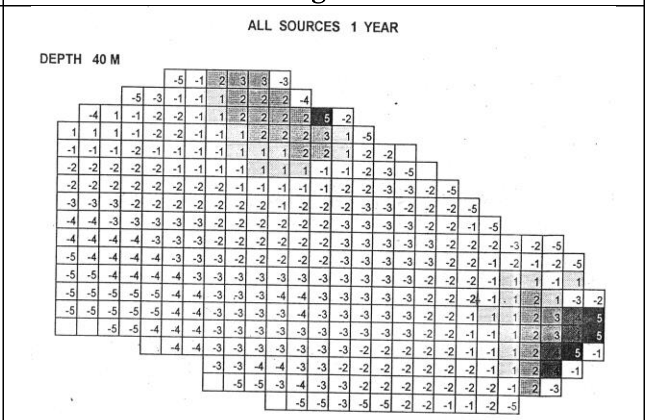


Fig. E

Picture 1. (A - Calculated Area; B - Source is in the Batumi area; C - Source is in the Novorossiisk area, D - Sources is in the rivers Rioni, Inguri, Bzib area; E - All sources work together).

Conclusion

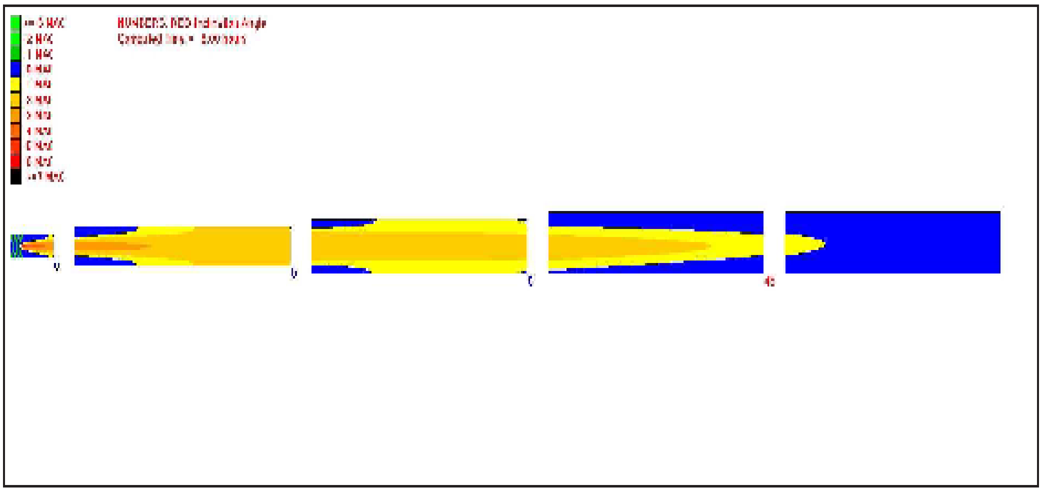
Thus the state independence and free market economics made actual not only creation of juridical basis, but international unification as well. Climatic unification may be made according the following scheme: 1) coastal regions with high humidity, 2) regions with average humidity, 3) highlands, 4) regions with low humidity and desert-like climate. Such regioning for standardization need sources and a lot of time. In this sphere the international cooperation may be very effective. On the other hand, from the standpoint of the international unification of the standards there is also a need to consider ways in which economic instruments may be employed as policy tools for improving atmosphere quality, especially in the most cost effective manner, possible under free market economics. That will improve regional economic situation. Finally, the coordination between economy-wide policies, including micro and micro-economic as well as sectoral policies should also be evaluated.

Analysis of medicoepidemiological data in separate regions of the studied area, the approach of estimation of ecological loading with arbitrary multiplicative parameters allowed to estimate ecological loading on population and carry out the regional mapping of contaminated areas.

The numeral models are worked out to forecast the molismological condition of the Black Sea coasts zone and water permithing to carry out the integral management of the coastal zone depending on the variability of anthropogenic pollutants.

3. Numerical tests, for yielding discharge of waste water into the river (the worst conditions of pollution).

The numerical tests were done. The model high-speed stream consisting of 5 sections with wight from 300 till 800 m was taken. The admixtures source is working constantly at one point at the beginning of the high-speed stream. The fluid speed is 1 m/sec along the fluid axis and it is decreasing to 0 at the banks of river. The depth is 10 m at the centre of high-speed stream and is decreasing to 0 at the banks (Picture 2).



Picture 2.

The 2-step MacCormack numerical scheme was used. The tests shows scheme stability.

As illustration is shown the result of 8 hours of expansion calculation. Numbers of Maximum allowable concentration - MACs - is taken as levels at the picture.

References

[1] Modeling of Marine systems, ed. by J. C. J. Nihoul, Elsevier Oceanography Series, 10, 1975, 269 p.

[2] Bowden K. F. J. Fluid Mech., **21**, 1965, 21:83.

[3] Peyret R., Taylor T. D. Computational Methods for Fluid Flow. Springer-Verlag, New-York, Heidelberg, Berlin, 1983, 358 p.

დაჭუჭყიანებული წყლების მოდელირება შავი ზღვის გოგირდწყალბადის მოპოვებისას

მ. ციცქიშვილი, ა. შაფთოშვილი

რეზიუმე

რიცხვითი მოდელები, კონტროლის ძირითადი პარამეტრები, მდინარეში „ჩაშვების“ შემთხვევის მოდელირება, მოდელის პარამეტრები, მაკ-კორმიკის პრედიქტორ - კორექტორი. რიცხვით სქემებში პარამეტრების რეალური მნიშვნელობების შერჩევით, კოლმოგოროვის აპროქსიმაციის გამოყენებით დიფუზიის აღწერისას, მიღებულია პრაქტიკულად ღირებული მნიშვნელობები დაჭუჭყიანების ველებისა, დამაჭუჭყიანებელი წყაროების სხვა და სხვა განლაგებისათვის. სამუშაოში მოყვანილია დაჭიუჭყიანების ველების გათვლის შედეგები.

Моделирование отработанных (сточных) вод при добыче сероводорода Черного моря

М.С. Цицкишвили, А.Е. Шаптошвили

Резюме

Численные модели, ‘‘основные параметры контроля’’, моделирование для случая сброса сточных вод в реку, параметры модели, предиктор-корректор Мак-Кормака. За счет подбора более реальных значений параметров в численных схемах, использования Колмогоровского приближения турбулентной диффузии, получены практически значимые величины полей загрязнения для различного размещения источников загрязнения. В работе приведены результаты расчетов полей загрязнения.