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Modeling and Development of a Software Complex for Calculating Pollution Propagation in a Water Bodies

S. D. Kurakbayeva¹, Zh. R. Umarova^{1,*}, G. A. Besbayev² and S. B. Botayeva¹

¹ Information Systems Department, M. Auezov South Kazakhstan State University, Kazakhstan.
 ² Computing Systems and Software Department, M. Auezov South Kazakhstan State University, Kazakhstan.

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Abstract: The main purpose of this paper was to describe new models of pollution discharge into water reservoirs. Unlike some known models, this new approach surmounts mathematical difficulties related to setting the correct boundary conditions. Specifically, this method shows that these difficulties can be partially overcome using local sources that have been suggested for describing the liquid phase distribution over the volume of the packed tower. Consequently, one-, two- and three-dimensional models defining the process of pollution discharge into nearby water bodies were developed. An estimation of dynamic characteristics of pollution dispersion in closed water bodies has been made.

Keywords: Mathematical model, water objects, local sources, technogeny discharges, relaxation influence, evaluation of relaxation impact, software interface.

1 Introduction

The presence of toxic substances in industrial effluent is a major source of water pollution. Presently, several mathematical methods are used to describe the distribution of pollution in the environment. It is clear that the effectiveness of a method increases when the physical nature of phenomena and processes are sufficiently studied. However, the problem of creating an adequate mathematical description of the dynamics of the spread of contamination from local sources remains current [1] -[5]. This is due to the serious mathematical difficulties that arise when setting the correct boundary conditions and when finding solutions to the problem. Previously, we described how these difficulties could be partially overcome using local sources to describe the liquid phase distribution over the volume of the packed tower [6]. Specifically, the main advantage of this method lies in overcoming vagueness when setting the boundary conditions at the tower walls, which restrict the liquid flow. Supporting this idea, adapting this method to the given process consists, in our opinion, of a mathematical similarity in the diffusion process and the process of liquid spreading over the packing layer [7]. As a result of our work, a method for calculating the propagation of pollutants in the water reservoir over a certain period of time after a pollution discharge event, taking into account the diffusion coefficient and reservoir size as well as allowing for the location of pollution sources and patterns of pollutant dispersion, are presented.

The development of the given method was carried out to solve one-, two- and three-dimensional problems of pollution propagation. Each of these problems involves an applied purpose. The results, achieved while solving a one-dimensional diffusion problem in a closed area, allow for the reconstruction and analysis of the pattern of pollution dispersion in tubes and drains. The calculation method of pollution propagation in a two-dimensional case was suitable for researching the surface layer of the water reservoir. The solution of the three-dimensional problem allowed definition of the pollution level in the closed reservoir.

2 Formulation of The Problem

2.1 One-dimensional diffusion problem

Primarily, the one-dimensional diffusion problem in a closed area was researched. The solution to the

^{*} Corresponding author e-mail: zhanat.umarova@gmail.com

one-dimensional problem is traditionally applied to running water in tubes, rivers or drains, and this situation can be described by the equation of convective diffusion:

$$\frac{\partial C}{\partial t} + V \frac{\partial C}{\partial z} = D \frac{\partial^2 C}{\partial z^2}$$

The substitution of x = z - Vt, t transforms the initial equation onto the following form:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

which allows it to pass from movable to fixed coordinates. The given problem is presented in Fig. 1 (a, b). Two possible locations of the pollution source with respect to the center of the area were considered: a shifted and non-shifted location. The pollution source can either coincide with the middle point of the researched water area or be located some distance from it.







(b)

Fig. 1: Shifted (a) and non-shifted (b) locations of the pollution source in one-dimensional space

Where 2A is the area width, 2n is the size of the area of the original pollution source, h is a distance from the center

of the source to the center of the area, D is the diffusion coefficient, and t is the observation period. The impurity concentration is described by a one-dimensional diffusion equation [8]:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \tag{1}$$

2.2 Modeling pollution propagation in the surface layer of water reservoirs (two-dimensional problem)

The two-dimensional problem, in the case of one pollution source, was initially considered for analyzing the surface layer condition. Graphically this problem can be presented as in Fig. 2. The following variables have been set: 2B is a field length (m); 2A is a field width, m; 2k and 2n are values of the initial pollution source in length and width, respectively (m); s is the distance from the pollution source center to the middle of the field at length (m); D is the diffusion coefficient; h is the distance from the pollution source center to the middle of the field at width (m); t is the observation period (s).



Fig. 2: Two-dimensional problem for analyzing the water body surface layer condition in the presence of one pollution source.

The appropriate two-dimensional diffusion equation [9] is as follows:

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right) \tag{2}$$

2.3 Model of pollution propagation in the reservoir (three-dimensional problem)

Instances where there are two possible locations of a pollution source in relation to a water body, depending on the type of pollutants in the wastewater, has also been



studied (see Fig. 3 (a, b)). Here 2A, 2B, and 2M are indicators characterizing the reservoir size (width, length, height); s, h, q are the distances from the source middle to the reservoir middle k length, width and height; 2k, 2n, 2p are the pollution source length, width, height, respectively; t is the observation period; γ is a coefficient of impurity dispersion through the surface of water in the reservoir.





Fig. 3: The possible locations of pollution sources in relation to the water body: at the bottom (a), and at a certain distance from the bottom (b)

The pollution spread in the reservoir is described by a three-dimensional diffusion equation:

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right)$$
(3)

3 Problem Solutions

3.1 Solution of the one-dimensional problem of pollution propagation.

In accordance with the approach of using local sources [7] [p.125-128], the general concentration of the pollution in the one-dimensional non-shifted case can be calculated by formula 4 and, for the shifted pollution source by formula 5:

$$\tilde{C}^*(x,t) = \eta \left(C_1(x,t) + \tilde{C}_{h\nu} \right) \tag{4}$$

$$\tilde{C}(x,t) = \eta (C_1(x,t) + C_2(x,t) + C_3(x,t))$$
(5)

where values $C_1(x,t), C_2(x,t), C_3(x,t), \tilde{C}_{hv}$ were determined by using the formulas:

$$C_1(x,t) = C(x_1,t) = \frac{1}{2} \left[erf\left(\frac{x+n}{2\sqrt{D*t}}\right) - erf\left(\frac{x-n}{2\sqrt{D*t}}\right) \right]$$

$$C_2(x,t) = C(x_2,t) = C[2(A-h)-x,t] =$$

$$\frac{1}{2} \left[erf\left(\frac{2(A-h)-x+n}{2\sqrt{D*t}}\right) - erf\left(\frac{2(A-h)-x-n}{2\sqrt{D*t}}\right) \right],$$

$$C_{3}(x,t) = C(x_{3},t) = C[-2(A+h) - x,t] =$$

$$\frac{1}{2} \left[erf\left(\frac{-2(A+h) - x + n}{2\sqrt{D*t}}\right) - erf\left(\frac{-2(A+h) - x - n}{2\sqrt{D*t}}\right) \right]$$

$$\tilde{C}_{hv} = \frac{S}{A} = \frac{\int_{A}^{\infty} C_{1}(x,t)dx}{A}$$

Correction η is calculated using the following formula:

$$\eta = \frac{S_1}{S_2}$$

Where $S_1 = \int_{-1000}^{1000} C_1(x,t) dx$ when calculating S_2 , one should pay attention to the integral borders. For S_2 in the non-shifted source of pollution, it is necessary to use formula 6, whereas formula 7 is used in the second case.

$$S_2 = \int_{-A}^{A} \tilde{C}^*(x,t) dx \tag{6}$$

$$S_2 = \int_{-(A+h)}^{A-h} \tilde{C}(x,t) dx \tag{7}$$

Therefore, substituting various values for D, A, n, h, and t in formulas 4 or 5, depending on the particular studied case, we can find values for pollutant concentrations in the studied closed area. Figures 4 and 5 depict the graphics, characterizing the pollution propagation in a water body from a bias source of pollution over 10, 15, 100, 200, 300, 400 s and in the following sets of initial data: n = 2 m, h = 6 m, A = 10 m, D = 0.3; n = 1 m, h = 4 m, A = 10 m, D = 0.3.



Fig. 4: Graphics of pollution propagation in the water environment for the shifting pollution source over 10, 15, 100, 200, 300, 400 s and at n=2 m, h=6 m, A=10 m, D=0,3.



Fig. 5: Graphics for pollution propagation in the water environment for the non-shifted pollution source over 10, 15, 100, 200, 300, 400 s and at n=1 m, h=4 m, A=10 m, D=0,3.

It should be noted that the patterns of pollution dispersion in the above-mentioned cases are quite different. First, they are connected to the value of the general concentration of pollution. Second, they are connected with the peculiarities of the dispersion pattern near wall 2. Patterns of pollution dispersion have been studied at the above-mentioned times and following sets of initial data: n=3 m, h=7 m, A=10 m, D= 0,3; n=4 m, h=2 m, A= 10 m, D= 0,3; n=2 m, h=5 m, A= 10 m, D= 0,3; n=3 m, h=5 m, A= 10 m, D= 0,3; n=4 m, h=1 m, A=10 m, D= 0,3; n=4 m, h=7 m, A=10 m, D= 0,3.

The time after which the non-uniformity of the concentration distribution did not exceed 5% was calculated. This level of non-uniformity is estimated by the ratio $\frac{C_{\text{max}}}{C_{\text{min}}} \leq 1,05$. The maximum concentration of the pollutant is focused on the point x = 0 because the coordinate area coincides with the center of the pollution source. The value of the impurity concentration in the water environment at the shifted source of pollution in the given enclosed area is minimal near wall 1, as the given area is the most remote from the pollution source. The water environment was available for an exact calculation of the value of the pollutant concentration in the drain, depending on the location of the pollution source relating to the center of the water body, the time and other parameters that influence this process[9].

3.2 Calculation of pollution propagation in the surface layers of the water body (two-dimensional problem solution)

It has been proven that, in accordance with the method of using local sources, the general concentration of the pollutant in a given problem is calculated by the following formula [10]:

$$\tilde{C}(x,y,t) = \eta (C_1(x,y,t) + C_2(x,y,t) + C_3(x,y,t) + C_4(x,y,t) + C_5(x,y,t))$$
(8)

Where values, $C_1(x, y, t)$, $C_2(x, y, t)$, $C_3(x, y, t)$, $C_4(x, y, t)$, $C_5(x, y, t)$ are in the following formulas:

$$C_1(x, y, t) = \left(\frac{1}{2\sqrt{\pi \cdot D \cdot t}}\right)^2 \times \int_{-k-n}^k \int_{-k-n}^n e^{-\left[\frac{(x-\xi)^2 + (y-\eta)^2}{4\cdot D \cdot t}\right]} d\xi \, d\eta$$

$$C_2(x, y, t) = \left(\frac{1}{2\sqrt{\pi \cdot D \cdot t}}\right)^2 \\ \times \int_{-k-n}^k \int_{-k-n}^n e^{-\left[\frac{[2(B-s)-x-\xi]^2+(0-\eta)^2}{4\cdot D \cdot t}\right]} d\xi \, d\eta$$

$$C_{3}(x,y,t) = \left(\frac{1}{2\sqrt{\pi \cdot D \cdot t}}\right)^{2}$$
$$\times \int_{-k-n}^{k} \int_{-k-n}^{n} e^{-\left[\frac{\left[-2(B+s)-x-\xi\right]^{2}+(0-\eta)^{2}}{4\cdot D \cdot t}\right]} d\xi \, d\eta$$



$$C_4(x,y,t) = \left(\frac{1}{2\sqrt{\pi \cdot D \cdot t}}\right)^2 \\ \times \int_{-k-n}^k \int_{-k-n}^n e^{-\left[\frac{(0-\xi)^2 + [-2(h+A)-y-\eta]^2}{4\cdot D \cdot t}\right]} d\xi \, d\eta$$

$$C_5(x,y,t) = \left(\frac{1}{2\sqrt{\pi \cdot D \cdot t}}\right)^2 \\ \times \int_{-k-n}^k \int_{-k-n}^n e^{-\left[\frac{(0-\xi)^2 + [2(A-h)-y-\eta]^2}{4\cdot D \cdot t}\right]} d\xi \, d\eta$$

The impurity dispersion pattern and value of the general pollutant concentration in the water body will differ depending on the observation period. This method is efficient for analyzing the surface layer condition in the presence of only one pollutant source. This approach allows for the calculation of a pollutant concentration over a certain period of time, and also for visualization of the impurity dispersion pattern from the initial data. The case of two pollutant sources at the surface of a landlocked reservoir was also considered. In particular, a method for calculating the impurity concentration depending on the location of both pollution sources was studied. Diagrams characterizing the impurity dispersion in the water environment of a two-dimensional space in the presence of two pollution sources located at different levels during time periods of 10, 100, and 400 s are presented in Fig. 6.

Fig. 6 indicates that the impurity dispersion pattern and size of the general pollutant concentration in the water body will be different depending on the extent of observation. Furthermore, we complicated the problem by adding one more pollutant source. We have studied a method for calculating the impurity concentration depending on the location of both pollution sources. The pollution sources can be located at a certain distance on one level or can be spread apart at different levels. Each above-mentioned case has its own differences and similarities. When calculating the general pollutant concentration of the second pollution source, factors such as the size, distance separating both sources, and location in relation to the middle of the water space under study should be considered. The concentration of the pollutant from the second source using a local source method [7] [p.125-128] was also calculated. The impurity dispersion patterns in the water environment for a two-dimensional diffusion problem in the presence of two pollution sources located on one level (a, b, c), and on different levels (d, e, f) over 10, 100, and 400 s are shown in Fig. 7.







(b)



(c)

Fig. 6: Diagrams of the impurity dispersion in the water environment for a two-dimensional problem during periods of time of 10 s (a), 100 s (b), and 400 s (c)

















(c)



Fig. 7: Diagrams of pollution dispersion in the water environment for a two-dimensional diffusion problem located on one level (a, b, c), and on different levels (d, e, f) over 10, 100, and 400 s.

The constructed diagrams illustrate show the expansion of the observation period influences the pollutant concentration in the given environment in the presence of two pollution sources and will gradually equalize.

3.3 Solution of the problem of pollution propagation in the reservoir (three-dimensional problem)

In accordance with the local source method, the general pollutant concentration in the reservoir in the two cases under study can be calculated with the following formula:

$$\tilde{C}(x,y,z,t) = \eta(C_1(x,y,z,t) + C_2(x,y,z,t) + C_3(x,y,z,t) + C_4(x,y,z,t) + C_5(x,y,z,t) + C_6(x,y,z,t) + \gamma \cdot C_7(x,y,z,t)$$
(9)

Where values, $C_1(x,y,z,t)$, $C_2(x,y,z,t)$, $C_3(x,y,z,t)$, $C_4(x,y,z,t)$, $C_5(x,y,z,t)$ are calculated by the following formulas:

$$C_1(x, y, z, t) = \left(\frac{1}{2\sqrt{\pi \cdot D \cdot t}}\right)^3 \\ \times \int_{-k-n-p}^k \int_{-p}^n e^{-\left[\frac{(x-\xi)^2 + (y-\eta)^2 + (z-\theta)^2}{4\cdot D \cdot t}\right]} d\xi \, d\eta \, d\theta$$

$$C_2(x,y,z,t) = \left(\frac{1}{2\sqrt{\pi \cdot D \cdot t}}\right)^3$$
$$\times \int_{-k-n-p}^{k} \int_{-p}^{n} \int_{p}^{p} e^{-\left[\frac{[2(B-s)-x-\xi]^2+(0-\eta)^2+(0-\theta)^2}{4\cdot D \cdot t}\right]} d\xi d\eta d\theta$$

$$C_{3}(x,y,z,t) = \left(\frac{1}{2\sqrt{\pi \cdot D \cdot t}}\right)^{3} \\ \times \int_{-k}^{k} \int_{-n-p}^{n} \int_{p}^{p} e^{-\left[\frac{[-2(B+s)-x-\xi]^{2}+(0-\eta)^{2}+(0-\theta)^{2}}{4\cdot D \cdot t}\right]} d\xi \, d\eta \, d\theta$$

$$C_4(x,y,z,t) = \left(\frac{1}{2\sqrt{\pi \cdot D \cdot t}}\right)^3$$
$$\times \int_{-k-n-p}^{k} \int_{-p}^{n} e^{-\left[\frac{(0-\xi)^2 + [-2(h+A)-y-\eta]^2 + (0-\theta)^2}{4\cdot D \cdot t}\right]} d\xi \, d\eta \, d\theta$$

$$C_{5}(x,y,z,t) = \left(\frac{1}{2\sqrt{\pi \cdot D \cdot t}}\right)^{3}$$
$$\times \int_{-k}^{k} \int_{-n-p}^{n} \int_{p}^{p} e^{-\left[\frac{(0-\xi)^{2}+[2(A-h)-y-\eta]^{2}+(0-\theta)^{2}}{4\cdot D \cdot t}\right]} d\xi d\eta d\theta$$

$$C_{7}(x,y,z,t) = \left(\frac{1}{2\sqrt{\pi \cdot D \cdot t}}\right)^{3}$$
$$\times \int_{-k-n-p}^{k} \int_{-p}^{n} \int_{p}^{p} e^{-\left[\frac{(0-\xi)^{2}+(0-\eta)^{2}+[2(M+q)-z-\theta]^{2}}{4\cdot D \cdot t}\right]} d\xi \, d\eta d\theta$$

It should be noted that the formula for determining value $C_6(x, y, z, t)$ depends on the pollution source location. Therefore, in the case when the pollution source is located at a certain distance from the bottom, the value $C_6(x, y, z, t)$ can be determined from the following formula:

$$C_{6}(x, y, z, t) = \left(\frac{1}{2\sqrt{\pi \cdot D \cdot t}}\right)^{3} \\ \times \int_{-k}^{k} \int_{-n-p}^{n} \int_{-p}^{p} e^{-\left[\frac{(0-\xi)^{2} + (0-\eta)^{2} + [-2(M-q)-z-\theta]^{2}}{4\cdot D \cdot t}\right]} d\xi \, d\eta \, d\theta \quad (10)$$

The pollution source location in the water body can be determined with the following formula:

$$C_{6}(x, y, z, t) = \left(\frac{1}{2\sqrt{\pi \cdot D \cdot t}}\right)^{3} \\ \times \int_{-k}^{k} \int_{-n-p}^{n} \int_{-p}^{p} e^{-\left[\frac{(0-\xi)^{2}+(0-\eta)^{2}+(-2p-z-\theta)^{2}}{4\cdot D \cdot t}\right]} d\xi \, d\eta \, d\theta \quad (11)$$

By calculating the operations, we can plot the diagrams characterizing the pollution spread in reservoir from defined initial data. For example (Fig. 8), there were given diagrams for the spread of pollutants at 5 meters in the two above mentioned cases with the following initial data: A = 10 m, B = 12 m, M= 15 m, D = 0.3, $\gamma = 0.3$, k =3 m, n =2 m, p =4 m, s =5 m, h =4 m, q1 =6 m, q2 =11 m and t = 15 s. As a result of numerical experiments in a three-dimensional case, the estimates of dynamic characteristics for pollutants spread in a landlocked water body have been obtained. Data obtained allow for evaluation of the level of pollution in the defined segment of the water environment depending on the surpassed period, type of pollutants, location and scale of the pollution source and reservoir.

3.4 Development of a software complex for calculating pollution propagation in a water body

Here, we present the software complex that has been developed in the DELPHI environment [11]. For the convenience of the user, the software interface was unified and can be arranged under the Windows XP operating system. A main menu has been created, and special symbols, reflecting the essence of the implemented commands, has been used. Using 'Help' in



(b)

Fig. 8: Diagrams of the spread of pollutants at a depth of 5 m during the observation period at 15 s at the location of the pollutant source at a certain distance from the source (a) and at the source (b)

the menu, the user becomes acquainted with information connected with the application field and the principles of using the given software complex as well as the additional data that are necessary in the framework of the given project. The menu item "Pollution propagation from the local source" contains the following commands: "Location of the pollution source", "Conventional signs", and "Exit". The command "Location of the pollution source" contains a submenu, allowing for the choice of one of two possible variants: "at the bottom of the reservoir" or "at a certain distance from the bottom". The command "At some distance from the bottom" the window "Window for analyzing pollutant propagation for sources located at some distance from the bottom" is presented. The window provided contains the following "Problem settlement", commands: "Calculate", "Graphics", and "Back". However, to create the given form, the following components were used: LabeledEdit,

Label, MainMenu, Bitbutton, etc. To operate the software, it was necessary to assign the data by defining the following: the width, length, and reservoir height; the coefficients of diffusion and impurity dispersion throughout the water surface in the reservoir; the distance from the middle of the pollution sources up to the middle of the reservoir based on the length, width and height; the observation period; the size of the pollution source; and the point coordinates, for which it was necessary to calculate the pollutant concentrations. Each field was checked for the correctness of the input data. In this case, two types of dialogue message are possible: "Data have been entered incorrectly" and "Data have not been entered". All of the computing operations were carried out on the basis of calculation methods for pollution diffusion in the water body. Furthermore, the computation of a triple integral, which is one of the main steps in our method, was realized on the basis of the Simpson formula (parabola formula), which is exact for multinomials up to the third degree, inclusively. The command "Graphics" allows for the construction of three-dimensional graphics, characterizing the dependence of the concentration of the pollution source location within the volume of the reservoir. To construct the graphics, the software appeals to the Mathcad application documents. This operation was organized with the help of the function ShellExecute. The command "Problem settlement" was applied to change the form, which contained three tabs: Problem settlement, Picture, Close, all of which provide information about the theoretical aspects of the researched object. The tab "Picture" allows for the graphical interpretation of the problem settlement. For the convenience of browsing, auxiliary tools are used with all of the software tools. All of the operations are analogous to the window "Analysis of pollutant propagation, located at the bottom of the water body". The only difference is that within the intermediate calculations, the concentration $C_6(x, y, z, t)$ was defined by formula (11). In the given window, it was also not necessary to enter the value of the pollution source height because it is automatically calculated when filling fields such as the height of the reservoir and the distance from the middle of the pollution source up to the middle of the reservoir in height. The working capacity of the software complex was determined for definite input data, and the received result was compared with the result of the application method in Mathcad software. Therefore, the software complex created could be widely used to calculate the pollution dispersion in water reservoirs, and it allowed for a large-scale array of input data with accurate results[12]. The program is applicable to modeling and monitoring industrial pollutant discharges in the water environment. The given program was registered as intellectual property with the Ministry of Intellectual Property Rights Committee of Justice in the Republic of Kazakhstan[13].



4 Conclusion

In this work, the local source method [7] applied to the problem of pollution propagation in water reservoirs was substantiated. One-, two- and three-dimensional models defining the process of pollution dispersion in the water bodies were developed. An estimation of the dynamic characteristics of pollution prevalence in a closed water body was described. The obtained results allow for estimation of the contamination rate in existing water bodies from industrial influence and can be used for monitoring, modeling and forecasting technogenic accidental discharge in different branches of industry; furthermore, related software was developed in the DELPHI environment for computing these methods^[14]. To use local sources, a special software complex was developed as known software products had not been adapted for this method. Program testing was carried out at defined initial conditions for problems with analytical solutions and also by comparing the calculation results with numerical data obtained by using other programs (Mathcad Prime 2.0, MS Excel 2010). The developed software complex, in contrast to the range of other available programs for calculating polluting discharge, allowed for a substantiated estimation of a dispersion effect from water body discharges.

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Sevara Dzhumagaliyevna Kurakbayeva received the candidate of technical science degree in mathematical modeling in ecology from the M. Auezov South Kazakhstan State University, Kazakhstan in 2010. Currently she is working as an associated professor of

Information Systems department at M. Auezov South Kazakhstan State University. Her research interests include mathematical and computer modeling, computer science, computer graphics.



Zhanat Rysbayevna Umarova received the PhD degree in Computer Science from Kazakh National Technical University. Almaty in 2012. Currently she is working as an associate professor of Information Systems department South M. Auezov at

Kazakhstan State University. Her research interests include mathematical modeling, computer simulation, information security and data protection in information systems, renewable recourses.



Gani Abzelbekovich **Besbavev** received the candidate of Physics and Mathematics science degree in mathematics from the Auezov South Kazakhstan State University, Kazakhstan in 2004.Currently he is working as associated professor of Computing

Systems and Software department at M. Auezov South Kazakhstan State University. His research interests include differential equations and applications, creation software package, mathematical and computer modeling, mathematical physics.



Saule Bayzahovna Botayeva received the candidate of technical science degree in Management in social and economic systems from the Kazakh National Technical University, Almaty in 2010. Currently she is working as an associated professor of Information

Systems department at M. Auezov South Kazakhstan State University. Her research interests include databases, logistics systems, and programming languages.