2D - MODEL OF CONTAMINANT WATER TRANSMISSION PROCESSES AND NUMERICAL SIMULATION ON A NATURAL LAKE

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Abstract. Nowadays, the water pollution problems in the lakes are urgent matters. The simulation of contaminant water transmission process plays important role in reality to improve people's life qualities. In this paper the 2D- mathematical model simulating transmission processes of some contaminant substances in one lake of Hanoi is studied. The finite volume method is used in model. The actions between substances are considered and the simulation results are compared with the measurements.

1. INTRODUCTION

Present-day in our country, water pollution is one of the most serious problems. Water quality is influenced directly to health of people. In this paper the 2D hydraulic and pollution models are used to simulate the transmissions of the pollution substances. The linear 2D water pollution model is studied by semi group method in [5]. The nonlinear 2D-Imech water pollution model is begun establishing in 2005 [1] by the group of Assoc. Prof. Hoang Van Lai. In this paper this model is developed to simulate transmission of the pollution substance combination acting each with others in water.

2. FORMULATION OF THE WATER POLLUTION PROBLEM

2D Pollution water model is consisted of hydraulic model and transmission - diffusion of pollution substances. The Saint - Vernant equation is written as follows:

$$\frac{\partial z}{\partial t} + \frac{\partial}{\partial x}(uh) + \frac{\partial}{\partial y}(vh) = 0 \quad (\text{in } \Omega) \tag{1}$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + g\frac{\partial z}{\partial x} = -\frac{gu(u^2 + v^2)^{1/2}}{K_x^2 h^{4/3}} \quad (\text{in } \Omega) \tag{2}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + g\frac{\partial z}{\partial y} = -\frac{gv(u^2 + v^2)^{1/2}}{K_y^2 h^{4/3}} \quad (\text{in } \Omega) \tag{3}$$

We suppose that there are m substances dissolved in water. Then the transmission and diffusion processes of pollution substances are described by the following equation:

$$\frac{\partial C_i}{\partial t} + \frac{\partial}{\partial x}uC_i + \frac{\partial}{\partial y}vC_i = f_i + D_i(\frac{\partial^2}{\partial x^2}C_i + \frac{\partial^2}{\partial y^2}C_i) \quad (\text{in } \Omega), \quad (i = 1...m) \tag{4}$$

Here:

$\Omega-$is a bounded domain of R^2 with a boundary Γ

$z-$ Free surface elevation,

$h-$ Water height

$u-$ Average velocity by x direction

$v-$ Average velocity by y direction

$g-$ Gravity acceleration

K_x- Strickler coefficient by x direction

K_y- Strickler coefficient by y direction

$S_{o,x}-$ Bottom slope by x direction

$S_{o,y}-$ Bottom slope by y direction

C_i- Concentration of i-substance

f_i- Pollution source of i-substance

D_i- the diffusion coefficient of i-substance

$m-$ The number of substances in water

$U = (u, v)-$ water velocity vector

The boundary and initial conditions of Saint - Vernant and water pollution equations are:

$U(x, y).\vec{n}|_\Gamma = \bar{U}(t)$, where $\vec{n}$ is the normal out orthogonal vector onto the perimeter of the region Ω,

$U(x, y, 0) = U_o(x, y), \quad z(x, y, 0) = z_o(x, y), \quad z|_\Gamma = \bar{z}(t), \quad C_i(x, y, 0) = C_{i,0}(x, y),$

$C_i(x, y, t)|_{(x,y)\in\Gamma_1} = \bar{C}_i(t)$ and $\left.\frac{\partial C_i}{\partial n}\right|_{\Gamma_2} = 0$, $\Gamma = \Gamma_1 \cup \Gamma_2$.

3. MATHEMATICAL ALGORITHM CALCULATED 2D WATER POLLUTION

3.1. Algorithm of 2D flow system.

In this model the finite volume method is used with the calculated triangular mesh. In the regions with complicated topography the flows are well simulated by this grid board. In finite volume method the calculated area is divided by the small simple elements as triangles. The triangular mesh is unstructured and represented as in Fig. 1. The mesh's unstructured properties are represented that the numbering of grids and elements are considered by any rule.

To apply the finite volume the equations (1) - (3) are rewritten as follows:

$$\frac{\partial V}{\partial t} + \frac{\partial A}{\partial x} + \frac{\partial B}{\partial y} = F \tag{5}$$

In the equation (5)

$$V = \begin{pmatrix} z \\ q_x \\ q_y \end{pmatrix}, \quad A = \begin{pmatrix} q_x \\ \frac{1}{2}u^2 + gz \\ uv \end{pmatrix}, \quad B = \begin{pmatrix} q_x \\ uv \\ \frac{1}{2}v^2 + gz \end{pmatrix}, \quad F = \begin{pmatrix} 0 \\ -gu\frac{\sqrt{u^2+v^2}}{K_y^2 h^{4/3}} + u\frac{\partial v}{\partial y} \\ -gv\frac{\sqrt{u^2+v^2}}{K_y^2 h^{4/3}} + v\frac{\partial u}{\partial x} \end{pmatrix}$$
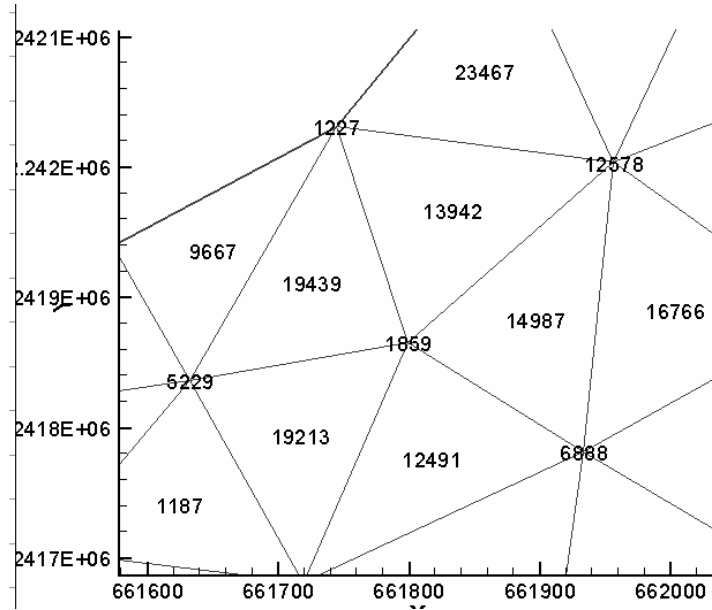
Fig. 1. The unstructured mesh

Integrating two sides of equation system (5) by small element S we have the formula:

$$\int_S \frac{\partial V}{\partial t} dS + \int_S \nabla.(A, B) dS = \int_S F dS$$

To approximate these integrals we assume that in small element S the functions z, u, v can be the constants. Therefore, using Green formula the above formula can be rewritten as following:

$$\frac{dV}{dt}S + \oint_{\partial S} (A, B).\vec{n} d(\partial S) = \int_S F dS \tag{6}$$

In (6), S is the area of element, ∂S is the perimeter of element, n is the out normal orthogonal vector onto ∂S. In the slow changing process problem to calculate the integrals we can use the average values for the functions in S element.

3.2. Mathematical algorithm for transmission-diffusion equations

The transmission pollution substance equation (4) can be rewritten as follows:

$$\frac{\partial C_i}{\partial t} + u\frac{\partial C_i}{\partial x} + v\frac{\partial C_i}{\partial y} - \frac{\partial}{\partial x}\left(D_i\frac{\partial C_i}{\partial x}\right) - \frac{\partial}{\partial y}\left(D_i\frac{\partial C_i}{\partial y}\right) = f_i$$

Or

$$\frac{\partial C_i}{\partial t} + U grad C_i - \nabla.D_i grad C_i = f_i \tag{7}$$

here $U = (u, v)$.

The pollution process model is depending on the combination of substances and number of them. The following substances and the conversion terms are considered:

Table 1. The substances and conversion terms

Variable	Conversion term
SS	Er - De
BOD	Hyd + FastCoxid - $R_{ON_{Denitri}}$ Denitri + Sed_{BOD} - $Sett_{BOD}$
CHL	$Growth_{CHL}$ - $Death_{CHL}$ - $Resp_{CHL}$ - $Settl_{CHL}$
DO	$R_{OC_{CHL}}$ $Growth_{CHL}$ - $R_{OC_{CHL}}$ $Death_{CHL}$ - SOD - FastCOxid - $R_{ON_{Nitri}}$ Nitri + Reae O_2
NH_4	$R_{NO_{Hyd}}$ Hyd - $R_{NC_{CHL}}$ P_{ap} $Growth_{CHL}$ - $R_{NC_{CHL}}$ Re sp_{CHL} - Nitri + Sed_{NH_4}
NO_3	Nitri - Denitri - $R_{NO_3C_{CHL}}$ $(1 - P_{ap})$ $Growth_{CHL}$ - Sed_{NO_3}
C_T	$R_{CC_{FastCOxid}}$ FastCOxid + $R_{CC_{Re\ sp}}$ Re sp_{CHL} - $R_{CC_{Growth}}$ $Growth_{CHL}$ + $Reae_{CO_2}$ + Sed_{CO_2} - $Prep_{CO_3}$
ALK	$R_{ALK,\ CHL}$ $Resp_{CHL}$-$(R_{ALK,\ CHL}$ P_{ap}-$R_{ALK,\ N}$ $(1-P_{ap}))$ $Growth_{CHL}$-$R_{ALK,\ Nitri}$ Nitri+$R_{ALK,\ Denitri}$ Denitri
pH/[H$_+$]	f ([H$_+$])

In the right side of equation (7) the combination of substances are considered and represented by the source functions $f_i (i = 1, ..., m)$. These functions f_i are called by conversion terms and written as follows: $f_i = \sum_{j=1}^{m} k_{i,j} C_j (i, j = 1, m)$. Here, m is the number of pollution substances and $k_{i,j}(i, j = 1, .., m)$ are the coefficients depending on temperatures and different substances.

Integrating two sides of equation (7) by dx and dy we have:

$$\int_S \frac{\partial C_i}{\partial t} dxdy + \int_S \left(div\left(UC_i \right) - C_i divU \right) dxdy - \int_S \nabla \left(D_i gradC_i \right) dxdy = \int_S \sum_{j=1}^{m} k_{i,j} C_j dxdy$$

Using the Green formula for the above equation we have:

$$\int_S \frac{\partial C_i}{\partial t} dxdy + \int_{\partial S} UC_i \vec{n} \partial S - \int_S C_i divU dxdy - \oint_{\partial S} D_i gradC_i . \vec{n} \partial S = \int_S \sum_{j=1}^{m} k_{i,j} C_j dxdy$$

Then the equation can be discrete by the following equation:

$$\frac{C_i - C_{i,t}}{\Delta t} dS + (uC_{i,t} - D_i \frac{\partial C_{i,t}}{\partial x}) n_x . \partial S + (vC_{i,t} - D_i \frac{\partial C_{i,t}}{\partial y}) n_y . \partial S - C_{i,t} \frac{z_i - z_{i,t}}{h\Delta t} dS = \sum_{j=1}^{n} k_{i,j} C_{j,t} dS$$

Here the functions are calculated at the center point of element; dS is the area of element; ∂S is the perimeter of element; C_t is the concentration in the last step; $\vec{n} = (n_x, n_y)$ out normal orthogonal vector of element; u, v and z are the values solving from (6); z_t is the value of z in the previous step. Then the concentration of substance C_i can be calculated by the following formula:

$$C_i = (k_{i,1}C_{i,t} + k_{i,2}C_{2,t} + ... + k_{i,n}C_{n,t})\Delta t + C_{i,t}(\frac{z - z_t}{h} + 1) -$$

$$-(uC_{i,t} - D_i\frac{\partial C_{i,t}}{\partial x})\frac{n_x \partial S\Delta t}{dS} - (vC_{i,t} - D_i\frac{\partial C_{i,t}}{\partial y})\frac{n_y \partial S\Delta t}{dS}$$

4. EXPERIMENTAL SIMULATION FOR THANH NHAN LAKE

Thanh Nhan lake is located behind Thanh Nhan hospital. Its area, water height, water capacity respectively are 8.1 ha, 1.5m - 3m and 162.0000m^3. Waste water flowing into lake is about 2100 m^3 per day-night.

a. Physical hydro properties

- Temperature of lake is oscillated from 23.4 ^{o}C to 23.8^o C in dry season.
- pH level is oscillated from 7.88mg/l to 8.57mg/l
- Muddy level is oscillated from 9mg/l to 34 mg/l.
- Salt level (NaCL) isn't changed in at the stations getting samples 0.01%
- Oxygen concentration dissolved in water is oscillated from 7.9 mg/l to 11.6 mg/l.

b. Chemical hydro properties:

* Organic element group:

- The contents of elements that have the origin Nitrogen such as NO_2, NO_3, and NH_3 having the following development processes:

+ The content of NO_2 is oscillated from 0,055mg to 0.062 mg/l higher than permitted critical value of surface water standard in Vietnam (0.01- 0.05mg/l)

+ The content of NO_3 is oscillated from 0.76mg to 0.81 mg/l lower very much than permitted critical value of surface water standard in Vietnam (10 - 15 mg/l).

+ The content of NH_3 is oscillated from 0.51mg to 0.62 mg/l not higher than permitted critical value of surface water standard in Vietnam (1 mg/l).

+ The content of PO_4 dissolved in water is oscillated from 0.44mg/l to 0.46 mg/l

+ The content of salt that has origin SO_4 is oscillated from 25mg/l to 27 mg/l.

+ The content of substances that have origin H_2S is oscillated from 0.116mg/l to 0.151 mg/l.

+ The need of chemical biology oxygen BOD_5 is oscillated from 15.5mg/l to 24.0 mg/l less than Vietnamese critical standard of surface water quality (less than 25 mg/l).

+ The need of chemical oxygen COD is oscillated from 345mg/l to 400 mg/l. Therefore, the chemical oxygen need is higher than Vietnamese critical standard of surface water quality about 10 times (less than 35 mg/l).

* The group of chemical toxin is consisted of some elements that have heavy metals such as catmint, mercury, leaden and mange. In general, the average contents of elements, that have heavy metals, are less than Vietnamese critical standard of surface water quality (1995).

Table 2. Water quality of Thanh Nhan lake in 11/2001

	P1 Gate into the north of lake	P2 Area in the middle of lake	P3 Gate out	Vietnamese critical standards	Remarks
Temperature ^{o}C	23.4	23.8	23.8		
Oxygen concentration dissolved (mg/l)	7.9	10.9	11.6	≥ 6 ≥ 2	
PH	7.88	8.48	8.57	6-8 5.5-9	
Derivative level (S/m)	0.04	0.04	0.04		
NaCL(%)	0.01	0.01	0.01		
Muddy level (mg/l)	9	25	34		
NO_2-N (mg/l)	0.055	0.057	0.062	0.01 0.05	Over the critical standards
NO_3-N (mg/l)	0.81	0.78	0.76	10 15	
NH_3 (mg/l)	0.52	0.51	0.62	0.05 1	
SO4(mg/l)	27	25	25		
PO4 (mg/l)	0,44	0,46	0,46		
COD(mg/l)	400	380	345	<10 <35	Over the critical standard about 10 times
$BOD_5 20^{o}$C (mg/l)	24.0	15.5	17.0	<4 <25	
Total Coli form(MPN/100ml)	280			5000	
Fecalcoliform(MPN/100ml)	200			5000	
Cu (mg/l)	0,00	0,00	0,00	0.1 1	
Mn (mg/l)	0.001	0,003	0,005	0.1 mg/l 0.8 mg/l	
Pb (μg/l)	2,740	2,370	3,140	0.05 mg/l 0.1 mg/l	
Cd (μg /l)	0,228	0,316	0,325	0.01 mg/l 0.02 mg/l	
Hg (μg /l)	0,089	0,076	0,091	0.001 mg/l 0.02 /l	

c. Geographical data

The geographical data of Thanh Nhan Lake are collected on the map 1:5.000 with the correction corresponding to real condition.
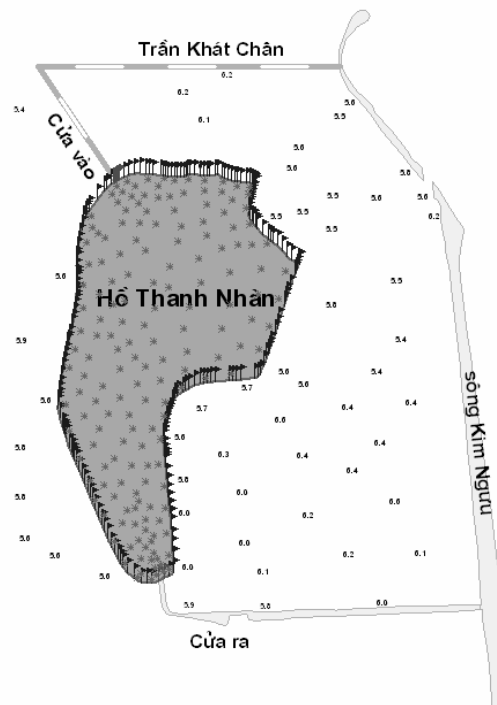

Fig. 2. Geographical map of Thanh Nhan lake

We only use norms of substances in the model such as BOD_5, SO_4, and COD. BOD's indicator shows the oxygen quantity needing for bacterium in oxygen reactions of organic substances in water. COD's indicator shows the chemical oxygen's quantity needing for oxygen reactions of organic substances in disintegration processes into CO_2 and H_2O. High contents of SO_4 influence to the processes introducing H_2S in water that makes bad smell and poison to fishes.

The substances BOD_5, SO_4, COD have exchanging relation. The chemical process disintegrated pollution substances are described as follows:

S_i (BOD_5) = - k_1 .BOD_5; S_i(SO_4) = - k_7 SO4; S_i (COD) = k_6 COD.

On the collected data, we establish the input data for the model. The geographical data are divided into the boundary and inside area of lake. These data are divided by the unstructured net with 1964 triangular elements and 1058 nodes. This geographical map and unstructured net are described as the following Fig. 3 and Fig. 4.

The data of discharges, water height and substance contents in the gate into the lake are as following:

The discharges in and out of lake are 2100 m^3per day-night.

The average water height is 4m.

The content of BOD_5 in the gate into lake is equal to the measurement value 24 mg/l.

The content of SO_4 in the gate into lake is equal to the measurement value 27 mg/l.

The content of COD in the gate into lake is equal to the measurement value 400 mg/l.
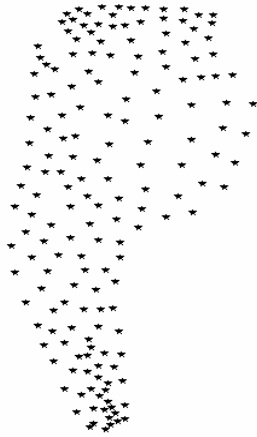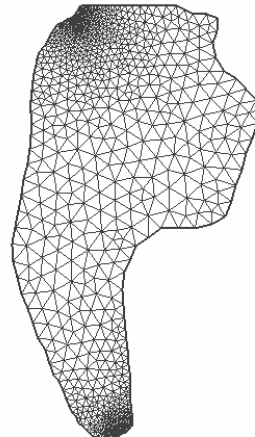

Fig. 3. Geographical data

Fig. 4. Unstructured net with triangular elements

On the gate out there are the conditions of concentration: $\partial C_i/\partial n = 0$ (i=1... m) where n is the out orthogonal vector onto the gate out of lake.

The measurement positions are described in the following figure
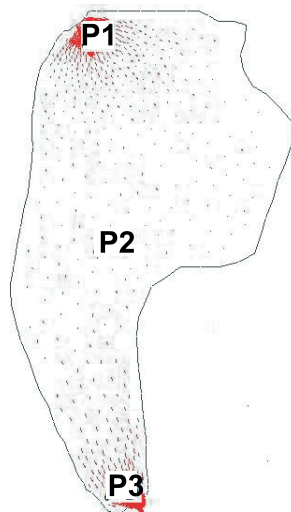
Fig. 5. The measurement positions on the lake

With the previous algorithm, the concentration results of BOD_5, SO_4, COD are obtained and described in the Figures 6-9
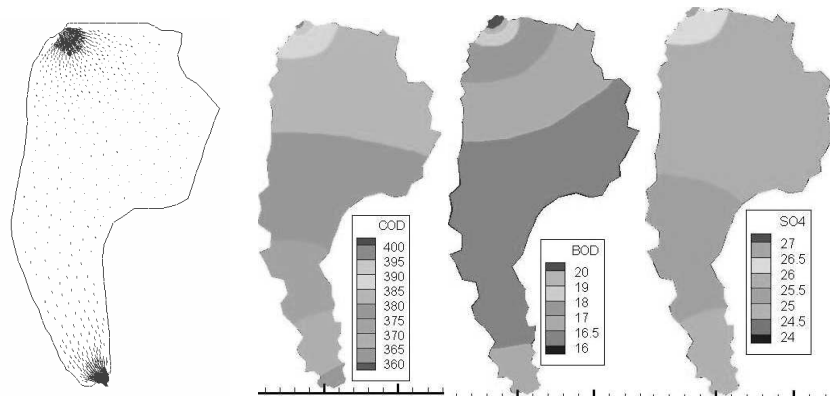
Fig. 6. Velocity and substance concentration fields COD, BOD$_5$, and SO4
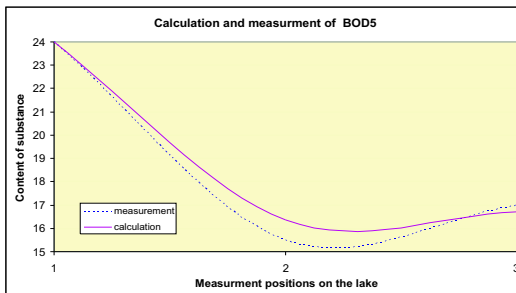

Fig. 7. Calculation and measurement of BOD$_5$ contents at some points on the lake
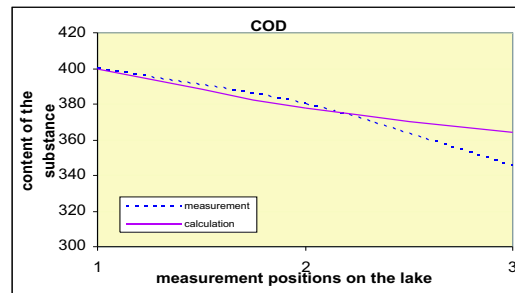

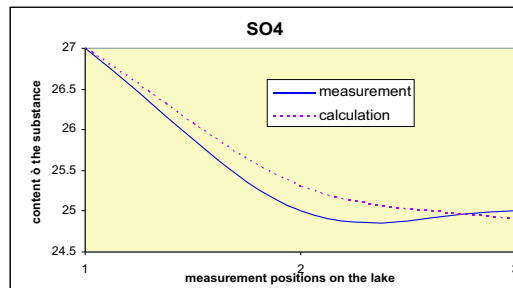*Fig. 8.* Calculation and measurement of COD contents at some points on the lake

Fig. 9. Calculation and measurement of SO$_4$ contents at some points on the lake

5. CONCLUSION

From the calculation results described by the transmission pictures of BOD$_5$, COD SO$_4$, it is easily to see that the calculation contents of these substances are closed to the measurements. In the middle of lake there are some errors between measurements and simulations of BOD$_5$, COD, and SO$_4$. These errors can be explained that the contents of

pollution substances are also depending on lake's temperatures, alga activates, and sunshine... These influences aren't considered in simulation process. The model can be used to simulate the transmission of substance combination in water with unlimited number of them if we have enough data. For the values of coefficients $k_{i,j}$ $(i, j = 1, \ldots, m)$ in combination pollution sources f_i $(i = 1, .., m)$ from the right side of equation (7) we need to get the experimental results from the Institute of Chemistry.

With the results of simulation, the model can be developed and considered as a supported tool to calculate substance contents and study water quality for the pollution problems in our country.

ACKNOWLEDGEMENT

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MÔ HÌNH LAN TRUYỀN Ô NHIỄM NƯỚC HAI CHIỀU VÀ TÍNH MÔ PHỎNG CHO MỘT HỒ CHỨA TỰ NHIÊN

Ngày nay, vấn đề ô nhiễm nước trong hồ chứa trở nên rất cấp thiết. Việc mô tả quá trình lan truyền chất trong hồ chứa đóng vai trò rất quan trọng trong việc nâng cao chất lượng cuộc sống của nhân dân. Trong bài báo này mô hình toán hai chiều mô tả quá trình lan truyền chất trong một hồ chứa ở Hà Nội được nghiên cứu. Phương pháp phần tử khối được sử dụng. Các ảnh hưởng tương tác của các chất trong hồ được nghiên cứu và các kết quả tính toán được so sánh với thực đo.