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Convection-diffusion modelling for chemical pollutant dispersion in the joint of artificial lake using finite element method

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Abstract. A convection-diffusion mathematical model is adopted to describe the chemical contamination dispersion problem in the joint of artificial lake. We consider the problem into 2-dimensional discussion limited to the surface of the joint. Under this assumption, the mathematical formulation of the pollution model comprises the mass conservation, which describes convection, turbulent diffusion and emission of the pollutant, illustrated by a convection-diffusion equation. We construct and analyse (discrete) boundary conditions for an implicit difference scheme. The finite element method is used to get the numerical solution of the convection-diffusion equation to insight into the variation of temperature and concentration fields. Especially, different with other similar research, a stochastic model of Lévy flights is employed to calculate the dispersion tensor coefficients, which heavily relies on the soil orography, stability class, distance of pollutant source and surface roughness. Consider the degradation of chemicals, we can also get form the concentration of time and space distribution by the instantaneous source of pollution. The experimental result of simulation shows that the progress of chemical pollutant dispersion in the joint of artificial lake is not only related to the velocity of water fluid, degradation rate, dispersion coefficient, and initial concentration, but also to the geometrical shape of the a horn mouth to the main body of the artificial lake. It also can be concluded that the Finite Element Method of Convection-Diffusion model is suitable, accurate and efficient for this kind of pollution problem.

***Key words*:** Environmental Impact, Chemical Pollutant Dispersion, Convection-Diffusion Problem, Finite Element Method

INTRODUCTION

Nowadays, the common fact that the release of waste materials from chemical and industrial facilities into water bodies could harm heavily the human health and the environment is broadly accepted in both academia and industry. According to literature [1,2] one typical environmental problem in current due to the dispersion of solutes in water bodies is the fate of the total residual chlorine in rivers. Unfortunately, in most developing countries, this kind of phenomenon is very common especially in inland rivers and lakes.

An artificial lake, sometimes called reservoir, is often a storage pond or impoundment from a dam which is used to store water. Artificial lakes may be created in river valleys by the construction of a dam or may be built by excavation in the ground or by conventional construction techniques such as brickwork or cast concrete. It is characterized by the neat geometric shapes that composed by a rectangular cavity connected to the river and a horn mouth to the main body reservoir as shown in Fig. 1. Due to the trait of large capacity and decreasing velocity of the fluid, the pollution is usually very serious in the joint of artificial lake [3]. In this research our aim is to investigate the dispersion of chemical contamination in the joint which is only related to the upstream pollution detection, but also affects the human and animal health downstream.

Fig. 1. The landscape of the joint of artificial lake.

Then, we should establish the strict mathematical model for the proposed problem. In general, modeling of contamination dispersion often plays an important role in environmental science, not only because of its capability to assess the importance of the relevant processes, but also to describe the deterministic relationship between emissions and concentrations/depositions. Typical modeling and techniques include non-reactive (e.g., dispersion modeling) and reactive (e.g., photochemical modeling); deterministic models (e.g., Gaussian, Lagrangian and Eulerian ones) and stochastic models [4,5].

Among these models, convection- diffusion problem [6-11], launched by the research in fluid science, also concentrate on the physical/chemical quantities carried by mass points in fluid flow, such

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as the concentration of the substance in the dissolved fluid flow in the process of change rule. These changes generally include convection, diffusion, and its attenuation of physical measurement of some physical and/or chemical causes or growth process. Convection diffusion phenomenon in the research of environmental protection is often met in fluid mechanics. In the research of fluid science, convection-diffusion equation is a consolidation of the diffusion and convection equations, and describes physical /chemical phenomena where particles, energy, or other physical/chemical quantities are transferred inside a physical/chemical system due to two processes: diffusion and convection. Under some contexts, it could be also called the advection-diffusion equation, drift-diffusion equation, Smoluchowski equation [12] or scalar transport equation [13].

In this article, we use the finite element method to get the numerical solution of the convection-diffusion equation to insight into the variation of temperature and concentration field. Specially, different with other similar research in [5,14], a stochastic model of Lévy flights is employed to calculate the dispersion tensor coefficients according to the concrete stochastic models, which are heavily rely on the soil orography, stability class, distance of pollutant source and surface roughness. Consider the degradation of chemicals, we can also get form the concentration of time and space distribution by the instantaneous source of pollution.

PROBLEM FORMULATION

Rationale and assumption

The rationale of the finite element method for convection-diffusion problem is shown below. First, denote the physical quantity fields (such as concentration field, velocity field temperature field, and so forth) as a finite collection of discrete points. According the initial and boundary conditions mesh the grid and generate the boundary conditions. Then establish and solve the algebraic equation on these discrete points to acquire the approximate solutions. Note that the convergence of the solution should be discussed. When the solution is not convergent, it is necessary to establish new discrete control equation to be resolved until the convergent one.

Before formalizing the problem, we should give some preliminary assumptions. Firstly, we consider the problem into 2-dimensional discussion limited to the surface of the lake. Therefore the pollutant's density has to be lower than the water's to make this assumption valid, for instance, the oil pollutant often taken as the example. Moreover, in this article, we present an Eulerian model of pollutant which on this scale never reacts significantly with other composites similar to the literature [15].

Dispersion of the pollutant

Here we adopt a non-reactive model for one pollutant in order to simplify the numerical method proposed, but it is not difficult to generalize to several reactive pollutants. At last, we assume the water flows are steady, so the first stage is used to compute the velocity field of the lake surface, while the second stage determines the flow of the pollutant measured by a local and time-dependent concentration: $C(x,y,t)$.

The mathematical formulation of the water bodies' pollution model is the equation of mass conservation, which describes convection, turbulent diffusion and emission of the pollutant, illustrated by the following convection- diffusion equation:

$$\frac{\partial C}{\partial t} + \vec{\nabla}.\left(-k\vec{\nabla}C + \vec{V}C\right) = f \quad in\,\Omega \times \left(0, t_f\right)$$

s.t.

$$\frac{\partial C}{\partial t} + \vec{\nabla}.\vec{q} = 0, \forall (x,y) \epsilon A, \vec{q} = -k\vec{\nabla}C + \vec{V}C$$

endowed with proper initial and boundary condition for the pollutant concentration $C(x,y,t)$, which stands for the concentration of pollutant [kg] per [m^3] water. The vector $\vec{q}$ stands for the flow [kg/m2-s]. The equation $\vec{q} = -k\vec{\nabla}C + \vec{V}C$ demonstrates the flow and the concentration of the pollutant obeying the relationship called behavior law, which is a mathematical relation between the gradients of a function and its dual function. In this work, boundary conditions are artificial specified since the river estuary never owns a nature boundary. The turbulent diffusivity tensor k could be employed into Guassian perturbation or Lévy flights which will be explained in the latter subsection. The contamination source f is standing for a term of generation/elimination [kg/m3-s]. The space domain of water bodies $S \in R^2$ lays over a given surface, and t_f denotes the final time. The vector $\vec{V}$ is the local field velocity of the flow.

Diffusivity tensor using Lévy flights

For the diffusivity tensor, we only consider the model on the transport and diffusion of pollutants emitted by industrial wastewater; hence we adopt the stochastic models (Gaussian perturbation, random walk and so forth). By diffusion, we understand an aggregation of dispersive processes which are of diffusion type in a mathematical sense, i.e. resulting from a random walk (Brownian motion, Einsteinian diffusion). For a good introduction into the research, see e.g. [16].

Under these premises, the concentration of the pollutants assumes the form of a stochastic distribution in two-dimensional space, and let it fit the coefficients of turbulent diffusivity tensor hereunder:

$$k = \begin{bmatrix} k_{xx} & 0 \\ 0 & k_{yy} \end{bmatrix}$$

where x and y are those associated with the horizontal plane.

The stochastic models could be used to obtain the empirical coefficients k_{xx} and k_{yy} on basis of orography, fluid stability and so forth. The value of them could be calculated as,

$$k_{xx} = k_{yy} = \frac{\sigma^2 det(\vec{V})}{2r}$$

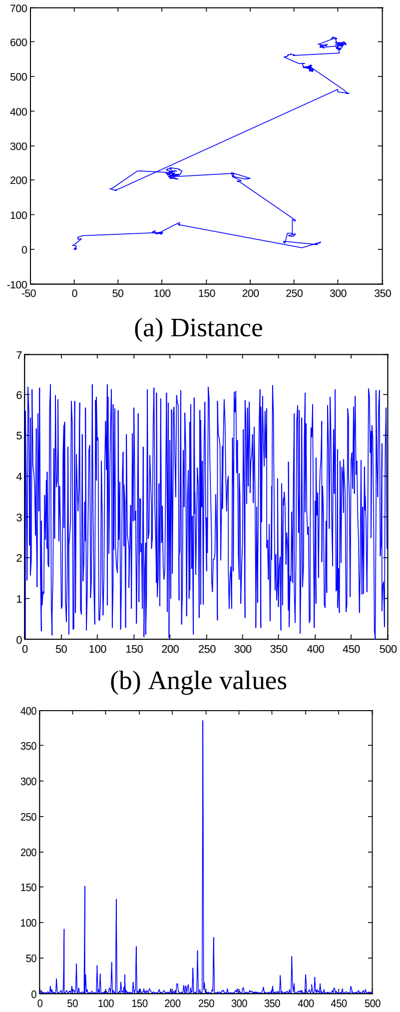
where r is the distance from the pollutant source and σ is the dispersion tensor coefficients according to the concrete stochastic models, which are heavily rely on the soil orography, stability class, distance of pollutant source and surface roughness (c.f. [17]).

In recent related researches, Gaussian models are used to be the stochastic model to generate the empirical coefficients in paper [5]. However, compared to Gaussian distribution, Lévy distribution is advantageous since the probability of returning to a previously visited site is smaller than for a Gaussian distribution, irrespective of the value of μ chosen. So in our research, another random walk method, Lévy flights, is employed to this work. Lévy flights, named after the French mathematician Paul Pierre Lévy, are Markov processes [18]. After a large number of steps, the distance from the origin of the random walk tends to a stable distribution. Lévy flights, which can be characterized by an inverse square distribution of step length, may optimize the random search process when targets are scarce and scarcity of resources. In contrast, Brownian motion is usually suited for the case when there is a need to locate abundant prey or targets.

Mathematically, Lévy flights are a kind of random walk whose step lengths meet a heavy-tailed Lévy alpha-stable distribution, often in terms of a power-law formula, $L(s)\sim|s|^{-1-\beta}$ where $0<\beta\leq 2$ is an index. A typical version of Lévy distribution can be defined as according to reference [19]

$$L(s,\gamma,\mu) = \begin{cases} \sqrt{\frac{\gamma}{2\pi}} exp\left[-\frac{\gamma}{2(s-\mu)}\right]\frac{1}{(s-\mu)^{3/2}}, 0<\mu<s<\infty; \\ 0, s\leq 0. \end{cases}$$

As the change of β, this can evolve into one of Lévy distribution, normal distribution and Cauchy distribution. Taking the 2D-Lévy flights for instance, the steps following a Lévy distribution as in Fig. 2(b), while the directions of its movements meet a uniform distribution as in Fig. 2(a). As shown in Fig. 2(c), an instance of the trajectory of 500 steps of random walks obeying a Lévy distribution. Note that the Lévy flights are often efficient in exploring unknown and large-scale search space than Brownian walks. One reason for this argument is that the variance of Lévy flights $\delta^2(t) \sim t^{3-\beta}$ increases faster than that of Brownian random walks, i.e., $\delta^2(t) \sim t$.



(a) Distance

(b) Angle values

(c) Step lengths

Fig. 2. 2D Lévy flights in 500 steps

Velocity field of the water body

The following assumptions are made in order to compute the water speed field: one is incompressible flow and the other is non-viscous flow. These could result into the consequence described by the following equations:

$$\vec{\nabla}\vec{V} = 0, \overrightarrow{rot\vec{z}} = 0$$

where the unit vector $\vec{z}$ is the direction vector normal to the lake. Now, we assume another function ψ, called stream-function, defined by :

$$u = \frac{\partial\psi}{\partial y}, v = -\frac{\partial\psi}{\partial x}$$

where *u* and *v* are the two horizontal components of the water speed field. Thus, if such a potential exists, then insertion into the rotational equation gives a single governing equation (Laplace equation) to be solved:

$$\Delta\psi = 0, \forall\ (x, y) \epsilon A$$

For a steady-state flow, the trajectories of the fluid-particles are within the streamlines.

It is possible to demonstrate that these streamlines are simply described by the equality:

$$\psi = \overline{\psi}$$

Coming from this last relationship, the boundary conditions are easily set when prescribing a different value to each boundary limited by two successive mouths similar to a 'wall' forbidding any crossover (the shore for instance). One of the boundary has to be prescribed as a zero value for ψ. The value of ψ will be defined according to the inflow/outflow of the relevant separating mouth in nearby boundaries. To each inflow and to each outflow corresponds a 'jump' of the value of ψ. A constant value for ψ defines a streamline

Variational form

The finite element method is based on the discretization of a variational form corresponding to each equation of the problem.

Based on the Eq. (1), the Galerkin variational problem [20] is corresponding to the mechanical principle of virtual work, i.e., for a static equilibrium of the system, the virtual work about the forces of all external forces along with the virtual displacement could be expressed as the following equation,

$$\begin{aligned} W = \iint_S \varphi(x, y) \left(\vec{\nabla}.\left(-k\vec{\nabla}C + \vec{V}C\right) + \frac{\partial C}{\partial t}\right) dxdy \\ = \sum \iint_{Se} k\vec{\nabla}\varphi(x,y).\left(\vec{\nabla}C\right) dxdy \\ - \oint_{\partial S} k\varphi(x,y).\left(\vec{\nabla}C\right)\ \vec{n}\ ds \\ + \sum \iint_{Se} \varphi(x,y)\left(\vec{\nabla}.\left(\vec{V}C\right)\right) dxdy \\ + \sum \iint_{Se} \varphi(x,y) \frac{\partial C}{\partial t} dxdy \end{aligned}$$

where $\varphi(x,y)$ stands for any trial function, S is the total lake surface and ∂S the limit of the lake. Once the division of the domain (called meshing) into elementary surfaces (called finite elements) is done, then the weak form is discretized and appears as a sum of elementary terms. Because the numerical solution of the above pollution model is critical to use accurate and stable numerical methods. In our work, we use a combination of Galerkin and upwind finite element method to simulate the chemical pollutant dispersion in river estuary.

Discrete forms of FEM

Let us discuss the Discrete forms of FEM. Firstly, *T* is a collection of continuous piecewise linear function under triangulation, which is a linear space on real number field. Every function *T(x,y)* in *T* could be expressed as:

$$T(x,y) = \sum_{i=1}^{Np} T_i N_i(x,y) = \langle N_1, N_2, N_3 \rangle \begin{Bmatrix} T_1 \\ T_2 \\ T_3 \end{Bmatrix}, (x,y) \in \bar{S}$$

where T_i is the value of *T(x,y)* on the spot of P_i. $N_i(x,y)$ are called the linear interpolation functions on element *e*. The linear interpolation function $N_i(x,y)$ get the value 1 on the spot of Pi, but around P_i get nonzero values.. Based on these interpolation function, any trail function $\varphi(x,y)$ could be expressed linearly as below:

$$\varphi(x,y) = \langle \varphi_1, \varphi_2, \varphi_3 \rangle \begin{Bmatrix} N_1 \\ N_2 \\ N_3 \end{Bmatrix}$$

Then the linear interpolation functions on element *e* have the solution as follows:

$$\begin{cases} N_1(x,y) = \dfrac{1}{2A^e}\left[y_{32}(x_2 - x) - x_{32}(y_2 - y)\right] \\ N_2(x,y) = \dfrac{1}{2A^e}\left[y_{13}(x_3 - x) - x_{13}(y_3 - y)\right] \\ N_3(x,y) = \dfrac{1}{2A^e}\left[y_{21}(x_1 - x) - x_{21}(y_1 - y)\right] \end{cases}$$

Thus, the gradient vector of T could be expressed as:

$$\vec{\nabla}T = \begin{Bmatrix} \dfrac{\partial T}{\partial x} \\ \dfrac{\partial T}{\partial y} \end{Bmatrix} = \begin{bmatrix} \dfrac{\partial N_1}{\partial x} & \dfrac{\partial N_2}{\partial x} & \dfrac{\partial N_3}{\partial x} \\ \dfrac{\partial N_1}{\partial y} & \dfrac{\partial N_2}{\partial y} & \dfrac{\partial N_3}{\partial y} \end{bmatrix} \begin{Bmatrix} T_1 \\ T_2 \\ T_3 \end{Bmatrix}^e = [B]\{T\}^e\ ;$$

$$\vec{V} = \begin{Bmatrix} \dfrac{\partial \psi}{\partial y} \\ -\dfrac{\partial \psi}{\partial x} \end{Bmatrix} = \begin{bmatrix} \dfrac{\partial N_1}{\partial y} & \dfrac{\partial N_2}{\partial y} & \dfrac{\partial N_3}{\partial y} \\ -\dfrac{\partial N_1}{\partial x} & -\dfrac{\partial N_2}{\partial x} & -\dfrac{\partial N_3}{\partial x} \end{bmatrix} \begin{Bmatrix} \psi 1 \\ \psi 2 \\ \psi 3 \end{Bmatrix}^e = \langle \psi \rangle^e \begin{bmatrix} B(2,:) \\ -B(1,:) \end{bmatrix}^T$$

$$\vec{\nabla}\varphi = \langle \varphi_1, \varphi_2, \varphi_3 \rangle^e \begin{bmatrix} \dfrac{\partial N_1}{\partial x} & \dfrac{\partial N_1}{\partial y} \\ \dfrac{\partial N_2}{\partial x} & \dfrac{\partial N_2}{\partial y} \\ \dfrac{\partial N_3}{\partial x} & \dfrac{\partial N_3}{\partial y} \end{bmatrix} = \langle \varphi \rangle^e [B]^T$$

Besides, we can write the gradient matrix $[B]$ as follows:

$$[B] = \begin{bmatrix} \dfrac{\partial N_1}{\partial x} & \dfrac{\partial N_2}{\partial x} & \dfrac{\partial N_3}{\partial x} \\ \dfrac{\partial N_1}{\partial y} & \dfrac{\partial N_2}{\partial y} & \dfrac{\partial N_3}{\partial y} \end{bmatrix} = \frac{1}{2A^e} \begin{bmatrix} y_{23} & y_{31} & y_{12} \\ x_{32} & x_{13} & x_{21} \end{bmatrix}$$

Hence, the elementary weak form, which is necessary to calculate the speed field, can be discretized as follows:

$$W_\psi = \sum_{e=1}^{nelt} W_\psi^e = \sum \iint_{Se} k\vec{\nabla}\varphi(x,y).\left(\vec{\nabla}C\right))dxdy$$
$$= \sum \iint_{Se} \langle\varphi\rangle^e [B]^T k [B]\{C\}^e\, dxdy$$
$$= \sum \langle\varphi\rangle^e \iint_{Se} [B]^T k [B]\, dxdy\, \{C\}^e$$
$$= \sum \langle\varphi\rangle^e [K]_\psi^e\, \{C\}^e$$

with the elementary stiffness matrix being defined by the relation :

$$[K]_\psi^e = A^e k [B]^T [B]$$

where A^e is the surface of the relevant element.

The weak form corresponding to the equation of diffusion-transport can be discretized as

$$W_C = W_{C1} + W_{C2}$$

Where:

$$W_{C1} = \sum_{e=1}^{nelt} W_{C1}^e$$
$$= \sum \iint_{Se} \varphi(\mathrm{x},\mathrm{y})\left(\vec{\nabla}.\left(\vec{V}\, C\right)\right))\mathrm{dxdy}$$
$$= \sum \iint_{Se} \varphi(\mathrm{x},\mathrm{y})\vec{V}.\left(\vec{\nabla}\, C\right)\mathrm{dxdy}$$
$$= \sum \iint_{Se} \langle\varphi\rangle^e \begin{Bmatrix} N1 \\ N2 \\ N3 \end{Bmatrix} \langle\psi\rangle^e \begin{bmatrix} B(2,:) \\ -B(1,:) \end{bmatrix}^T [B]\{C\}^e \mathrm{dxdy}$$
$$= \sum \langle\varphi\rangle^e \iint_{Se} \begin{Bmatrix} N1 \\ N2 \\ N3 \end{Bmatrix} \mathrm{dxdy}\, \langle\psi\rangle^e \begin{bmatrix} B(2,:) \\ -B(1,:) \end{bmatrix}^T [B]\{C\}^e$$
$$= \sum \langle\varphi\rangle^e \frac{A^e}{3} \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix} \langle\psi\rangle^e [B]^T \begin{bmatrix} B(2,:) \\ -B(1,:) \end{bmatrix} \{C\}^e$$
$$= \langle\varphi\rangle^e [K]_C^e \{C\}^e$$

Then the definition of the transport matrix $[K]_C^e$ could be written as following:

$$[K]_C^e = \frac{A^e}{3} \begin{Bmatrix} 1 \\ 1 \\ 1 \end{Bmatrix} \langle\psi\rangle^e [B]^T \begin{bmatrix} B(2,:) \\ -B(1,:) \end{bmatrix}$$

The components of the vector $\langle\psi\rangle^e$ are the nodal values of the triangular element, which outputs are resulting from the first step of the solving procedure (water velocity field).

$$W_{C2} = \sum_{e=1}^{nelt} W_M^e = \sum \iint_{Se} \varphi(\mathrm{x},\mathrm{y}) \frac{\partial \mathrm{C}}{\partial t} \mathrm{dxdy}$$
$$= \sum \langle\varphi\rangle^e \iint_{Se} \begin{Bmatrix} N1 \\ N2 \\ N3 \end{Bmatrix} \langle N1, N2, N3\rangle \mathrm{dxdy} \{\dot{C}\}^e$$
$$= \sum \langle\varphi\rangle^e [M]^e \{\dot{C}\}^e = \sum \langle\varphi\rangle^e \frac{A^e}{12} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix} \{\dot{C}\}^e$$

where the mass matrix is relevant to the temporal term and defined by :

$$[M]^e = \frac{A^e}{12} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$$

What's more, the components of the vector $\{\dot{C}\}^e$ are the temporal derivatives of the concentration value at the nodes.

At the end of the assembly step, which consists in summing up the whole set of elementary contributions for the global system, we can write the two equations systems hereunder:

(1) Solving the water speed field:

$$W_\psi = 0$$

(2) Transport of the pollutant with the help of the water field speed:

$$W_C = 0$$

Considering stablility of function, we use an explicit schema to the diffusion of the pollutant in the lake corresponds one equations system. There are no boundary conditions of the Dirichlet's type for this equations system. The necessary and boundary condition for the pollutant is over the whole contour of the lake: there must be a reflexion of the pollutant over the whole contour. This is a Neumann's type of boundary condition.

The system to be solved is therefore the following:

$$[M]\{\dot{C}\} + \left[K_\psi + K_C\right]\{C\} = \{F_C\}$$

where vector $\{F\}$ results of the introduction of the initial condition.

$$[M]\frac{\{C\}^{n+1} - \{C\}^n}{\Delta t} + \left[K_\psi + K_C\right]\{C\}^n = \{F_C\}^n$$
$$\{C\}^{n+1} = \left([I] - \Delta t[M]^{-1}\left[K_\psi + K_C\right]\right)\{C\}^n + \Delta t[M]^{-1}\{F_C\}^n$$
$$[G] = [I] - \Delta t[M]^{-1}\left[K_\psi + K_C\right]$$

We put l_i the eigenvalues of the matrix $[M]^{-1}\left[K_\psi + K_C\right]$, with $l_i \geq 0$. Therefore: $\lambda_i = 1 - l_i$ is the stable scheme if

$$0 \le \lambda_i \le 1,\ \Delta t \le \frac{1}{l_i^{max}}$$

To the diffusion of the pollutant in the joint corresponds one equations system. There is no boundary condition of the Dirichlet's type for this equation system. The necessary and boundary condition for the pollutant is over the whole contour of the joint surface: there must be a reflexion of the pollutant over the whole contour. This is a Neumann's type of boundary condition.

$$\mathrm{e}\vec{q}\cdot\vec{n} = -75\ \mathrm{W/m} \quad \text{(Neumann)}$$

$$-\oint_{\partial s} \mathrm{ke}\ \varphi(\mathrm{x},\mathrm{y}).\left(\vec{\nabla}\mathrm{T}\right)\ \vec{n}\ ds = \sum \int_{l^e} \varphi(-75)\,\mathrm{ds}$$
$$= \sum \langle \varphi 1, \varphi 2\rangle^e \frac{l^e(-75)}{2}\begin{Bmatrix}1\\1\end{Bmatrix}$$

However, in the other cases, the Cauchy's type of boundary condition is considered.

$$\mathrm{e}\vec{q}\cdot\vec{n} = \mathrm{he}(\mathrm{T}-\mathrm{Tair})$$

So the last component of Eq. (3) could be written as :

$$-\oint_{\partial s} \mathrm{ke}\ \varphi(\mathrm{x},\mathrm{y}).\left(\vec{\nabla}\mathrm{T}\right)\ \vec{n}\ ds$$
$$= \sum \int_{l^e} \varphi\mathrm{he}\,(\mathrm{T}-\mathrm{Tair})\mathrm{ds}$$
$$= \sum \int_{l^e} \langle \varphi \rangle^e \begin{Bmatrix}N1\\N2\end{Bmatrix} \mathrm{he}\,\langle N1 \quad N2\rangle \{T\}^e \mathrm{ds}$$
$$- \sum \int_{l^e} \langle \varphi \rangle^e \begin{Bmatrix}N1\\N2\end{Bmatrix} \mathrm{heTair}\,\mathrm{ds}$$
$$= \sum \langle \varphi 1, \varphi 2\rangle^e \frac{hel^e}{6}\begin{bmatrix}2 & 1\\1 & 2\end{bmatrix}\begin{Bmatrix}T1\\T2\end{Bmatrix}^e$$
$$- \sum \langle \varphi 1, \varphi 2\rangle^e \frac{hel^e\mathrm{Tair}}{2}\begin{Bmatrix}1\\1\end{Bmatrix}$$
$$= \sum \langle \varphi 1, \varphi 2\rangle^e \left(\frac{hel^e}{6}\begin{bmatrix}2 & 1\\1 & 2\end{bmatrix}\begin{Bmatrix}T1\\T2\end{Bmatrix}^e - \frac{hel^e\mathrm{Tair}}{2}\begin{Bmatrix}1\\1\end{Bmatrix}\right)$$

SOLVING STAGES

To calculate the solving procedure, the transport modeling of the chemical pollutant by the speed field has to satisfy the following stages:

Step 0. Preprocessing of the parameters.

Step 1. Soling the speed field equation:

$$[K_\psi]\{\psi\} = \{F_\psi\}$$

Step 2. Regulating the initial condition on C:

$$C(x_0, y_0, t=0) = C_0$$

Step 3. Choosing the time step Δt.

Step 4. Iterating on the discrete time.

Step 4.1 Resolution of the concentration increment between time 'n' and time 'n+1' :

$$\{[M] + \Delta t[K_\psi + K_C]\}\{\Delta C_n^{n+1}\} = \Delta t(\{F_C\} - [K_\psi + K_C]\{C^n\})$$

Step 4.2 Update the solution:

$$\{C^{n+1}\} = \{C^n\} + \{\Delta C_n^{n+1}\}$$

Step 5. Postprocessing of the results.

EXPERIMENTAL RESULTS AND ANALYSIS

Time and space distribution of pollutant concentration formed by transient source

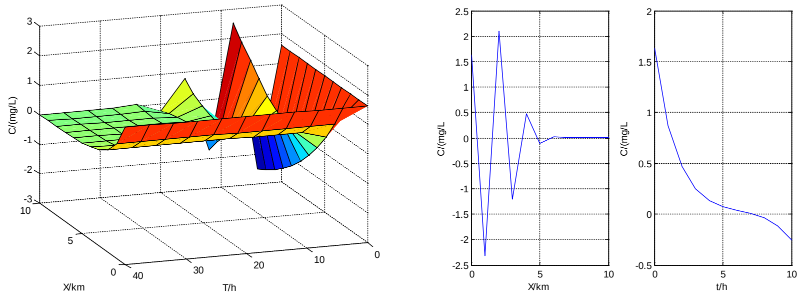
In this simulation, we investigate the time and space distribution of pollutant concentration formed by transient source. As shown in Table 1, the experiment is divided into two groups. Group I presents the case with a low flow velocity of 0.05km/h, while Group II with a high flow velocity of 0.5km/h. Each group consists of two tries with different pollutants degradation rate constant, i.e., 0.16 and 0.84. The initial concentration C0 is fixed to 1.63mg/L.

Table 1. Time and space distribution of concentration by transient source.

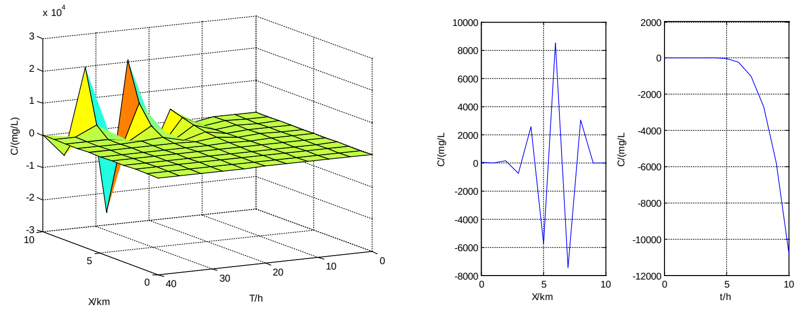
Group	Type	u [km/h]	p	C_0 [mg/L]
Group I	(a)	0.05	0.16	1.63
	(b)	0.05	0.84	1.63
Group II	(a)	0.5	0.16	1.63
	(b)	0.5	0.84	1.63

Fig. 3 (a)-(d) illustrates the time and space distribution of pollutant concentration formed by transient source. The vertical coordinates denote the pollutant concentration. From Fig. 3 (a) and (b), we can clearly see that concentration shocks up and down about 0, and declines rapidly with the time elapses, regardless of degradation rate constant. However, in the Fig. 3 (c) and (d), the concentration varies with the change of distance obviously. Moreover, the fluid may carry the pollutant downstream fast so that the concentration is large when far from the transient source.

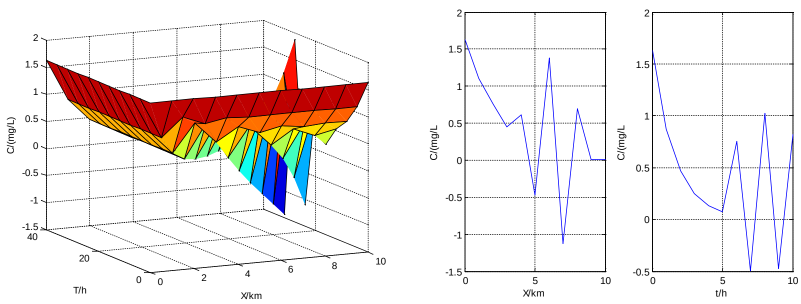
Concentration of suspended particles increases near the bed with increase of settling velocity, as it proceeds towards downstream. It is interesting to note that with increase of settling velocity the elongation in the concentration profiles is mostly prominent near the bed surface. This is because the heavier particles travel most of the time very close to the bottom, where the velocity gradient is greater than any other region; this means, that the greater the velocity gradient, the larger the longitudinal dispersion [27].



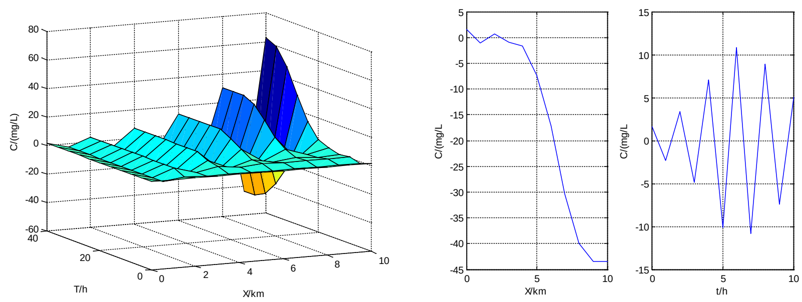
(a) Group I (a)



(b) Group I (b)

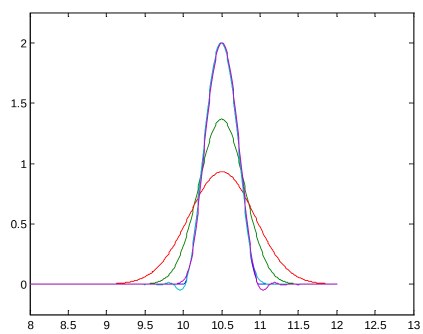


(c) Group II (a)

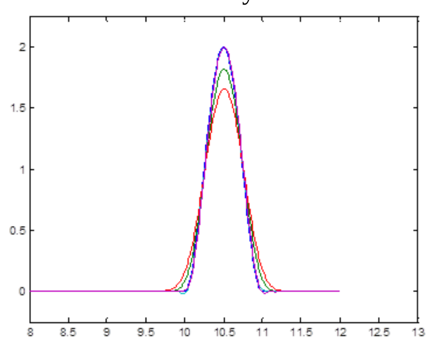


(d) Group II (b)

Fig. 3. Time and space distribution of pollutant concentration formed by transient source.



(a)



(b)

Fig. 4. Dimensionless, steady, concentration profiles at various downstream distances from the source.

Temperature transport and heat flow of chemical pollutants

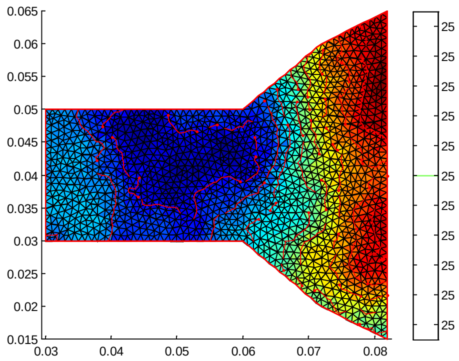
In this subsection, we are investigating the joint geometry's the influence for the temperature transport of chemical pollutants. This facet of research is meaningful as the downstream creature such as fishes and other stream biota are very sensitive to the variation of temperature. On the other hands, the chemical pollutants in industrial wastewater, such as, metallurgical or chemical fibre wastewater, always take higher temperature than the water bodies.

In reality, according to the different geometrical morphology, the joint of artificial lake can be classified as into two types, i.e., Parabolic Joint and Hyperbolical Joint, which own different kind of horn mouth to the main body reservoir.

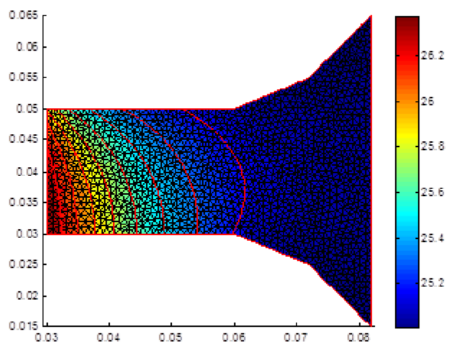
The parameter setting of simulation is shown in Table 2, where N_{nt} is the number of nodes, N_{elt} the number of elements, and N_{barres} the number of barriers elements. It also presents the numerical solutions of pollutants temperature in PJ and HJ.

Table 2. Numerical solutions of diffusion of pollutants temperature

Joint Type	N_{nt}	N_{elt}	N_{barres}	Minimum field solution	Maximum field solution
Parabolic Joint (PJ)	1496	2990	181	25	25
Hyperbolical Joint (HJ)	1408	2823	202	25.00859600	26.37535877



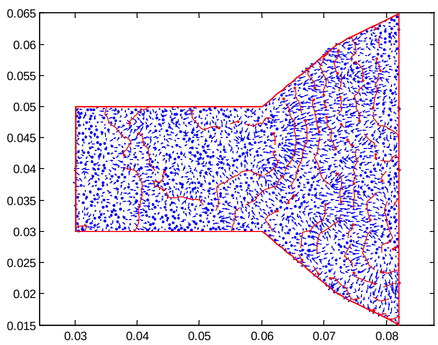
(a)



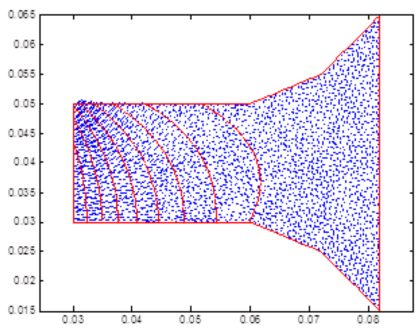
(b)

Fig. 5. Temperature transport of chemical pollutants in PJ and HJ

Fig. 5 describes the temperature transport of chemical pollutants in PJ and HJ. In Fig. 5(a), the temperature field is non-gradient because the chemical pollutants present a different diffusion and the diversity of directions. It also can be seen that the temperature in the horn mouth of PJ is higher than the rectangular cavity. Therefore, in this kind of joint, the temperature transport and heat flow of chemical pollutants may seriously affect the survival of the downstream creature. Whereas in the case depicted by Fig. 5(b), the temperature field of pollutants decrease rapidly because of the uniform thermal plume. Hence, the water body of this kind of horn mouth is not easy to be affected by the variation of temperature. The Fig. 6 illustrates the heat flow of chemical pollutants with isothermal in PJ and HJ.



(a)



(b)

Fig. 6. Heat flow of chemical pollutants with isothermal in PJ and HJ.

Consider for the coefficients of turbulent diffusivity under the cases of PJ and HJ, the landscape of the global stiffness matrices are shown in Fig. 7(a) and (b) respectively. Note that the matrices are block-tridiagonal, clearly showing the random distribution on the N_{nts}. It can be seen that the block before Nbarres (with green diagonal line) is sparser than the block after N_{barre}s (with red diagonal line) in both Fig. 7(a) and (b). Moreover, in Fig. 7 (a), there exist some discontinuous blocks but continuous in Fig. 7(b). According to our treatment to the coefficients of turbulent diffusivity, the matrices should follow a distribution by Lévy flights.

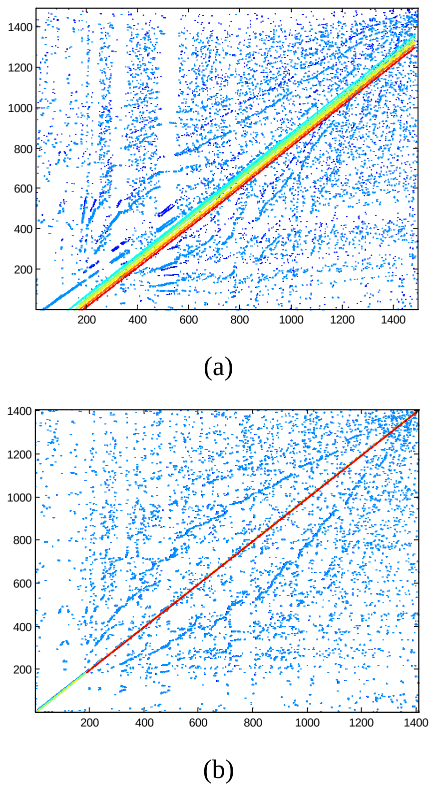


Fig. 7 .Heat flow of chemical pollutants with isothermal in PJ and HJ.

This can be verified in both Fig. 8 (a) and (b), where the temporal residue vectors are illustrated. In this figures, the coefficients of turbulent diffusivity is transformed as the 1-dimesion steps.

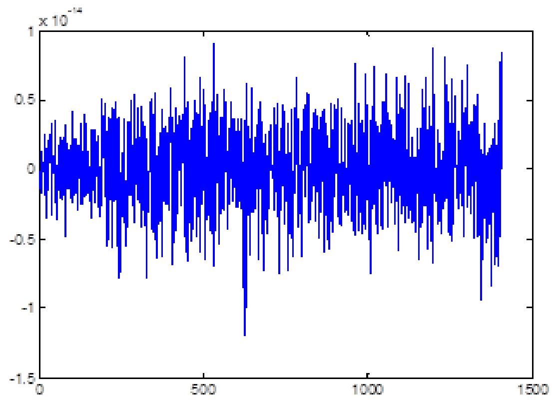


Fig. 8. Coefficients of turbulent diffusivity following a distribution by Lévy flights.

CONCLUSIONS

In this paper, we investigate the chemical contamination dispersion problem in the joint of artificial lake; a convection-diffusion mathema- tical model is adopted to describe it. We consider the problem into 2-dimensional discussion limited to the surface of the joint. Firstly, for the diffusivity tensor, we only consider the model on the transport and diffusion of pollutants emitted by industrial wastewater; hence we adopt a new kind of stochastic models, Lévy flights, to model it. The latter simulation proved this the correctness of the random distribution. Then we also investigate the time and space distribution of pollutant concentration formed by transient source and found that the fluid may carry the pollutant downstream fast so that the concentration is large when far from the transient source. Concentration of suspended particles increases near the bed with increase of settling velocity, as it proceeds towards downstream. It is interesting to note that with increase of settling velocity the elongation in the concentration profiles is mostly prominent near the bed surface. At last, we investigate the joint geometry's the influence for the temperature transport of chemical pollutants. In the kind of PJ, the temperature transport and heat flow of chemical pollutants may seriously affect the survival of the downstream creature. Whereas, the water body of the kind of horn mouth of HJ is not easy to be affected by the variation of temperature.

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МОДЕЛИРАНЕ ПО МЕТОДА НА КРАЙНИТЕ РАЗЛИКИ НА КОНВЕКТИВНАТА ДИФУЗИЯ ПРИ РАЗСЕЙВАНЕТО НА ХИМИЧЕСКИ ЗАМЪРСИТЕЛИ В ИЗКУСТВЕН ВОДОЕМ

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(Резюме)

Разработен е математичен модел за описанието на дисперсията на химични замърсители в устието на изкуствен водоем, основан на конвективната дифузия. Разгледана е двумерната задача в област, ограничена до повърхността на канала. При тези предпоставки моделът се основава на уравнението за съхранение на масата с отчитане на конвективната и турбулентната диффузия. Съставени са и са анализирани гранични условия с помощта на неявана диференчна схема. Методът на крайните елементи е използван за да се получи числено решение на уравнението на конвективната дифузия и да се получат полетата на разпределение на концентрациите и на температурата. Успоредно с това е използван стохастичният метод на Lévy за определянето на коефициентите в дисперсионния тензор, който силно зависи от орографията на почвата, класа на стабилност, разстоянието от източника на замърсяване и повърхностната грапавина. Отчитайки разлагането на химическите вещества може да се открие времевото и пространственото разпределение на моментен източник на замърсяване. Симулационните експерименти показват, че разпространението на замърсяването в устието на водоема зависи не само от скоростта на флуида, скоростта на разлагане, дисперсионния коефициент и началната концентрация, но и геометричната форма на устието.

Може да се заключи, че методът на крайните елементи е подходящ в случая на конвективна дифузия; той е точен и ефикасен в този клас проблеми на замърсяването.