The influence of mixed derivatives on the mathematical simulation of pollutants transfer
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Abstract

Both turbulent diffusion and dissolved matter dispersion are anisotropic processes. From the formal point of view this fact is expressed by the tensor form of the transfer coefficients. As a result, mixed derivatives of concentration appear in the transport equations. However many authors, for the sake of simplicity, neglect these derivatives. The paper deals with investigation of the influence of cross-derivatives, exerted on the results of calculations. Theoretical and numerical analyses lead to the conclusion, that investigated terms are of great importance and should not be neglected.

1 Governing equations

Two main versions of the dissolved matter conservation law are commonly used for description of the mass transfer processes. The first one describes the time-averaged turbulent transfer, and can be written as follows (see e.g. TASK Committee [1]):

\[ \frac{\partial \bar{c}}{\partial t} + (\bar{u} \nabla)\bar{c} = D \Delta \bar{c} - \text{div} \ m_T + \sum S_{fi} \]  

where: \( \bar{c} \), \( \bar{u} \) - time-averaged concentration and velocity, \( D \) - molecular diffusivity, \( S_{fi} \) - source functions (i = 1,...,Is), \( m_T \) - turbulent unit mass flux, defined as the time-averaged product of concentration \( c' \) and velocity fluctuations \( u' \):

\[ m_T = u' c' \]  

The second relation is the depth-averaged version of the Eq.1 (see e.g. Rutherford [2]):

\[
\frac{\partial s}{\partial t} + v_x \frac{\partial s}{\partial x} + v_y \frac{\partial s}{\partial y} = -\frac{1}{H} \frac{\partial (Hm_M)}{\partial x} - \frac{1}{H} \frac{\partial (Hm_D)}{\partial y} + \sum S_{fi} \tag{3}
\]

where: \( s, v \) - depth-averaged concentration and velocity, \( H \) - depth of the water layer, \( m_M \) - total relative unit mass flux, containing fluxes due to the molecular diffusion (\( m_M \)), turbulent diffusion (\( m_T \)) and dispersion (\( m_D \)):

\[
m_E = m_M + m_T + m_D = -D \nabla \bar{c} + \bar{u}'c' + \bar{u}c' \tag{4}
\]

(doubled bar denotes depth-averaging).

The relative mass fluxes are usually described by the generalised Fick’s law, which can be written in two forms - containing scalar coefficients for isotropic processes, or containing tensor coefficients for anisotropic phenomena (Wang [3], Sawicki [4]). Both processes discussed in this paper are anisotropic (e.g. Tennekes and Lumley [5], Fischer et al. [6]), especially the second one (i.e. dispersion). Analysing the experimental data, accessible in the problem bibliography, one can state, that the turbulent diffusion (Eq.1) has three characteristic directions (i.e. principal axes) - parallel to the flow boundary and to the velocity vector (\( L \)), parallel to the boundary and transversal to the velocity vector (\( T \)) and normal to the boundary (\( N \)). According to this we can write:

\[
m_T = -[D_T] \nabla \bar{c} \tag{5}
\]

The process of plane dispersion (Eq. 3) in turn proves two characteristic directions - parallel (\( L \)) and transversal (\( T \)) to the depth-averaged velocity vector, so we can write:

\[
m_E = -[K] \nabla s \tag{6}
\]

Determination of the tensors \([D_T]\) and \([K]\) components is a difficult problem, so in practice it is very often assumed that the process of transport is isotropic. As a result scalar transport coefficients can be introduced:

\[
m_T = -D_T \left( \frac{\partial \bar{c}}{\partial x} i + \frac{\partial \bar{c}}{\partial y} j + \frac{\partial \bar{c}}{\partial z} k \right) \tag{7}
\]

\[
m_E = -K \left( \frac{\partial s}{\partial x} i + \frac{\partial s}{\partial y} j \right) \tag{8}
\]

However this assumption is discordant with a physical sense of turbulent and dispersive mixing. Some authors try to correct this incompatibility, introducing something, what can be called „a para-isotropy”, writing for turbulent diffusion (e.g. Lin and Falconer [7]):

\[
-\text{div} \, \mathbf{m}_T = \frac{\partial}{\partial x} \left( D_{tx} \frac{\partial \bar{c}}{\partial x} \right) + \frac{\partial}{\partial y} \left( D_{ty} \frac{\partial \bar{c}}{\partial y} \right) + \frac{\partial}{\partial z} \left( D_{tz} \frac{\partial \bar{c}}{\partial z} \right) \tag{9}
\]

and for dispersion (e.g. Rutherford [2]):

\[
-\text{div} \, (H \mathbf{m}_E) = \frac{\partial}{\partial x} \left( HK_{\alpha} \frac{\partial s}{\partial x} \right) + \frac{\partial}{\partial y} \left( HK_{\beta} \frac{\partial s}{\partial y} \right) \tag{10}
\]

Two latest equations are simplified versions of general relations (5) and (6), in which cross-derivatives of concentration were neglected. It can be seen in comparison of Eq. 9 and Eq. 10 with the following forms of Eq. 5 and Eq. 6:
The expressions (11, 12) receive the forms (9,10) only in one case - when the coordinate system axes coincide with principal axes of the turbulent diffusion tensor (for Eq. 11) or dispersion tensor (for Eq. 12). With such a situation we can have to do in 1D-flows.

Many authors are aware of the fact, that making use of Eq 9 (or Eq. 10), instead of Eq. 11 (or Eq. 12), they introduce an error. However the order of magnitude of this error has not been evaluated so far, and simplified models are applied in practice without any deeper discussion (e.g. Chatwin and Allen [8], Fischer et al [6]). The purpose of this paper is a determination of the influence, exerted by the cross-derivatives on the advection-dispersion equation.

2 Theoretical analysis of the problem

In the course of this paper, the process of dispersion will be considered. As it was mentioned above, in this process we can distinguish two principal axes, determined by the local coordinates L0T (L || v, T ⊥ v). In order to eliminate the influence of the advective effects, we will analyse the case of constant velocity and depth. In a local coordinates we can rewrite Eq 3 as follows (source functions were neglected, as they do not influence the process):

\[
\frac{\partial s}{\partial t} + v_L \frac{\partial s}{\partial L} = \frac{\partial}{\partial L} (K_L \frac{\partial s}{\partial L}) + \frac{\partial}{\partial T} (K_T \frac{\partial s}{\partial T})
\]

(13)

A mathematical analysis of this equation leads to the conclusion, that in a simple case, when the polluted area in the initial moment of time has a circular shape, the transformation of this area consists in elongation of its initial shape along the OL-axis (when \(K_L > K_T\) - Fig. 1a), or along the OT-axis (when \(K_L < K_T\) - Fig. 1b).

Application of local coordinates is not very convenient, so we have to define one system for whole the problem (e.g. a Cartesian one, x0y), and to solve Eqs. 3, 6 instead of Eq. 13. In such a situation we have (Sawicki [4]):
Water Pollution

Figure 1: Transformation of a polluted area - accurate model (a: $K_L > K_T$, b: $K_L < K_T$)

\[ K_{xx} = K_L n_x^2 + K_T n_y^2 \]
\[ K_{xy} = (K_L - K_T) n_x n_y \]
\[ K_{yy} = K_L n_y^2 + K_T n_x^2 \] (14)

where:
\[ n_x = \frac{v_x}{|v|}, n_y = \frac{v_y}{|v|} \] (15)

Coefficients $K_L$ and $K_T$ in Eqs. 15 can be determined for example from classical formulas of Elder ($v^\star$ - shear velocity):
\[ K_L = 5.93 Hv^\star, \quad K_T = 0.23 Hv^\star \] (16)

However if we apply a simplified relation (10) instead of Eq. 12, the role of 0L - and 0T-axes (Fig. 1) will be played by axes 0x and 0y respectively. As a result we can suspect, that the transformation of a polluted area will consist in elongation in 0x (when $K_{xx} > K_{yy}$) or 0y (when $K_{xx} < K_{yy}$) direction (Fig. 2). Such a situation would be discordant with the physical meaning of the dispersion proc-

Figure 2: Transformation of a polluted area - simplified model (a: $K_{xx} > K_{yy}$, b: $K_{xx} < K_{yy}$)
3 Numerical analysis of the problem

In order to investigate the dispersion process and its dependence on the model accuracy, the full (Eqs. 3,12) and the simplified (Eqs. 3,10) models were solved numerically. The isotropic model (Eqs. 3,8) was solved in the first turn, for evaluation of the numerical method influence. Assuming $\nu=\text{const.}$ and $K=\text{const}$, the isotropic equation can be written as follows:

$$\frac{\partial s}{\partial t} + v_x \frac{\partial s}{\partial x} + v_y \frac{\partial s}{\partial y} = K_{xx} \frac{\partial^2 s}{\partial x^2} + K_{yy} \frac{\partial^2 s}{\partial y^2}$$  \hspace{1cm} (17)

and for initial conditions:

$$s(x,y,t=0) = \begin{cases} S_0 & \text{for } -\frac{a}{2} \leq x \leq -\frac{a}{2}, -\frac{b}{2} \leq y \leq -\frac{b}{2} \\ 0 & \text{for residual field} \end{cases}$$  \hspace{1cm} (18)

The Eq. 17 have the following analytical solution:

$$s(x,y,t) = \frac{S_0}{4} \left[ \text{erf} \left( \frac{a-x+v_xt}{\sqrt{4K_{xx}t}} \right) + \text{erf} \left( \frac{a+x-v_xt}{\sqrt{4K_{xx}t}} \right) \right]$$

$$\left[ \text{erf} \left( \frac{b-y+v_yt}{\sqrt{4K_{yy}t}} \right) + \text{erf} \left( \frac{b+y-v_yt}{\sqrt{4K_{yy}t}} \right) \right]$$  \hspace{1cm} (19)

where: $S_0$ - depth-averaged concentration of pollutants for $t=0$, erf - error function, $a,b$ - dimensions of concentration wave along x and y axes for $t=0$.

Numerical solution is based on the decomposition method. The transport equation was decomposed on two independent processes (Szymkiewicz [9]): advection and dispersion. Dispersion equation was solved by finite difference method and the solution was transferred along the flow direction. The results of numerical solution of isotropic equation are shown in Fig. 3.

Figure 3: Solution of advection-dispersion equation for isotropic case ($K_{xx}=K_{yy}$)
The concentration profile along \( \mathbf{L} \) direction (in local coordinates) for initial time \( t=0 \), after time \( t=50 \) sec and \( t=100 \) sec is shown in Fig. 4. There is a comparison of analytical and numerical solution. The analytical solution is represented by solid line and numerical - by dotted line. First concentration wave is initial condition (for \( t=0 \)) and it is a solution of Eq. 19 for \( t=0.8 \) sec, \( a=2m \), \( b=2m \), \( S_0=20 \text{ mg/l} \), \( v_x=v_y=0 \). This wave is an initial condition of numerical solution for all cases. As we can see in Fig. 4, this numerical method gives good results.

The next step was numerical solution of full advection-dispersion equation (Eq. 12), and then - simplified equation when 'para - isotropy' is assumed (Eq. 10). For the initial condition assumed as before, and for \( v_x=v_y=\text{const}=0.2 \text{ m/s} \), \( H=\text{const}=1 \text{ m} \), \( v^* =0.017 \text{ m/s} \) (\( K_L=0.1 \text{ m}^2/\text{s} \) and \( K_T=0.004 \text{ m}^2/\text{s} \)), the following cases were considered:

1). solution of full advection-dispersion equation, which, if we consider Eq. 12, has the following shape:

\[
\frac{\partial s}{\partial t} + v_x \frac{\partial s}{\partial x} + v_y \frac{\partial s}{\partial y} = \frac{\partial}{\partial x} \left[ K_{xx} \frac{\partial s}{\partial x} + K_{xy} \frac{\partial s}{\partial y} \right] + \frac{\partial}{\partial y} \left[ K_{yx} \frac{\partial s}{\partial x} + K_{yy} \frac{\partial s}{\partial y} \right]
\]  

(20)

where coordinates of \([ \mathbf{K} ]\) are described by Eq. 14. Because tensor \([ \mathbf{K} ]\) is constant, the equation has the form:

\[
\frac{\partial s}{\partial t} + v_x \frac{\partial s}{\partial x} + v_y \frac{\partial s}{\partial y} = K_{xx} \frac{\partial^2 s}{\partial x^2} + 2K_{xy} \frac{\partial^2 s}{\partial x \partial y} + K_{yy} \frac{\partial^2 s}{\partial y^2}
\]  

(21)

The result of numerical solution of Eq. 21 is shown in Fig. 5 and 6. The first case, presented in Fig. 5, was obtained under the assumption \( K_L>K_T \), and second case (Fig. 6) for \( K_L<K_T \).
solution of simplified advection-diffusion equation, which, if we consider Eq. 10, has the following form:

\[ \frac{\partial s}{\partial t} + v_x \frac{\partial s}{\partial x} + v_y \frac{\partial s}{\partial y} = K_{xx} \frac{\partial^2 s}{\partial x^2} + K_{yy} \frac{\partial^2 s}{\partial y^2} \]  

(22)

The result of numerical solution of Eq. 22 is shown in Fig. 7 and 8. The first case, presented in Fig. 7, is for $K_{xx} > K_{yy}$, and second case (Fig. 8) for $K_{xx} < K_{yy}$. Theoretical and numerical analyses lead to the conclusion, that mixed derivatives of concentration in the transport equations are of great importance and should not be neglected.
Fig. 7: Solution of simplified advection-dispersion equation for $K_{xx} > K_{yy}$.

Fig. 8: Solution of simplified advection-dispersion equation for $K_{xx} < K_{yy}$.

References:


4. Sawicki J. M., Plane Dispersion of Pollutants, Hydrological, Chemical and Biological Processes of Transformation and Transport of Contaminants in


