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A 2D NUMERICAL MODEL FOR THE TRANSPORT OF POLLUTANTS. THE INFLUENCE OF BOUNDARY CONDITIONS.

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ABSTRACT: The pollutants transport phenomena in a 2D unsteady free surface flow has been studied. The weighted residual method has been used for the integration of the transport equations, applying the Galerkin formulation for the spatial integration and a differentiation scheme for the time integration. The variation of the dispersion coefficient with the direction has been taken into account by the use of a dispersion tensor. The code allows to impose Dirichlet, Neumann, Mixed and Open boundary condition types. Several solutions have been carried out for a numerical test with known analytical solution so as to validate the numerical model and to check the behaviour of open boundary condition type.

KEYWORDS: 2D Free Surface Flow, Pollutants Dispersion, Finite Elements Method, Boundary Conditions.

1. GOVERNING EQUATIONS

The problem we are dealing with is the transport of pollutants in a two-dimensional free surface flow. The general transient equation that models the transport of a contaminant can be written as:

$$h\frac{\partial C}{\partial t} + h\mathbf{u}\cdot\nabla C = \nabla\cdot\left(h\mathbf{D}\cdot\nabla C\right) - kCh + S$$

where h is the depth, C is the solute concentration, **u** is the velocity vector, **D** is the dispersion tensor, k is the decay ratio and S is the mass of solute injected per unit area.

In the coordinate system x′y′, such that the x′ axis is parallel to the velocity vector, tensor **D** can be writen as the diagonal tensor

$$\mathbf{D}' = \begin{pmatrix} D_L & 0 \\ 0 & D_T \end{pmatrix}$$

Where the longitudinal dispersion coefficient, D_L, and the transverse dispersion coefficient, D_T, can be calculated from the hydrodynamics variables with the following expressions (Lin and Falconer, 1997):

$$D_L = \frac{k_l\,\mathbf{v}\,h\sqrt{g}}{C_z}\;;\; D_T = \frac{k_t\,\mathbf{v}\,h\sqrt{g}}{C_z}$$

being C_z the Chezy bed roughness coefficient, k_l the longitudinal dispersion constant and k_t the turbulent diffusion constant.

By means of a coordinate rotation the dispersion tensor can be expressed in the coordinate system x,y.

$$\mathbf{D} = \begin{pmatrix} D_{xx} & D_{xy} \\ D_{yx} & D_{yy} \end{pmatrix} \quad \text{being} \quad \begin{aligned} D_{xx} &= D_L \cos^2\alpha + D_T \operatorname{sen}^2\alpha \\ D_{xy} &= D_{yx} = \left(D_L - D_T\right)\operatorname{sen}\alpha\,\cos\alpha \\ D_{yy} &= D_L \operatorname{sen}^2\alpha + D_T \cos^2\alpha \end{aligned} \qquad (12)$$

1.1 Boundary conditions

The boundary condition types that have been considered are Dirichlet, Neumann, Mixed and Open type. The three first conditions are widely explained in the literature. The fourth type consists in considering that contaminants go out by dispersion through the outflow boundaries.

Classically the treatment of the outflow borders has been done choosing a numerical domain big enough, so that the borders where outflow exist, will be far from the source point and a Neumann boundary condition can be imposed there. Using an Open boundary condition on outflow boundaries the numerical domain can be smaller without any accuracy loss.

1.1.1 Dirichlet type:

The pollutant concentration is imposed on the boundaries or in a point of the domain.

$$C(x,y,t) = C_e \text{ on } \Gamma_1$$

1.1.2 Neumann type:

The component of the gradient of concentration normal to the boundary is imposed. This condition is equivalent to fix the dispersive mass flux trough the border.

$$h(\mathbf{D} \cdot \nabla C) \cdot \vec{n} = F \text{ on } \Gamma_2$$

F is mass of pollutant flux per unit length of the boundary. In impervious boundaries, such as river or channels sides, F=0.

1.1.3 Mixed or Robin type:

Total flux of mass through the boundary Γ_3 is imposed.

$$Cq_e \cdot n + h(\mathbf{D} \cdot \nabla C) \cdot n = C_e q_e \cdot n + F_e \text{ on } \Gamma_3$$

q_e is the water flow per unit length, C_e is the pollutant concentration of this flow and F_e is the mass flux of polluntants, with no fluid contribution, through the boundary.

It can be observed that the Neumann boundary condition is a particular case of this type with q_e equal to zero.

1.1.4 Open border type:

The fourth type consists in considering that contaminants go out by dispersion through permeable boundaries. The flux of contaminants that go out is given by the following expression:

$$\int_{\Gamma} h(\mathbf{D}\cdot\nabla C)\mathbf{d\Gamma}$$

The concentration field is the unknown variable of the transport problem but its gradient can be expressed as a linear combination of the shape functions gradient, when using the Finite Element Method.

With an isoparametric coordinate system, making use of the Finite Element Method:

$$C=\sum_{i=1}^{n} C_i(t)N_i(x,y)$$

Therefore:

$$\nabla C=\sum_{i=1}^{n} C_i(t)\nabla N_i(x,y)$$

and

$$h\mathbf{D}\nabla C=\sum_{i=1}^{n} hC_i(t)\mathbf{D}\nabla N_i(x,y)=\begin{pmatrix}\sum_{i=1}^{n} hC_i(t)\left(D_{xx}\dfrac{\partial N_i}{\partial x}+D_{xy}\dfrac{\partial N_i}{\partial y}\right)\\ \sum_{i=1}^{n} hC_i(t)\left(D_{yx}\dfrac{\partial N_i}{\partial x}+D_{yy}\dfrac{\partial N_i}{\partial y}\right)\end{pmatrix}$$

On outflow boundaries the type of boundary condition that can be used is of the Neumann type, with F=0. In such case the domain has to be big enough so the hypothesis of gradient of the pollutant concentration being null can be done.

Another option is to use the open boundary condition on outflow boundaries. The advantage of using this last type of boundary condition is that the numerical domain can be much smaller than the one produced by a Neumann type.

2. NUMERICAL METHOD

The transport equation has been solved using the Finite Element Method. The use of a Galerkin formulation for the spatial discretization and a differentiation scheme for the time discretization leads to the equation:

$$\left[\frac{1}{\Delta_k t}\left(\mathbf{A}^{k-1}W^{k-1}+\mathbf{A}^{k}W^{k}\right)+\left(\mathbf{B}^{k}W^{k}\right)\right]\mathbf{C}^{k}=\left[\frac{1}{\Delta_k t}\left(\mathbf{A}^{k-1}W^{k-1}+\mathbf{A}^{k}W^{k}\right)-\left(\mathbf{B}^{k-1}W^{k-1}\right)\right]\mathbf{C}^{k-1}+\left(\mathbf{E}^{k-1}W^{k-1}+\mathbf{E}^{k}W^{k}\right)$$

Where the superscript refers to the instant of time in which the matrices are calculated. With the time interval being $\Delta_k t=t^k-t^{k-1}$.

With:

$$A_{ij}=\int_{\Omega_e} hN_jN_i\,d\Omega$$

$$B_{ij}=\int_{\Omega_e}\left(hu_x\frac{\partial N_j}{\partial x}+hu_y\frac{\partial N_j}{\partial y}\right)N_i\,d\Omega+\int_{\Omega_e}\left(khN_j\right)N_i\,d\Omega+\int_{\Gamma_1}\mathbf{q_e}N_jN_i\,\mathbf{d}\Gamma+$$
$$+\int_{\Omega_e}\left(hD_{xx}\frac{\partial N_j}{\partial x}\frac{\partial N_i}{\partial x}+hD_{yx}\frac{\partial N_j}{\partial y}\frac{\partial N_i}{\partial x}+hD_{xy}\frac{\partial N_j}{\partial x}\frac{\partial N_i}{\partial y}+hD_{yy}\frac{\partial N_j}{\partial y}\frac{\partial N_i}{\partial y}\right)d\Omega-$$
$$-\int_{\Gamma_1}h\left[\left(D_{xx}\frac{\partial N_j}{\partial x}+D_{xy}\frac{\partial N_j}{\partial y}\right)n_x+\left(D_{yx}\frac{\partial N_j}{\partial x}+D_{yy}\frac{\partial N_j}{\partial y}\right)n_y\right]d\Gamma$$
$$E_i=\int_{\Gamma_1}\mathbf{q_e}C_e N_i\,\mathbf{d}\Gamma+\int_{\Gamma_2}FN_i\,d\Gamma+\int_{\Omega}SN_i\,d\Omega$$

where N_i, N_j are shape funcions, (n_x,n_y) is the unitary vector normal to the boundary, W^k and W^{k-1} are the values of the weighting function for the time integration.

In the next table the values of W^{k-1} and W^k for some known schemes are shown:

scheme	W^{k-1}	W^k
Forward Difference	1.0	0.0
Crank-Nicholson	0.5	0.5
Backward Difference	0.0	1.0

The element types considered are the lineal rectangle (4nodes), the quadratic rectangle (8 nodes), the lineal triangle (3 nodes) and the quadratic triangle (6 nodes).

3. NUMERICAL TEST: Advection-Dispersion from a continuous injection into a channel flow

To validate the numerical model the results for a problem with analytical solution has been calculated. This problem is the injection of a mass flux S, in the central point of a channel. For simplicity the flow will be parallel, uniform and steady.

The governing equation is:

$$h\frac{\partial C}{\partial t} + u_x h\frac{\partial C}{\partial x} = hD_{xx}\frac{\partial^2 C}{\partial x^2} + hD_{yy}\frac{\partial^2 C}{\partial y^2} - kCh + S\delta(x - x_F, y - y_F)$$

with the initial condition:

$$C(x, y, 0) = 0$$

and the boundary condition:

$$C(\pm\infty, \pm\infty, t) = 0$$

δ is the Dirac function defined as: $\delta = 0 \; \forall (x, y) \neq (x_F, y_F)$ and $\int_\Omega \delta(x - x_F, y - y_F) d\Omega = 1$

S is the mass injected per unit time in the source point, with coordinates (x_F, y_F).

3.1 Analytical solution

The analytical solution for this problem with unlimited domain can be written as (Sauty, 1980):

$$C(x, y, t) = \frac{\frac{S}{h}\exp\left(\frac{x - x_F}{B}\right)}{4\pi\sqrt{D_{xx}D_{yy}}} W\left(U, \frac{r}{B}\right)$$

being

$$B = \frac{2D_{xx}}{u_x}, \quad \gamma = 1 + \frac{2B\lambda}{u_x}, \quad r = \sqrt{\left((x - x_F)^2 + \frac{D_{xx}}{D_{yy}}(y - y_F)^2\right)\gamma}, \quad U = \frac{r^2}{4\gamma D_{xx} t},$$

$$W\left(U, \frac{r}{B}\right) = \int_u^\infty \frac{1}{\theta}\exp\left(-\theta - \frac{r^2}{4B^2\theta}\right) d\theta \cong \sqrt{\frac{\pi B}{2r}}\exp\left(-\frac{r}{B}\right)\left(1 - erf\left(\frac{2U - \frac{r}{B}}{2\sqrt{U}}\right)\right)$$

The approximation done for $W(U, r_B)$ is accurate within 10% for r/B>1 and accurate within 1% for r/B>10.

The analytical solution for the continuous injection in the central point of a channel, $C_T(x, y, t)$, can be obtained by means of the image sources method starting from the analytical solution for an unlimited domain $C(x, y, t)$

$$C_T(x, y, t) = \sum_{m=-\infty}^{\infty} C(x, y - mB, t)$$

where B is the width of the channel.

3.2 Numerical solution

Different boundary condition types have been introduced on the outflow borders to check which one yields a better solution.

The element type used in this test has been the lineal rectangle and a Crank Nicholson differentiation has been applied for the time integration.

Given that the boundaries A_1A_2 and A_3A_4 are impervious a Neumann boundary condition (F=0) is going to be used on them. Trough boundary A_1A_4 a fresh water influx is produced and thus a Mixed Boundary condition will be applied on it. On side A_2A_3 , in a first case (see fig.1) a Neumann boundary condition (F=0) is going to be imposed, and in a second case (see fig.2) an open boundary condition will be fixed. Both solutions will be compared to prove that the use of an Open boundary condition in outflow boundaries improves the numerical solution.

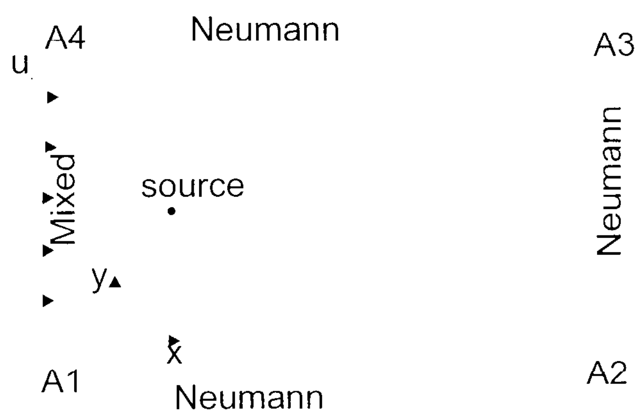


Fig. 1: **Case 1**: Boundary condition types imposed on each side.

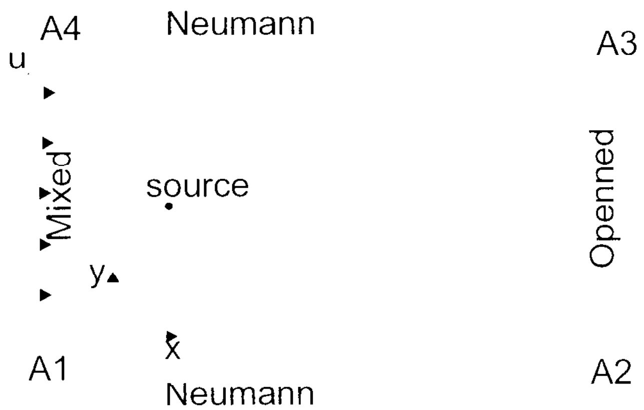


Fig. 2: **Case 2**: Boundary condition types imposed on each side.

The values of the hydrodynamic variables adopted for this test are: u_x=1m/s and h=1m.

The mass per unit time injected in the point of coordinates (0.2647,0) meters is S=0.0417kg/s. The longitudinal and transverse dispersion coefficient are D_L=0.05m^2/s and D_T= 0.05m^2/s.

The coordinates for the corners of the domain are A1(0,-0.5), A2(L,-0.5), A3(L,0.5) and A4(0,0.5), where L is the length of the numerical domain. The validity of the open boundary condition is going to be proved using two different numerical domains, one of 1m length and another of 6 m length.

For this data the analytical solution is within 1% accurate for r>1m thus it will be taken as the exact solution to check numerical results only for the 6 m long domain.

3.2.1 Case 1. L=6m.

The numerical solution with a Neumann boundary condition on side A2A3 has been calculated for a domain of length L=6m.

Numerical and analytical solution after 1 and 3 s can be seen in figures 3 and 4.

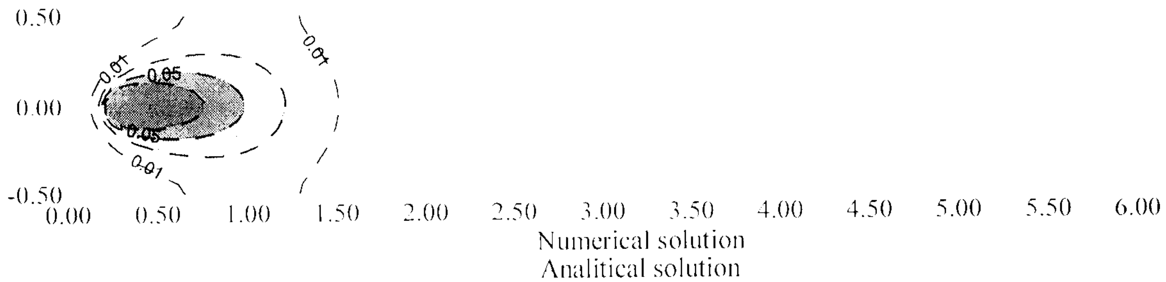


Fig. 3: Isoconcentration cuves (mg/cm^3) for analytical and numerical solution after 1s

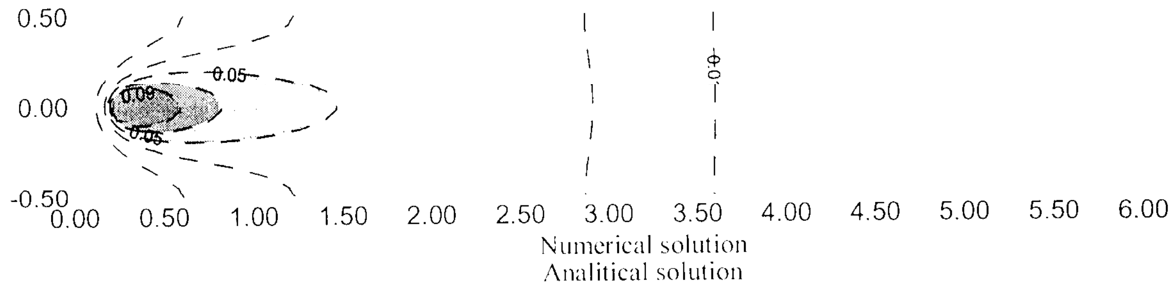


Fig. 4: Isoconcentration cuves (mg/cm^3) for analytical and numerical solution after 3s

For this case, the gradient of the analytical solution concentration field after 1 and 3 seconds is zero on the outflow boundary, so the Neumann type of boundary condition on this border is used properly.

For this test, numerical and analytical solutions can be hardly distinguished because of their proximity.

3.2.2 Case 2. L=6m.

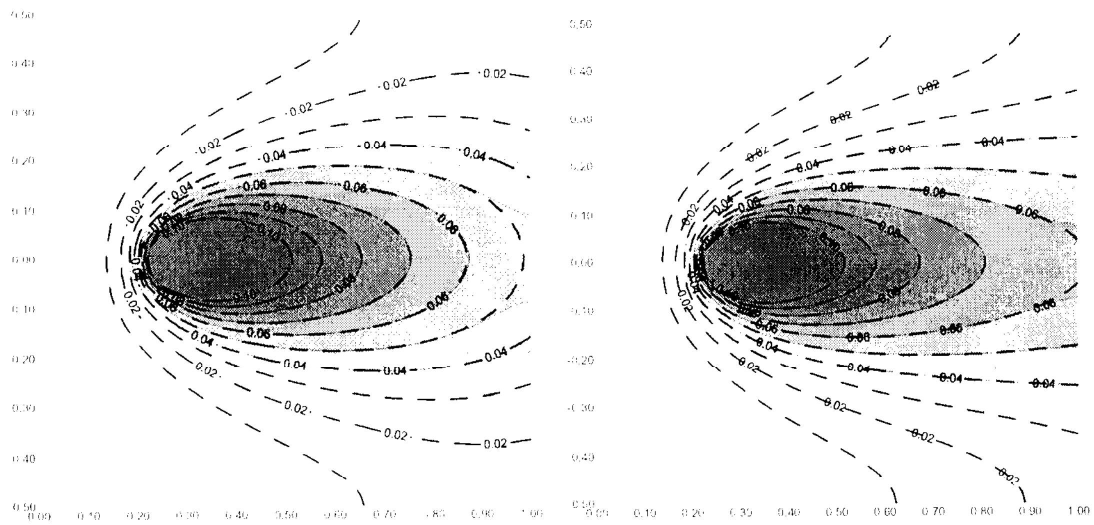
The numerical solution with an open boundary condition on side A2A3 has been calculated in a numerical domain of length L=6m.

This solution has been proved to be the same as the solution obtained with Neumann boundary condition for case 1, represented in figures 3 and 4.

When using an open boundary condition the dispersive flux of mass going out of the domain is taken into account. In this case the gradient is zero on the boundary, so the dispersive outflux of mass will be zero, which is the hypothesis done by the Neumann boundary condition used in the previous section.

3.2.3 Case 1. L=1m

For this domain length, the distance from the source point to any point in the domain is less than 1 m, thus, the error in calculation of analytical solution is bigger than 1%. The numerical solution obtained with the 6 m long domain will be used as the exact solution to check the numerical one obtained in this new domain.



Numerical solution
Exact solution

Fig. 5 and 6: Numerical solutions after 1 and 3s for L=6 and for L=1m.

When the domain length is reduced to 1m, the imposition of a Neumann boundary condition on outflux boundary will cause an error in the numerical solution since the component of the gradient normal to the boundary can not be neglected.

So the iso-concentration curves obtained in the numerical solution are forced to be normal to this boundary, as can be seen in Fig. 5 and 6. Physically this implies that there is no dispersive transport trough outflow borders where Neumann boundary condition is applied.

In Fig. 5 and 6 it can be seen that in spite of the use of Neumann boundary condition in outflow boundary, the difference between the numerical and the exact solutions is only of a certain importance in the area close to that border.

3.2.4 Case 2. L=1m

In this case using an open boundary condition on the outflow boundary produces a numerical solution better than the one obtained with Neumann boundary condition, as can be seen by the comparison of figures 7 and 8 with figures 5 and 6.

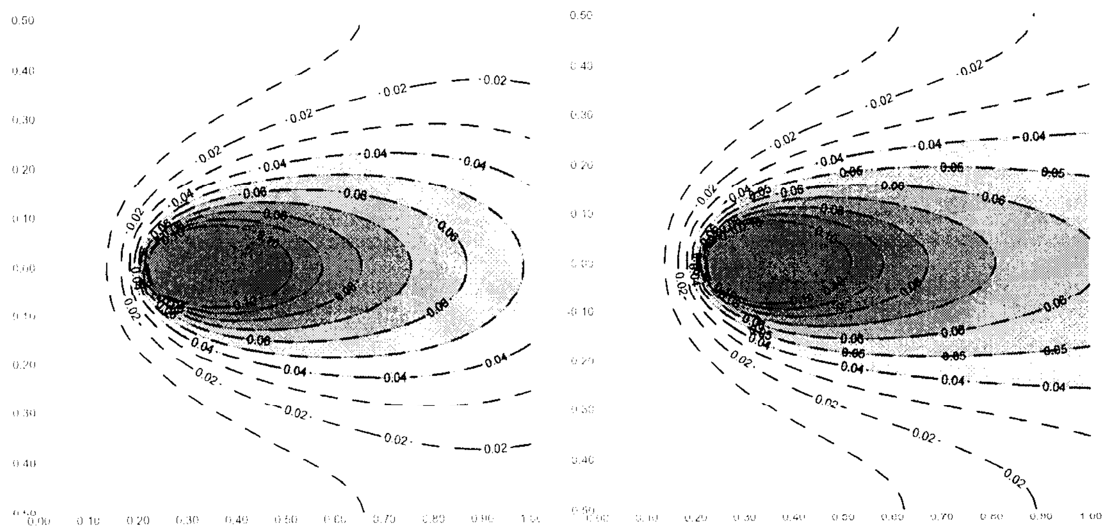


Fig. 7 and 8: Isoconcentration cuves (mg/cm^3) for analytical and numerical solution after 1 and 3s

In the area close to the outflow border the solution after 1s is much better than the solution obtained with Neumann boundary condition. After 3s the solution near the border, in relation with the one obtained when using Neumann boundary condition, is better too.

4. CONCLUSIONS

On outflux boundaries the use of the open condition instead of the Neumann condition improves the numerical solution nearby these borders.