CHAPTER 3.- NUMERICAL SOLUTION

3.1.- COMPONENTS OF A NUMERICAL SOLUTION METHOD.

Characteristics of the model

In the second chapter it has been shown the complex and unsuccessful possibility to obtain an analytical solution for the transport process in a “real case”. So it is necessary to use a numerical tool to solve the problem. The purpose of this chapter is to describe the numerical modelling adopted for the transport equation of pollutant in stratified coastal waters. So, a numerical model for the advection diffusion equation in 3 dimensional, assuming possibility of the stratification flow, has been described. This numerical model analysis is according to the computer software that has been used. This computational software is the MIKE 3 developed by DHI (Denmark Hydraulic Institute) in the frame of MIKE ZERO packages. The purpose is to describe only superficially the code basis, even the pre-processing and post-processing. However, a reference about the components of the numerical solution will be done. Although, this chapter is focused on the numerical improvement achieved due the application by two numerical tools. The first component is the unstructured mesh for the discretization of the domain. The scheme used for this discretization is the triangulation of Delaunay that allows to obtain a triangular mesh in the domain. The density of the mesh is according of the accuracy required and the stability analysis given by the Courant number. The other tool is the finite volume method as a finite approximation used in the scheme of the transport equation. Summarizing, in this chapter and in the general report has been tried to demonstrate the suitability of this numerical model.

This computational software solves the necessary hydrodynamic equations as a previous step for the resolution of the equation of the transport. However only a summary about the hydrodynamics numerical module has been presented. The possibilities of this software, even the hydrodynamic and the transport module, will be described in the next chapter. The main characteristics of the software are the next:
Component
Numerical solution: MIKE 3 FM

<table>
<thead>
<tr>
<th>Dimension work</th>
<th>3D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Integral method</td>
<td>Eulerian</td>
</tr>
<tr>
<td>Coordinate vector system</td>
<td>Cartesian</td>
</tr>
<tr>
<td>Cell element</td>
<td>Prisms: triangular extrusion</td>
</tr>
<tr>
<td>Method generation mesh.</td>
<td>Triangulation Delaunay</td>
</tr>
<tr>
<td>Finite approx. for transport equation.</td>
<td>FVM</td>
</tr>
<tr>
<td>Method for resolution for transport equations.</td>
<td>UPWIND</td>
</tr>
<tr>
<td>Finite approx. for hydrodynamics equations.</td>
<td>FEM/FVM</td>
</tr>
<tr>
<td>Method for resolution for hydrodynamic equations.</td>
<td>GMRES</td>
</tr>
</tbody>
</table>

Table 3.1. Characteristics of MIKE 3 FM

So, the MIKE 3D allows to solve the hydrodynamic and transport problem in 3 dimensional axis. As well, it is a Eulerian method, so it is focused on a fixed control volume and the changes in proprieties of the fluid that pass in and out of the volume. The other point of view is the Lagrangian integral method, where the integral formulation considers a coordinate system that moves with the plume. The different components of the mathematical model have been described in the next chapters emphasising the components associated at Mesh generation and the finite approximation for the transport equation.

Mathematical equations of transport phenomena.

The convection-diffusion phenomenon is given by the next partial equation, showed in the previous chapter, as:

\[
\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} \left[ (D_x) \frac{\partial C}{\partial x} \right] + \frac{\partial}{\partial y} \left[ (D_y) \frac{\partial C}{\partial y} \right] + \frac{\partial}{\partial z} \left[ (D_z) \frac{\partial C}{\partial z} \right] + S \tag{3.1}
\]

The first analyse shows that the problem is lineal and the solution described for this equation is unsteady. These characteristics will have an influence in the different components in the modelisation of the problem.

Manel Grifoll i Colls (ETSECCPB, UPC) 38
Numerical grid: approach unstructured grids.

It is known that a good distribution in the points in the domain where is required solve any problem in numerical methods is indispensable to obtain a good numerical solution. However, the distribution points should consider the behaviour of the solution in the domain, thus set up the point in the suitable position. For example large gradients in the parameter solution will require more points density than a uniform solution zone. So, the local accuracy and the geometric boundary required will determine the final distribution of nodes and cells in the domain. With the purpose of enhance the points distribution has been developed different techniques in mesh generation. One type of mesh that allows to achieve this purpose is the unstructured mesh, in opposite at the classical structured or regular mesh. The unstructured mesh has an irregular connectivity, so any node or point can has different number of neighbour’s points or nodes. This characteristic allows use for complex geometry and domain boundary, so is the most flexible type of grid.

The fact to distribute suitably the nodes will be important to obtain a good solution in the problem of the transport process in those points, which is suspected that they can be interesting in the domain. In this it is able to save cost of the computational point of view. Another consequence is that an unstructured mesh allows a progressive change of the size of the element without an excessive distortion (using refined mesh tools) so the transition big-small elements are staggered. Finite volume and finite element method can be applied to unstructured grids. This is because the governing equations in these methods are written in the integral form and the numerical integration can be carried out directly on unstructured grid domain in which no coordinate transformation is no required. This is contrary to the finite difference method which a structured mesh can be used. A wide range in possible ways exists for the shape of the cells: triangles, squares, tetrahedrons, hexahedrons, prisms, pyramids,… however, the shapes that are used to generate meshes in the software used are triangles in 2D and extruded in the vertical dimension.
According (Chung 2001) there are two majors unstructured grid generation methods: Delaunay method or Delaunay-Voronoi method (DVM) and advancing front methods (AFM). Being the Delaunay method for describing the mesh in the software, a general form of this generation method has been described in the following lines.

Delaunay Method (DVM)

Given a discrete group of points and once defined a diagram of Voronoi around each point, the resulting mesh defined by the Delaunay’s method or triangulations is the dual one to the diagram. For practical effects the mesh would be obtained uniting with lines right neighbouring points whose Voronoi polyhedrons share an edge. In the next figure has been shown the definition in 2D:

![3.2. Delaunay triangulations (solid lines) and Voronoi diagram (dashed lines)](image)

The Delaunay triangulations are obtained drawing connecting lines between nodes perpendicular to the edges of the Voronoi diagram. When four nodes are co-cyclic, quadrangular elements are produced but they can be correctly divided into two triangles. The Delaunay method has several properties that will be interesting in the generation mesh:

- The first is that the result about the Delaunay’s triangulations is only.

- Another property is the consideration that the method maximised the minimum angle (*min max criterion*) in all triangular elements (notice you that this is required for a good quality of finite methods (FEM, FVM)).

- The last one is a geometric property than in 2D is given by the fact that it’s possible to define a interior circle that it goes by the three points of the triangle without any other point of the domain to be in the interior (*empty circle criterion*). Analogously we can defined the same property in 3D using a sphere for 5 points. This proprieties are all important in the fact which is possible to affirm that the mesh generated is not degenerated and will be able to find an algorithm...
that allows generated the mesh easily, quickly and with quality to use after the numerical approach considered.

There exist different algorithms to define the mesh generation Delaunay’s method as Bowyer (1981), Watson (1984)...The algorithm used by MIKE 3 is called Triangle and it will be explained in the next lines. The Triangle’s speed for generate mesh is one of the most important property that it have.

Triangle Algorithm

This is the algorithm used to develop the Triangulation of Delaunay and has been developed by Computer Science Division (University of California at Berkeley) but in DHI have introduced some considerations to define inner points in the triangulation process. The final method is an incremental method. The reason of the incremental meaning is that each inner point is added every time in the triangulation process. In opposite of the Incremental methods exist the non-Incremental method, which require all vertex positions to be known in advance. The advantage of the incremental methods is that we can control the generation process, useful if, for example we want to refine a zone where there is a source term introducing more inner points or block domain (in the chapter 2.3 is explained the different types refined process). Triangle is specialized for creating two-dimensional finite element meshes. The steps are the next:

- Set up a maximum area of the triangle as restriction.
- Set up the contour of the water domain are defined a vertex points and a straight-line points.
- A first Delaunay triangulation of its points has been done.
- Impose maxim area criteria per triangle and generated inner points and triangles.
- Regenerated at the points, and the triangles, with no angle smaller than twenty-five degrees (standard angle) as criteria between the edges.

Also their creators sustain that this method is one of the most efficient carrying out triangulation of Delaunay.
Vertical approach

The spatial discretization is based on an unstructured mesh of linear triangular elements in the horizontal and a layered vertical mesh using a generalized sigma transformation explained in DHI manual (2003). So, like a extrusion has been done. The result of the volume cell, where the finite approximation will be applied, are prisms with a triangular shape.

3.3. Vertical extrusion

Refining mesh in MIKE 3.

In the last chapter have been exposed techniques for the generation of unstructured meshes. However once resolved the problem it is possible not to be satisfied with the solution obtained. In this case it will be convenient to regenerate the mesh again for improve the approach. Another reason of the regeneration of the mesh is associated to the stability of the method used. The fact to consider a numerical approach sometimes the discretization in time-step and length-step is not suitable and the result is the instability of the scheme. The stability of the model is explained in the chapter 4.2, but now is necessary to emphasize that the stability can be a reason to regenerate the mesh. MIKE 3 allows refining mesh manually through a toolbar implemented especially as a mesh editor. For example, in the next figure it is shown a unstructured mesh generated for a channel in the lagoon according with the bathymetry, where is shown the accuracy is in function of the channel presence, which affects the final solution as has been explained in the chapter before.
3.4. Detail of a channel with high accuracy

Finite approximations.

In the next lines, the three methods more common have been shortly described to solve PDE’s systems. Also, an analysing has been made to study their advantages and disadvantages on the application in the water bodies problems.

Finite difference method (FDM)

The finite element difference method (FDM) is the easiest method to use for simple geometry. The start point is to consider conservation equation in differential form. This differential form is approximated by replacing the partial derivatives by approximations in terms of the nodal values of the functions. The result is one algebraic equation per grid node. Therefore, the FDM is adequate to apply in rectangular grids (structured grids), and impossible in a unstructured grids. However, this method has difficulties in application to complex geometries. Another disadvantage is that, in principle, the conservation is not enforced in the procedure.

Finite element method (FEM)

The finite element difference method (FDM) is the easiest method to use for simple geometry. The start point is to consider conservation equation in differential form. This differential form is approximated by replacing the partial derivatives by approximations in terms of the nodal values of the functions. The result is one algebraic equation per grid node. Therefore, the FDM is adequate to apply in rectangular grids (structured grids), and impossible in a unstructured grids. However, this method has difficulties in application to complex geometries. Another disadvantage is that, in principle, the conservation is not enforced in the procedure.

The finite element method. (FEM) is similar to FVM. Also is appropriate to apply in unstructured meshes and with complex geometries. The concept of FEM is the equation of solution is multiplied for a weight function before they are integrated over entire domain. Then the equation is substituted into the integral of the conservation law and, finally the equation in overall is derived and imposes zero in each node, which is the same to impose the best solution (the one with minimum residual). The result is a set of non-linear algebraic equations. The principal disadvantage, which is shared by any method that uses unstructured grids, is that the matrices of the linerized equations are not as well structured as those for regular grid. Consequently it’s more difficult to efficient solution method. So in FEM underlying principles and formulations require a mathematical rigor. In the chapter 3.3 a practical reduced comparison has been done between FVM and FEM in general terms.
Finite volume method (FVM)

The finite volume method uses the integral form of the conservation equations as its starting point. The domain is subdivided in elemental cells whose applies the conservation equations. The elemental cells or volume is denoted by its centroid, and in this faces is applied the integral form that establish a relation between neighbour cells. This method is conservative by construction because the surface integral of normal fluxes guarantee the conservation proprieties through the domain, so is suitable to apply in the diffusion-convection equation. As well is appropriate to be applied in a complex geometry using unstructured grids. However this method is difficult to apply in 3D in order higher than second. In this case the approach requires two levels of approximation: interpolation and integration. Also, the FVM, the characteristic of the transport equation, where only two arguments appear, the velocity is known and the concentration is unknown, allows that this method is the most appropriate according with the final system equations. This method is used in the program analysed.

Finite volume method for transport equation

Another point of view of the FVM is: the transformation of the partial differential equation into a new equation where the variable in one cell is a function of the variable in the neighbour cells. The new function can be thought of as a weighted average of the concentration in the neighbouring cells. For example in 2D situation with the nort-south-est-west notation the formula becomes:

\[ c_p = \frac{a_w c_w + a_e c_e + a_s c_s}{a_p} \]  

(3.2)

3.5. nort-south-est-west

To obtain the weight coefficients the transport equation has to be applied. The convective flux and the diffusive flux in 2D will be calculated as follows:

\[ F_{\text{convective}} = U \cdot A \cdot C \]  

(3.3)
\[ F_{\text{diffusive}} = D_i \cdot A \cdot \frac{\partial C}{\partial x} \]  \hspace{1cm} (3.4)

Where \( A \) is the cell face. The values of the variables are given in the centre of the cells, but for the convective and diffusive flows must be evaluated in the cell surfaces. The result is a non-staggered grid. So, it's necessary to estimate the variables on the cell surface. In this case the first order upstream approximation is usually used. In the upstream the concentration of the cell surface is the same as the concentration in the cell on the upstream side of the cell side. So:

If \( U = U_{\text{int}} \Rightarrow C_j = C_j \)  \hspace{1cm} (3.5)
Else \( U = U_{\text{out}} \Rightarrow C_j = C_i \)  \hspace{1cm} (3.6)

The fluxes, according to the direction, in the computational molecule are:

\[ F_w = U_w \cdot A_w \cdot C_w + D_w \frac{A_w \cdot (C_w - C_p)}{dx} \]  \hspace{1cm} (3.7)

\[ F_v = U_v \cdot A_v \cdot C_p + D_v \frac{A_v \cdot (C_p - C_e)}{dx} \]  \hspace{1cm} (3.8)

\[ F_s = U_s \cdot A_s \cdot C_p + D_s \frac{A_s \cdot (C_p - C_s)}{dy} \]  \hspace{1cm} (3.9)

3.6. Molecular notation
\[ F_n = U_n \cdot A_n \cdot C_n + D_n \frac{A_n \cdot (C_n - C_p)}{dy} \]  \hspace{1cm} (3.10)

Imposing continuity:

\[ F_w - F_e + F_n - F_s = 0 \]  \hspace{1cm} (3.11)

The equation is the next:

\[ C_p \left( D_w \frac{A_w}{dx} + U_e A_e + D_e \frac{A_e}{dx} + U_s A_s + D_s \frac{A_s}{dy} + D_n \frac{A_n}{dy} \right) = \]
\[ C_w \left( D_w \frac{A_w}{dx} + U_w A_w \right) + C_e \left( D_e \frac{A_e}{dx} \right) + \left( U_n A_n + D_n \frac{A_n}{dy} \right) C_n + \left( D_s \frac{A_s}{dy} \right) C_s \]  \hspace{1cm} (3.12)

Where it is possible to identify the weighting factors:

\[ a_p = \left( D_w \frac{A_w}{dx} + U_e A_e + D_e \frac{A_e}{dx} + U_s A_s + D_s \frac{A_s}{dy} + D_n \frac{A_n}{dy} \right) \]  \hspace{1cm} (3.13)

\[ a_w = \left( D_w \frac{A_w}{dx} + U_w A_w \right) \]  \hspace{1cm} (3.14)

\[ a_e = \left( D_e \frac{A_e}{dx} \right) \]  \hspace{1cm} (3.15)

\[ a_n = \left( U_n A_n + D_n \frac{A_n}{dy} \right) \]  \hspace{1cm} (3.16)

\[ a_s = \left( D_s \frac{A_s}{dy} \right) \]  \hspace{1cm} (3.17)

Where is easy to check:

\[ a_p = a_e + a_w + a_s + a_n \]  \hspace{1cm} (3.18)

Finally is necessary to introduce the unsteady term. In this case, the mass change, \( m \), in cell P can be written by:

\[ \Delta m = \left( c_{p,s} - c_{p,s-1} \right) \cdot V_p \]  \hspace{1cm} (3.19)
Where $V_p$ is the volume. Otherwise for continuity is written:

$$\Delta t(F_w - F_e + F_a - F_s) = \Delta m$$

(3.20)

So, combining both equations gives:

$$F_w - F_e + F_a - F_s = \frac{(C_{p,j} - C_{p,j-1})V_p}{\Delta t}$$

(3.21)

That is the same:

$$a_p c_p = a_w c_w + a_e c_e + a_a c_a + a_s c_s = \frac{(C_{p,j} - C_{p,j-1})V_p}{\Delta t}$$

(3.22)

The additional term on the right side is the source term on the right side and can be divided into two terms.

$$S_0 = \left(\frac{C_{p,j-1}}{\Delta t}\right) V_p ; \quad S_1 = \frac{V_p}{\Delta t}$$

(3.23)

So the final equation weighted is.

$$c_p = \frac{1}{a_p + S_1}(a_w c_w + a_e c_e + a_a c_a + a_s c_s + S_0)$$

(3.24)

Check that in the derivation has been impose continuity. So, always that will be filled. This property is an important advantage of the FVM, overcoat in the problems about conservative lows.

**FVM for transport equation in unstructured mesh**

The numerical approach to solve the transport equation unsteady, considering the diffusion and the convection, is the Finite Volume Method. There are a several algorithms and schemes to approach the solution such as showed in 2 dimensional case. The scheme used by MIKE 3 is the QUICKEST (*Quadratic upstream interpolation for convective kinematics*). This method has been extended according QUIK, which has developed, by Leonard (1978). This method is accurate at third-order, so the error should be small. It isn’t unconditionally stable but in comparison with the upwind scheme and the central differencing scheme the stability is better in the QUICK. However in the flexible version of the program actually only has been developed the UPWIND scheme for the convection and CENTRAL scheme for the diffusion term.
UPWIND-CENTRAL scheme

The fact to use a triangular mesh has an influence in the scheme to implement in the advection diffusion equation. Actually the software analysed uses a simple approximation based on the upwind scheme for convection and central for the diffusion. This scheme is a first order accuracy in the first case and second order accuracy in the second case.

Given the conservation form:

$$\frac{\partial \bar{C}}{\partial t} + u \frac{\partial \bar{C}}{\partial x} + v \frac{\partial \bar{C}}{\partial y} + w \frac{\partial \bar{C}}{\partial z} = \frac{\partial}{\partial x} \left[ (D + Ec_x) \frac{\partial \bar{C}}{\partial x} \right] + \frac{\partial}{\partial y} \left[ (D + Ec_y) \frac{\partial \bar{C}}{\partial y} \right] + \frac{\partial}{\partial z} \left[ (D + Ec_z) \frac{\partial \bar{C}}{\partial z} \right] + S$$

(3.25)

in a compact form is:

$$\frac{\partial C}{\partial t} + u_j \frac{\partial C}{\partial x_j} - D_j \frac{\partial^2 C}{\partial x_j^2} = 0$$

(3.26)

after

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x_j} \left( u_j \cdot C - D_j \frac{\partial C}{\partial x_j} \right) = 0$$

(3.27)

And the differential form is:

$$\frac{\partial}{\partial t} \int_V C dV + \int_C \left( u_n \cdot C - D_j \frac{\partial C}{\partial n} \right) dS = 0$$

(3.28)

In the prismatic mesh with triangular shape it is possible to rewrite more compactly:

$$\frac{\partial}{\partial t} \int_V C dV + \sum_{j=1}^s F_j = 0$$

(3.29)

3.7. Prismatic mesh
and finally:

\[
\frac{\partial C}{\partial t} + \frac{1}{V_i} \sum_{j=1}^{5} F_j = 0 \tag{3.30}
\]

where the local flows \( F \) are, according to the notation where in the \( i \)-cell has a horizontal neighbours as \( j,k,l \) and vertical \( p,s \):

\[
F_1 = F_{ij} = u_{ij} \cdot C_{ij} - D \cdot \frac{C_j - C_{ij}}{\Delta l_{ij}} \tag{3.31}
\]

\[
F_2 = F_{ik} = u_{ik} \cdot C_{ik} - D \cdot \frac{C_k - C_{ik}}{\Delta l_{ik}} \tag{3.32}
\]

\[
F_3 = F_{ij} = u_{ij} \cdot C_{ij} - D \cdot \frac{C_i - C_{ij}}{\Delta l_{ij}} \tag{3.33}
\]

\[
F_4 = F_{ip} = u_{ip} \cdot C_{ip} - D \cdot \frac{C_j - C_{ip}}{\Delta l_{ip}} \tag{3.34}
\]

\[
F_5 = F_{is} = u_{is} \cdot C_{is} - D \cdot \frac{C_j - C_{is}}{\Delta l_{is}} \tag{3.35}
\]

Remark that has been considered a particular problem in the coastal water body where \( D_x = D_y \). To evaluate the concentration in the cell’s face in the diffusion term has been considered upwind scheme as follows, for example in the face between \( i,j \) centroids:

\[
\text{If } U = U_{\text{int}} \Rightarrow C_{ij} = C_j \tag{3.36}
\]

\[
\text{Else } U = U_{\text{out}} \Rightarrow C_{ij} = C_i \tag{3.37}
\]

In the diffusion term is used a central difference, so a gradient has appeared. So finally the equation scheme is:

\[
C_i^{t+1} = C_i^t + \Delta t \cdot \frac{1}{V_i} \sum_{j=1}^{5} F_j - C_i^t \tag{3.38}
\]

This scheme is an explicit one, so the \( i \)-concentration in next time step only depends on the time step before. This scheme is the simplest that can be set up in partial equation and is not unconditionability stable.

**Stability and convergence**

The fact to use an explicit scheme means that it is conditionally stable, so fill up the convergence condition. This property is given by CFL condition, introduced in 1928 by Courant, Friederichs and Lewy. Although, according to the study carried out by Abbot (1989) this method appears numerical damping or numerical diffusion, also called false diffusion, that makes the result inaccurate. This error evaluate by Abbot (1989) is:
\[ T.E. = \left( -\frac{u^2 \cdot \Delta t}{2} + \frac{u \cdot \Delta x}{2} \right) \frac{\partial^2 C}{\partial x^2} \]  

(3.39)

However, the fact to apply the next relation in the scheme between the variables involved in the truncation error the numerical diffusion disappears.

\[ \frac{u \cdot \Delta t}{\Delta x} = 1 \]  

(3.40)

This relation is called the **Transport Curant number** and will have a primordial influence in the stability process. Otherwise appears a maximum limit in time step size that represents a serious limitation for the explicit scheme. Continuing in the Abbot (1989) studies and considering central differences to determine \( C_{ij} \), the solution only will be accurately stable in the next situations, so the solution will not blow up above these conditions.

\[ Cr = \frac{u \cdot \Delta t}{\Delta x} < 1 \]  

(3.41)

for the convection term, and according with Abott (1989) the diffusion term:

\[ \frac{D \cdot \Delta t}{\Delta x^2} < \frac{1}{2} \]  

(3.42)

In the **chapter 5** is shown the numerical discuss to choose a suitable time step to avoid stability problems.

**Boundary conditions**

In the numerical transport solution in the transport equation only two boundaries conditions can appear:

**Absorbent condition.** When a accumulation or a free continuity of the concentration is given. For example free open sea boundaries or even zones of high residence time such as wetlands, depending of the time scale of the problem (Dirichlet condition).

\[ C_{ij} = cte. \]  

(3.43)

**Impermeable condition.** When a flow concentration in the direction is zero. The land boundary should be an example of this boundary condition (Newman condition).

\[ \frac{\partial C_{ij}}{\partial n} = cte \]  

(3.44)
3.2.- COMPARISION FVM VS. FEM

A reduced comparison between FVM and FEM are presented here. The comparison is in the hydrodynamic module, where both schemes are implemented for unstructured mesh. The first is implemented in the experimental phase the second in the commercial software.

<table>
<thead>
<tr>
<th></th>
<th>Stability: Max. Cr.</th>
<th>Time computing</th>
</tr>
</thead>
<tbody>
<tr>
<td>FVM</td>
<td>0.5</td>
<td>4 hours</td>
</tr>
<tr>
<td>FEM</td>
<td>1</td>
<td>7 hours</td>
</tr>
</tbody>
</table>

Table 3.2. FVM vs. FEM

It’s shown that the FVM requires a Currant number smaller, which implies a time step smaller and in principle less fast. Therefore, in overall the FEM is slower than FVM. The reason is in the concept of the FEM (see chapter 4.4), which the implementation requires more code lines due to the approach and interpolation process, so the computational time increase. According to that, the implementation of FEM is more complex. Otherwise, in FVM there are only schemes of interpolation between cells and nodes. However the computational time depends the order of accuracy for the scheme used. The fact to be easier the implementation in FVM allows set up the models for example in flood and dry analyses, where the resolutions via FEM present a high difficult, or water quality modelling, even cycle of nutrients in aquatic ecosystem where involve large number of variables (chapter 5.10).

3.3.- SOLUTION IN HYDRODYNAMIC EQUATIONS

Formulation

The advection diffusion equation needs as a previous step a solution of the velocity field. The commercial software that has been used also gives this solution. The computational features and application areas of this software is described more accuracy in the next part (chapter 4), so in this chapter only has been described the equations to solve the hydrodynamic problem. The hydrodynamic module is based on the solution of 3-dimensional incompressible Reynolds averaged Navier-Stokes equations, subject to the assumptions of Boussinesq (the density variation can be negligible except the terms where appears multiplying by g term) and of a hydrostatic pressure (vertical accelerations negligible against acceleration of gravity). These assumptions give the Shallow water equations.

\[
\frac{1}{\rho} \frac{\partial p}{\partial z} = -g \quad (3.45)
\]

\[
\rho = \rho_0 + \rho'(x, y, z) \rightarrow \rho' << \rho_0 \quad (3.46)
\]
The general approach is to use a generalised wave equation, derived from the depth averaged continuity and momentum equation, to describe the free surface while the local momentum equations for the two horizontal components describe the vertical profiles, given the pressure gradients. Therefore, in the start point the local continuity equation is written as:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$

(3.47)

and the two horizontal momentum for x and y component respectively:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = -\frac{\partial}{\partial x} \left( g \eta + \frac{p}{\rho} \right) + fV - \frac{\partial}{\partial z} \left( \nu_r \frac{\partial u}{\partial z} \right) + A_x - \frac{g}{\rho} \eta \frac{\partial \rho}{\partial z}$$

(3.48)

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = -\frac{\partial}{\partial y} \left( g \eta + \frac{p}{\rho} \right) + fU - \frac{\partial}{\partial z} \left( \nu_r \frac{\partial v}{\partial z} \right) + A_y - \frac{g}{\rho} \eta \frac{\partial \rho}{\partial z}$$

(3.49)

where

$p$ : density
$u, v, w$ : velocities in x, y, z direction
$f$ : Coriolis parameter
$\nu_r$ : turbulent eddy viscosity
$\eta$ : Elevation
$p$: Pressure
$U, V$: velocity in deep averaging
$A_x, A_y$: horizontal stress terms associated to Eddy viscosity horizontal

$$A_x = \frac{\partial}{\partial x} \left( \nu_r \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \nu_r \frac{\partial u}{\partial y} \right); \quad A_y = \frac{\partial}{\partial x} \left( \nu_r \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial y} \left( \nu_r \frac{\partial v}{\partial y} \right)$$

(3.50)

The vertical dimension can be considered easily if is considered vertical hydrostatic pressure approach, so the vertical velocity will be described by continuity. Depth averaging of the local equations reads for the continuity equations are:

$$U = \frac{u}{H}, \quad V = \frac{v}{H}$$

(3.51)

then the continuity equations and the two horizontal moments equations are (introducing stresses caused by the bed resistance and the wind explained in the chapter 2.2):

$$\frac{\partial \eta}{\partial t} + \frac{\partial UH}{\partial x} + \frac{\partial VH}{\partial y} = 0$$

(3.52)
\[
\frac{\partial U}{\partial t} + U \frac{\partial U}{\partial x} + V \frac{\partial V}{\partial y} = -g \frac{\partial}{\partial x} (\eta_A + \eta) + fV + \frac{\tau_{sx} - \tau_{sx}}{\rho} + A_x + B_x
\]  
(3.53)

\[
\frac{\partial V}{\partial t} + U \frac{\partial V}{\partial x} + V \frac{\partial V}{\partial y} = -g \frac{\partial}{\partial y} (\eta_A + \eta) - fV + \frac{\tau_{sv} - \tau_{sv}}{\rho} + A_y + B_y
\]  
(3.54)

Where:

\( \tau_S \): surface stress (see chapter 2.2):
\[
\tau_{s} = \rho \cdot \nu_T \cdot \frac{\partial u}{\partial z} = \rho \cdot \nu_T \cdot C_{W} \cdot W_{x}
\]  
(3.55)

\( \tau_B \): bed stress (see chapter 2.2):
\[
\tau_{B} = \rho \cdot C_{D} \cdot |Q(z) \cdot u(z)|
\]  
(3.56)

\( B_x, B_y \): depth averaged baroclinic pressure gradients.

\[
B_x = -\frac{g}{\rho} \int_0^\eta \frac{\partial \rho}{\partial z} dz ; B_y = -\frac{g}{\rho} \int_0^\eta \frac{\partial \rho}{\partial y} dz
\]  
(3.57)

So, have been shown the features included in the software. In conclusions the numerical modelling system simulates unsteady three-dimensional flows taking into account density variations, bathymetry and external forcing such as meteorology, tidal elevations, currents and other hydrographic conditions.

**Influence of stratified presence**

Remark the effects of the baroclinic gradients. These effects are in the modification of the turbulent eddy viscosity that will inhibit under stratification presence gradients. As well in the term \( B_x \) and \( B_y \) that corresponds to the baroclinic gradients.

### 3.4.- VERIFICATION, CALIBRATION AND VALIDATION

The calibration is the process when the model is adjusted to the real measurements. During the set up of the numerical model several assumptions have been made that can move the results away from the reality. The usual parameters to be calibrated are the bed roughness for the hydrodynamic model or the Prandtl number for the transport model. However sometimes is not sufficient, then there are more parameters, which can be calibrated for example in the turbulence model. Although sometimes it’s usual run the new model in another different turbulent closure to achieve the minimum difference between the numerical results and the real measurements. However in overall there are three steps in the model calibration:

1.- Model verification: Here it is checked that the model results are expected. This is usually done by a comparison with sample examples where the analytical solution is known, for example the expressions explained in the chapter 2.2.

2.- Model calibration: where the model parameters are adjusted.
3.- Model validation: where the calibrated model is used to predict a situation, which the results can be compared with observations. This is done to ensure the capabilities of the model.

3.5.- OTHERS UTILITIES:

The transport equation has closer similarities with another process of transport. As well this process is links to the hydrodynamic behaviour, as will be shown.

Water quality model

The fact to solve the transport process can be considered as a first step to solve a water quality model. The purpose of the water quality model is to determine the variation of concentrations of difference substances that has an influence on the ecosystem. Usually these substances are linked to the biological reaction that changes their concentration. The biochemical reactions are called reaction kinetics of the substance. Usually these reactions can be of the zero-order kinetics, first-order kinetics or second order kinetics.

- Zero-order kinetics:
  \[
  \frac{dC}{dt} = -k \Rightarrow C = C_0 - kt
  \]  (3.58)

- First-order kinetics:
  \[
  \frac{dC}{dt} = -kC \Rightarrow C = C_0 \exp^{-kt}
  \]  (3.59)

- Second order kinetics:
  \[
  \frac{dC}{dt} = -kC^2 \Rightarrow C = C_0 \frac{1}{1 + KC_0t}
  \]  (3.60)

Reactions of high order are rare. The result must be included in the source term. However these equations describe the situation with only one variable. For some cases there are multiple water quality constituents. So, the change in one variable is a function of the concentration of the other variables. However there is a limiting variable concentration determining which process is taken place. In addition most biochemical processes depend on the temperature. One example is the nutrient cycle that involves oxygen, phosphorus, nitrogen and algae/bacteria (or phytoplankton).
3.8. Cycle algae growth

This cycle determines the algae growth. These problems can be predicted using a numerical modelling, called water quality model, where the hydrodynamic model (flow, temperature and salinity), even the transport behaviour model, is necessary to implement the water quality model. So a utility of the numerical model of the transport has been shown.

**Sediment transport in estuaries**

The estuaries are important in the geological cycle because much of the sediment that found the ocean floor is derived from land and reaches the ocean through rivers and their estuaries. In principle the sediment reaches the ocean difficulties but is necessary to do a few considerations. First of all, the sediment is denser than the freshwater and salt water, so the sediment tends to sink to the bottom. If this sediment must be moved it has to be kept in suspension. In the river this occurs through the turbulence. However this turbulence is minimum in a short period of time between rising and falling time. In this cases the heavier sediment particles have a chance to settles at the bottom. So, a part of the sediment never will reach to the sea, and will accumulate in the estuary. However the current will be in function as well of the turbulence, influenced by the salinity structure of the estuary. For example, in the salt wedge structure, the accumulate sediment upstream can not leave the estuary. Another factor of the process of transport of the sediment in the estuary is the river discharge. In this case under river flood conditions the river discharge will promote the particle transport. Summarising the hydrodynamic behaviour will determine the transport of the sediment in the estuaries.

In the similar way of the transport pollutant or water quality, the equations that govern the problem are linked to the hydrodynamic behaviour. And the transport sediment equation keeps similarities with the transport substances process. According to Van Rijn (1993) the governing equations in this case:

\[
\text{fluid: } \frac{\partial}{\partial t} (1-C) + \frac{\partial}{\partial x_i} \left( (1-C) \mu_{f,i} + \epsilon_{f} \frac{\partial C}{\partial x_i} \right) = 0
\]
\[
\text{sediment: } \frac{\partial}{\partial t} (C) + \frac{\partial}{\partial x_i} \left( C (u_{f,i} - w_s) - \varepsilon_f \frac{\partial C}{\partial x_i} \right) = 0
\]

in which:

- \( C \): local volume concentration
- \( \varepsilon_f \): fluid mixing coefficient (m²/s)
- \( \varepsilon_s \): sediment mixing coefficient (m²/s)
- \( w_s \): vertical fall velocity

The sediment velocity is assumed to be equal to the fluid velocity (mixiture velocity) with exception of the vertical direction where a constant velocity equal to particle fall velocity is assumed (\( w_s \)). The complexities of these equations induce to solve the transport process of sediment using also a numerical way.