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A Study Case of Hydrodynamics and Water Quality Modelling: Coatzacoalcos River, Mexico

Franklin Torres-Bejarano, Hermilo Ramirez and Clemente Rodríguez
*Mexican Petroleum Institute
Mexico*

1. Introduction

The common basis of the modeling activities is the numerical solution of the momentum and mass conservation equations in a fluid. For hydrodynamic modeling, the Navier-Stokes equations are usually simplified according to the specific water body properties, obtaining, for example, the shallow water equations, so called because the horizontal scale is much larger than the vertical. Therefore, in cases where the river has a relation width-depth of 20 or more and for many common applications, variations in the vertical velocity are much less important than the transverse and longitudinal direction (Gordon et al., 2004). In this sense, the equations can be averaged to obtain the vertical approach in two dimensions in the horizontal plane, which adequately describes the flow field for most of the rivers with these characteristics.

At the same time, the contaminant transport models have evolved from simple analytical equations based on idealized reactors to sophisticated numerical codes to study complex multidimensional systems. Since the introduction of the classic Streeter-Phelps model in the 1920 to evaluate the Biochemical Oxygen Demand and dissolved oxygen in a steady state current, contaminant transport and water quality models have been developed to characterize and assist the analysis of a large number of water quality problems.

This chapter presents the numerical solution of the two-dimensional Saint-Venant and Advection-Diffusion-Reaction equations to calculate the free surface flow and contaminant transport, respectively. The solution of both equations is based on a second order Eulerian-Lagrangian method. The advective terms are solved using the Lagrangian scheme, while the Eulerian scheme is used for diffusive terms. The specific application to the Coatzacoalcos River, Mexico is discussed, having as a main building block the water quality assessment supported on mathematical modelling of hydrodynamics and contaminants transport. The solution method here proposed for the two-dimensional equations, yields appropriate results representing the river hydrodynamics and contaminant behaviour and distribution when comparing with field measurements.

In this work is presented the structure of a numerical model giving an overview of the program scope, the conceptual design and the structure for each hydrodynamic, pollutants transport and water quality modules that includes ANAITE/2D model (Torres-Bejarano and Ramirez, 2007). The numerical solution scheme is detailed explained for both Saint-Venant and the Advection-Diffusion-Reaction equation. To validate the model, some comparisons were made between model results and different field measurements.

2. The numerical model

The developed model is a scientific numerical hydrodynamic and water quality model written in FORTRAN; the model has been named ANAITE/2D. The current version of this model solves the Saint-Venant equations for hydrodynamics representation and the Advection-Diffusion-Reaction (A-D-R) equation using a two-dimensional approach to simulate the pollutants fate.

2.1 The hydrodynamic module

In order to obtain a better representation of the hydrodynamics reproduced by the ANAITE model (Torres-Bejarano & Ramirez, 2007), this work presents the solution to change from one-dimensional steady state approach to unsteady two-dimensional flow approximation, solving the two-dimensional Saint-Venant equations (eqs. 1, 2 and 3); these equations describe two-dimensional unsteady flow vertically averaged, representing the principles of conservation of mass and momentum and are obtained from the Reynolds averaged Navier-Stokes equations under certain simplifications (Chaudhry, 1993). These equations have a wide applicability in the study of free surface flow. For example, the flow in open channels with steep slopes (Salaheldin et al., 2000), flows over rough infiltrating surfaces (Wang et al., 2002), propagation of flood waves Rivers (Ying et al., 2003), dam break flow (Mambretti et al., 2008), among others.

$$\frac{\partial h}{\partial t} + \frac{\partial(hu)}{\partial x} + \frac{\partial(hv)}{\partial y} = 0 \quad (1)$$

$$\frac{\partial u}{\partial t} = -u \frac{\partial u}{\partial x} - v \frac{\partial u}{\partial y} - g \frac{\partial h}{\partial x} + \nu_t \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + g(S_{ox} - S_{fx}) \quad (2)$$

$$\frac{\partial v}{\partial t} = -u \frac{\partial v}{\partial x} - v \frac{\partial v}{\partial y} - g \frac{\partial h}{\partial y} + \nu_t \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + g(S_{oy} - S_{fy}) \quad (3)$$

where:

- S_f = friction slope, (·)
- h = water depth, (m)
- u = longitudinal velocity, x direction (m/s)
- v = transversal velocity, y direction (m/s)
- ν_t = turbulent viscosity, (m²/s)
- g = acceleration due to gravity, (m/s²)

In this equations system, it was assumed that the effect of the Coriolis force and tensions due to wind at the free surface are negligible given the nature of the problems that focus this work, although their inclusion in the numerical scheme can be done without difficulty.

2.2 The water quality module

The water quality model, adapted to the main stream of Coatzacoalcos river, simulates the behaviour and concentration distributions for different water quality parameters. The water quality module solves the following parameters, grouped according to the chemical properties:

- **Physics:** Temperature, Salinity, Suspended Solids, Electric Conductivity.
- **Biochemical:** Dissolved Oxygen (DO), Biochemical Oxygen Demand (BOD), Fecal Coliforms (FC).
- **Eutrophication:** Ammonia Nitrogen (NH₃), Nitrates (NO₃), Organic Nitrogen (N_{org.}), Inorganic phosphorous (phosphate, PO₄), organic Phosphorous (P_{org.}).
- **Metals:** Cadmium, Chromium, Nickel, Lead, Vanadium, Zinc.
- **HAPs:** Acenaphthene, Phenanthrene, Fluoranthene, Benzo(a)anthracene, Naphthalene.

The transport and transformation of the different environmental parameters was carried out by applying the two-dimensional approach of A-D-R (eq. 4):

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = \frac{\partial}{\partial x} \left(E_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(E_y \frac{\partial C}{\partial y} \right) \pm \Gamma_c \quad (4)$$

where:

C = Concentration of any water quality parameter, (mg/L)

E_x = Coefficient of longitudinal dispersion, (m²/s)

E_y = Coefficient of transversal dispersion (m²/s)

Γ_c = Reaction mechanism (specified for each parameter) (m⁻¹)

The reaction mechanism, Γ_c , is used to represent the water quality parameters, and it is solved individually for each of them.

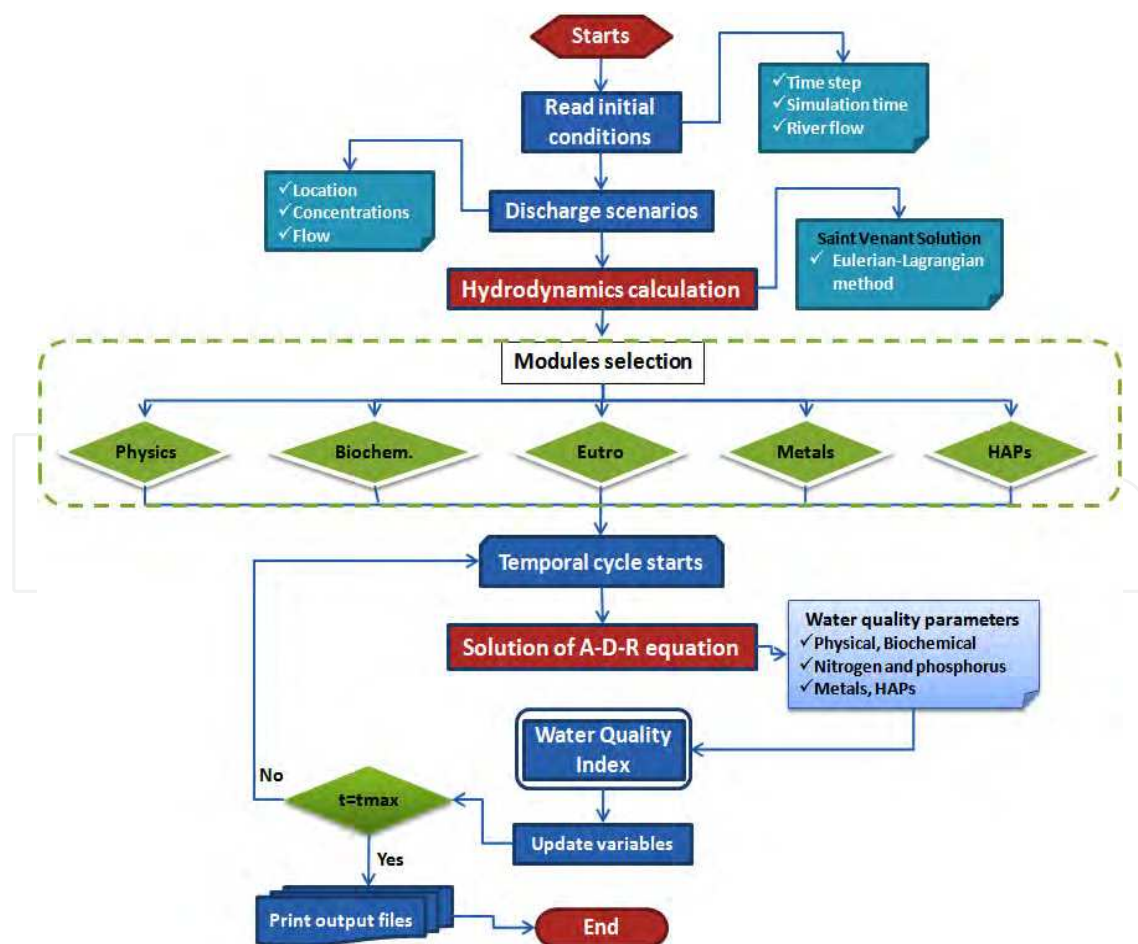


Fig. 1. Flow diagram of ANAITE/2D numerical model

2.3 Numerical solutions

The Saint-Venant and A-D-R equations are numerically solved using a second order Eulerian-Lagrangian method; a detailed explanation of the solution is presented in this work. The method separates the equations into its two main components: advection and diffusion, which are solved using a combination of Lagrangian and Eulerian techniques, respectively. In this way, the entire equations are solved. Fig. 1 shows the flow diagram for the model general solution.

2.3.1 Numerical grid

A numerical grid Staggered Cell type is used (Fig. 2). In this grid the scalars are evaluated in the center of the cell and vector magnitudes on the edges.

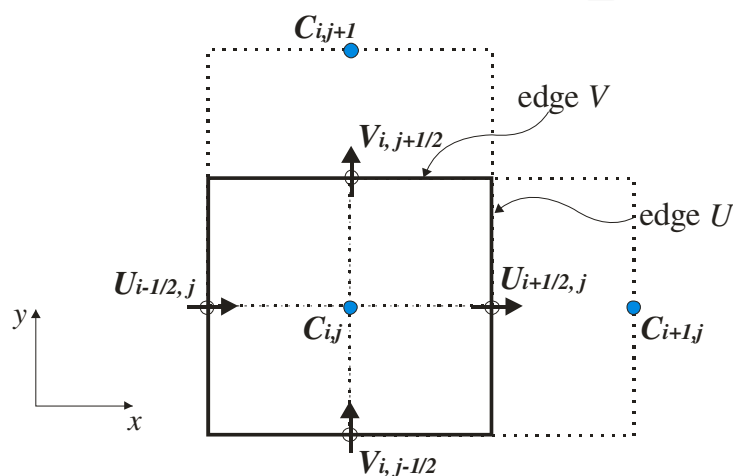


Fig. 2. Notation for Staggered cell grid

2.3.2 Advection (Lagrangian method)

The advection solution uses a Lagrangian method whose interpolation/extrapolation principle is based on the characteristics method. In the characteristics method is assigned to each node at t^{n+1} a particle that does not change its value as it moves along a characteristic line defined by the flow. It locates its position in the previous time t^n by the interpolation of adjacent values of a characteristic value, in this case the Courant number, which is assigned to node t^{n+1} . For simplicity, the method is exemplified in one dimension, but is similar for two or three dimensions (Fig. 3).

Assuming that the value of the variable at point P (φ_p^n), can be calculated by interpolating between the values φ_{i-1}^n y φ_i^n from the adjacent points x_0 and x_1 respectively (Rodriguez et al., 2005).

If a particle at the point P travels at a constant velocity U will move a distance $x + U \Delta t$ at time $t + \Delta t$, so it is:

$$\varphi(x, t) = \varphi(x + u\Delta t, t + \Delta t) = \varphi(x + p\Delta x, t + \Delta t) \quad (5)$$

if we apply the modified Gregory-Newton interpolation:

$$f(P) \equiv f(x + p\Delta x) = f_1 - p[f_1 - f_0] + \frac{p(p-1)}{2!}[f_2 - 2f_1 + f_0] - \Lambda \quad (6)$$

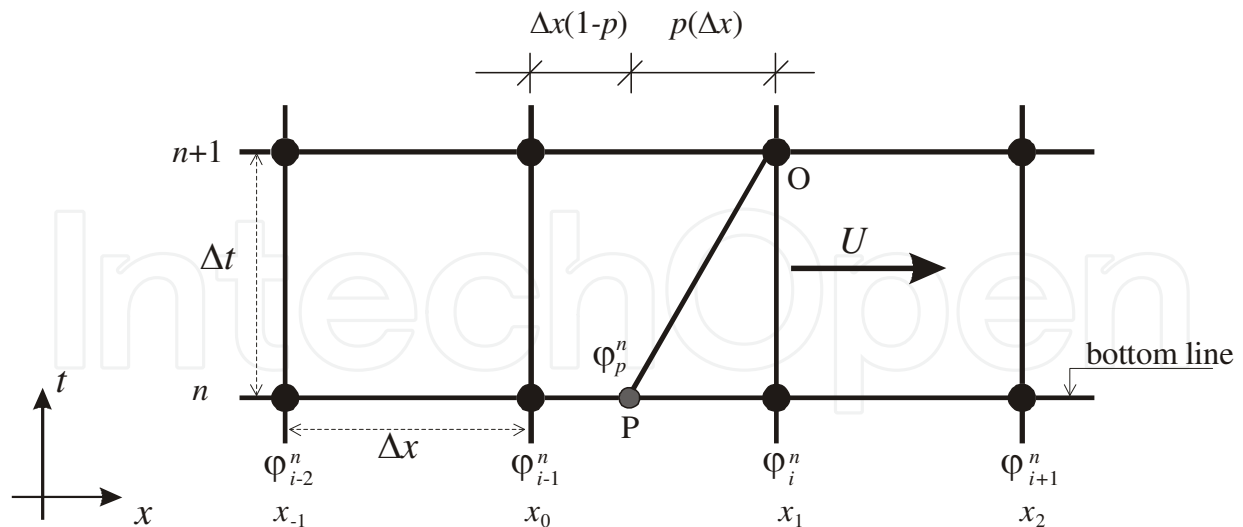


Fig. 3. Notation used, shown in one-dimensional mesh

Where $f(P)$, f_1 , f_0 y f_2 are the values at points P , x_1 , x_0 , and x_2 respectively, p is a weight coefficient which positions the point P with respect to φ_i^n and φ_{i-1}^n . Since the polynomial is a second-degree interpolation, the three terms of equation (6) are used. Substituting the known values for the three points:

$$\varphi_p^n = (1 - p^2)\varphi_i^n + (0.5p^2 + 0.5p)\varphi_{i-1}^n + (0.5p^2 - 0.5p)\varphi_{i+1}^n$$

As the value at point P is required in a two dimensional grid, the solution is expressed as shown in equation (7).

$$\begin{aligned} \varphi_{i-a,j-b} = & (1 - p^2) \left[(1 - q^2)\varphi_{i,j}^n + (0.5q^2 + 0.5q)\varphi_{i,j-1}^n + (0.5q^2 - 0.5q)\varphi_{i,j+1}^n \right] \\ & + (0.5p^2 + 0.5p) \left[(1 - q^2)\varphi_{i-1,j}^n + (0.5q^2 + 0.5q)\varphi_{i-1,j-1}^n + (0.5q^2 - 0.5q)\varphi_{i-1,j+1}^n \right] \\ & + (0.5p^2 - 0.5p) \left[(1 - q^2)\varphi_{i+1,j}^n + (0.5q^2 + 0.5q)\varphi_{i+1,j-1}^n + (0.5q^2 - 0.5q)\varphi_{i+1,j+1}^n \right] \end{aligned} \quad (7)$$

where p and q , are the Courant numbers in x and y directions, respectively. The calculation of the Courant numbers for u and v is as follows:

$$C_u(p) = \frac{u_{i,j}^* \Delta t}{\Delta x_i} ; C_v(q) = \frac{v_{i,j}^* \Delta t}{\Delta y_j} \quad (8)$$

where:

$$u_{i,j}^* = (1 - \alpha)u_{i,j} + \frac{\alpha}{4}(u_{i+1,j+1} + u_{i-1,j+1} + u_{i+1,j-1} + u_{i-1,j-1}) \quad (9)$$

$$v_{i,j}^* = (1 - \alpha)v_{i,j} + \frac{\alpha}{4}(v_{i+1,j+1} + v_{i-1,j+1} + v_{i+1,j-1} + v_{i-1,j-1}) \quad (10)$$

α is coefficient of relaxation with typical values between 0 – 1. In this work 0.075 was used. $u^*_{i,j}$ and $v^*_{i,j}$ are spatial velocities in x and y direction respectively.

The solution method is applied in a similar way to the advective terms presents in the continuity (Eq. 1), momentum (Eqs. 2 and 3) and A-D-R (Eq. 4) equations; $\varphi = h, u, v$ y C , are the advective variables, obtained by the lagrangian method in its second order approximation.

2.3.3 The diffusion (Eulerian method)

Turbulent diffusion. The turbulent viscosity coefficient present in the Saint-Venant equations is evaluated with a zero order model or mixing length model in two dimensions (vertically averaged):

$$\nu_t = l_m^2 \sqrt{2 \left(\frac{\partial u}{\partial x} \right)^2 + 2 \left(\frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 + \left(2.34 \frac{u_f}{\kappa h} \right)^2} \quad \therefore l_m \approx 0.267 \kappa h \quad (11)$$

where:

l_m = mixing length

u_f = friction velocity, $u_f = \sqrt{ghS}$

κ = von Kármán constant

Thus, the diffusion terms in x and y are solved respectively by the following formulas:

$$Dift_u = \nu_t \left\{ \left[\left(\frac{u_{i+1,j} - u_{i,j}}{\Delta x_i} \right) - \left(\frac{u_{i,j} - u_{i-1,j}}{\Delta x_{i-1}} \right) \right]^n + \left[\left(\frac{u_{i,j+1} - u_{i,j}}{\Delta y_j} \right) - \left(\frac{u_{i,j} - u_{i,j-1}}{\Delta y_{j-1}} \right) \right]^n \right\} \quad (12)$$

$$Dift_v = \nu_t \left\{ \left[\left(\frac{v_{i+1,j} - v_{i,j}}{\Delta x_i} \right) - \left(\frac{v_{i,j} - v_{i-1,j}}{\Delta x_{i-1}} \right) \right]^n + \left[\left(\frac{v_{i,j+1} - v_{i,j}}{\Delta y_j} \right) - \left(\frac{v_{i,j} - v_{i,j-1}}{\Delta y_{j-1}} \right) \right]^n \right\} \quad (13)$$

Detailed analysis of turbulence, their interpretation and mathematical treatment can be found at Rodi, (1980), Rodríguez et al., (2005).

Longitudinal and transverse dispersion in rivers. The A-D-R equation evaluates the dispersion process by Ex and Ey coefficients.

In this work the longitudinal dispersion coefficient proposed by Seo and Cheong (1998) has been implemented (Eq. 14):

$$\frac{Ex}{hu_f} = 5.915 \left(\frac{W}{h} \right)^{0.620} \left(\frac{u}{u_f} \right)^{1.428} \quad (14)$$

The expression for estimating the transverse dispersion coefficient in a river is given by (adapted from Martin and McCutcheon, 1999):

$$Ey = 0.023 h U^* \quad (15)$$

The 0.023 value was specifically obtained for the studied river. The dispersion terms in equation (4) are numerically solved as follow:

$$\begin{aligned} Disp_C = & \frac{\Delta t}{\Delta x_i} \left[\frac{Ex_{i+1,j}}{\Delta x_i} (C_{i+1,j} - C_{i,j}) - \frac{Ex_{i,j}}{\Delta x_{i-1}} (C_{i,j} - C_{i-1,j}) \right]^n \\ & + \frac{\Delta t}{\Delta y_j} \left[\frac{Ey_{i,j+1}}{\Delta y_j} (C_{i,j+1} - C_{i,j}) - \frac{Ey_{i,j}}{\Delta y_{j-1}} (C_{i,j} - C_{i,j-1}) \right]^n \end{aligned} \quad (16)$$

2.3.4 The pressure terms

This is the term that takes into account the external forces in the Saint-Venant equations, in this case the gravitational forces. It is solved with a centered difference of depth values in the calculation grid (Eq. 17).

$$Pres_u = -g \left[\frac{h_{i+1,j} - h_{i-1,j}}{2\Delta x} \right]^n ; Pres_v = -g \left[\frac{h_{i,j+1} - h_{i,j-1}}{2\Delta y} \right]^n \quad (17)$$

2.3.5 The continuity equation

Expanding the derivative and rearranging terms in equation (1), the continuity equation is as follows:

$$h_{i,j}^{n+1} = Advect_h - \Delta t \left[h_{i,j}^* \left(\frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x_i} \right) + h_{i,j}^* \left(\frac{v_{i,j+1} - v_{i,j-1}}{2\Delta y_j} \right) \right]^n \quad (18)$$

where:

$$h_{i,j}^* = \frac{1}{4} (h_{i+1,j+1} + h_{i-1,j+1} + h_{i+1,j-1} + h_{i-1,j-1}) \quad (19)$$

2.3.6 General solution for velocities

Grouping the obtained terms, the following general equations for velocities are reached:

$$[u_{i,j}]^{n+1} = Advect_u + \Delta t [Dift_u - Pres_u]^n - \Delta t g [S_{ox} + S_{fx_{i,j}}]^n \quad (20)$$

$$[v_{i,j}]^{n+1} = Advect_v + \Delta t [Dift_v - Pres_v]^n - \Delta t g [S_{oy} - S_{fy_{i,j}}]^n \quad (21)$$

The first element of the last term is the free surface slope, which multiplied by the gravity represents the action of gravitational forces. This term can be expressed as:

$$S_{ox} = -\partial z_0 / \partial x ; S_{oy} = -\partial z_0 / \partial y \quad (22)$$

The second element of the last term represents the bottom stress, which causes a nonlinear effect of flow delay and is calculated by the Manning formula:

$$S_{fx} = \frac{n^2 u \sqrt{u^2 + v^2}}{h^{4/3}} ; S_{fy} = \frac{n^2 v \sqrt{u^2 + v^2}}{h^{4/3}} \quad (23)$$

where:

S_f = friction slope, (·)

n = Manning roughness coefficient

2.3.7 General solution for A-D-R equation

Finally, grouping term for A-D-R equation the solution is obtained with:

$$[C_{i,j}]^{n+1} = Adv_{ec_c} + \Delta t [Disp_C]^n \pm \Delta t [\Gamma_C]^n \quad (24)$$

As mentioned in section 2.2, Γ_C is solved individually for each parameter.

2.3.8 Stability requirements

Because a finite difference scheme is used, should be considered the linear stability criteria. The selection of the time step and space must satisfy the condition of Courant-Friedrichs-Lewy (CFL) for a stable solution. The CFL condition for two-dimensional Saint-Venant equations can be written as (Bhallamudi and Chaudhry, 1992):

$$C_n = \frac{(R + \sqrt{gh}) \cdot \Delta t}{\Delta x \cdot \Delta y} \sqrt{\Delta x^2 + \Delta y^2} < 1 \quad (25)$$

where: R = magnitude of the resultant velocity, (m/s)

3. Study case: Coatzacoalcos River

The last stretch of the Coatzacoalcos River located in the Minatitlan-Coatzacoalcos Industrial Park (MCIP), with about 40 km length, is part of an area of vast natural diversity, where the high population concentration creates important environmental changes, due to pressures arising mainly from consumption and industrial activities. Currently, insufficient information exists for MCIP regarding hydrodynamics and water quality at the river stretch. This is one of the most polluted rivers in Mexico and is consequently a critical area in terms of industrial pollution.

Coatzacoalcos is a commercial and industrial port that offers the opportunity to operate a transportation corridor for international traffic, the site is the development basis for industrial, agricultural, forestry and commercial in this region; by the volume of cargo is considered the third largest port in the Gulf of Mexico (Fig. 4). The area of Coatzacoalcos river mouth has had a rapid urban and industrial growth in the last three decades. In this area, the largest and most concentrated industrial chemical complex, petrochemical and derivatives has been developed in Latin-America.

The importance of this industrial park, formed mainly by the Morelos petrochemical complex, Cangrejera, Cosoloacaque and Pajaritos, is such that 98% of the petrochemicals used throughout the country are produced there. Fig. 5 shows the industrial and petrochemical facilities located in this area.

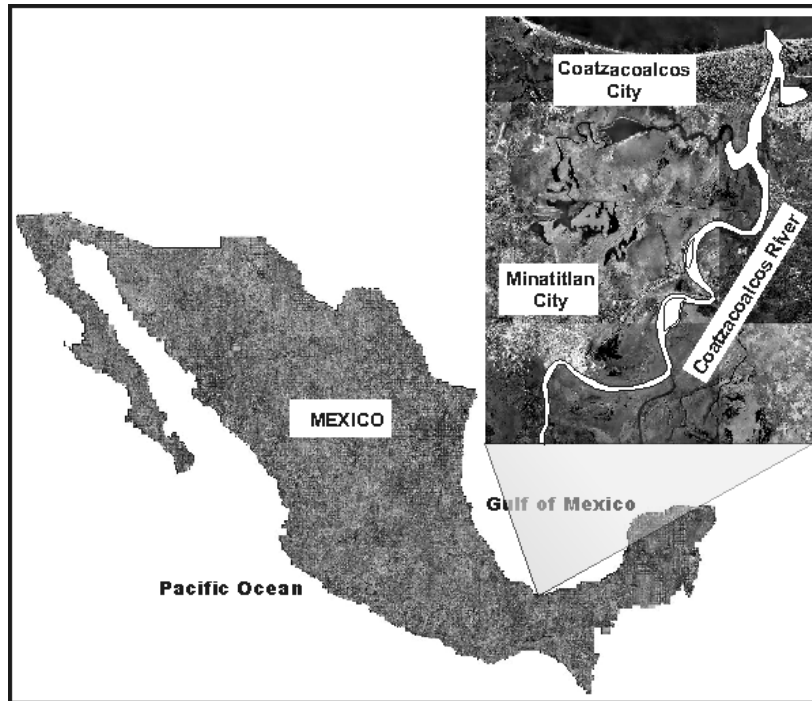


Fig. 4. Location of Coatzacoalcos River

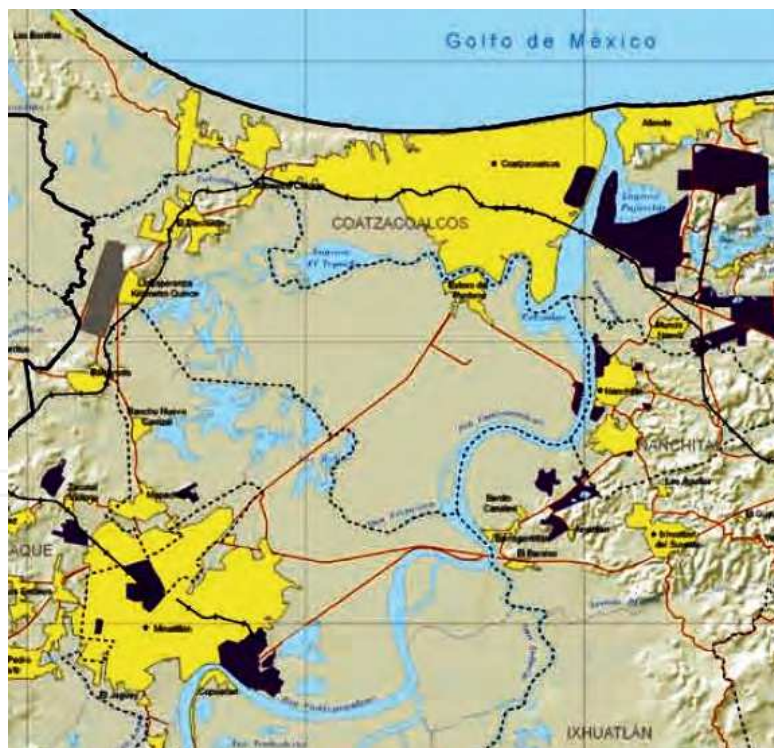


Fig. 5. Minatitlan-Coatzacoalcos industrial park and study zone

4. Results and discussion

We have developed a numerical model that solves the two-dimensional Saint-Venant equations and the Advection-Diffusion-Reaction equation to study the pollutants transport.

The model results show agreement with measurements of velocity direction and magnitude, as well with water quality parameters. Therefore, it is considered that the developed model can be implemented and applied to different situations for this study area and others rivers with similar characteristics.

4.1 Model validation

For validation purpose, a sampling and measurement campaign was carried out in the Coatzacoalcos river stretch from upstream of Minatitlan city ($17^{\circ} 57' 00''$ N - $94^{\circ} 33' 00''$ W) to its mouth in Gulf of Mexico ($18^{\circ} 09' 32''$ N - $94^{\circ} 24' 41.33''$ W). The main objective was to obtain velocities, bathymetry and water quality at 10 points of the Coatzacoalcos River (Fig. 6). The information obtained through direct measurements and chemical analysis is primarily used for testing and numerical model validation.



Fig. 6. Measurements and sampling sites

Table 1 shows the water velocity magnitude, direction and location measured on the ten stations. These values were compared with the model results. Fig. 7 and Fig. 8 show a comparison between measured and calculated water velocities.

As shown in Fig. 7 and 8, the hydrodynamics numerical results correspond fairly well with field measurements. The model results show agreement in direction and magnitude of the measured velocity, which demonstrate that the model results are consistent and reliable to the real river behaviour. Therefore, it is considered that the developed model can be implemented and applied to different situations for the studied area.

Likewise, the water quality modules were validated by comparison with field measurements, observing that the model results are consistent with these measurements

and they are in the same order of magnitude. Fig. 9 shows some of the obtained results (each point represents a measurement station and the solid line the model result).

Station	Latitude	Longitude	East Vel. (cm/s)	North Vel. (cm/s)	Resultant (m/s)	Direction (°)
1	17.96468	-94.5529350	-24.06	-42.34	0.49	60.39
2	17.97063	-94.4749317	4.75	23.65	0.24	78.65
3	18.01482	-94.4479867	-43.56	-8.69	0.44	11.28
4	18.06698	-94.4156000	-11.32	58.24	0.59	-79.00
5	18.08841	-94.4215717	-10.74	39.62	0.41	-74.83
6	18.1023	-94.4374683	9.38	-5.57	0.11	-30.69
7	18.1117	-94.4217833	36.78	-58.26	0.69	-57.74
8	18.12396	-94.4148883	34.06	-1.98	0.34	-3.33
9	18.13607	-94.4112700	6.62	-16.16	0.17	-67.72
10	18.16384	-94.4154150	-7.14	1.02	0.07	-8.15

Table 1. Measurements of water velocity

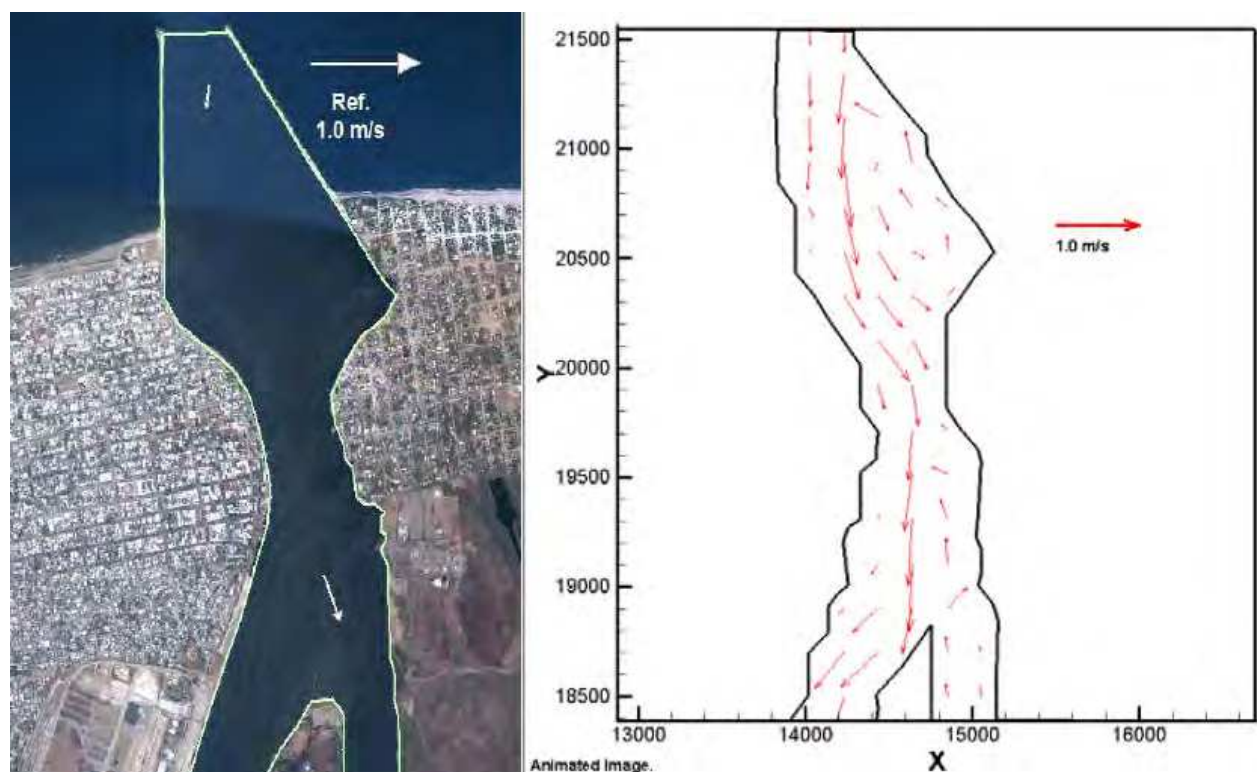


Fig. 7. Comparison between measured and calculated velocities for the river mouth

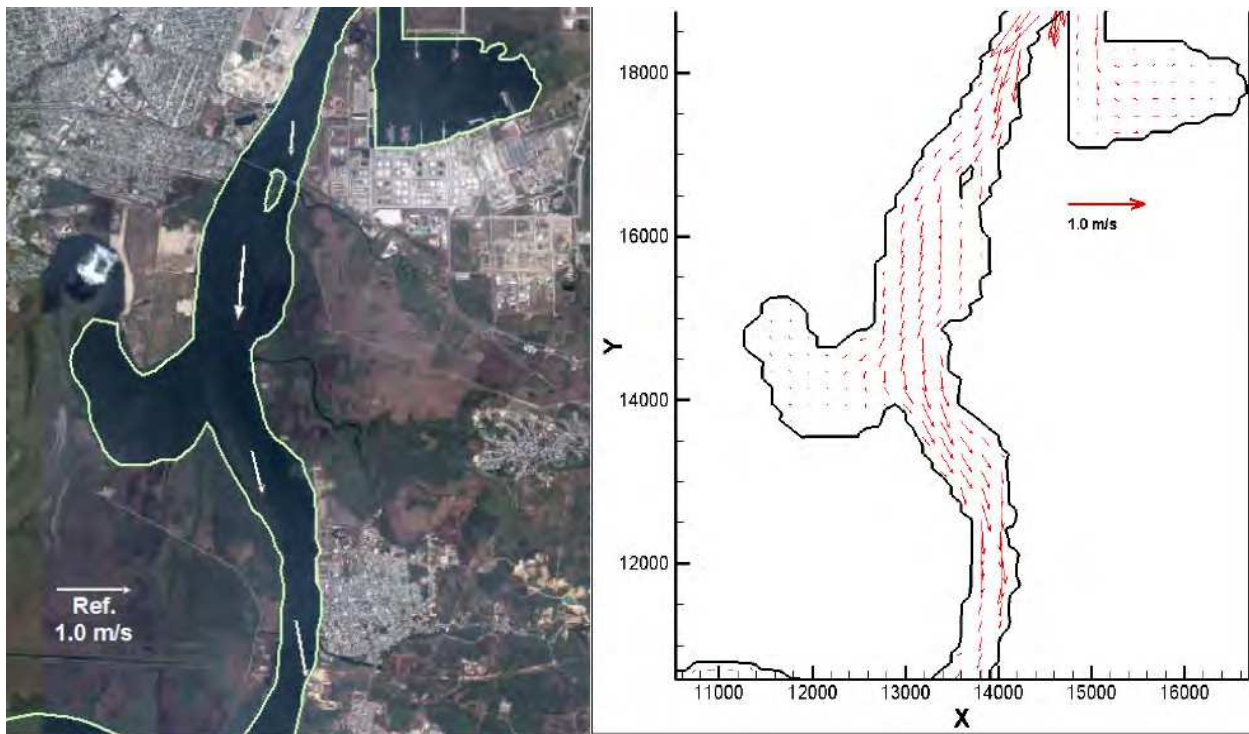


Fig. 8. Comparison between measured and calculated velocities for the river middle part

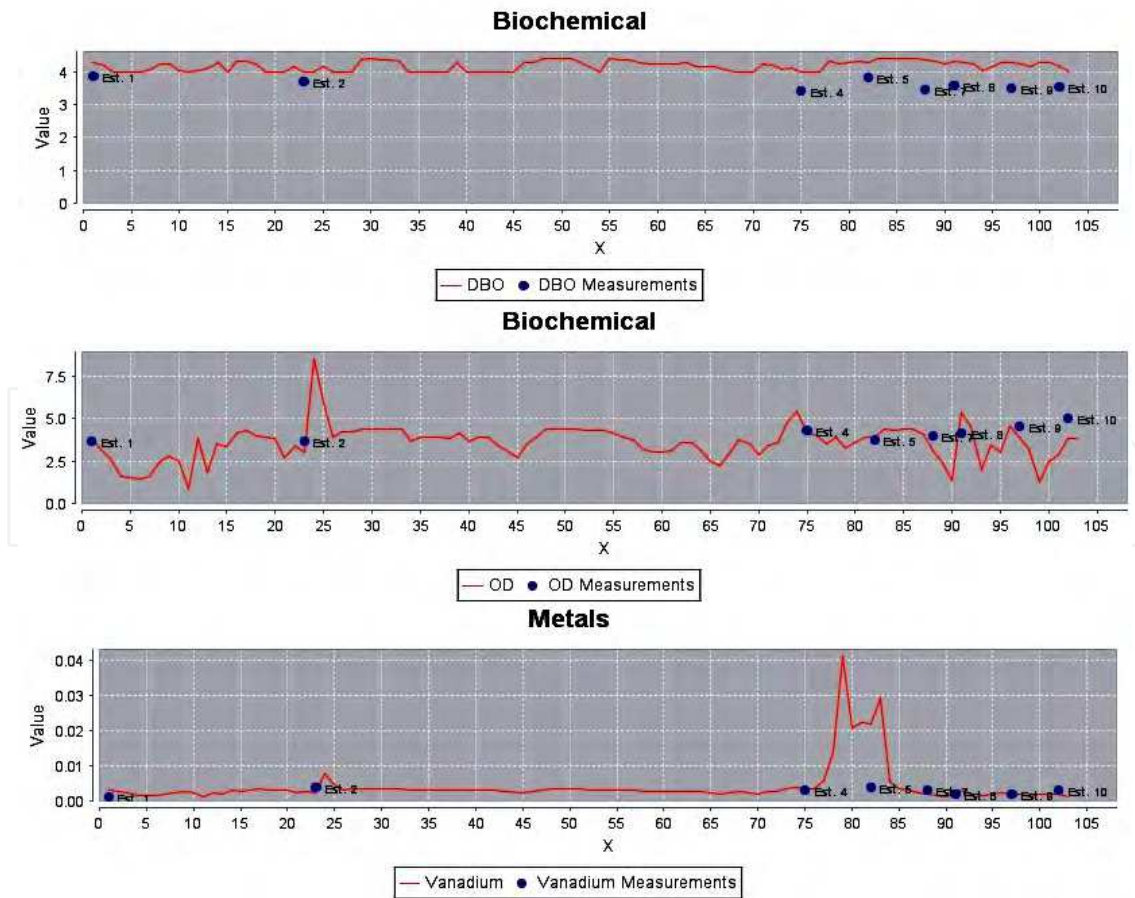


Fig. 9. Concentration profiles for measured and calculated DO, BOD and Vanadium

4.2 Numerical modeling

The initial step in the methodology implemented was the numerical grid generation, using specialized software. Initial and boundary conditions (tide, the level of free water surface, and hydrodynamic condition) were imposed; the model was set up with information gathered in the measurement campaigns, as well as water balances to determine the river dynamics.

The mesh or numerical grid was created using the program ARGUS ONE (<http://www.argusint.com>), Fig. 10 shows the calculation grid system for Coatzacoalcos river stretch, which has a length of about 25 km, spacing of $\Delta x = \Delta y = 100$ m. The grid has 163 element in the X direction and 211 points in Y direction, giving a total of 34393 elements.



Fig. 10. Grid configuration

Two simulation scenarios were performed representing dry season and rain season. The input data required are shown in Table 2: Manning roughness coefficient, hydrological flow, cross-sectional area, flow velocity and direction.

Parameter	Dry season	Rain season
Flow rate (m ³ /s)	405	1104.9
Cross section (m ²)	812.4	2216.7
Flow velocity (m/s)	0.5	0.5
Flow direction (°)	58.78°	60.39
Manning coefficient	0.025	0.025

Table 2. Initial data for simulations

4.3 Results of hydrodynamics simulations

The simulation represents 30 days corresponding to dry and rain season. The numerical integration time or time step was, $\Delta t = 2.0$ s. Fig. 11 shows the obtained result for resultant velocity.

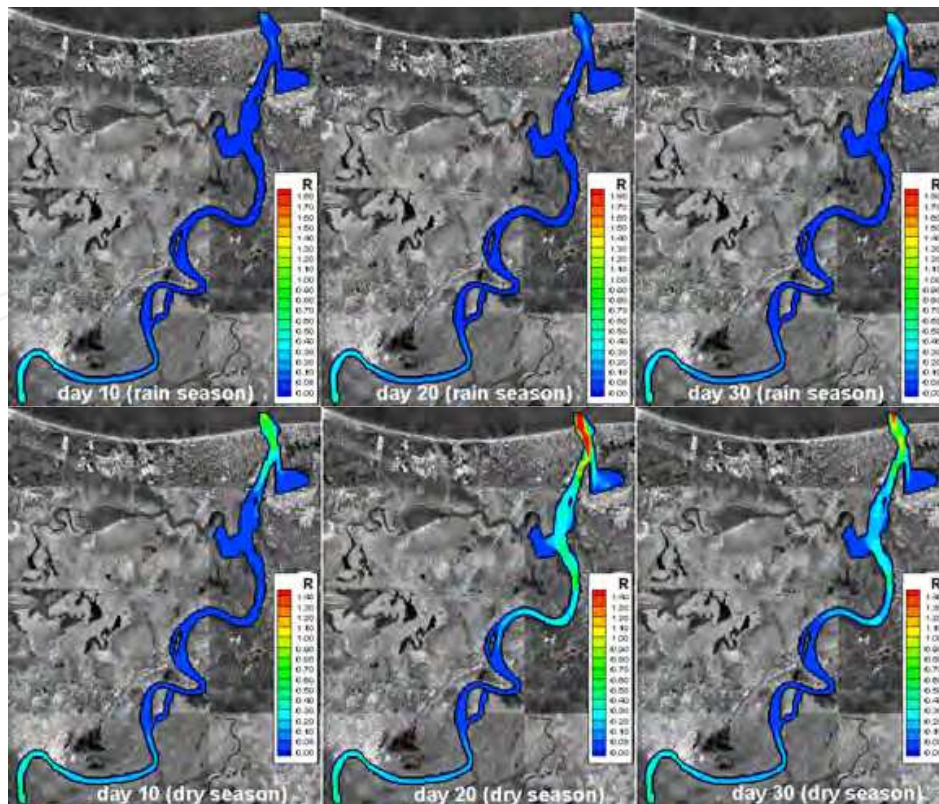


Fig. 11. Velocity contours of Coatzacoalcos River (rain and dry season) over time

4.4 Modeling of pollutant transport

This section presents some of the simulated parameters. Initially we describe the simulation scenario solved to provide a better idea and understand clearly what the simulations are representing.

4.4.1 Simulation scenario

To assess the water quality in Coatzacoalcos River, a representative discharge scenario was initially defined, highlighting the main activities and characteristics over this area (Fig. 12). The idea was study the river environmental behaviour, influenced by the oil activity developed on this area, six discharges were located representing the industrial activity and the influence of urban areas where such facilities industry are seated.

The discharge conditions for every simulated water quality parameter are presented in Table 3.

Discharge	Temp. (°C)	DO (mg/L)	BOD (mg/L)	Faecal Col. (NMP/100 ml)
Minatitlan	26.70	3.70	290.71	21,5000
Refinery	25.70	3.70	190.86	21,3000
Uxpanapa R.	24.70	3.70	190.70	21,7000
Nanchital	27.70	3.70	290.43	31,5000
Pajaritos P.C.	26.70	3.70	290.83	22,4100
Coatzacoalcos	25.70	3.70	110.60	21,4300

Table 3. Discharges conditions



Fig. 12. Discharge scenario

The following figures show the model results for these water quality parameters.

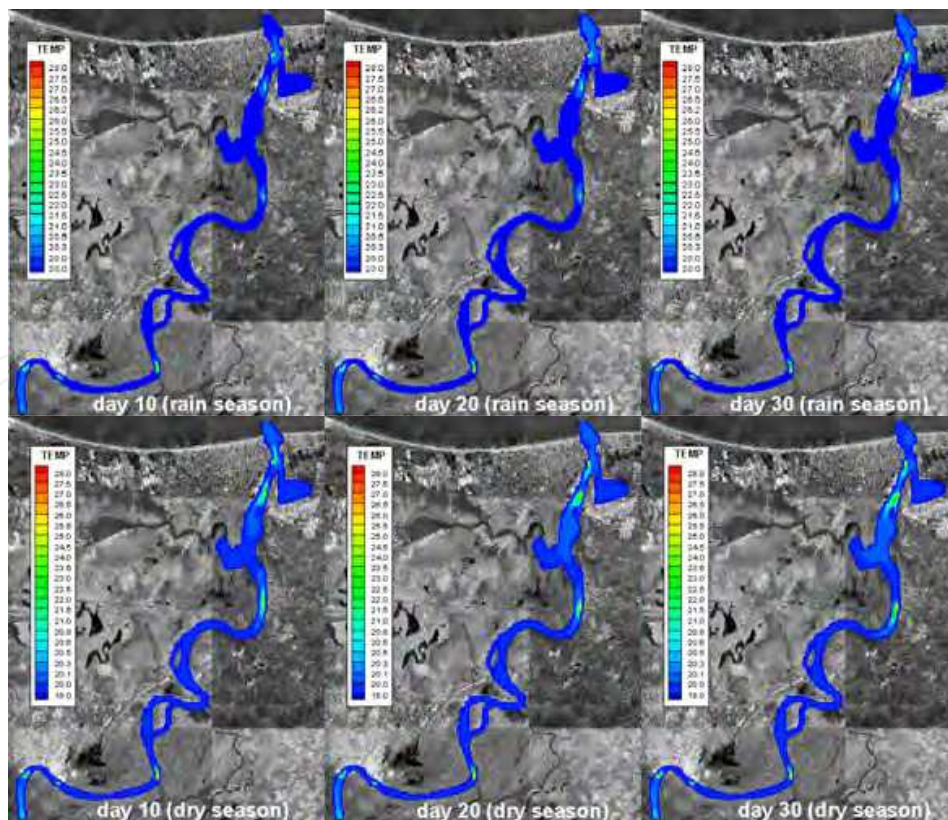


Fig. 13. Temperature simulations over time

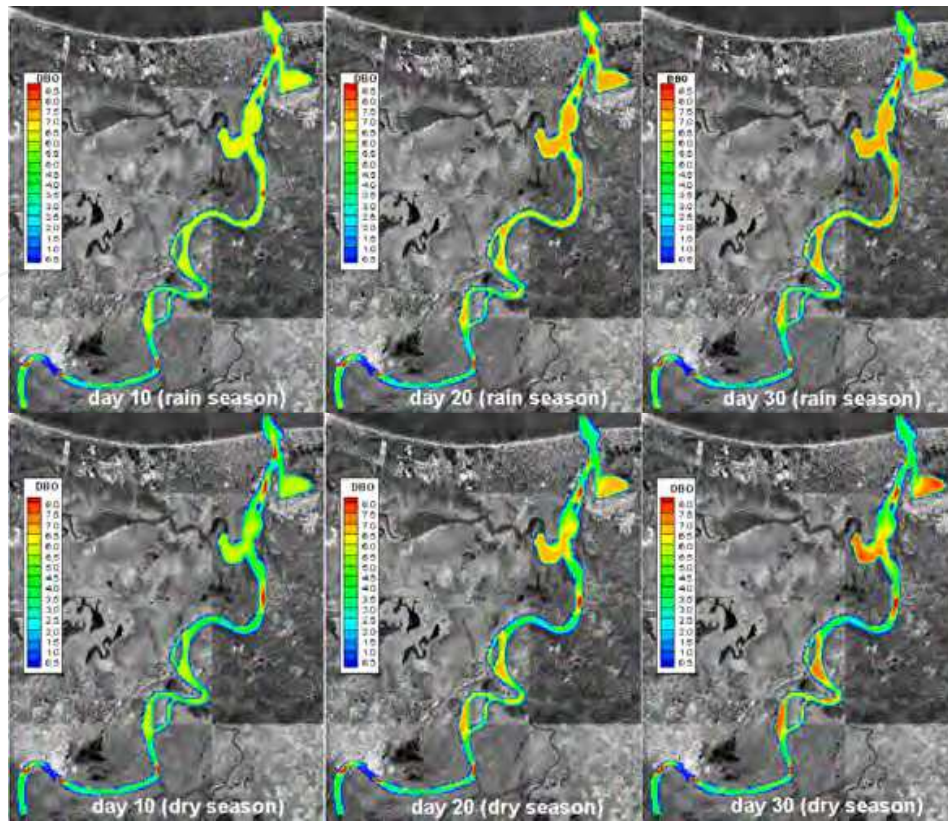


Fig. 14. Biochemical Oxygen Demand simulations over time

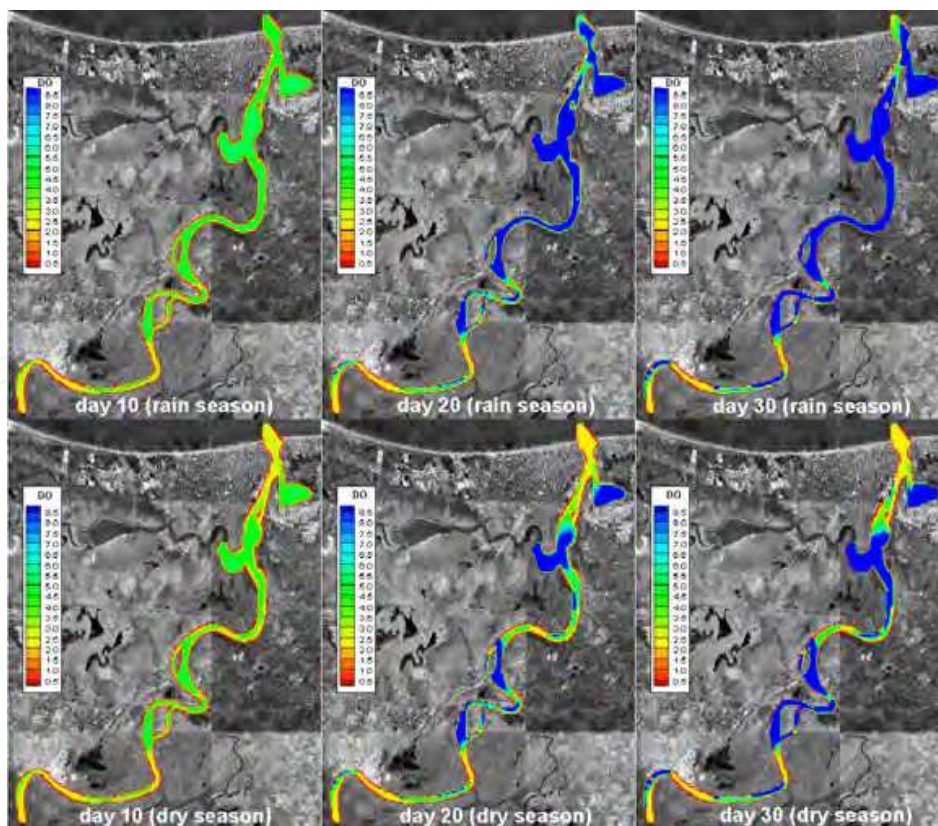


Fig. 15. Dissolved Oxygen simulations over time

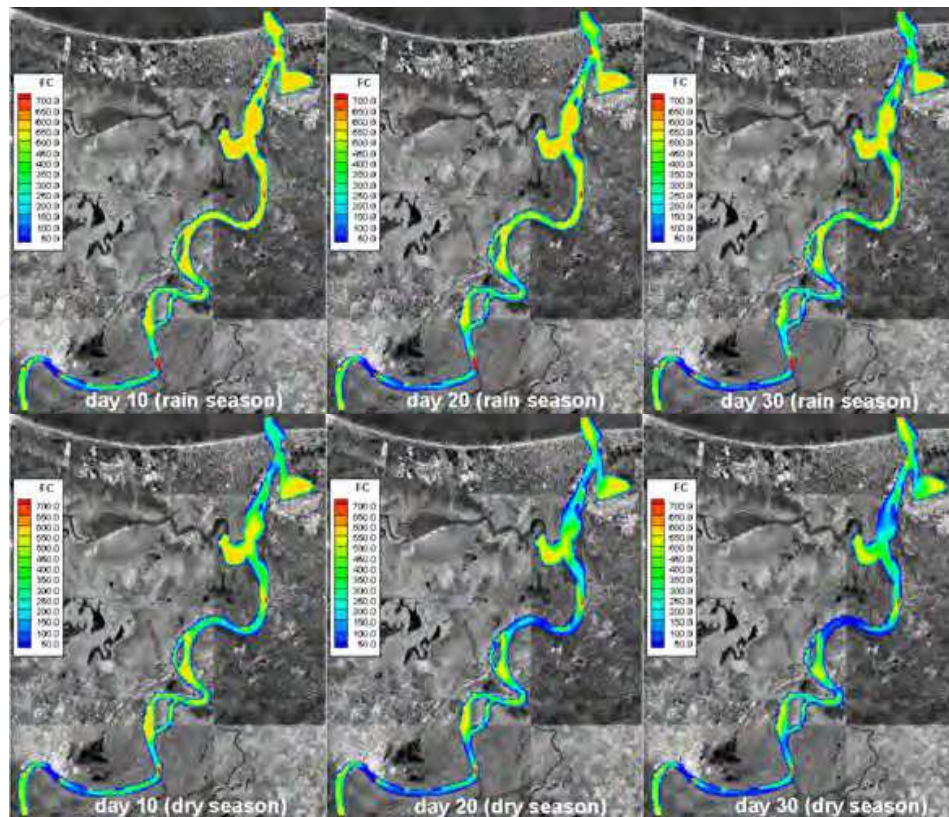


Fig. 16. Faecal Coliforms simulations over time

5. Conclusions

The solution obtained for the two-dimensional Saint-Venant and A-D-R equations using an Eulerian-Lagrangian method has great versatility, obtaining consistent and satisfactory results for different types of flow and open channel conditions. The considered scheme provides numerical stability that avoids numerical oscillations of the obtained solutions and also allows significant larger time steps (Δt). The combination with the Eulerian solution for diffusive terms is always guaranteed satisfying the C-F-L condition.

About the hydrodynamics study of Coatzacoalcos river, it was determined that the river behaviour is influenced by several factors, being the most important the hydrological aspect, which varies depending on the time of the year. Because of this, it was observed that dry season presents an important tide penetration towards the mainland of the river, while for rain season when the river flow increase, the penetration is less significant and the water mainly flows downstream to the mouth in the Gulf of Mexico.

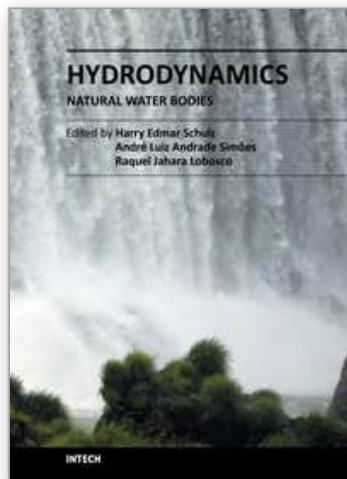
On the other hand, the pollutants transport is dominated strongly by the hydrodynamics, and the difference for the two simulated seasons was observed. This simulation shows higher concentrations and also a more significant dispersion in dry season, because the tide penetration occurs intermittently upstream and downstream in the area near to the river mouth. While for rain season there is no significant contaminant dispersion, with a local effect of the simulated discharges.

Thus, a solution algorithm has been proposed to the study open channel hydrodynamics, which together with the A-D-R equation solution allows the study of transport,

transformation and reaction of pollutants, being the basis of the water quality model proposed.

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The knowledge of the characteristics of the fluids and their ability to transport substances and physical properties is relevant for us. However, the quantification of the movements of fluids is a complex task, and when considering natural flows, occurring in large scales (rivers, lakes, oceans), this complexity is evidenced. This book presents conclusions about different aspects of flows in natural water bodies, such as the evolution of plumes, the transport of sediments, air-water mixtures, among others. It contains thirteen chapters, organized in four sections: Tidal and Wave Dynamics: Rivers, Lakes and Reservoirs, Tidal and Wave Dynamics: Seas and Oceans, Tidal and Wave Dynamics: Estuaries and Bays, and Multiphase Phenomena: Air-Water Flows and Sediments. The chapters present conceptual arguments, experimental and numerical results, showing practical applications of the methods and tools of Hydrodynamics.

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Slavka Krautzeka 83/A
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Phone: +86-21-62489820
Fax: +86-21-62489821

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