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Modelling Water Quality with Iber

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WP4: Accidental water pollution

Practical exercise I

Wastewater discharge of CBOD and ammonia in a river (Iber)

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1 Practical Example I: Wastewater discharge of BOD and ammonia in a river modelled with Iber

1.1 Objectives

This example introduces the options available in Iber's nitrogen cycle, dissolved oxygen cycle, and organic matter modules (Cea et al., 2016). We will look at the evolution of discharge from a wastewater treatment plant into a river reach. This plant releases a continuous discharge of organic matter and nitrogen in the form of ammonia and nitrate. We will analyse the levels of DO (dissolved oxygen), NH3-H (ammoniacal nitrogen), NO3-N (nitrate-nitrite nitrogen) and CBOD (carbonaceous biochemical oxygen demand) in the river once a steady state is achieved. We will then compare the concentrations predicted in Iber with the observed concentrations presented in Thomann & Mueller (1987).

1.2 Description of the case study and input data

The example consists of a river with an annual discharge of 100 ft3/s (2.83 m3/s) in which a wastewater treatment plant discharges effluent containing organic matter, ammonia and nitrates. We want to analyse the evolution of dissolved oxygen, organic matter and nitrogen over 50 km of the river under steady state conditions.

The example is presented in Thomann & Mueller (1987) (Figure 1).

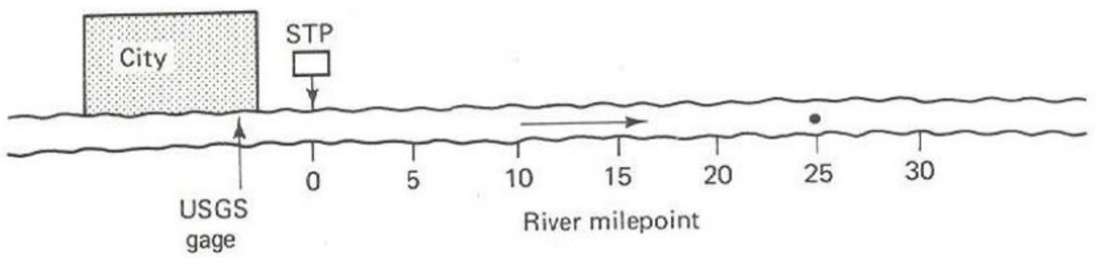

Figure 1.Schematic diagram of the case study from Thomann & Mueller (1987).

Since the length of the river reach is much larger than its width, the geometry will be conceptualized as a straight channel with a rectangular cross section, with uniform slope and dimensions along the reach, as proposed in Thomann & Mueller (1987). Figure 2 schematically represents the geometry of this example. Note that in this figure the scales on the longitudinal and transverse directions are different.

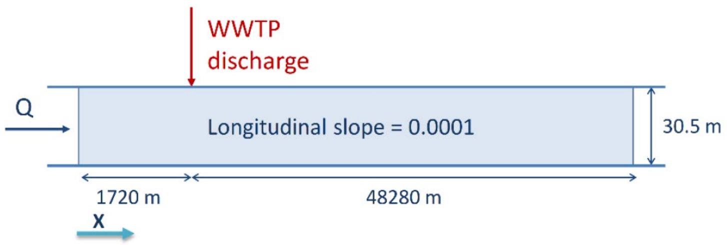

Figure 2. Schematic diagram of the case study from Thomann & Mueller (1987).

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The complete scheme for this exercise, with the characteristics of the effluent from the wastewater treatment plant and the river, is shown in Figure 3. Please note that the variable units in the scheme are different to those used in the Iber model.

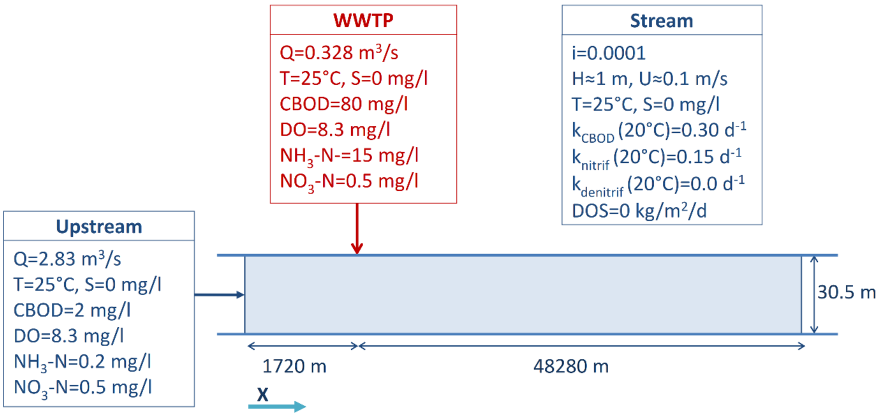

Figure 3. Schematic diagram of the case study.

We will ignore the denitrification process ($k_{denitrif}$ = 0 d^{-1}), since it only occurs in anoxic conditions, and dissolved oxygen concentrations are relatively high throughout the reach (we will later verify in the results that this is the case). Values for the **CBOD** degradation rate (k_{CBOD}) and the nitrification rate (k_{nitrif}) are taken directly from Thomann & Mueller (1987).

The salinity and temperature equations will not be calculated. Instead, we will directly assign the values of these variables (**S** and **T** in Figure 3), assuming they are uniform along the reach and constant over time.

The observed in-stream concentrations of **DO**, **CBOD**, **NH_3-N** and **NO_3-N** downstream from the discharge as presented in Thomann & Mueller (1987) provide a benchmark comparison for the numerical results obtained with Iber. These point measurements are shown in Table 4 and are included in the file **field_data.grf**.

Table 1.Observed in-stream concentrations along the reach (distance X is measured as indicated in Figure 3).

X(m)	CBOD(mg/l)	NH_3-N(mg/l)	NO_3-N(mg/l)	DO(mg/l)
1300	2.4	0.3	0.5	7.6
4500	9.8	1.6	0.6	6.4
8300	7.0	1.7	0.6	6.5
12800	5.8	1.5	1.1	5.4
19000	6.0	1.0	0.9	6.1
26900	4.4	0.9	1.1	6.3
35100	3.4	1.1	1.7	6.3
47700	0.6	0.8	1.7	7.2

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1.3 Model set-up

1.3.1 Geometry

After launching the model and creating a new project (**Files>>Save**) we are ready to set up the model. The basic steps are described in this section. First, we create the geometry of the model. This consists of a single rectangular surface with a slope of **0.0001** in the longitudinal direction.

We manually introduce the coordinates of the start and end point of each line (**Geometry>>Create>>Straight line**). The elevation of the inlet and outlet boundaries are **Z=5** m and **Z=0** m, respectively. Once the four sides of the rectangle have been defined according to the scheme shown in Figure 4, we create a rectangular **NURBS** surface (**Geometry>>Create>>NURBS surface**).

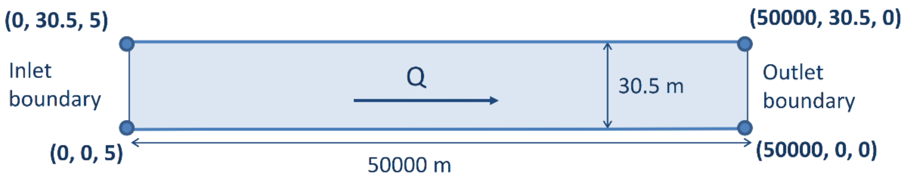

Figure 4. Definition of the rectangular surface in the model.

1.3.2 Hydrodynamics

The next step is to assign the **hydrodynamic boundary** and **initial conditions** (**Data>>Hydrodynamics>>Boundary Conditions**). At the upstream boundary, we assign a discharge of **Q=2.83 m³/s**. At the downstream boundary we set a water surface elevation **1 m**. As the initial condition we impose a water depth to **1 m** throughout the domain (**Data>>Hydrodynamics>>Initial Conditions**).

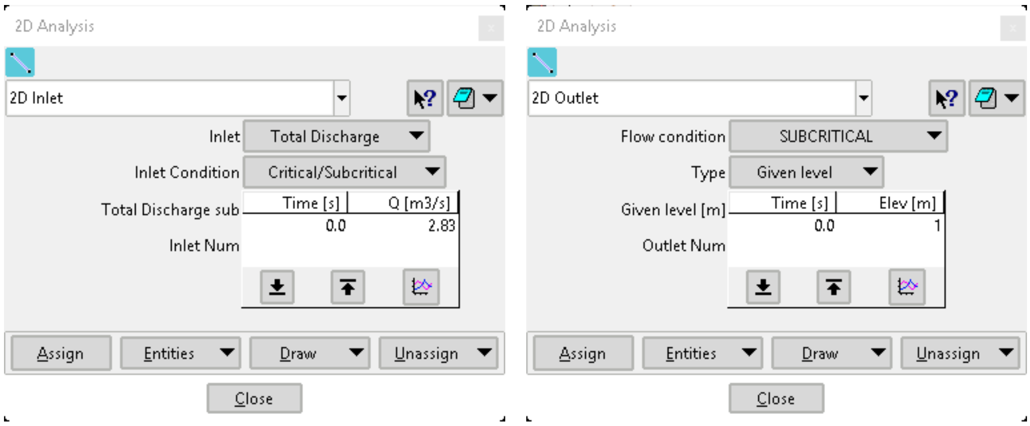

Figure 5. Boundary conditions tab to introduce the upstream discharge and the downstream water level.

As indicated in Figure 3, the water depth and velocity in the reach are approximately **1 m** and **0.1 m/s**. In order to satisfy these values of **velocity** and **depth**, we have to define a suitable **Manning roughness coefficient (n)**, according to:

$$U = \frac{1}{n} \cdot R_h^{3/2} \cdot i^{1/2} = \frac{1}{n} \cdot h^{3/2} \cdot i^{1/2} \tag{1}$$

where ***U*** is the water velocity, ***R***R_h is the hydraulic radius, ***h*** is the depth and ***i*** is the slope. For **U=0.1** m/s, **h=1** m, given the slope of **i=0.0001**, we have to set a Manning coefficient of **0.10** s·m$^{-1/3}$ throughout the domain (**Data>>Roughness>>Land Use**). These values correspond to the lowest part of the river reach, downstream of the **WWTP discharge**. At the point where the discharge occurs there will be a local variation of depth and velocity.

1.3.3 Water quality

We now introduce the water quality data. We first define the boundary conditions of the model (**Data>>Water Quality>>Boundary Conditions**). We assign separately the conditions referring to the dissolved oxygen, the **CBOD** and the nitrogen cycle, only at the upstream boundary (vertical left line of the channel). In accordance with Figure 3, we introduce the following values in the corresponding tabs (Figure 6): **CBOD=0.002 kg/m^3**, **DO=0.0083 kg/m^3**, **NH_3-N=0.0002 kg/m^3** and **NO_3-N=0.0005 kg/m^3**.

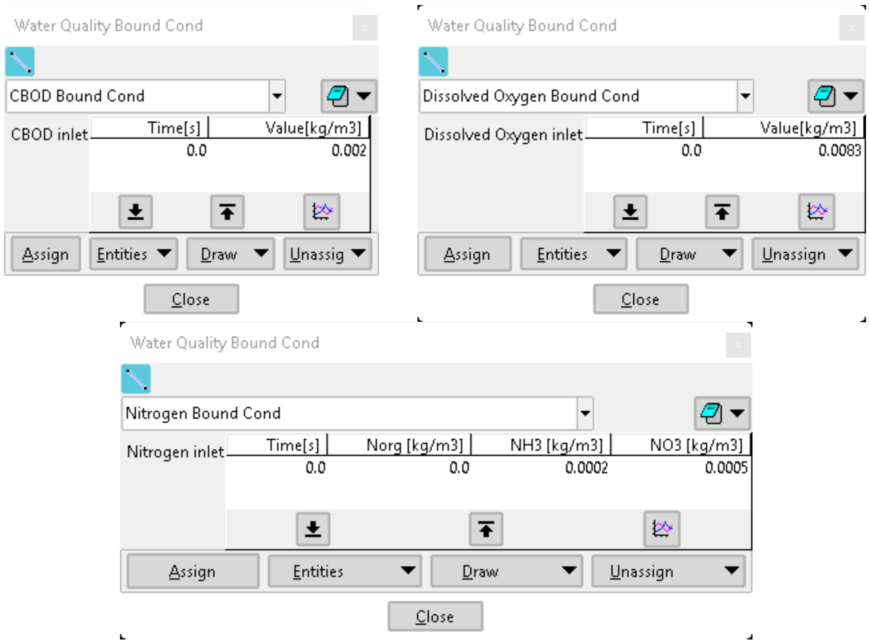

Figure 6. Water quality boundary conditions tab to introduce the upstream DO, CBOD, NH_3-N and NO_3-N concentrations.

We then specify the initial water quality conditions in the whole reach (**Data>>Water Quality>>Initial Conditions**). As with the previous step, we introduce separately the conditions for the dissolved oxygen, the CBOD and the nitrogen cycles (Figure 7). We use the same values as for the upstream boundary condition. However, this choice is not relevant for the current example, since we are only interested in the final results, when the steady state is reached, these being independent of the initial conditions.

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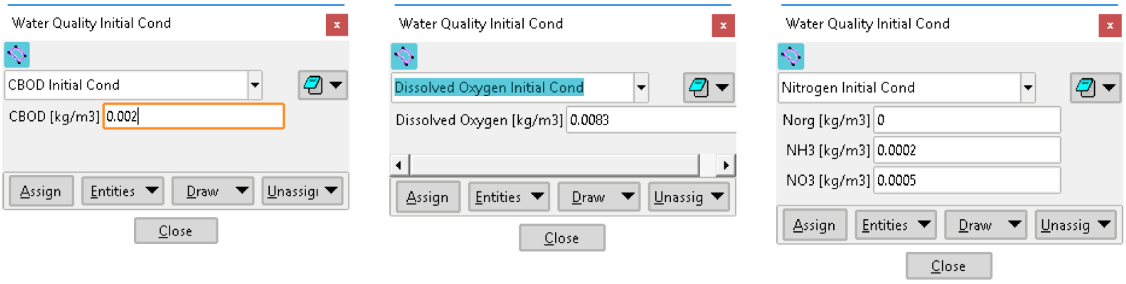

Figure 7. Water quality initial conditions tab to introduce the DO, CBOD, NH_3-N and NO_3-N initial concentrations.

We are not interested in the sediment oxygen demand, and therefore we set a value of **0 kg/m²/d** throughout the domain (**Data>>Water Quality>>Sediment Oxygen Demand**) (Figure 8).

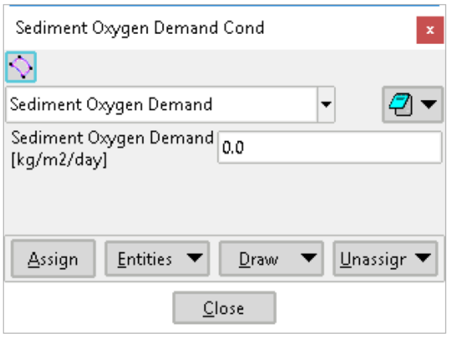

Figure 8. Sediment oxygen demand tab.

Finally, we introduce into the model the discharge of the wastewater treatment plant. To do this, we create a new discharge (**Data>>Water Quality>>Discharges**) and manually specify its location. According to Figure 3, the discharge is located at **X=1720 m**. In the transverse direction, we introduce the discharge in the middle of the river (**Y=15.25 m**). This is in fact not relevant here, since we will create a mesh with a single element in the transverse direction, therefore assuming complete mixing in this direction. Given that Iber is a depth-averaged model, the location of the discharge on the **Z axis** is also not relevant here. We arbitrarily set it at **Z=0 m**.

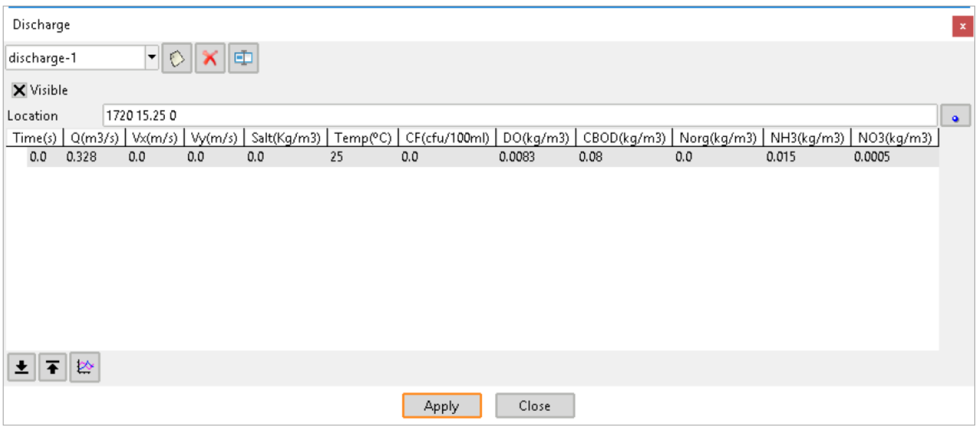

Figure 9. Discharge tab to introduce the location and water quality characteristics of the effluent of the wastewater treatment plant.

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We must also introduce the flow rate and the water quality characteristics of the effluent of the wastewater treatment plant (Figure 9). According to Figure 3, we introduce the following values: **Q=0.328 m³/s**, **CBOD=0.08 kg/m³**, **DO=0.0083 kg/m³**, **NH_3-N=0.015 kg/m³** and **NO_3-N=0.0005 kg/m³**.

Once the discharge data has been introduced, its location will be displayed in the model geometry (with points on the **X** and **Y** coordinates indicated above).

1.3.4 Mesh

The next step is to create a computational mesh to spatially discretize the domain. We use a structured mesh made of rectangular elements. Since the length of the river reach is three orders of magnitude larger than the river width, the mesh has a single element in the transverse direction. In the longitudinal direction, the spatial domain covers a total distance of **50 km**, and we select a mesh size of **100 m**. We therefore assign the following number of cells in the surface: **1 cell** in the transverse direction and **500 cells** in the longitudinal direction (**Mesh>>Structured>>Surfaces>>Assign number of cells**). When we generate the mesh (**Mesh>>Generate**) we obtain **500 elements** of **30.5 m x 100 m**.

1.3.5 Calculation data

Before running the model we need to set the computation parameters (**Data>>Problem Data**). First, we select the time parameters (Figure 10). We choose a maximum simulation time of **7 days (604,800 s)** to allow the model to reach a steady state. Bear in mind that the total length of the reach is **50 km** and that velocities are in the order of **0.1 m/s**, so that the time it takes the water to traverse the reach is around **500,000 s**. This value is an approximation, since the concentration of organic matter, dissolved oxygen and nitrogen depends not only on its advection by the mean flow along the channel, but also on the interaction processes between these components. Therefore, we need to check in the post-processing that a steady state has really been achieved. We will use time evolution graphs of the different variables for this. Given that we are not interested in the transient results, we choose a wide time interval of **10,800 s** for storing the results (i.e., one result every **3 hours**).

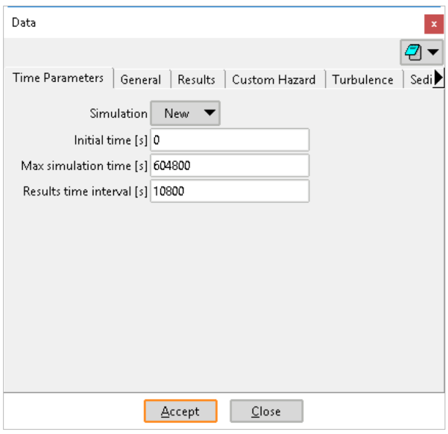

Figure 10. Time parameters tab to assign the initial time, maximum simulation time and results time interval.

We then establish the parameters and kinetics related to water quality. First, we set the temperature and salinity values at **25 °C** and **0 kg/m³**, respectively (Figure 11). Second, we activate

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the dissolved oxygen, **CBOD** and nitrogen modules and define the reaction kinetic constants (Figure 11 and Figure 12). As indicated in Figure 3, the first order kinetic coefficients for organic matter degradation, nitrification and denitrification are **k_{CBOD}=0.30 d^{-1}**, **k_{nitrif}=0.15 d^{-1}** and **$k_{denitrif}$=0 d^{-1}**.

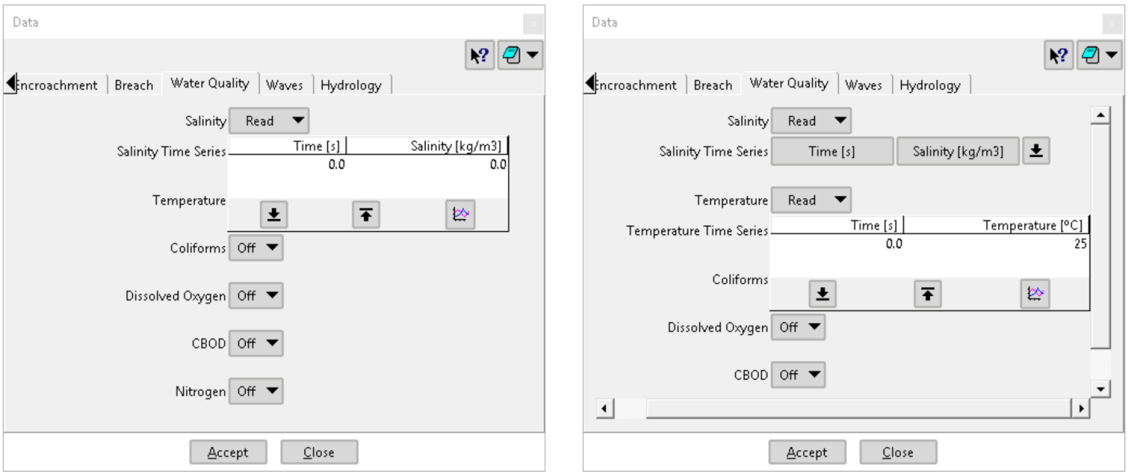

Figure 11. Water quality tab to assign the salinityand temperature values.

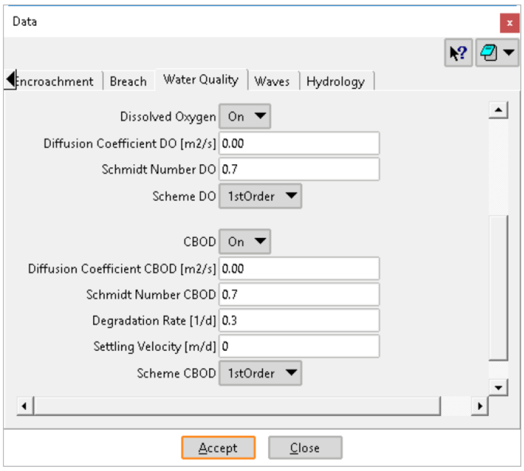

Figure 12. Water quality tab to define the DO and CBOD kinetics.

The organic nitrogen hydrolysis rate does not influence the results, since the concentration of organic nitrogen is zero throughout the domain. The same is true for the settling velocity of organic nitrogen. We can thus leave the default values for the ammonification rate and the organic nitrogen setting velocity. The settling for the organic matter also has little influence on the **CBOD** concentrations compared to the degradation process. We can thus ignore this process and enter a setting velocity of **0 m/d** (Figure 12).

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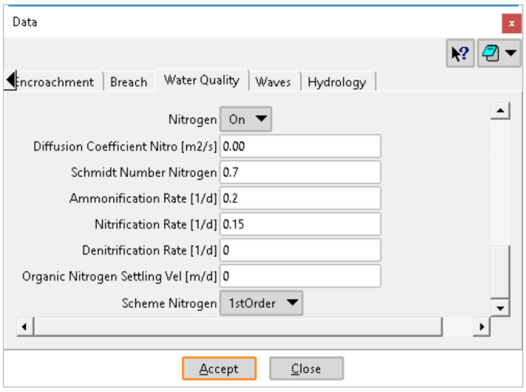

Figure 13. Water quality tab to define the nitrogen kinetics.

We are now ready to run the model (**Calculate>>Calculate**). Although the mesh has only **500 elements**, we will simulate **7 days**, so the calculation may take a few minutes. Once the calculation is finished, we can go to the post-processing tab to analyse the results.

1.4 Analysis of results

1.4.1 Initial checks

The results are first checked to ensure that a steady state is achieved at the end of the simulation. We plot the time evolution of all variables (**DO**, **CBOD**, **NH_3-N** and **NO_3-N**) at a point close to the downstream boundary (e.g., **X=49050 m**) (Figure 121). In order to do this, we open the **View graphs** window and click on the **Create tab**. **Select View: Point Evolution, Analysis**: **Water Quality**. Then choose the variable to plot on the **Y-axis**, starting for example with the **dissolved oxygen concentration (DO)**. Press **Apply** and introduce the coordinates of the point in the command line (**e.g., 49050,15**). Once we have repeated the procedure for the other variables (**CBOD, NH_3-N and NO_3-N**), we obtain a figure like the one shown in Figure 14. We can see how a steady state is achieved for all variables around **t=500,000 s** (dotted line in Figure 14).

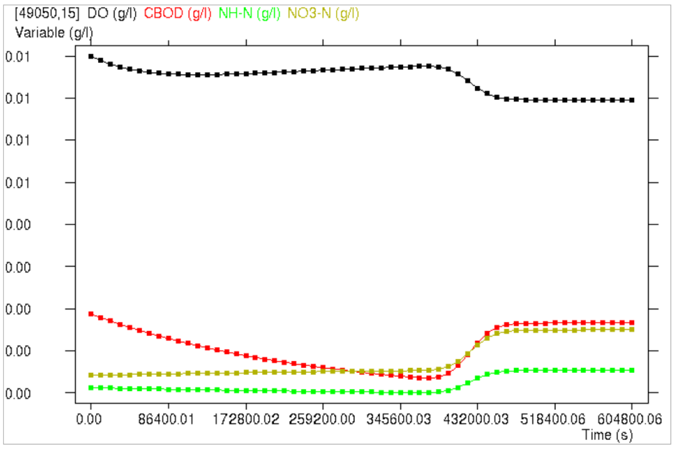

Figure 14. Temporal evolution of DO, CBOD, NH3-N and NO3-N concentrations at X=49050 m.

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1.4.2 Hydrodynamic results

Before analysing the water quality results, it is a good idea to check the hydrodynamic results. Water velocity and depth in the river should be in the order of **0.1 m/s** and **1 m**, respectively. We create a longitudinal profile using the **create profiles** icon ( ) on the Iber toolbar (**located at the left part of the interface**), and manually enter the coordinates of the start and end points of the profile, as shown in Figure 15.

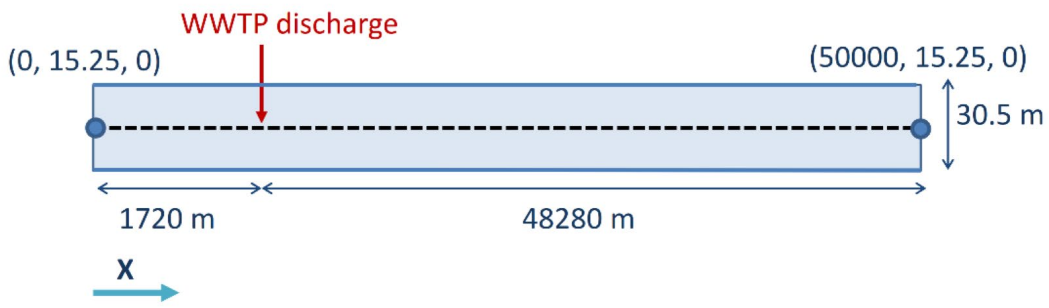

Figure 15. Definition of the longitudinal profile of the river.

Once the profile is created, we open the **Graph** window (**Window>>View graphs>Create**). With the **Border graph** tool, we plot the **water depth** and **velocity** along the profile at the last time step of the simulation. The depth and velocity values should be in the range of **0.92 - 1 m** and **0.090 - 0.096 m/s**, respectively, downstream of the discharge (Figure 123).

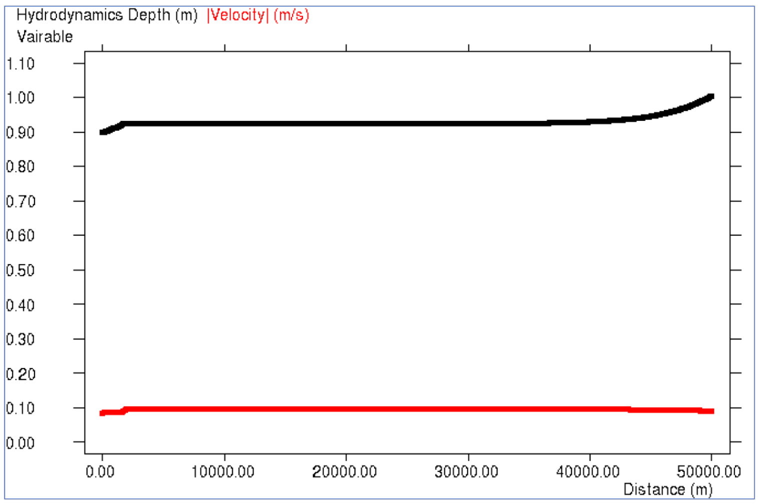

Figure 16. Depth and velocity profiles along the longitudinal axis of the river at the end of the simulation.

1.4.3 Water quality results

We now begin the analysis of the water quality results. We plot the longitudinal profiles of **DO**, **CBOD**, **NH_3-N** and **NO_3-N** concentration, using the profile that we created in the previous step (Figure 15). We select the last time step of the simulation to plot the results under steady state conditions. The results should look like the image below (Figure 17).

The WWTP discharge has higher **CBOD** and **NH_3-N** concentrations than the river in its natural state (the upstream boundary conditions). Therefore, the **WWTP** discharge produces a sudden change in **NH_3-N** and **CBOD** concentrations. The same does not apply for **DO** and **NO_3-N**, given that the effluent from the **WWTP** and the river have the same concentrations.

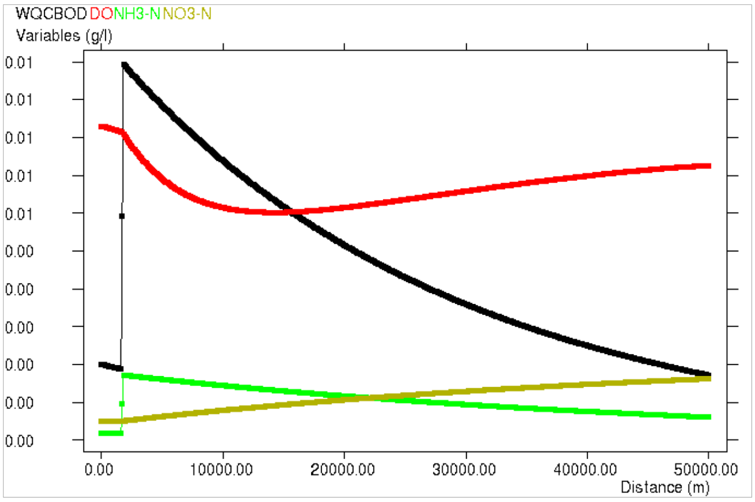

Figure 17. Concentration profiles of DO, CBOD, NH3-N and NO3-N along the longitudinal axis of the river at the end of the simulation.

The discharge of **CBOD** and ammonia induces a decay in the concentration of **DO** along the first **10 km** downstream of the discharge due to the oxygen demand of the processes of biodegradation and nitrification. **DO** concentration reaches a minimum value of around **6 mg/l**. Further downstream the biodegradation and nitrification rates diminish due to the lower concentration of **CBOD** and **ammonia**, and the concentration of **DO** increases progressively by surface reaeration. However, the **DO** at the downstream end of the reach has not yet recovered to the original **DO** levels.

As explained in the input data section, we have ignored the denitrification process due to the relatively high **DO** concentrations throughout the reach. We have now verified that this was indeed the case by means of the **DO** profile shown in Figure 17.

We will now compare the concentrations predicted by the model with the observed concentrations presented in Thomann & Mueller (1987) (shown in Table 1). In order to do so, we must change the name of the **graph-set to "WQ"** and then import the file **field_data.grf** (**Files>>Import>>Graph**). Note that the values shown in **Table 1** have been converted to the **International System of Units**.

We compare the simulated and measured concentrations using **graphs**. We plot the simulated **concentrations** as **continuous** lines and the **measured** concentrations as data **points** (Figure 18).

It can be seen how the numerical model correctly reproduces the observed spatial evolution of the four variables considered, despite the simplifications made in the geometry of the river. There are of course some errors and dispersion in the field measurements, but the trend over the analysed section is well captured by the numerical model.

The differences between the model data and the field data are to some extent due to the simplification of a **50 km river reach** to a rectilinear channel of a rectangular section with a constant width and slope.

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In this exercise we have taken directly the values of the reaction constants proposed in Thomann & Mueller (1987), which have been previously calibrated. In a real case we would need to calibrate these to achieve a good level of agreement between the numerical results and the measurements.

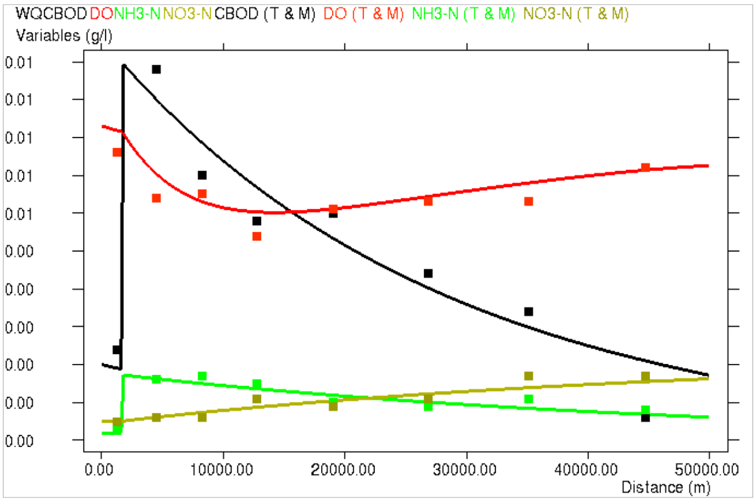

Figure 18. Longitudinal concentration profiles of DO, CBOD, NH3-N and NO3-N obtained with Iber and comparison with measured concentrations.

1.5 Conclusions

In this exercise we have analysed the evolution of dissolved oxygen, organic matter and nitrogen in a 50 km river reach. Due to the length of the reach, we have simplified the geometry to a rectilinear channel of a rectangular cross section, and we have assumed that there is complete mixing in the transverse direction of the river. The calculation mesh in Iber thus has a single element in this direction. The reaction kinetic constants have already been calibrated for this test case in Thomann & Mueller (1987).

Despite the simplifications made, the model correctly reproduces the observed evolution of the water quality variables along the reach.

1.6 Data

Data for the exercise can be downloaded from this link: https://hydroeurope.upc.edu/wp-content/uploads/2024/10/Data_WQ_E1.zip

1.7 References

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