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Micropollutant and sediment interaction models using WAQTEL-MICROPOL module

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Abstract – **The MICROPOL sub-module of WAQTEL simulates the exchanges of micropollutants between three compartments of the water column: Water (dissolved form), suspended sediment (adsorbed) and bed sediments (deposited). Micropollutant transport is mainly impacted by sediment processes (transport, deposition, and resuspension) and chemical reactions (sorption, desorption and decay) in 2D/3D. This article presents recent model development allowing to simulate transport of micropollutant considering one or two-step adsorption/desorption reversible reactions. In the first case, the dissolved form of micropollutant exchanges through direct adsorption or desorption with suspended sediments, forward and reverse kinetics being pseudo-1st order. In the second case, slowly reversible internal sediment sites are considered as an additional micropollutant tracer, exchanging concentration with surfacic sediment sites, internalisation and externalisation kinetics being pseudo-1st order. This new version of MICROPOL was integrated into the TELEMAC system and validated with analytical solutions on multiple test-cases available on the TELEMAC validation manual. A real study case of the use of this WAQTEL module in the Loire Estuary is also presented. A fixed concentration of sediment and micropollutant was injected in the upstream boundary condition, decay and kinetic parameters were chosen to study the impact of the different model hypothesis available in the MICROPOL settings.**

Keywords: Micropollutant, Sediment transport, pollutant transport, WAQTEL-MICROPOL.

I. INTRODUCTION

Hydrodynamic modelling is an effective tool to assist decision making related to continuous or accidental micropollutant release. Model complexity must be adjusted to match intricated settings such as uneven topography, stratified water bodies or interactions between multiple components. Evaluating the effect of sediments on pollutant transport in 2D or 3D is necessary to accurately locate pollutant concentrations [1]. Previous studies were made on the subject using the TELEMAC system for bacterial [2] and radionuclide [3] release models, on account of the high spatiotemporal resolution and user-defined processes.

The MICROPOL sub-module of WAQTEL simulates the evolution of micropollutants (metals or radioelements) and their interaction with sediments (suspended or deposited). Concentrations of particles (pollutants or sediments) are represented as advected tracers in the water column. In the V8P3 version of TELEMAC, WAQTEL-MICROPOL module was able to correctly model micropollutant transport in 2D using 1st order kinetic exchanges. The 3D model could not properly model sediment settling, erosion of bed sediments and carried unstable operations on pollutant tracers. TELEMAC solves tracer advection diffusion equation:

$$F(C) = \frac{\partial c}{\partial t} + \boldsymbol{U}.\boldsymbol{\nabla C} - \nabla.(\mathrm{k}\boldsymbol{\nabla C}) = S, \qquad (1)$$

with $C(x; y; z; t)$ is the tracer concentration, t is time, $(x; y; z)$ the coordinates, k the diffusion coefficient (m²/s), U the velocity vector (m/s), $S(x; y; z; t)$ the internal source term.

Suspended Particulate Matter (SPM) can adsorb micropollutants in rivers and estuaries [4]. In WAQTEL, suspended sediments are advected and dispersed as tracers while bed sediments remain stationary. Two main sedimentary physical phenomena can occur depending on the sediment and water conditions: settling in smooth waters and erosion/re-suspension in high flow areas ([6], [7] and [8]). Combining micropollutant and sediment transport, TELEMAC considers 5 tracers:

- suspended matter (SS),
- bottom sediments (SF),
- dissolved species of micropollutant (C),
- the fraction of micropollutant adsorbed on suspended particulate matter (C_{ss}),
- the fraction of micropollutant adsorbed on bottom sediments (C_{ff}).

Whether in suspension or deposited on the bottom, the matter is a passive tracer: in other words, it does not influence the flow (no feedback). This hypothesis involves that the deposits depth must be negligible compared to the water depth (the bed is assumed to be unmodified).

There is no direct adsorption/desorption of dissolved micropollutants on the deposited matter, only on SPM (the model assumes a preponderance of water – SPM exchanges over direct water – bottom sediment exchanges). Contaminated particles from SPM can deposit in bottom sediments.

Multiple models can be used to predict the micropollutant interactions at the interface water-SPM particles. The most common model uses the "equilibrium" approach, where interactions are considered instantaneous. Those models are

well-suited for chronic continuous contaminations with small spatiotemporal variations. However, more complex models are required when facing acute pollution events. Considering one or two-step kinetic exchanges can have a large impact on the concentration's outcome, in view of the fact that sorption speed of micropollutant on SPM depends on the pollutant and sediment characteristics. Accurately representing kinetic models in the 2D and 3D components of the TELEMAC system would then allow studies of SPM-micropollutant interactions on large-scale high-resolution cases. It is also essential to study the impact of choosing more complex models on the propagation of pollutants.

The aim of this paper is firstly to present the model development of 2D and 3D SPM-micropollutant interactions, validation test-cases were then used to verify this model. Lastly, the model was tested on a real test-case scenario in the Loire estuary, this allowed the comparison of simple one-step reversible kinetic model and more complex two-step reversible model.

II.   MODEL DESCRIPTION

A.   Suspended matter

The model describing the evolution of SPM and bottom sediments involved in MICROPOL is a classic representation of the deposition laws and re-suspension of cohesive SPM [5], that are the laws of Krone [6] and Partheniades [7], [8]. Both processes require the knowledge of characteristic constants:

- deposition occurs when bottom shear stress τ_b, which varies according to the flow conditions, becomes lower than a threshold value τ_s, known as the critical shear stress for sedimentation. It is then assumed that the SPM settles at a constant velocity w (known as the settling velocity or velocity of sedimentation),

- re-suspension occurs when a threshold τ_r, known as the critical shear stress for re-suspension, is exceeded. Its importance is weighted by a constant e, the rate of erosion characteristic of deposited SPM (also known as the Partheniades constant).

These phenomena translate into the following expressions of deposition flux SED and erosion RS (kg/m²/s):

$$SED = \begin{cases} w.SS\left(1 - \frac{\tau_b}{\tau_s}\right) & \text{if } \tau_b < \tau_s, \\ 0 & \text{if } \tau_b \geq \tau_s \end{cases} \qquad (2)$$

$$RS = \begin{cases} e\left(\frac{\tau_b}{\tau_r} - 1\right) & \text{if } \tau_b > \tau_r. \\ 0 & \text{if } \tau_b \leq \tau_r \end{cases} \qquad (3)$$

The bottom shear stress τ_b (in Pa) is given by

$$\tau_b = \frac{1}{2}\rho C_f U^2 \qquad (4)$$

with C_f the friction coefficient, ρ the density of water and U^2 the square of the velocity. The equations of the evolution of SPM tracers (variable SS) and bottom sediments (variable SF) write as follows:

- First tracer: suspended particulate matter

$$F(SS) = \frac{RS - SED}{h}. \qquad (5)$$

With F as defined in equation (1).

- Second tracer: fixed bottom sediments

$$\frac{\partial(SF)}{\partial t} = SED - RS. \qquad (6)$$

The model relating to SPM has four parameters: the velocity of sedimentation w, the erosion rate e, the critical shear stress for deposition τ_s and the critical shear stress for erosion τ_r.

B.   Micropollutants

1)   One-step reversible model

The model representing the evolution of micropollutants assumes that the transfers of micropollutants (radioelement, metal) between the dissolved and particulate phases correspond to either direct adsorption or ionic exchanges modelled by a reversible reaction, of pseudo-1st kinetic order [9]. In the case of direct adsorption, the reaction can be represented in the form of the following chemical equation:

$$\text{R} + \cdot - S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \text{R} - S \qquad (7)$$
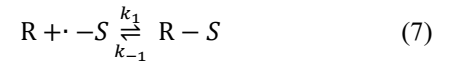
with R the micropollutant in dissolved form, $-S$ the surface site associated with SPM, $R-S$ the adsorbed micropollutant. It is a reversible reaction, controlled by adsorption (k_1 in m³/kg/s) and desorption velocities (k_{-1} in s⁻¹). It leads to an equilibrium state, and then a distribution of micropollutants between the dissolved and particulate phase described by the distribution coefficient K_d (in m³/s):

$$K_d = \frac{[R-S]}{[R]} = \frac{k_1}{k_{-1}}, \qquad (8)$$

where $[R]$ is the activity (or concentration of micropollutant) in dissolved phase (in Bq/m³ or kg/m³), $[R-S]$ is the activity (or concentration of micropollutant) associated to SPM (in Bq/kg or kg/kg). Once adsorbed, the fixed micropollutants act like SPM (deposition, re-suspension) and can then produce areas of polluted sediment. The model includes an exponential decay law (radioactive decay type) of micropollutant concentrations in each compartment of the modelled ecosystem, through a constant written L (expressed in s⁻¹). One-step reversible model can be schematically represented as in Figure 1:
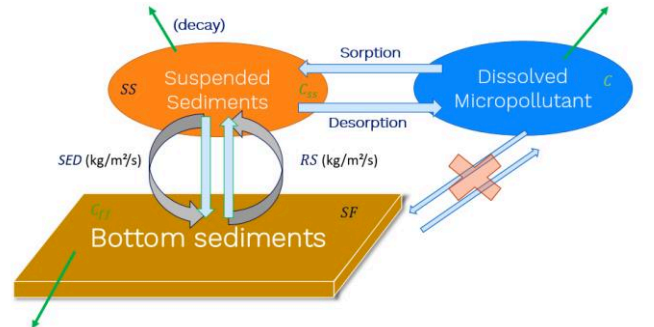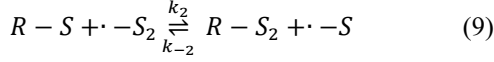
Figure 1. One-step reversible model exchanges.

2) Two-step reversible model

A new feature in MICROPOL allows the user to consider a two successive-step reversible model. In this case, a second reaction of pseudo-1st order introducing a slowly reversible site is considered [10]. This new reaction can be represented by the following chemical equation:

$$R - S + \cdot -S_2 \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} R - S_2 + \cdot -S \qquad (9)$$

with $R- S_2$ the adsorbed micropollutant bound to slowly reversible sites $-S_2$ of the suspended particle. It is a reversible reaction, controlled by adsorption (k_2 in s^{-1}) and desorption velocities (k_{-2} in s^{-1}). It leads to an equilibrium state, and then a distribution of micropollutants between the "non-specific" and "specific" sites ($-S$ and $-S_2$ respectively) described by the distribution coefficient K_{d2}:

$$K_{d2} = \frac{[R-S_2]}{[R-S]} = \frac{k_2}{k_{-2}}, \qquad (10)$$

where $[R - S_2]$ is the activity (or concentration of micropollutant) in the internal "specific" sites (in Bq/kg or kg/kg), $[R - S]$ is the activity (or concentration of micropollutant) associated to SPM surfacic "non-specific" sites (in Bq/kg or kg/kg). Two-step reversible model can be schematically represented as in Figure 2:
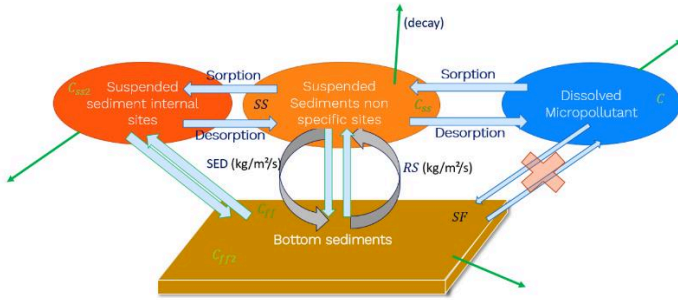

Figure 2. Two-step reversible model exchanges.

3) Equations

The system includes an equation for each micropollutant phase, namely 5 tracers:

- C : concentration of micropollutants in water (Bq/m^3),

- C_{ss1}: concentration of micropollutants adsorbed on SPM "non-specific sites" (Bq/m^3),

- C_{ff1}: concentration of micropollutants adsorbed on bottom sediments "non-specific sites" (Bq/m^2),

- C_{ss2}: concentration of micropollutants adsorbed on SPM "specific sites" (Bq/m^3),

- C_{ff2}: concentration of micropollutants adsorbed on bottom sediments "specific sites" (Bq/m^2).

The unit of concentration chosen for the demonstration is Bq/m^3, but it could also be written in kg/m^3 (for example, in

the case of a metal). The internal sources for sediment tracers SS and SF are the same as in the previous section.

Taking the two-step reversible model into account leads to the following equations for each micropollutant phases:

- Third tracer: dissolved micropollutant:

$$F(C) = -k_1.SS.C + k_{-1}.C_{SS1} - L.C. \qquad (11)$$

- Fourth tracer: micropollutant associated to SPM "non-specific" sites

$$F(C_{ss1}) = k_1.SS.C - k_{-1}.C_{ss1} + \frac{\frac{RS}{SF}C_{ff1} - \frac{SED}{SS}C_{ss1}}{h} - \\ k_2.C_{ss1} + k_{-2}.C_{ss2} - L.C_{ss1}. \qquad (12)$$

- Fifth tracer: micropollutant associated to bottom sediments "non-specific" sites

$$\frac{\partial C_{ff1}}{\partial t} = \frac{SED}{SS}C_{ss1} - \frac{RS}{SF}C_{ff1} - k_2.C_{ff1} + k_{-2}.C_{ff2} \\ -L.C_{ff1}. \qquad (13)$$

- Sixth tracer: micropollutant associated to SPM "specific" sites

$$F(C_{ss2}) = \frac{\frac{RS}{SF}C_{ff2} - \frac{SED}{SS}C_{ss2}}{h} + k_2.C_{ss1} - k_{-2}.C_{ss2} \\ -L.C_{ss2}. \qquad (14)$$

- Seventh tracer: micropollutant associated to bottom sediments "specific" sites

$$\frac{\partial C_{ff2}}{\partial t} = \frac{SED}{SS}C_{ss2} - \frac{RS}{SF}C_{ff2} + k_2.C_{ff1} - k_{-2}.C_{ff2} \\ -L.C_{ff2}. \qquad (15)$$

Terms with SF as denominator are nullified when SF is close to 0. Two-step kinetic exchanges tracers C_{ss2}, C_{ff2} and parameters k_2 and k_{-2} are nullified when the keyword KINETIC EXCHANGE MODEL is set to the value 1 (default).

Therefore, there are five parameters of the micropollutant model: the distribution coefficient at equilibrium K_d between the dissolved and particulate non-specific phase, the kinetic constant of desorption k_{-1} between the dissolved and particulate non-specific phase, the distribution coefficient at equilibrium K_{d2} between the "non-specific" and "specific" sites, the kinetic constant of desorption k_{-2} , and the exponential decay constant L (radioactive decay, for example).

III. TEST CASES

Multiple test cases for WAQTEL-MICROPOL module are now available on the V8P4 version of the TELEMAC system. The MICROPOL model was compared to analytic solutions in the case of a simple basin at rest for 2D and 3D models. More advanced interactions are also qualitatively studied to ensure that exchange processes are consistent.

A. 2D Basin at rest

In 2D, a basin at rest is considered (length and width = 10 m) with flat bathymetry and elevation at 0 m. The triangular mesh is

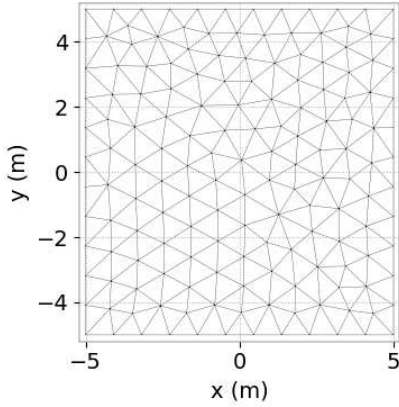composed of 272 triangular elements and 159 nodes as in Figure 3.

Figure 3. 2D square basin at rest mesh.

The initial conditions, settling velocity w (m/s) and the exponential decay constant L (s-1) are adapted in each test case in order to individually model sedimentation, sorption, desorption and decay. The distribution coefficient K_d (L/g) is set at a value of 1 and the constant of kinetic desorption k_{-1} at the value of 2.5E-7 s^{-1} for all test cases. All other parameters are taken with the default values in the WAQTEL STEERING FILE. The time step is 1h = 3,600 s for a simulated period of 3,200 h $\simeq$ 133 days.

The first test case is a simple sorption with no sedimentation or erosion: initial tracer conditions $(SS, SF, C, C_{ss}, C_{ff}) = (1, 0, 1, 0, 0)$ and parameter values $(w, L) = (0, 0)$. An analytical solution can be calculated in the case of simple steady hydrodynamic conditions using (11) and (12). In the case where the settling velocity w is nil, there is no sediment evolution, and the exchanges remain exclusively in the micropollutant tracers. By setting the initial concentration of micropollutants adsorbed by SPM (C_{ss}) at 1 Bq/m3 and 0 otherwise, an analytical solution under these conditions is:

$$\begin{cases} C_{ss}(t) = \frac{SS_0}{SS_0+1}(1 - e^{-k_{-1}(SS_0+1)t}) \\ C(t) = \frac{1}{SS_0+1}(SS_0 + e^{-k_{-1}(SS_0+1)t}) \end{cases} \quad (16)$$

Figure 4 shows the comparison between simulated simple sorption and the analytic solution (16).
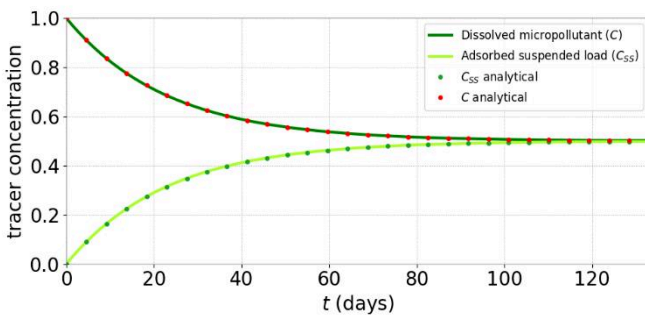

Figure 4. Tracer evolution on simple sorption test case.

The second test case evaluates deposition of SPM in the basin at rest: $(SS, SF, C, C_{ss}, C_{ff}) = (1, 0, 0, 0, 0)$ and $(w, L) = $ (4E-7, 0). An analytical solution can be calculated in the case of simple steady hydrodynamic conditions using (5) and (6). With a unitary constant water depth ($h = 1$ m) and no erosion ($U = 0$ m/s) the deposition flux SED follows:

$$SED = w.SS, \quad (17)$$

and the suspended sediment concentration (SS) is:

$$SS(t) = SS_0 e^{-wt}. \quad (18)$$

Similarly, the bottom sediments follow:

$$SF(t) = SF_0 + SS_0(1 - e^{-wt}). \quad (19)$$

Figure 5 shows that simple sediment is modelled correctly according to the analytic solution (18) and (19).
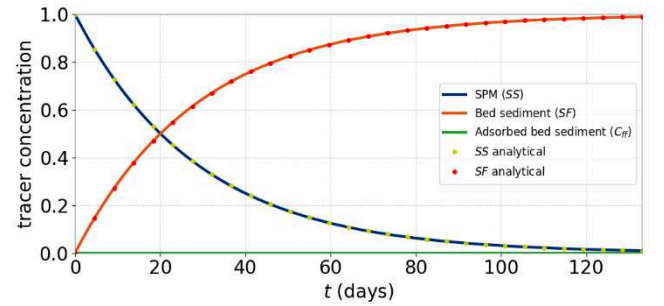

Figure 5. Tracer evolution on simple sedimentation test case.

When combining the first two test cases (sorption and sedimentation), we can qualitatively assess that the model correctly represents more complex dynamics with: $(SS, SF, C, C_{ss}, C_{ff}) = (1, 0, 1, 0, 0)$ and $(w, L) = $ (4E-7, 0). Under steady hydrodynamic conditions, the model reaches an equilibrium state when all sediments are deposited as shown in Figure 6.
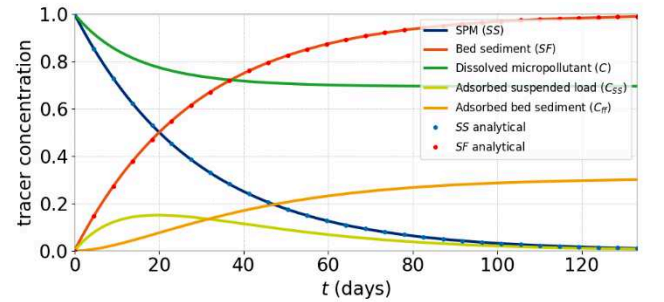

Figure 6. Tracer evolution on sedimentation and sorption test case.

Decay and desorption can also be studied in the fourth test case: $(SS, SF, C, C_{ss}, C_{ff}) = (1, 0, 0, 1, 0)$ and $(w, L) = $ (4E-7, 1.13E-7). Once the suspended sediment tracer is fully deposited, concentrations of micropollutants in water and in bed sediments decreases with the appropriate rate as shown in Figure 7.
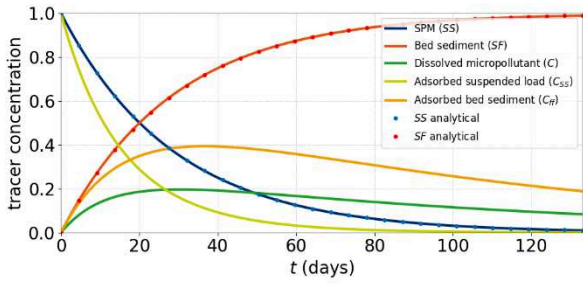
Figure 7. Tracer evolution on sedimentation and sorption test case with decay.

Two-step reversible model can be activated by setting the keyword KINETIC EXCHANGE MODEL = 2 in the WAQTEL STEERING FILE. In the next test cases, the distribution coefficients K_d and K_{d2} are set at a value of 2 L/g and 2. The sorption reaction rates k_1 and k_2 are set at a value of 0.1 L.g^{-1}.s^{-1} and 0.1 s^{-1}. All other parameters are taken with the default values in the WAQTEL STEERING FILE. The initial water depth is 1 m with a fluid at rest. The initial values for tracers are homogeneous in each test cases.

In the case where the settling velocity w is nil, there is no sediment evolution, and the exchanges remain exclusively in the micropollutant tracers in the water column. By setting the initial concentration of micropollutants in the water (C) at 1 Bq/m^3 and 0 otherwise, an analytical solution under these conditions is:

$$\begin{cases} C(t) = \frac{1}{7}\left(1 + (3+\sqrt{2})e^{\frac{-3+\sqrt{2}}{10}t} + (3-\sqrt{2})e^{-\frac{3+\sqrt{2}}{10}t}\right) \\ C_{ss1}(t) = \frac{1}{7}\left(2 - (1-2\sqrt{2})e^{\frac{-3+\sqrt{2}}{10}t} - (1+2\sqrt{2})e^{-\frac{3+\sqrt{2}}{10}t}\right) \\ C(t) = \frac{1}{7}\left(4 - (2+3\sqrt{2})e^{\frac{-3+\sqrt{2}}{10}t} - (2-3\sqrt{2})e^{-\frac{3+\sqrt{2}}{10}t}\right) \end{cases} \quad (20)$$

This analytical solution corresponds to a simple sorption using two-step kinetic scheme with no sedimentation or erosion with $(SS, SF, C, C_{SS1}, C_{ff1}, C_{ss2}, C_{ff2}) = (1, 0, 1, 0, 0, 0, 0)$ and $(w, L) = (0, 0)$. Figure 8 shows the comparison between simulated simple sorption and the analytic solution (16).
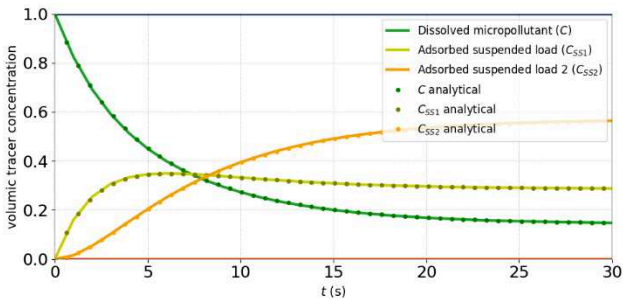

Figure 8. Tracer evolution on simple sorption test case using two-step reversible model.

The two-step reversible model can be used to model more complex transfers. In this second test case, both desorption of micropollutants from SPM toward dissolved form, deposition, and decay are evaluated with

$(SS, SF, C, C_{ss1}, C_{ff1}, C_{ss2}, C_{ff2}) = (1, 0, 0, 1, 0, 0, 0)$ and $(w, L) = (4E-7, 1.13E-7)$. Once the suspended sediment tracer is fully deposited, concentrations of micropollutants in water and bed sediments specific and non-specific sites decreases with the appropriate rate as shown in Figure 9.
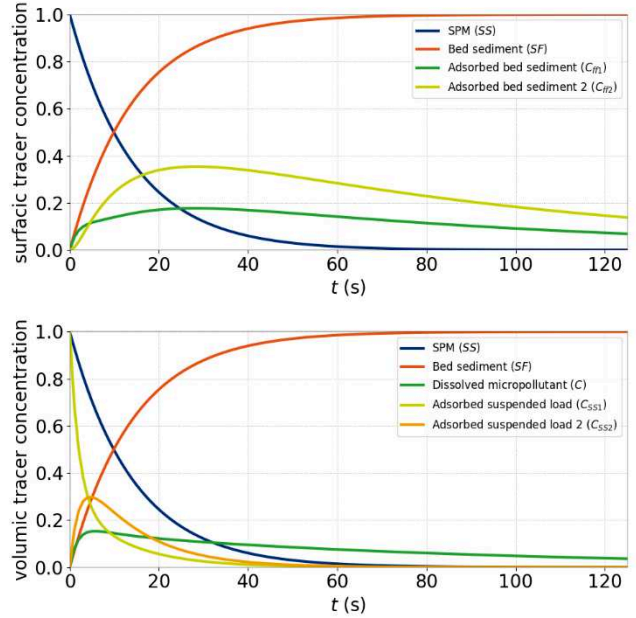

Figure 9. Tracer evolution on sedimentation and desorption test case with decay using two-step reversible model.

B. 3D Basin with various hydrodynamic conditions

Exchanges between suspended sediments and bed sediments are studied here. A concentration of suspended sediment is initially placed on top of the water column and settling, and deposition processes are observed. A 50 m long and 2.5 m wide rectangular basin at rest is considered with flat bathymetry and elevation at 0 m. Five superimposed layers are regularly spaced vertically. The triangular mesh is composed of 500 triangular elements and 306 nodes as showed in Figures 10 and 11.
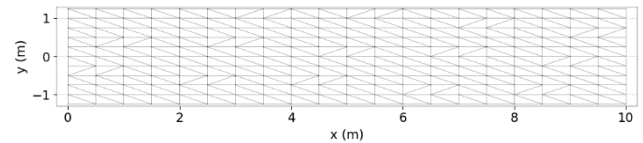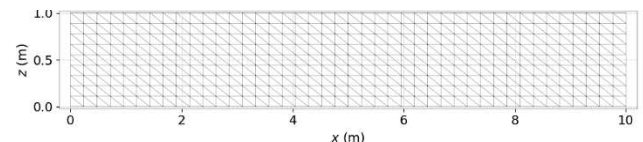

Figure 10. Horizontal mesh

Figure 11. Vertical mesh.

In this test case, only suspended sediments (SS) and bed sediments (SF) are studied. The settling velocity w is set at 4.E−3 m/s in the WAQTEL STEERING FILE. The initial water depth is 1 m with a fluid at rest. The initial value for

the suspended sediment tracer is set at a concentration of 1 kg/m3 in the top layer ($z = 1$ m) as in Figure 12. The bed sediment tracer is initially set to zero. The time step is 1 s for a simulated period of 1,000 s $\approx$ 17 min.
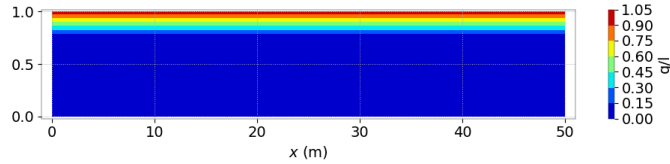

Figure 12. Suspended sediment initial concentrations.

Figure 13 shows the suspended sediment (SS) (kg/m3) and bed sediment (SF) (kg/m2) evolution along time at different water depths. The blue dashed line represents the water depth divided by the sediment settling velocity, it can help to estimate the time magnitude for the SPM to reach the bottom layer.
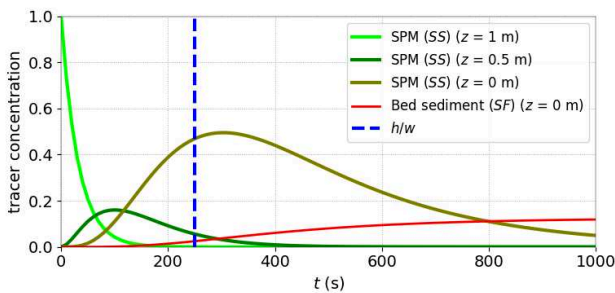

Figure 13. Suspended sediment and bed sediment evolution.

At $t = 1,000$ s only residual suspended sediments are still being deposited in the bottom layer as in the vertical cross section of Figure 14.
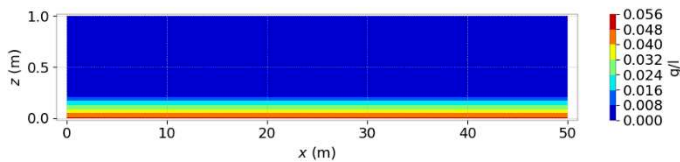

Figure 14. Suspended sediment concentrations at t = 1000 s.

In the next test case, an initial bump of bed sediment is placed at the bottom layer under a constant water velocity, erosion process is observed. The mesh is identical as the previous test case, except it is vertically divided in 10 superimposed layers. The settling velocity w is set at 0.02 m/s in the WAQTEL STEERING FILE. Critical shear stresses of resuspension and sedimentation τ_r and τ_s are set to 0.01 Pa. The erosion rate (or Partheniades constant) e is set at 1.E-3 kg/m2/s. The initial water depth is 1 m. The initial values for the suspended sediment tracer is set to zero and the initial values of the bed sediment are placed as a polynomial concentration:

$$SF(t=0) = \max(0,5(x-7)(3-x)). \qquad (21)$$

For the solid walls, a slip condition is used. Upstream flowrate equal to 1.5 m3/s is imposed. Downstream, the water level boundary condition is equal to 1 m.
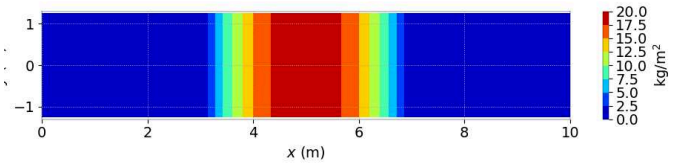

Figure 15. Bed sediment initial concentrations.

The time step is 0.1 s for a simulated period of 150 s. Figures 16 and 17 show the suspended sediment (SS) and bed sediment (SF) evolution along time on a vertical cross section and bed sediment final concentrations.
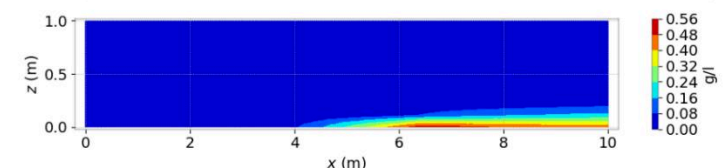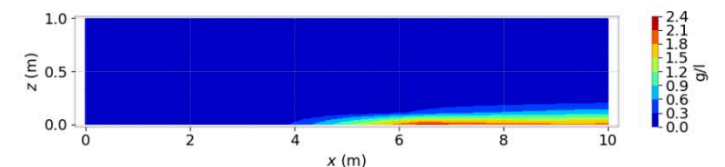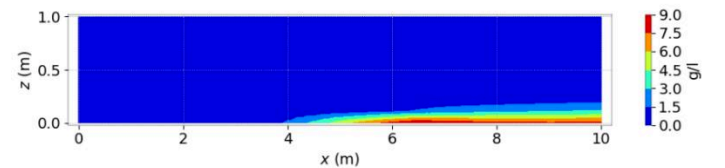

Figure 16. Suspended sediment concentrations at t = 5, 75 and 150 s.
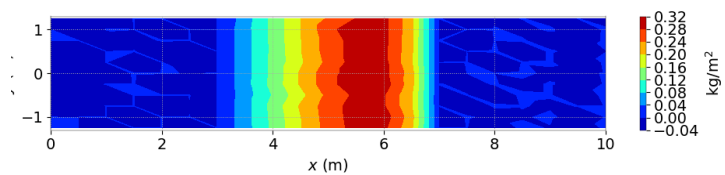
Figure 17. Bed sediment final concentrations.

Having verified that sediment and erosion processes are now properly represented, micropollutant transport can be studied as in the 2D test cases.

Decay and desorption can also be studied in the next test case in 3D: $(SS, SF, C, C_{ss}, C_{ff}) = (1, 0, 0, 1, 0)$ and $(w, L) = (0,07, 8.3E-3)$. Once the suspended sediment tracer is fully deposited, concentrations of micropollutants in water and in bed sediments decreases with the appropriate rate as shown in Figure 18.

Figure 18. Tracer evolution on sedimentation and desorption test case with decay in 3D.

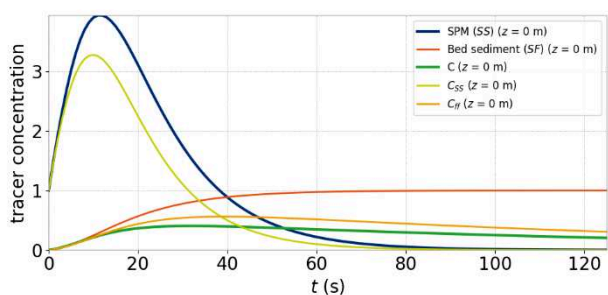Depending on the bottom layer thickness, suspended sediments concentration accumulates before reaching the bed sediment layer.

Next test case uses two-step reversible model with distribution coefficients K_d and K_{d2} set at a value of 2 L/g, sorption reaction rates k_1 and k_2 set at a value of 0.1 L.g^{-1}.s^{-1}, sediment settling velocity w to 4E-7 m/s and exponential decay constant L to 1.13E-7 s^{-1}. Initial concentrations are as follows: $(SS, SF, C, C_{ss1}, C_{ff1}, C_{ss2}, C_{ff2})$ = (1, 0, 0, 1, 0, 0, 0). Figure 19 illustrate the evolution of surfacic (top) and volumic tracer concentrations. The model was able to simulate the exchanges between specific and non-specific sites along with desorption of micropollutant towards the dissolved form, sedimentation process and decay.
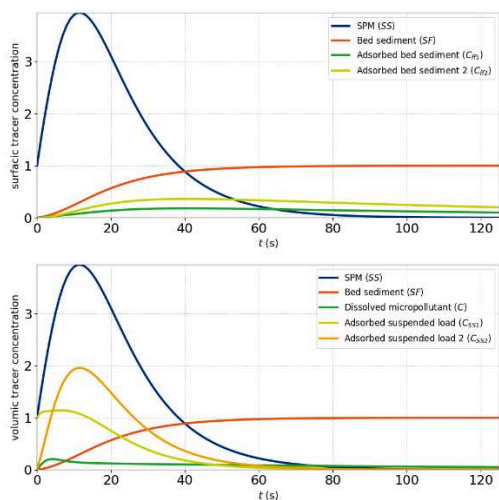

Figure 19. Tracer evolution on sedimentation and desorption test case with decay using two-step reversible model in 3D.

IV. REAL CASE: LOIRE ESTUARY

The model was tested on the Loire Estuary domain coupling TELEMAC-2D and WAQTEL module. The study area extends from 40 km upstream of the Saint-Nazaire Port and up to 100 km offshore. In view of limiting computing costs, the grid was refined in the Loire riverbed and coarsened on Atlantic Ocean side. For all simulations, a numerical time step of 5 s was considered. A triangular mesh of 45 000 nodes and 90 000 elements was mapped on a 100 m resolution bathymetric dataset as shown in Figure 20.
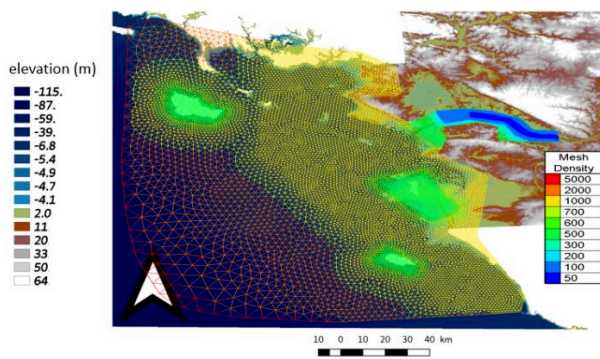

Figure 20. Model mesh and bathymetry.

The hydrodynamic model solves shallow water equations in the non-conservative form using finite element method. A Strickler law of bottom friction was chosen with a coefficient of 50 m$^{1/3}$ s^{-1}. Sediment settling velocity was set at the value of 0.4 cm/h, sedimentation critical shear stress and critical stress of resuspension were respectively set at 0.1 and 0.5 Pa. A constant prescribed flowrate of 900 m^3/s was imposed on the upstream boundary condition. A semi-diurnal tidal flow is introduced by means of a sinusoidal free surface elevation in time with a mean value of 3 m and an amplitude of 2 m. A first run with no micropollutant concentration was used to reach a stable periodic state on a one-year period. In Figure 21 is presented the spatial distribution and time evolution of suspended sediment and bed sediments at five locations. These locations are near the upstream boundary condition (+35km), in the riverbed (+26km, +18km), at the estuary (Saint-Nazaire) and offshore (+15km).
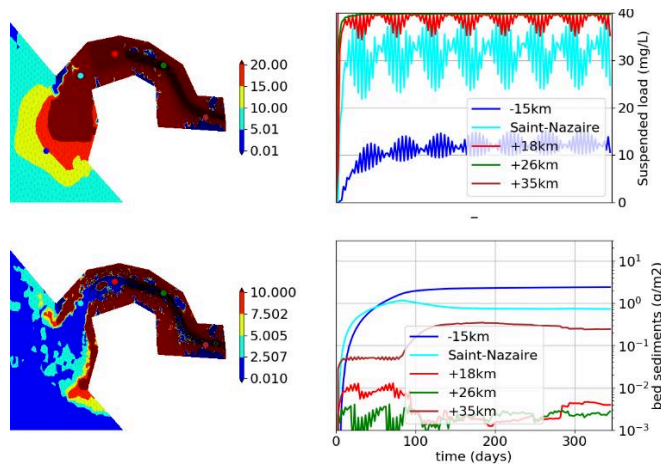
Figure 21. Sediment initialisation in the Loire estuary.

After this initialisation, a micropollutant discharge was injected as an upstream boundary condition with a concentration of 100 L^{-1}. In this case, the micropollutant can be viewed as any type of contaminant. The exponential decay constant was set at the value of 7.3E-10 s^{-1}, the distribution coefficient at 63 L/g, and the kinetic desorption coefficient at the value of 4.E-4 s^{-1}. The choice of these parameters is aimed to replicate the characteristics magnitude measured of ^{137}Cs in the Loire Estuary in [11]. Transport, sorption, and deposition of micropollutant was observed on a period of 4

days. Figure 22 demonstrate the model ability to simulate the transfers of micropollutant to sediments while being advected by the river. It was observed that dissolved concentrations were reduced by the presence of sediments. In this case, the low sediment settling velocity and the short simulation duration only allowed a small fraction of micropollutant to be deposited in the bottom sediments.
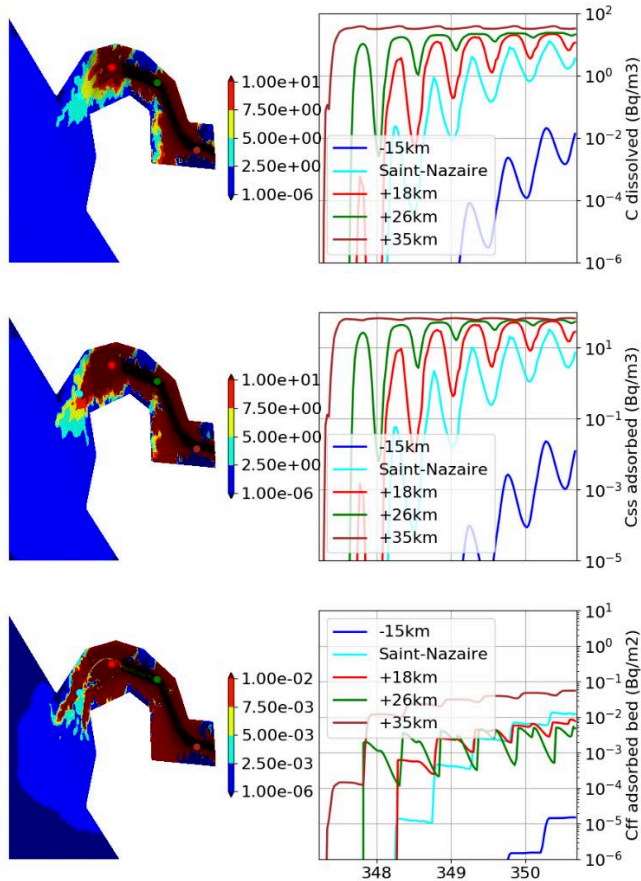

Figure 22. Micropollutant concentrations in dissolved form, adsorbded by suspended load and deposited in bed sediments. Colormaps show the final concentrations in the estuary.

As a way to assess the impact of considering two-step reversible model for micropollutant and sediment interactions, another test case was implemented with the same hydrodynamic and sediment parameters. In this case however, the two-step reversible option was activated, and two new parameters were added: The second distribution coefficient K_2 was set at the value of 2.5, and the kinetic desorption coefficient k_{-2} at the value of 2.E-5 s^{-1}. Propagation of micropollutant was observed on the same time scale as before on Figure 23.
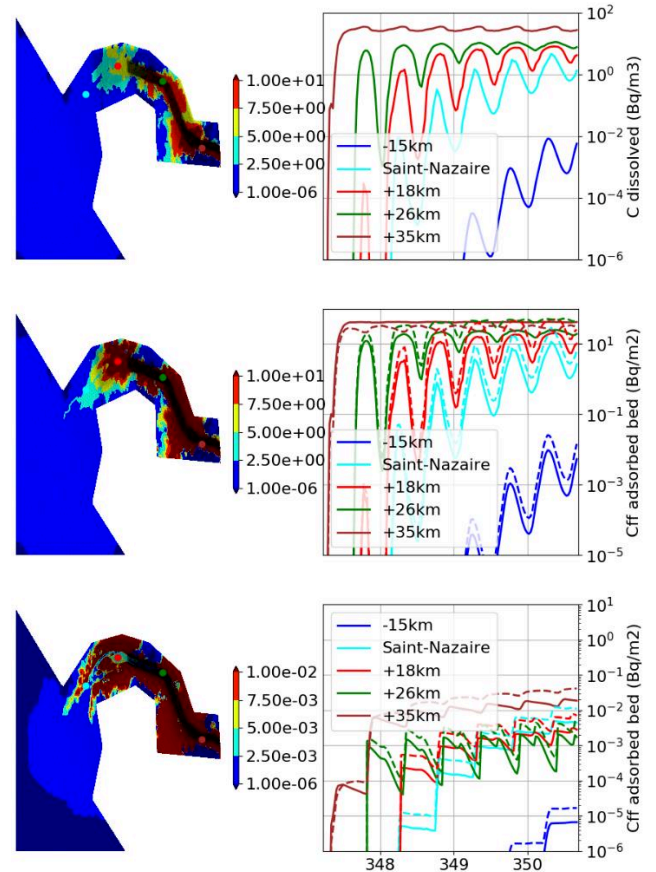

Figure 23. Micropollutant concentrations in dissolved form, adsorbded by suspended load and deposited in bed sediments in sediment surfacic sites (colored lines) and internal sites (dashed lines). Colormaps show the final concentrations in the estuary.

A qualitative analysis of the two previous figures shows that considering the two-step reversible model reduces the spatial dispersion of micropollutant and their concentration in surfacic sites. As expected, the micropollutant are transferred towards sediment "specific" sites, thus reducing dissolved concentrations in the water column. Comparison of final concentrations between one-step and two-step kinetic exchange models are shown in Table I. Final concentrations in the points distant from the inlet were more impacted by the different models. At some points, the concentrations were reduced by up to two-thirds.

Table I Dissolved micropollutant concentration comparison at the five study points.

Points	One-step reversible model		Two-step reversible model		Relative differences
	Final concentration C_{f1}	Dilution coefficient $C_i/C_{f1}{}^a$	Final concentration C_{f2}	Dilution coefficient $C_i/C_{f2}{}^a$	$\frac{C_{f2}-C_{f1}}{C_{f1}}$ (%)
-15 km	2.2E-02	4.5E+03	9.0E-03	1.1E+04	-59%
Saint-Nazaire	4.3	2.3E+01	1.57	6.4E+01	-63%
+18 km	1.5E+01	6.7	5.3	1.9E+01	-65%

Points	One-step model	reversible	Two-step model	reversible	Relative differences
	Final concentration C_{f1}	*Dilution coefficient* $C_i/C_{f1}{}^a$	*Final concentration* C_{f2}	*Dilution coefficient* $C_i/C_{f2}{}^a$	$\frac{C_{f2}-C_{f1}}{C_{f1}}$ (%)
+26 km	2.2E+01	4.5	8.1	1.2E+01	-63%
+35 km	3.4E+01	2.9	2.8E+01	3.6	-18%

a. $C_i = 100\ L^{-1}$ the injected concentration at the inlet

V.   CONCLUSIONS AND PERSPECTIVES

The goal of this study was to present and assess the developments of pollutant and sediment interactions in the TELEMAC system and to experiment on different modelling approaches.

In this paper, the implementation of the WAQTEL-MICROPOL module of TELEMAC is presented on theoretical and real test-cases. It was demonstrated that the TELEMAC software can now model conservative sediment and micropollutant transport in 2D and 3D with decay law and using one or two step reversible model. The test case on the Loire Estuary demonstrated that the model is usable on more complex domains and for intricated boundary conditions. Moreover, the results demonstrated that the model selection has a great impact on the final concentrations. Considering one or two pollutant sites in sediments affect the transfer rates from dissolved form to adsorbed micropollutant state.

This work provides a basis for further usage of the WAQTEL-MICROPOL model, while demonstrating application of the documentation test case and an application on a fictive scenario. The model developed is now ready to be tested on industrial and scientific studies.

Some additional work could improve the model by implementing salinity laws and concentration laws for sensitive parameters, namely the distribution coefficient and the kinetic desorption velocity. Another development could see the link between the sediments of this module and the sediments used in the GAIA module.

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