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***Abstract*—As part of the PCB-AXELERA research program, a simple model of PCBs (polychlorinated biphenyl) contamination in the Rhone river has been developed. The main objective is to assess the distribution of PCBs under various hydraulic regimes. This model uses TELEMAC-3D to simulate the water flow, and is coupled to DELFT3D-WAQ to simulate the transport of sediment and PCBs. The vertical resolution of the grid is 10 layers. The transport of sediments is modelled using the Krone and Partheniades formulation. The PCBs distribution between organic matter and water is treated as an equilibrium portioning, which accounts for the processes of adsorption and desorption of PCBs on the sediment. The model is run on an idealised channel. A sensitivity analysis is made to assess the impact of the numerical scheme and the vertical diffusion on the distribution of sediment in the water column using DELFT3D-WAQ. The modelled PCBs concentrations are in the same order of magnitude that the observations, which validates the set of parameters and the processes selected**

## I. INTRODUCTION

PCBs are a class of micropollutant widely used in industry since the late 1930s, due to their specific properties of high stability and low reactivity. They are released in the environment through the processes of evaporation in the atmosphere by incineration of PCB-contaminated wastes, discharge of industrial wastewater effluents in rivers, and accidental spillage of PCB-contaminated hydraulic fluid. They have been identified as presenting public health and ecosystem risk due to their toxicity even at low level. For this reason, PCBs have been banned in France since 1987. Some commercial mixtures of PCBs are highly persistent, which explained why they are still found at high level in rivers and fishes. Water quality standards for PCB have been established and the PCB contamination in fish, river water, and sediment is regularly monitored. Processes affecting PCBs in the environment are [1]:

- bioaccumulation,
- volatilisation,
- adsorption and desorption to organic matter, and
- biodegradation and transformation.

Through this various processes, they contaminated the compartments of the aquatic system: water, soil, air and fishes. PCBs are characterized by a low solubility, and bind strongly to organic particles in sediments and soils. Therefore most PCBs are found adsorbed on the sediments.

The main objective of this study was to develop a model of PCB transport at the scale of a river segment to understand the mechanisms of transport and fate of PCBs. The study area is located approximately 50km downstream of Lyon, in southern-east of France, near Condrieu (Fig. 1). This site is formed by two side-arms of the main stream of the Rhone river, called 'lône', which are favourable to sediment deposition (Fig. 2).

At first, an inventory of datasets available to determine the concentration of dissolved PCB and adsorbed PCB is presented. Then the model is run on an idealised channel, based on the geometry of a part of the side-arm. A sensitivity analysis is made to assess the impact of the numerical scheme and vertical diffusion on the distribution of sediment in the water column. Finally the results of the model are compared against dataset to validate the set of parameters determining the transport of sediments and PCBs.


Figure 1. Study site.

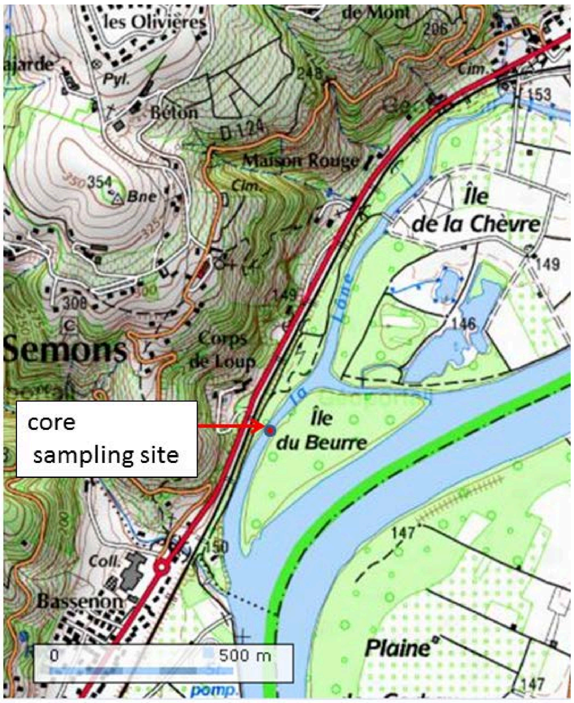


Figure 2. Location of the core sampling site.

## II. AVAILABLE DATA

Datasets of adsorbed PCB on SPM (suspended particulate matter) are available through the Regional Water Agency (Table I) at the station of Chasse-sur-Rhône (Fig. 1), upstream Condrieu. Datasets of dissolved PCB were only available at the station of Arles (Fig. 1), another study site of the research project. In addition, a sediment core from the side-arm (location on Fig. 2) was collected in 2008 and gives PCB concentration and organic matter content of the river bed sediment (Table II) [2, 3]. The core gives a record of the PCB concentration adsorbed on sediment deposited from 1965 to 2008. This dataset gives the level of PCB contamination of the sediment at the study site.

## III. MODEL DESCRIPTION

### A. Model grid and topography

The model is formed from the side-arm delineating the island of Beurre (Fig. 3). It includes 527 nodes on the horizontal plan. The vertical resolution is 10 layers. Triangles are of 15 meters size approximately. Topography is lowered to 144.4 m NGF along the river bank to always get a minimum water depth over the whole domain and avoid spurious effects due to uncovered nodes.

### B. Modelling hydrodynamic and sediment using TELEMAC-3D

Simulation with the model TELEMAC-3D using a constant flow rate upstream and imposing a constant water level downstream is made during 6 hours. Sediment transport is modelled using the Krone and Partheniades formula for sedimentation and re-suspension. Sediment bed is not erodible, but sediment deposited during the previous time-step can be re-suspended. Friction at the bottom is modelled by the law of Nikuradse with the Nikuradse length set at 0.15 m after validation against data [4].

The parameters of the law of Krone and Partheniades are the Partheniades constant, settling velocity, the critical shear stress for sedimentation, the critical shear stress for erosion. These values are set after calibration against datasets [4, 5]. They are given in Table III. The model is forced upstream with a constant flow of 5 $m^3s^{-1}$, a constant value for inorganic matter of 10 mg/L and a PCB total concentration of $10^{-7}$ mg/L. The water level imposed downstream is 144.7m NGH.

### C. Modelling sediment and PCB distribution using DELFT3D-WAQ

PCB distribution is modelled using the results of the hydrodynamics modelled by TELEMAC-3D coupled to the

TABLE I. DATASETS FROM THE FRENCH WATER AGENCY

| Type of measurement | Sampling frequency | year | average | Standard Deviation | Total number of measurements |
|---|---|---|---|---|---|
| Dissolved PCB at Arles | 3 measurements ( march, april and december) | 2010 | 0.0039 µg/L | 0.0028 µg/L | 3 |
| PCB in SPM at Chasse sur Rhone | Every 3 months | 1991-2009 | 0.014 mg/kg DM | 0.015 mg/kg DM | 33 |
| PCB in sediment of the river bed at Chasse sur Rhône | Once a year | 1994-2009 | 75.11 µg/kg DM | 183.16 µg/kg DM | 7 |

TABLE II. DATASETS FROM THE SEDIMENT CORE

| Type of measurement | Age of sediment collected | average | Standard Deviation | Total number of sub samples after sectioning of the core |
|---|---|---|---|---|
| PCB in sediment of the river bed | 1965-2008 | 0.0605 mg/kg DM | 0.065 mg/kg DM | 20 |
| Total Organic Carbon of sediment | 1965-2008 | 11598.63 mg/kg DM | 3696 mg/kg DM | 20 |

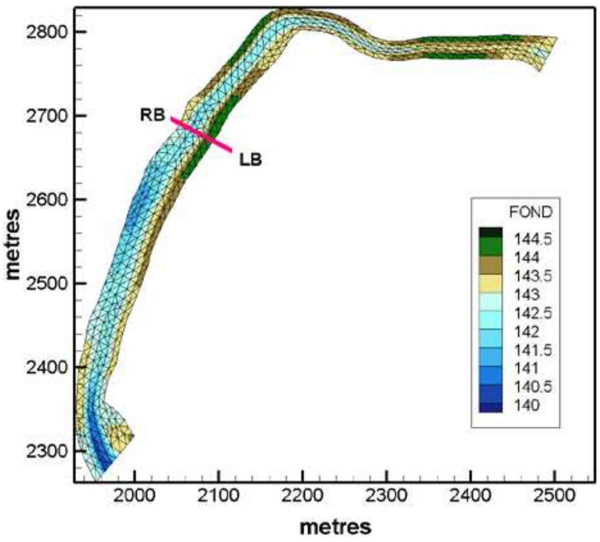


Figure 3. Model grid, bathymetry and position of the vertical slice.

TABLE III. PARAMETERS FOR SEDIMENTATION AND RE-SUSPENSION IN TELEMAC-3D

| Parameter | Value | Unit |
|---|---|---|
| Partheniades constant | $6.50\ 10^6$ | $kg\ m^{-2}\ s^{-1}$ |
| Critical shear stress for sedimentation | 10000 | $N\ m^{-2}$ |
| Critical shear stress for erosion | $5.33\ 10^{-2}$ | $N\ m^{-2}$ |
| Settling velocity | 0.0001 | $m\ s^{-1}$ |
| Porosity | 0.45 | % |
| Nikuradse length | 0.15 | m |

DELFT3D-WAQ module. The following variables are modelled in DELFT3D-WAQ: IM1 (inorganic matter), POM (particulate organic matter), PCB-par (PCB adsorbed on sediment particle), PCB-dis (PCB dissolved in water). The model accounts for the PCB and sediment deposited at the bed layer. The variables representing the content of the bed layer are the following: IM1S1, POMS1, PCB-disS1, PCB-parS1. The processes accounted for the transport of sediment, organic matter and adsorbed PCB are sedimentation and re-suspension following the law of Krone and Partheniades. Adsorption and desorption of PCB on the SPM (suspended particulate matter) is modelled by partition coefficients, following the Langmuir law. The fraction of PCB adsorbed (fpoc) and the fraction of PCB dissolved (fdf) is therefore calculated at each time step. We assume that the chemical reaction is at equilibrium, therefore Koc is a constant. The following equations (1) (2) (3) (4) determine the distribution between the PCB adsorbed (PCB-par) and the PCB dissolved (PCB-dis), as fraction of the total PCB concentration (PCB-tot):

$$\text{PCB-par=fpoc PCB-tot} \quad (1)$$

$$\text{PCB-dis =fdf 153-tot = (1-fpoc) PCB-tot} \quad (2)$$

$$\text{PCB-tot = PCB-par+PCB-dis} \quad (3)$$

$$\text{fdf = (1/Kp SS)=1/(1+Koc POC)} \quad (4)$$

We also assume that adsorption occurs only on the organic matter content of the sediment. The content of Particulate Organic Matter (POM) in the sediment is expressed as a fraction of inorganic matter (5):

$$\text{POM = \%OM\_IM1} \times \text{IM1} \quad (5)$$

The suspended solid (SS) is the sum of inorganic matter and particulate organic matter (POM) (6):

$$\text{SS=suspended solid = IM1+POM} \quad (6)$$

The particulate organic matter is expressed as a ratio of the particulate organic carbon using the coefficient fdm (7):

$$\text{POM = fdm POC} \quad (7)$$

The equation of Karickhoff (8) links Koc, the octanol/water partition coefficient, with Kow, the octanol/water partition coefficient [6]:

$$\text{log(Koc)=log(Kow)} \quad (8)$$

The values of the parameters are given in Table IV.

The variables IM1, IM1S1, POM, POMS1 are subject to the processes of re-suspension and sedimentation, with the same parameter values than in TELEMAC-3D (Table III). A representation of model structure (processes and variables) is given Fig. 4.

TABLE IV. PARAMETERS FOR SORPTION AND DESORPTION OF PCB IN DELFT3D-WAQ

| Parameter | Value | Unit | Reference |
|---|---|---|---|
| Kow | $10^{6.11}$ | L/kg | [6] |
| %OM_IM1 | 0.01 | - | Data from Table II |
| fdm | 2.6 | gDM/gC | [7] |

## IV. SENSITIVITY ANALYSIS

### A. *Influence of vertical diffusion*

Simulation with DELFT3D-WAQ was made over 8 hours. The spin up time, which is the time to reach an

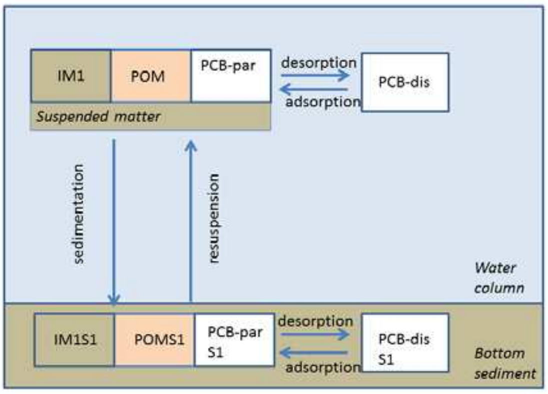


Figure 4. Variables and processes activated in DELFT3D-WAQ to simulate PCB transport and reactions.

equilibrium state under a permanent regime on this small domain, is 3 hours. Several values of the vertical diffusion were tested. Sediment distribution modelled with DELFT3D-WAQ varies depending on the vertical diffusion. The objective was to calibrate the coefficient of vertical diffusion in DELFT3D-WAQ to approach the results of the sediment distribution over the vertical obtained with TELEMAC-3D, as previous work has been made to calibrate and validate a numerical model of sediment transport using TELEMAC-3D on this area [4, 5]. Results were compared for a vertical slice B going from the left bank (LB) to the right bank (RB) (Fig. 3). Sediment distribution modelled with TELEMAC-3D is presented Fig. 5. It shows a vertical gradient in sediment distribution, with higher concentration near the bed (around 2 mg/L). DELFT3D-WAQ can account for the vertical diffusion calculated by TELEMAC-3D. In this case the results produce non-homogeneous distribution of sediment with spikes of concentration. Therefore a constant vertical diffusion coefficient was selected. Results for various values of the coefficient of vertical diffusion are shown on Fig. 6. The raising of the vertical diffusion results in the smoothing of the vertical gradient of sediment concentration. A value of vertical diffusion of $10^{-4} m^2 s^{-1}$ in DELFT3D-WAQ was then selected as it avoids spikes on the vertical distribution compared to lower values, and gives results similar qualitatively to the vertical distribution obtained with TELEMAC-3D.

### *B. Comparison between numerical schemes*

In a second stage, a comparison between two numerical schemes (n°16 and n°21) was made (Fig. 7). The numerical scheme n°16 is an implicit upwind scheme in horizontal, centrally discretised vertically, with an iterative solver [8]. The numerical scheme n°21 is a local-theta flux-corrected transport scheme [8]. The highest differences are shown on the left bank (X=2090m), with concentration reaching 35mg/L when using numerical scheme 21 instead of 30mg/L with numerical scheme n°16. The numerical scheme n°21 seems to reduce the effect of smoothing of the vertical

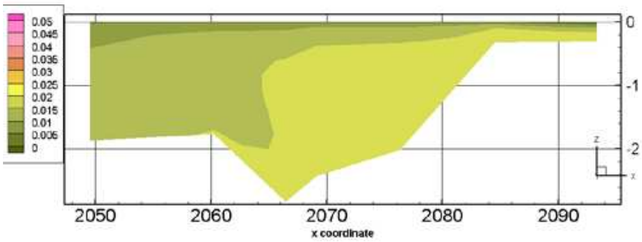


Figure 5. Vertical distribution of suspended sediment using TELEMAC-3D in g/L.

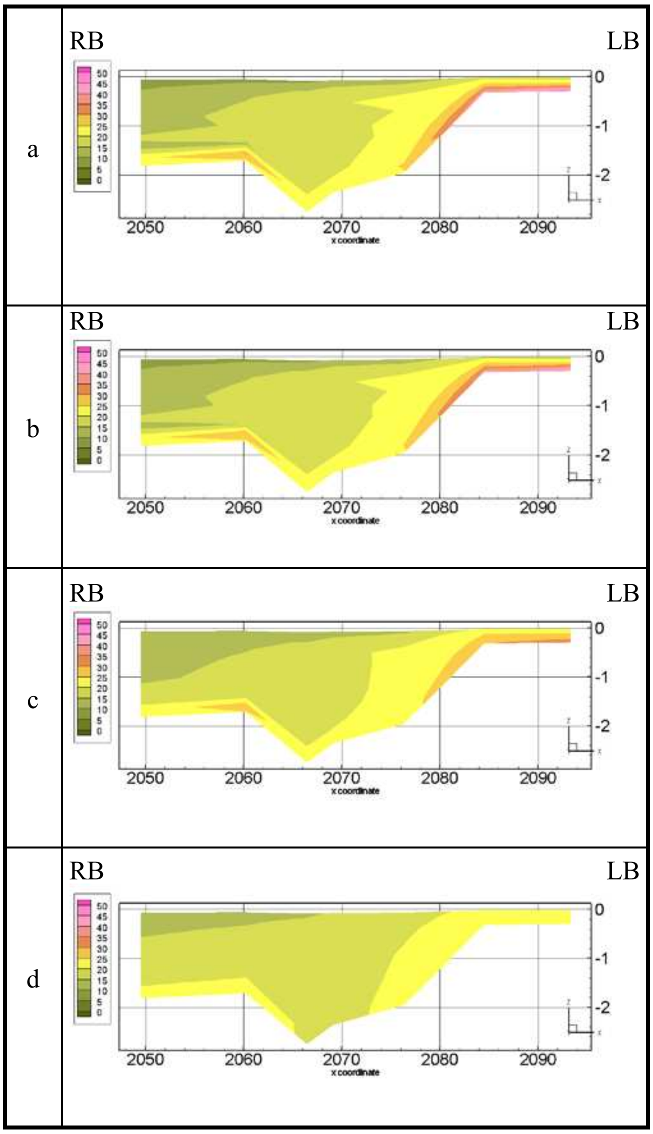


Figure 6. Vertical distribution of suspended sediment in mg/L using TELEMAC-3D a) $10^{-7} m^2s^{-1}$, b) $10^{-6} m^2s^{-1}$, c) $10^{-5} m^2s^{-1}$, d) $10^{-4} m^2s^{-1}$.

gradient induced by the use of the vertical dispersion of $10^{-4} m^2 s^{-1}$.

## V. VALIDATION OF THE NUMERICAL MODEL OF PCB TRANSPORT

In the second stage, DELFT3D-WAQ was run over 2 months under permanent flow. We use the numerical scheme 21 and a time-step of 10s. Fig. 8 shows the result of the vertical distribution of PCB-par, PCB-dis and PCB-tot in the water column. The model shows that PCB-dis varies from $5.10^{-6}$ to $7.10^{-6}$ mg/L (Fig. 8a). This order of magnitude is in agreement with the dataset (Table I). PCB-par varies from $1.3\ 10^{-6}$ to $5\ 10^{-7}$ mg/L (Fig. 8b). PCB-dis is therefore the main contributor of PCB-tot, compared to the other component PCB-par. PCB-tot varies from $7\ 10^{-6}$ to $6.2\ 10^{-6}$mg/L and shows vertical variations (Fig. 8c).

The modelled POC concentration varies from 0.2 to 0.4 mgC/L (Fig. 9a), which is lower than the order of magnitude generally found in rivers (from 1 mgC/L to 2 mgC/L) [9, 10]. The comparison between Figs. 9a and 9b shows that the vertical distribution of POC is correlated to IM1, the inorganic fraction, in agreement with the model equation (5). The highest concentration in IM1 and POC are found at the bottom of the left bank side and the right bank side. The PCB content of the sediment Q153SS is defined as the ratio of PCB adsorbed divided by the suspended solid, equation (9):

$$Q153SS = 10^6\ PCB\text{-}par / SS = 10^6\ PCB\text{-}par/(IM1+POM) \quad (9)$$

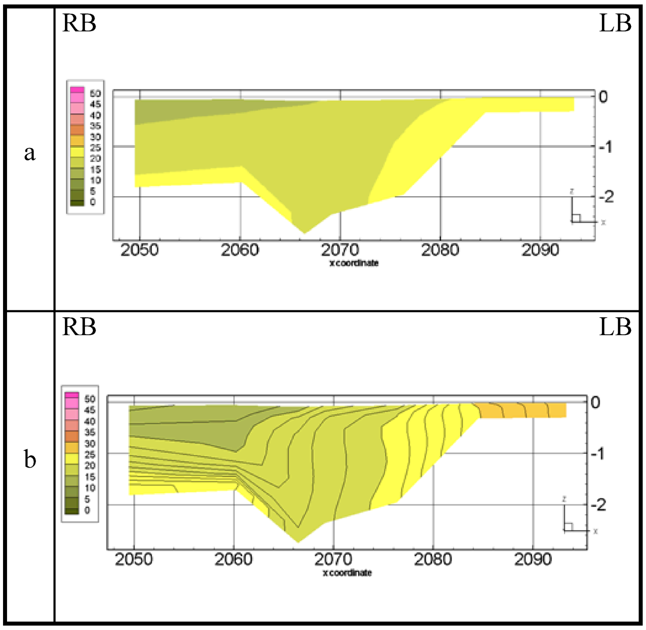


Figure 7. Comparison between 2 numerical scheme : a) scheme 16, b) scheme 21. The vertical diffusion is $10^{-4}\ m^2 s^{-1}$ in both case.

The modelled PCB content in the sediment varies from 0.042 to 0.048 mg/kgDM (Fig. 9c). This value is also in the order of magnitude of the core data (Table I). Modelled vertical distribution indicates that higher PCB content in the sediment is found near the water surface of the right bank.

## VI. CONCLUSION AND OUTLOOK

A numerical model of PCB transport has been developed using DELFT3D-WAQ. The model simulates the transport of sediment and PCB in a small channel, representative of a portion of a side-arm of the Rhone River. Comparison between sediment modelled with TELEMAC-3D and DELFT3D-WAQ has shown that a constant vertical diffusion of $10^{-4}\ m^2 s^{-1}$and the choice of the numerical scheme 21 was giving results similar to the sediment distribution modelled with TELEMAC-3D.

In a second stage, simulation over 2 months to simulate sediment transport and PCB transport was made. Results of the dissolved PCB and PCB adsorbed on sediment were compared against data available. It shows that modelled results are in the same order of magnitude than the datasets, which validates the PCB transport model processes and the parameters selected.

Future work will consist in running realistic simulation on a wider grid covering the main Rhone and both side-arms. The main objective is to assess the preferential area of deposition of PCB during high hydraulic flow.


## ACKNOWLEDGEMENT

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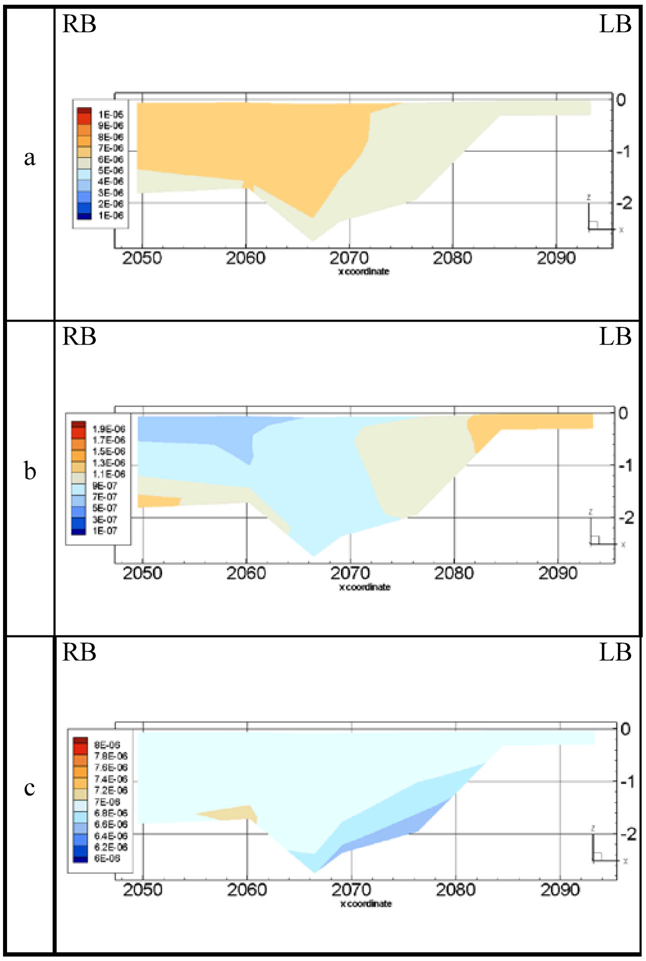


Figure 8. Vertical distribution of : a) PCB-dis (mg/L) b) PCB-par (mg/L), c) PCBtot=PCB-par+PCB-dis (mg/L).

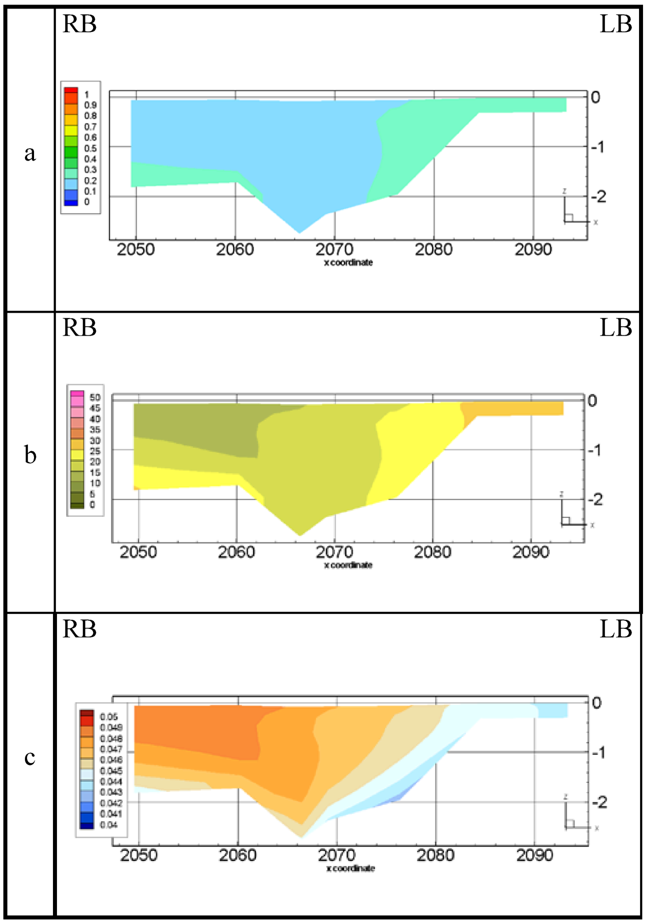


Figure 9. Vertical distribution of: a) POC (mgC/L), b) IM1 (mg/L), c) Q153SS (mg/kg DM).

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