2D NUMERICAL CODE TO SIMULATE THE TRANSPORT AND DEPOSITION OF DISSOLVED AND PARTICULATE CONTAMINANTS IN A FLOOD RETENTION RESERVOIR

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ABSTRACT

Pollutants such as heavy metals are adsorbed to fine suspended particles, which are transported through the river system and deposited in near bank groyne fields, harbors, headwater sections and reservoirs. Sedimentation of sediment bound contaminants in reservoirs plays an important role in water resources management. Therefore, it is a challenging task to model and predict the fate of contaminated suspended sediment particles in terms of their spatial and temporal distribution in river system, particularly in reservoirs aiming to find out optimum operation rules for mitigation. Therefore, a contaminated transport model CTM-SUBIEF-2D has been developed based on the module SUBIEF-2D which is a part of numerical the code TELEMAC-2D System. The new code describes the transport of dissolved and particulate substances in the water body and the river bed with emphasis on the interaction between aqueous and dissolved phases by first order sorption kinetics.

The developed model was applied to a representative flood retention reservoir in southern Germany. Jacoub et.al. (2002a,b) showed that the unsteadiness of the flow field during the flood retention periods controls the transport and sedimentation in the flood retention reservoir. In this study, numerical simulations under unsteady state conditions are performed for a representative fraction size and two different outlet operation rules in terms of outflow discharge to predict the behavior of contaminants as a function of space and time. The numerical results show the transport behavior of contaminants, suspended sediments and the spatial and temporal distribution of contaminated deposits under different reservoir operation rules. It can be shown that the amount of sediments and contaminants deposited in the reservoir can be reduced by appropriate operation of the bottom outlet without losing the flood retention efficiency.

1. INTRODUCTION

Fine sediments, that have particle sizes ranging between 1-80 micrometer, are a major component of the suspended load in river systems, lakes, estuaries, and reservoirs. These fine-grained sediments have strong capacity to adsorb contaminants, such as heavy metals and organic chemicals released to the aquatic system. Thus, contaminated suspended sediments can eventually be deposited on the

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river bed where they can accumulate and build up a hazardous potential sources for contaminants that might be eroded during flood events. Though contaminants are generally associated with cohesive sediments, their transport and fate are essential to adequately characterize the sediment and contaminant distribution in water bodies.

The transport of the contaminated suspended sediments is governed by physical and chemical processes. The physical processes include the advection and dispersion mechanisms while the chemical processes are driven by sorption kinetics between the dissolved and particulate matters. The distribution between the adsorbed and dissolved phase concentrations in both the water body and the sub-surface zone is necessary for the mobility of reactive substances. This distribution can be chemically defined in terms of equilibrium distribution and sorption kinetics. It is still an important issue to numerically model these processes considering all parameters that are relevant in predicting the temporal and spatial distribution of contaminated and pure suspended sediments. The numerical studies that tried to address the above mentioned problem, Westrich (1988), Margvelashily et.al. (1997), Margvelashily et.al. (2000) and Jonhsson and Wörman (2001), did not consider either diffusion or sorption kinetics in the sub-surface zone and some studies only considered one-dimensional modeling.

Therefore, the aim of this study is to develop a contaminated transport code based on the numerical code TELEMAC-2D System. The new developments were done for the module SUBIEF-2D, part of the TELEMAC System, which dealt with suspended sediments only. The new code, called CTM-SUBIEF-2D, describes the two dimensional transport of suspended sediments (SS), dissolved and particulate substance concentrations in the water body (C_D and C_A, respectively) and the sub-surface zone (G_D and G_A, respectively), with emphasis on the interaction between dissolved and absorbed phases by first order sorption kinetics, Figure 1, unlike the previous studies.

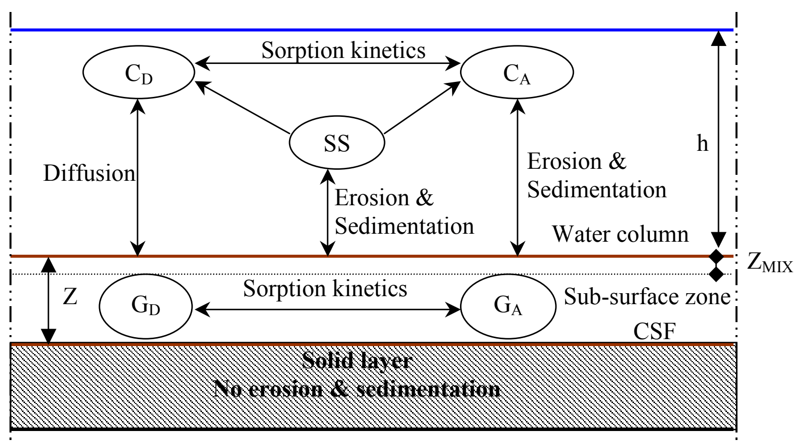

Figure 1 The physical concept of the new code CTM-SUBIEF-2D.

2. THE NUMERICAL CODE

2.1 Transport Model SUBIEF-2D

SUBIEF-2D is a two dimensional finite element model in horizontal plane and is designed based on the TELEMAC-2D System, EdF (2000). The module deals with suspended sediments transport which can be described by the advection-dispersion equation taking into account sedimentation/erosion processes as given in eq. 1. The suspended sediments concentration (SS) and the velocities in x,y directions are integrated over the average water depth. The erosion and deposition rates can be calculated from eq. 2, Krone (1962) and Partheniades and Asce (1965).

$$\frac{\partial SS}{\partial t}+\vec{u}.gradSS=div\left(\vec{K}.gradSS\right)+\frac{Q_e-Q_d}{h}+Source/Sink \tag{1}$$

$$Q_d=V_s.SS.\left[1-\left(\frac{u^*}{u_d^*}\right)^2\right] \qquad \& \qquad Q_e=M.\left[\left(\frac{u^*}{u_e^*}\right)^2-1\right] \tag{2}$$

2.2 Contaminant Transport Model CTM-SUBIEF-2D

The new code, Figure1, depends on the k-d concept. It deals with five variables, that are suspended sediment concentration (SS), dissolved and particulate concentrations in both the water body (C_D and C_A, respectively) and the sub-surface zone (G_D and G_A, respectively) . Each variable is expressed in a mass conservation transport equation that includes the interaction terms, (i.e sorption, diffusion, sedimentation and erosion). The diffusion mechanism takes place between the dissolved phases in the water body (C_D) and sub-surface zone (G_D). While the sorption kinetics occurs between the dissolved and particulate phases in the water body and the sub-surface zone as well. These five transport equations are given below:

1-Mass conservation for suspended sediments (SS) in the water body :

$$\frac{\partial SS}{\partial t}+\underline{u}.gradSS=div(\vec{K}.gradSS)-\underbrace{\frac{Q_d-Q_e}{h}}_{Sedimentation/Erosion}+Source/Sink \tag{3}$$

2-Mass conservation for dissolved phase (C_D) in the water body :

$$\frac{\partial C_D}{\partial t}+\underline{u}.gradC_D=div(\vec{K}.gradC_D)-\underbrace{K_1(K_D.SS.C_D-C_A)}_{SorptionKinetics}-\underbrace{\frac{D_S}{Z_{AB}}.\frac{(C_D-G_D)}{h}}_{Diffusion}+Source/Sink \tag{4}$$

3-Mass conservation for adsorbed phase (C_A) in the water body :

$$\frac{\partial C_A}{\partial t}+\underline{u}.gradC_A=div(\vec{K}.gradC_A)+\underbrace{K_1(K_D.SS.C_D-C_A)}_{SorptionKinetics}-\underbrace{\frac{Q_d^*-Q_e^*}{h}}_{Sedimentation/Erosion}+Source/Sink \tag{5}$$

4-Mass conservation for dissolved phase (G_D) in the sub-surface zone :

$$\frac{\partial G_D}{\partial t}=\underbrace{\frac{D_S}{Z_{AB}}.\frac{(C_D-G_D)}{Z_{MIX}}}_{Diffusion}-\underbrace{K_2(K_B.CSF.G_D-G_A)}_{SorptionKinetics} \tag{6}$$

5-Mass conservation for particulate phase (G_A) in the sub-surface zone :

$$\frac{\partial G_A}{\partial t}=\underbrace{K_2(K_B.CSF.G_D-G_A)}_{SorptionKinetics}+\underbrace{\frac{Q_d^*}{Z_{MIX}}}_{Sedimentation}-\underbrace{\frac{Q_e^*}{Z_{MIX}}}_{Resuspension} \tag{7}$$

and,

$$Q_d^*=Q_d\cdot\frac{C_A}{SS} \qquad \& \qquad Q_e^*=Q_e\cdot\frac{G_A}{CSF} \tag{8}$$

These equations are solved numerically using linear schemes since the non-linearity is always weak in the transport equation, Press et.al. (1992). Therefore the transport equations 3 to 7 are only coupled through the interaction terms (i.e sorption kinetics, diffusion, sedimentation and erosion).

3. CASE STUDY: FLOOD RETENTION RESERVIOR

3.1 Introduction

The flood retention reservoir considered in this study, Figure 2, has a dimension of 307 m x 257 m with a total storage capacity of 550,000 m^3. Its catchment area is 15 km^2 and is located in southern Germany. The reservoir can be considered as a representative reservoir because of its typical size and shape, Schultz (2002). Jacoub et.al (2002a) showed that the unsteadiness with high mixing turbulence controls the flow behavior in the chosen flood retention reservoir because of the complex geometry and outlet operation rules. They also showed the effect of different outlet operation rules, under unsteady state conditions, on the suspended sediments behavior, sedimentation patterns and total sediments budget during a flood event. The outlet operation rules used in this study can be summarized as follows, Figure 3:
Case 1: short emptying phase.
Case 2: long emptying phase.

The outflow discharges for case 1 and 2 are a function of time. The simulations are done for a real hydrograph occurred from 28th January 2000 to 5th February 2000, which was modified to a simple linear inflow function for the numerical simulations, Figure 3.

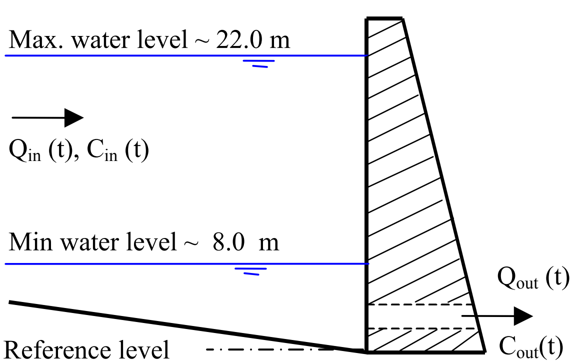

Figure 2 Vertical section of the reservoir.

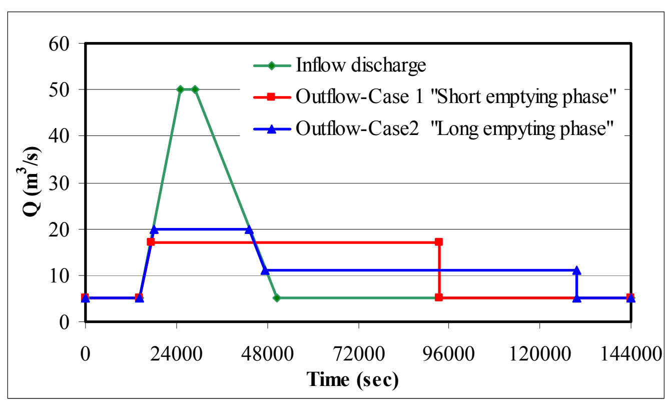

Figure 3 The inflow and outflow hydrographs.

3.2 The Numerical Domain and Parameters Used

According to the model concept shown in Figure 1, some hydraulic, physical and numerical parameters should be defined. These parameters concerning discharge, hydrograph, sediments and contaminants properties are taken from some laboratory tests, field measurements and pertinent literature and are specified as given below:

Geometry: size of the model is approximately 307 m x 257 m; water level elevation at rest is 8.0 m (~ 3.0 m average water depth).

Mesh: an irregular mesh is generated since the k-ε turbulence model is used. Triangular elements are elongated in the direction of the flow. Number of elements is 2328 and number of nodes is 1241. The element size varies from 3.0 m^2 to 13.8 m^2, Figure 4.

Shear stress: critical deposition shear stress of 0.064 N/m^2, critical erosion shear stress of 2.5 N/m^2 and settling velocity of 0.00035 m/s for suspended particles were used.
Bottom: according to the filed data, Strickler formula with coefficient of 50.0 $m^{1/3}/s$ was chosen since the reservoir bed consists of very fine sediments.
Sorption parameters: the equilibrium distribution coefficients in the water body (K_D)and the sub-surface zone (K_B) are 10.0 m^3/kg and 100.0 m^3/kg, respectively. Sorption kinetic rates between the dissolved and particulate phases in the water body (K_1) and sub-surface zone (K_2) are chosen as $1.0x10^{-4}$ s^{-1} and $4.0x10^{-8}$ s^{-1} , respectively. The mixing layer thickness (Z_{MIX}) is $5.5x10^{-3}$ m while the diffusion is taking place through a thickness of $5.5x10^{-4}$ m (Z_{AB}).
Boundary condition: the inflow discharge hydrograph, Figure 3, was prescribed by the formatted data files,. Suspended sediments inflow concentration (SS) at the upstream boundary varies between 0.2 kg/m^3 and 2.0 kg/m^3, Figure 5, whereas the inflow concentration of dissolved phase contaminants (C_D) is a constant value of 0.01 kg/m^3.
Time discretization: time step was 5 s for hydrodynamic simulations and 2.5 s for transport simulations to ensure that the courant number is less than 1. Simulation duration was 40 hrs.

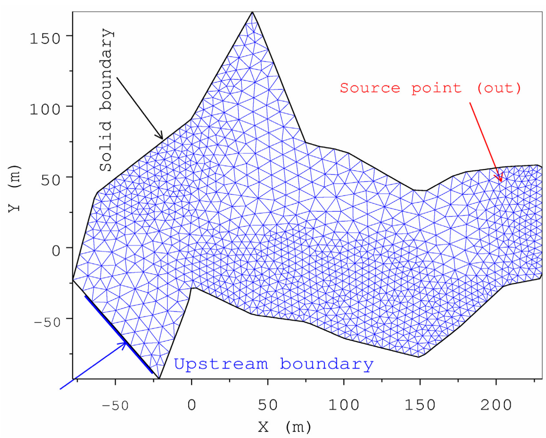

Figure 4 Numerical domain of the reservoir.

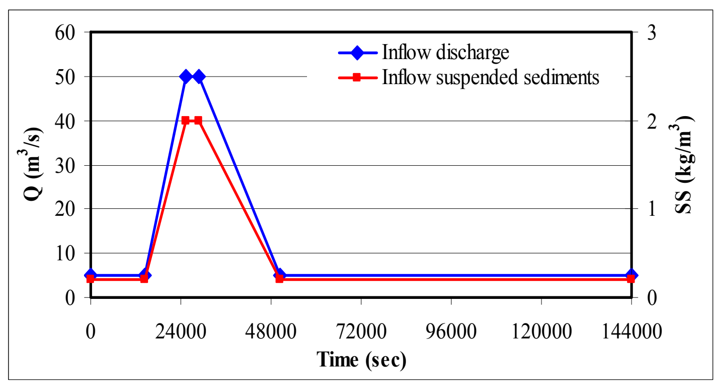

Figure 5 Discharge and suspended sediments inflow.

4. NUMERICAL RESULTS AND THEIR INTERPRETATION

4.1 Hydrodynamic Results

According to the inflow and outflow hydrographs, Figure 3, the average water elevations varied between 8.0 m and 22.3 m and between 8.0 and 18.5 m for short and long emptying phases, respectively, Figure 6.

During the flood peak, a main stream flow with adjacent large scale eddies in the domain were observed due to high mixing turbulence, high momentum and kinetic energy (**unsteady state case**), Figure 7. The flow pattern does not much differ in both phases, cases 1 and 2, since the hydraulic conditions during the flood peak remain almost the same. The water elevations were reduced and reached to the initial elevations after 26 and 36 hours for short and long emptying phases, respectively because of $Q_{out}>Q_{in}$.

After the emptying phases, the generated eddies had almost disappeared due to energy dissipation and a steady state eddy configuration was reestablished at the end of the simulations (**steady state case),** Figure 7. More details about the flow behavior can be obtained from Jacoub and Westrich (2002b).

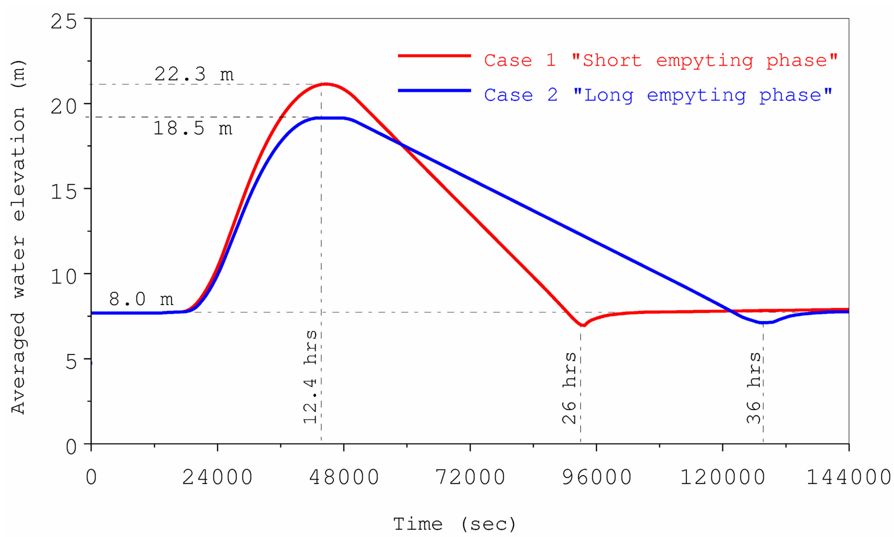

Figure 6 The averaged water elevations for cases 1 and 2 during the simulations.

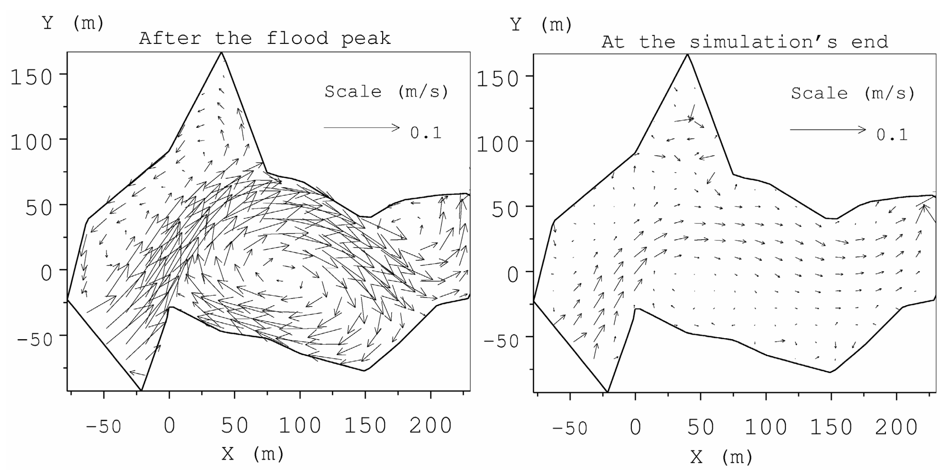

Figure 7 The velocity vectors for cases 1 and 2 after the flood peak and at the end of simulation.

4.2 Sediments and Contaminants Transport Results

Since the suspended sediment particles (SS) and the particulate phase (C_A) are bound together, the behavior of both is identical, Figures 8 and 9. The following interpretation is used for cases 1 and 2 since they have the same behavior and patterns but with different concentrations, Table 1:

During the flood peak, the water elevations were raised and large scale eddies due to turbulence were established. That leads to strong mixing with advection and diffusion mechanisms of suspended sediments and particulate contaminants in the water body. At the eddies center, the concentrations of (SS) and (C_A) are relatively small, because the turbulent mixing is a major phenomena and it controls the behavior of (SS) and (C_A).

After the peak time the water elevations were gradually reduced, the stored energy was dissipated and less inflow of suspended sediments was applied, Figures 5 and 6. That resulted in narrow suspended sediment plume with low concentration and high sedimentation with bound contaminants. After the emptying period, i.e. at time $Q_{out}=Q_{in}$, the water levels were constant with no changes in the hydraulic conditions, and almost a steady state case has been established, resulting in a central plume associated with high suspended sediment and particulate contaminant concentrations.

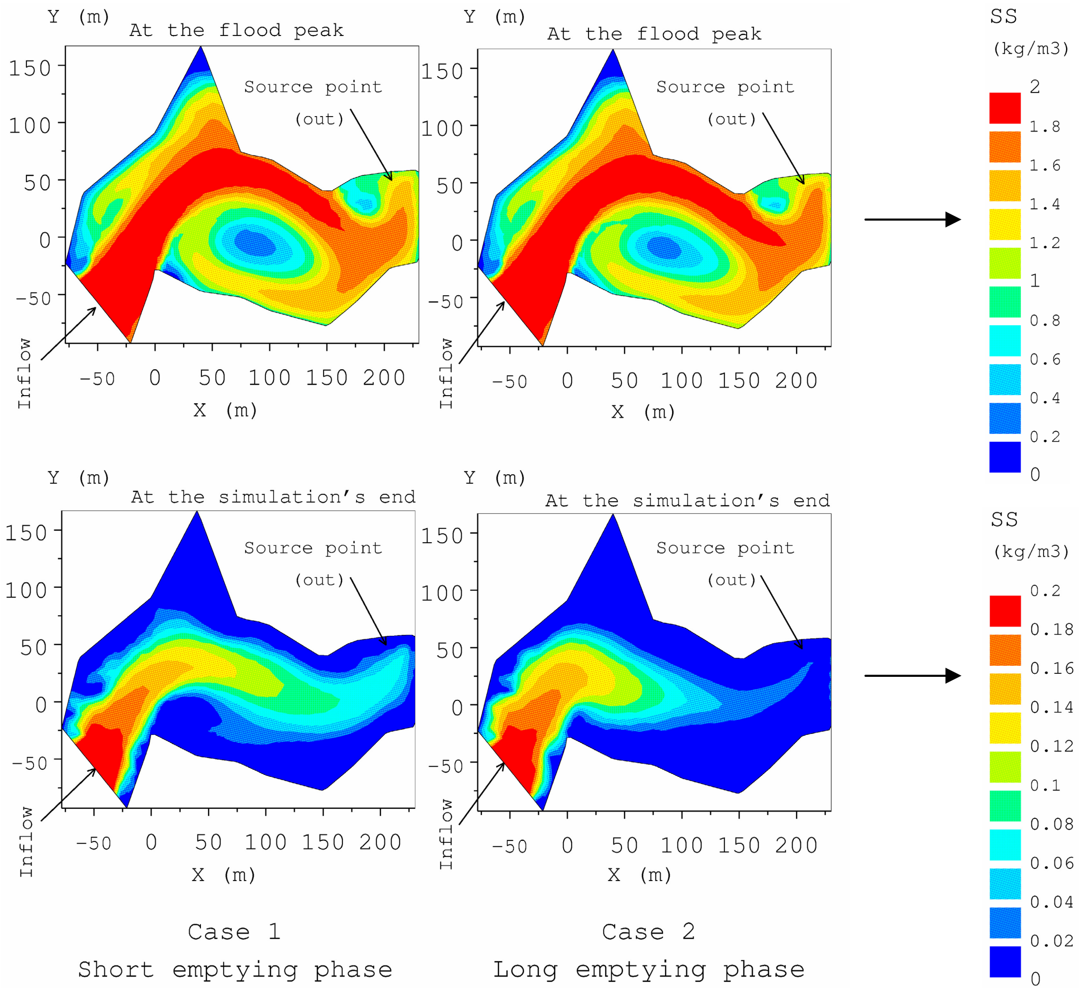

Figure 8 The suspended sediment behavior at the flood peak and at the simulation's end.

At the end of simulation, i.e at time = 40 hrs, high suspended sediment and particulate phase concentration plume at the middle and less concentrations at the boundaries (where high sedimentation, bounded sediments occurred) were obtained. Because the flow was tending to reach steady state case and the advection became a major mechanism, Figures 8 and 9. The suspended sediment and particulate contaminant plumes for case 2 was shorter than case 1 since the time taken after equalizing the inflow and outflow discharge is less for case 2 than case 1, therefore case 2 is further away from steady state case than case 1.

The sedimentation pattern looks similar for short and long emptying phases cases 1 and 2, Figure 10, but with different amounts, Table 1. That is due to the different outlet discharge functions. High sedimentation but lower contaminant deposition is obtained for long emptying phase as compared to short emptying phase. That is because the suspended sediment concentration is smaller in the long emptying phase simulation than the short phase. Therefore, the concentration of particulate contaminants, through sorption kinetics, in the water body (C_A) decreases and consequently the particulate contaminants concentration, through sedimentation process, at the sub-surface zone (G_A) is reduced as well and vice versa, eqs. 4, 5 and 7. In this case study, the dissolved contaminants phase (G_D) in the sub-surface zone has almost no significant influence on the particulate contaminants concentration (G_A) since the sorption kinetics parameters used are very small, Sect. 3.2. Therefore the concentration of (G_A) at the sub-surface is mainly affected by sedimentation processes, Figure 1.

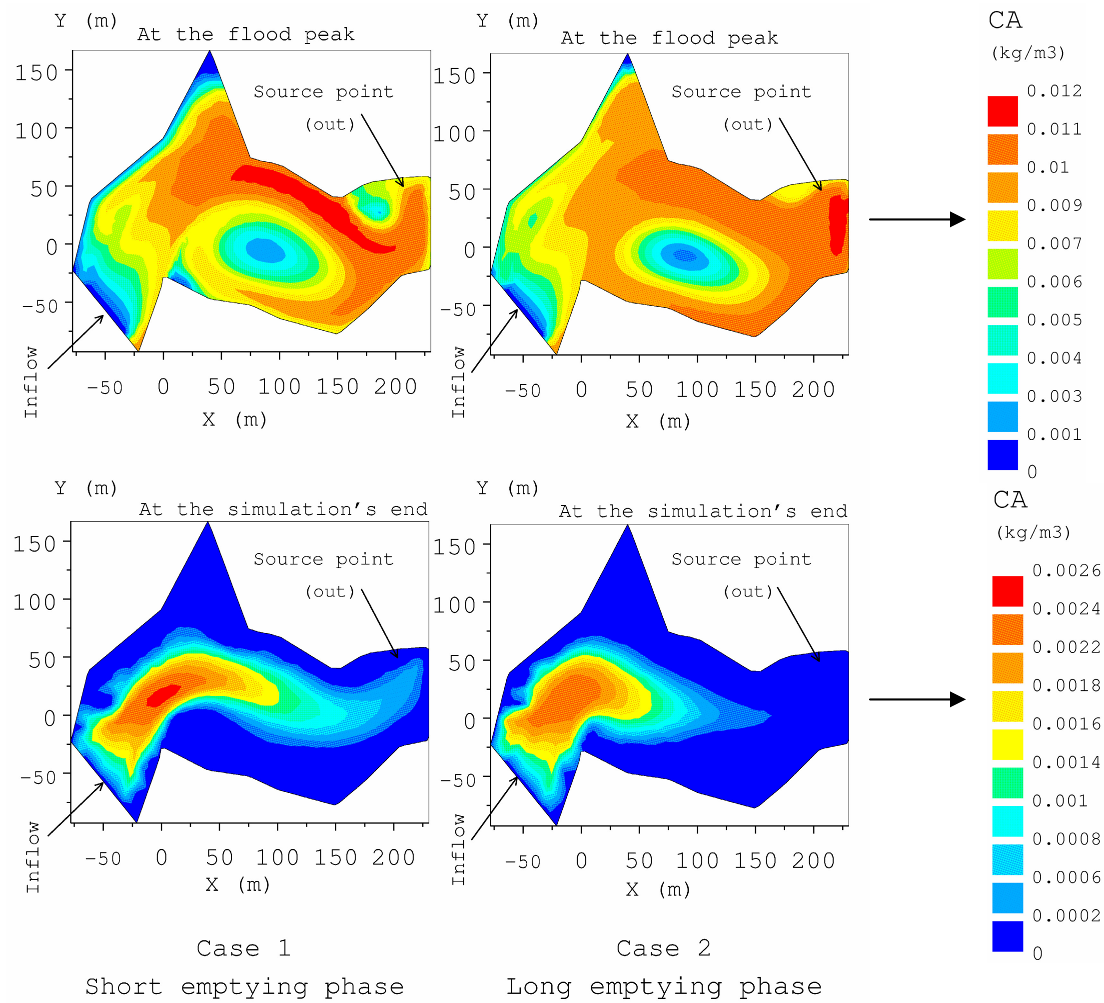

Figure 9 The particulate contaminants concentrations for short and long emptying phases.

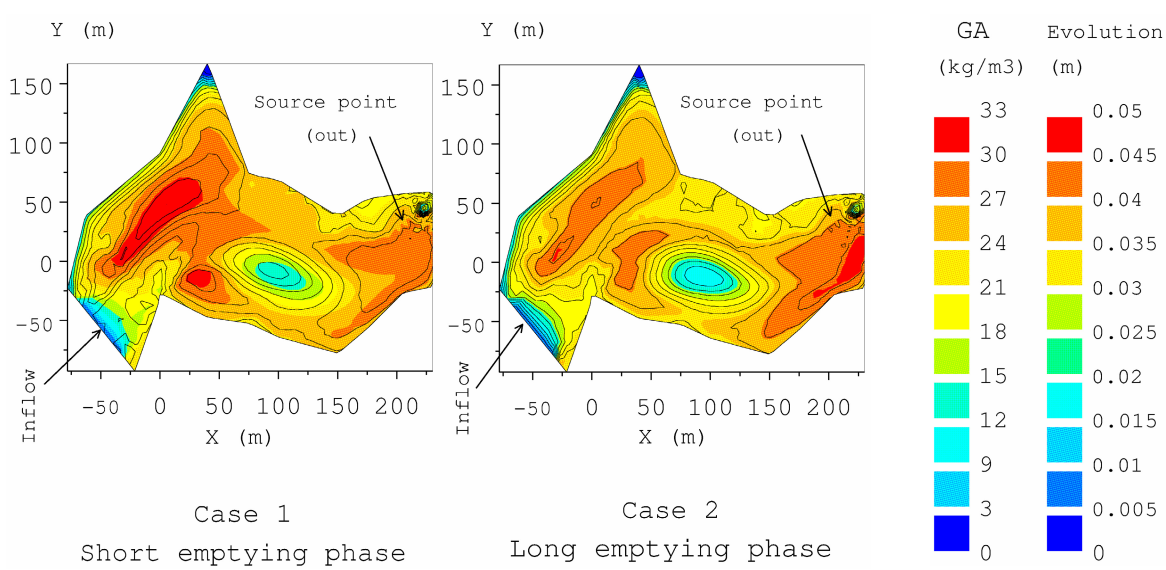

Figure 10 The particulate concentrations, evolutions and sedimentation patterns at the reservoir bed.

Table 1 Mass balance of suspended sediments and particulate contaminants in the sub-surface zone.

Mass	Suspended sediments (kg)				GA	
	Into domain	Out of domain	Suspended	Deposited	Mass (kg)	Concentration (g/kg)
Short phase (Case 1)	1667381	1000248	14247	652886	397	0.607
Long phase (Case 2)	1667381	994793	11103	661413	334	0.505

5. CONCLUSION

In this paper, a two dimensional, horizontal plane, numerical contaminant transport model CTM-SUBIEF-2D is presented for fine suspended sediment and contaminants transport in fluvial systems. The model employs k-d concept to describe the interactions between dissolved and particulate phases by first order sorption kinetic in both the water body and the sub-surface zone. The new developed code CTM-SUBIEF-2D was applied to a representative flood retention reservoir in southern Germany to predict the behavior of contaminants in space and time. Due to lack of data, no calibration was done and therefore, the model parameters could be directly taken from available literature.

The results show that the new developed code is able to deal with all processes mentioned in Figure 1 for contaminant transport problems. The numerical results also show the transport behavior of contaminants, suspended sediments and the spatial and temporal distribution of contaminated deposits under different reservoir operation rules with respect to the outlet discharge.

Two cases of reservoir operation rules, long and short emptying phases, were chosen to determine the best operation for reducing the amounts of sedimentation and contaminants. Higher sedimentation but lower contaminant deposition is obtained for the long emptying as compared to short empting phase, Sect. 4.2. The numerical calculations also indicated less sedimentation but higher contaminant deposition in the reservoir for increased outflow discharges.

Therefore, it could be concluded that the amount of sediments and deposited contaminants need not always have a proportionality. As seen in this study, the two quantities, i.e sedimentation and deposited contaminants, follow in an inverse proportionality.

As for the sedimentation mitigation, short emptying phase (case 1) is more effective in reducing reservoir sedimentation while long emptying phase (case 2) is better for less contaminants at the sub-surface zone in the reservoir.

NOTATION

All symbols are mentioned according to their appearance in the equations:

SS	kg/m^3	Suspended sediment concentration.
C_D, C_A	kg/m^3	Dissolved and particulate concentrations in the water body, respectively.
G_D, G_A	kg/m^3	Dissolved and particulate concentrations in the sub-surface zone, respectively.
K	m^2/s	Dispersion coefficient in the water body.
V_s	m/s	Settling velocity of sediment particles.
u^*_d, u^*_e	m/s	Critical shear stress velocities for deposition and erosion, respectively.
u,v	m/s	Depth averaged velocity components in x and y directions, respectively.
Q_d, Q_e	kg/m^2 s	Deposition and erosion rate fluxes, respectively.

h	m	Average water depth.
M	$kg/m^2\ s$	Partheniades constant for erosion.
K_1,K_2	s^{-1}	Sorption rates in the water body and the sub-surface zone, respectively.
K_D,K_B	m^3/kg	Equilibrium distribution coefficients in the water body and the sub-surface zone, respectively.
CSF	kg/m^3	Bottom concentration of the deposited/eroded layer.
Z_{MIX},Z_{AB}	m	Mixing layer and adsorption thickness at the sub-surface zone, respectively.
D_s	m^2/s	Diffusion coefficient into the sub-surface zone.
t	s	Time.
Z	m	Layer thickness which can be eroded or deposited.

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