



Simulation on release of heavy metals Cd and Pb in sediments

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Abstract: The re-release process and the release rate of heavy metals, cadmium and plumbum, which are rich in sediments of a certain water area, were investigated using a combined experimental and numerical method. Results show that the release law of Cd and Pb in sediments is divided into two stages: rapid release and dynamic equilibrium, which is in great agreement with the pseudo second-order kinetic equation with a correlation coefficient R^2 above 0.99. As the flow velocity accelerates, the release rate of heavy metals increases. The analysis results indicate that the water quality in the area can exceed the surface water Class V standard less than 3 h, and all but one of the relative deviations between the simulation value and the field survey result are within $\pm 10\%$.

Key words: sediment; heavy metal pollution; re-release rate; numerical simulation

1 Introduction

The river pollution left over from history will affect the surrounding biota for a lasting period of time [1–3]. Heavy metals are considered as the major component of pollutants in the aquatic environment because of the toxicity, bio-accumulation and stability against the degradation, which seriously threatens the well-being of human [4–6]. Toxic metals are transported into water through both natural sources and anthropogenic sources, such as sewage discharge, atmospheric deposition and surface runoff. After adsorption, desorption and precipitation processes, heavy metals are accumulated in the sediments continuously [7,8] and may be released into the water due to the sediment resuspension, desorption reactions, oxidation or reduction reactions [9,10]. As a potential sink of various pollutants, the sediments will cause secondary pollution to the overlying water in the form of a new source [11].

Therefore, researches focusing on the release of heavy metal pollutants in sediments are of great significance for the control and prevention of heavy metal pollution in rivers.

With the field measurement method, NICKEL et al [12] and CHAI et al [13] selected multiple test points in the research basin for heavy metal pollution assessment and pollution status analysis. However, this method is restricted to the development of measuring techniques. In order to better control the experimental condition and conduct targeted research, many scholars [14,15] completed the study of heavy metal contamination in sediments through indoor experiments. TSAI and LICK [14] designed a portable device for measuring sediment resuspension, which enables a rapid and accurate resuspension measurement. Since the 1980s, numerical simulation method has been gradually introduced into the study of heavy metal pollution in sediments [16]. In numerical simulations, the mathematical description of the interacting mechanism between heavy metals and

water, suspended sediments and sediments is of crucial importance. MAHDAVI et al [17] and SERRANO-PACHECO et al [18] took the water body as a whole to describe the kinetic process of heavy metal transport and transformation by numerical models. With the MeRiMod modelling tool, ŽAGAR et al [19] established a 1-D aquatic model to investigate mercury cycling processes in the river system. Nevertheless, most of the existing studies are limited to the historical sedimentation and pollution processes of heavy metals [20–22], which are lack of prediction for heavy metal release and re-pollution phenomena. Few studies have considered the relationship between the release rate of heavy metals and hydrodynamic conditions. Therefore, the numerical transformation of release phenomenon still needs further investigation.

In this study, in order to characterize the diffusion behavior of heavy metal pollutants in the sediment-overlying water system, indoor experiments are conducted to investigate the effect of flow velocity on the release rates of heavy metals Cd and Pb in the sediments of a certain water area. The re-release process of heavy metals in the actual river section is numerically simulated to study the distribution of heavy metals in the water body for pollution control.

2 Experimental

The re-release process of heavy metal in sediments includes the entering of particulate pollutants into water and the transformation of heavy metals from the sedimentary to the dissolved state. In this work, the riverbed sediment in the downstream section of a certain water area was selected as the study object. Based on the indoor experiment, the contents of Cd and Pb in the overlying water was measured under the condition that the sediment was considered as a pollution source. The release and diffusion discipline of Cd and Pb at different flow velocities were described by the release kinetic formulas of Cd and Pb, which improved the concentration equation of heavy metal pollutants diffusion in aquatic environment.

2.1 Materials preparation

The sediments are sampled by grab in a downstream section of an actual river. The collected

samples were dried in an electric oven at 60 °C for 14 d and 110 °C for 2 d until they attained constant mass, and ground into powder by agate mortar and pestle until fine particles (<150 μm). Next, 40 g sample was placed into clean Teflon vial, digested with 1 mL HNO₃ and 3 mL HF and heated on a hot plate at 130 °C for about 72 h. After the sample was cooled, 0.5 mL HClO₄ was added, and heated on a hot plate at 120 °C for 12 h with the lid opened until the white smoke disappeared. Afterwards, 1 mL HNO₃ and 1 mL deionized water were added and heated on a hot plate at 120 °C for 12 h for re-dissolution. Finally, the cooled solutions were transferred to a Teflon beaker and diluted with deionized water to a final volume of 40 mL. The concentrations of dissolved metals (Cd and Pb) in the water samples were measured by the inductively coupled plasma mass spectrometry (Agilent 7500 ICP-MS) under the standard operating conditions.

2.2 Experimental device and principle

Due to the data sensitivity, the data concerning metal content in the paper were all divided by a uniform base value. In order to obtain a stable experimental environment, an indoor circulating water tank was used, which was 50 cm in length and 40 cm in height, as shown in Fig. 1. The experimental circulating water was pure water, and the sediment was taken from the downstream section of a certain water area. By means of artificial pollution, the initial values of Cd and Pb in the sediment were set as 123.505 and 2944 mg/kg respectively based on the measured value in the actual river section. The mud layer was evenly spread 10 cm thick and the water layer was 20 cm. The experiment lasted for three weeks. In the first week, the experimental reagents and the sediment samples were prepared. The contents of Cd and Pb

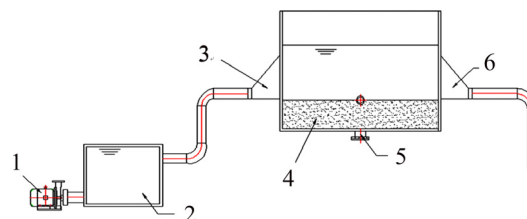


Fig. 1 Schematic diagram of experimental device used in this study (1–Water circulating pump; 2–Water tank; 3–Circulating outlet; 4–Sediments; 5–Emptying outlet; 6–Circulating inlet)

in samples were measured by ICP-MS. In the second week, the pump was started to stabilize the water tank with a flow velocity of 0.1 km/h, which was the average annual flow velocity of the river. During the process, heavy metals in the sediment would be freely released and reached a dynamic equilibrium. In the third week, the flow velocity was adjusted to 0.3, 0.5, 0.7, 0.9 and 1.1 km/h successively for the experimental conditions, so that the release dynamics of heavy metals Cd and Pb in the sediment under the disturbance of different flow rates can be investigated.

2.3 Samples collection and analysis

2.3.1 Samples collection

The experimental analysis index is the content of heavy metals in the overlying water. Five sampling locations were set in the water tank, located in the center of water 10 cm-deep from the water surface, which are shown in Fig. 2. In each site, 20 mL sample was collected and centrifuged for 10 min to obtain the supernatant. After mixing with HNO_3 , the solution was adjusted to pH value less than 2, and then placed in the refrigerator for later testing. The contents of Cd and Pb in water were measured by ICP-MS.

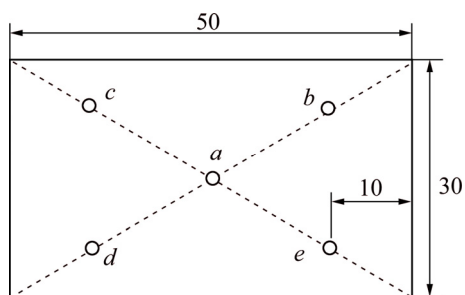


Fig. 2 Distribution of sampling locations (Unit: cm)

2.3.2 Analysis of experimental results

As shown in Figs. 3 and 4, the release disciplines of heavy metals Cd and Pb in sediments at different flow velocities are basically the same, which are divided into two stages, consisting of a rapid release stage and a dynamic equilibrium stage. The concentrations of Cd and Pb in the overlying water were boosted with time, then reached a state of dynamic equilibrium. With the acceleration of flow velocity, the release rates of Cd and Pb in the sediment gradually increased, and the concentrations of heavy metals in the overlying water increased as well in the dynamic equilibrium stage.

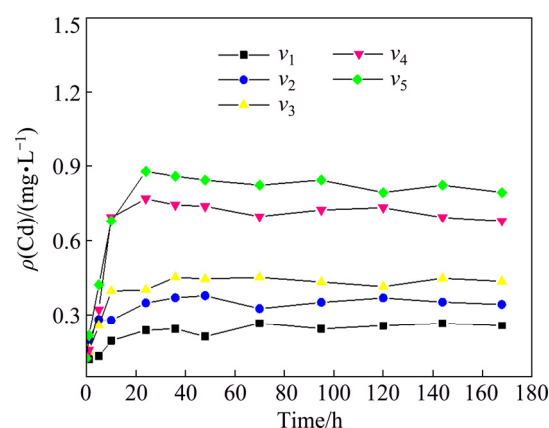


Fig. 3 Concentration of Cd in overlying water ($v_1=0.3$ km/h, $v_2=0.5$ km/h, $v_3=0.7$ km/h, $v_4=0.9$ km/h and $v_5=1.1$ km/h)

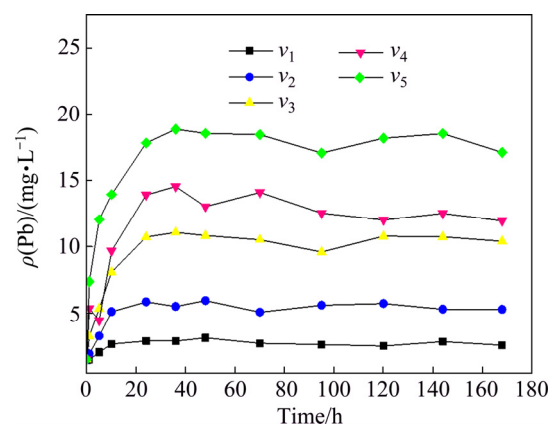


Fig. 4 Concentration of Pb in overlying water ($v_1=0.3$ km/h, $v_2=0.5$ km/h, $v_3=0.7$ km/h, $v_4=0.9$ km/h and $v_5=1.1$ km/h)

According to previous studies [23,24], the pseudo second-order kinetic equation and the Elovich equation were adopted to fit the concentrations of Cd and Pb in the above experiment, which are shown in Tables 1 and 2. The release processes of Cd and Pb in the certain river sediment had a good matching degree with the pseudo second-order kinetic equation with a correlation coefficient R^2 above 0.99; whereas the equation fitted according to the Elovich equation is not ideal. By comparing the reaction mechanisms represented by the two fitting forms [25,26], a conclusion can be drawn that the release process of heavy metals Cd and Pb in sediments tends to obey the single reaction mechanism, and does not require a high activation energy.

Considering the influence of the flow velocity and the time, the contents of Cd and Pb in the overlying water can be described as follows:

Table 1 Kinetic formula for Cd release process

Velocity/(km·h ⁻¹)	$t/c=at+b$			$c=a\ln(t-c)+b$			
	a	b	R^2	a	b	c	R^2
0.3	24.04	8.821	0.9982	0.00273	0.0298	0.889	0.681
0.5	13.21	4.321	0.998	0.00309	0.0636	1.000	0.719
0.7	10.38	1.33	0.998	0.0071	0.0673	0.994	0.832
0.9	7.105	2.001	0.9966	0.0128	0.0876	0.987	0.706
1.1	6.212	0.7134	0.9973	0.0154	0.0965	0.969	0.768

c is the amount of adsorption/release at time t ; a and b are coefficients of the kinetic equation

Table 2 Kinetic formula for Pb release process

Velocity/(km·h ⁻¹)	$t/c=at+b$			$c=a\ln(t-c)+b$			
	a	b	R^2	a	b	c	R^2
0.3	1.809	1.444	0.9933	0.0184	0.477	1.000	0.607
0.5	0.901	1.071	0.9961	0.0776	0.768	0.992	0.745
0.7	0.4701	0.6353	0.9962	0.226	1.121	0.877	0.778
0.9	0.403	0.1689	0.9944	0.299	1.236	0.519	0.532
1.1	0.2802	0.0936	0.9966	0.288	2.326	0.947	0.829

$$t/c=41.95e^{-2v}+4.23e^{-2v} \text{ (for Cd)} \quad (1)$$

$$t/c=4.343e^{-3v}+3.17e^{-3v} \text{ (for Pb)} \quad (2)$$

Equation (1) denotes the content of Cd in water and Eq. (2) denotes the content of Pb in water with the correlation coefficient R^2 of 0.9832 and 0.9841, respectively. The formulas can be adopted to predict the release amount of Cd and Pb in sediments when the flow velocity reaches any point between 0.3 and 1.1 km/h. With a single adsorption/release constant, the release rate χ of Cd and Pb in sediments during the dynamic process can be deduced by

$$C_s(t, v) = -C(t, v) \cdot V_w / M \quad (3)$$

$$\chi = \frac{\partial C_s}{\partial t} \quad (4)$$

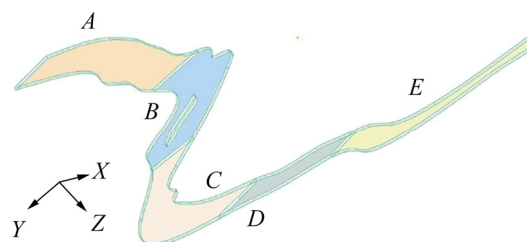
where $C(t, v)$ denotes the function of the content of Cd or Pb in the water, and $C_s(t, v)$ denotes the function of the content of the corresponding elements in the sediment, V_w is the volume of water in the tank; M is the amount of dry sediment under the corresponding area.

3 Numerical simulation

3.1 Physical model

In order to fully reflect the release characteristics of Cd and Pb in sediments, a representative river section of about 25 km in a

certain water area was selected with an annual average depth of 31.3 m measured by the local hydrological station. As shown in Fig. 5, the physical model of the river section was built by ArcGIS10.2 and ICEM software, which is 1:1 ratio to the real size and is divided into 5 regions (A, B, C, D and E) bounded by the middle section of two adjacent sampling sections.

**Fig. 5** Physical model of selected water area

3.2 Mathematical model

The river flow exists in the form of turbulence in nature. The mathematical model can be derived under the assumption that the fluid is incompressible.

(1) Continuity equation

$$\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} = 0 \quad (5)$$

where u_x , u_y and u_z denote the average velocity components in the x , y and z directions, respectively.

(2) Momentum equation

On the riverbed and river bank of real rivers, flowing water is subject to a strong viscous shearing stress due to the presence of sediments. Therefore, considering the effect of sediments at the bottom, the momentum equation is established with the water-level depth (h) as the characteristic quantity under the condition of three-dimension [27]:

$$\frac{\partial u_x}{\partial t} + u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_x}{\partial y} + u_z \frac{\partial u_x}{\partial z} = -g \frac{\partial h}{\partial x} + \nu_\varepsilon \left(\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2} \right) - \frac{\partial \tau_{sx}}{\rho H} \quad (6)$$

$$\frac{\partial u_y}{\partial t} + u_x \frac{\partial u_y}{\partial x} + u_y \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_y}{\partial z} = -g \frac{\partial h}{\partial y} + \nu_\varepsilon \left(\frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_y}{\partial y^2} + \frac{\partial^2 u_y}{\partial z^2} \right) - \frac{\partial \tau_{sy}}{\rho H} \quad (7)$$

$$\frac{\partial u_z}{\partial t} + u_x \frac{\partial u_z}{\partial x} + u_y \frac{\partial u_z}{\partial y} + u_z \frac{\partial u_z}{\partial z} = -g \frac{\partial h}{\partial z} + \nu_\varepsilon \left(\frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial y^2} + \frac{\partial^2 u_z}{\partial z^2} \right) - \frac{\tau_{sz}}{\rho H} \quad (8)$$

where the first term on the right side of the equation denotes the volume force, the second term denotes the turbulent shear stress, the third term denotes the viscous shearing stress at the riverbed, H is the average depth of water-level, g denotes the gravitational acceleration; h denotes the depth of the water; ν_ε denotes the kinematic viscosity of turbulence; ρ denotes the density of river, and τ_{sx} , τ_{sy} and τ_{sz} denote the viscous shearing stress at the riverbed.

$$\frac{\tau_{sx}}{\rho} = C_f u_x (u_x^2 + u_y^2 + u_z^2)^{1/2} \quad (9)$$

$$\frac{\tau_{sy}}{\rho} = C_f u_y (u_x^2 + u_y^2 + u_z^2)^{1/2} \quad (10)$$

$$\frac{\tau_{sz}}{\rho} = C_f u_z (u_x^2 + u_y^2 + u_z^2)^{1/2} \quad (11)$$

where C_f is the friction coefficient.

(3) Turbulence model

Considering that the influence of the sediment viscosity to the near-wall water area is significant, the standard k - ε turbulence model is modified according to the previous study [28]:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho u_j k) =$$

$$\frac{\partial}{\partial x_j} \left[\frac{\mu_e}{\delta_k} \cdot \frac{\partial k}{\partial x_j} \right] + G_k - \rho \varepsilon + \rho P_k \quad (12)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_j}(u_j \rho \varepsilon) = \\ \frac{\partial}{\partial x_j} \left(\frac{\mu_e}{\delta_\varepsilon} \cdot \frac{\partial \varepsilon}{\partial x_j} \right) + \frac{\varepsilon}{k} (C_1 G_k - C_2 \rho \varepsilon) + \rho P_\varepsilon \quad (13) \end{aligned}$$

$$G_k = \mu_t \left\{ 2 \left[\left(\frac{\partial u_x}{\partial x} \right)^2 + \left(\frac{\partial u_y}{\partial y} \right)^2 + \left(\frac{\partial u_z}{\partial z} \right)^2 \right] + \right.$$

$$\left. \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right)^2 + \left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x} \right)^2 + \left(\frac{\partial u_y}{\partial z} + \frac{\partial u_z}{\partial y} \right)^2 \right\} \quad (14)$$

where C_1 , C_2 , δ_k and δ_ε are coefficients of the k - ε model, respectively; G_k is the generation item; k denotes the turbulence kinetic energy; ε denotes the turbulence kinetic energy dissipation ratio; μ_e denotes the effective viscosity, μ_t denotes the eddy viscosity; P_k and P_ε are the modified terms of friction resistance for the turbulence kinetic energy, related to the viscous shearing stress and the depth of water [29].

$$P_k = C_f^{-1/2} \frac{u_*^3}{h} \quad (15)$$

$$P_\varepsilon = C_\varepsilon \frac{u_*^4}{h^2} \quad (16)$$

$$C_\varepsilon = C_{\varepsilon f} \frac{C_2}{C_f^{3/4}} \sqrt{C'_\mu} \quad (17)$$

where C'_μ , $C_{\varepsilon f}$ are coefficients of the k - ε model, respectively, u_* denotes the friction velocity. The relevant coefficients are listed in Table 3.

Table 3 Coefficients of standard k - ε turbulent model

C_1	C_2	C_f	$C_{\varepsilon f}$	C'_μ	δ_k	δ_ε
1.43	1.92	6.22×10^{-3}	3.6	0.09	1.0	1.3

(4) Vertical velocity profile of river

Flow velocity is one of the vital hydraulic elements that reflect turbulent characteristics, denoted as [30]

$$u = u_m \left(\left[\frac{2z}{h} - \left(\frac{z}{h} \right)^2 \right] \left(\frac{1}{1-\beta} \right) \right)^{1/a} \quad (18)$$

where z is the height from the riverbed; a is the index; u_m denotes the maximum flow velocity;

$\beta = u_m 2\nu / (gJh^2)$, in which ν denotes the kinematic viscosity of water and J denotes the hydraulic gradient.

(5) Concentration equation

Without the participation of external pollution sources, the concentration equation is established by

$$\begin{aligned} \frac{\partial c}{\partial t} = & \frac{\partial(u_x c_x)}{\partial x} + \frac{\partial(u_y c_y)}{\partial y} + \frac{\partial(u_z c_z)}{\partial z} + \\ & \frac{\partial}{\partial x} \left[(D_{mx} + D_{tx} + D_d) \frac{\partial c}{\partial x} \right] + \\ & \frac{\partial}{\partial y} \left[(D_{my} + D_{ty}) \frac{\partial c}{\partial y} \right] + \frac{\partial}{\partial z} \left[(D_{mz} + D_{tz}) \frac{\partial c}{\partial z} \right] + R \end{aligned} \quad (19)$$

$$R = \frac{\chi M}{Ah} \quad (20)$$

where D_m is the molecular diffusion coefficient of heavy metals; D_t is the turbulent diffusion coefficient of heavy metals; D_d is the longitudinal dispersion diffusion coefficient of heavy metals; R is the source item; χ is the release rate of heavy metals; A denotes the effective area of the sediment surface in the control body.

In the numerical simulation, the relevant parameters are shown in Table 4.

3.3 Analysis of simulation results

Results of the numerical simulation are shown in Figs. 6 and 7. Under the flow disturbance, the heavy metals in sediments re-released. Over time, the contents of Cd and Pb on the sediment surface of a certain water area gradually decreased. After an interval of 24 h, the simulation values of the heavy metal contents in sediments in regions *A*, *B*, *C*, *D* and *E* were compared with the field survey result, as illustrated in Table 5. The relative deviations were all within $\pm 10\%$ except for one individual value, which demonstrates that the mathematical model and simulation method used in this work have certain theoretical significance, and can manage to simulate the dynamic process of re-release of heavy metals in sediments due to the change of flow velocity in a certain period of time.

As shown in Fig. 8, the heavy metals released from the sediment has a great influence on the water body. The average concentrations of Cd and Pb in the river section were taken as the analysis

Table 4 Relevant parameters in numerical simulation

Parameter	Value or formula
Density of water/(kg·m ⁻³)	1000
Kinematic viscosity of water/(m ² ·s ⁻¹)	1.006×10 ⁻⁶
Molecular diffusion coefficient/(m ² ·s ⁻¹)	2.88×10 ⁻⁸
	$D_{tx} = I u'^2 b^2 / D_{ty}$
Turbulent diffusivity [31]	$D_{ty} = 3 D_{tz} = (1/2) \kappa u_* h$ $D_{tz} = (1/6) \kappa u_* h$
Longitudinal dispersion coefficient [32]	$D_d = 0.6 B^2 (1/H) u_*$
Concentration of Cd in overlying water/(mg·L ⁻¹)	0.13
Concentration of Pb in overlying water/(mg·L ⁻¹)	1.42
Maximum section velocity/(km·h ⁻¹)	0.79
Iteration method	Multigrid V loop iteration

$I_{\text{const}} = 0.1$; $b' = 0.7B$; $u'^2 = 0.2u^2$, u is the average velocity; B is the width of river

index, which increased nearly linearly within 24 h under flow disturbance. The ratio of the average content of Cd at 24 h to the initial average content is: $0.185 \div 0.002 = 92.5$, while the ratio of the average content of Pb to the initial average content is: $5.9 \div 0.012 = 491.7$. Under the flow disturbance for 2 h, the concentration of Cd in the water is ten times of the initial content. Compared with the surface water environmental quality standard [33] shown in Table 6, it can be observed that the concentration of Cd exceeds surface water Class I standard; meanwhile, the content of Pb exceeds surface water Class V standard. Under the flow disturbance for 3 h, the concentration of Cd in water exceeds surface water Class V standard. In conclusion, when the release of heavy metals in sediments occurs, it can quickly affect the overlying water in a short time, and result in a significant deterioration of the water quality. Furthermore, the influence will gradually deepen as the disturbance continues.

In order to explore the spatial and temporal distribution of heavy metals Cd and Pb released into water from the sediment, the average concentration of heavy metals in vertical direction

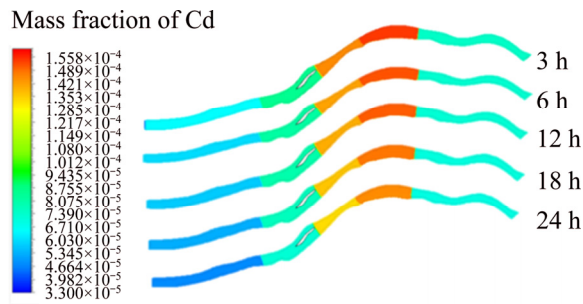


Fig. 6 Content of Cd in sediments at different time

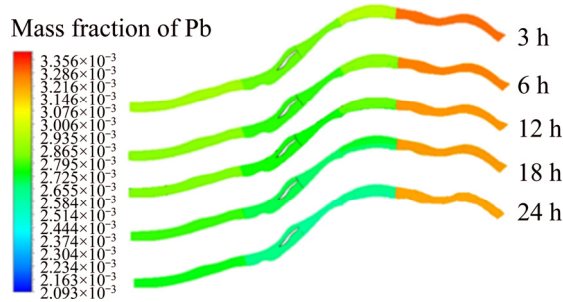


Fig. 7 Content of Pb in sediments at different time

Table 5 Relative deviation between simulation value and field survey result

Region	Relative deviation/%	
	Cd	Pb
A	14.4	0.8
B	1.6	1.5
C	1.7	0.5
D	2.19	5.1
E	−0.9	6.1

was investigated at 3, 6, 12, 18 and 24 h after the disturbance of water flow, as shown in Fig. 9. The distribution discipline of the heavy metals in the vertical direction is basically the same at different time. The diffusion range of Cd is mainly concentrated in the water body within 8 m above the sediment, and before 6 h, the water body more than 15 m above the sediments can meet surface water Class V standard. Since then, Cd has continued to diffuse upward. At 24 h, the water body more than 18 m high from the bottom of the riverbed can reach surface water Class V standard.

The distribution of Pb in the vertical direction can be divided into three regions according to the magnitude of the average concentration: 10^3 , 10^2

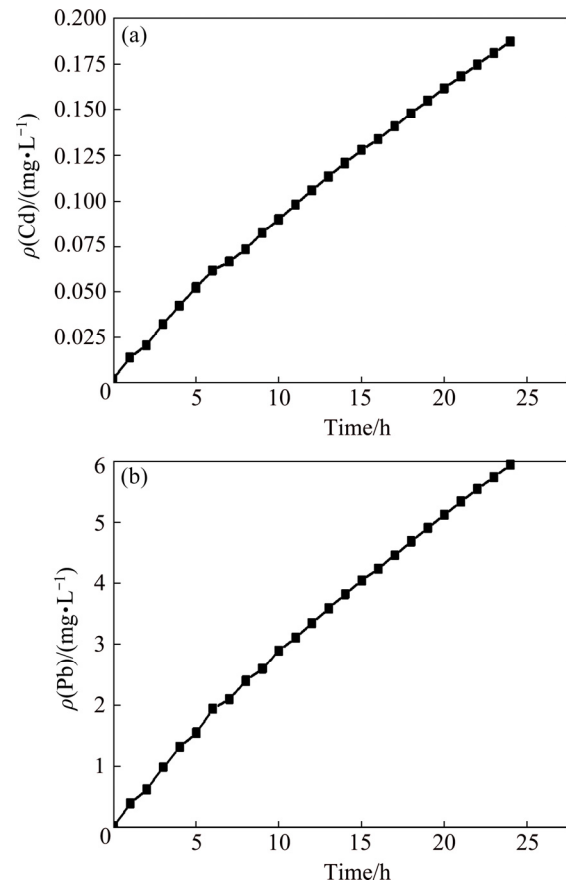


Fig. 8 Average concentration of heavy metals in water body: (a) Cd; (b) Pb

Table 6 Environmental quality standards for surface water at pH 6–9 (mg/L)

Class	Cd	Pb
I	≤0.001	≤0.01
II	≤0.005	≤0.01
III	≤0.005	≤0.05
IV	≤0.005	≤0.05
V	≤0.01	≤0.1

and 10^1 . Before 3 h, the average concentration of Pb was in the magnitude of 10^3 within 3 m above the sediment, the magnitude of 10^2 from 3 to 8 m and the concentration at other heights is in the third range. From 3 to 24 h, the diffusion area with a magnitude of 10^3 further increased in the calculation area, and the concentration increase is obvious in the heights of 3 to 7 m from the sediment, where the Pb concentration at 24 h is more than 1.5 times that at 3 h. Within 24 h of monitoring, the average concentration of Pb in water will reach surface water Class V standard more than 18 m above the sediment.

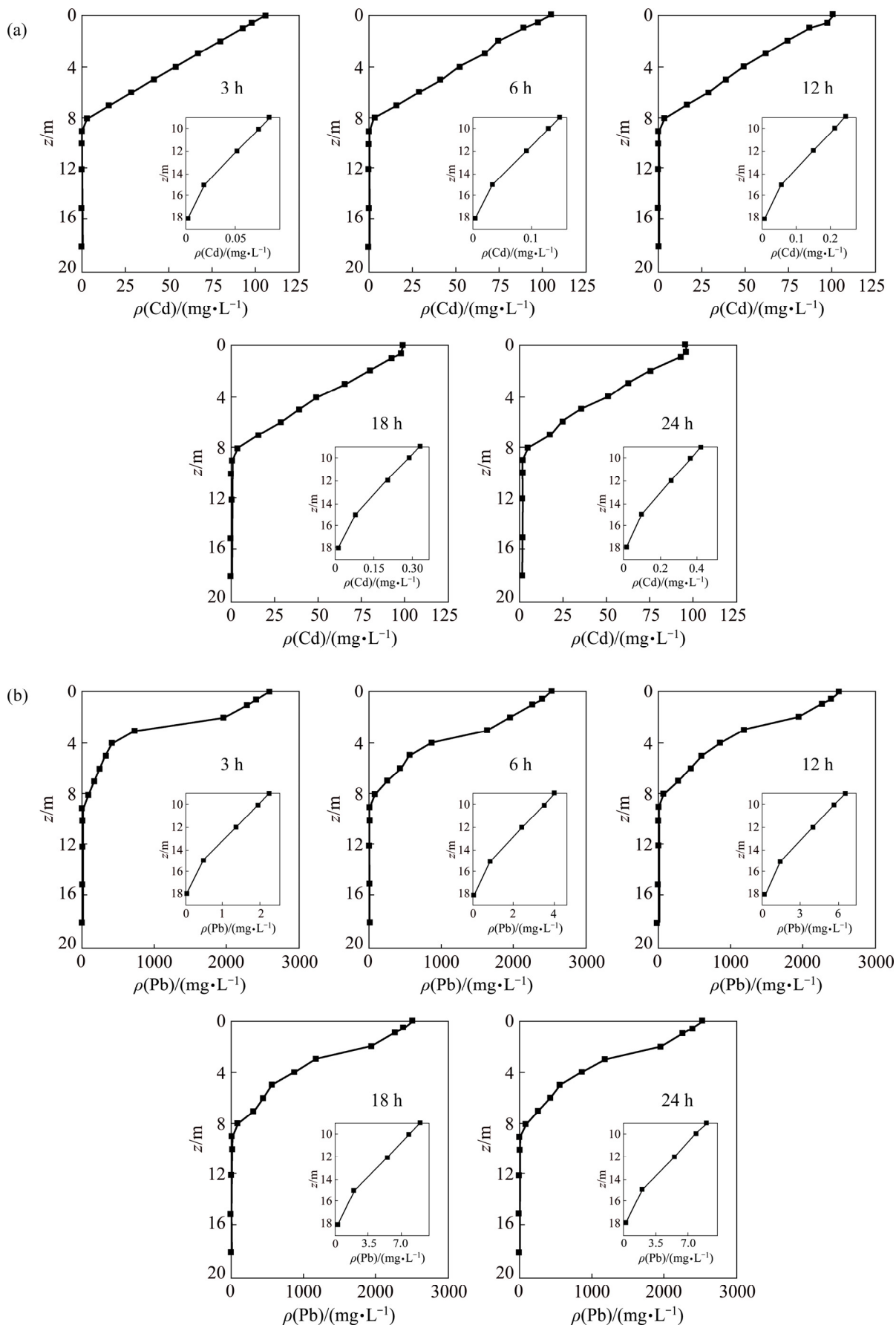


Fig. 9 Vertical distribution of heavy metals in river at different time: (a) Cd; (b) Pb

The average concentration of heavy metals in water body 8 m high from the bottom of the riverbed is analyzed by zoning. As shown in Fig. 10, regions *A*, *B*, *C*, *D* and *E* are the overlying waters corresponding to the riverbed sediment subsection area, in which *E* is the upstream and *A* is the downstream. Because of the difference in heavy metal contaminants in sediments, there is a significant difference in pollutant content in each water area during the release process. At the early stage of release, the heavy metal concentration in the corresponding upper water is directly related to that in the sediment, where the concentrations of Cd and Pb in sediments are large, the concentration in the water above is also large. Over time, the concentration in the water will change significantly due to the migration and diffusion of heavy metals. In the waters above the sediment with large heavy metal concentration, the concentration tends to decrease. However, in the adjacent downstream waters, the concentration will slowly increase with time. It can be concluded that concentration of the

heavy metals in the sediment is the main reason affecting the degree of heavy metals pollution in water within 24 h after the release of heavy metals from the sediment. After a dynamic equilibrium is reached from the release process, the migration and diffusion of heavy metals in water gradually play a leading role carried by suspended particles in the river environment [34].

4 Conclusions

(1) Based on the indoor experiment, the release law of heavy metals Cd and Pb in sediments at different flow rates was observed to be basically the same, which is divided into two stages, the rapid release section and the dynamic equilibrium section.

(2) With the increase of the flow rate, the release rates of Cd and Pb in the rapid release section gradually increase, and the heavy metal content in the overlying water body increases at dynamic equilibrium. The release processes of Cd and Pb in sediments are well matched with the pseudo second-order kinetic equation.

(3) The numerical simulation demonstrates that the heavy metals Cd and Pb in the sediments can rapidly diffuse into the overlying water body. The water quality in the area can exceed the surface water Class V standard less than 3 h and does not meet the surface water Class V standard until the height of 18 m above the sediment at 24 h.

(4) The content of heavy metals Cd and Pb in sediments after 24 h in the numerical simulation results are in good agreement with the field survey results. All but one of the relative deviations are within $\pm 10\%$, which verifies the reasonability and feasibility of the mathematical model established.

Acknowledgments

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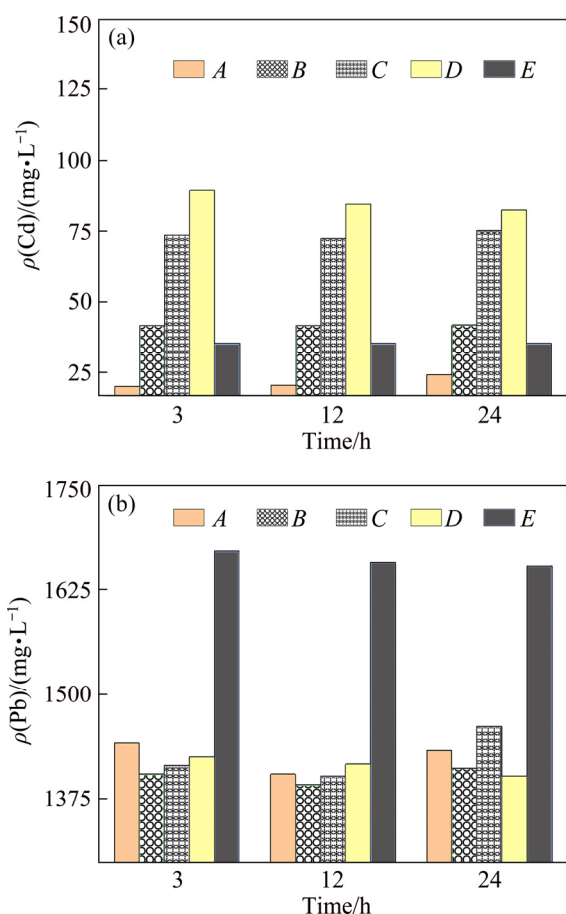


Fig. 10 Average concentration of heavy metals in water body 8 m high from bottom of riverbed within 24 h: (a) Cd; (b) Pb

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水域底泥中重金属 Cd 与 Pb 释放规律的数值模拟

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摘要: 采用实验研究与数值模拟相结合的方法, 研究某水域底泥中典型重金属污染物 Cd 与 Pb 再释放过程和释放速率。结果表明, 底泥中 Cd 和 Pb 的释放规律分为快速释放和动态平衡两个阶段, 与准二级动力学方程具有较好的匹配度, 相关系数 R^2 大于 0.99。随着河流流速的加快, 底泥中重金属的释放速率增大。分析表明, 该区域水质可以在 3 h 内超过地表水环境质量 V 类标准。数值模拟结果与实测值之间的相对偏差除一项外均在 $\pm 10\%$ 以内。

关键词: 底泥; 重金属污染; 再释放率; 数值模拟

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