Supplementary Materials

for

Evaluation of nano-silver concentrations using multi-media fate and transport models with different spatial resolutions

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Supplementary Materials Include:

- **Tables S1-5**
- **Figures S1**
- **Equation S1-12**
- **Section A & Section B**

Table S1

Some river parameters are not recorded in the Hunan Hydrological Bureau official website database and have no major influence on the calculation of the main process parameters of AgNPs migration in the river, so the parameters in the research of Praetorius et al.(1) and Ding et al.(2) are used instead.

Table S1 Hydrological Parameters table of Xiangjiang River Basin

Parameter	*Symbol*	*Value*	*Unit*	*ref.*
river flow velocity	$v_{river,flow}$	0.65	m s^{-1}	(2)
water temperature	T_{water}	287	K	(1)
water density	ρ_{water}	1000	kg m^{-3}	(1)
shear rate	G	10	s^{-1}	(1)
dynamic viscosity of water	μ_{water}	1.002×10^{-3}	Pa·s	(1)
velocity of sediment transfer (bed load shift)	$v_{Sed\text{-}transf}$	3	kg s^{-1}	(1)
sediment resuspension velocity	v_{resusp}	3.17×10^{-12}	m s^{-1}	(1)
sediment burial velocity to deep sediment	v_{burial}	9.50×10^{-12}	m s^{-1}	(1)
sediment density	ρ_{Sed}	2.60×10^{3}	kg m^{-3}	(2)
Boltzmann constant	k_B	1.38×10^{-23}	J K^{-1}	(1)
gravitational acceleration on earth	g	9.81	m s^{-2}	(1)

Table S2

Table S2 Table of model size and compartment division of Xiangjiang main stream

Parameter	*Symbol*	*Value*	*Unit*
length of the river	l_{River}	768.1（770）	km
Model 1			
number of boxes in the river model	n_{boxes}	6	
River segmentation and compartment division method			
box length for boxes n = 1 (Yongzhou)	$l_{box,1}$	2.27×10^5	m
box length for boxes n = 2 (Hengyang)	$l_{box,2}$	2.26×10^5	m
box length for boxes n = 3 (Zhuzhou)	$l_{box,3}$	8.96×10^4	m
box length for boxes n = 4 (Xiangtan)	$l_{box,4}$	4.25×10^4	m
box length for boxes n = 5 (Changsha)	$l_{box,5}$	7.40×10^4	m
box length for boxes n = 6 (Yueyang)	$l_{box,6}$	1.09×10^5	m
Model 2			
length of river box n	$l_{box,n}$	increasing*	
number of boxes in the river model	n_{boxes}	527	
depth of flowing water (W1)	h_{W1}	41.98	m
depth of stagnant water (W2)	h_{W2}	5.14	m
depth of sediment (Sed)	h_{Sed}	0.26	m
cross sectional area of first box of flowing water	$A_{W1,1}$	7.78×10^3	m^2

cross sectional area of last box of flowing water	$A_{W1,\ n\ boxes\ +1}$	$4{*}\ A_{W1,1}$	m^2
volume of box n of flowing water (W1)	$V_{W1,n}$	$(A_{W1,n}+A_{W1,n+1})/2\cdot l_{box,n}$	m^3
volume of box n of stagnant water (W2)	$V_{W2,n}$	12% of $V_{W1,n}$	m^3
volume of box n of sediment (Sed)	$V_{Sed,n}$	5% of $V_{W1,n}$	m^3
River segmentation and compartment division method			
box length for boxes n = 1,...,100 (0 to 10 m)	$l_{box,n}$	0.1	m
box length for boxes n = 101,...,190 (10 to 100 m)	$l_{box,n}$	1	m
box length for boxes n = 191,...,280 (100 m to 1 km	$l_{box,n}$	10	m
box length for boxes n = 281,...,370 (1 km to 10 km)	$l_{box,n}$	100	m
box length for boxes n = 371,...,460 (10 km to 100 km)	$l_{box,n}$	1	km
box length for boxes n = 461,...,527 (100 km to 770 km)	$l_{box,n}$	10	km

Table S3

Table S3 Nanoparticles and natural colloid parameters

	Parameter	*Symbol*	*Value*	*Unit*	*ref.*
AgNPs	particle diameter	d_{AgNPs}	9.05×10^{-8}	m	(3)
	density	ρ_{AgNPs}	8478	kg m^{-3}	(3)
NCs	particle diameter	d_{NCs}	2.91×10^{-7}	m	(3)
	density	ρ_{NCs}	1250	kg m^{-3}	(3)
	concentration (determined by dry weight after filtration)	C_{NCs}	1.03E $\times 10^{-2}$	kg m^{-3}	(3)

Table S4

Table S4 Table for calculating the life process rate constant of AgNPs

Parameter	*Symbol*	*Value*	*Unit*	*ref.*
deposition rate constant of AgNPs in flowing water	$k_{\mathrm{dep,AgNPs,W1}}$	$\frac{v_{\mathrm{dep,AgNPs}}}{h_{W1}}$	s^{-1}	(1)
deposition rate constant of AgNPs in stagnant water	$k_{\mathrm{dep,AgNPs,W2}}$	$\frac{v_{\mathrm{dep,AgNPs}}}{h_{W2}}$	s^{-1}	(1)
deposition rate constant of NCs in flowing water	$k_{\mathrm{dep,NCs,W1}}$	$\frac{v_{\mathrm{dep,NCs}}}{h_{W1}}$	s^{-1}	(1)
deposition rate constant of NCs in stagnant water	$k_{\mathrm{dep,NCs,W2}}$	$\frac{v_{\mathrm{dep,NCs}}}{h_{W2}}$	s^{-1}	(1)

heterogeneous aggregation rate constants of AgNPs and NCs in water	k_{het}	$k_{het} = k_{het,crit}$ * (	s^{-1}	(3)
water exchange rate constant between flowing and stagnant water	$k_{exch,1\text{-}2}$	1.00E-05	s^{-1}	(4, 5)
water exchange rate constant between stagnant and flowing water	$k_{exch,2\text{-}1}$	$k_{exch,1\text{-}2} * \frac{V_{W1}}{V_{W2}}$	s^{-1}	(4, 5)
sediment burial rate constant to deep sediment	k_{burial}	$\frac{v_{burial}}{h_{Sed}}$	s^{-1}	(1)
sediment resuspension rate constant	k_{resusp}	$\frac{v_{resusp}}{h_{Sed}}$	s^{-1}	(1)
rate constant of horizontal sediment transfer (bed load shift) of box n	$k_{Sed\text{-}trans,n}$	$(\frac{v_{Sed - trans}}{\rho_{Sed}})/V_{Sed,n}$	s^{-1}	
river flow rate constant of box n	$k_{river,flow,n}$	$v_{river,flow,n} * \frac{A_W}{V_W}$	s^{-1}	

In Table S4, v_{dep} represents the sedimentation rate (m s^{-1}) of AgNPs or NCs particles in the water, which can be calculated according to the Stokes equation.

$$v_{dep} = \frac{2r^2(\rho_P - \rho_{water})g}{9\mu}$$

where ρ_P represents the density of AgNPs or NCs (kg m^{-3}), and g represents the gravitational acceleration on earth (m s^{-2}).

Eq. S1-Eq. S12

The concentration conservation equations of free AgNPs in each phase of the first compartment:

- flowing water (W1): (Eq. S1)

$$\frac{dc^{\mathrm{AgNPs}}_{W1,1}}{dt} =- \left(k_{\mathrm{exch},1-2} + k_{\mathrm{river,flow},1} + k_{\mathrm{dep,AgNPs},W1} + k_{\mathrm{het}}\right) * c^{\mathrm{AgNPs}}_{W1,1}(t) + k_{\mathrm{exch},2-1} * \ldots$$

- stagnant water (W2): (Eq. S2)

$$\frac{dc^{\mathrm{AgNPs}}_{W2,1}}{dt} =- \left(k_{\mathrm{exch},2-1} + k_{\mathrm{dep,AgNPs},W2} + k_{\mathrm{het}}\right) * c^{\mathrm{AgNPs}}_{W2,1}(t) + \left(k_{\mathrm{exch},1-2} + k_{\mathrm{dep,A}}\ldots\right.$$

$$(t) + k_{\mathrm{resusp}} * \frac{V_{\mathrm{Sed},1}}{V_{W2,1}} * c^{\mathrm{AgNPs}}_{\mathrm{Sed},1}(t)$$

- sediment (Sed): (Eq. S3)

$$\frac{dc^{\mathrm{AgNPs}}_{\mathrm{Sed},1}}{dt} =- \left(k_{\mathrm{resusp}} + k_{\mathrm{burial}} + k_{\mathrm{Sed-transfer},1}\right) * c^{\mathrm{AgNPs}}_{\mathrm{Sed},1}(t) + k_{\mathrm{dep,AgNPs},W2} * \frac{V_{W2,1}}{V_{\mathrm{Sed},1}} * c^{\mathrm{AgNPs}}_{W2,1}(t)$$

The concentration conservation equations of AgNPs aggregated with NCs in each phase of the first compartment:

- flowing water (W1): (Eq. S4)

$$\frac{dc^{\mathrm{AgNPs+NCs}}_{W1,1}}{dt} =- \left(k_{\mathrm{exch},1-2} + k_{\mathrm{river,flow},1} + k_{\mathrm{dep,NCs},W1}\right) * c^{\mathrm{AgNPs+NCs}}_{W1,1}(t) + k_{\mathrm{het}} * c^{\mathrm{AgNPs}}_{W1,1}(t\ldots$$

$$\frac{V_{W2,1}}{V_{W1,1}} * c^{\mathrm{AgNPs+NCs}}_{W2,1}(t)$$

- stagnant water (W2): (Eq. S5)

$$\frac{dc^{\mathrm{AgNPs+NCs}}_{W2,1}}{dt} =- \left(k_{\mathrm{exch},2-1} + k_{\mathrm{dep,NCs},W2}\right) * c^{\mathrm{AgNPs+NCs}}_{W2,1}(t) + k_{\mathrm{het}} * c^{\mathrm{AgNPs}}_{W2,1}(t) + \left(k_{\mathrm{exch},1}\ldots\right. \frac{V_{W1,1}}{V_{W2,1}} *$$

$$c^{\mathrm{AgNPs+NCs}}_{W1,1}(t) + k_{\mathrm{resusp}} * \frac{V_{\mathrm{Sed},1}}{V_{W2,1}} * c^{\mathrm{AgNPs+NCs}}_{\mathrm{Sed},1}(t)$$

- sediment (Sed): (Eq. S6)

$$\frac{dc_{\mathrm{Sed,1}}^{\mathrm{AgNPs+NCs}}}{dt} = -\left(k_{\mathrm{resusp}} + k_{\mathrm{burial}} + k_{Sed\text{-}\mathrm{transfer,1}}\right) * c_{\mathrm{Sed,1}}^{\mathrm{AgNPs+NCs}}(t) + k_{\mathrm{dep,NCs},W2} * \frac{V_{W2,1}}{V_{\mathrm{Sed,1}}} * c^{\mathrm{AgN}} \ldots (t)$$

The concentration conservation equations of free AgNPs in each phase of the 2-n compartments:

- flowing water (W1): (Eq. S7)

$$\frac{dc_{W1,\mathrm{n}}^{\mathrm{AgNPs}}}{dt} = -\left(k_{\mathrm{exch,1-2}} + k_{\mathrm{river,flow,n}} + k_{\mathrm{dep,AgNPs},W1} + k_{\mathrm{het}}\right) * c_{W1,\mathrm{n}}^{\mathrm{AgNPs}}(t) + k_{\mathrm{exch,2-1}} * \frac{V_{W2,\mathrm{n}}}{V_{W1,\mathrm{n}}} * c_{W2,\mathrm{n}}^{\mathrm{AgNPs}}(t) +$$

$$k_{\mathrm{riverflow,n-1}} * \frac{V_{W1,\mathrm{n-1}}}{V_{W1,\mathrm{n}}} * c_{W1,\mathrm{n-1}}^{\mathrm{AgNPs}}(t)$$

- stagnant water (W2): (Eq. S8)

$$\frac{dc_{W2,\mathrm{n}}^{\mathrm{AgNPs}}}{dt} = -\left(k_{\mathrm{exch,2-1}} + k_{\mathrm{dep,AgNPs},W2} + k_{\mathrm{het}}\right) * c_{W2,\mathrm{n}}^{\mathrm{AgNPs}}(t) + \left(k_{\mathrm{exch,1-2}} + k_{\mathrm{dep,AgNPs},W1} \ldots\right.$$

$$k_{\mathrm{resusp}} * \frac{V_{\mathrm{Sed,n}}}{V_{W2,\mathrm{n}}} * c_{\mathrm{Sed,n}}^{\mathrm{AgNPs}}(t)$$

- sediment (Sed): (Eq. S9)

$$\frac{dc_{\mathrm{Sed,n}}^{\mathrm{AgNPs}}}{dt} = -\left(k_{\mathrm{resusp}} + k_{\mathrm{burial}} + k_{\mathrm{sed-transfer,n}}\right) * c_{\mathrm{Sed,n}}^{\mathrm{AgNPs}}(t) + k_{\mathrm{dep,AgNPs},W2} * \frac{V_{W2,\mathrm{n}}}{V_{\mathrm{Sed,n}}} * c_{W2,\mathrm{n}}^{\mathrm{AgNPs}}(t) +$$

$$k_{\mathrm{sed-transfer,n-1}} * \frac{V_{\mathrm{Sed,n-1}}}{V_{\mathrm{Sed,n}}} * c_{\mathrm{Sed,n-1}}^{\mathrm{AgNPs}}(t)$$

The concentration conservation equations of AgNPs aggregated with NCs in each phase of the 2-n compartment:

- flowing water (W1): (Eq. S10)

$$\frac{dc_{W1,\mathrm{n}}^{\mathrm{AgNPs+NCs}}}{dt} = -\left(k_{\mathrm{exch,1-2}} + k_{\mathrm{river,flow,n}} + k_{\mathrm{dep,NCs},W1}\right) * c_{W1,\mathrm{n}}^{\mathrm{AgNPs+NCs}}(t) + k_{\mathrm{het}} * c_{W1,\mathrm{n}}^{\mathrm{AgNPs}}(t) +$$

$$k_{\mathrm{exch,2-1}} * \frac{V_{W2,\mathrm{n}}}{V_{W1,\mathrm{n}}} * c_{W2,\mathrm{n}}^{\mathrm{AgNPs+NCs}}(t) + k_{\mathrm{riverflow,n-1}} * \frac{V_{W1,\mathrm{n-1}}}{V_{W1,\mathrm{n}}} * c_{W1,\mathrm{n-1}}^{\mathrm{AgNPs+NCs}}(t)$$

- stagnant water (W2): (Eq. S11)

$$\frac{dc_{W2,\mathrm{n}}^{\mathrm{AgNPs+NCs}}}{dt} = -\left(k_{\mathrm{exch,2-1}} + k_{\mathrm{dep,NCs},W2}\right) * c_{W2,\mathrm{n}}^{\mathrm{AgNPs+NCs}}(t) + k_{\mathrm{het}} * c_{W2,\mathrm{n}}^{\mathrm{AgNPs}}(t) + (k_{\mathrm{exc}}$$

$$\frac{V_{W1,\mathrm{n}}}{V_{W2,\mathrm{n}}} * c_{W1,\mathrm{n}}^{\mathrm{AgNPs+NCs}}(t) + k_{\mathrm{resusp}} * \frac{V_{\mathrm{Sed,n}}}{V_{W2,\mathrm{n}}} * c_{\mathrm{Sed,n}}^{\mathrm{AgNPs+NCs}}(t)$$

- sediment (Sed): (Eq. S12)

$$\frac{dc_{\mathrm{Sed,n}}^{\mathrm{AgNPs+NCs}}}{dt} = -\left(k_{\mathrm{resusp}} + k_{\mathrm{burial}} + k_{\mathrm{sed-transfer,n}}\right) * c_{\mathrm{Sed,n}}^{\mathrm{AgNPs+NCs}}(t) + k_{\mathrm{dep,NCs},W2} * \frac{V_{W2,}}{V_{\mathrm{Sed,}}} (t) +$$

$$k_{\mathrm{sed-transfer,n-1}} * \frac{V_{\mathrm{Sed,n-1}}}{V_{\mathrm{Sed,n}}} * c_{\mathrm{Sed,n-1}}^{\mathrm{AgNPs+NCs}}(t)$$

Section A. Establishment of mass conservation equation

The whole life process of free AgNPs and AgNPs bound NCs are established to form first-order rate constant concentration balance equations, as shown in Eq.S1-S12. It is assumed that AgNPs are in a steady state in each compartment, which is reflected in the equation as $dc_i/dt=0$. Furthermore, each equation is equivalent to the multivariate linear equation $q-a_1*c_1+a_2*c_2+a_3*c_3+....=0$, which contains multiple unknowns, where q is the emission rate of AgNPs (kg s^{-1}) , a_i represents the coefficient term, and c_i

represents the concentration term.

Extract all a_1, a_2, a_3... to form a coefficient matrix A, which represents the rate constant of migration and transformation in the medium (s^{-1}); c_1, c_2, c_3... are all proposed to form an unknown matrix C, which represents the steady-state concentration of AgNPs; extracting q_1, q_2, q_3... to form a constant matrix Q, and the equation $A*C=-Q$ can be obtained.

$A_1=$

$$\begin{bmatrix} -(k_{\text{exch},1-2}+k_{\text{river,flow},1}+k_{\text{dep,AgNPs},W1}+k_{\text{het}}) & k_{\text{exch},2-1}*\frac{V_{W2,1}}{V_{W1,1}} & 0 & \cdots \\ (k_{\text{exch},1-2}+k_{\text{dep,AgNPs},W1})*\frac{V_{W1,1}}{V_{W2,1}} & -(k_{\text{exch},2-1}+k_{\text{dep,AgNPs},W2}+k_{\text{het}}) & k_{\text{resusp}}*\frac{V_{\text{sed},1}}{V_{W2,1}} & \cdots \\ 0 & k_{\text{dep,AgNPs},W2}*\frac{V_{W2,1}}{V_{\text{sed},1}} & -(k_{\text{resusp}}+k_{\text{burial}}+k_{\text{sed-transfer},1}) & \cdots \\ k_{\text{het}} & 0 & 0 & -(k_{\text{exch},1-2}+k_{\text{riv}}\cdots \\ 0 & k_{\text{het}} & 0 & (k_{\text{exch},1-2}+k_{\text{d}}\cdots \\ 0 & 0 & 0 & \cdots \end{bmatrix}$$

$$C_1=\begin{bmatrix} c_{W1,1}^{\text{AgNPs}}(t) \\ c_{W2,1}^{\text{AgNPs}}(t) \\ c_{\text{Sed},1}^{\text{AgNPs}}(t) \\ c_{W1,1}^{\text{AgNPs+NCs}}(t) \\ c_{W2,1}^{\text{AgNPs+NCs}}(t) \\ c_{\text{Sed},1}^{\text{AgNPs+NCs}}(t) \end{bmatrix}; \quad Q_1=\begin{bmatrix} e_{\text{AgNPs}}^{\text{input}} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

In compartment 2-n, the constant matrix A_n, the unknown number matrix C_n, and the constant matrix Q_n are as follows:

$A_n=$

$$\begin{bmatrix} -(k_{\text{exch},1-2}+k_{\text{river,flow},n}+k_{\text{dep,AgNPs},W1}+k_{\text{het}}) & k_{\text{exch},2-1}*\frac{V_{W2,n}}{V_{W1,n}} & 0 & 0 & \cdots \\ (k_{\text{exch},1-2}+k_{\text{dep,AgNPs},W1})*\frac{V_{W1,n}}{V_{W2,n}} & -(k_{\text{exch},2-1}+k_{\text{dep,AgNPs},W2}+k_{\text{het}}) & k_{\text{resusp}}*\frac{V_{\text{sed},n}}{V_{W2,n}} & 0 & \cdots \\ 0 & k_{\text{dep,AgNPs},W2}*\frac{V_{W2,n}}{V_{\text{sed},n}} & -(k_{\text{resusp}}+k_{\text{burial}}+k_{\text{sed-transfer},n}) & 0 & \cdots \\ k_{\text{het}} & 0 & 0 & -(k_{\text{exch},1-2}+k_{\text{river},}\cdots \\ 0 & k_{\text{het}} & 0 & (k_{\text{exch},1-2}+k_{\text{dep},}\cdots \\ 0 & 0 & 0 & 0 & \cdots \end{bmatrix}$$

$$C_n=\begin{bmatrix} c_{W1,n}^{AgNPs}(t) \\ c_{W2,n}^{AgNPs}(t) \\ c_{Sed,n}^{AgNPs}(t) \\ c_{W1,n}^{AgNPs+NCs}(t) \\ c_{W2,n}^{AgNPs+NCs}(t) \\ c_{Sed,n}^{AgNPs+NCs}(t) \end{bmatrix};\quad Q_n=\begin{bmatrix} k_{riverflow,n-1} * \dfrac{V_{W1,n-1}}{V_{W1,n}} * c_{W1,n-1}^{AgNPs}(t) \\ 0 \\ k_{sed-transfer,n-1} * \dfrac{V_{Sed,n-1}}{V_{Sed,n}} * c_{Sed,n-1}^{AgNPs}(t) \\ k_{riverflow,n-1} * \dfrac{V_{W1,n-1}}{V_{W1,n}} * c_{W1,n-1}^{AgNPs+NCs}(t) \\ 0 \\ k_{sed-transfer,n-1} * \dfrac{V_{Sed,n-1}}{V_{Sed,n}} * c_{Sed,n-1}^{AgNPs+NCs}(t) \end{bmatrix}$$

Section B. R language programming calculation

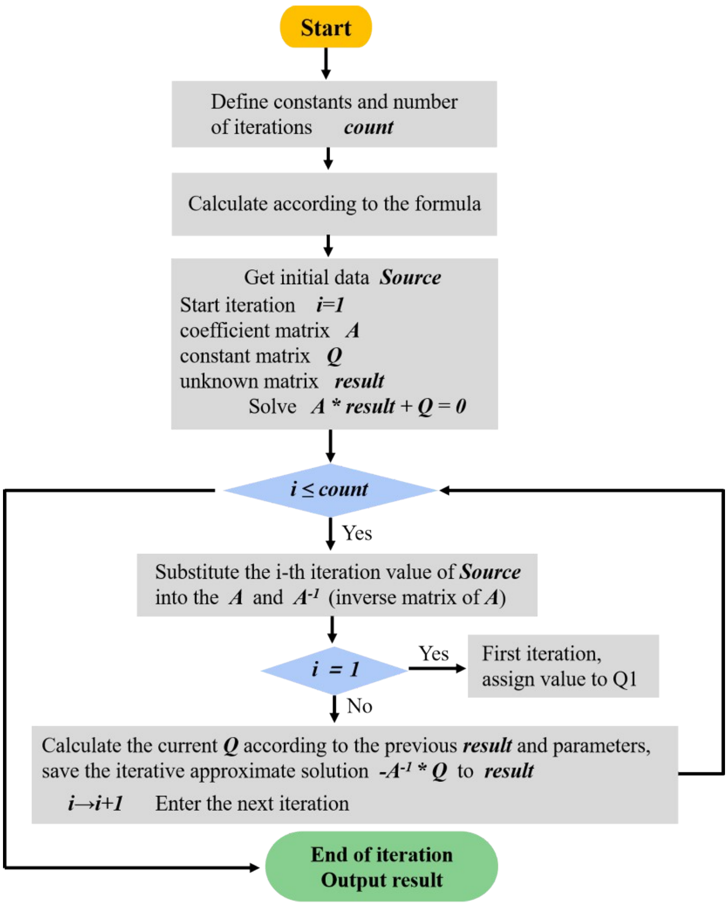

Figure S1 Model calculation programming flow chart

Use R language programming to assist the calculation. The programming flowchart is shown in Figure S1. According to the relevant calculation formula, the value of the rate constant of AgNPs life process is shown in Table S5.

Table S5 Table for life process rate constant calculation numerical of AgNPs

Parameter	*Symbol*	*Value*	*Unit*
deposition rate constant of AgNPs in flowing water	$k_{(dep,AgNPs\ W1)}$	7.94×10^{-10}	s^{-1}
deposition rate constant of AgNPs in stagnant water	$k_{(dep,AgNPs\ W2)}$	6.48×10^{-9}	s^{-1}
deposition rate constant of NCs in flowing water	$k_{(dep,NCs,W1)}$	1.10×10^{-9}	s^{-1}
deposition rate constant of NCs in stagnant water	$k_{(dep,NCs,W2)}$	8.96×10^{-9}	s^{-1}
heterogeneous aggregation rate constants of AgNPs and NCs in water	$k_{(het)}$	3.03×10^{-6}	s^{-1}
water exchange rate constant between flowing and stagnant water	$k_{(exch,1-2)}$	1.00×10^{-5}	s^{-1}
water exchange rate constant between stagnant and flowing water	$k_{(exch,2-1)}$	8.33×10^{-5}	s^{-1}
sediment burial rate constant to deep sediment	$k_{(burial)}$	3.65×10^{-11}	s^{-1}
sediment resuspension rate constant	$k_{(resusp)}$	1.22×10^{-11}	s^{-1}
rate constant of horizontal sediment transfer (bed load shift) of box n	$k_{(sed\text{-}trans,n)}$	9.61×10^{-10}	s^{-1}
river flow rate constant of box n	$k_{(river,flow,n)}$	7.17×10^{-6}	s^{-1}

Reference

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