说明书

流域重金属行为模拟模型输入输出系统 V1.0

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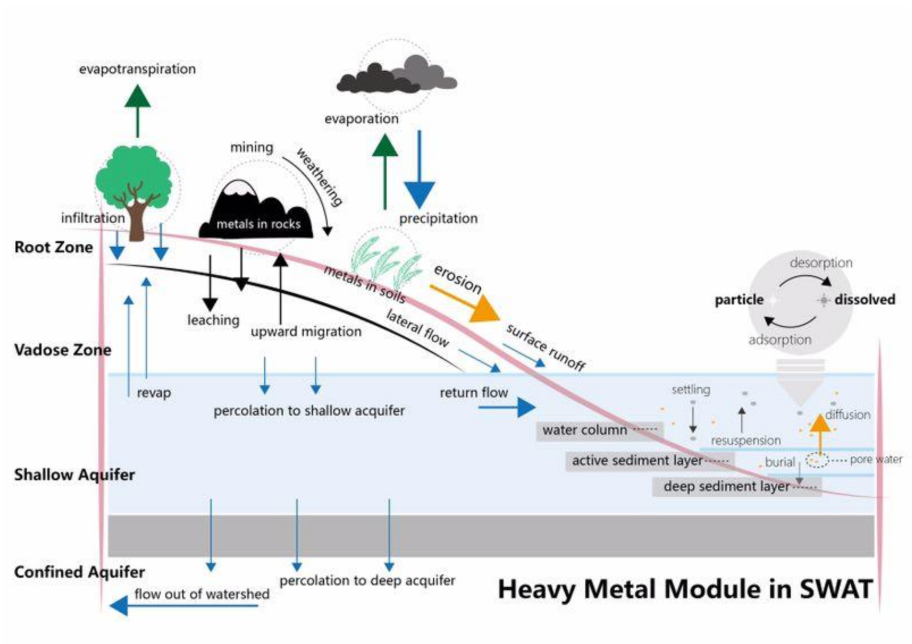
2022 年 8 月

SWAT-HM

User’s manual

August 2022



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1. SWAT-HM description

SWAT-HM (Soil and Water Assessment Tool – Heavy Metal) was developed to simulate the fate and transport of heavy metals (HM) at the watershed scale. SWAT-HM provides a process-based representation of the metal behavior from uplands to streams and down to the watershed outlet. Fig. 1 illustrates a schematic diagram of the main processes (upland and channel processes) of the SWAT-HM. SWAT-HM operates at a daily time step, tracking the stores and fluxes of dissolved and particulate metals in both the land and in-stream phases of a catchment. Fig 2 displays the command loop of SWAT-HM code.

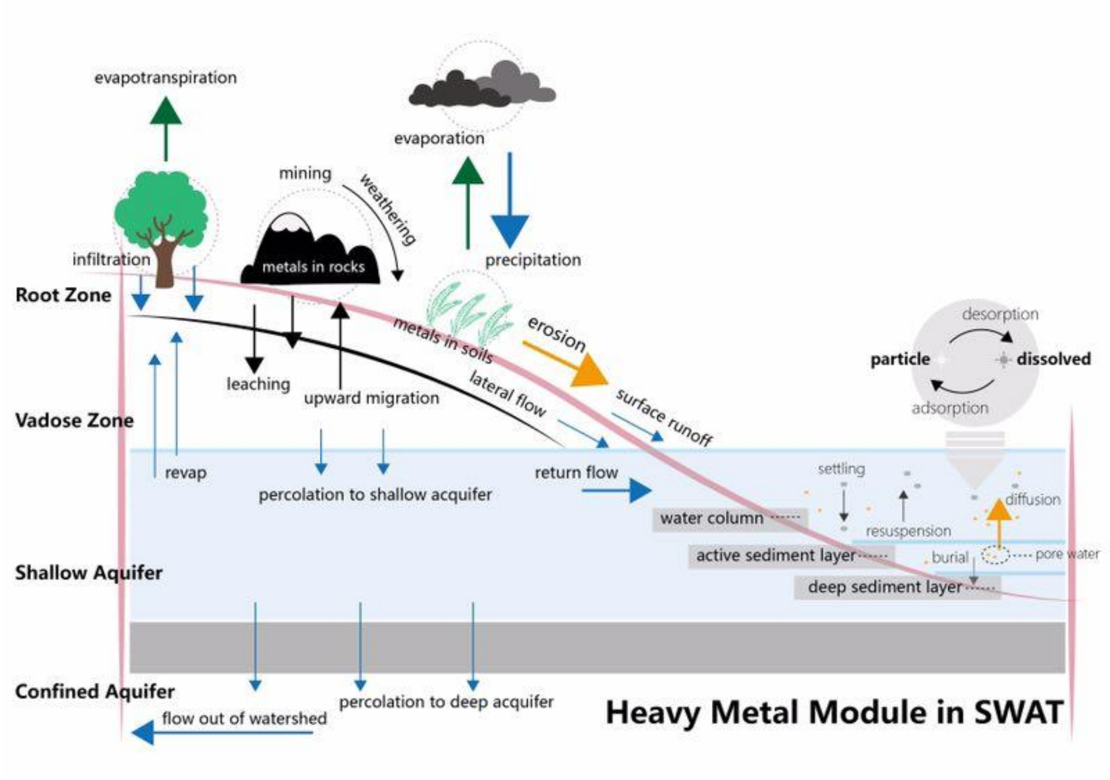

Fig. 1 - Schematic framework of heavy metal module coupled with the SWAT model

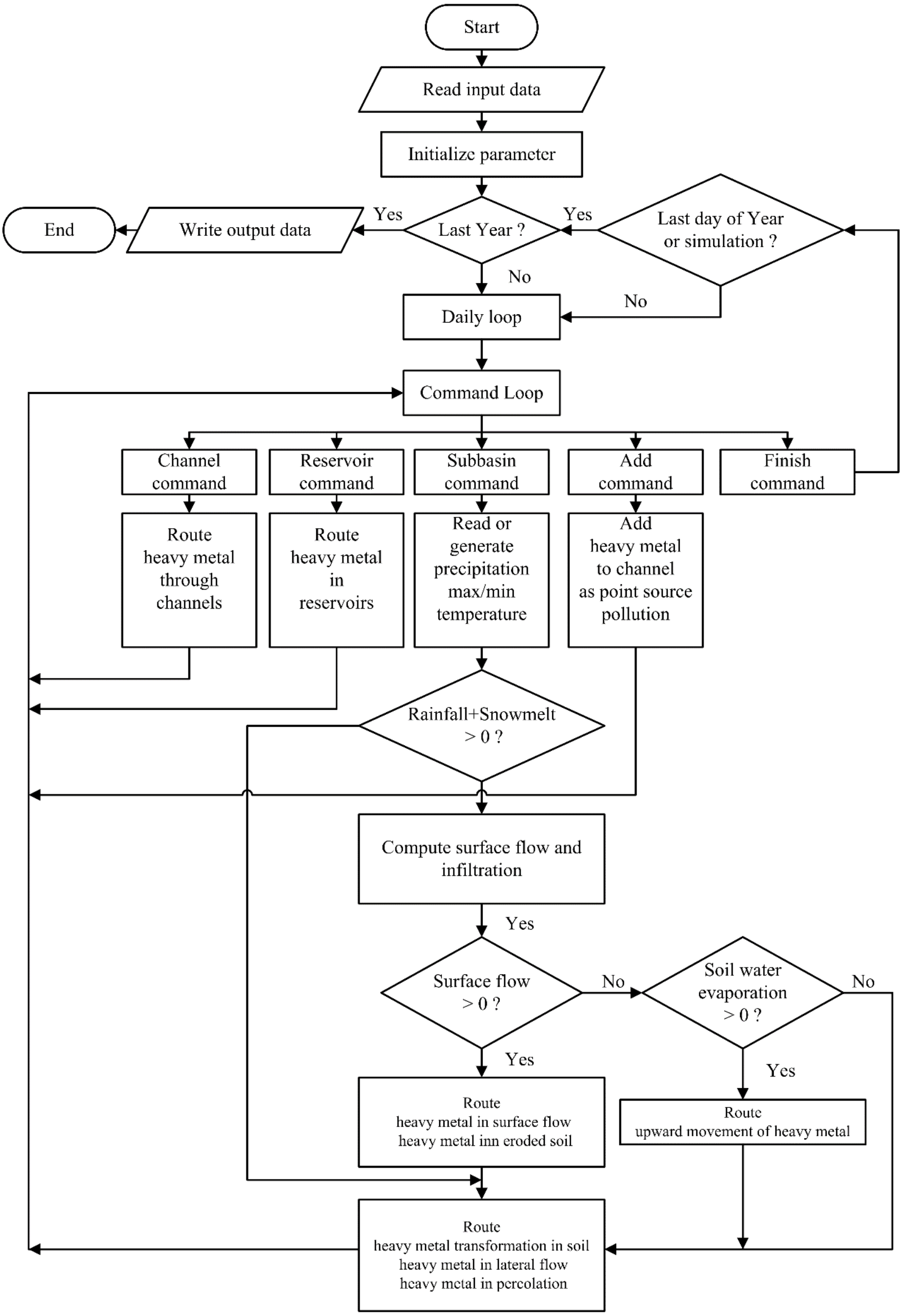

Fig. 2 – SWAT-HM command loop

1.1. Heavy metal transformation module

In this section, we first introduce the transformations module followed by the transport module specifications because of the dependence of metal mobility and bioavailability on its chemical speciation. In the natural environment, there are numerous reactions that affect the speciation of metals, such as sorption (adsorption/desorption), complexation (association/dissociation), precipitation, diffusion into carbonates and oxyhydroxides. In the solid phase, metals are present as labile, non-labile, and inert metal. Labile metal is part of the solid-phase metal that is rapidly exchangeable with the solution phase. Inert solid metal is the case for metals present in parent minerals, which is unlikely to control the ion activity in soil solution. The metal of 'labile' pool on the solid phase can be slowly transferred from/to a non-labile pool. The transfer from labile to non-labile pool is a slow process takes years or longer. In the solution phase, metals are present as free ions, as complexes with inorganic or organic ligands, or associated with mineral colloids. The free ion in solution is generally the most reactive species in terms of reaction with the solid phase. Metal ions adsorb to organic matter, oxyhydroxides and clay minerals. Similar to the inert solid metal, some metals in solution may be equally non-reactive, such as metals in colloidal minerals.

Fig. 3s a-d illustrate different levels (level 0-3) of complexity about potential reaction mechanisms, in increasing order of simplicity. The level 3 scheme (Fig. 3a) represents all the main processes mentioned above. It is conceptually attractive, but requires extensive input information, which is often not available in routine research. In the level 2 scheme, the differences between non-labile and inert metals, in both solid and solution phase, are not considered. However, the successful application of level 2 scheme requires the accurate modeling or observation of dissolved organic matter (DOM). As a watershed-scale model, we consider level 1 and level 0 scheme are practically useful. The level 1 SWAT-HM model consists of 3 pools: dissolved metal (M_d), labile metal (M_l), and non-labile metal (M_n), in which free metal ions (M^{n+}) and metal complexes (ML) in solution are regarded together as dissolved metal (M_d). The last, most simplified, level 0 SWAT-HM transformation module consists of 2 pools: dissolved metal (M_d) and particulate metal (M_p), in which labile metal (M_l) and non-labile metal (M_n) are further regarded together as particulate phase metal (M_p).

In level 1 model, two major types of reactions are taken into account in the heavy metal transformation model: (1) sorption, and (2) slow reaction (details in Table 1). Sorption reaction refers to the adsorption-desorption processes between the dissolved metal in the solution phase and the labile metal in the solid phase. Many studies have demonstrated that adsorption-desorption is the most important process affecting the mobility and bioavailability of metals (Degryse et al., 2009). The "slow reaction" refers to all the slow chemical processes (between labile and non-labile phases) in the solid phase, such as the intra-particle diffusion of metals in carbonates and oxyhydroxides. This is included in SWAT-HM because of its importance for long-term metal prediction

(Buekers et al., 2008; Crout et al., 2006). Generally, the sorption reaction is much faster than the solid phase slow reaction, which occurs over months or years. Ernstberger et al. (2002) measured the adsorption and desorption rates of Zn, Cd, Ni, and Cu and found that the sorption response time ranges within several minutes (T_{1_c} = 300-3,000 s in Table 1). For the solid phase slow reaction, Buekers et al. (2008) used the simple first-order reversible reaction to measure response time and reaction rates (T_{2_c} = 124-800 d in Table 1). Therefore, for the sorption reactions, we adapted the classical local equilibrium assumption (Bahr and Rubin, 1987; Chapra, 2008; Rubin, 1983), i.e., the equilibrium constant (K_d) is used in modeling sorption reaction. In contrast, for the slow reactions, the kinetic approach characterized by reaction rates (k_1, k_{-1}) has to be followed to describe the slow reaction, as the slow reaction is too vanishingly slow to attain an equilibrium within the daily time scale (T_{2_c} >> 1 d).

Dissolved metals (solution phase, [M_d]) are reversibly adsorbed onto solids and become labile adsorbed metals (solid phase, M_l). The solid-solution partition coefficient (K_d) is defined as the ratio of the labile metal concentration in the solid phase to the dissolved metal concentration in the solution phase when equilibrium is attained:

$$K_{\mathrm{d}} = \frac{M_{\mathrm{l}}}{[M_{\mathrm{d}}]} \tag{1}$$

where K_d is the solid-solution partition coefficient (L kg^{-1}), and M_l and [M_d] denote the labile metal concentration in the solid phase (mg kg^{-1}) and dissolved metal concentration in the solution phase (mg L^{-1}), respectively.

Furthermore, the kinetic rates (k_1, k_{-1}) of the slow reaction are specified to allow for the reversible conversion between the labile adsorbed metals (M_l) and their non-labile counterpart (solid phase, M_n).

$$\begin{aligned} \frac{dM_l}{dt} &= -k_1 M_l + k_{-1} M_n \\ \frac{dM_n}{dt} &= k_1 M_l - k_{-1} M_n \end{aligned} \tag{2}$$

where k_1 and k_{-1} are forward and backward rates of slow reaction (d^{-1}), and M_l and M_n denote the labile and non-labile metal concentration in the solid phase (mg kg^{-1}).

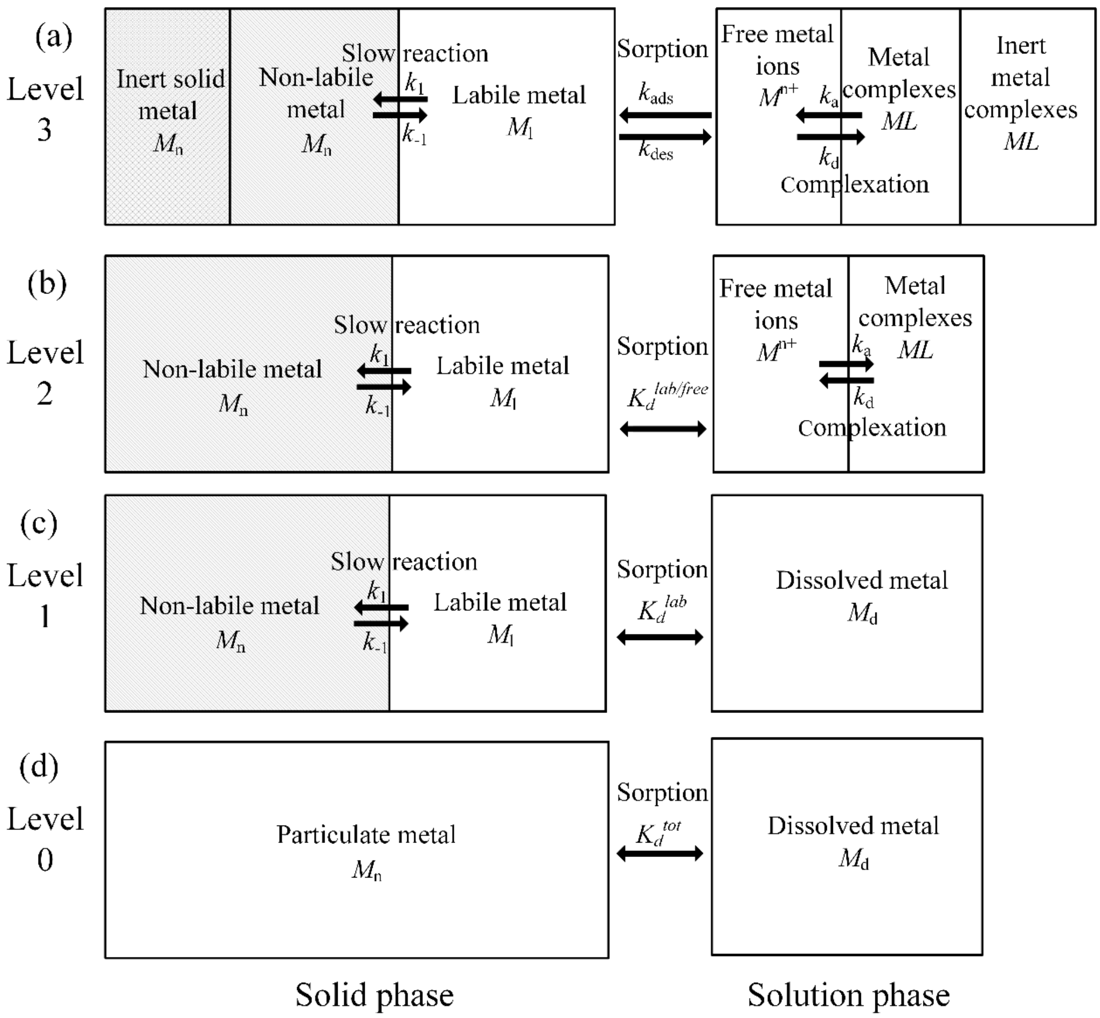

Fig. 3 - Graphical descriptions of the metal transformation model in the soil-water environment. K_d, k_a, k_d, k_{ads}, k_{des}, k_1 and k_{-1} denote the equilibrium and rate constants.

Table 1 - Two major reactions in the soil-water environment and their kinetics equations, equilibrium constants, response times and reaction rates.

Reaction	Formulation	Kinetics equation/Equilibrium constant /response time	Reaction rate					Reference
(1)		$\theta \frac{d[M_d]}{dt} = -k_{\text{ads}}\theta[M_d] + k_{\text{des}}\rho M_l$		**Zn**	**Cd**	**Ni**	**Cu**	
Sorption	$M_l \underset{k_{\text{ads}}}{\overset{k_{\text{des}}}{\rightleftarrows}} [M_d]$	$\rho \frac{dM_l}{dt} = k_{\text{ads}}\theta[M_d] - k_{\text{des}}\rho M_l$	k_{ads} (10^3 s^{-1})	3.31	1.41	1.24	33.2	Ernstberger et al. (2002)
		$K_d = \frac{M_l}{[M_d]} = \frac{k_{\text{des}}}{k_{\text{ads}} \cdot \frac{\rho}{\theta}}$	$k_{\text{des}} \cdot \rho/\theta$ (10^6 s^{-1})	25	16	1.5	9.5	
		$T_c^1 = \frac{1}{k_{\text{des}} + k_{\text{ads}} \cdot \frac{\rho}{\theta}}$	T_c^1 (s)	300	700	800	3000	
(2)		$\frac{dM_l}{dt} = -k_1 M_l + k_{-1} M_n$		**Zn**	**Cd**	**Ni**	**Cu**	
Slow reaction	$M_n \underset{k_1}{\overset{k_{-1}}{\rightleftarrows}} M_l$	$\frac{dM_n}{dt} = k_1 M_l - k_{-1} M_n$	k_1 (10^4 d^{-1})	8.37	7.25	48.4	32.6	Buekers et al. (2008)
		$K_s = \frac{M_l}{M_m} = \frac{k_{-1}}{k_1}$	k_{-1} (10^4 d^{-1})	12.6	5.25	32.3	22.7	
		$T_c^2 = \frac{1}{k_{-1} + k_1}$	T_c^2 (d)	478	800	124	181	

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Table 2 - Selected regression models for logK_d (in L kg^{-1}), derived from pore-water based K_d values. The regression equations were fitted with K_d values that were based on total solid phase concentrations ($K_d^{tot/free}$) or on labile solid phase concentration (K_d^{lab})

Metal	K_d	Regression equation	N	R^2
Cd	K_d^{tot}	$\log K_d = 0.56 \cdot pH - 0.83$	123	0.65
Cd	K_d^{tot}	$\log K_d = 0.55 \cdot pH + 0.70 \cdot \log\%OC - 1.04$	122	0.72
Cd	K_d^{lab}	$\log K_d = 0.65 \cdot pH - 1.59$	86	0.66
Cd	K_d^{lab}	$\log K_d = 0.62 \cdot pH + 0.61 \cdot \log\%OC - 1.7$	86	0.71

1.2. The framework of the heavy metal module in the upland

A framework of the heavy metal module on land is depicted in 错误!未找到引用源。a. Within this frame, the SWAT model undertakes the hydrological and sediment processes that serve as external driving forces of the heavy-metal module. The mass balance equation of metals in the soil profile is expressed as Eq. (3).

$$\Delta M_{\text{soil}} = M_{\text{atmo}} + M_{\text{weth}} + M_{\text{fer}} - M_{\text{surf}} - \sum_{\text{ly}=1}^{\text{n}} M_{\text{lat,ly}} - M_{\text{perc,ly=n}} - M_{\text{ero}} - M_{\text{pu}} \qquad (3)$$

Where M_{atmo} is the metal input from atmospheric deposition, M_{weth} is the metal input from weathering of waste rocks, M_{fer} is the metal input from chemical fertilizer and manure; while metal outputs include plant metal uptakes (M_{pu}), metal leached down out of soil profile ($M_{perc,ly=n}$, bottom soil layer), and metal exports from upland to the river channel with surface runoff (M_{surf}), lateral flow ($\sum_{ly=1}^{n} M_{lat,ly}$, all soil layers) and soil erosion (M_{ero}).

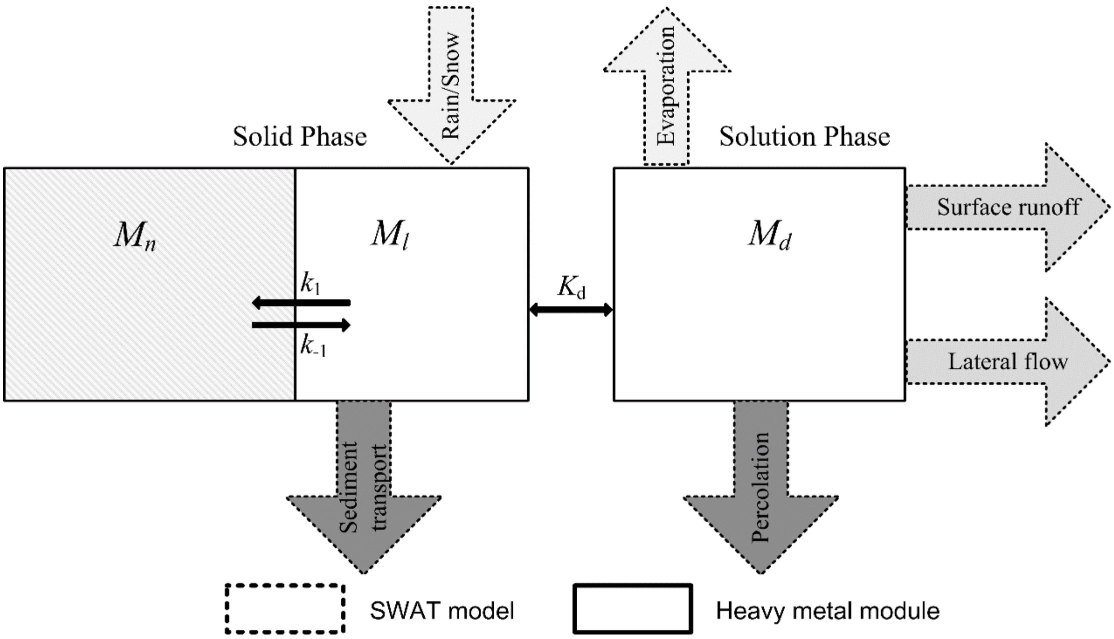


Fig. 4 - Schematic framework of heavy metal transport and transformation in the upland. Metals in the solution phase transport with surface runoff, lateral flow, percolation and upward migration with evaporation; metals in the solid phase transport with soil erosion.

1.1.1. Leaching

Heavy metal in the solution phase of soil layers can be transported with surface runoff Q_{surf}, lateral flow Q_{lat} and percolation Q_{perc}. For each soil layer, the amount of metal moved with water flow M_{flow}, is a function of time, initial metal concentration and flow rate w_{mobile} (surface runoff, lateral flow and percolation for the topsoil layer,

$w_{\text{mobile}} = Q_{\text{surf}} + Q_{\text{lat}} + Q_{\text{perc}}$; lateral flow and percolation for the lower soil layers, $w_{\text{mobile}} = Q_{\text{lat}} + Q_{\text{perc}}$), as shown in Eq. (4).

$$M_{\text{flow,ly}} = M_{0,\text{ly}} \cdot \left(1 - \exp\left(\frac{-w_{mobile}}{SAT + K_d \rho d} t\right)\right) \tag{4}$$

where M_{flow} is the amount of heavy metal transported with flow in the soil per hectare (kg ha^{-1}), for the top soil layer ly = 1, $M_{\text{flow,ly}} = M_{\text{surf,ly}} + M_{\text{lat,ly}} + M_{\text{perc,ly}}$; for the lower soil layers ly = 2,...,n, $M_{\text{flow,ly}} = M_{\text{lat,ly}} + M_{\text{perc,ly}}$. $M_{0,\text{ly}}$ is the initial amount of mobile heavy metal for each soil layer per hectare (the sum of the M_{d} and M_{l} amounts, kg ha^{-1}), t is the time, w_{mobile} is the amount of mobile water (mm), SAT is the saturated soil moisture (mm), d is the depth of the soil layer (mm), and ρ is the soil bulk density (kg m^{-3}).

1.1.2. *Movement with soil erosion*

When soil erosion occurs, heavy metals in the solid phase migrate with the solids, and the amount of transported metal with eroded soil M_{ero} is expressed as shown in Eq. (5).

$$M_{\text{ero}} = \left(M_{\text{l}} + M_{\text{n}}\right) \cdot sed_{\text{ero}} \cdot \varepsilon \tag{5}$$

where M_{ero} is the amount of heavy metal transported with eroded soil per hectare (kg ha^{-1}), M_{l} and M_{n} are the concentration of labile or non-labile metal in soil (mg kg^{-1}), respectively, sed_{ero} is the amount of sediment transported to the channel per hectare (kg ha^{-1}), ε is the enrichment ratio of heavy metal (Quinton and Catt, 2007).

1.1.3. *Plant uptake*

SWAT simulates crop growth by a simplified method of the Erosion-Productivity Impact Calculator (EPIC) model (Williams, 1990). In SWAT, the phenological plant development is based on daily accumulated heat units, potential biomass is based on a method developed by Monteith (Monteith et al., 1977). We used the common approach called plant uptake factor (*PUF*) to model the plant uptake process. Being straightforward, this approach relies on the *PUF* factor which is defined as the ratio of metal concentration in the plant (mg kg^{-1}) to that of soil (mg kg^{-1}). The amount of metal uptake by plant M_{plt} is expressed as Eq. (6).

$$M_{\text{pu}} = \left(M_l + M_n\right) \cdot PUF \cdot bio\_ms \tag{6}$$

where M_{pu} is the amount of heavy metal transported from soil to plant per hectare (kg ha^{-1}), M_{l} and M_{n} are the concentration of labile or non-labile metal in soil (mg kg^{-1}), respectively, *PUF* is the plant uptake factor (-), and *bio_ms* is the plant biomass per hectare (kg ha^{-1}).

1.3. The framework of heavy metal module in the water body

Adapted to the framework of SWAT, which assumes a well-mixed and 1-D water body (Debele et al., 2008), a simple mass balance method is used to simulate the in-stream processes including settling, resuspension, diffusion, and burial (Fig. 5). The mass balance equations of metals in water column and bed sediment are expressed as Eq. (7) and (8).

$$\Delta M_{wtr} = M_{\text{in}} - M_{\text{out}} - M_{\text{set}} + M_{\text{rsp}} - M_{\text{dif}} \quad (7)$$

$$\Delta M_{sed} = M_{\text{set}} - M_{\text{rsp}} + M_{\text{dif}} \quad (8)$$

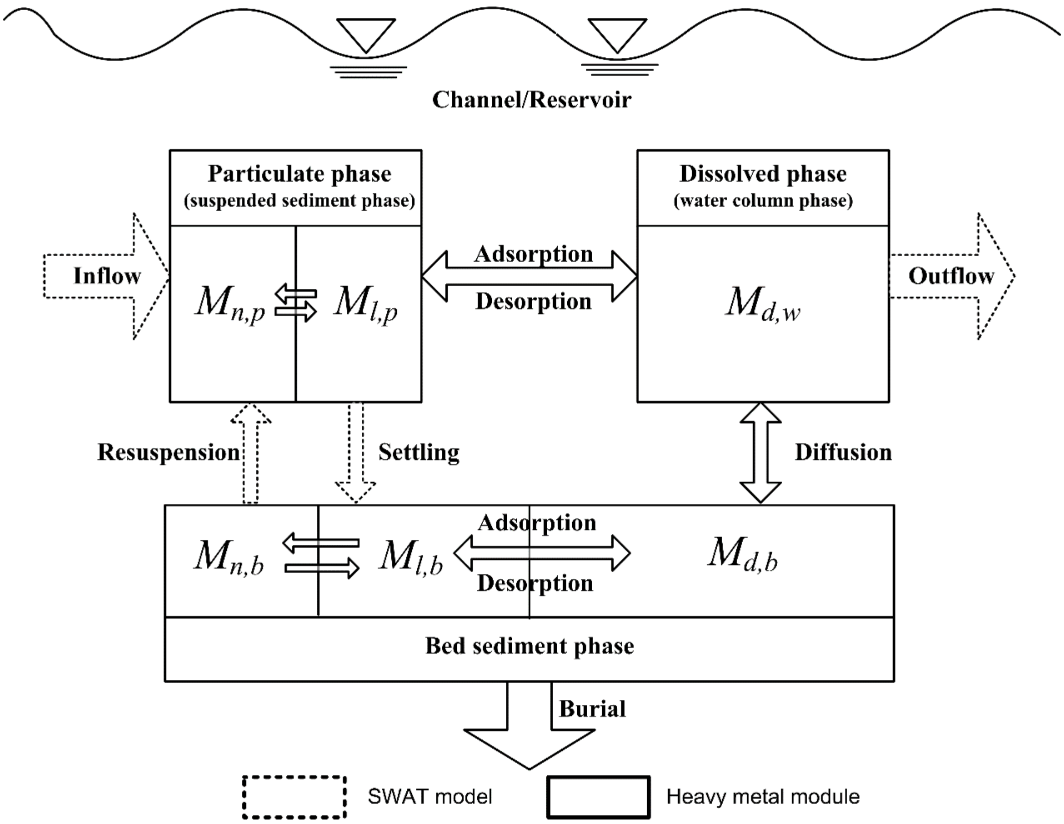


Fig. 5 - Schematic framework of heavy metal transport and transformation in the water body. The processes of adsorption and desorption, settling and resuspension, diffusion, and burial are included.

1.1.4. Settling and resuspension

The sediment budget obtained in SWAT is used to determine the settling or resuspension amount of heavy metal:

$$M_{\text{set}} = sed_{\text{set}} \cdot \left(M_{\text{l,p}} + M_{\text{n,p}}\right) \quad (9)$$

$$M_{\text{res}} = sed_{\text{res}} \cdot \left(M_{\text{l,b}} + M_{\text{n,b}}\right) \tag{10}$$

where M_{set} and M_{res} are the amounts of settled and resuspended heavy metal (kg), respectively; sed_{set} and sed_{res} are the amounts of settled and resuspended sediment (kg), respectively; $M_{\text{l,p}}$ and $M_{\text{n,p}}$ are the concentrations of the labile and non-labile metal in the suspended sediment (particulate phase, mg kg^{-1}), respectively; $M_{\text{l,b}}$ and $M_{\text{n,b}}$ are the concentrations of the labile and non-labile metal in the bed sediment (mg kg^{-1}), respectively.

1.1.5. Diffusion

The transport of dissolved metal species between the water column and riverbed pore water is a diffusion process controlled by the concentration gradient (Lick, 2008). That is, the dissolved metal in the water column can diffuse into or from the pore water when it has relatively higher or lower concentrations, which is quantitatively expressed by Eq. (11):

$$M_{\text{dif}} = V_{\text{d}} \cdot \left(\left[M_{\text{d,w}}\right] - \left[M_{\text{d,b}}\right]\right) \tag{11}$$

where M_{dif} is the diffusion flux of heavy metal (kg m^{-2} d^{-1}), positive M_{dif} means the diffusion is from the water column to bed sediment and negative M_{dif} means the opposite diffusion direction. V_{d} is the diffusion velocity (m d^{-1}), $[M_{\text{d,w}}]$ and $[M_{\text{d,b}}]$ are the concentrations of dissolved metal in the water column and the pore water of bed sediment (mg L^{-1}), respectively.

1.1.6. Burial

Burial refers to the movement of solids downward from the active sediment layer to the deep sediment (Gualtieri, 1999). The burial flux of heavy metal transport is expressed, as shown in Eq. (12):

$$M_{\text{bur}} = V_{\text{b}} \cdot \left(M_{\text{l,b}} + M_{\text{n,b}}\right) \cdot \rho_{\text{b}} \tag{12}$$

where M_{bur} is the burial flux of heavy metal (kg m^{-2} d^{-1}), V_{b} is the burial velocity (m d^{-1}), ρ_{b} is the bulk density of bed sediment (kg m^{-3}), $M_{\text{l,b}}$ and $M_{\text{n,b}}$ are the concentrations of the labile and non-labile metal in the bed sediment (mg kg^{-1}), respectively.

2. Inputs of SWAT-HM model

Three kinds of extra input data are needed to run the SWAT-HM including metal property data, point source data and non-point source data. Metal property data refer to the parameters used in the metal simulation. The heavy metal module combined into SWAT can model metal behavior loaded as point and non-point pollution. Hence, the point and non-point source input files should be prepared to comply with the format as required by the SWAT.

2.1. Metal parameter file (metal.dat)

In SWAT-HM (Fig. 3), dissolved metal (solution phase, M_d) are reversibly adsorbed onto solids and become labile adsorbed metal (solid phase, M_l). In the solution phase, dissolved metal (M_d) and dissolved ligands (solution phase, L) are reversibly associated to form metal complexes (solution phase, ML). In the solid phase, a slow reaction is specified to allow for the reversible conversion between the labile adsorbed metal (M_l) and its non-labile counterpart (solid phase, M_n). The kinetic rate constants for the three types of reaction are denoted by k_{ads}, k_{des}, k_a, k_d, k_1 and k_{-1}, respectively. All these parameters are summarized in metal.dat file.

Table 3 - Parameters of metal property file.

Parameters	Definition	File
K_{d1}	solid-solution partition coefficient in soil (L kg^{-1})	metal.dat
K_{d2}	solid-solution partition coefficient in channel water (L kg^{-1})	metal.dat
K_{d3}	solid-solution partition coefficient in bed sediment (L kg^{-1})	metal.dat
k_1	kinetics rate of forward slow reaction (d^{-1})	metal.dat
k_{-1}	kinetics rate of backward slow reaction (d^{-1})	metal.dat
k_{sol}	solubility of heavy metal in the solution	metal.dat
r_w	weathering rate (--)	metal.dat

The file format for the metal.dat is:

Table 4 - The file format of metal property file.

Parameters	Line #	Position	Format	F90 Format
ID	2	Space1-3	integer	i3
Name	2	Space4-13	charset	a10
level	2	Space14-16	integer	i3
K_{d1}	2	Space15-26	float	f10.3
K_{d2}	2	Space27-36	float	f10.3
K_{d3}	2	Space37-46	float	f10.3
k_1	2	Space47-56	float	f10.3
k_{-1}	2	Space57-66	float	f10.3

k_{sol}	2	Space67-76	float	f10.3
r_w	2	Space77-86	float	f10.3

2.2. Point source data (xp.dat)

The original version of the heavy metal module in SWAT only routes simple mass balance through the channel network loaded as point sources without any in-stream and upland processes. Consistent with the original SWAT model, SWAT-HM also allows point source files to be read in at any sub-basin inlet along the channel network.

The point source input files (e.g., xxp.dat) should be created by user, and it should be mentioned that, in the current version of SWAT-HM, only one metal can be simulated at a time. Following is a brief description of the variables in the daily point source input file (Table 5).

Table 5 - Point source data

Variable	**Definition**
Title	The first six lines of the file are reserved for user comments; the comments may take up to 80 spaces per line.
DAY	Julian date for record
YEAR	Four-digit year for record
FLODAT	Contribution to the streamflow for the day (m^3)
SEDDAY	Sediment loading to the reach for the day (tons/d)
……	……
HMLDAY	Loading of heavy metal to the reach for the day (kg/d)

The file format for the xp.dat is:

Table 6 - The file format for the xp.dat

Parameters	**Line #**	**Position**	**Format**	**F90 Format**
DAY		Space1-5	integer	i3
YEAR		Space6-9	integer	f10.3
FLOCNST	2	Space10-26	float	
SEDCNST	2	Space27-43	float	
ORGNCNST	2	Space44-60	float	
ORGPCNST	2	Space61-77	float	
NO3CNST	2	Space78-94	float	
NH3CNST	2	Space95-111	float	
NO2CNST	2	Space112-128	float	
MINPCNST		Space129-145	float	
CBODCNST		Space146-162	float	

DISOXCNST		Space163-179	float	
CHLACNST		Space180-196	float	
SOLPSTCNST		Space197-213	float	
SRBPSTCNST		Space214-230	float	
BACTPCNST		Space231-247	float	
BACTLPCNST		Space248-264	float	
CMTL1CNST		Space265-281	float	
CMTL2CNST		Space282-298	float	
CMTL3CNST		Space299-315	float	

2.3. Nonpoint source data

2.3.1. hml files

SWAT-HM accounts for sorption and slow reactions among metal species; the heavy metals in the upland are allowed to transport vertically through percolation and evaporation-induced water rising as well as horizontally through soil erosion and surface/subsurface runoff; the heavy metals in the water body, in contrast, are modeled to undergo settling, resuspension diffusion and burial processes. So boundary conditions and parameters are required to run the SWAT-HM model. For example, the initial concentration of metal species in different environmental medias (e.g., soil, sediment).

The nonpoint source input files (e.g., 000010001.hml, 000010000.swq) should be created by user. Following is a brief description of the variables in the daily point source input file.

Table 7 - Non-point source data - hml file

Variable	Definition	File
ID	Metal ID	.hml
hmfraction[a]	fraction of waste rock dumps/tailings area contained in a HRU	.hml
hmsrc[a]	Source strength of the waste rock dumps, tailings after weathering, ready for rain-washing-out (kg/ha)	.hml
hmrock[a]	Metal in rock to be weathered (kg/ha)	.hml
Sol_M_l	Labile metal concentration in 1st soil layer (mg/kg)	.hml
Sol_M_n	Non-labile metal concentration in 1st soil layer (mg/kg)	.hml
ε	Enrichment ratio of heavy metal (-)	hml
Sol_pH	Soil pH (-)	.hml

a) hmfraction, hmsrc and hmrock are three variables related to the process of metal weathering. In SWAT-HM. The released metals from weathering of waste rocks are added to the labile metal pool in soils. If waste rocks do not exist in HRU, these variables can be set as 0.

Table 8 - The file format for the .hml

Parameters	Line #	Position	Format	F90 Format
HML_P1	3	Space1-10	integer	i10
HML_P2	4	Space1-10	float	f3.6
HML_P3	5	Space1-10	float	f6.3
HML_P4	6	Space1-10	float	f6.3
HML_P5	7	Space1-10	float	f6.3
HML_P6	8	Space1-10	float	f6.3
HML_P8	9	Space1-10	float	f6.3
HML_P9	10	Space1-10	float	f6.3

HML_P10	11	Space1-10	float	f6.3
HML_P11	12	Space1-10	float	f6.3
HML_P12	13	Space1-10	float	f6.3

2.3.2. Swq files

Table 9 - Non-point source data - swq file

	Definition	File
Sed_M_l	Initial labile metal concentration in sediment (kg/m^3)	.swq
Sed_M_n	Initial non-labile metal concentration in sediment (kg/m^3)	.swq
Sed_HML_STL[a]	Settling velocity for Heavy Metal (m/d)	.swq
Sed_HML_RSP[a]	Resuspension velocity for Heavy Metal (m/d)	.swq
Sed_HML_MIX	Mixing velocity for Heavy Metal (m/d)	.swq
Sed_HML_BRY	Burial velocity for Heavy Metal (m/d)	.swq
Sed_HML_ACT	Depth of active sediment layer for heavy metal (m)	swq

a) Sed_HML_STL and Sed_HML_RSP are the settling velocity and resuspension velocity of Heavy Metal, respectively. In the current version of SWAT, if you have the sediment data to calibrate the soil erosion process, these two parameters will not be used any more.

Table 10 - The format of the .swq file

Parameters	Line #	Position	Format	F90 Format
Sed_HML_STL[a]	32	Space1-15	float	f10.4
Sed_HML_RSP[a]	33	Space1-15	float	f10.4
Sed_HML_MIX	34	Space1-15	float	f10.4
Sed_HML_BRY	35	Space1-15	float	f9.5
SWQ_HML_LabileCONC	36	Space1-15	float	f10.4
SWQ_HML_NonLabileCONC	37	Space1-15	float	f10.4
Sed_HML_ACT	38	Space1-15	float	f10.4

3. Outputs of SWAT-HM model

3.1. Subbasin level heavy metal output file (outhml.sub)

The subbasin heavy metal file contains output data about concentration and amount of dissolved metal, metal complexes, labile adsorbed metal and non-labile metal, the value are the total amount of all the HRUs within the subbasin.

Table 11 - Subbasin heavy metal file (outhml.sub)

	Definition	**File**
Sub	Subbasin number	outhml.sub
GIS	GIS number reprinted from watershed configuration file	outhml.sub
Date	Daily time step : the Julian date Monthly time step : the month (1 - 12) Annual time step : 4-digit year	outhml.sub
Area	Area of the subbasin (km^2)	outhml.sub
M_d_Sub	Dissolved metal transported from the subbasin to the reach through surface runoff (kg)	outhml.sub
M_d_Sub	Dissolved metal transported from the subbasin to the reach through lateral flow (kg)	outhml.sub
M_l_Sub	Labile adsorbed metal transported from the subbasin to the reach through soil erosion (kg)	outhml.sub
M_n_Sub	Non-labile metal transported from the subbasin to the reach through erosion (kg)	outhml.sub
M_{total}_Sub	Total amount of heavy metal transported from the subbasin to the reach (kg)	outhml.sub

Table 12 - The format of the output.sub file

Parameters	Line #	Position	Format	F90 Format
SUB		Space1-4	integer	i4
YEAR		Space5-12	integer	i4
MON		Space13-18	integer	I3
AREAkm2		Space19-31	float	f9.5
HM_SURQkg		Space32-44	float	f10.4
HM_LATkg		Space45-57	float	f10.4
HM_PERCkg		Space58-70	float	f10.4
HM_PLANTkg		Space71-83	float	f10.4
HM_GWkg		Space84-96	float	f10.4
LabHM_EROkg		Space97-109	float	f10.4
NLabHM_EROkg		Space110-122	float	f10.4
HM_ATMOkg		Space123-135	float	f10.4
HM_WETHkg		Space136-148	float	f10.4
HM_AGRkg		Space149-161	float	f10.4
HM_OUTkg		Space162-174	float	f10.4
HM_INkg		Space175-187	float	f10.4

3.2. HRU level heavy metal output file (outhml.hru)

The HRU heavy metal file contains output data about concentration and amount of free metal ions, metal complexes, labile adsorbed metal and non-labile metal in HRU. In the current version of SWAT-HM, only the metal concentrations of first layer are allowed to be output.

Table 13 - HRU heavy metal file (outhml.hru)

	Definition	File
CROP	Four letter character code for the cover/plant on the HRU	outhml.hru
HRU	HRU number	outhml.hru
SUBHRU	Subbasin to which the HRU belongs	outhml.hru
SUB	Subbasin number	outhml.hru
MGT	Management code	outhml.hru
Date	Daily time step : the Julian date Monthly time step : the month (1 - 12) Annual time step : 4-digit year	outhml.hru
Area	Drainage area of the HRU (km^2)	outhml.hru
M_d_Sub	Dissolved metal concentration in first soil layer (kg)	outhml.hru
M_l_Sub	Labile adsorbed metal concentration in first soil layer (kg)	outhml.hru
M_n_Sub	Non-labile metal concentration in first soil layer (kg)	outhml.hru

Table 14 - The format of the output.rch file

Parameters	Line #	Position	Format	F90 Format
CROP		Space1-6	integer	a4
HRU		Space7-12	integer	i5
MONSUBNAME		Space13-19	integer	i5
HRUNO		Space20-25	float	i4
SUB		Space26-30	float	i5
MGE		Space31-35	float	i5
DAY		Space36-40	float	i4
AREAkm2		Space41-51	float	f10.4
DisHMkg/ha		Space52-64	float	f10.4
LabHMLkg/ha		Space65-77	float	f10.4
NLabHMkg/ha		Space78-90	float	f10.4
HM_SURQkg		Space91-103	float	f10.4
HM_LATkg		Space104-116	float	f10.4
HM_PERCkg		Space117-129	float	f10.4

HM_PLANTkg		Space130-142	float	f10.4
HM_GWkg		Space143-155	float	f10.4
LabHM_EROkg		Space156-168	float	f10.4
NLabHM_EROkg		Space169-181	float	f10.4
HM_ATMOkg		Space182-194	float	f10.4
HM_WETHkg		Space195-207	float	f10.4
HM_AGRkg		Space208-220	float	f10.4

3.3. Main channel heavy metal output file (outhml.rch)

The main channel heavy metal file contains output data about concentration and amount of free metal ions, metal complexes, labile adsorbed metal, and non-labile metal in three different environmental media (water, suspended sediment and bed sediment). Only one metal can be routed through the stream network at one time.

Table 15 - Main channel heavy metal file (outhml.rch)

	Definition	**File**
RCH	Reach number	outhml.rch
GIS	GIS number reprinted from watershed configuration file	outhml.rch
Date	Daily time step : the Julian date Monthly time step : the month (1 - 12) Annual time step : 4-digit year	outhml.rch
Area	Area drained by reach (km^2)	outhml.rch
M_d_IN	Dissolved metal transport into reach during time step	outhml.rch
M_l_IN	Labile adsorbed metal transport into reach during time step	outhml.rch
M_n_IN	Non-labile metal transport into reach during time step	outhml.rch
M_{set}	Amounts of settled heavy metal (kg)	outhml.rch
M_{res}	Amounts of resuspended heavy metal (kg)	outhml.rch
M_{bur}	The burial flux of heavy metal ($kg\ m^{-2}\ d^{-1}$)	outhml.rch
M_{dif}	The diffusion flux of heavy metal ($kg\ m^{-2}\ d^{-1}$)	outhml.rch
M_d_OUT	Dissolved metal transport out of reach during time step	outhml.rch
M_l_OUT	Labile adsorbed metal transport out of reach during time step	outhml.rch
M_n_OUT	Non-labile metal transport out of reach during time step	outhml.rch

M_d_Bed	Dissolved metal concentration in the pore water of bed sediment (mg L^{-1})	outhml.rch
M_l_ Bed	Labile adsorbed metal concentration in bed sediment (mg kg^{-1})	outhml.rch
M_n_ Bed	Non-labile metal concentration in bed sediment (mg kg^{-1})	outhml.rch

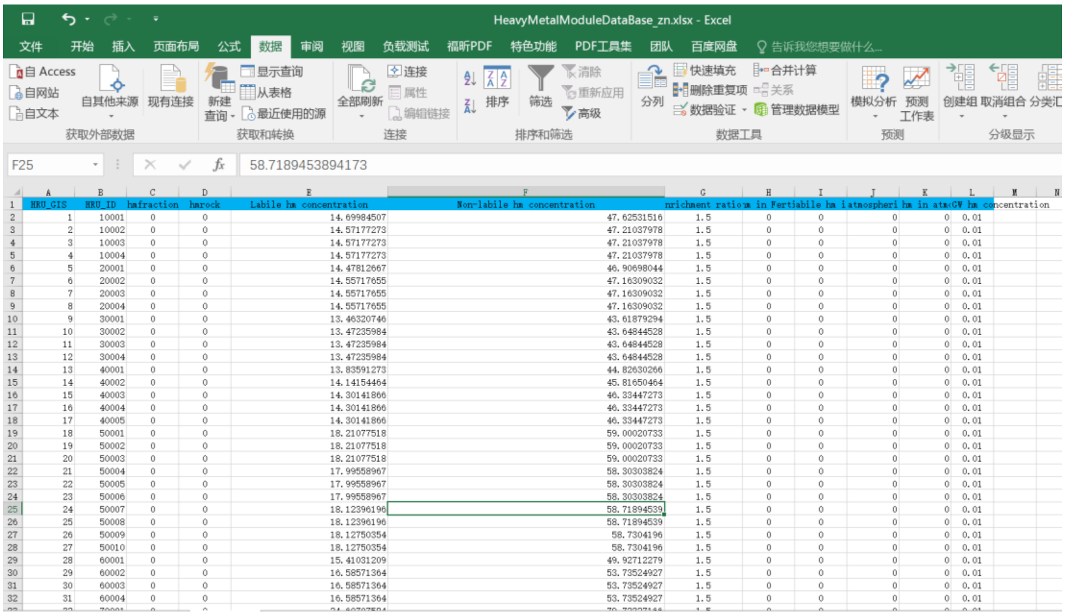
a) Free metal ions and Metal complexes
b) Metal complexes

Table 16 - The format of the output.rch file

Parameters	**Line #**	**Position**	**Format**	**F90 Format**
RCH		Space1-4	integer	i4
YEAR		Space5-12	integer	i4
MON		Space13-18	integer	I3
AREAkm2		Space19-31	float	f9.5
DisHM_INkg		Space32-46	float	f10.4
LabHM_INkg		Space47-61	float	f10.4
NLabHM_INkg		Space62-76	float	f10.4
DisHM_OUTkg		Space77-91	float	f10.4
LabHM_OUTkg		Space92-106	float	f10.4
NLabHM_OUTkg		Space107-121	float	f10.4
HMSETTLkg		Space122-136	float	f10.4
HMRESUSPkg		Space137-151	float	f10.4
HMLBURYkg		Space152-166	float	f10.4
HMLDIFFkg		Space167-181	float	f10.4
SedDisHMkg/m3		Space182-196	float	f10.4
SedLabHMkg/m3		Space197-211	float	f10.4
SedNLabHMkg/m3		Space212-226	float	f10.4

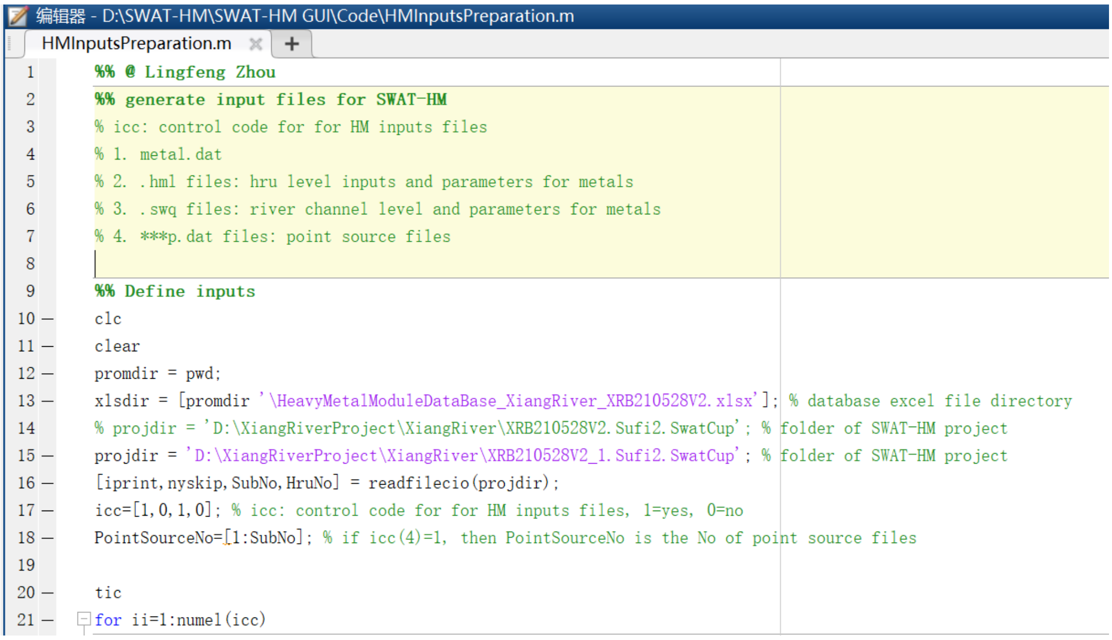
4. How to prepare the SWAT-HM input files

A Excel SWAT-HM database plus Python/Matlab scripts are provided for SWAT-HM users to create the input files required for running SWAT-HM model. Take Matlab scripts as an example, After assigning the values of parameters and inputs for SWAT-HM in the Excel database file. Using Matlab scripts to creating the input files. Python/Matlab code are posted on Github (https://github.com/LyntonZhou/SWAT-HM-pre-post-processing)



HRU_GIS	HRU_ID	hmfraction	hmrock	Labile hm concentration	Non-labile hm concentration	nrichment ratio	m in Fert	iabile hm i	atmospheri	hm in atm	GW hm concentration
1	10001	0	0	14.69984507	47.62531516	1.5	0	0	0	0	0.01
2	10002	0	0	14.57177273	47.21037978	1.5	0	0	0	0	0.01
3	10003	0	0	14.57177273	47.21037978	1.5	0	0	0	0	0.01
4	10004	0	0	14.57177273	47.21037978	1.5	0	0	0	0	0.01
5	20001	0	0	14.47812667	46.90698044	1.5	0	0	0	0	0.01
6	20002	0	0	14.55717655	47.16309032	1.5	0	0	0	0	0.01
7	20003	0	0	14.55717655	47.16309032	1.5	0	0	0	0	0.01
8	20004	0	0	14.55717655	47.16309032	1.5	0	0	0	0	0.01
9	30001	0	0	13.46320746	43.61879294	1.5	0	0	0	0	0.01
10	30002	0	0	13.47235984	43.64844528	1.5	0	0	0	0	0.01
11	30003	0	0	13.47235984	43.64844528	1.5	0	0	0	0	0.01
12	30004	0	0	13.47235984	43.64844528	1.5	0	0	0	0	0.01
13	40001	0	0	13.83591273	44.82630266	1.5	0	0	0	0	0.01
14	40002	0	0	14.14154464	45.81650464	1.5	0	0	0	0	0.01
15	40003	0	0	14.30141866	46.33447273	1.5	0	0	0	0	0.01
16	40004	0	0	14.30141866	46.33447273	1.5	0	0	0	0	0.01
17	40005	0	0	14.30141866	46.33447273	1.5	0	0	0	0	0.01
18	50001	0	0	18.21077518	59.00020733	1.5	0	0	0	0	0.01
19	50002	0	0	18.21077518	59.00020733	1.5	0	0	0	0	0.01
20	50003	0	0	18.21077518	59.00020733	1.5	0	0	0	0	0.01
21	50004	0	0	17.99558967	58.30303824	1.5	0	0	0	0	0.01
22	50005	0	0	17.99558967	58.30303824	1.5	0	0	0	0	0.01
23	50006	0	0	17.99558967	58.30303824	1.5	0	0	0	0	0.01
24	50007	0	0	18.12396196	58.71894539	1.5	0	0	0	0	0.01
25	50008	0	0	18.12396196	58.71894539	1.5	0	0	0	0	0.01
26	50009	0	0	18.12750354	58.7304196	1.5	0	0	0	0	0.01
27	50010	0	0	18.12750354	58.7304196	1.5	0	0	0	0	0.01
28	60001	0	0	15.41031209	49.92712279	1.5	0	0	0	0	0.01
29	60002	0	0	16.58571364	53.73524927	1.5	0	0	0	0	0.01
30	60003	0	0	16.58571364	53.73524927	1.5	0	0	0	0	0.01
31	60004	0	0	16.58571364	53.73524927	1.5	0	0	0	0	0.01

Fig. 6 - Excel database of SWAT-HM model



```
%% @ Lingfeng Zhou
%% generate input files for SWAT-HM
% icc: control code for for HM inputs files
% 1. metal.dat
% 2. .hml files: hru level inputs and parameters for metals
% 3. .swq files: river channel level and parameters for metals
% 4. ***p.dat files: point source files

%% Define inputs
clc
clear
promdir = pwd;
xlsdir = [promdir '\HeavyMetalModuleDataBase_XiangRiver_XRB210528V2.xlsx']; % database excel file directory
% projdir = 'D:\XiangRiverProject\XiangRiver\XRB210528V2.Sufi2.SwatCup'; % folder of SWAT-HM project
projdir = 'D:\XiangRiverProject\XiangRiver\XRB210528V2_1.Sufi2.SwatCup'; % folder of SWAT-HM project
[iprint,nyskip,SubNo,HruNo] = readfilecio(projdir);
icc=[1,0,1,0]; % icc: control code for for HM inputs files, 1=yes, 0=no
PointSourceNo=[1:SubNo]; % if icc(4)=1, then PointSourceNo is the No of point source files

tic
for ii=1:numel(icc)
```

Fig. 7 - Matlab script to create the input files of SWAT-HM model.

5. Visualization

Python/Matlab code are posted on Github (https://github.com/LyntonZhou/SWAT-HM-pre-post-processing)

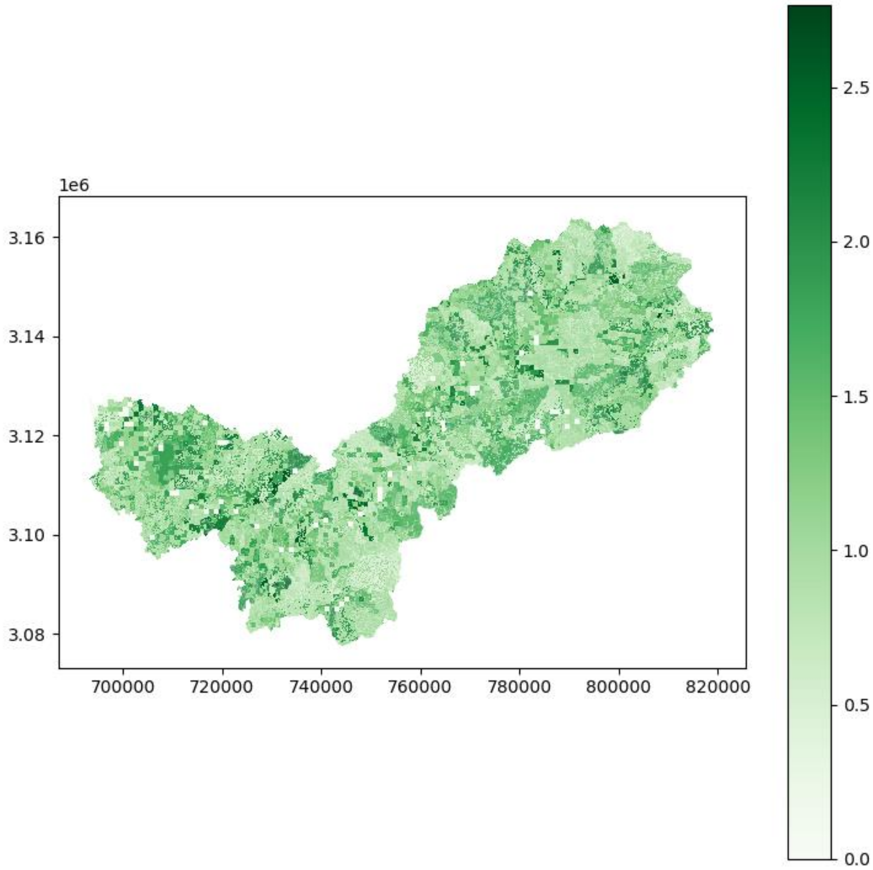


Fig. 8 – Example of HRU output of SWAT-HM

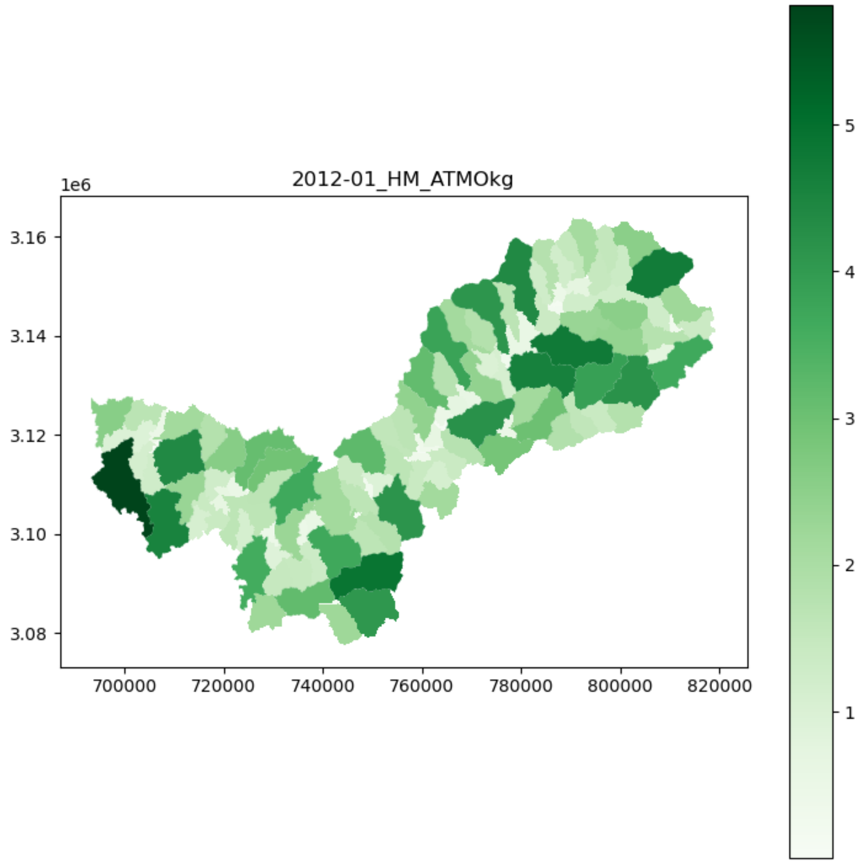


Fig. 9 – Example of subbasin output of SWAT-HM

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