A Heavy Metal Module Coupled in SWAT Model and Its Application

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3. Demonstrative implementation
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1. Introduction

Heavy metal pollution in mining area
1. Introduction

[1]. Statements E I. Comparison of Predicted and Actual Water Quality at Hardrock Mines[J].
1. Introduction

SWAT model

The soil and water Assessment Tool (SWAT) has been proven to be an effective tool for nonpoint-source pollution problem, such as nitrogen and phosphorus and pesticide. However, as far as heavy metals is concerned, the SWAT model, by its own version, only allows point source loading inputs and includes no algorithms to model in-stream processes but simple mass balance equations\(^2\), which addresses a small part of heavy metal pollution issues.

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2. Heavy Metal module -- Challenges

- **Primary Source identification**
  - Drains
  - Waste rocks
  - Tailings
  - Contaminated soil
  - ...

- **Chemical speciation**
  - Solid phase: labile (adsorbed); non-labile (strong bonded, minerals)
  - Aqueous phase: free ions, complexes, colloids

- **Physical movement**
  - Wind erosion, transport
  - Soil erosion, transport
  - Surface runoff
  - Lateral flow
  - Groundwater flow
2. Heavy Metal module -- Challenges

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  - Groundwater flow
2. Heavy Metal module

Fig. Molecular-scale environmental processes of metals in soils and aquatic systems[3]

2. Heavy Metal module – Transformation model

Tab. Three major reactions in soil-water environment

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Formulation</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adsorption &amp; desorption</td>
<td>$M_l \xrightleftharpoons[k_{ads}]^{k_{des}} M^{n+}$</td>
<td>$\theta \frac{d\left[M^{n+}\right]}{dt} = -k_{ads} \theta\left[M^{n+}\right] + k_{des} \rho M_l$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\rho \frac{dM_l}{dt} = k_{ads} \theta \left[M^{n+}\right] - k_{des} \rho M_l$</td>
</tr>
<tr>
<td>Complexation</td>
<td>$M^{n+} + L \xrightarrow[k_{d}]{k_{a}} ML$</td>
<td>$\frac{d\left[ML\right]}{dt} = k_a \left[M^{n+}\right] \cdot [L] - k_d \left[ML\right]$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\frac{d\left[M^{n+}\right]}{dt} = -k_a \left[M^{n+}\right] \cdot [L] + k_d \left[ML\right]$</td>
</tr>
<tr>
<td>Slow reaction</td>
<td>$M_n \xrightarrow[k_1]{k^{-1}_1} M_l$</td>
<td>$\frac{dM_l}{dt} = -k_1 M_l + k^{-1}_1 M_n$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\frac{dM_n}{dt} = k_1 M_l - k^{-1}_1 M_n$</td>
</tr>
</tbody>
</table>
2. Heavy Metal module – Land phase process

Chemical transformation:
- Sorption
- Complexation
- Slow(aging) reaction

Physical transport:
- Leaching
- Upward migration
- Erosion
- …
2. Heavy Metal module – Channel phase process

Chemical transformation:
- Sorption
- Complexation
- Slow(aging) reaction

Physical transport:
- Settling
- Resuspension
- Diffusion
- Burial
- ...
2. Heavy Metal module -- Module framework

**Heavy metal module**

**Input**
- Metal property data
- Point source data
- Non-point source data

**Land phase**
- Weathering
- Leaching
- Upward migration
- Movement of the sorbed

**Channel phase**
- Adsorption & Desorption
- Settling & Resuspension
- Diffusion
- Burial

**Output**
- outhml.hru
- outhml.sub
- outhml.rch
- outhml.rsv
2. Heavy Metal model

Flow chart
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3. Demonstrative Implementation

Location: south-central China

Study area: 1990 km²

Precipitation: 1290-1840 mm (yearly)

Hydrology: Daxi river (blue), Xiaoxi river (green), Baoshan stream (yellow)

Mining area: Qibaoshan mine, 6.5 km²

Metal: Zn, Pb, Cu, Cd
3. Demonstrative Implementation

<table>
<thead>
<tr>
<th>Material</th>
<th>pH</th>
<th>OC (%)</th>
<th>Total (ug L⁻¹)</th>
<th>Acid-Soluble (ug L⁻¹)</th>
<th>Reducible (ug L⁻¹)</th>
<th>Oxidizable (ug L⁻¹)</th>
<th>Residual (ug L⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Zn</td>
<td>Cd</td>
<td>Zn</td>
<td>Cd</td>
<td>Zn</td>
</tr>
<tr>
<td>waste rock</td>
<td>— a)</td>
<td>1</td>
<td>3110-6175 (4797)</td>
<td>15-250 (97)</td>
<td>1026-3953 (2822)</td>
<td>6.1-204.7 (76.60)</td>
<td>27-219 (105)</td>
</tr>
<tr>
<td>Soils (near the waste rock)</td>
<td>3.0-5.4</td>
<td>2</td>
<td>466-1017 (756)</td>
<td>1.5-4.1 (2.7)</td>
<td>51-80 (69)</td>
<td>0.25-0.65 (0.40)</td>
<td>5-50 (20)</td>
</tr>
<tr>
<td>Soils(near the drain outlet)</td>
<td>3.1-4.9</td>
<td>2</td>
<td>457-688 (538)</td>
<td>0.6-2.2 (1.4)</td>
<td>47-107 (70)</td>
<td>0.02-0.93 (0.35)</td>
<td>5-28 (12)</td>
</tr>
<tr>
<td>undisturbed soils</td>
<td>5.6-6.8</td>
<td>2</td>
<td>118-262 (157)</td>
<td>0.2-0.9 (0.45)</td>
<td>1-15 (9)</td>
<td>0.01-0.41 (0.15)</td>
<td>1-10 (5)</td>
</tr>
</tbody>
</table>
3. Demonstrative Implementation

### Basic data for SWAT model

<table>
<thead>
<tr>
<th>Type</th>
<th>Description</th>
<th>Data source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Digital elevation model (DEM)</td>
<td>90 m</td>
<td>Data Center for Resources and Environmental Sciences, Chinese Academy of Sciences (RESDC)</td>
</tr>
<tr>
<td>Land use data</td>
<td>90 m</td>
<td>The Institute of Soil Science, Chinese Academy of Sciences</td>
</tr>
<tr>
<td>Soil data</td>
<td>1:1000000</td>
<td>Hydrology bureau of hunan province; <a href="http://data.cma.cn">http://data.cma.cn</a></td>
</tr>
<tr>
<td>Meteorological data</td>
<td>Daily</td>
<td>Hydrology bureau of hunan province</td>
</tr>
<tr>
<td>Hydrological data</td>
<td>Daily</td>
<td>Hydrology bureau of hunan province</td>
</tr>
</tbody>
</table>
### 3. Demonstrative Implementation

#### Additional data of heavy metal module

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Metl</th>
<th>typical(initial) value/ fitted value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_d$ (in soil)</td>
<td>L kg$^{-1}$</td>
<td>Zn</td>
<td>1.0-10.0/1.5$^a$</td>
<td>(Sauve et al., 2000; Allison and Allison, 2005)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cd</td>
<td>1.0-10.0/3.4</td>
<td></td>
</tr>
<tr>
<td>$K_d$ (in channel)</td>
<td>L kg$^{-1}$</td>
<td>Zn</td>
<td>1000.0-5000.0/1020.3</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cd</td>
<td>500-10000/2153.0</td>
<td></td>
</tr>
<tr>
<td>$K_d$ (in riverbed sediment)</td>
<td>L kg$^{-1}$</td>
<td>Zn</td>
<td>1.0-50.0/38.0</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cd</td>
<td>1.0-80.0/270.7</td>
<td></td>
</tr>
<tr>
<td>$k_1$</td>
<td>d$^{-1}$</td>
<td>Zn</td>
<td>1.3*10$^{-3}$</td>
<td>(Crout et al., 2006; Buekers et al., 2008)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cd</td>
<td>5.2*10$^{-4}$</td>
<td></td>
</tr>
<tr>
<td>$k_1$</td>
<td>d$^{-1}$</td>
<td>Zn</td>
<td>8.4*10$^{-4}$</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Cd</td>
<td>7.3*10$^{-4}$</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
<th>Typical range/Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Point source$^a$)</td>
<td>Flow Flow of point source for a day(m$^3$ d$^{-1}$)</td>
<td>9600/9600/2040</td>
<td>Average</td>
</tr>
<tr>
<td></td>
<td>Point-Zn Point loading of Zn to reach for the day(kg)</td>
<td>6.5/6.5/17.5</td>
<td>Average</td>
</tr>
<tr>
<td></td>
<td>Point-Cd Point loading of Cd to reach for the day(kg)</td>
<td>0/0/0</td>
<td>Average</td>
</tr>
<tr>
<td></td>
<td>$M_l$ Labile metal concentration in the 1st layer soil(mg kg$^{-1}$)</td>
<td>Zn:300/10/0.5 Cd:15/1/0.2</td>
<td>Average</td>
</tr>
<tr>
<td></td>
<td>$M_n$ Non-labile metal concentration in the 1st layer soil(mg kg$^{-1}$)</td>
<td>Zn:3000/400/100 Cd:30/3/1</td>
<td>Average</td>
</tr>
<tr>
<td></td>
<td>Hmfr Fractions of waste dumps and tailings area in HRUs (%)</td>
<td>1.0%-43.6%(10.0%)$^c$</td>
<td>remote sensing</td>
</tr>
<tr>
<td></td>
<td>hmrock Heavy metal in waste rock (kg ha$^{-1}$)</td>
<td>Zn:1000 Cd:10</td>
<td>Average</td>
</tr>
<tr>
<td></td>
<td>Weathering rate$^b$ Weathering rate of waste rocks and tailings (d$^{-1}$)</td>
<td>10$^{-5}$-10$^{-4}$</td>
<td>(Bennett et al., 2000)</td>
</tr>
</tbody>
</table>
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4. Results—Calibration and validation of flow and sediment

<table>
<thead>
<tr>
<th></th>
<th>Period</th>
<th>Time resolution</th>
<th>$E_{ns}$</th>
<th>$r^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Stream flow</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Calibration</td>
<td>(2009-2011)</td>
<td>monthly</td>
<td>0.81</td>
<td>0.89</td>
</tr>
<tr>
<td></td>
<td></td>
<td>daily</td>
<td>0.81</td>
<td>0.86</td>
</tr>
<tr>
<td>Validation</td>
<td>(2012-2014)</td>
<td>monthly</td>
<td>0.93</td>
<td>0.95</td>
</tr>
<tr>
<td></td>
<td></td>
<td>daily</td>
<td>0.84</td>
<td>0.84</td>
</tr>
<tr>
<td><strong>Sediment</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Calibration</td>
<td>(2009-2011)</td>
<td>monthly</td>
<td>0.70</td>
<td>0.72</td>
</tr>
<tr>
<td></td>
<td></td>
<td>daily</td>
<td>0.73</td>
<td>0.85</td>
</tr>
<tr>
<td>Validation</td>
<td>(2012-2014)</td>
<td>monthly</td>
<td>0.64</td>
<td>0.74</td>
</tr>
<tr>
<td></td>
<td></td>
<td>daily</td>
<td>0.50</td>
<td>0.56</td>
</tr>
</tbody>
</table>
4. Results—Calibration and validation of HM module

Dissolved Zn output (watershed outlet)
4. Results—Zn (two rainfall events)
4. Results—Cd (two rainfall events)
4. Results – Different transport paths

[Images showing precipitation and pollutant loadings on different dates from June 19, 2014 to June 23, 2014]
4. Results—Model outputs at watershed outlet

Precipitation

Flow

Suspended sediment

Dissolved Zn

Solid Zn

day from January 1st, 2009
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5. Conclusion and discussion

- The simulation of stream flow and suspended sediment is good both on monthly basis and daily basis.

- A heavy metal module coupled with SWAT model is established to simulate the Zn, Cd dynamics in Liuyang river upstream basin.

- This modified model contains the processes of weathering, leaching, sorption, complexation and so on, which embodies the process of source release, migration and transformation of heavy metal at the watershed scale.

- More measured data are needed to test and improve the heavy metal module.
Thank you very much!

zhou_lingfeng@mail.bnu.edu.cn
Key parameter: partition coefficient $K_d$

$$K_d = \frac{M_s}{[M]}$$

Different $K_d$ in different processes

1. Partition between soil and water
2. Partition between suspended sediment and water
3. Partition between bottom sediment and water

Determine the appropriate $K_d$ for various medium
recognize the mine/tailing/piling area in the remote sensing image