

Supplementary information for

The optimal relationships between As and Cd of porewater in paddy soils

with variation in pe+pH: An insight from trade-off value

Table S1. The definition and significance of the DOM characteristic parameters [1]

Characteristic parameters	Definition	Interpretation
Absorption coefficient [$\alpha(\lambda)$]	$\alpha(\lambda) = 2.303 \times A(\lambda) / l$ Where $a(\lambda)$ is wavelength λ absorption coefficient (M^{-1}), $A(\lambda)$ is absorbance, and l is the optical path (m).	Represent the relative concentration of chromophoric dissolved organic matter (CDOM) in DOM and was positively correlated with the concentration of CDOM.
SUVA ₂₅₄	$SUVA_{254} = \alpha(254) / DOC$ Where DOC is the concentration of dissolved organic matter in paddy soil porewater, SUVA ₂₅₄ is reported in units of $L / (mg \cdot m)$.	Indicate the aromaticity of DOM, which is positively correlated with the aromaticity of the DOM.
SUVA ₂₆₀	$SUVA_{260} = a(260) / DOC$ Where DOC is the concentration of dissolved organic matter in paddy soil porewater, SUVA ₂₆₀ is reported in units of $L / (mg \cdot m)$.	Indicate the hydrophobicity of DOM, which positively correlates with the DOM hydrophobic group.
Humification index (HIX)	The ratio of areas under the Em at 435-480 nm and 300-345 nm plus 435-480 nm at an Ex wavelength 254 nm ($f_{435-480} / f_{300-345}$)	reflecting the humification index of DOM

Table S2. Subregions of 3D-EEMs according to the FRI theory and the corresponding components [2].

Region	Ex (nm)	Em (nm)	Substance
I	200–250	280–330	tyrosine
II	200–250	330–380	tryptophan
III	200–250	380–500	fulvic acids
IV	250–440	280–380	soluble microbial by-products
V	250–440	380–500	humic acids

8 Table S3. The minimum trade-off of As and Cd in soils corresponds to the optimal pH, Eh, and pe+pH.

No.	Optimal pH	Optimal Eh (mV)	Optimal pe+pH	Objects	Soil pH	Soil As (mg/kg)	Soil Cd (mg/kg)	Soil Fe (%)	Soil SOC (g/kg)	Reference
1	7.25 /	-140 /	4.9 (c) 3.25	Total dissolved As and Cd	5.08	96.00	1.20	2.78	34.00	[3]
2	6.80	-130	4.6(c)	Bioavailable As and Cd	5.73-6.49	27.47-72.59	0.71-2.82	/	11.02-33.68	[4]
3	7.31	-130	5.1(c)	Bioavailable As and Cd	6.60	143.58	24.12	/	46.00	[5]
4	6.2	-73	5.0(c)	Total dissolved As and Cd	5.80	2.49 (a)	0.84 (a)	/	16.20	[6]
5	/	/	6.6	Total dissolved As and Cd	6.56	47.65	4.03	3.45	55.60	In this study

9 Note: letter “a” represents the available As and Cd extracted by the 0.1 M HCl; letter “b” represents the value from the calculation via pe+Eh/59.2mV; letter “c” represents the the result calculated by

10 Optimal Eh and pH.

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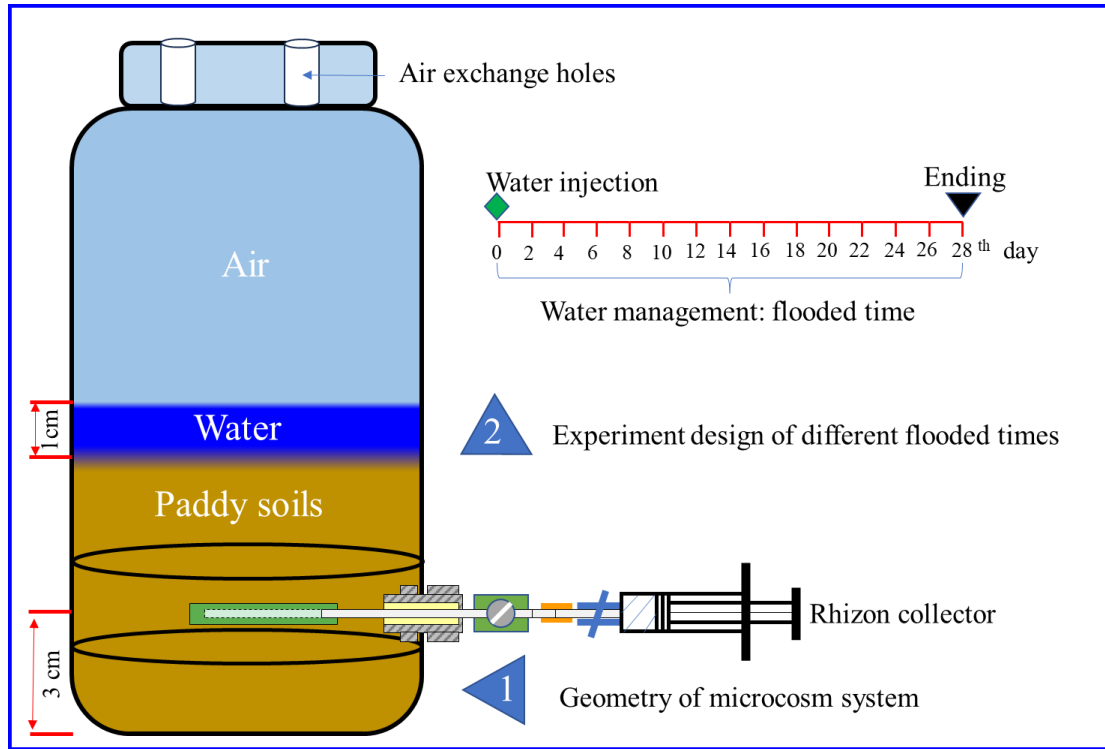


Figure S1. Experiment design of different flooded times (Experiment 1). The Microcosm system is equipped with a porewater collector with a 0.60 μm pore size of sampling head, which is set at approximately 3cm up the soil bottom. Microcosm systems can measure soil temperature, Eh, and pH in situ. Three caps of polyethylene plastic bottles were opened in two holes using the 5mm drill bit to ensure that the overlying water was connected with the atmosphere and the evaporation was negligible. After opening the hole, the bottle cap was padded with nylon cloth to prevent other pollutants from entering the bottle. The experimental design of water management: different flooded times. The incubation experiment lasted 28 days, and porewater samples were collected every two days (2d, 4d, 6d, 8d, 10d, 12d, 14d, 16d, 18d, 20d, 22d, 24d, 26d and 28d).

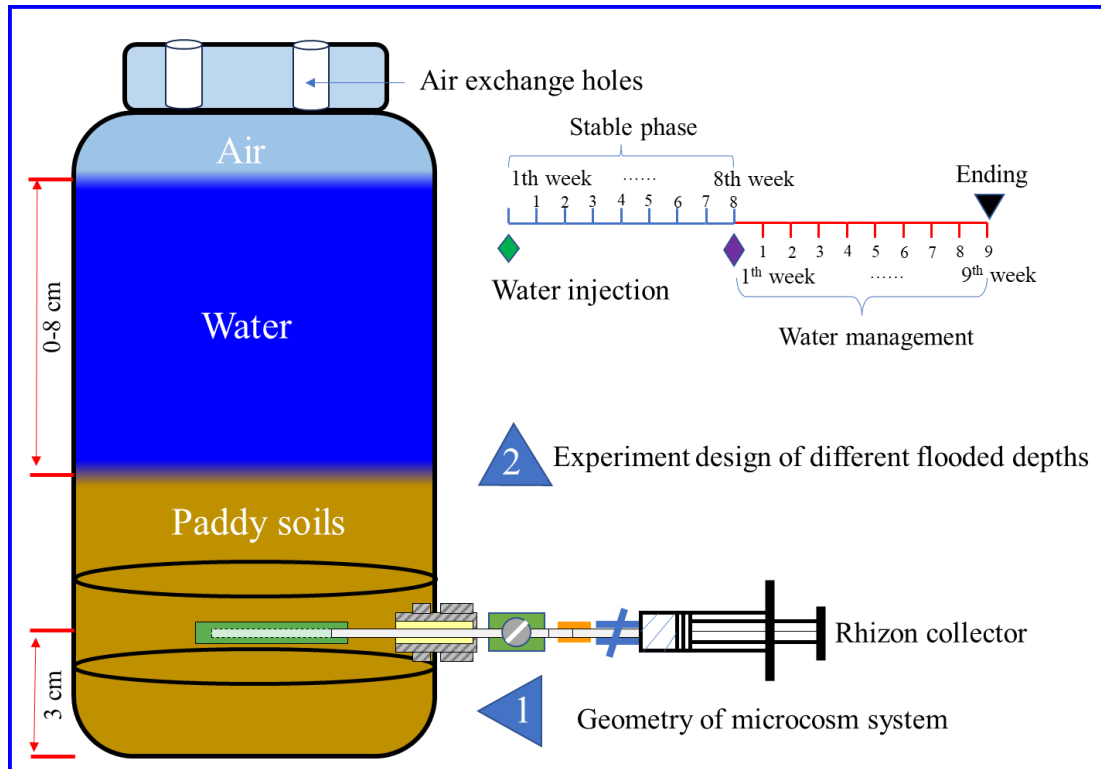


Figure S2. Experiment design of different flooded depths (Experiment 2). Experimental design of water management: the experimental water level was regulated and maintained at flooding (8 cm, 6 cm, 4 cm, 2 cm, 1cm), wetting (0 cm), and drainage (dry1, dry2, and dry3) for one week.

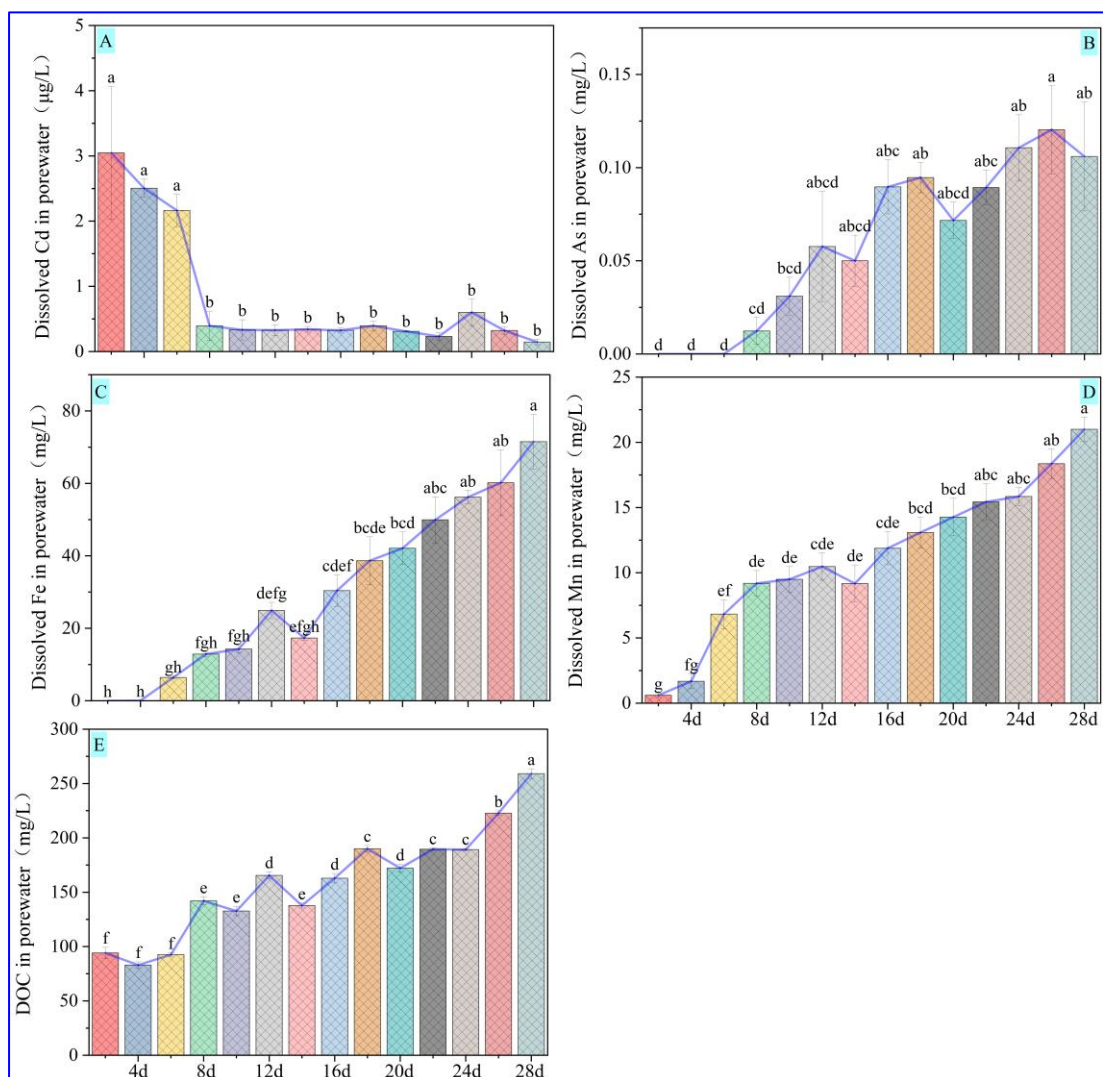


Figure S3. Dissolution characteristics of dissolved elements/substances in porewater of paddy soils under the flooding period. A-E shows the dynamic changes of dissolved Cd, As, Fe, Mn, and DOC in the porewater of paddy soils during flooding.

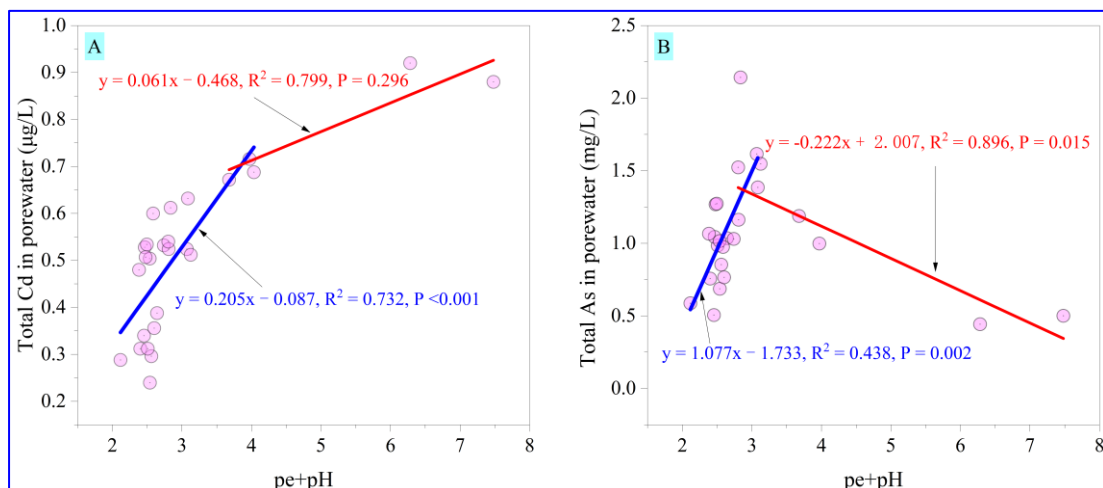


Figure S4. Quantitative relationships between total Cd (A)/As(B) in porewater and soil redox capacity (pe+pH) under flooding depths. The piecewise fit method with the liner function was used to determine the relationships between total Cd/As in porewater and pe+pH.

Reference

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