Supplementary Material Cover Sheet

Mobility of antipyretic drugs with different molecular structures in saturated soil porous media

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Number of tables: 2

Number of figures: 5

S1. Particle size distribution (PSD) of soil

In this work, soil grain particle size distribution (PSD) was measured by the sieve-pipette method (SPM). The SPM is based on Stokes' Law. [1] The soil was dispersed using an ultrasonic vibrator (ca. 20 g soil and ca. 60 mL water in a beaker; sonicated for 2 min). The sand fraction was collected by passing the soil-water suspension through a 53-μm sieve. A 50 mL sample of suspension (< 53 μm) was collected to measure silt plus clay. The suspension was allowed to settle for 8 h in a temperature-controlled room (20 °C), and a sample was collected with a 50-mL pipette from a depth of 10 cm to determine clay. [1] Clay (< 2 μm), silt (2–53 μm), and sand (53–2 000 μm) contents were calculated as the percentage (%) of recovered sample mass based on the USDA soil texture classification system.

S2. Determination of the CEC of soil

The soil's cation exchange capacity (CEC) was measured by following the previously reported method. [2] In brief, 500 mL of $CaCl_2$ (1eq/L) are injected through a column filled with 10 g of soil from bottom to top. Then, 150 mL of $CaCl_2$ (0.05 eq/L) is injected, followed by 500 mL of KNO_3 (1eq/L). The percolate was collected in a 500 mL flask, and the total calcium was titrated with EDTA (0.02eq/L) at pH 12 using the Eriochrome Black T as an indicator. At the same time, the chloride is titrated with $AgNO_3$ (0.05eq/L) using the K_2CrO_4 as an indicator. The CEC is given by:

CEC (meq /100g) = 2*v*-5V

Where *v* is the volume (mL) of EDTA required for calcium titration and V is the volume (mL) of $AgNO_3$ required for chloride titration.

Table S1. ζ-potential of soil under different solution chemistry conditions

No.	electrolyte solution	pH	ζ-potential of soil (mV)
1	10 mM NaCl	5.0	-20.1 ± 1.2
2	10 mM NaCl	7.0	-25.9 ± 0.7
3	10 mM NaCl	9.0	-31.6 ± 2.1
4	0.5 mM $CaCl_2$	5.0	-21.7 ± 0.5

Table S2. Fitted parameters of two-site nonequilibrium transport model from breakthrough results of column experiments.

Column No.	Antipyretic drugs [a]	electrolyte solution	pH	Parameters of two-site nonequilibrium transport model						
				R (-)	β (-)	ω (-)	f (-)	α (1/d)	K_d (L/kg)	r^2
1	IMC	10 mM NaCl	7.0	5.13 ± 0.12	0.312 ± 0.009	0.477 ± 0.003	0.145 ± 0.007	2.51 ± 0.03	1.69 ± 0.07	0.993
2	IBF	10 mM NaCl	7.0	3.76 ± 0.15	0.387 ± 0.013	0.332 ± 0.027	0.164 ± 0.012	2.27 ± 0.07	1.15 ± 0.02	0.986
3	APAP	10 mM NaCl	7.0	3.39 ± 0.08	0.421 ± 0.015	0.263 ± 0.032	0.178 ± 0.010	2.10 ± 0.05	0.97 ± 0.05	0.999
4	IMC	0.5 mM $CaCl_2$	5.0	6.53 ± 0.17	0.269 ± 0.007	0.495 ± 0.035	0.136 ± 0.017	2.70 ± 0.06	2.26 ± 0.13	0.977
5	IBF	0.5 mM $CaCl_2$	5.0	4.56 ± 0.09	0.337 ± 0.011	0.427 ± 0.021	0.151 ± 0.010	2.31 ± 0.11	1.44 ± 0.11	0.992
6	APAP	0.5 mM $CaCl_2$	5.0	3.68 ± 0.05	0.401 ± 0.014	0.395 ± 0.023	0.175 ± 0.013	2.19 ± 0.09	1.09 ± 0.15	0.993
7	IMC	10 mM NaCl	5.0	5.55 ± 0.11	0.295 ± 0.006	0.481 ± 0.017	0.135 ± 0.008	2.62 ± 0.09	1.82 ± 0.13	0.987
8	IBF	10 mM NaCl	5.0	3.87 ± 0.07	0.362 ± 0.013	0.411 ± 0.021	0.139 ± 0.012	2.43 ± 0.15	1.34 ± 0.07	0.998
9	APAP	10 mM NaCl	5.0	3.56 ± 0.09	0.392 ± 0.015	0.359 ± 0.017	0.155 ± 0.017	2.21 ± 0.13	1.06 ± 0.05	0.999
10	IMC	10 mM NaCl	9.0	4.37 ± 0.08	0.351 ± 0.012	0.452 ± 0.013	0.158 ± 0.012	2.32 ± 0.07	1.38 ± 0.10	0.993
11	IBF	10 mM NaCl	9.0	3.11 ± 0.02	0.447 ± 0.017	0.278 ± 0.015	0.185 ± 0.017	2.26 ± 0.16	0.83 ± 0.02	0.995
12	APAP	10 mM NaCl	9.0	2.69 ± 0.07	0.495 ± 0.003	0.172 ± 0.003	0.198 ± 0.019	1.95 ± 0.12	0.71 ± 0.01	0.996

[a] IMC, IBF, and APAP represent indometacin, ibuprofen, and acetaminophen, respectively.

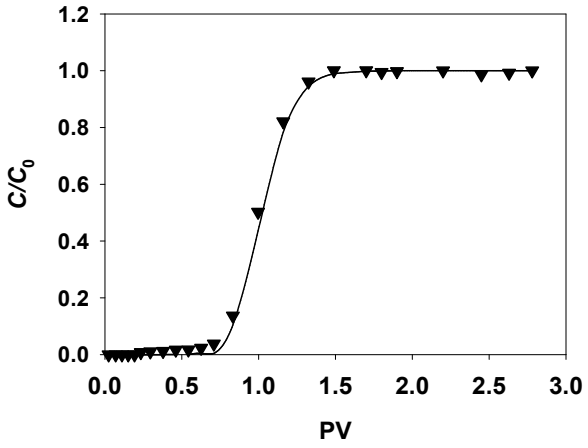

Fig. S1. The representative breakthrough curve of conservative tracer (Br^-). The line was plotted by fitting the breakthrough data with the one-dimensional steady-state advection–dispersion equation**.**

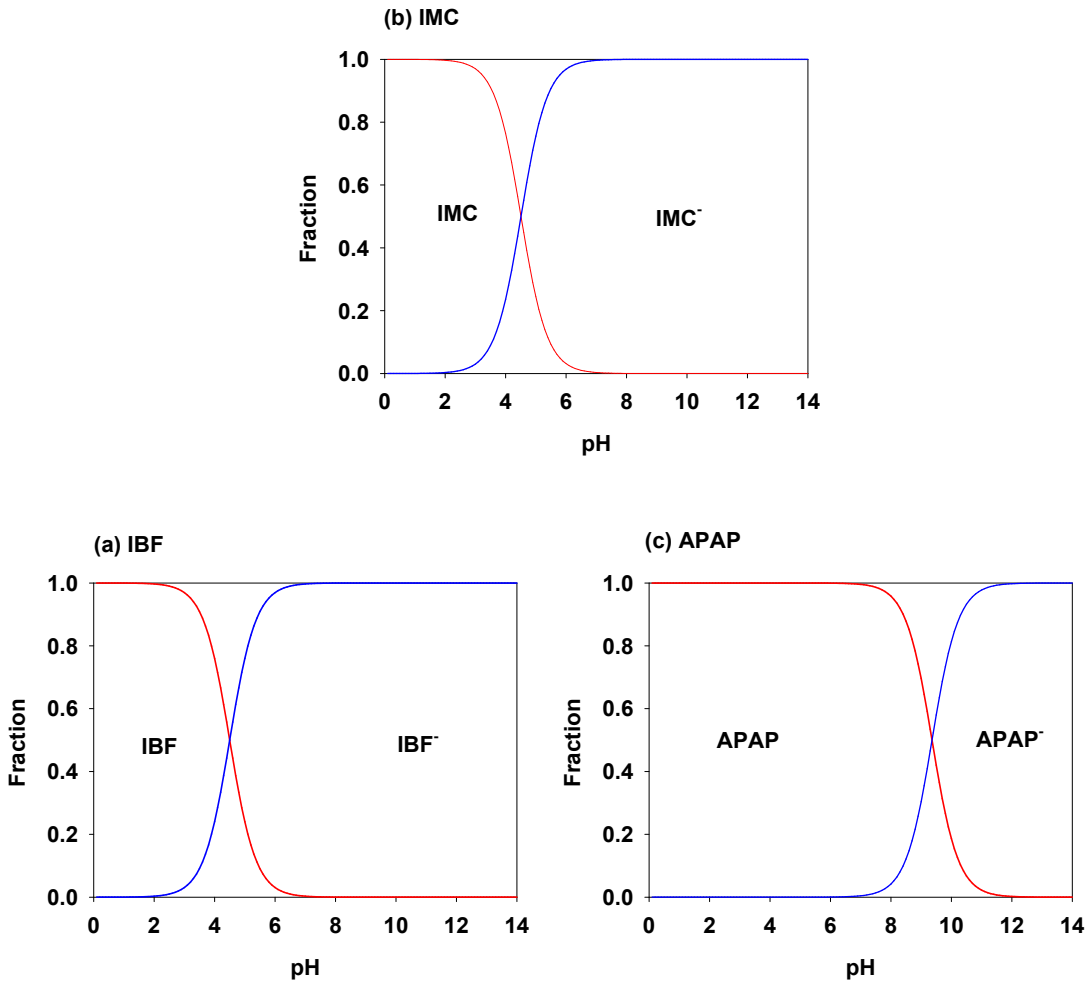

Fig. S2. pH-dependent speciation of the whole organic acid molecular and the functional groups, respectively: (a) IMC; (b) IBF; and (c) APAP.

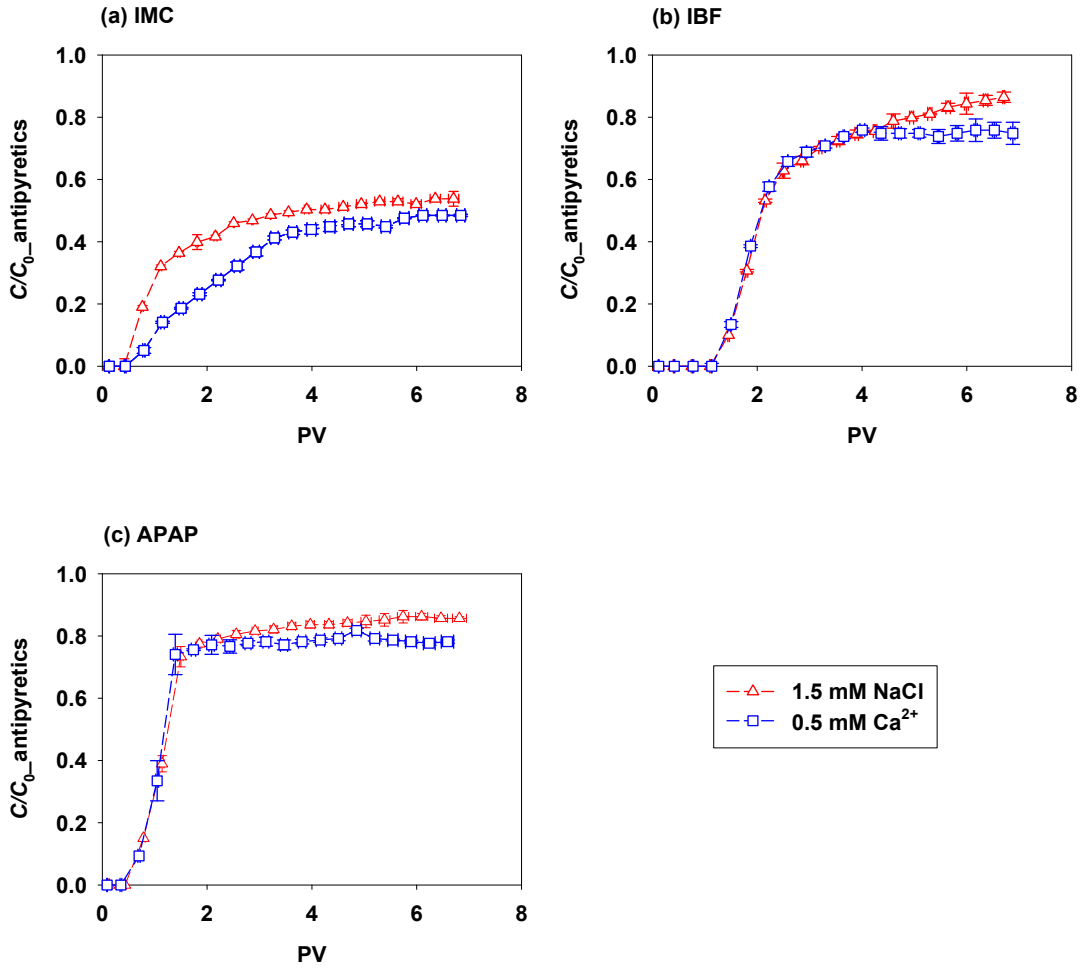

Fig. S3. Transport of SNM in saturated soil columns in the presence of 1.5 mM Na^{+} and 0.5 mM Ca^{2+} at pH 5.0: (a) IMC; (b) IBF; and (c) APAP.

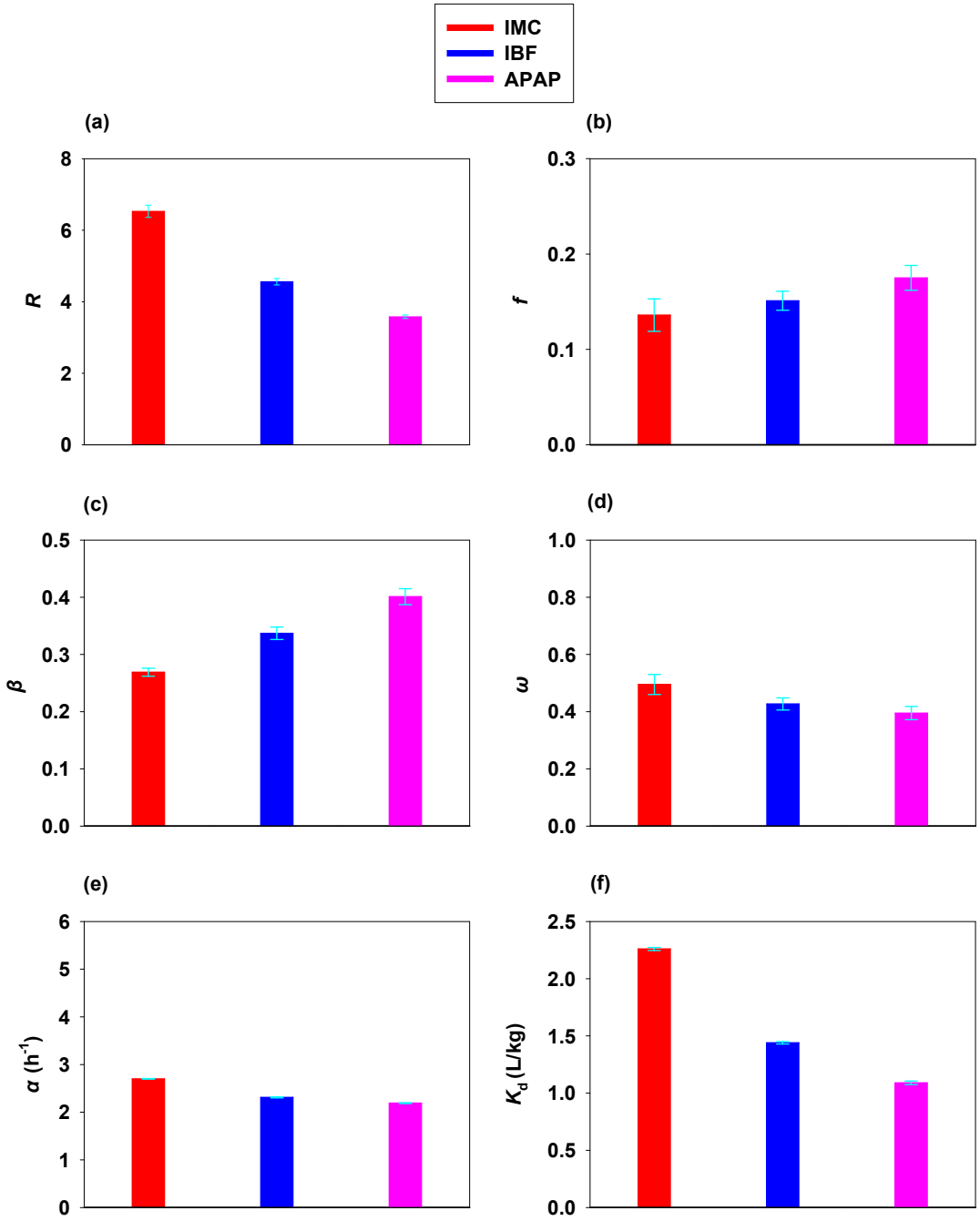

Fig. S4. Fitted parameters of two-site nonequilibrium transport model from breakthrough results of column experiments (in the presence of 0.5 mM Ca^{2+}, pH 5.0): (a) Retardation factor (R); (b) the fraction of Type 1 sites (f); (c) the fraction of instantaneous retardation to the total retardation (β); and (d) the coefficient of partitioning between the equilibrium and nonequilibrium phases (ω); (e) the first-order rate for kinetics at Type 2 sites (α); (f) K_d values.

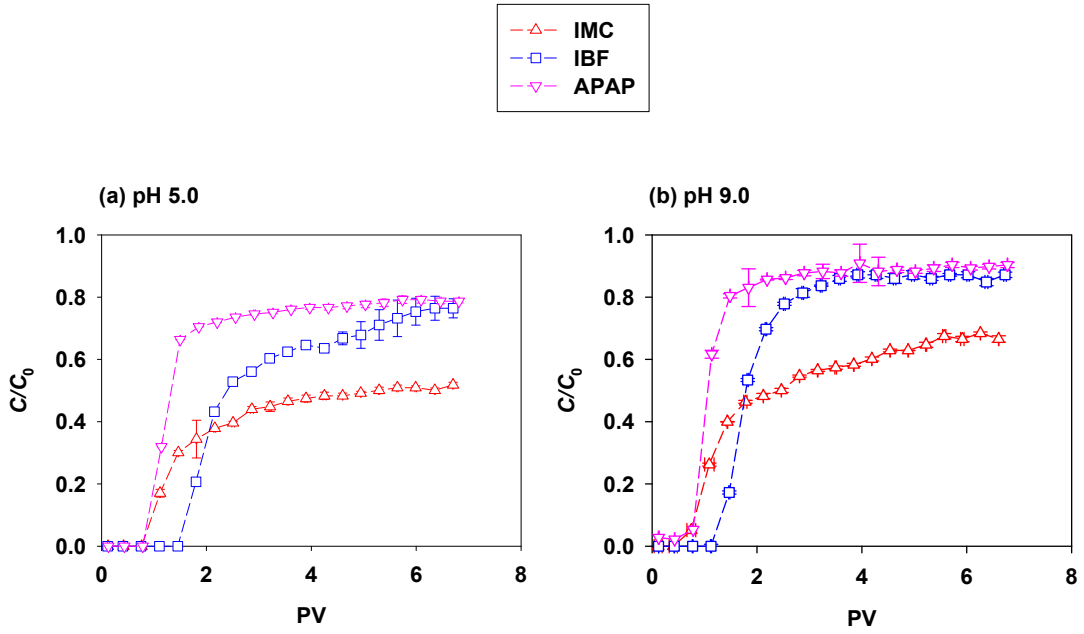

Fig. S5. Transport of antipyretic drugs in saturated soil columns at different pH conditions: (a) pH 5.0, (columns 7–9, Table 2); (b) pH 9.0 (columns 10–12, Table 2).

References:

[1] G. W. Gee, D. Or, *Particle size analysis*. In Dane J, Topp C (eds.) Methods of Soil Analysis, *Soil Sci. Soc. Am. Madison.*, 2002, pp. 255–293.

[2] M. Abdelwaheb, K. Jebali, H. Dhaouadi, S. Dridi-Dhaouadi, Adsorption of nitrate, phosphate, nickel and lead on soils: risk of groundwater contamination. *Ecotox. Environ. Safe.* 2019, **179,** 182–187.