Supporting Information

Modeling Bioaccumulation of Metallic Engineered Nanomaterials in a Freshwater Ecosystem

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The following information is provided in the Supporting Information:

Data selection tiers

Parameter selection for each species and each ENM was conducted in a tiered process where the preference ranking was as follows:

1. parameter measured for specific ENM and specific species
2. parameter measured for specific ENM for similar species
3. parameter measured for any ENM for specific species
4. parameter measured for any ENM for similar species
5. parameter measured for metal ion of ENM for specific species
6. parameter measured for metal ion of ENM for similar species
7. parameter measured for similar metal ion for specific species
8. parameter measured for similar metal ion for similar species
9. parameter measured for any metal ion for specific species
10. parameter measured for any metal ion for similar species

The search process started by looking for the specific parameter for each individual organism for each ENM. If no ENM specific parameters could be identified, the metal ion equivalent was explored. If parameters for the specific metal ion could not be found, then other commonly studied metal ions (e.g. mercury, cadmium, etc.) were investigated. This was done separately species by species for each parameter and ENM. When a parameter for the specific species could not be identified, the parameter for a similar species (e.g. *D. pulex* instead of *D. magna*) was substituted. The uncertainty increases moving down the ranking table.

Bioaccumulation Equations by Species (parameters are defined in Tables S2-S4)

1. *S. capricornutum*

$$\frac{dC_{b,1}}{dt} = k_{u1,1}C_w - k_{e,1}C_{b,1} - k_{dis}C_{b,1} - D_1C_{b,1}$$

$$\frac{dC_{dis,1}}{dt} = k_{u3,1}\alpha_{bio1}C_{w,dis} + k_{dis}C_{b,1} - k_{e_{dis},1}C_{dis,1} - D_1C_{b,1}$$

2. *F. crotonensis*

$$\frac{dC_{b,2}}{dt} = k_{u1,2}C_w - k_{e,2}C_{b,2} - k_{dis}C_{b,2} - D_2C_{b,2}$$

$$\frac{dC_{dis,2}}{dt} = k_{u3,2}\alpha_{bio2}C_{w,dis} + k_{dis}C_{b,2} - k_{e_{dis},2}C_{dis,2} - D_2C_{b,2}$$

3. *D. magna*

$$\frac{dC_{b,3}}{dt} = k_{u1,3}C_w + k_{u2,3}C_{ss} + \alpha_3\alpha_{ENM,3}k_{d,3}C_{b,1} - k_{e,3}C_{b,3} - k_{dis}C_{b,3} - D_3C_{b,3}$$

$$\frac{dC_{dis,3}}{dt} = k_{u3,3}\alpha_{bio3}C_{w,dis} + k_{dis}C_{b,3} - k_{e_{dis},3}C_{dis,3} - D_3C_{b,3}$$

4. *H. azteca*

$$\frac{dC_{b,4}}{dt} = k_{u1,4}C_w + k_{u2,4}C_{sed} + \alpha_4\alpha_{ENM,4}k_{d,4}C_{b,1} - k_{e,4}C_{b,4} - k_{dis}C_{b,4} - D_4C_{b,4}$$

$$\frac{dC_{dis,4}}{dt} = k_{u3,4}\alpha_{bio4}C_{w,dis} + k_{dis}C_{b,4} - k_{e_{dis},4}C_{dis,4} - D_4C_{b,4}$$

5. *V. constricta*

$$\frac{dC_{b,5}}{dt} = k_{u1,5}C_w + k_{u2,5}C_{sed} + \alpha_5\alpha_{ENM,5}k_{d,5}C_{b,3} - k_{e,5}C_{b,5} - k_{dis}C_{b,5} - D_5C_{b,5}$$

$$\frac{dC_{dis,5}}{dt} = k_{u3,5}\alpha_{bio5}C_{w,dis} + k_{dis}C_{b,5} - k_{e_{dis},n}C_{dis,5} - D_5C_{b,5}$$

6. *P. promelas*

$$\frac{dC_{b,6}}{dt} = k_{u1,6}C_w + \alpha_6\alpha_{ENM,6}k_{d,6}C_{b,3} - k_{e,6}C_{b,6} - k_{dis}C_{b,6} - D_6C_{b,6}$$

$$\frac{dC_{dis,6}}{dt} = k_{u3,6}\alpha_{bio6}C_{w,dis} + k_{dis}C_{b,6} - k_{e_{dis},6}C_{dis,6} - D_6C_{b,6}$$

7. *O. mykiss*

$$\frac{dC_{b,7}}{dt} = k_{u1,7}C_w + \alpha_7\alpha_{ENM,7}k_{d,7}C_{b,6} - k_{e,7}C_{b,7} - k_{dis}C_{b,7} - D_7C_{b,7}$$

$$\frac{dC_{dis,7}}{dt} = k_{u3,7}\alpha_{bio7}C_{w,dis} + k_{dis}C_{b,7} - k_{e_{dis},7}C_{dis,7} - D_7C_{b,7}$$

Table S1. Environmental parameter values used in nanoBio model for San Francisco Bay

Definition	Parameter	Value	Units
Volume of water compartment	V_W	1.5956E+12	L
Volume of suspended sediment compartment	V_{ss}	1.5956E+07	kg
Volume of sediment solids compartment	V_{sed}	3.8295E+10	kg
Volume Sediment Water compartment	V_{sedw}	6.3825E+10	L

Table S2. ENM dissolution rates considered in nanoFate and nanoBio

ENM	Dissolution Rate (1/day)	Metal ion Bioavailability (α_{bio})	References
CuO	0.00195	0.116	[1–13]
TiO_2	0	0	
ZnO	0.08675	0.7542	[1,6,10,11,13–30]

Table S3. Species specific parameter values considered in nanoBio

Definition	Parameter	Units	*S. capricornutum*	*F. crotonensis*	*D. magna*	*H. azteca*	*V. constricta*	*P. promelas*	*O. mykiss*
Wet body mass of individual organism	M_i	mg	$3.58*10^{-8}$	$6.8*10^{-7}$	3	8	$2.657*10^{3}$	$3*10^{3}$	$4*10^{6}$
Lifespan	L_n	days	2	3	60	365	3650	912.5	2920
Biomass density	B_n	mg/m^3	1	1	12.39	52.17	40.83	1.67	$2.65*10^{-2}$
Species pH	pH	--	7.32	7.32	7.32	6	7	4.5	5
Assimilation Efficiency	α_n	--	NA	NA	0.2	0.5	0.5	0.35	0.8

Table S4. ENM-specific parameter values for the various species used in nanoBio

CuO									
Definition	Parameter	Units	*S. capricornutum*	*F. crotonensis*	*D. magna*	*H. azteca*	*V. constricta*	*P. promelas*	*O. mykiss*
Uptake from water	$k_{u1,n}$	L/mg-day	$2.78*10^{-2}$	$2.78*10^{-1}$	$1.6*10^{-1}$	$5.79*10^{-4}$	$7.68*10^{-3}$	$9.6*10^{-4}$	$4.32*10^{-5}$
Uptake of solids	$k_{u2,n}$	L/mg-day	NA	NA	$1.6*10^{-14}$	$4.8*10^{-5}$	$7.68*10^{-5}$	0	0
Uptake of dissolved ion from water	$k_{u3,n}$	L/mg-day	$1.41*10^{-7}$	$1.41*10^{-7}$	$1.6*10^{-2}$	$8.66*10^{-1}$	$7.29*10^{-3}$	$5.13*10^{-3}$	$6.3*10^{-2}$
Ingestion rate	$k_{d,n}$	g/mg-day	NA	NA	$1.6*10^{-8}$	$4.8*10^{-5}$	$7.68*10^{-6}$	$7.02*10^{-6}$	$7.69*10^{-2}$
ENM/Metallic Assimilation Efficiency	α_{ENM}	--	NA	NA	0.332	0.72	0.41	0.06	0.06
Fecal elimination rate	$k_{e,n}$	g/mg-day	$1.73*10^{-4}$	$3*10^{-3}$	0.029	$6.38*10^{-5}$	$7.68*10^{-6}$	$7.02*10^{-7}$	$2*10^{-6}$
Fecal elimination rate of dissolved ion	$k_{edis,n}$	g/mg-day	0	0	0.29	$2.52*10^{-3}$	1.92	$1.9*10^{-2}$	$1.7*10^{-2}$
TiO_2									
Definition	Parameter	Units	*S. capricornutum*	*F. crotonensis*	*D. magna*	*H. azteca*	*V. constricta*	*P. promelas*	*O. mykiss*
Uptake from water	$k_{u1,n}$	L/mg-day	$3.25*10^{-3}$	$3.25*10^{-3}$	$1.6*10^{-1}$	$5.79*10^{-4}$	$7.68*10^{-3}$	$9.6*10^{-4}$	$4.32*10^{-5}$
Uptake of solids	$k_{u2,n}$	L/mg-day	0	0	$1.6*10^{-4}$	$4.8*10^{-5}$	$7.68*10^{-5}$	0	0
Uptake of dissolved ion from water	$k_{u3,n}$	L/mg-day	$1.41*10^{-7}$	$1.41*10^{-7}$	$1.6*10^{-2}$	$4.44*10^{-1}$	$7.29*10^{-3}$	$5.13*10^{-3}$	$2*10^{-6}$
Ingestion rate	$k_{d,n}$	g/mg-day	NA	NA	$1.6*10^{-8}$	$4.8*10^{-5}$	$7.68*10^{-6}$	$7.02*10^{-6}$	$7.69*10^{-2}$
ENM/Metallic Assimilation Efficiency	α_{ENM}	--	NA	NA	0.326	0.137	0.03	0.3	0.3
Fecal elimination rate	$k_{e,n}$	g/mg-day	$1.73*10^{-4}$	$3*10^{-4}$	$1.6*10^{-3}$	$6.38*10^{-5}$	$7.68*10^{-6}$	$7.02*10^{-7}$	$2*10^{-6}$
Fecal elimination rate of dissolved ion	$k_{edis,n}$	g/mg-day	0	0	0.29	$1.04*10^{-2}$	1.92	$1.9*10^{-2}$	$2*10^{-3}$
ZnO									
Definition	Parameter	Units	*S.*	*F.*	*D. magna*	*H. azteca*	*V.*	*P.*	*O. mykiss*

			capricornutum	*crotonensis*			*constricta*	*promelas*	
Uptake from water	$k_{u1,n}$	L/mg-day	3.19*10^{-2}	3.19*10^{-2}	1.6*10^{-2}	5.79*10^{-4}	7.68*10^{-3}	9.6*10^{-4}	4.32*10^{-5}
Uptake of solids	$k_{u2,n}$	L/mg-day	0	0	1.5*10^{-4}	4.8*10^{-5}	7.68*10^{-2}	0	0
Uptake of dissolved ion from water	$k_{u3,n}$	L/mg-day	1.41*10^{-7}	1.41*10^{-7}	2.1*10^{-4}	0.44	7.29*10^{-3}	5.13*10^{-3}	2*10^{-6}
Ingestion rate	$k_{d,n}$	g/mg-day	NA	NA	1.6*10^{-8}	4.8*10^{-5}	7.68*10^{-6}	7.02*10^{-6}	7.69*10^{-2}
ENM/Metallic Assimilation Efficiency	α_{ENM}	--	NA	NA	0.33	0.49	0.332	0.3	0.3
Fecal elimination rate	$k_{e,n}$	g/mg-day	1.73*10^{-4}	3*10^{-4}	1.6*10^{-2}	6.38*10^{-5}	7.68*10^{-6}	7.02*10^{-7}	2*10^{-6}
Fecal elimination rate of dissolved ion	$k_{edis,n}$	g/mg-day	0	0	0.29	1.04*10^{-2}	1.92	1.9*10^{-2}	1.1*10^{-2}

References CuO: [31–67]; TiO_2: [31–35,37–70]; ZnO: [31–35,37–69,71–75]

#adsorption rate of nanoparticle to particulate matter

Table S5. Summary of exposure conditions and concentrations in biological tissue for laboratory experiments

ENM	Species	Medium	Exposure (mg/L or mg/kg for dietary and/or sediment exposure)	Time Period (days)	Concentration in Biological Tissue (mg/g)	Ref.
CuO	*M. balthica*	Sed.	147.7 mg/kg DW	35	0.9 – 2.4 DW	[76]
CuO	*P. antipodarum*	Sed.	240 mg/kg DW	14	0.05 – 0.065 DW	[77]
CuO	*L. variegatus*	Sed.	40 mg/kg DW	10	0.058 DW	[78]
CuO	*C. carpio*	FW	100 mg/L	30	0.07 – 0.13 DW	[79]
CuO	*L. stagnalis*	FW	0.013 mg/L	3-5	0.26 DW	[9]
CuO	*C. Vulgaris*	FW	50 mg/L	1	3.5 mg Cu/g C	[79]
CuO	*D. magna*	FW	0.07 mg/L	9	1.84 DW	[79]
TiO_2	*D. magna*	FW	0.1 mg/L	1	4.52 DW	[80]
TiO_2	*D. magna*	FW	1 mg/L	1	61.1 DW	[80]
TiO_2	*D. magna*	FW	2 mg/L	4	92.3 DW	[81]
TiO_2	*D. rerio*	FW	4,520 mg/kg DW^	14	0.107 DW	[82]
TiO_2	*D. rerio*	FW	61,086 mg/kg DW ^	14	0.522 DW	[82]
TiO_2	*C. carpio*	FW	10 mg/L	10	1.60 DW	[83]
TiO_2	*C. carpio*	FW	10 mg/L	25	3.39 DW	[83]
TiO_2	*C. carpio*	FW	10 mg/L	10	4.95 DW	[84]
TiO_2	*O. Mykiss*	FW	0.1 mg/L	14	0.12 – 0.16 DW	[85]
TiO_2	*O. Mykiss*	FW	5.0 mg/L	14	0.39 – 0.88 DW	[86]
ZnO	*M. galloprovincialis*	Mar.	0.1 mg/L	84	0.16 – 0.18 DW	[87]
ZnO	*M. galloprovincialis*	Mar.	0.5 mg/L	84	0.18 – 0.31 DW	[87]
ZnO	*M. galloprovincialis*	Mar.	0.1	112	0.40 DW	[88]
ZnO	*O. Mykiss*	FW	0.5 mg/L	14	0.34 – 0.51 DW	[86]

^ Dietary exposure
§ Wet weight
¶ DW = Dry weight
ND – no data/not reported
Bioaccumulation not reported, estimated by authors based on reported exposure and accumulation
& BMF = Biomagnification factor
*Dietary exposure plus ambient exposure
FW = freshwater
Sed. = sediment
Mar. = marine water
Ref. = reference

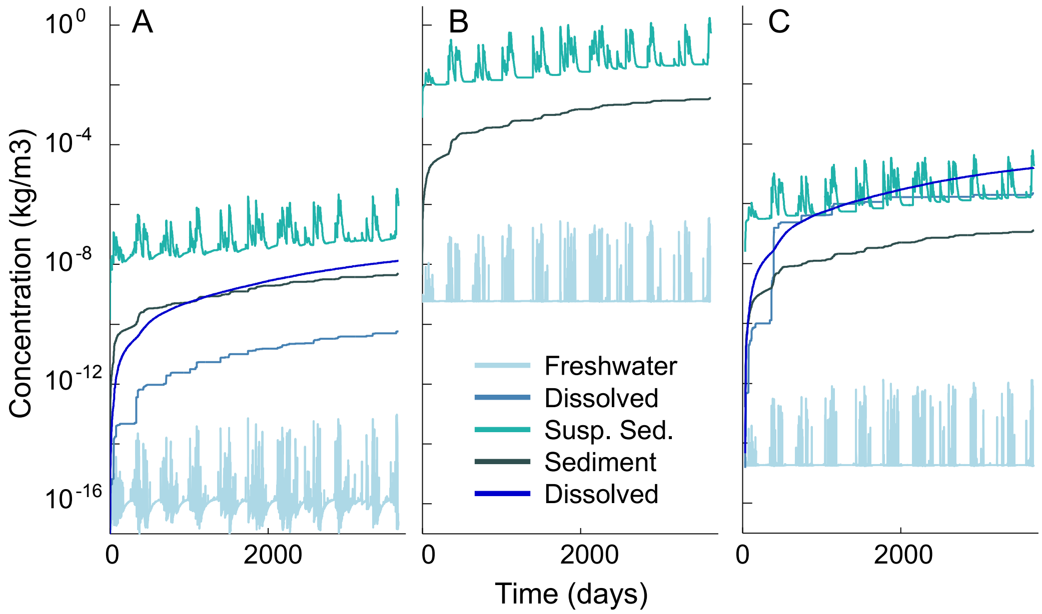

Figure S1. Environmental exposure concentrations from nanoFate model for (A) nCuO, (B) $nTiO_2$, and (C) nZnO.

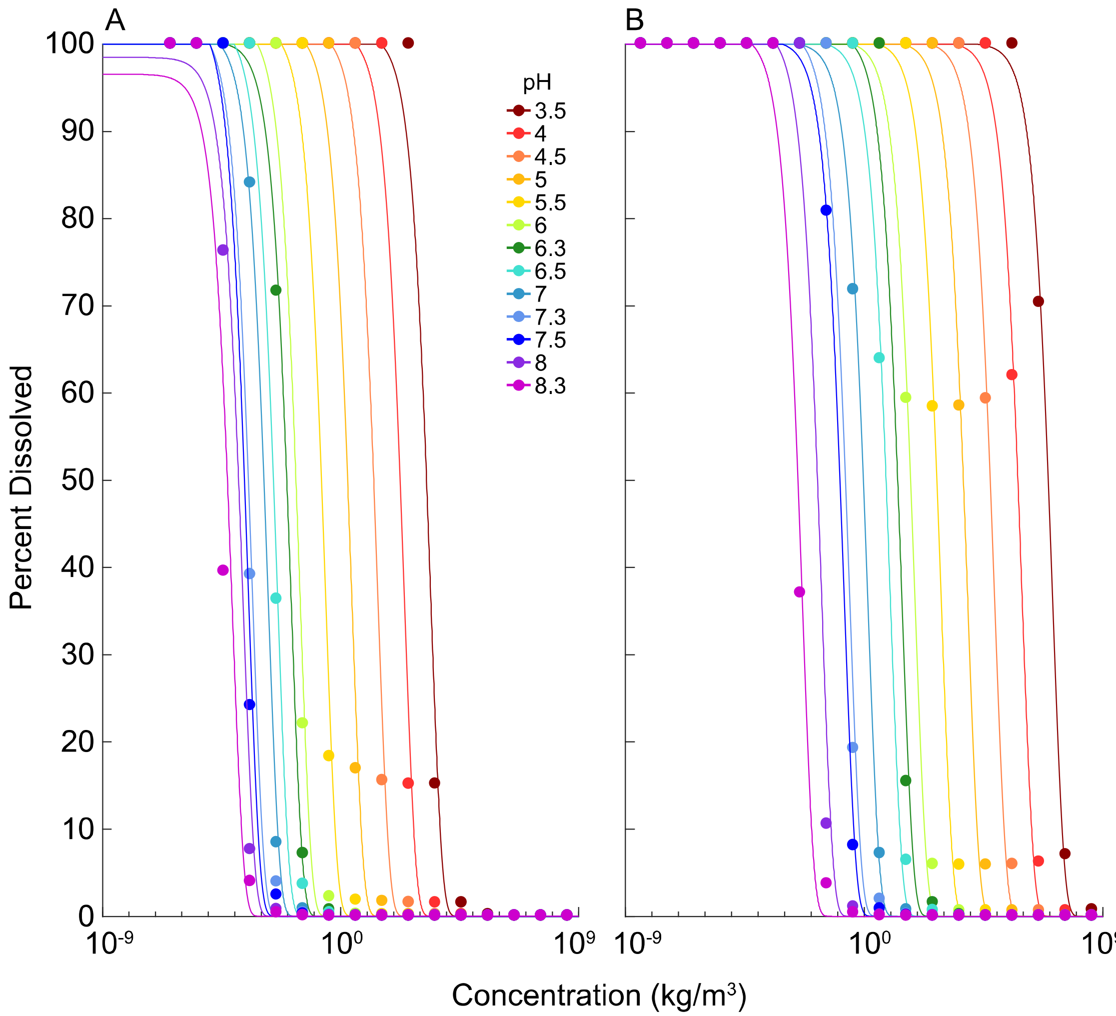

Figure S2. Dissolution curves from *MINTeq*. (A) CuO to Cu^{2+}; and (B) ZnO to Zn^{2+}.

Table S6. Pseudo-steady state mean concentration and time to mean for nCuO

Species	nCuO		Cu^{2+}	
	Time to Pseudo-Steady-State (d)	Pseudo-State-State Concentration (ug/mg)	Time to Pseudo-Steady-State (d)	Pseudo-State-State Concentration (ug/mg)
S. capricornutum	46	1.02E-13	1100	9.03E-16
F.crotonensis	46	1.02E-13	1508	1.19E-15
D.magna	352	2.95E-13	3327	2.76E-15
H. Azteca	3327	1.16E-12	3327	2.76E-15
V.constricta	3327	1.16E-12	3327	2.76E-15
P.promelas	1748	1.01E-12	3327	2.76E-15
O. mykiss	2282	2.10E-10	3327	2.76E-15

Table S7. Pseudo-steady state mean concentration and time to mean for $nTiO_2$

Species	$nTiO_2$		Ti^+	
	Time to Pseudo-Steady-State (d)	Pseudo-State-State Concentration (ug/mg)	Time to Pseudo-Steady-State (d)	Pseudo-State-State Concentration (ug/mg)
S. capricornutum	335	7.52E-08	NA	0
F.crotonensis	335	7.52E-08	NA	0
D.magna	352	1.32E-07	NA	0
H. Azteca	2893	5.17E-07	NA	0
V.constricta	2660	3.06E-07	NA	0
P.promelas	1881	1.30E-07	NA	0
O. mykiss	2660	3.06E-07	NA	0

Table S8. Pseudo-steady state mean concentration and time to mean for nZnO

Species	nZnO		Zn^{2+}	
	Time to Pseudo-Steady-State (d)	Pseudo-State-State Concentration (ug/mg)	Time to Pseudo-Steady-State (d)	Pseudo-State-State Concentration (ug/mg)
S. capricornutum	335	2.69E-12	2892	2.15E-10
F.crotonensis	335	2.69E-12	2893	2.19E-10
D.magna	352	4.81E-12	2891	2.07E-10
H. Azteca	3328	1.21E-11	2891	2.07E-10
V.constricta	2892	1.57E-11	2891	2.07E-10
P.promelas	2240	8.54E-12	2891	2.07E-10
O. mykiss	2243	1.96E-12	2891	2.07E-10

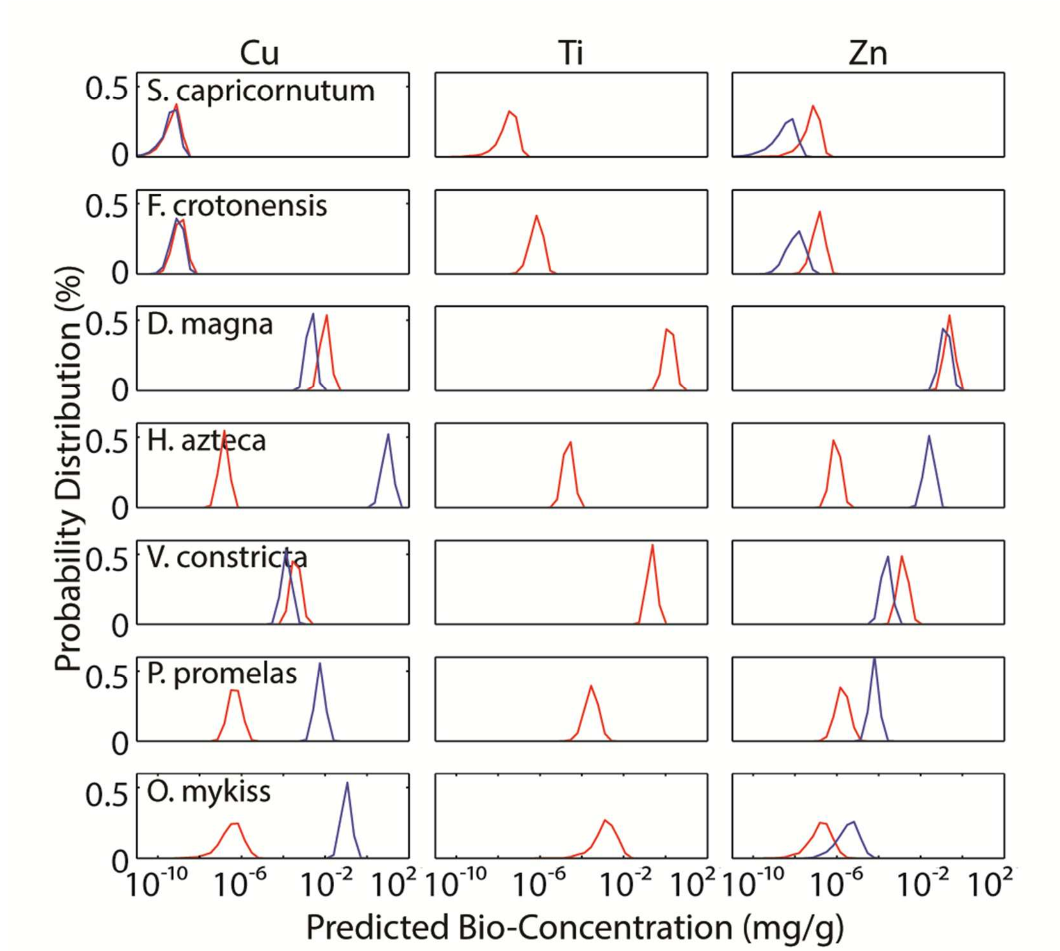

Figure S3. Probability distribution of predicted organism ENM (red) and dissolved ion (blue) concentrations. Each row is for a single species. The x-axis of each graph shows the predicted body-burden (mg/g) and the y-axis shows the frequency predicted over 10,000 Monte Carlo simulations.

Table S9. Geometric standard deviations for each chemical and biological species

Species	nCuO	Cu	$nTiO_2$	nZnO	Zn
S. capricornutum	3.007	3.090	3.094	3.000	4.155
F. crotonensis	1.946	1.958	1.953	1.902	2.582
D. magna	1.609	1.525	1.689	1.630	1.718
H. azteca	1.606	1.683	1.686	1.672	1.670
V. constricta	1.667	1.654	1.563	1.713	1.692
P. promelas	1.964	1.609	2.063	2.026	1.531
O. mykiss	3.632	1.643	3.5053	3.505	3.328

Table S10. Sensitivity ranking of all model parameters for each ENM

CuO								
Definition	Parameter	S. capricornutum	F. crotonensis	D. magna	H. azteca	V. constricta	P. promelas	O. mykiss
Assimilation efficiency	α_n	0.0000	0.0000	0.0983	0.0964	0.1021	0.2144	0.3235
Biomass density	B_n	0.0951	0.0926	0.1006	0.0950	0.0998	0.0901	0.1008
Dissolution rate	k_{dis}	0.1007	0.0995	0.0953	0.1707	0.2392	0.1723	0.1502
Dissolved Ion concentration in water	C_{wdis}	0.0983	0.1015	0.0963	0.1001	0.0955	0.1087	0.1001
Elimination rate	$k_{e,n}$	0.1051	0.0947	0.1624	0.1005	0.0938	0.1062	0.0962
Elimination rate of dissolved ion	$k_{edis,n}$	0.0000	0.0000	0.0918	0.0961	0.0998	0.0962	0.1016
ENM concentration in sediment	C_{sed}	0.0992	0.0967	0.1047	0.2934	0.2627	0.1076	0.1058
ENM concentration in suspended sediment	C_{ss}	0.0928	0.1134	0.2903	0.1061	0.1019	0.2105	0.1497
ENM concentration in water	C_w	0.1815	0.2081	0.1010	0.1017	0.1012	0.1125	0.1029
Ingestion rate	$k_{d,n}$	0.0000	0.0000	0.0934	0.1009	0.0963	0.2092	0.1501
Lifespan	L_n	0.4223	0.3510	0.1361	0.1493	0.0986	0.1150	0.0930
Uptake by water	$k_{u1,n}$	0.1946	0.2242	0.0954	0.0889	0.0882	0.0993	0.1053
Uptake of dissolved ion	$k_{u3,n}$	0.0945	0.0780	0.1011	0.0981	0.0994	0.0893	0.0995
Uptake of solids	$k_{u2,n}$	0.0000	0.0000	0.2908	0.2790	0.2718	0.0000	0.0000
Wet body mass of individual organism	M_i	0.0938	0.0957	0.0906	0.1115	0.1001	0.0984	0.0957
Cu^{2+}								
Definition	Parameter	S. capricornutum	F. crotonensis	D. magna	H. azteca	V. constricta	P. promelas	O. mykiss
Assimilation efficiency	α_n	0.0000	0.0000	0.0966	0.1001	0.1019	0.1036	0.1046
Biomass density	B_n	0.1010	0.1007	0.1069	0.0943	0.0958	0.1002	0.0979
Dissolution rate	k_{dis}	0.0915	0.0975	0.1526	0.0986	0.1009	0.0995	0.0936
Dissolved Ion concentration in water	C_{wdis}	0.1918	0.2190	0.1993	0.2700	0.2539	0.2703	0.2754
Elimination rate	$k_{e,n}$	0.1030	0.1015	0.1171	0.0996	0.0972	0.0975	0.1009
Elimination rate of dissolved ion	$k_{edis,n}$	0.0000	0.0000	0.2114	0.1000	0.2626	0.1838	0.2137
ENM concentration in sediment	C_{sed}	0.1155	0.0900	0.0889	0.0972	0.1071	0.0952	0.0965
ENM concentration in suspended sediment	C_{ss}	0.0964	0.1022	0.1625	0.1058	0.0890	0.0998	0.1065
ENM concentration in water	C_w	0.0981	0.0907	0.1003	0.0989	0.0967	0.0958	0.0933
Ingestion rate	$k_{d,n}$	0.0000	0.0000	0.1010	0.1016	0.0922	0.0936	0.0990

Lifespan	L_n	0.4421	0.3619	0.1908	0.2411	0.0959	0.1350	0.1085
Uptake by water	$k_{u1,n}$	0.1033	0.1053	0.1038	0.0963	0.0974	0.0905	0.0907
Uptake of dissolved ion	$k_{u3,n}$	0.1848	0.1972	0.1910	0.2754	0.2572	0.2800	0.2785
Uptake of solids	$k_{u2,n}$	0.0000	0.0000	0.1564	0.0927	0.1000	0.0000	0.0000
Wet body mass of individual organism	M_i	0.1009	0.1018	0.1004	0.1024	0.1021	0.1053	0.0935
TiO_2								
Definition	Parameter	S. capricornutum	F. crotonensis	D. magna	H. azteca	V. constricta	P. promelas	O. mykiss
Assimilation efficiency	α_n	0.0000	0.0000	0.0880	0.1066	0.1037	0.1932	0.3366
Biomass density	B_n	0.1002	0.0893	0.0906	0.0984	0.1007	0.0987	0.1069
Dissolution rate	k_{dis}	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Dissolved Ion concentration in water	C_{wdis}	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Elimination rate	$k_{e,n}$	0.0961	0.0952	0.0989	0.0985	0.0929	0.0919	0.1004
Elimination rate of dissolved ion	$k_{edis,n}$	0.0000	0.0000	0.0970	0.0995	0.1001	0.0985	0.1003
ENM concentration in sediment	C_{sed}	0.0914	0.1033	0.1058	0.2486	0.2917	0.1048	0.1089
ENM concentration in suspended sediment	C_{ss}	0.1006	0.1010	0.2606	0.1081	0.0963	0.1985	0.1545
ENM concentration in water	C_w	0.1772	0.1993	0.1004	0.0927	0.1030	0.0996	0.0991
Ingestion rate	$k_{d,n}$	0.0000	0.0000	0.0865	0.0939	0.0881	0.2002	0.1531
Lifespan	L_n	0.4409	0.3567	0.2413	0.2592	0.1537	0.1765	0.1146
Uptake by water	$k_{u1,n}$	0.1970	0.2153	0.0917	0.0969	0.0908	0.0989	0.1035
Uptake of dissolved ion	$k_{u3,n}$	0.0911	0.0875	0.0992	0.0888	0.0951	0.1071	0.1048
Uptake of solids	$k_{u2,n}$	0.0000	0.0000	0.2708	0.2417	0.2986	0.0000	0.0000
Wet body mass of individual organism	M_i	0.0966	0.1091	0.1012	0.1008	0.1007	0.1088	0.0940
ZnO								
Definition	Parameter	S. capricornutum	F. crotonensis	D. magna	H. azteca	V. constricta	P. promelas	O. mykiss
Assimilation efficiency	α_n	0.0000	0.0000	0.0995	0.0985	0.1048	0.2007	0.3223
Biomass density	B_n	0.0915	0.1000	0.0950	0.0992	0.1010	0.1094	0.0987
Dissolution rate	k_{dis}	0.0929	0.1017	0.1791	0.2549	0.2620	0.1901	0.1418
Dissolved Ion concentration in water	C_{wdis}	0.1025	0.0892	0.0964	0.1014	0.0992	0.1050	0.0964
Elimination rate	$k_{e,n}$	0.1103	0.1000	0.1020	0.0993	0.1049	0.1053	0.0948
Elimination rate of dissolved ion	$k_{edis,n}$	0.0000	0.0000	0.1001	0.0931	0.0929	0.0942	0.0933

ENM concentration in sediment	C_{sed}	0.1035	0.0943	0.1070	0.2704	0.2695	0.1110	0.0982
ENM concentration in suspended sediment	C_{ss}	0.0922	0.0935	0.2958	0.1045	0.0965	0.2076	0.1402
ENM concentration in water	C_w	0.1818	0.2107	0.0941	0.0982	0.1145	0.1079	0.0984
Ingestion rate	$k_{d,n}$	0.0000	0.0000	0.0899	0.0895	0.0905	0.2028	0.1550
Lifespan	L_n	0.4295	0.3431	0.1343	0.1070	0.1073	0.0976	0.1006
Uptake by water	$k_{u1,n}$	0.2065	0.2100	0.0913	0.1062	0.1005	0.0966	0.0911
Uptake of dissolved ion	$k_{u3,n}$	0.0802	0.0968	0.1043	0.1046	0.1049	0.1012	0.0953
Uptake of solids	$k_{u2,n}$	0.0000	0.0000	0.2845	0.2542	0.2588	0.0000	0.0000
Wet body mass of individual organism	M_i	0.1056	0.0943	0.0927	0.0994	0.1114	0.0930	0.0973
Zn^{2+}								
Definition	Parameter	S. capricornutum	F. crotonensis	D. magna	H. azteca	V. constricta	P. promelas	O. mykiss
Assimilation efficiency	α_n	0.0000	0.0000	0.0903	0.0980	0.0979	0.1280	0.3308
Biomass density	B_n	0.0993	0.0966	0.0846	0.1071	0.1033	0.1086	0.0939
Dissolution rate	k_{dis}	0.1427	0.1507	0.1347	0.1053	0.1062	0.0991	0.0979
Dissolved Ion concentration in water	C_{wdis}	0.1036	0.0928	0.1036	0.2591	0.0990	0.2469	0.1011
Elimination rate	$k_{e,n}$	0.1097	0.1025	0.0967	0.0920	0.0941	0.0932	0.0967
Elimination rate of dissolved ion	$k_{edis,n}$	0.0000	0.0000	0.1616	0.1249	0.2523	0.1995	0.1373
ENM concentration in sediment	C_{sed}	0.1020	0.0945	0.1032	0.1047	0.2735	0.1088	0.0972
ENM concentration in suspended sediment	C_{ss}	0.0928	0.0941	0.2650	0.1110	0.0992	0.1451	0.1511
ENM concentration in water	C_w	0.1449	0.1658	0.0953	0.0942	0.1078	0.0958	0.1013
Ingestion rate	$k_{d,n}$	0.0000	0.0000	0.0873	0.1062	0.0880	0.1429	0.1591
Lifespan	L_n	0.4786	0.4130	0.1980	0.2177	0.0898	0.1553	0.1111
Uptake by water	$k_{u1,n}$	0.1597	0.1565	0.0940	0.0978	0.1065	0.0905	0.0963
Uptake of dissolved ion	$k_{u3,n}$	0.0815	0.0947	0.1044	0.2875	0.0886	0.2200	0.0949
Uptake of solids	$k_{u2,n}$	0.0000	0.0000	0.2472	0.0981	0.2578	0.0000	0.0000
Wet body mass of individual organism	M_i	0.1054	0.0932	0.1003	0.1003	0.1086	0.0979	0.0960

Visual MINTEQ simulation

The Visual MINTEQ model was used to predict the equilibrium concentration of free metal ion (Cu^{2+} or Zn^{2+}) in the various compartments. For the freshwater compartment, the details are presented in Table S10 – S12, since this is most relevant for the analysis presented for a freshwater aquatic food chain. To setup the Visual MINTEQ model, the composition of freshwater is presented in Table S10. The chemical species and solid phases considered for the Cu and Zn systems are presented in Table S10, as well as the equilibrium distribution at an initial concentration of 4.4E-06 M for zincite (ZnO) and 4.5E-06 M for tenorite (CuO). The solubility equilibrium constants (Kso) was adjusted to reflect particle size via the surface area. Table S12 presents the fraction of dissolved metal ion (Cu^{2+} or Zn^{2+}) in this freshwater system at different initial concentrations of CuO or ZnO. The fraction of dissolved metal ion decreases markedly as the initial concentrations increase. These responses were then built into the nanoFate model to predict the available concentration of nanoCuO and free Cu^{2+}, or nanoZnO and free Zn^{2+}.

Table S11. Freshwater composition considered in MINTEQ

pH	7.63	
IS	1.84E-02	equiv/kg
HCO_3^-	3.30E-03	mol/kg
TOC	1.64E-04	mol/kg
Al	4.74E-05	mol/kg
As (V)	0.00E+00	mol/kg
B	3.42E-05	mol/kg
Ba	0.00E+00	mol/kg
Ca^{2+}	2.76E-03	mol/kg
Cl-	3.53E-03	mol/kg
Fe	0.00E+00	mol/kg
I	0.00E+00	mol/kg
K+	7.95E-05	mol/kg
Li	4.32E-06	mol/kg
Mn^{2+}	0.00E+00	mol/kg
Mg^{2+}	1.40E-03	mol/kg
Na^+	2.18E-03	mol/kg
NO_3-	7.01E-05	mol/kg
NO_2-	0.00E+00	mol/kg
PO_4^{3-}	5.90E-06	mol/kg

Table S12. Cu and Zn speciation considered in MINTEQ

% of total concentration	Species name	% of total concentration	Species name
0.944	Cu^{+2}	38.608	Zn^{+2}
0.235	Cu DOM1	0.383	Zn DOM1
4.298	$CuOH^{+}$	5.558	$ZnOH^{+}$
0.014	$Cu(OH)_3^{-}$	13.115	$Zn(OH)_2$ (aq)
1.48	$Cu(OH)_2$ (aq)	0.01	$Zn(OH)_3^{-}$
0.019	$Cu_2(OH)_2^{+2}$	0.228	$ZnCl^{+}$
0.159	$CuSO_4$ (aq)	6.192	$ZnSO_4$ (aq)
0.013	$CuHPO_4$ (aq)	0.116	$Zn(SO_4)_2^{-2}$
82.906	$CuCO_3$ (aq)	0.084	$ZnHPO_4$ (aq)
0.102	$CuHCO_3^{+}$	33.11	ZnCO3 (aq)
9.804	$Cu(CO3)_2^{-2}$	2.084	$ZnHCO_3^{+}$
0.022	$CuH_2BO_3^{+}$	0.504	$Zn(CO3)_2^{-2}$

Table S13. Fraction of dissolved Cu^{2+} or Zn^{2+} in freshwater as calculated using MINTEQ and the freshwater composition from Table S10

Cu^{2+} Concentration kg/m^3	Molality	% Dissolved	Zn^{2+} Concentration kg/m^3	Molality	% Dissolved
3.57E-05	4.49E-07	100.000%	3.57E-04	4.39E-06	100.000%
3.57E-04	4.49E-06	27.287%	3.57E-03	4.39E-05	37.468%
3.57E-03	4.49E-05	2.792%	3.57E-02	4.39E-04	3.747%
3.57E-02	4.49E-04	0.273%	3.57E-01	4.39E-03	0.375%
1.00E-01	1.26E-03	0.097%	4.88E-01	6.00E-03	0.274%
2.00E-01	2.51E-03	0.049%	5.70E-01	7.00E-03	0.235%
			6.10E-01	7.50E-03	0.219%

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