Supplementary Materials

Using a multimedia aquivalence model to evaluate the environmental fate of Fe, Mn and trace metals in an industrial city, China

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Table S1 The descriptive statistics of observed concentration of metals in multimedia in Nanjing

	ng/m³	Fe	Mn	Zn	Cr	Ni	Cu	Pb	Cd	Reference data source
Atmosphere PM2.5	AM	492.36	48.34	287.92	15.59	9.37	65.80	140.55	2.91	(Kong et al., 2015; Li et al., 2016; Ming et al., 2017; Zheng et al., 2019)
	N	30	25	30	30	30	30	30	25	
	SD	398.44	31.68	196.14	11.33	6.51	48.45	117.69	2.09	
	Median	444.50	47.00	244.50	12.50	7.60	63.35	107.50	2.84	
	Min	0.36	1.30	1.30	1.30	1.30	1.30	1.00	0.22	
	Max	1100.00	115.00	824.00	39.80	25.20	176.00	427.00	7.86	
	GM	123.58	33.58	183.22	10.97	7.13	42.04	84.45	2.17	
River water	μg/L	Fe	Mn	Zn	Cr	Ni	Cu	Pb	Cd	(Wu et al., 2009; Cai et al., 2016)
	AM	67.25	6.17	43.15	5.94	14.43	20.01	22.00	0.83	
	N	43	3	43	43	3	43	43	43	
	SD	59.77	2.35	21.69	4.46	9.39	9.32	111.62	1.20	
	Median	49.00	5.40	42.00	5.10	13.40	21.00	2.90	0.40	
	Min	23.00	4.30	7.60	2.10	5.60	4.00	1.50	0.10	
	Max	350.50	8.80	92.00	24.30	24.30	41.00	734.00	6.40	
	GM	54.55	5.89	36.99	5.07	12.22	17.47	3.59	0.52	
Sediment	mg/kg	Fe (%)	Mn	Zn	Cr	Ni	Cu	Pb	Cd	(Huang et al., 2006; Ma et al., 2011; Song et al., 2011; Shen et al., 2014; Yuan et al., 2014; Zhang et al., 2015; Wang et al., 2018)
	AM	6.49	777.38	120.35	78.23	40.20	44.90	38.91	1.72	
	N	14	4	41	41	25	41	41	37	
	SD	4.39	568.30	180.87	42.67	12.73	32.12	34.94	3.50	
	Median	5.77	628.26	95.40	87.68	43.60	43.60	27.30	0.37	
	Min	2.11	301.00	0.24	0.01	6.40	0.25	0.35	0.03	
	Max	20.70	1552.00	1191.79	161.30	63.70	139.81	173.20	16.45	
	GM	5.65	634.05	63.08	36.00	37.20	28.96	25.01	0.57	
SPM	mg/kg	Fe (%)	Mn	Zn	Cr	Ni	Cu	Pb	Cd	(Hua et al., 2011; Yuan et al., 2011; Ma et al., 2011)
	AM	7.25	958.40	196.96	109.95	56.06	81.87	66.49	127.68	
	N	12	18	25	25	7	25	25	25	
	SD	2.47	148.41	108.18	35.77	5.76	36.25	29.81	278.06	
	Median	6.40	989.65	172.30	101.00	53.70	70.90	60.30	1.32	
	Min	5.69	512.00	91.90	79.70	50.20	38.10	27.90	0.57	
	Max	14.70	1157.00	658.00	265.00	67.90	205.00	146.00	1145.00	
	GM	6.99	944.99	179.94	106.37	55.82	75.56	61.01	5.36	
Soil	mg/kg	Fe (%)	Mn	Zn	Cr	Ni	Cu	Pb	Cd	(Lu et al., 2003; Yin et al., 2005; Lu et al., 2006; Wang et al., 2006; Wang et al., 2018)
	AM	3.51	646.14	170.42	79.07	35.57	67.91	88.51	0.35	
	N	31	35	65	61	31	65	60	12	
	SD	1.03	178.06	156.58	35.69	9.34	115.65	81.77	0.32	
	Median	3.66	684.70	120.10	81.15	37.70	39.97	63.25	0.28	
	Min	1.31	100.20	41.82	6.89	9.90	12.20	9.83	0.10	
	Max	6.47	927.47	851.70	232.00	54.63	869.40	472.60	1.20	
	GM	3.35	610.02	131.76	69.98	34.03	44.48	63.68	0.26	

Road dust	mg/kg	Fe (%)	Mn	Zn	Cr	Ni	Cu	Pb	Cd	This study
	AM	5.10	678.91	333.12	119.53	45.21	100.75	336.08	0.65	
	N	23	23	23	23	23	23	23	23	
	SD	1.58	128.13	182.96	78.74	16.55	41.51	628.59	0.27	
	Median	4.69	672.74	261.80	104.21	43.33	100.78	103.65	0.57	
	Min	2.85	416.23	84.87	54.70	23.22	19.72	31.99	0.25	
	Max	10.75	947.36	788.60	454.96	90.15	177.65	2626.05	1.48	
	GM	4.92	667.39	289.68	107.20	42.65	90.88	141.64	0.61	

Notes: AM: arithmetic mean; N: the number of data in the references; SD: standard deviation; GM: geometric mean

Table S2 Discharge of heavy metal pollutants

Water			**Air**		
Discharge standard of pollutants (mg/L)	Quantity of wastewater effluent (10^4 L)	Heavy metals discharge （kg/a）	Maximum acceptable emission concentration (mg/m^3)	Industrial waste gas emissions （10^4 m^3）	Heavy metals emissions （kg/a）
3.00E+00*	8.96E+07	268.91	25.00*	6.96E+07	1.74E+07
2.00E+00	8.96E+07	179.28	20.00	6.96E+07	1.39E+07
1.00E+00	8.96E+07	89.64	5.00*	6.96E+07	3.48E+06
1.00E-01	8.96E+07	8.96	5.00	6.96E+07	3.48E+06
5.00E-02	8.96E+07	4.48	4.30	6.96E+07	2.99E+06
5.00E-01	8.96E+07	44.82	5.00*	6.96E+07	3.48E+06
1.00E-01	8.96E+07	8.96	0.70	6.96E+07	4.87E+05
1.00E-02	8.96E+07	0.90	0.85	6.96E+07	5.92E+05

Sources: Discharge standard of pollutants for municipal wastewater treatment plant (GB 18918-2002); and Nanjing statistical bureau, 2012; and Air pollutant release standard. The asterisk* was self-defined.

Table S3 Summary of partition coefficients used in the model.

Element	Molar mass (g/mol)	LogK$_r$ (L/kg)	Log K$_{so}$ (L/kg)	Log K$_{se}$ (L/kg)	Log K$_p$ (L/kg)
Fe	55.845	5.97	5.22	5.64	5.80
Mn	54.94	4.47	3.08	4.79	5.00
Zn	65.409	4.68	3.86	3.65	4.30
Cr	51.996	4.00	4.65	3.42	4.41
Ni	58.69	4.34	4.19	3.76	3.90
Cu	63.546	4.23	3.54	3.82	4.10
Pb	207.2	5.61	4.04	4.04	5.20
Cd	112.41	5.03	2.97	2.98	4.15

MATLAB Live Script

Z value —fugacity capacities

```
K1=table2array(K)
%
```

Fe	**630957.3**	**436515.8**	**165958.7**	**933254.3**
Mn	100000	61659.5	1202.264	29512.09
Zn	19952.62	4466.836	7244.36	47863.01
Cr	25703.96	2630.268	44668.36	10000
Ni	7943.282	5754.399	15488.17	21877.62
Cu	12589.25	6606.934	3467.369	16982.44
Pb	158489.3	10964.78	10964.78	407380.3
Cd	14125.38	954.9926	933.2543	107151.9

```
Z=double(K1)
Z_Air=1*10^(-6)
Z_water=1
Z_particle=Z(:,2)
Z_sediment=Z(:,3)
Z_soil=Z(:,4)
Z_roaddust=Z(:,5)
Z_aerosol=10^8
Z1=Z_Air.*(1-v13)+Z_aerosol.*v13          % Bulk air (dimensionless)
Z2=Z_water*(1-v23)+Z_particle*v23          % Bulk water (dimensionless)
Z3=Z_Air*v31+Z_water*v32+Z_soil*v33        % Bulk soil (dimensionless)
Z4=Z_water*(1-v43)+Z_sediment*v43          % Bulk sediment (dimensionless)
```

Parameters

```
% The area of each environmental compartment in Nanjing, unit: m^2
A_air=6412.81*10^6      % Surface area of air
```

```
A_water=7.42E+08       % Surface area of water
A_soil=3.08E+09        % Surface area of urban soil
A_road=2.10E+09        % Road surface area
% Transport parameters
I_R=1107               % Annual precipitation（mm）
G_Rain=I_R/1000/(365*24)       % Raining rate (m/h)
G_DD=10.8              % Dry deposition velocity of solids in air (m/h)
Q02=2.90E-02           % water advection flow rate into Nanjing(m3/h)
G_v=0.0000744            % Evaporation rate (m/h)
Q20=Q02+A_water*G_Rain-A_water*G_v
                       % water flow out of Nanjing (m3/h)
V_P=2.08*10^(-7)       % Volume fraction of water particle
V_Q=15*10^(-12)        % Volume fraction of aerosols
v13=3.00*10^(-11)      % Volume fraction of solids in air
v23=2.70*10^(-3)       % Volume fraction of solids in water
v31=2.00*10^(-1)       % Volume fraction of air in soil
v32=3.00*10^(-1)       % Volume fraction of water in soil
v33=5.00*10^(-1)       % Volume fraction of solids in soil
v43=7.00*10^(-1)       % Volume fraction of solids in sediment
p13=1.5                % Density of solids in air (t/m3)
p23=1.25               % Density of solids in water (t/m3)
p33=2.49               % Density of solids in soil (t/m3)
p43=2.49               % Density of solids in sediment (t/m3)
p53=1.80               % Density of solids in road dust (t/m3)

G_WW=4.41*10^(-5)      % Water runoff rate from soil (m/h)
G_SW=2.30*10^(-8)      % Soil Loss rate from soil (m/h)
G_SD=3.42*10^(-6)      % Sediment deposition rate (m/h)
G_RS=1.1*10^(-8)       % Sediment resuspension rate (m/h)
G_SB=3.4*10^(-8)       % Sediment burial rate (m/h)
G_LS=3.9*10^(-5)       % Leaching rate (soil to ground water) (m/h)
G_ST=0.01              % Diffusion rate to stratosphere (m/h)
G_RR=G_Rain*0.9        % Road runoff (m/h)
G_DW =G_RR*10^(-4)     % Road dust washoff (m/h)

kAW=3                  % Air side mass transfer coefficient over water (m/h)
kWA=0.03               % Water side mass transfer coefficient over air (m/h)
kAS=1                  % Air side mass transfer coefficient over soil (m/h)
kSA=0.02               % Soil side mass transfer coefficient over air (m/h)
kAR=46.5               % Air side mass transfer coefficient over road dust (m/h)
kT=4*10^(-4)           % Sediment-water diffusion mass transfer coefficient (m/h)
k24=2*10^(-2)          % Water side mass transfer coefficient over sediment (m/h)
Q=200000               % Scavenging ratio
Y3=5*10^(-2)           % Diffusion path length in soil (m)
```

```
Y4=5*10^(-3)            % Diffusion path length in sediment (m)
B1=4*10^(-2)            % Molecular diffusion coefficient in air (m2/h)
B2=4*10^(-6)            % Moleculat diffusion coefficient in water (m2/h)
B4=2.49*10^(-6)         % Molecular diffusion coefficient in sediment pore water (m2/h)
```

D values

```
D2R=A_water.*Z_water.*G_Rain
% Air to water for wet gas deposition
D2W=A_water.*Z_aerosol.*G_Rain.*Q.*v13
% Air to water for wet particle deposition
D2D=A_water.*Z_aerosol.*G_DD.*v13
% Air to water for Dry particle deposition
D21B=1./(1./(kAW.*A_water.*Z_Air)+1./(kWA.*A_water.*Z_water))
% Diffusion for Air-water
D12B=D21B
D3R=A_soil.*Z_water.*G_Rain
% Air to soil for wet gas deposition
D3W=A_soil.*Z_aerosol.*G_Rain.*Q.*v13
% Air to soil for wet particle deposition
D3D=A_soil.*Z_aerosol.*G_DD.*v13
% Air to soil for dry particle deposition
D13B=1./(1./(kAS.*A_soil.*Z_Air)+Y3./(A_soil.*(B1.*Z_Air+B2.*Z_water))) % Diffusion for Air-soil
D31B=D13B
DRL=A_soil.*Z_water.* G_WW              % Soil run-off
D3L=A_soil.*Z_soil.*G_SW                % Soil erosion
D24I=A_water.*Z_particle.*G_SD          % Water particle deposition
DRS=A_water.*Z_sediment.*G_RS.*v43      % Sediment resuspension
D42B=1/(1/(k24*A_water*Z_water)+Y4/(B4*A_water*Z_water))
% Diffusion between sediment and water
D24B=D42B
D5R=A_road.*Z_water.*G_Rain
% Air to road for wet gas deposition
D5W=A_road.*Z_aerosol.*G_Rain.*Q.*v13
% Air to road for wet particle deposition
D5D=A_road.*Z_aerosol.*G_DD.*v13
% Air to road for dry particle deposition
D15B=1./(1./(kAR.*A_road.*Z_Air))       % Diffusion for Air-road dust
D51B=D15B
D52R=A_road.*Z_water.*G_RR              % road runoff
D52D=A_road.*Z_roaddust.*159./(1.8*10^6)./(365*24)   % road dust runoff
DSB=A_water.*Z_sediment.*G_SB           % Sediment burial
DLS=A_soil.*Z_water.*G_LS               % Soil leaching to groudwater
DST=A_air.*Z_Air.*G_ST                  % Diffusion to stratosphere
D_water=[268.91 179.28 89.64 8.96 4.48 44.82 8.96 0.90]'
%Discharge to water (kg/a)
```

```
D_air=[1.74E+07 1.39E+07 3.48E+06 3.48E+06 2.99E+06 3.48E+06 4.87E+05 5.92E+05]'   % Discharge to air (kg/a)
M=[55.845 54.94 65.409 51.996 58.69 63.546 207.2 112.41]'
% Molar mass (g/mol)
E_water=D_water.*1000./M./(365*24)
% Heavy metals emissions to water (mol/h)
E_air=D_air.*1000./M./(365*24)
% Heavy metals emissions to air (mol/h)
```

The discharge flux of pollutants and the inflow and outflow flux of atmosphere and water

```
Q01=1.08*10^6      % Air advection flow into Nanjing (m³/h)
Q10=Q01            % Air advection flow out of Nanjing (m³/h)
D10V=Q10.*Z1
PM=[492.36 48.34 287.92 12.5 7.13 65.8 107.5 2.17]'
% Atmospheric PM2.5 concentration（ng/m³）
CA=PM./(10^9)./M                % aerosol concentration（mol/m³）
E01V=Q01.*CA                    % Atmospheric flux into Nanjing
RW=[0.23982 0.00617 0.04315 0.00594 0.014443 0.02001 0.0029 0.00083]'
% Concentration of river water into Nanjing（mg/L）
CW=RW./M          % Concentration of river water into Nanjing（mol/m³）
E02V=Q02.*CW                    % water advection input (mol/h)
D20V=Q20.*Z2                    % water advection output
```

Coefficient of system of equations — Factor

```
U=[1 1 1 1 1 1 1 1]'
% Equations for Air
F_Air1=-(D2R+D2W+D2D+D3R+D3W+D3D+D5R+D5W+D5D+D12B+D13B+D15B+D10V+DST).*U
F_Air2=D21B.*U
F_Air3=D31B.*U
F_Air4=0.*U
F_Air5=D51B.*U
F_Aircon=-(E01V+E_air)
% Equations for water
F_water1=(D2R+D2W+D2D+D12B).*U
F_water2=-(D21B+D24I+D24B+D20V)
F_water3=D3L+DRL
F_water4=DRS+D42B
F_water5=D52R+D52D
F_watercon=-(E02V+E_water)
% Equations for Soil
F_soil1=(D3R+D3W+D3D+D13B).*U
F_soil2=0.*U
F_soil3=-(D3L+DRL+D31B+DLS)
F_soil4=0.*U
F_soil5=0.*U
F_soilcon=0.*U
```

```
% Equations for Sediment
F_sediment1=0.*U
F_sediment2=D24I+D24B
F_sediment3=0.*U
F_sediment4=-(D42B+DRS+DSB)
F_sediment5=0.*U
F_sedimentcon=0.*U
% Equations for Road dust
F_road1=(D15B+D5R+D5W+D5D).*U
F_road2=0.*U
F_road3=0.*U
F_road4=0.*U
F_road5=-(D51B+D52R+D52D)
F_roadcon=0.*U
```

Establishment and solution of system of equations

```
% Fe
for i=1:8
A=[F_Air1(i) F_Air2(i) F_Air3(i) F_Air4(i) F_Air5(i);
    F_water1(i) F_water2(i) F_water3(i) F_water4(i) F_water5(i);
    F_soil1(i) F_soil2(i) F_soil3(i) F_soil4(i) F_soil5(i);
    F_sediment1(i) F_sediment2(i) F_sediment3(i) F_sediment4(i) F_sediment5(i);
    F_road1(i) F_road2(i) F_road3(i) F_road4(i) F_road5(i)]
B=[F_Aircon(i);F_watercon(i);F_soilcon(i);F_sedimentcon(i);F_roadcon(i)]
% X=A\B means the solution to the equation AX=B
if i==1
    X_Fe=A\B
elseif i==2
    X_Mn=A\B
elseif i==3
    X_Zn=A\B
elseif i==4
    X_Cr=A\B
elseif i==5
    X_Ni=A\B
elseif i==6
    X_Cu=A\B
elseif i==7
    X_Pb=A\B
elseif i==8
    X_Cd=A\B
end
end
X=[X_Fe X_Mn X_Zn X_Cr X_Ni X_Cu X_Pb X_Cd]
Q1=X(1,:)'                          % Aquivalence for air (mol/m^3)
```

```
Q2=X(2,:)'                % Aquivalence for water (mol/m3)
Q3=X(3,:)'                % Aquivalence for soil (mol/m3)
Q4=X(4,:)'                % Aquivalence for sediment (mol/m3)
Q5=X(5,:)'                % Aquivalence for road dust (mol/m3)

C1=Q1.*Z1                 % Molar concentration of metals for air (mol/m3)
C2=Q2.*Z2                 % Molar concentration of metals for water (mol/m3)
C2p=Q2.*Z_particle         % Molar concentration of metals for particle (mol/m3)
C3=Q3.*Z3                 % Molar concentration of metals for soil (mol/m3)
C4=Q4.*Z4                 % Molar concentration of metals for sediment (mol/m3)
C5=Q5.*Z_roaddust         % Molar concentration of metals for road dust (mol/m3)

Bwmass=[215.5 19.31 4.18 0.9 0.61 1.26 0.71 0.019]'
% Background values of elements in river water of Yangtze river system（μg/L)
Bwmol=Bwmass./1000000./M.*1000
% Background values of elements in river water（mol/m3）
C2mol=C2+Bwmol            % Total molar concentration of metals for water

Bsmass=[30200 585 62.6 77.8 26.7 22.3 26.2 0.126]' % Soil background value（mg/kg）
Bsmol=Bsmass./1000./M./(1/1000/p33)
Brmol=Bsmass./1000./M./(1/1000/p53)
C3mol=C3+Bsmol            % Total molar concentration of metals for soil
C4mol=C4+Bsmol            % Total molar concentration of metals for sediment
C5mol=C5+Brmol            % Total molar concentration of metals for road dust
```

Notes: Subscript are defined as follows: 1: air; 2: water; 3: soil; 4: sediment; 5: road dust

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