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Reactive Transport Modelling of the Long-Term Interaction between Carbon Steel and MX-80 Bentonite at 25 °C

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Supplementary material

Table S1. Log K at 25 °C and stoichiometric coefficients of homogeneous reactions.

Reaction	log K	Primary species												
		Ca^{2+}	Mg^{2+}	Na^{+}	K^{+}	Fe^{2+}	Cl^{-}	HCO_3^{-}	SO_4^{2-}	$SiO_2(aq)$	$Al(OH)_4^{-}$	$O_2(aq)$	H^{+}	X^{-}
OH^{-}	13.9878	0	0	0	0	0	0	0	0	0	0	0	-1	0
CO_3^{2-}	10.3240	0	0	0	0	0	0	1	0	0	0	0	-1	0
$CaCO_3(aq)$	7.0069	1	0	0	0	0	0	1	0	0	0	0	-1	0
$CaSO_4(aq)$	-2.1007	1	0	0	0	0	0	0	1	0	0	0	0	0
$CaOH^{+}$	12.8484	1	0	0	0	0	0	0	0	0	0	0	-1	0
$CaCl^{+}$	0.7003	1	0	0	0	0	1	0	0	0	0	0	0	0
$CaHCO_3^{+}$	-1.0430	1	0	0	0	0	0	1	0	0	0	0	0	0
$CaCl_2(aq)$	0.6538	1	0	0	0	0	2	0	0	0	0	0	0	0
$CaH_3SiO_4^{+}$	8.7916	1	0	0	0	0	0	0	0	1	0	0	-1	0
$MgCO_3(aq)$	7.3548	0	1	0	0	0	0	1	0	0	0	0	-1	0
$MgHCO_3^{+}$	-1.0330	0	1	0	0	0	0	1	0	0	0	0	0	0
$MgSO_4(aq)$	-2.3833	0	1	0	0	0	0	0	1	0	0	0	0	0
$MgOH^{+}$	11.7778	0	1	0	0	0	0	0	0	0	0	0	-1	0
$MgCl^{+}$	0.1387	0	1	0	0	0	1	0	0	0	0	0	0	0
$MgH_3SiO_4^{+}$	8.5416	0	1	0	0	0	0	0	0	1	0	0	-1	0
$NaOH(aq)$	14.7955	0	0	1	0	0	0	0	0	0	0	0	-1	0
$NaCO_3^{-}$	9.8160	0	0	1	0	0	0	1	0	0	0	0	-1	0
$NaHCO_3(aq)$	-0.1549	0	0	1	0	0	0	1	0	0	0	0	0	0
$NaCl(aq)$	0.7818	0	0	1	0	0	1	0	0	0	0	0	0	0
$NaSO_4^{-}$	-0.8120	0	0	1	0	0	0	0	1	0	0	0	0	0
$CO_2(aq)$	-6.3409	0	0	0	0	0	0	1	0	0	0	0	1	0

Table S2. Log K at 25 °C and stoichiometric coefficients of homogeneous reactions.

Reaction	log K	Primary species												
		Ca^{2+}	Mg^{2+}	Na^{+}	K^{+}	Fe^{2+}	Cl^{-}	HCO_3^{-}	SO_4^{2-}	$SiO_2(aq)$	$Al(OH)_4^{-}$	$O_2(aq)$	H^{+}	X^{-}
Fe^{3+}	-8.4837	0	0	0	0	1	0	0	0	0	0	0.25	1	0
$FeHCO^{+3}$	-2.0423	0	0	0	0	1	0	1	0	0	0	0	0	0
$FeCO_3(aq)$	5.5306	0	0	0	0	1	0	1	0	0	0	0	-1	0
$FeCl^{+}$	0.1648	0	0	0	0	1	1	0	0	0	0	0	0	0
$FeCl^{2+}$	-7.6712	0	0	0	0	1	1	0	0	0	0	0.25	1	0
$FeCl_2(aq)$	2.4632	0	0	0	0	1	2	0	0	0	0	0	0	0
$FeOH^{+}$	9.6327	0	0	0	0	1	0	0	0	0	0	0	-1	0
$FeOH^{2+}$	-6.2937	0	0	0	0	1	0	0	0	0	0	0.25	0	0
$Fe(OH)_2(aq)$	20.5884	0	0	0	0	1	0	0	0	0	0	0	-2	0
$Fe(OH)_3(aq)$	3.6487	0	0	0	0	1	0	0	0	0	0	0.25	-2	0
$Fe(OH)_4^{-}$	13.1166	0	0	0	0	1	0	0	0	0	0	0.25	-3	0
$Fe(OH)_2^{+}$	-2.5888	0	0	0	0	1	0	0	0	0	0	0.25	-1	0
$Fe(SO_4)_2^{-}$	-11.7305	0	0	0	0	1	0	0	2	0	0	0.25	1	0
$FeSO_4(aq)$	-2.1894	0	0	0	0	1	0	0	1	0	0	0	0	0
$Fe_2(OH)_2^{4+}$	-14.0174	0	0	0	0	2	0	0	0	0	0	0.5	0	0
KOH(aq)	14.4600	0	0	0	1	0	0	0	0	0	0	0	-1	0
KSO_4^{-}	-0.8752	0	0	0	1	0	0	0	1	0	0	0	0	0
KCl(aq)	1.4995	0	0	0	1	0	1	0	0	0	0	0	0	0
HSO_4^{-}	-1.9767	0	0	0	0	0	0	0	1	0	0	0	1	0
HS^{-}	138.2709	0	0	0	0	0	0	0	1	0	0	-2	1	0
$AlOH^{2+}$	-11.5489	0	0	0	0	0	0	0	0	0	1	0	2	0
$Al(OH)_3(aq)$	-5.9897	0	0	0	0	0	0	0	0	0	1	0	1	0
$Al(OH)_2^{+}$	-17.1837	0	0	0	0	0	0	0	0	0	1	0	3	0
Al^{3+}	-22.1372	0	0	0	0	0	0	0	0	0	1	0	4	0

Table S3. Log K at 25 °C and stoichiometric coefficients of mineral reactions.

Reaction	log K	Primary species												
		Ca^{2+}	Mg^{2+}	Na^{+}	K^{+}	Fe^{2+}	Cl^{-}	HCO_3^{-}	SO_4^{2-}	$SiO_2(aq)$	$Al(OH)_4^{-}$	$O_2(aq)$	H^{+}	X^{-}
Iron	59.0116	0	0	0	0	1	0	0	0	0	0	-0.5	-2	0
Montmorillonite	-18.0198	0.02	0.9	0.15	0.2	0.45	0	0	0	3.75	1.25	0.04	-1.84	0
Quartz	-4.0037	0	0	0	0	0	0	0	0	1	0	0	0	0
Calcite	1.8527	1	0	0	0	0	0	1	0	0	0	0	-1	0
Illite	-41.9211	0	0.25	0	0.6	0	0	0	0	3.5	2.3	0	1.2	0
Pyrite	217.3379	0	0	0	0	1	0	0	2	0	0	-3.5	2	0
Muscovite	-52.8588	0	0	0	1	0	0	0	0	3	3	0	2	0
Albite	-19.3942	0	0	1	0	0	0	0	0	3	1	0	0	0
Magnetite	-6.5069	0	0	0	0	3	0	0	0	0	0	0.5	-6	0
Siderite	-0.1888	0	0	0	0	1	0	1	0	0	0	0	-1	0
Nontronite-Na	-35.8238	0	0	0.33	0	2	0	0	0	3.67	0.33	0.5	-4	0
Nontronite-Mg	-35.9180	0	0.165	0	0	2	0	0	0	3.67	0.33	0.5	-4	0
Cronstedtite	-0.7260	0	0	0	0	4	0	0	0	1	0	0.5	-8	0
Greenalite	22.6499	0	0	0	0	3	0	0	0	2	0	0	-6	0

Table S4. Log K at 25 °C and stoichiometric coefficients of cation exchange reactions.

Reaction	log K	Primary species											
		Ca^{2+}	Mg^{2+}	Na^{+}	K^{+}	Fe^{2+}	Cl^{-}	HCO_3^{-}	SO_4^{2-}	SiO_2(aq)	$Al(OH)_4^{-}$	O_2(aq)	H^{+}	X^{-}
X-Na	0.0	0	0	1	0	0	0	0	0	0	0	0	0	1
X-K	-0.7	0	0	0	1	0	0	0	0	0	0	0	0	1
X2-Ca	-0.8	1	0	0	0	0	0	0	0	0	0	0	0	2
X2-Mg	-0.6	0	1	0	0	0	0	0	0	0	0	0	0	2
X2-Fe	-0.5	0	0	0	0	1	0	0	0	0	0	0	0	2