Table 2. Major chemical reactions used in reactive-transport simulations.

[Modified from Parkhurst and others (2003); *C*, concentration; *k*, rate constant; *SI*, saturation index—log ion activity product divided by the solubility product; *DOC*, dissolved organic carbon; | | indicates absolute value]

Reaction number	Reaction	Reaction type	Equation
1	Phosphorus sorption	Equilibrium	$SiteOH + PO_4^{3-} + 2H^+ = SiteHPO_4^- + H_2O$
2	Phosphorus-sorption site protonation	Equilibrium	$SiteOH + H^+ = SiteOH_2^+$
3	Phosphorus-sorption site deprotonation	Equilibrium	$SiteOH = SiteO^- + H^+$
4	Cation sorption	Equilibrium	$Cation\_siteOH + Cat^{x+} = Cation\_siteOCat^{x-1} + H^+$
5	Cation-sorption site protonation	Equilibrium	$Cation\_siteOH + H^+ = Cation\_siteOH_2^+$
6	Cation-sorption site deprotonation	Equilibrium	$Cation\_siteOH = Cation\_siteO^- + H^+$
7	$Fe(OH)_3$(amorphous)	Equilibrium	$Fe(OH)_3 + 3H^+ = Fe^{+3} + 3H_2O$
8	Pyrolusite	Equilibrium	$MnO_2 + 4H^+ + 2e^- = Mn^{+2} + 2H_2O$
9	Decomposition of dissolved organic carbon (DOC), reactant is CH_2O	Kinetic	$Rate = -kC_{DOC}$
10	Decomposition of sorbed organic carbon, reactant is CH_2O (applies after cessation of wastewater disposal)	Kinetic	$Rate = -k_{O_2}C_{O_{2,\ aq}} - k_{NO_3}C_{NO_{3,\ aq}}$
11	Vivianite precipitation and dissolution, reactant is $Fe_3(PO_4)_2$	Kinetic	$Rate = -kC_{PO_4}\left(\frac{SI_{vivianite}}{1 + \lvert SI_{vivianite}\rvert}\right)$
12	Strengite precipitation and dissolution, reactant is $FePO_4$	Kinetic	$Rate = -kC_{PO_4}\left(\frac{SI_{strengite}}{1 + \lvert SI_{strengite}\rvert}\right)$
13	Removal of dissolved N_2 (prevents N_2 reoxidation to nitrate), reactant is N_2	Kinetic	$Rate = -kC_{N_{2,\ aq}}$