Hydroxyl Radical AOP: Scavenging by NOM, Carbonate and Iron, Half-Life

Share of hydroxyl radicals reacting with a target compound against NOM, bicarbonate, carbonate, Fe(II) and Mn(II), with the half-life and contact time needed.

Input parameters

Unit system: SI

Parameter	Value	Unit
Target rate constant with HO•, L/(mol·s)	4.2000e+09	
Target concentration	100.00	µg/L
Target molar mass	131.39	kg/kmol
NOM as dissolved organic carbon	1.0000	mg/L
NOM rate constant, L/(mol C·s)	3.9000e+08	
Total carbonate	4.0000	mmol/L
pH	8.0000	
Iron(II)	0.50000	mg/L
Manganese(II)	0.10000	mg/L
Hydroxyl radical concentration, mol/L	1.0000e-10	
Target removal	99.000	%

Calculated results

Parameter	Value	Unit
Target concentration, mol/L	7.6109e-07	
Rate of HO• use by the target, 1/s	3,196.6	
HO• scavenging by NOM, 1/s	32,470	
HO• scavenging by carbonate species, 1/s	40,800	
HO• scavenging by Fe(II) and Mn(II), 1/s	3,009.2	
Share of HO• reacting with the target	4.0221	%
Pseudo-first-order rate k_R C_HO•	0.42000	1/s
Half-life of the target	1.6504	s
Time for the target removal (batch or PFR)	0.18274	min

Notes for this case

• Rate constants with HO•: HCO_3^- 8.5 × 10^6, CO_3^{2-} 3.9 × 10^8, Fe(II) 3.3 × 10^8, Mn(II) 3.0 × 10^7 L/(mol·s) (Buxton et al.); carbonate speciation with pK_a 6.3 and 10.3. The half-life assumes a steady HO• concentration; 1/Q_R is the slow-down caused by the scavengers.

Formula and method

$$Q_R = \frac{k_R C_R}{k_R C_R + k_{NOM} C_{DOC} + k_{HCO_3^-} C_{HCO_3^-} + k_{CO_3^{2-}} C_{CO_3^{2-}} + k_{Fe} C_{Fe} + k_{Mn} C_{Mn}}$$

$$t_{1/2} = \frac{\ln 2}{k_R C_{HO\bullet}}, \quad t_X = \frac{-\ln(1-X)}{k_R C_{HO\bullet}}$$

Variables

k_R	Target rate constant with HO•, L/(mol·s)	-
C_R	Target concentration	kg/m³
M_R	Target molar mass	kg/kmol
C_{DOC}	NOM as dissolved organic carbon	kg/m³
k_{NOM}	NOM rate constant, L/(mol C·s)	-
C_{T,CO_3}	Total carbonate	mol/m³
pH	pH	-
$C_{Fe(II)}$	Iron(II)	kg/m³
$C_{Mn(II)}$	Manganese(II)	kg/m³
$C_{HO\bullet}$	Hydroxyl radical concentration, mol/L	-
X	Target removal	-
$k_R C_R$	Rate of HO• use by the target, 1/s	-
$k_{NOM} C_{DOC}$	HO• scavenging by NOM, 1/s	-
$k_{HCO_3}[HCO_3^-] + k_{CO_3}[CO_3^{2-}]$	HO• scavenging by carbonate species, 1/s	-
$k_{Fe} C_{Fe} + k_{Mn} C_{Mn}$	HO• scavenging by Fe(II) and Mn(II), 1/s	-
Q_R	Share of HO• reacting with the target	-
k	Pseudo-first-order rate k_R C_HO•	1/s
$t_{1/2}$	Half-life of the target	s
t_X	Time for the target removal (batch or PFR)	s

Method and standards

Competition kinetics for hydroxyl radicals between the target and background scavengers.

Assumptions and limits

- Second-order kinetics; scavengers in excess and unchanged.

Report details

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This calculator online

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Reopens the calculator with the inputs of this report.