

Table_1_suppl

Simple outcomes from the tool, a set of equations and reactions

Parameters:	Equation/reaction used in the calculation
Radius of influence / Total flow path in model	$\lg R = \frac{k(h^2 - H^2)}{0.733Q} + \lg r$ <p>Where R – radius of influence, k – hydraulic conductivity, h – water table level after the injection, H – water table level before the injection, Q – injection rate, r – radius of well.</p>
Total bulk treatment volume	$V = Am, \text{ where } A = \pi R^2$ <p>Where V – total bulk treatment volume, A – area, R – ROI (radius of influence), m – thickness of polluted layer.</p>
Maximum oxidant concentration	$C_{\max} = M_{ox} * 1000000 / V_{liq} * 1000$ <p>Where C_{max} – maximum concentration of oxidant, M_{ox} – mass of the injected oxidant(real data in kg), V_{liq} – volume of injected liquid in m³.</p>
Mass of porous media	$M = dV$ <p>Where M – mass of porous medium, V – total bulk treatment volume, d – dry bulk density.</p>
Volume of oxidant to be delivered	$V_{ox} = Vn$ <p>Where V_{ox} – volume of oxidant must be delivered, V – total bulk treatment volume, n – porosity.</p>
Dose of oxidant	$D = (C_{\max} V_{ox}) / M$ <p>Where D - dose of oxidant, V_{ox} – volume of oxidant must be delivered, C_{max} – maximum concentration of oxidant, M – mass of porous medium.</p>
Effective porosity, usually 10 to 48% smaller than porosity	$n_e = (0.1 \div 0.48)n$

	<p>Where</p> <p>n_e – effective porosity,</p> <p>n – porosity.</p>
Velocity of water for max effective porosity	$v_{\min} = kI / n_{e\max}, \text{ where } I = \text{delta}H / R$ <p>Where</p> <p>v_{\min} – minimum velocity,</p> <p>I – hydraulic gradient,</p> <p>$\text{delta}H$ – pressure equal $(703,069679 \cdot \text{pressure in psi}) / 1000$,</p> <p>$n_{e\max}$ – maximum effective porosity,</p> <p>k – hydraulic conductivity,</p> <p>R – ROI.</p>
Velocity of water for min effective porosity	$v_{\max} = kI / n_{e\min}, \text{ where } I = \text{delta}H / R$ <p>Where</p> <p>v_{\max} – maximum velocity,</p> <p>I – hydraulic gradient,</p> <p>$\text{delta}H$ – pressure equal $(703,069679 \cdot \text{pressure in psi}) / 1000$,</p> <p>$n_{e\min}$ – minimum effective porosity,</p> <p>k – hydraulic conductivity,</p> <p>R – ROI.</p>
pE of groundwater	$pe = (Eh * 96485) / (2.303 * 8.314 * (283.15 + T))$ <p>Where</p> <p>T – temperature in Celsius degrees,</p> <p>Eh – oxidation-reduction potential in V.</p>
Time of reaching the ROI for max effective porosity	$t_{\max} = R / v_{\min}$ <p>Where</p> <p>t_{\max} – maximum time of reaching ROI,</p> <p>R – ROI,</p> <p>v_{\min} – minimum velocity.</p>
Time of reaching ROI for min effective porosity	$t_{\min} = R / v_{\max}$ <p>Where</p> <p>t_{\min} – minimum time of reaching ROI,</p> <p>R – ROI,</p> <p>v_{\max} – maximum velocity.</p>
Number of wells for max effective porosity	$N_{\min} = V_{ox} / Qt_{\max}$ <p>Where</p> <p>N_{\min} – minimum number of wells,</p> <p>V_{ox} – volume of oxidant must be delivered,</p> <p>Q – injection rate,</p> <p>t_{\max} – maximum time of reaching ROI.</p>
Numbers of wells for min effective porosity	$N_{\max} = V_{ox} / Qt_{\min}$ <p>Where</p>

	N_{\max} – maximum number of wells, V_{ox} – volume of oxidant must be delivered, Q – injection rate, t_{\min} – minimum time of reaching ROI.
Mass of KMnO_4 oxidant needed for calculated amount of pollutant [kg] (stoichiometric ratios):	
Toluene	$\text{C}_7\text{H}_8 + 2\text{H}^+ + 2\text{MnO}_4^- = \text{C}_7\text{H}_6\text{O}_2 + 2\text{MnO}_2 + 2\text{H}_2\text{O}$ $Y_{\text{MnO}_4^-/\text{Toluene}} = (2 \cdot 118.9)/(1 \cdot 92.14) = 2.58 \text{ (mg/mg)}$
Ethylbenzene	$\text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 + 4\text{MnO}_4^- + 4\text{HCl} = \text{C}_6\text{H}_5\text{CO}_2\text{H} + \text{CO}_2 + 4\text{MnO}_2 + 4\text{KCl} + 4\text{H}_2\text{O}$ $Y_{\text{MnO}_4^-/\text{Ethylbenzene}} = (4 \cdot 118.9)/(1 \cdot 106.17) = 4.48 \text{ (mg/mg)}$
Benzene	$\text{C}_6\text{H}_6 + 10\text{MnO}_4^- + 10\text{H}^+ = 10\text{MnO}_2 + 6\text{CO}_2 + 8\text{H}_2\text{O}$ $Y_{\text{MnO}_4^-/\text{Benzene}} = (10 \cdot 118.9)/(1 \cdot 78.11) = 15.22 \text{ (mg/mg)}$
PCE	$3\text{C}_2\text{Cl}_4 + 4\text{MnO}_4^- + 4\text{H}_2\text{O} = 6\text{CO}_2 + 12\text{Cl}^- + 4\text{MnO}_2 + 8\text{H}^+$ $Y_{\text{MnO}_4^-/\text{Pce}} = (4 \cdot 118.9)/(3 \cdot 165.7) = 0.96 \text{ (mg/mg)}$
TCE	$\text{C}_2\text{Cl}_3\text{H} + 2\text{MnO}_4^- = 2\text{CO}_2 + 3\text{Cl}^- + 2\text{MnO}_2 + \text{H}^+$ $Y_{\text{MnO}_4^-/\text{Tce}} = (2 \cdot 118.9)/131.29 = 1.81 \text{ (mg/mg)}$
DCE	$3\text{C}_2\text{Cl}_2\text{H}_2 + 8\text{MnO}_4^- = 2\text{CO}_2 + 3\text{Cl}^- + 2\text{MnO}_2 + \text{H}^+$ $Y_{\text{MnO}_4^-/\text{Dce}} = (8 \cdot 118.9)/(3 \cdot 96.88) = 3.27 \text{ (mg/mg)}$
VC	$3\text{C}_2\text{H}_3\text{Cl} + 10\text{MnO}_4^- = 6\text{CO}_2 + 10\text{MnO}_2 + 7\text{OH}^- + 3\text{Cl}^- + \text{H}_2\text{O}$ $Y_{\text{MnO}_4^-/\text{Vc}} = (10 \cdot 118.9)/(3 \cdot 62.47) = 6.34 \text{ (mg/mg)}$
NOD	$3\text{C}_7\text{H}_8\text{O}_4 + 28\text{MnO}_4^- + 28\text{H}^+ = 21\text{CO}_2 + 28\text{MnO}_2 + 26\text{H}_2\text{O}$ $Y_{\text{MnO}_4^-/\text{NOM}} = (28 \cdot 118.9)/(3 \cdot 156.07) = 7.11 \text{ (mg/mg)}$
TOTAL	Total mass of permanganate used for oxidation of COCs and NOD according to reactions described above