

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, 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, I – hydraulic gradient, $\text{delta}H$ – pressure equal $(703,069679 * \text{pressure in psi}) / 1000$, $n_{e\max}$ – maximum effective porosity, k – hydraulic conductivity, R – ROI.</p>
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pE of groundwater	$pe = (Eh * 96485) / (2.303 * 8.314 * (283.15 + T))$ <p>Where</p> <p>T – temperature in Celsius degrees, 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, R – ROI, v_{\min} – minimum velocity.</p>
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Number of wells for max effective porosity	$N_{\min} = V_{ox} / Qt_{\max}$ <p>Where</p> <p>N_{\min} – minimum number of wells, V_{ox} – volume of oxidant must be delivered, Q – injection rate, t_{\max} – maximum time of reaching ROI.</p>
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	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	$C_7H_8 + 2H^+ + 2 MnO_4^- = C_7H_6O_2 + 2MnO_2 + 2H_2O$ $Y_{MnO_4^-/Toluene} = (2*118.9)/(1*92.14) = 2.58 \text{ (mg/mg)}$
Ethylbenzene	$C_6H_5CH_2CH_3 + 4MnO_4^- + 4HCl = C_6H_5CO_2H + CO_2 + 4MnO_2 + 4KCl + 4H_2O$ $Y_{MnO_4^-/Ethylbenzene} = (4*118.9)/(1*106.17) = 4.48 \text{ (mg/mg)}$
Benzene	$C_6H_6 + 10 MnO_4^- + 10 H^+ = 10 MnO_2 + 6 CO_2 + 8 H_2O$ $Y_{MnO_4^-/Benzene} = (10*118.9)/(1*78.11) = 15.22 \text{ (mg/mg)}$
PCE	$3C_2Cl_4 + 4MnO_4^- + 4H_2O = 6CO_2 + 12Cl^- + 4MnO_2 + 8H^+$ $Y_{MnO_4^-/Pce} = (4*118.9)/(3*165.7) = 0.96 \text{ (mg/mg)}$
TCE	$C_2Cl_3H + 2MnO_4^- = 2CO_2 + 3Cl^- + 2MnO_2 + H^+$ $Y_{MnO_4^-/Tce} = (2*118.9)/131.29 = 1.81 \text{ (mg/mg)}$
DCE	$3C_2Cl_2H_2 + 8MnO_4^- = 2CO_2 + 3Cl^- + 2MnO_2 + H^+$ $Y_{MnO_4^-/Dce} = (8*118.9)/(3*96.88) = 3.27 \text{ (mg/mg)}$
VC	$3C_2H_3Cl + 10MnO_4^- = 6CO_2 + 10MnO_2 + 7OH^- + 3Cl^- + H_2O$ $Y_{MnO_4^-/Vc} = (10*118.9)/(3*62.47) = 6.34 \text{ (mg/mg)}$
NOD	$3C_7H_8O_4 + 28MnO_4^- + 28H^+ = 21CO_2 + 28MnO_2 + 26H_2O$ $Y_{MnO_4^-/NOM} = (28*118.9)/(3*156.07) = 7.11 \text{ (mg/mg)}$
TOTAL	Total mass of permanganate used for oxidation of COCs and NOD according to reactions described above