RegenOx™

Advanced Chemical Oxidation

Thermodynamics and Kinetics

To understand the complete oxidation picture, one must also consider the thermodynamics and the kinetics of the reaction. Thermodynamics tells us the likelihood or potential that a reaction will take place and kinetics tells us how fast it will happen.

Thermodynamics

Voltages are commonly used when comparing chemical oxidants; however, they are typically derived from hydrogen oxidation half-cell reactions, which are both inaccurate (we are not interested in oxidizing hydrogen to water) and incomplete. When interpreting completely balanced equations in terms of the thermodynamics, the relative Gibb's Free Energy is a more valid approach for comparing reactions than voltages based on half-cell reactions alone. Gibb's Free Energy and voltage are linked by the following equation, where E is the voltage, n is the number of electron-equivalents per mole and F is Faraday's constant:

$$E = \frac{-\Delta G}{nF}$$

In Table 1 below, we present data for the comparative oxidation of PCE (C_2Cl_4) rather than hydrogen and use Gibbs Free Energy (ΔG) as a measure of the energy that is available from the reaction. The lower the free energy, the more negative the ΔG and the more likely the reaction will occur. When compared with three other chemical oxidation products in Table 1, RegenOx (which runs under basic conditions) yields the lowest free energy (and highest voltage). This means that the RegenOx reaction is the most favorable oxidation reaction.

Table 1. Comparitive Oxidation of PCE

Chemical Oxidant	Balanced Equation	Gibbs Free Energy (ΔG)
RegenOx™	$C_2Cl_4 + 2\ H_2O_2 + 4\ NaOH \Leftrightarrow 2\ CO_2 + 4\ NaCl + 4\ H_2O$	-338 kcal/mol
Potassium Permanganate	$C_2Cl_4 + 4\ KMnO_4 \Leftrightarrow 2\ CO_2 + 4\ MnO_2 + 4\ KCl + 2\ O_2$	-329 kcal/mol
Potassium Persulfate	$C_2Cl_4 + 2\ K_2S_2O_8 + 4\ H_2O \Leftrightarrow 2\ CO_2 + 4\ KCl + 4\ H_2SO_4$	-271 kcal/mol
Hydrogen Peroxide	$C_2Cl_4 + 2\ H_2O_2 \Leftrightarrow 2\ CO_2 + 4\ HCl$	-261 kcal/mol

Kinetics

The oxidation rates of toluene and PCE were compared (by using average pseudo-first order rate coefficients as measured in laboratory studies) with RegenOx and permanganate. Toluene was most quickly oxidized by RegenOx (Figure 1). RegenOx oxidized PCE at a similar rate as permanganate (Figure 2). RegenOx oxidation is kinetically favorable with a range of environmental contaminants, including chlorinated aliphatics such as PCE and hydrocarbons such as toluene.

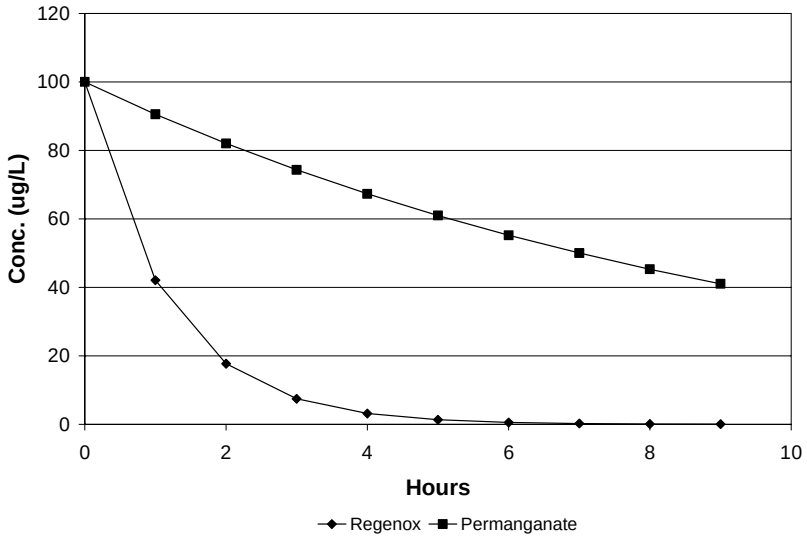

Figure 1. Comparison of Toluene Oxidation

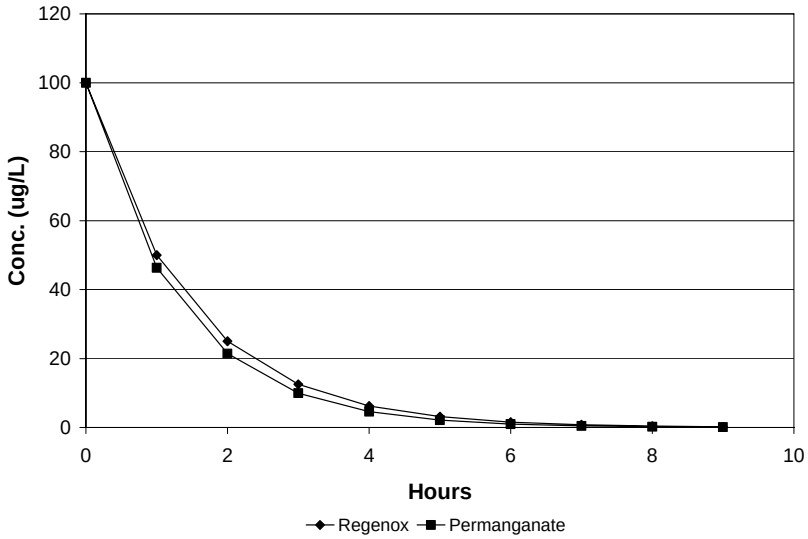

Figure 2. Comparison of PCE Oxidation