

Differential Equations for the Chemical Mechanism - Chlorine

$$O_2 \quad r_1 \quad r_2 \quad r_3 \quad r_4 \quad r_5 \quad r_8$$

$$O_3 \quad r_2 \quad r_3 \quad r_4$$

$$ClO_2 \quad r_6 \quad r_7$$

$$ClOO \quad r_7 \quad r_8$$

$$O \quad 2r_1 \quad r_2 \quad r_3 \quad r_5$$

$$Cl \quad r_4 \quad r_5 \quad r_7 \quad r_8$$

$$ClO \quad r_4 \quad r_5 \quad 2r_6$$

Reaction Expressions

$$r_1 \quad k_1 O_2$$

$$r_2 \quad k_2 O_2 \quad O$$

$$r_3 \quad k_3 O_3$$

$$r_4 \quad k_4 O_3 \quad Cl$$

$$r_5 \quad k_5 O \quad ClO$$

$$r_6 \quad k_6 ClO^2$$

$$r_7 \quad k_7 ClO_2$$

$$r_8 \quad k_8 ClOO$$

Applying a Pseudo-Steady-State Hypothesis

$$Cl \quad r_4 \quad r_5 \quad r_7 \quad r_8 \quad 0$$

$$r_7 \quad r_8 \quad r_4 \quad r_5$$

$$r_4 \quad r_5 \quad k_7 ClO_2 \quad k_8 ClOO$$

$$ClO \quad r_4 \quad r_5 \quad 2r_6 \quad 0$$

$$2r_6 \quad r_4 \quad r_5$$

$$2k_6 ClO^2 \quad k_7 ClO_2 \quad k_8 ClOO$$

$$2k_6 x^2 \quad k_7 ClO_2 \quad k_8 ClOO$$

$$x \quad \sqrt{\frac{k_7 ClO_2 \quad k_8 ClOO}{2k_6}}$$

$$ClO \quad \sqrt{\frac{k_7 ClO_2 \quad k_8 ClOO}{2k_6}}$$

$$O \quad 2r_1 \quad r_2 \quad r_3 \quad r_5$$

$$O \quad 2k_1 O_2 \quad k_2 O_2 \quad O \quad k_3 O_3 \quad k_5 O \quad ClO$$

$$O \quad 2k_1 O_2 \quad k_2 O_2 \quad O \quad k_3 O_3 \quad k_5 O \quad \sqrt{\frac{k_7 ClO_2 \quad k_8 ClOO}{2k_6}}$$

$$2k_1 O_2 \quad k_2 O_2 \quad O \quad k_3 O_3 \quad k_5 O \quad \sqrt{\frac{k_7 ClO_2 \quad k_8 ClOO}{2k_6}} \quad 0$$

$$\begin{array}{l}
2k_1 O_2 \quad k_2 O_2 \quad x \quad k_3 O_3 \quad k_5 x \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \quad 0 \\
2k_1 O_2 \quad k_3 O_3 \quad k_2 O_2 \quad x \quad k_5 x \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \\
2k_1 O_2 \quad k_3 O_3 \quad x \left[k_2 O_2 \quad k_5 \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \right] \\
x \frac{2k_1 O_2 \quad k_3 O_3}{\left[k_2 O_2 \quad k_5 \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \right]} \\
0 \frac{2k_1 O_2 \quad k_3 O_3}{\left[k_2 O_2 \quad k_5 \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \right]}
\end{array}$$

$$\begin{array}{l}
\text{Cl} \quad r_4 \quad r_5 \quad r_7 \quad r_8 \\
\text{Cl} \quad k_4 O_3 \quad \text{Cl} \quad k_5 O \quad \text{ClO} \quad k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO} \quad 0 \\
k_4 O_3 \quad \text{Cl} \quad k_5 O \quad \text{ClO} \quad k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO} \quad 0 \\
k_4 O_3 \quad \text{Cl} \quad k_5 O \quad \text{ClO} \quad k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO} \\
\text{Cl} \quad \frac{k_5 O \quad \text{ClO} \quad k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{k_4 O_3} \\
k_5 \frac{\frac{2k_1 O_2 \quad k_3 O_3}{\left[k_2 O_2 \quad k_5 \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \right]} \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \quad k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{k_4 O_3} \\
\text{Cl} \quad \frac{\frac{2k_1 O_2 \quad k_3 O_3}{\left[k_2 O_2 \quad k_5 \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \right]} \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \quad k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{k_4 O_3}
\end{array}$$

$$\begin{array}{l}
O_2 \quad r_1 \quad r_2 \quad r_3 \quad r_4 \quad r_5 \quad r_8 \\
O_2 \quad k_1 O_2 \quad k_2 O_2 \quad O \quad k_3 O_3 \quad k_4 O_3 \quad \text{Cl} \quad k_5 O \quad \text{ClO} \quad k_8 \text{ ClOO} \\
O_2 \quad -k_1(O_2) - k_2(O_2) \left(\frac{2k_1 O_2 \quad k_3 O_3}{\left[k_2 O_2 \quad k_5 \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \right]} \right) \quad k_3(O_3) \\
k_4(O_3) \left(\frac{k_5 \frac{\frac{2k_1 O_2 \quad k_3 O_3}{\left[k_2 O_2 \quad k_5 \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \right]} \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \quad k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{k_4 O_3}}{k_4 O_3} \right) \\
k_5 \left(\frac{2k_1 O_2 \quad k_3 O_3}{\left[k_2 O_2 \quad k_5 \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \right]} \right) \left(\sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \right) \quad k_8(\text{ClOO})
\end{array}$$

$$\begin{array}{l}
O_3 \quad r_2 \quad r_3 \quad r_4 \\
O_3 \quad k_2(O_2) \left(\frac{2k_1 O_2 \quad k_3 O_3}{\left[k_2 O_2 \quad k_5 \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \right]} \right) - k_3(O_3) \\
-k_4(O_3) \left(\frac{k_5 \frac{\frac{2k_1 O_2 \quad k_3 O_3}{\left[k_2 O_2 \quad k_5 \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \right]} \sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \quad k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{k_4 O_3}}{k_4 O_3} \right)
\end{array}$$

$$\begin{array}{l}
\text{ClO}_2 \quad r_6 \quad r_7 \\
\text{ClO}_2 \quad k_6 \left(\sqrt{\frac{k_7 \text{ ClO}_2 \quad k_8 \text{ ClOO}}{2k_6}} \right)^2 - k_7(\text{ClO}_2)
\end{array}$$

$$\text{ClOO} \quad r_7 \quad r_8$$

$\text{ClOO} \cdot \xrightarrow{k_7} \text{ClO}_2 + \text{ClOO} \cdot \xrightarrow{k_8} \text{ClOO} \cdot$