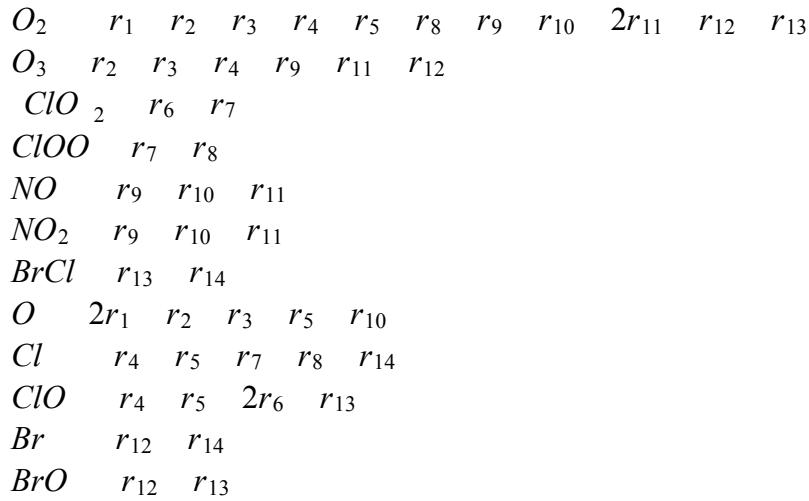
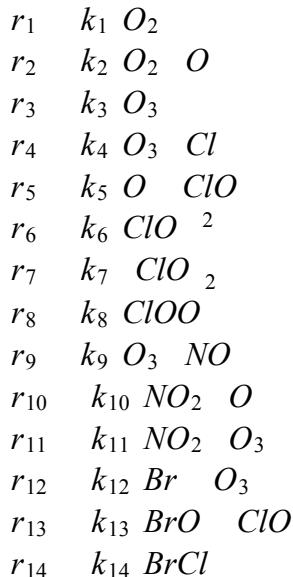


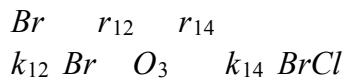
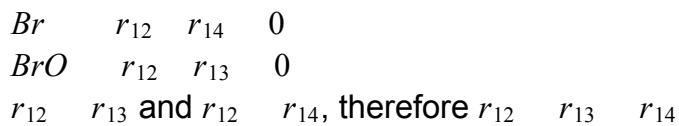
Differential Equations for the Chemical Mechanism



Reaction Expressions



Applying a Pseudo-Steady-State Hypothesis



$$\text{Br} \quad \frac{k_{14} \text{BrCl}}{k_{12} O_3}$$

$$\begin{array}{ccccccccc} BrO & r_{12} & r_{13} & & & & & & \\ k_{12} Br & O_3 & k_{13} BrO & ClO & k_{14} BrCl & & & & \\ \text{BrO} & \frac{k_{14} \text{BrCl}}{k_{13} \sqrt{\frac{k_7 \text{ClO}_2 k_8 \text{ClOO}}{2k_6}}} & & & & & & & \\ Cl & r_4 & r_5 & r_7 & r_8 & r_{14} & 0 & & \\ r_7 & r_8 & r_{14} & r_4 & r_5 & & & & \\ r_4 & r_5 & k_7 \text{ClO}_2 & k_8 \text{ClOO} & k_{14} \text{BrCl} & & & & \end{array}$$

$$\begin{array}{ccccccccc} ClO & r_4 & r_5 & 2r_6 & r_{13} & 0 & & & \\ 2r_6 & r_{13} & r_4 & r_5 & & & & & \\ 2k_6 \text{ClO}_2 & k_{14} \text{BrCl} & k_7 \text{ClO}_2 & k_8 \text{ClOO} & k_{14} \text{BrCl} & & & & \\ 2k_6 x^2 & k_7 \text{ClO}_2 & k_8 \text{ClOO} & & & & & & \\ x & \sqrt{\frac{k_7 \text{ClO}_2 k_8 \text{ClOO}}{2k_6}} & & & & & & & \\ \text{ClO} & \sqrt{\frac{k_7 \text{ClO}_2 k_8 \text{ClOO}}{2k_6}} & & & & & & & \end{array}$$

$$\begin{array}{ccccccccc} O & 2r_1 & r_2 & r_3 & r_5 & r_{10} & & & \\ O & 2k_1 O_2 & k_2 O_2 & O & k_3 O_3 & k_5 O & ClO & k_{10} NO_2 & O \\ O & 2k_1 O_2 & k_2 O_2 & O & k_3 O_3 & k_5 O & \sqrt{\frac{k_7 \text{ClO}_2 k_8 \text{ClOO}}{2k_6}} & k_{10} NO_2 & O \\ 2k_1 O_2 & k_2 O_2 & O & k_3 O_3 & k_5 O & \sqrt{\frac{k_7 \text{ClO}_2 k_8 \text{ClOO}}{2k_6}} & k_{10} NO_2 & O & 0 \\ 2k_1 O_2 & k_2 O_2 & x & k_3 O_3 & k_5 x & \sqrt{\frac{k_7 \text{ClO}_2 k_8 \text{ClOO}}{2k_6}} & k_{10} NO_2 & x & 0 \\ 2k_1 O_2 & k_3 O_3 & k_2 O_2 & x & k_5 x & \sqrt{\frac{k_7 \text{ClO}_2 k_8 \text{ClOO}}{2k_6}} & k_{10} NO_2 & x & \\ 2k_1 O_2 & k_3 O_3 & x \left[k_2 O_2 & k_5 \sqrt{\frac{k_7 \text{ClO}_2 k_8 \text{ClOO}}{2k_6}} & k_{10} NO_2 \right] & & & & & & \\ x & \frac{2k_1 O_2 k_3 O_3}{\left[k_2 O_2 k_5 \sqrt{\frac{k_7 \text{ClO}_2 k_8 \text{ClOO}}{2k_6}} k_{10} NO_2 \right]} & & & & & & & \\ O & \frac{2k_1 O_2 k_3 O_3}{\left[k_2 O_2 k_5 \sqrt{\frac{k_7 \text{ClO}_2 k_8 \text{ClOO}}{2k_6}} k_{10} NO_2 \right]} & & & & & & & \end{array}$$

$$\begin{array}{ccccccccc} Cl & r_4 & r_5 & r_7 & r_8 & r_{14} & & & \\ Cl & k_4 O_3 & Cl & k_5 O & ClO & k_7 \text{ClO}_2 & k_8 \text{ClOO} & k_{14} \text{BrCl} & 0 \\ k_4 O_3 & Cl & k_5 O & ClO & k_7 \text{ClO}_2 & k_8 \text{ClOO} & k_{14} \text{BrCl} & 0 & \\ k_4 O_3 & Cl & k_5 O & ClO & k_7 \text{ClO}_2 & k_8 \text{ClOO} & k_{14} \text{BrCl} & & \\ Cl & \frac{k_5 O \text{ClO}_2 k_7 \text{ClO}_2 k_8 \text{ClOO} k_{14} \text{BrCl}}{k_4 O_3} & & & & & & & \end{array}$$

$$\begin{aligned}
& \text{Cl} \frac{k_5 \frac{2k_1 O_2 k_3 O_3}{\left[k_2 O_2 k_5 \sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} k_{10} NO_2 \right]}}{\frac{k_4 O_3}{\sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} k_7 ClO_2 k_8 ClOO k_{14} BrCl}} \\
& O_2 r_1 r_2 r_3 r_4 r_5 r_8 r_9 r_{10} 2r_{11} r_{12} r_{13} \\
& O_2 k_1 O_2 k_2 O_2 O k_3 O_3 k_4 O_3 Cl k_5 O ClO k_8 ClOO \\
& k_9 O_3 NO k_{10} NO_2 O 2k_{11} NO_2 O_3 k_{12} Br O_3 k_{13} BrO ClO \\
& O_2 -k_1(O_2) -k_2(O_2) \left(\frac{2k_1 O_2 k_3 O_3}{\left[k_2 O_2 k_5 \sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} k_{10} NO_2 \right]} \right) k_3(O_3) \\
& k_4(O_3) \left(\frac{k_5 \frac{2k_1 O_2 k_3 O_3}{\left[k_2 O_2 k_5 \sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} k_{10} NO_2 \right]}}{\frac{k_4 O_3}{\sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} k_7 ClO_2 k_8 ClOO k_{14} BrCl}} \right) \\
& k_5 \left(\frac{2k_1 O_2 k_3 O_3}{\left[k_2 O_2 k_5 \sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} k_{10} NO_2 \right]} \right) \left(\sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} k_8(ClOO) k_9(O_3)(NO) \right. \\
& \left. k_{10}(NO_2) \left(\frac{2k_1 O_2 k_3 O_3}{\left[k_2 O_2 k_5 \sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} k_{10} NO_2 \right]} \right) 2k_{11}(NO_2)(O_3) k_{12}\left(\frac{k_{14} BrCl}{k_{12} O_3}\right)(O_3) \right. \\
& \left. k_{13}\left(\frac{k_{14} BrCl}{k_{13} \sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}}}\right) \left(\sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} \right) \right) \\
& O_3 r_2 r_3 r_4 r_9 r_{11} r_{12} \\
& O_3 k_2(O_2) \left(\frac{2k_1 O_2 k_3 O_3}{\left[k_2 O_2 k_5 \sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} k_{10} NO_2 \right]} \right) -k_3(O_3) \\
& -k_4(O_3) \left(\frac{k_5 \frac{2k_1 O_2 k_3 O_3}{\left[k_2 O_2 k_5 \sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} k_{10} NO_2 \right]}}{\frac{k_4 O_3}{\sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} k_7 ClO_2 k_8 ClOO k_{14} BrCl}} \right) \\
& -k_9(O_3)(NO) -k_{11}(NO_2)(O_3) -k_{12}\left(\frac{k_{14} BrCl}{k_{12} O_3}\right)(O_3) \\
& ClO_2 r_6 r_7 \\
& ClO_2 k_6 \left(\sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} \right)^2 -k_7(ClO_2) \\
& ClOO r_7 r_8 \\
& ClOO k_7(ClO_2) -k_8(ClOO) \\
& NO r_9 r_{10} r_{11} \\
& NO -k_9(O_3)(NO) k_{10}(NO_2) \left(\frac{2k_1 O_2 k_3 O_3}{\left[k_2 O_2 k_5 \sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} k_{10} NO_2 \right]} \right) k_{11}(NO_2)(O_3) \\
& NO_2 r_9 r_{10} r_{11} \\
& NO_2 k_9(O_3)(NO) -k_{10}(NO_2) \left(\frac{2k_1 O_2 k_3 O_3}{\left[k_2 O_2 k_5 \sqrt{\frac{k_7 ClO_2 k_8 ClOO}{2k_6}} k_{10} NO_2 \right]} \right) -k_{11}(NO_2)(O_3)
\end{aligned}$$

$$\begin{array}{cccccc}
BrCl & r_{13} & r_{14} \\
BrCl & k_{13} & BrO & ClO & k_{14} & BrCl \\
BrCl & k_{13} & \frac{k_{14} \ BrCl}{k_{13} \ \sqrt{\frac{k_7 \ ClO_2 \ k_8 \ ClOO}{2k_6}}} & \sqrt{\frac{k_7 \ ClO_2 \ k_8 \ ClOO}{2k_6}} & k_{14} & BrCl \\
BrCl & k_{14} & BrCl & k_{14} & BrCl & 0 \\
BrCl & 0
\end{array}$$