

## Supplementary material.

### Numerical procedure for $k_6$ and $k_7$ determination.

From Eqs. 35 and 38:

$$E = 1 + \frac{D_{ClOH}}{D_{H_2S}} \frac{C_{ClOH}}{C_{H_2S}^*} (1-x) + \frac{D_{ClO^-}}{D_{H_2S}} \frac{C_{ClO^-}}{C_{H_2S}^*} \left( 1 - \frac{1 - \frac{1}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} (1-x)}{1 + \frac{5}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} \frac{1-x}{x}} \right) \quad \text{Eq. A. 1}$$

$$\Rightarrow E = 1 + A - Ax + B \left( \frac{-\frac{1}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} x^2 - \frac{2}{3} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} x + \frac{5}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7}}{x \left( 1 - \frac{5}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} \right) + \frac{5}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7}} \right) \quad \text{Eq. A. 2}$$

$$\text{With } A = \frac{D_{ClOH}}{D_{H_2S}} \frac{C_{ClOH}}{C_{H_2S}^*} \text{ and } B = \frac{D_{ClO^-}}{D_{H_2S}} \frac{C_{ClO^-}}{C_{H_2S}^*} \quad \text{Eq. A. 3}$$

$$\Rightarrow x^2 \left( A \left( \frac{5}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} - 1 \right) - \frac{1}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} B \right) + x \left( \left( 1 - \frac{5}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} \right) (1-E) + A \left( 1 - \frac{5}{3} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} \right) - \frac{2}{3} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} B \right) + \frac{5}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} (1+A+B-E) = 0 \quad \text{Eq. A. 4}$$

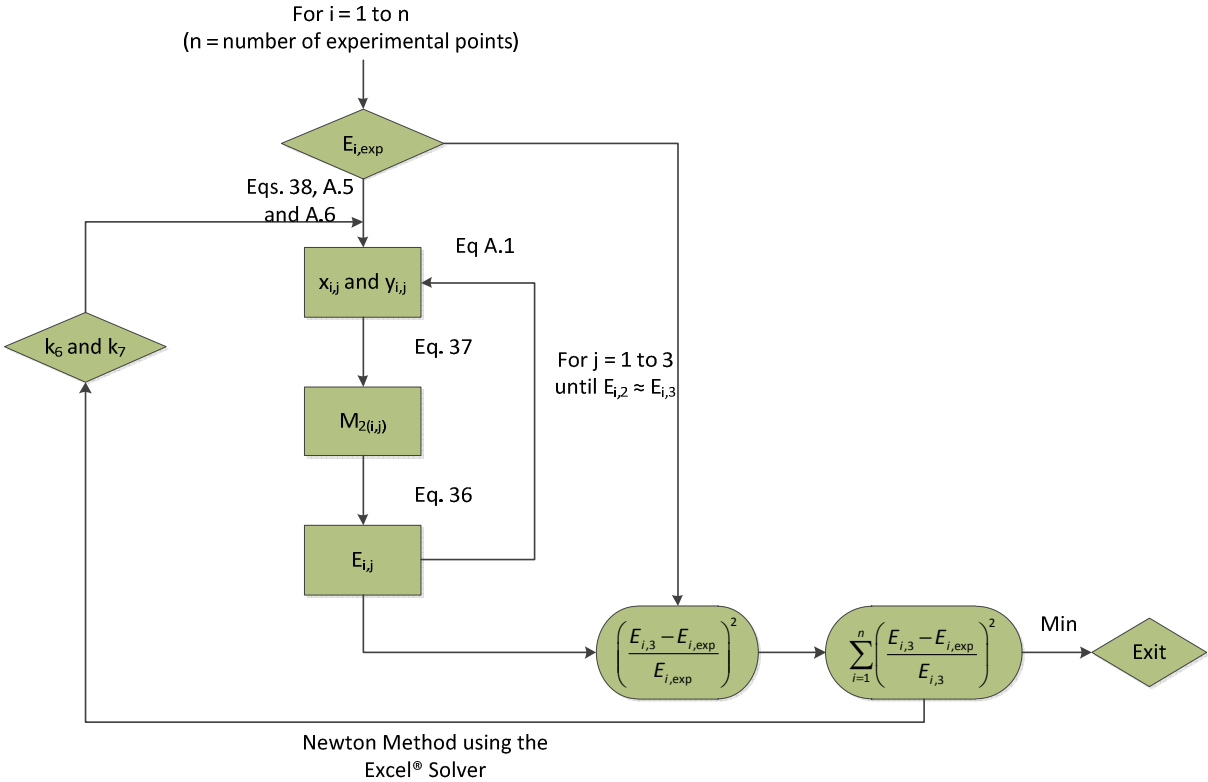
$$\Rightarrow ax^2 + bx + c = 0$$

$$\text{With } \begin{cases} a = A \left( \frac{5}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} - 1 \right) - \frac{1}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} B \\ b = \left( 1 - \frac{5}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} \right) (1-E) + A \left( 1 - \frac{5}{3} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} \right) - \frac{2}{3} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} B \\ c = \frac{5}{6} \frac{D_{ClOH}}{D_{ClO^-}} \frac{k_6}{k_7} (1+A+B-E) \end{cases} \quad \text{Eq. A. 5}$$

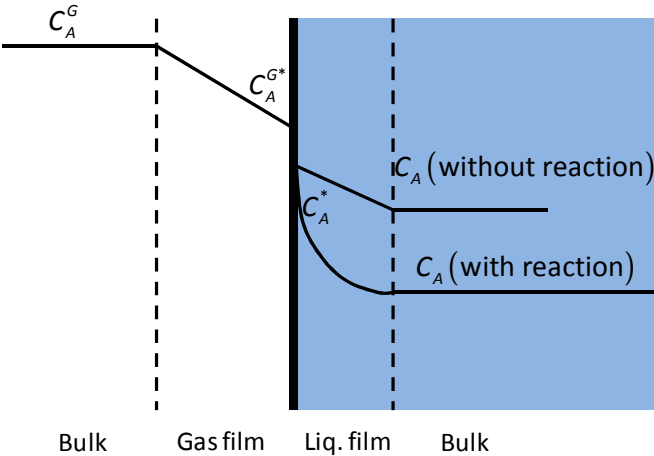
This second degree polynom admits only one possible root to respect the condition  $0 < x < 1$ :

$$\Rightarrow x = \frac{-b - \sqrt{b^2 - 4ac}}{2a} \quad \text{Eq. A. 6}$$

From one experimental value of  $E$  ( $E_{i,exp}$ ), for a given couple ( $k_6 ; k_7$ ),  $x$  and  $y$  can be deduced. An iterative calculation enables to calculate  $E_i$  until convergence (3 iterations of the parameter  $j$  are sufficient). The Excel<sup>®</sup> solver enables to determine the couple ( $k_6 ; k_7$ ) by the least square method using the procedure described by the following figure.



# Gas-liquid transfer and mass balance schemes



Physical absorption :

$$Q_L (C_{A,o} - C_{A,i}) = Q_G (C_{A,i}^G - C_{A,o}^G)$$

Chemical absorption :

$$Q_L (C_{A,o} - C_{A,i}) + \text{Reaction} = Q_G (C_{A,i}^G - C_{A,o}^G)$$

