

$$A_0 = 2 A_1 + A_2 \quad (0)$$

$$A_1 + A_3 = A_5 + A_4 \quad (1)$$

$$A_4 + A_6 = A_7 \quad (2)$$

$$A_7 + A_3 = A_8 + A_4 \quad (3)$$

$$2 A_7 = A_9 + A_{10} \quad (4)$$

$$A_7 + A_{11} = A_8 + A_{12} \quad (5)$$

$$A_7 + A_{12} = A_{13} \quad (6)$$

$$w_0 = k_0 \cdot C_0(t)$$

$$w_1 = k_1 \cdot C_1(t) \cdot C_3(t)$$

$$w_2 = k_2 \cdot C_4(t) \cdot C_6(t)$$

$$w_3 = k_3 \cdot C_7(t) \cdot C_3(t)$$

$$w_4 = 2 k_4 \cdot C_7(t)^2$$

$$w_5 = k_5 \cdot C_7(t) \cdot C_{11}(t)$$

$$w_6 = k_6 \cdot C_7(t) \cdot C_{12}(t)$$

$$k_0 = 10^{-6} - 10^{-4}$$

$$k_1 = 10^7 - 10^9$$

$$k_2 = 10^7 - 10^9$$

$$k_3 = 1 - 10$$

$$k_4 = 10^6 - 10^8$$

$$k_5 = 10^{-6} - 10^{-4}$$

$$k_6 = 0.01 - 100$$

Input data

$Data :=$	$\begin{bmatrix} 0 & 0.043 \\ 140 & 0.042764 \\ 280 & 0.042528 \\ 440 & 0.041938 \\ 560 & 0.041584 \\ 790 & 0.040994 \\ 1030 & 0.039578 \\ 1240 & 0.038988 \\ 1440 & 0.037454 \\ 1570 & 0.03592 \\ 1870 & 0.033442 \\ 2000 & 0.030964 \\ 2200 & 0.02943 \end{bmatrix}$
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$$te := Data^{(0)} \cdot s$$

$$C_{6e} := Data^{(1)} \cdot \frac{\text{mole}}{L}$$

$$t_{end} := \max(te) = 2200 \text{ s}$$

## ODEs solution

$$C_0'(t) = -(k_0 \cdot C_0(t))$$

$$C_1'(t) = 2 \cdot k_0 \cdot C_0(t) - k_1 \cdot C_1(t) \cdot C_3(t)$$

$$C_2'(t) = k_0 \cdot C_0(t)$$

$$C_3'(t) = -(k_1 \cdot C_1(t) \cdot C_3(t)) - k_3 \cdot C_3(t) \cdot C_7(t)$$

$$C_4'(t) = k_1 \cdot C_1(t) \cdot C_3(t) - k_2 \cdot C_4(t) \cdot C_6(t) + k_3 \cdot C_3(t) \cdot C_7(t)$$

$$C_5'(t) = k_1 \cdot C_1(t) \cdot C_3(t)$$

$$C_6'(t) = -(k_2 \cdot C_4(t) \cdot C_6(t))$$

$$C_7'(t) = k_2 \cdot C_4(t) \cdot C_6(t) - 4 \cdot k_4 \cdot C_7(t)^2 - k_3 \cdot C_3(t) \cdot C_7(t) - k_5 \cdot C_7(t) \cdot C_{11}(t) - k_6 \cdot C_7(t) \cdot C_{12}(t)$$

$$C_8'(t) = k_3 \cdot C_3(t) \cdot C_7(t) + k_5 \cdot C_7(t) \cdot C_{11}(t)$$

$$C_9'(t) = 2 \cdot k_4 \cdot C_7(t)^2$$

$$C_{10}'(t) = 2 \cdot k_4 \cdot C_7(t)^2$$

$$C_{11}'(t) = -(k_5 \cdot C_7(t) \cdot C_{11}(t))$$

$$C_{12}'(t) = k_5 \cdot C_7(t) \cdot C_{11}(t) - k_6 \cdot C_7(t) \cdot C_{12}(t)$$

$$C_{13}'(t) = k_6 \cdot C_7(t) \cdot C_{12}(t)$$

$$C_0(0 \mathbf{s}) = 0.013 \quad C_1(0 \mathbf{s}) = 0 \quad C_2(0 \mathbf{s}) = 0 \quad C_3(0 \mathbf{s}) = 11.72 \quad C_4(0 \mathbf{s}) = 0$$

$$C_5(0 \mathbf{s}) = 0 \quad C_6(0 \mathbf{s}) = C_6 e_0 \quad C_7(0 \mathbf{s}) = 0 \quad C_8(0 \mathbf{s}) = 0 \quad C_9(0 \mathbf{s}) = 0 \quad C_{10}(0 \mathbf{s}) = 0$$

$$C_{11}(0 \mathbf{s}) = 0.00007 \quad C_{12}(0 \mathbf{s}) = 0 \quad C_{13}(0 \mathbf{s}) = 0$$

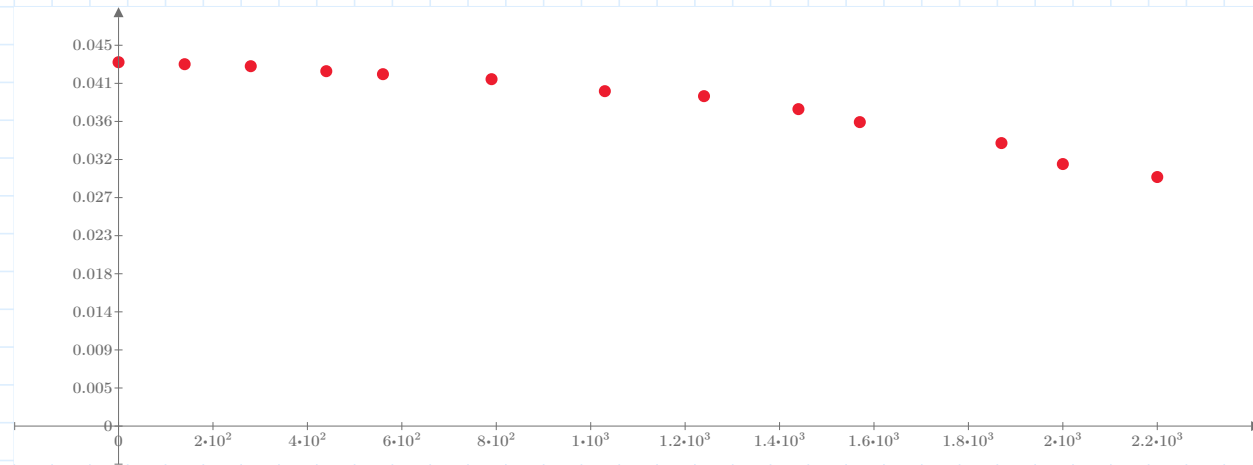
Решатель

$$S(k_0, k_1, k_2, k_3, k_4, k_5, k_6) := \text{odesolve} \left( \begin{array}{c} C_0(t) \\ C_1(t) \\ C_2(t) \\ C_3(t) \\ C_4(t) \\ C_5(t) \\ C_6(t) \\ C_7(t) \\ C_8(t) \\ C_9(t) \\ C_{10}(t) \\ C_{11}(t) \\ C_{12}(t) \\ C_{13}(t) \end{array} \right), t_{end}$$

$$C_6(t, k_0, k_1, k_2, k_3, k_4, k_5, k_6) := \left\| \begin{array}{l} C_6 \leftarrow S(k_0, k_1, k_2, k_3, k_4, k_5, k_6)_6 \\ C_6(t) \end{array} \right\|$$

$$t := 0 \text{ s}, \frac{t_{end}}{300} \dots t_{end}$$

$$\begin{bmatrix} k_0 \\ k_1 \\ k_2 \\ k_3 \\ k_4 \\ k_5 \\ k_6 \end{bmatrix} := \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \cdot \frac{1}{s}$$



$$S(k_0, k_1, k_2, k_3, k_4, k_5, k_6) := \sum_{i=0}^{\text{last}(te)} \left( (C_6(te_i, k_0, k_1, k_2, k_4, k_4, k_5, k_6) - C_6 e_i)^2 \right)$$

$$\begin{bmatrix} k_0 \\ k_1 \\ k_2 \\ k_3 \\ k_4 \\ k_5 \\ k_6 \end{bmatrix} := \text{Minimize } (S, k_0, k_1, k_2, k_3, k_4, k_5, k_6) = ? \frac{1}{s}$$