

The OpenFOAM class for reaction rate called Langmuir-Hinshelwood provided the reaction rate of a reaction with two reactants and a single active site.

The reaction rate is:

$$r = \frac{K_0}{(a + K_1 c_1^{m_1} + K_2 c_2^{m_2})^{m_0}} = \frac{K_0}{b^{m_0}} \quad (1)$$

With

$$K_i = A_i \cdot T^{\beta_i} \exp\left(-\frac{T_{a,i}}{T}\right) \quad (2)$$

$$b = a + K_1 c_1^{m_1} + K_2 c_2^{m_2} \quad (3)$$

Derivative with respect to temperature:

$$\frac{\partial r}{\partial T} = \frac{1}{b^{m_0}} \left(\frac{\partial K_0}{\partial T} - \frac{K_0}{b} m_0 \frac{\partial b}{\partial T} \right) \quad (4)$$

Where:

$$\frac{\partial K_0}{\partial T} = \frac{K_0}{T} \left(\beta_0 + \frac{T_{a,0}}{T} \right) \quad (5)$$

$$\frac{\partial b}{\partial T} = c_1^{m_1} \frac{\partial K_1}{\partial T} + c_2^{m_2} \frac{\partial K_2}{\partial T} \quad (6)$$

Derivative with respect to molar concentration:

$$\frac{\partial r}{\partial c_i} = -\frac{1}{b^{m_0}} \frac{K_0}{b} m_0 \frac{\partial b}{\partial c_i} \quad (7)$$

Where:

$$\frac{\partial b}{\partial c_i} = \frac{m_i K_i c_i^{m_i-1}}{c_i} \quad (8)$$

So, the derivative with respect to molar concentration is:

$$\frac{\partial r}{\partial [c_i]} = -\frac{K_0}{b^{m_0}} \frac{m_0}{b} \cdot \frac{m_i K_i [c_i]^{m_i-1}}{[c_i]} = -k \cdot \frac{m_0}{b} \cdot \frac{\partial b}{\partial c_i} \quad (9)$$