PRACTICAL SESSION 3

EXERCISE 1

$A \longrightarrow$ Products $\qquad r = k C_A^{\,n}$

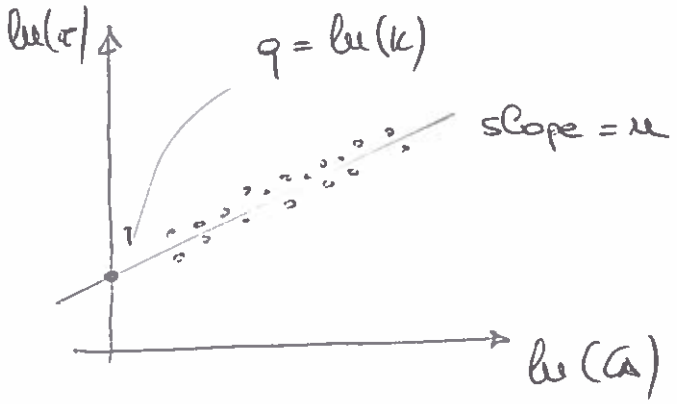
differential method $\qquad \frac{dC_A}{dt} = -r \Rightarrow -\frac{dC_A}{dt} = +kC_A^{\,n}$

$$\ln\left(-\frac{dC_A}{dt}\right) = \ln(kC_A^{\,n}) \Rightarrow \ln\left(-\frac{dC_A}{dt}\right) = \ln k + n \ln C_A$$

$$\ln(r) = \ln(k) + n \ln C_A$$

$$y = a_0 + a_1 x_1$$

$$\begin{cases} y = \ln(r) \\ a_0 = \ln(k) \\ a_1 = n \\ x_1 = \ln(C_A) \end{cases}$$



$$\underline{Y} = \begin{bmatrix} \ln(r) \\ \vdots \end{bmatrix} \qquad \underline{\underline{X}} = \begin{bmatrix} 1 & \ln C_A^{\,0} \\ 1 & \vdots \\ \vdots & \vdots \\ 1 & \end{bmatrix} \Big\} M_{exp}$$

$$\underbrace{\underline{\underline{X}}'\underline{\underline{X}}}_{\underline{\underline{A}}}\,\underline{a} = \underbrace{\underline{\underline{X}}'\underline{Y}}_{\underline{b}} \Rightarrow \underline{\underline{A}}\,\underline{a} = \underline{b} \qquad \begin{cases} \underline{\underline{A}} = \underline{\underline{X}}'\underline{\underline{X}} \\ \underline{b} = \underline{\underline{X}}'\underline{Y} \end{cases}$$

EXERCISE 2

$$3H_2 + CO \longrightarrow CH_4 + 2H_2O$$

$$r = f(C_0) \cdot g(H_2)$$

TEST 1 (Hypothesis)

$$r = K C_{CO}^{\mu_{CO}} \cdot C_{H2}^{\mu_{H2}}$$

$$\ln(r) = \ln K + \mu_{CO} \ln C_{CO} + \mu_{H2} \ln C_{H2}$$

$$y = a_0 + a_1 x_1 + a_2 x_2$$

$$\begin{cases} y = \ln(r) \\ a_0 = \ln(K) \\ a_1 = \mu_{CO} \\ a_2 = \mu_{H2} \\ x_1 = \ln C_{CO} \\ x_2 = \ln C_{H2} \end{cases}$$

$$\underline{Y} = \begin{bmatrix} \ln(r) \\ \vdots \end{bmatrix} \Big\} \mu_{exp}$$

$$\underline{\underline{X}} = \begin{bmatrix} 1 & \ln C_{CO} & \ln C_{H2} \\ 1 & \vdots & \vdots \\ \vdots & \vdots & \vdots \\ 1 & \vdots & \vdots \end{bmatrix} \mu_{exp}$$

$$\Downarrow$$

- $K = \exp(a_0) = 6.05 \cdot 10^{-3}$

$\underline{\mu_{CO} = 1.00}$

$\mu_{H2} = 0.0168$

$R^2 = 0.92$

↑

very bad — model not adequate

Look at experimental data

$r \sim P_{CO}^{\mu}$ is adequate

$r \sim P_{H2}^{\mu}$ is not adequate
opposite behavior at high and low pressure

$$r \sim \frac{P_{H2}^{\mu_{low}}}{1 + P_{H2}^{\mu_{high}}}$$

Hypothesis: $$r = \frac{b_1 \cdot P_{CO}^{\mu_{CO}} \cdot P_{H2}^{\mu_{H2}^{low}}}{1 + b_2 P_{H2}^{\mu_{high}}}$$

$$\ln(r) = \ln b_1 + \mu_{CO} \ln P_{CO} + \mu_{H2}^{low} \ln P_{H2} - \ln\left(1 + b_2 P_{H2}^{\mu_{high}}\right)$$

5 parameters
$$\begin{cases} a_1 = \ln b_1 \\ a_2 = \mu_{CO} \\ a_3 = \mu_{H2}^{low} \\ a_4 = \mu_{H2}^{high} \\ a_5 = b_2 \end{cases}$$

~~$\ln(r) = a_1 + \ln$~~

$$\ln(r) = a_1 + a_2 \ln P_{CO} + a_3 \ln P_{H2} - \ln\left(1 + a_5 P_{H2}^{a_4}\right)$$

non linear regression analysis
- 1 dependent variable $y = \ln(\cdot e)$
- 2 independent variables $\begin{cases} x_1 = P_{CO} \\ x_2 = P_{H2} \end{cases}$
- 5 parameters

$$y = a_1 + a_2 \ln(x_1) + a_3 \ln(x_2) - \ln\left(1 + a_5 x_2^{a_4}\right)$$