

PRACTICAL SESSION 4

EXERCISE 1



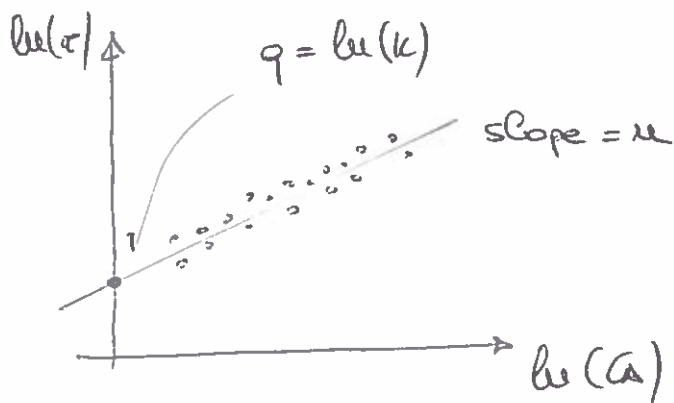
differential method $\frac{dC_A}{dt} = -r \Rightarrow -\frac{dC_A}{dt} = +k C_A^u$

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

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

$$y = a_0 + a_1 x_1$$

$$\left\{ \begin{array}{l} y = \ln(r) \\ a_0 = \ln(k) \\ a_1 = u \\ x_1 = \ln(C_A) \end{array} \right.$$



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

$$\underline{\underline{X}} = \begin{bmatrix} 1 & \ln C_A^0 \\ 1 & \vdots \\ 1 & \vdots \end{bmatrix} \quad \left. \vphantom{\begin{bmatrix} 1 & \ln C_A^0 \\ 1 & \vdots \\ 1 & \vdots \end{bmatrix}} \right\} n_{\text{exp}}$$

$$\underbrace{\underline{\underline{X}}' \underline{\underline{X}}}_{\underline{\underline{A}}} \underline{\underline{a}} = \underbrace{\underline{\underline{X}}' \underline{\underline{Y}}}_{\underline{\underline{b}}}$$

$$\Rightarrow \underline{\underline{A}} \underline{\underline{a}} = \underline{\underline{b}}$$

$$\left\{ \begin{array}{l} \underline{\underline{A}} = \underline{\underline{X}}' \underline{\underline{X}} \\ \underline{\underline{b}} = \underline{\underline{X}}' \underline{\underline{Y}} \end{array} \right.$$

EXERCISE 2



$$r = f(\text{CO}) \cdot g(\text{H}_2)$$

TEST 1 (Hypothesis)

$$r = K C_{\text{CO}}^{\mu_{\text{CO}}} \cdot C_{\text{H}_2}^{\mu_{\text{H}_2}}$$

$$\ln(r) = \ln K + \mu_{\text{CO}} \ln C_{\text{CO}} + \mu_{\text{H}_2} \ln C_{\text{H}_2}$$

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

$$\left\{ \begin{array}{l} y = \ln(r) \\ a_0 = \ln(K) \\ a_1 = \mu_{\text{CO}} \\ a_2 = \mu_{\text{H}_2} \\ x_1 = \ln C_{\text{CO}} \\ x_2 = \ln C_{\text{H}_2} \end{array} \right.$$

$$\underline{y} = \begin{bmatrix} \ln(r) \\ \vdots \\ \vdots \end{bmatrix} \quad \mu_{\text{exp}}$$

$$\underline{X} = \begin{bmatrix} 1 & \ln C_{\text{CO}} & \ln C_{\text{H}_2} \\ \vdots & \vdots & \vdots \\ 1 & \vdots & \vdots \end{bmatrix} \quad \mu_{\text{exp}}$$



$$\left\{ \begin{array}{l} K = \exp(a_0) = 6.05 \cdot 10^{-3} \\ \mu_{\text{CO}} = 1.00 \\ \mu_{\text{H}_2} = 0.0168 \end{array} \right.$$

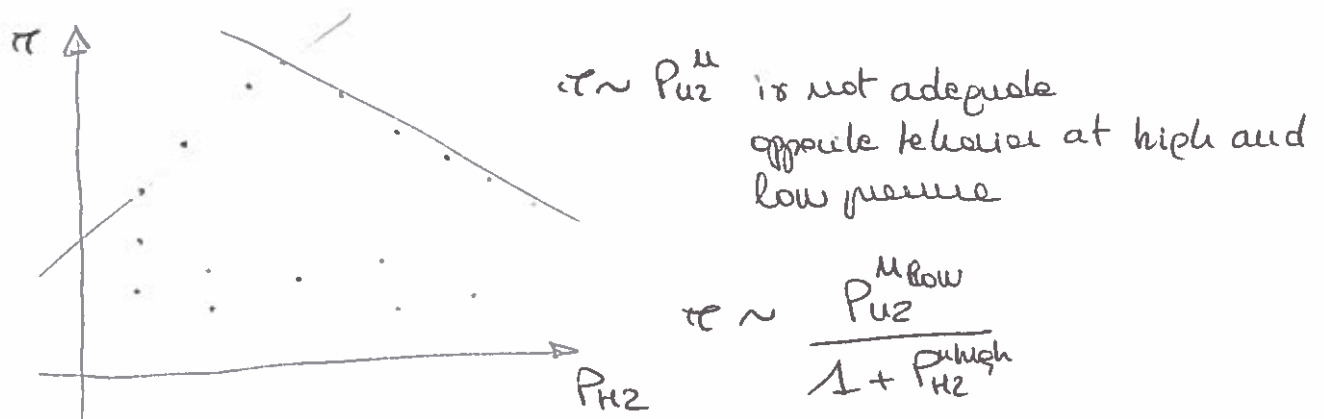
$$R^2 = 0.92$$



very bad

model not adequate

Look at experimental data



Hypothesis:
$$\pi = \frac{b_1 \cdot P_{CO}^{\mu_{CO}} \cdot P_{H_2}^{\mu_{H_2}^{low}}}{1 + b_2 P_{H_2}^{\mu_{H_2}^{high}}}$$

$$\ln(\pi) = \ln b_1 + \mu_{CO} \ln P_{CO} + \mu_{H_2}^{low} \ln P_{H_2} - \ln(1 + b_2 P_{H_2}^{\mu_{H_2}^{high}})$$

5 parameters

$$\left\{ \begin{array}{l} a_1 = \ln b_1 \\ a_2 = \mu_{CO} \\ a_3 = \mu_{H_2}^{low} \\ a_4 = \mu_{H_2}^{high} \\ a_5 = b_2 \end{array} \right.$$

~~$\ln(\pi) = a_1 + a_2$~~

$$\ln(\pi) = a_1 + a_2 \ln P_{CO} + a_3 \ln P_{H_2} - \ln(1 + a_5 P_{H_2}^{a_4})$$

non linear regression analysis

{	1 dependent variable	$y = \ln(\cdot)$
	2 independent variables	$\begin{cases} x_1 = P_{CO} \\ x_2 = P_{H_2} \end{cases}$
	5 parameters	

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