Chemical Reaction Engineering

Practical Session 3

29 November 2019

Analysis of experimental data

1. *Irreversible reaction of order n (linear regression analysis)*

The following irreversible reaction occurs in a batch reactor: $A \rightarrow Products$. The rate of consumption of species A (i.e. $-\frac{dC_A}{dt}$) was measured as a function of different initial concentrations of A itself, according to what reported in the table below.

Is a power-law reaction rate expression $r = kC_A^n$ able to correctly describe the experimental data? If yes, estimate the kinetic constant k and the reaction order n.

$C_A^0 \left(\frac{mol}{l}\right)$	0.1	0.3	0.5	0.8	1	2	4
$r \left(\frac{mol}{l\,min}\right)$	0.073e-2	0.32e-2	0.77e-2	1.43e-2	1.8e-2	4.7e-2	12.34e-2

2. *Formation of methane from carbon monoxide and hydrogen (non linear regression analysis)*

The formation of methane from carbon monoxide and hydrogen using a nickel catalyst was largely studied in the scientific literature. The reaction:

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

was carried out at $260\ °C$ in a differential reactor where the effluent concentration of methane was measured.

Determine the reaction rate law based on the measured data, reported in the attached table.

Assume that the reaction rate law is the product of a function $f(CO)$ of the partial pressure of CO and a function $g(H_2)$ of the partial pressure of H_2:

$$r = f(CO)g(H_2)$$

Run	P_{CO} $[atm]$	P_{H2} $[atm]$	$r \left[\frac{mol_{CH4}}{cat\ min}\right]$
1	1	1	0.0072
2	1.8	1	0.0129
3	4.08	1	0.0292
4	1	0.1	0.0049
5	1	0.5	0.0073
6	1	4	0.0053
7	2	0.1	0.0098
8	2	0.5	0.0146
9	2	4	0.0106
10	1	2	0.0064
11	1.8	2	0.0115
12	4.08	2	0.026
13	3	0.1	0.0147
14	3	0.5	0.0219
15	3	4	0.0159
16	1	3	0.0058
17	1.8	3	0.0104
18	4.08	3	0.0235