Chemical Reaction Engineering

Practical Session 5

9 December 2021

Analysis of experimental data

1. ***Irreversible reaction of order n (linear regression analysis, differential method)***
   The following irreversible reaction occurs in a batch reactor: $A \rightarrow Products$. The concentration of species A was measured at 9 different times, according to the table reported 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 using the differential method.

$\boldsymbol{t(min)}$	0	5	10	15	20	25	30	35	40
$\boldsymbol{C_A\ (mol/l)}$	10	8.0262	6.5575	5.4393	4.5708	3.8847	3.3346	2.8877	2.5203

2. ***Irreversible reaction of order n (non-linear regression analysis, integral method)***

   Repeat the previous exercise using the integral method.

3. ***Estimation of kinetic parameters for the Arrhenius' law***

   The kinetic constant of a chemical reaction was measured at different temperatures, according to the table reported below. Determine the kinetic parameters if we consider the kinetic constant can be described through the modified Arrhenius' law:

$$k(T) = AT^n \exp\left(-\frac{E}{RT}\right)$$

$\boldsymbol{T(K)}$	**300**	**350**	**350**	**400**	**450**
$\boldsymbol{k\ (1/min)}$	2.5197e-04	3.4984e-02	3.8545e-02	1.5634e+00	2.9993e+01
$\boldsymbol{T(K)}$	**450**	**500**	**500**	**550**	
$\boldsymbol{k\ (1/min)}$	2.5964e+01	3.3637e+02	2.9365e+02	2.1903e+03	

Suggested exercises

4. ***Irreversible reaction of order n (linear regression analysis, differential method)***

   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.

$C_A^0\ (mol/l)$	0.1	0.3	0.5	0.8	1	2	4
$r\ (mol/l/min)$	0.073e-2	0.32e-2	0.77e-2	1.43e-2	1.8e-2	4.7e-2	12.34e-2

5. ***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:

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

In particular, the following two hypotheses must be compared:

Hypothesis 1: $r = kP_{CO}^{n_{CO}}P_{H2}^{n_{H2}}$

Hypothesis 2: $r = k_1 \frac{P_{CO}^{n_{CO}}P_{H2}^{n_{H2,low}}}{1+k_2 P_{H2}^{n_{H2,high}}}$

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