Practical 12

Homogeneous Kinetics

Exercise 1

The following irreversible reaction occurs in a batch reactor in isothermal and isobaric conditions (330 °C and 1 atm):

$$A \rightarrow B \tag{1}$$

Is a power-law reaction expression $r = kC_A^n$ able to correctly describe the experimental data?

If yes, estimate the kinetic constant k and the reaction order n both with the integral approach and with the differential method.

time [s]	cA [mol m^{-3}]
0	10
5	9.60309
10	9.221919
15	8.855882
20	8.504348
25	8.16673
30	7.842528
35	7.531231
40	7.232217
45	6.945019
50	6.66923
55	6.404441
60	6.150217
65	5.90602
70	5.671484
75	5.446273
80	5.23005
85	5.022439
90	4.823012
95	4.631482
100	4.447574
105	4.271012
110	4.101462
115	3.938598

120	3.78219
125	3.632012
130	3.487834
135	3.349365
140	3.216362
145	3.088637
150	2.966002
155	2.848267
160	2.735181
165	2.626565
170	2.522263
175	2.422121
180	2.325976
185	2.233622
190	2.144922
195	2.059748
200	1.977974
205	1.899457
210	1.824034
215	1.751599
220	1.682046
225	1.615271
230	1.551156
235	1.489583
240	1.430457

Exercise 2

From an experimental campaign conducted in a batch reactor in isothermal and isobaric conditions (330 °C and 1 atm), data of concentrations in time have been registered. Determine the kinetic constants and the reaction orders by assuming a power-law expression.

time [s]	cA [mol m^{-3}]	cB [mol m^{-3}]	cC [mol m^{-3}]
0	10	0	0
5	8.704426	1.001806	0.293768
10	7.677792	1.77099	0.551218
15	6.844558	2.375893	0.779549
20	6.155117	2.860868	0.984015
25	5.575374	3.256035	1.168591
30	5.081415	3.582281	1.336305
35	4.655794	3.854643	1.489563
40	4.285085	4.084555	1.63036
45	3.959923	4.279909	1.760169
50	3.672077	4.447532	1.880391
55	3.4159	4.59205	1.992049

60	3.18658	4.717398	2.096022
65	2.97991	4.826891	2.193199
70	2.793139	4.922727	2.284134
75	2.623403	5.007142	2.369455
80	2.468477	5.081814	2.44971
85	2.326794	5.147951	2.525256
90	2.196684	5.206811	2.596505
95	2.076714	5.259421	2.663865
100	1.965956	5.306464	2.727579
105	1.863484	5.348624	2.787892
110	1.76827	5.386607	2.845124
115	1.67966	5.420859	2.899481
120	1.597114	5.451762	2.951124
125	1.520081	5.479699	3.00022
130	1.447936	5.505069	3.046995
135	1.380292	5.528122	3.091587
140	1.316828	5.549068	3.134104
145	1.257222	5.568121	3.174656
150	1.201106	5.585511	3.213383
155	1.148166	5.601415	3.250419
160	1.098208	5.615955	3.285837
165	1.051037	5.62925	3.319713
170	1.006456	5.641421	3.352122
175	0.964232	5.652598	3.38317
180	0.924195	5.66287	3.412935
185	0.886221	5.672308	3.441471
190	0.850185	5.680982	3.468833
195	0.815962	5.688963	3.495075
200	0.783402	5.696325	3.520273
205	0.752406	5.703116	3.544478
210	0.722892	5.709381	3.567727
215	0.694777	5.715161	3.590062
220	0.667975	5.7205	3.611525
225	0.64239	5.725441	3.632169
230	0.61796	5.730012	3.652027
235	0.594627	5.734242	3.671132
240	0.572332	5.738157	3.689512

Exercise 3

In order to derive the rate equation for the reaction A -> B (irreversible) a dedicated experimental campaign has been performed in a plug flow reactor in isothermal and isobaric conditions. The experimental data are reported in the tables below.

Derive the functional form of the rate equation together with the pre-exponential terms and the activation energy of the reaction constant(s).

1) Temperature: 206.85°C:

Test	$\mathbf{c_{A,IN}}$ $\mathbf{mol\ m^{-3}}$	$\mathbf{c_{B,IN}}$ $\mathbf{mol\ m^{-3}}$	$\mathbf{c_{A,OUT}}$ $\mathbf{mol\ m^{-3}}$	$\mathbf{c_{B,OUT}}$ $\mathbf{mol\ m^{-3}}$
1	0.75	0.1	0.73232	0.11768
2	1	0.1	0.97643	0.12357
3	1.25	0.1	1.2205	0.12946
4	1.5	0.1	1.4646	0.13535
5	1.75	0.1	1.7088	0.14125

2) Temperature: 226.85°C:

Test	$\mathbf{c_{A,IN}}$ $\mathbf{mol\ m^{-3}}$	$\mathbf{c_{B,IN}}$ $\mathbf{mol\ m^{-3}}$	$\mathbf{c_{A,OUT}}$ $\mathbf{mol\ m^{-3}}$	$\mathbf{c_{B,OUT}}$ $\mathbf{mol\ m^{-3}}$
1	0.75	0	0.71592	0.034082
2	1	0	0.954557	0.045443
3	1.25	0	1.1932	0.056804
4	1.5	0	1.4318	0.068165
5	1.75	0	1.6705	0.079526

3) Temperature 236.85°C:

Test	$\mathbf{c_{A,IN}}$ $\mathbf{mol\ m^{-3}}$	$\mathbf{c_{B,IN}}$ $\mathbf{mol\ m^{-3}}$	$\mathbf{c_{A,OUT}}$ $\mathbf{mol\ m^{-3}}$	$\mathbf{c_{B,OUT}}$ $\mathbf{mol\ m^{-3}}$
1	0.75	0.1	0.70379	0.14621
2	1	0.15	0.93839	0.21161
3	1.25	0.2	1.173	0.27701
4	1.5	0.25	1.4076	0.34242
5	1.75	0.3	1.6422	0.40782

4) Temperature 246.85°C:

Test	$c_{A,IN}$ $mol\ m^{-3}$	$c_{B,IN}$ $mol\ m^{-3}$	$c_{A,OUT}$ $mol\ m^{-3}$	$c_{B,OUT}$ $mol\ m^{-3}$
1	0.75	0.1	0.68826	0.16174
2	1	0.1	0.91768	0.18232
3	1.25	0.1	1.1471	0.20291
4	1.5	0.1	1.3765	0.22349
5	1.75	0.1	1.6059	0.24407

5) Temperature 277.85°C:

Test	$c_{A,IN}$ $mol\ m^{-3}$	$c_{B,IN}$ $mol\ m^{-3}$	$c_{A,OUT}$ $mol\ m^{-3}$	$c_{B,OUT}$ $mol\ m^{-3}$
1	0.75	0.1	0.61521	0.23479
2	1	0.1	0.82025	0.27975
3	1.25	0.1	1.0253	0.32472
4	1.5	0.1	1.2303	0.36969
5	1.75	0.1	1.4353	0.41466

Operating conditions and reactor configuration:

Feed flow rate at 298 K and 1atm = 0.02 Nm^3/s

Feed pressure = 1 atm

Reactor diameter = 0.02 m

Reactor length = 0.06 m

