Practical 13

Heterogeneous Kinetics

Exercise 1

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, isobaric conditions and all the mass transport phenomena proceed faster than the chemical reaction. 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: 220°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	0.728	0.022
2	1	0	0.97	0.029
3	1.25	0	1.214	0.036
4	1.5	0	1.456	0.044
5	1.75	0	1.699	0.051

2) Temperature: 240°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	0.713	0.038
2	1	0	0.95	0.05
3	1.25	0	1.188	0.062
4	1.5	0	1.425	0.075
5	1.75	0	1.663	0.087

3) Temperature 240°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	1	0.25	0.95	0.3
2	1	0.5	0.95	0.55
3	1	0.75	0.95	0.8
4	1	1	0.95	1.05
5	1	1.25	0.95	1.3

4) Temperature 260°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	0.689	0.061
2	1	0	0.918	0.082
3	1.25	0	1.148	0.102
4	1.5	0	1.377	0.123
5	1.75	0	1.607	0.143

Operating conditions and reactor configuration:

Feed flow rate at 298 K and 1atm = $4*10^{-6}$ Nm^3/s

Feed pressure = 1 atm

Reactor Volume = $2*10^{-7}$ m3

Exercise 2

In order to derive the rate equation for the catalytic reaction A→B (irreversible) a dedicated experimental campaign has been performed. The lab reactor has a volume of 1.18 10^{-7} m^3 with a void fraction of 0.4. Several tests have been conducted in chemical regime and isothermal conditions in the reactor. The flow rate was $3x10^{-6}$ $Nm^3 s^{-1}$. Pressure drops were negligible. Derive the functional form of the rate equation and pre-exponential terms and activation energy of the reaction constant(s).

The experimental data are reported in the following tables:

1) Temperature: 220°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	0.728	0.022
2	1	0	0.97	0.029
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5	1.75	0	1.699	0.051

2) Temperature: 240°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	0.713	0.038
2	1	0	0.95	0.05
3	1.25	0	1.188	0.062
4	1.5	0	1.425	0.075
5	1.75	0	1.663	0.087

3) Temperature 240°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	1	0.25	0.95	0.3
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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}
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