



**UNIVERSITY OF ROME “LA SAPIENZA”
NANOTECHNOLOGIES ENGINEERING**

EXERCISES 1

MICRO AND NANOPARTICLES

EXERCISE #1

REACTOR DESIGN

In a perfectly mixed reactor following chemical reaction takes place:



At given operating conditions, the kinetics of the reaction are described as:

$$-r_A = k \cdot c_A \cdot c_B^2$$

where $k = 0.3 \text{ l}^2 \cdot \text{mol}^{-2} \cdot \text{s}^{-1}$.

The feed flow rate is equal to 1.5 l/s with an average molar volume about 0.05 l/mol; composition is made by A, B and an inert bulk I; molar fractions are $x_{A0} = 0.06$ and $x_{B0} = 0.20$.

Calculate the volume of the reactor required to have C in the output stream at 1.0 mol/l.

Density of the liquid is constant.

SOLUTION TO EXERCISE #1

First step:

$d_m = \text{feed flow molar density} = 1/v_m$

$$c_{A0} = x_{A0} \cdot d_m$$

$$c_{B0} = x_{B0} \cdot d_m$$

Density is constant \rightarrow calculations are performed on the concentration values.

The required value of C_C is obtained solving these equations:

$$c_A = c_{A0} - c_C$$

$$c_B = c_{B0} - 2 \cdot c_C$$

Therefore:

$$-r_A = k \cdot c_A \cdot c_B^2$$

And finally:

$$V = Q \cdot \tau = 6.25 \text{ l}$$

EXERCISE #2

PARALLEL REACTIONS

Aqueous solution of A at 100 l/min, molar fraction 0.1, and of B in a reactor will give following reactions:

$A+B \rightarrow R$ (desired) (reaction 1)

$A \rightarrow C$ (undesired) (reaction 2)

Molar density is equal to 20 mol/l. At given operating conditions, following relationship holds:

$$-r_{A1} = k_1 \cdot C_A \cdot C_B$$

where $k_1 = 10 \text{ l} \cdot \text{mol}^{-1} \cdot \text{s}^{-1}$,

$$-r_{A2} = k_2 \cdot C_A$$

where $k_2 = 1 \text{ s}^{-1}$.

Calculate the flow rate of B such to obtain a conversion of A in R equal to 20%, with 50% of selectivity. Densities are equal to those of water.

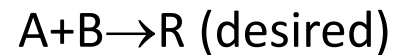
SOLUTION TO EXERCISE #2

By the value of R and the beginning concentration of A the concentration of A in the reactor is estimated. By adopting the selectivity value, from the two kinetics equation a estimation of the concentration of B is obtained. Therefore, the flow rate of B can be estimated and must be capable to “feed” both reactions: a value of 0.5 mol/l equal to 25 l/min (in case of B pure) is found.

EXERCISE #3

REACTION IN SERIES

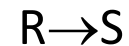
A feed stream of 400 l/min, where A and B are at 2 e 3 mol/l, respectively, is sent to a reactor where this reaction takes place:



$$-r_{A1} = k_1 \cdot C_A \cdot C_B$$

$$\text{where } k_1 = 2 \text{ l} \cdot \text{mol}^{-1} \cdot \text{min}^{-1},$$

And



$$-r_{R2} = k_2 \cdot C_R$$

$$\text{where } k_2 = 1 \text{ l} \cdot \text{mol}^{-1} \cdot \text{min}^{-1}.$$

Calculate the volume of the reactor in order to maximize the production of R.

SOLUTION TO EXERCISE #3

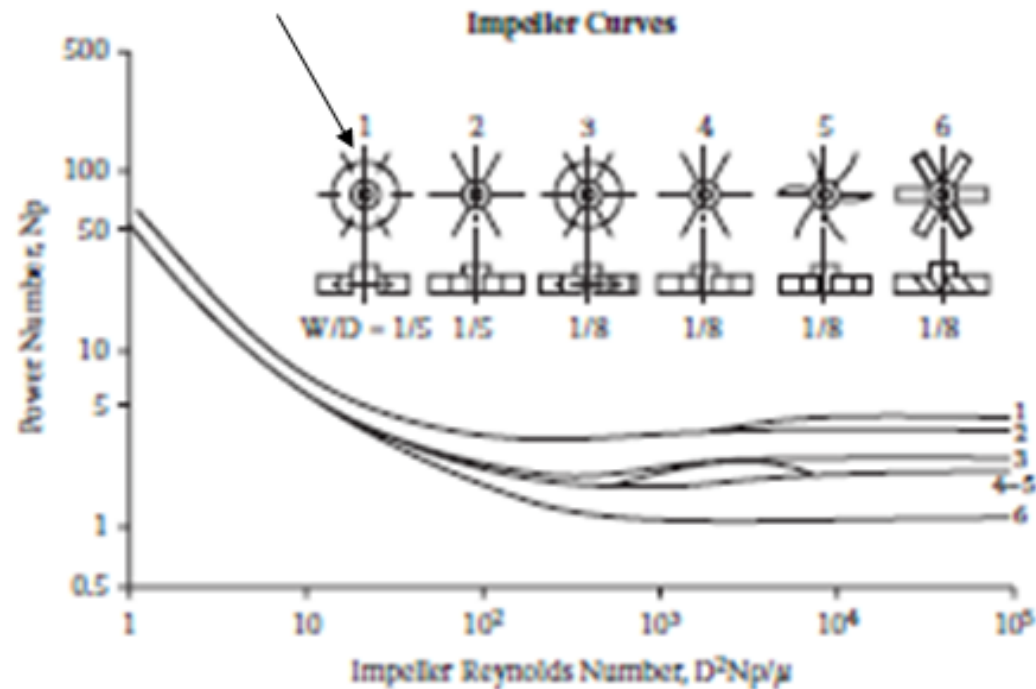
The material equation $C_R = -r_A t + r_S t$ is maximum when $dC_R/dt = 0$. In this case, a value of c_A equal to 0.5 mol/l is obtained, therefore $r_A = 1.5$ mol/l min and a residence time of 1h is required: the volume of the reactor should be equal to 400l.

EXERCISE #4

MIXING

A Rushton impeller is used to mix water in a reactor. The diameter is equal to 1m. Calculate the power consumption of the impeller system to keep a rotation speed of 60 rpm.

$$Re = \frac{\rho \cdot N \cdot D^2}{\mu}$$



SOLUTION TO EXERCISE #4

$$P = N_p \cdot \rho \cdot N^3 \cdot D^5$$

Therefore: $P = 5 \text{ kW}$.

EXERCISE #5

MICROMIXING

A micromixing time of 5 ms is required for a liquid solution having kinematic viscosity equal to 1 cSt and diffusivity D equal to $2.2 \cdot 10^{-9} \text{ m}^2/\text{s}$.

SOLUTION TO EXERCISE #5

$$t_m = 0.5 \cdot \frac{\lambda_k^2}{D} \quad \longrightarrow \quad \lambda_k = \left(\frac{V_f^3}{\varepsilon} \right)^{1/4}$$

Therefore: $\varepsilon = 2 \text{ kW/kg}$.