Process Systems Engineering
Prof. Davide Manca – Politecnico di Milano

Exercise 2

Reactor design of HDA process

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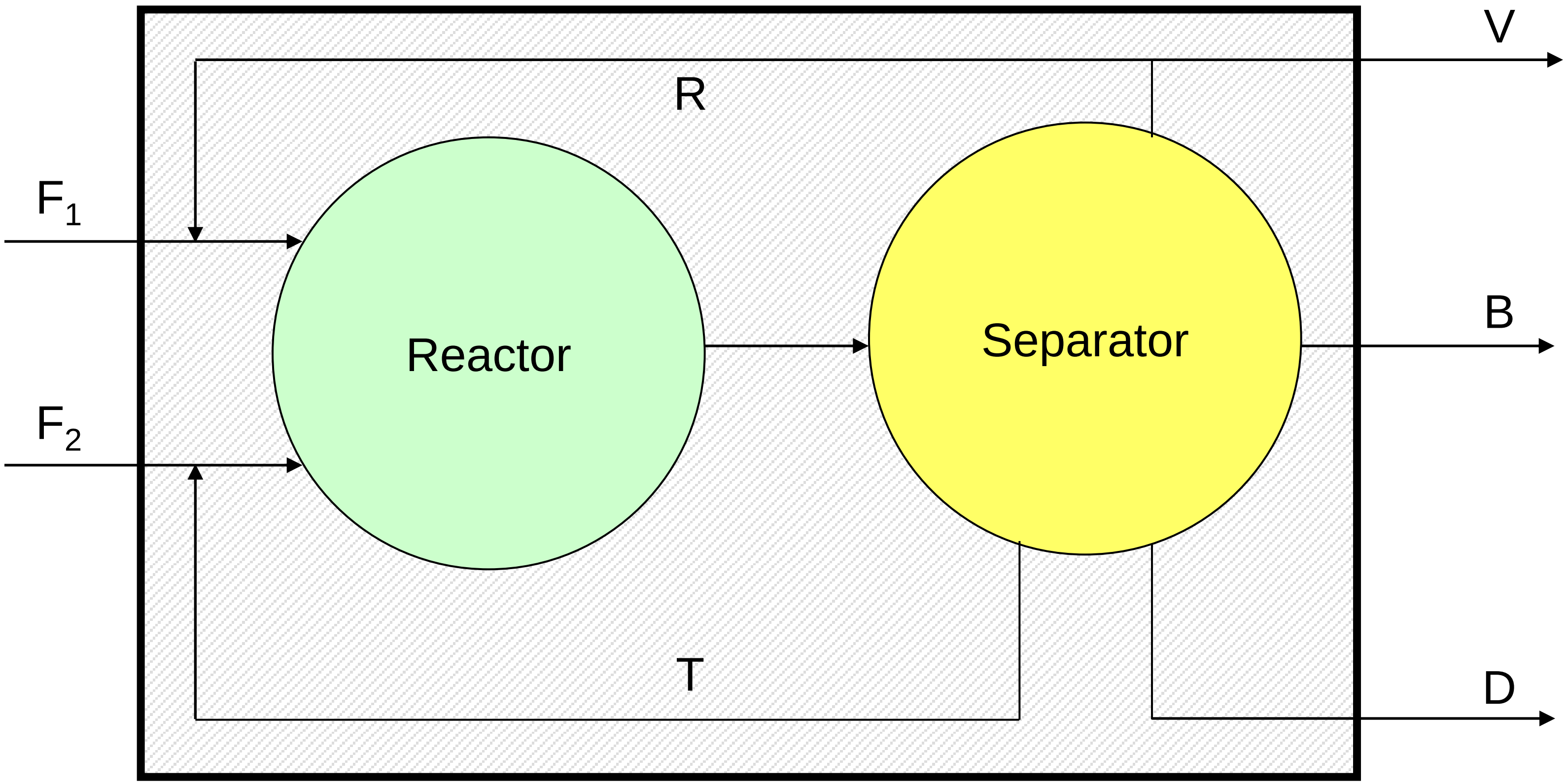
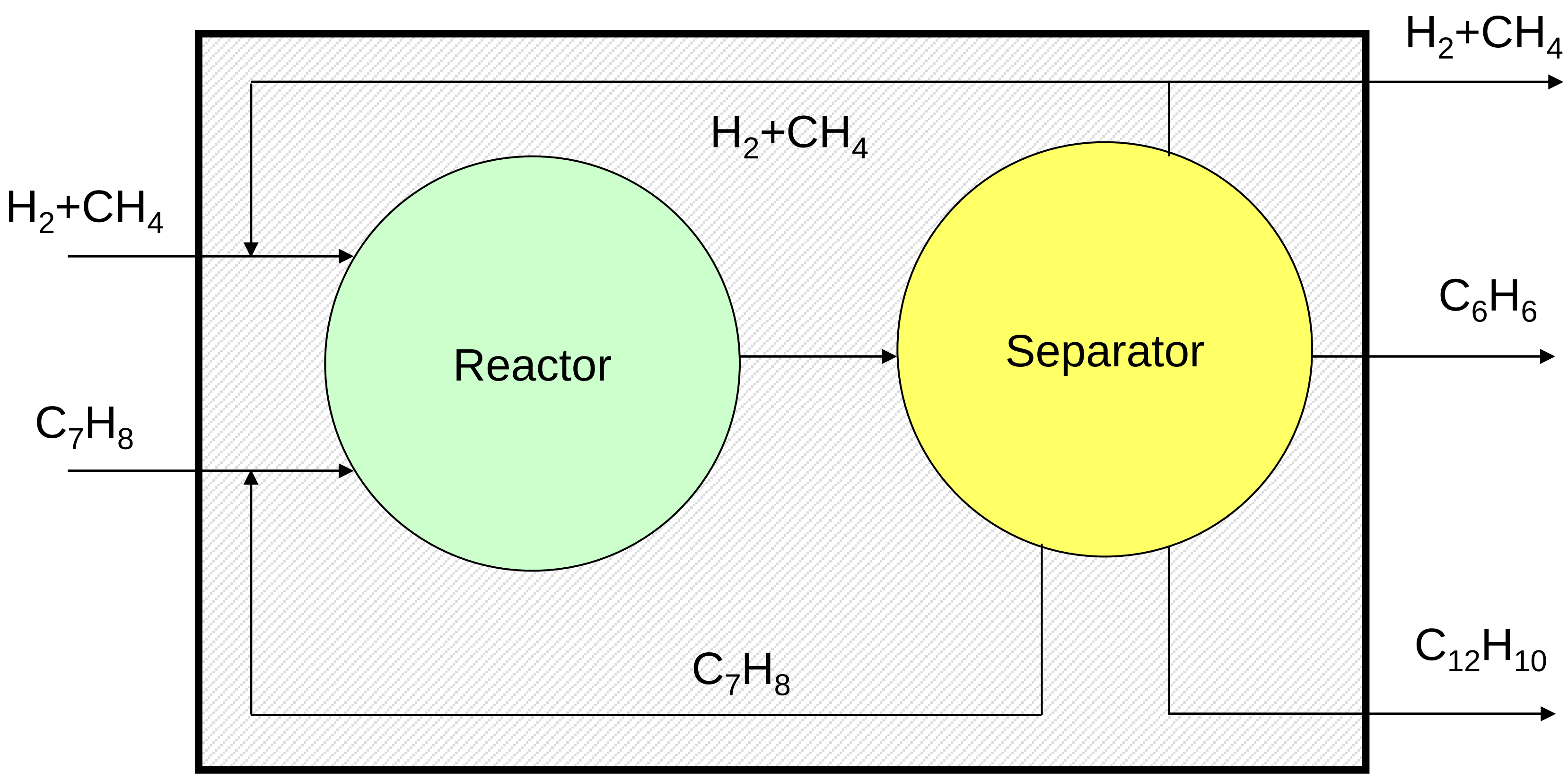
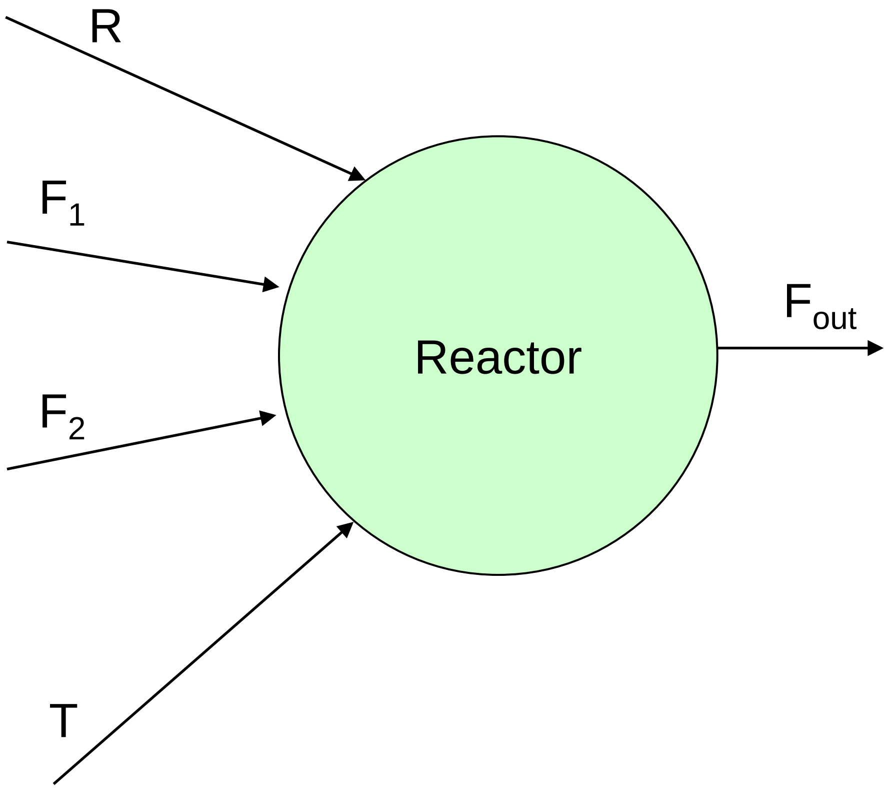
Process HDA



Process HDA



Selection of the reactor



Reactions

Main reactions

$$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$$

$$R_1 = k_1 c_T \sqrt{c_H} \qquad \left[kmol/m^3 s\right]$$

$$A_1 = 3.5\mathrm{E}+10 \quad \left[\left(m^3\right)^{0.5} \Big/ \left(kmol^{0.5}\cdot s\right)\right]$$

$$k_1 = A_1 \exp\left(-\frac{E_1}{RT}\right)$$

$$E_1 = 50900 \quad \left[kcal/\left(kmol\cdot K\right)\right]$$

Side reactions

$$2C_6H_6 \rightarrow C_{12}H_{10} + H_2$$

$$R_2 = k_2 c_B^2 \qquad \left[kmol/m^3 s\right]$$

$$A_2 = 2.1\mathrm{E}+12 \quad \left[m^3/\left(kmol\cdot s\right)\right]$$

$$k_2 = A_2 \exp\left(-\frac{E_2}{RT}\right)$$

$$E_2 = 60500 \quad \left[kcal/\left(kmol\cdot K\right)\right]$$

Degree of Freedom

Selection of Reactor

- Conditions of input streams
- Residence time or volume of the reactor
- Operating conditions (pressure and temperature)

Degrees of Freedom

Conditions of input streams

- The stream of fresh hydrogen contains 5% mol of methane
- The reactants are at room temperature
- The ratio between hydrogen and toluene in the inlet stream to the reactor must be on the one hand high enough to avoid coking and other hand sufficiently low to reduce the costs of recycling. It is suggested to use an optimal ratio equal to 5.

Residence time and reactor volume

Determined by the following specifications:

- The selectivity must be $\geq$ 96%
- The productivity of benzene must be = 265 kmol/h
- The purity of benzene must be ≥ 0.9997

Degrees of Freedom

Operating conditions

Pressure

The reactions are equimolar

PROS: by increasing the pressure there is an increase of concentration of products that speeds up the reaction

CONS: by increasing the pressure there is an increase in the operating costs of compression

$\Rightarrow$ P = 34 bar

Degrees of Freedom

Operating conditions

Operating temperature

There is no need of any catalyst.

- High temperature increases the reaction velocity
- The main reactions is exothermic
- The side reactions are faster at higher temperatures
  Becomes more important (higher activation energy)

  $\Rightarrow$ it is worth operating low temperature!

Range of economic interest : 600 – 750 °C
(Carry out tests at intervals of 50 °C)

Degrees of Freedom

Selection of the reactor

The reaction scheme is in series:

Toluene $\Rightarrow$ Benzene $\Rightarrow$ Biphenyl

Necessary to control contact time (while maintaining the selectivity above 96%)

Must use a Plug-Flow reactor!

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Matrix of streams/ compositions

	H_2	CH_4	C_6H_6	C_7H_8	$C_{12}H_{10}$
F_1	0.95	0.05	0	0	0
F_2	0	0	0	1	0
B	0	0	1	0	0
D	0	0	0	0	1
V	x_v	$1- x_v$	0	0	0
R	x_v	$1- x_v$	0	0	0
T	0	0	0	1	0

Definitions

- Selectivity: $$\sigma = \frac{\text{Desired moles of Product}}{\text{Moles converted}} = \frac{n_{C_6H_6}}{n_{C_7H_8}^{init} - n_{C_7H_8}^{end}}$$

- Conversion: $$\xi = \frac{\text{Moles reacted}}{\text{Initial moles}} = \frac{n_{C_7H_8}^{init} - n_{C_7H_8}^{end}}{n_{C_7H_8}^{init}} = 1 - \frac{n_{C_7H_8}^{end}}{n_{C_7H_8}^{init}}$$

- Residence Time: $$\tau = \frac{\text{Volume reactor}}{\text{Volumetric flow rate}}$$

Requirements

1. Determine the conversion, the selectivity and the residence time as a function of the operating temperature of the reactor using numerical integration of the plug-flow model, by assuming isothermal the reactor, and neglecting the presence of recycles in the evaluation of initial concentrations

2. Evaluate the adiabatic ΔT of the reaction so to assess if the reactor can be considered isothermal

3. Carry out the following diagrams:
    - Conversion / Selectivity
    - Temperature / Conversion
    - Temperature / residence time

Balance equations

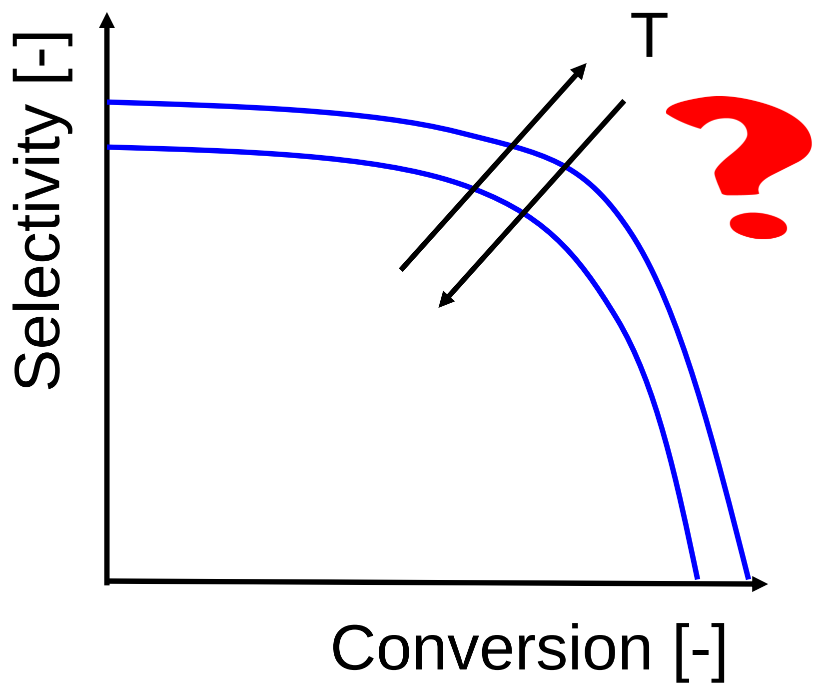
$$\frac{d[j]}{d\tau} = -\sum_{i=1}^{NR} \upsilon_{ji} R_i \qquad j = 1 \div NC$$

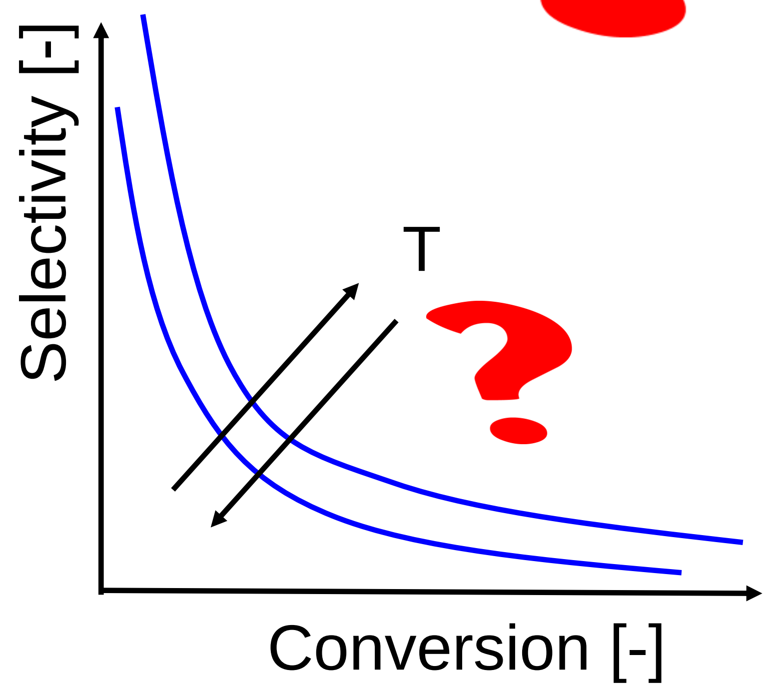
$$\begin{cases} \dfrac{d[H_2]}{d\tau} = -R_1 + R_2 \\ \dfrac{d[CH_4]}{d\tau} = R_1 \\ \dfrac{d[C_6H_6]}{d\tau} = R_1 - 2R_2 \\ \dfrac{d[C_7H_8]}{d\tau} = -R_1 \\ \dfrac{d[C_{12}H_{10}]}{d\tau} = R_2 \end{cases}$$

5 ODEs

Analysis of results

Diagram conversion / selectivity

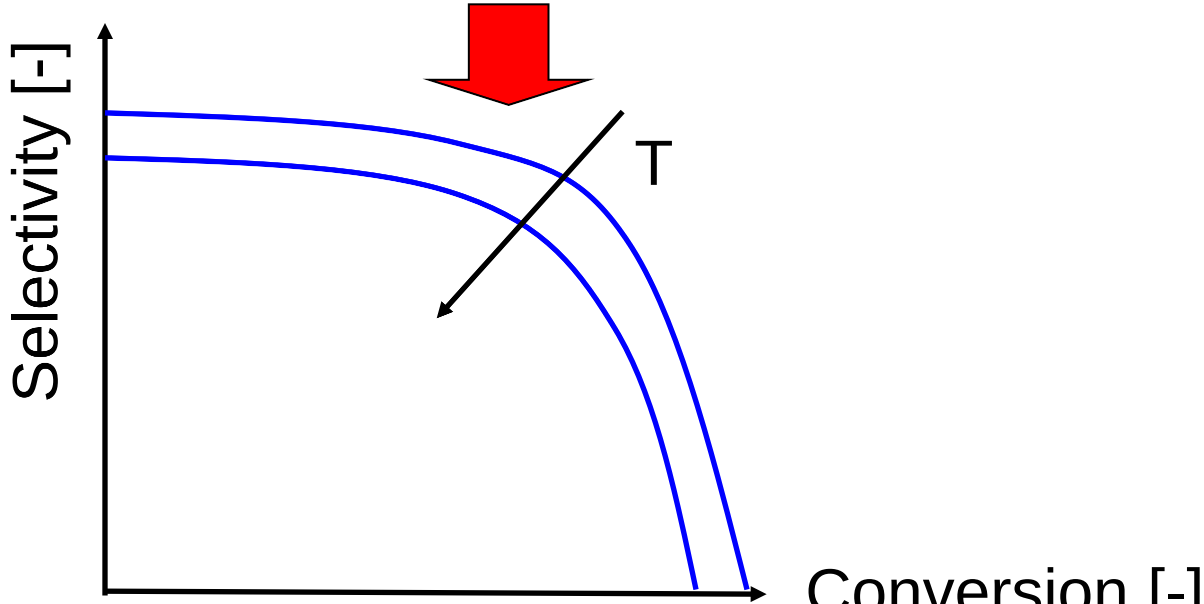




Some considerations

- The selectivity decreases by increasing the temperature because the side reaction plays an increasingly important role

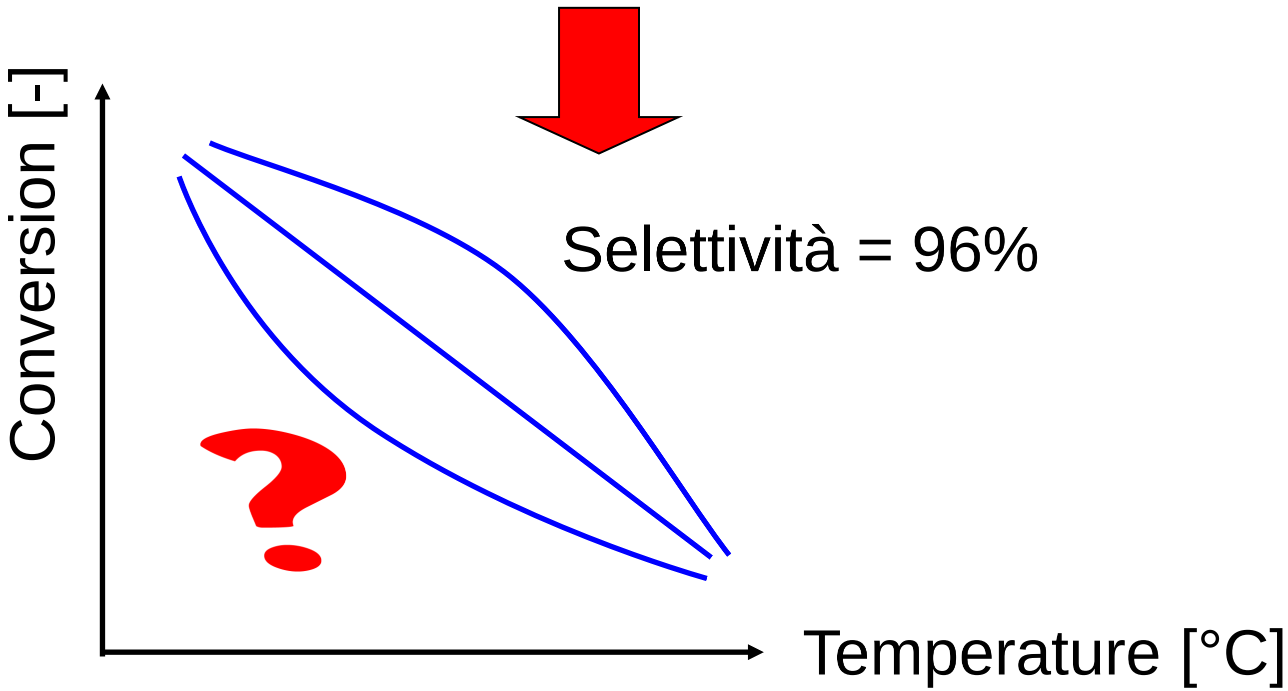
- Initially the selectivity tends to unity because, at low conversions, the reaction rate of side reaction is significantly lower than that of the main reaction



Analysis of results

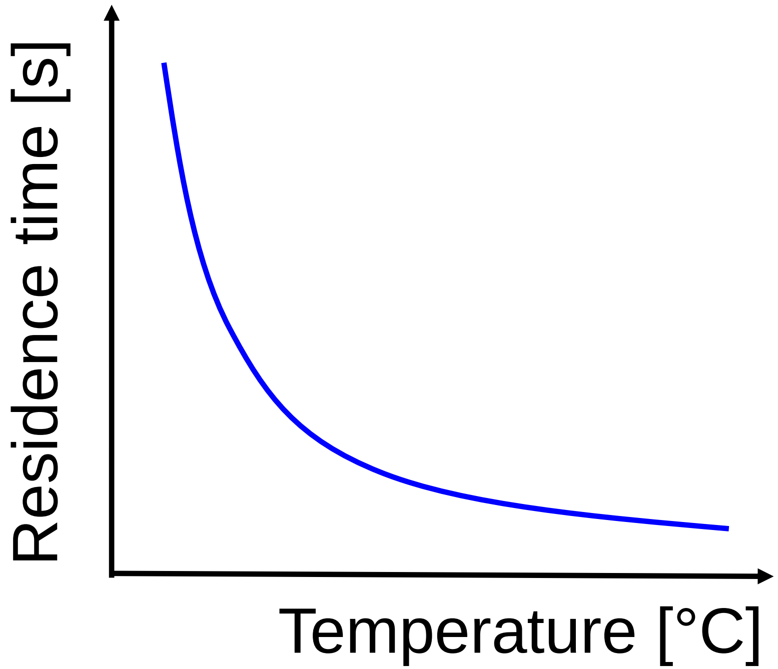
Diagram temperature/conversion

By increasing the temperature, the secondary reaction becomes increasingly important: therefore, working at high temperatures, it is necessary to limit the conversion in order to achieve a selectivity equal to 96%



Analysis of results

Residence time/temperature



Some suggestions

- Matlab Tutorial:

  http://www.chem.polimi.it/homes/dmanca/DECDPC/Ese%2000.pdf

- Useful Tips:
  - Using the "Find" function;
  - Formatting graphs.

Function"find"

- Consider the vector
- `a = [14 0.5 2 29 1];`

  `i = find(a > 3);`

  returns the index in the vector where the value satisfies the condition a(i) > 3
- In this case:

  `i = [1 4];`

Graphs (plot)

```
nf= nf+ 1;
figure(nf)
plot(x1,y1,'k-*',x2,y2,'r-. ', ...
'LineWidth',3);
set(gca,'FontSize',18)
xlabel('x [m]')
ylabel('y [kg]')
legend('Mod1', 'Mod2',1)
text(xText,yText,'testo')
saveas(figure(nf),'C:\MyFigure.emf')
```