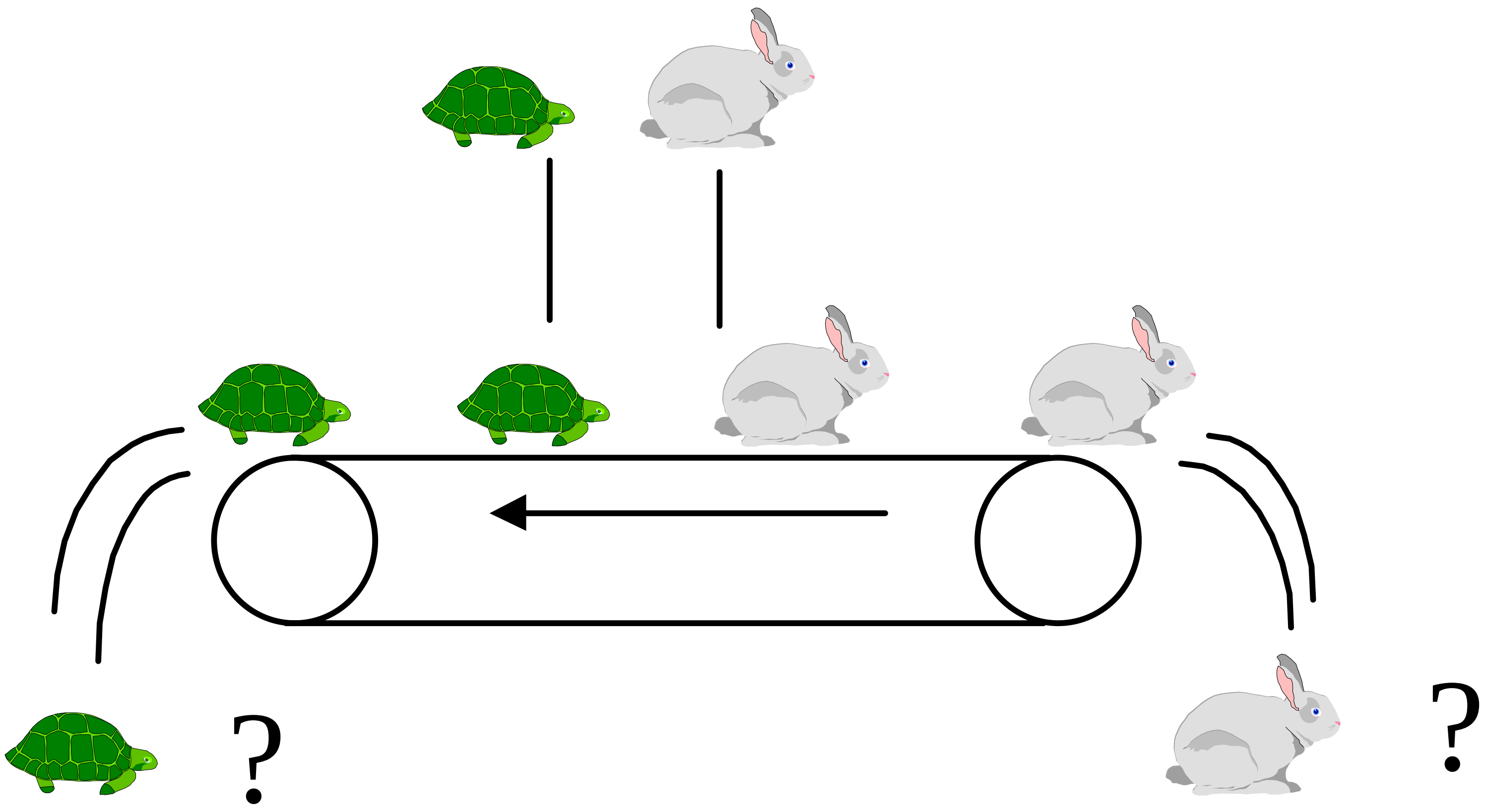
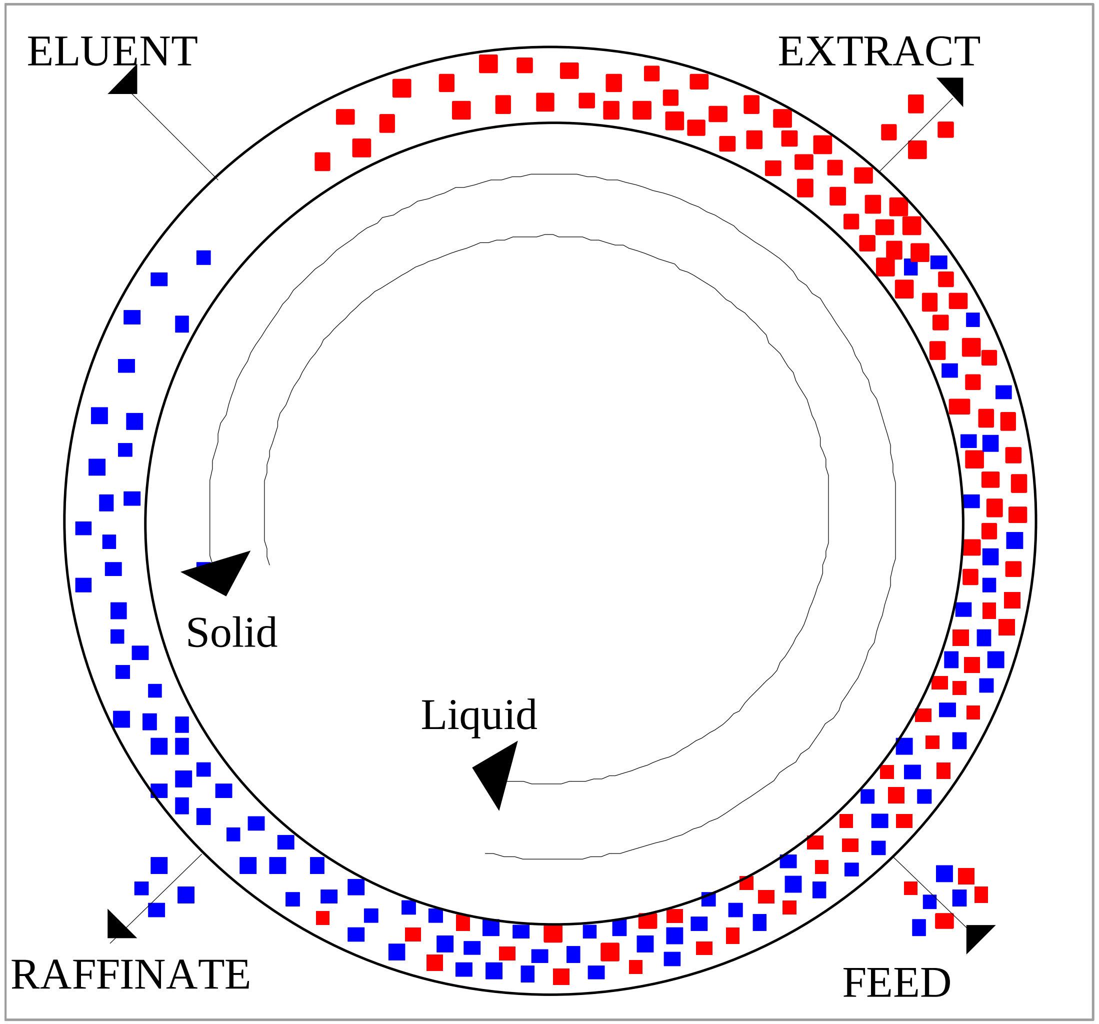
Moving Bed Concept

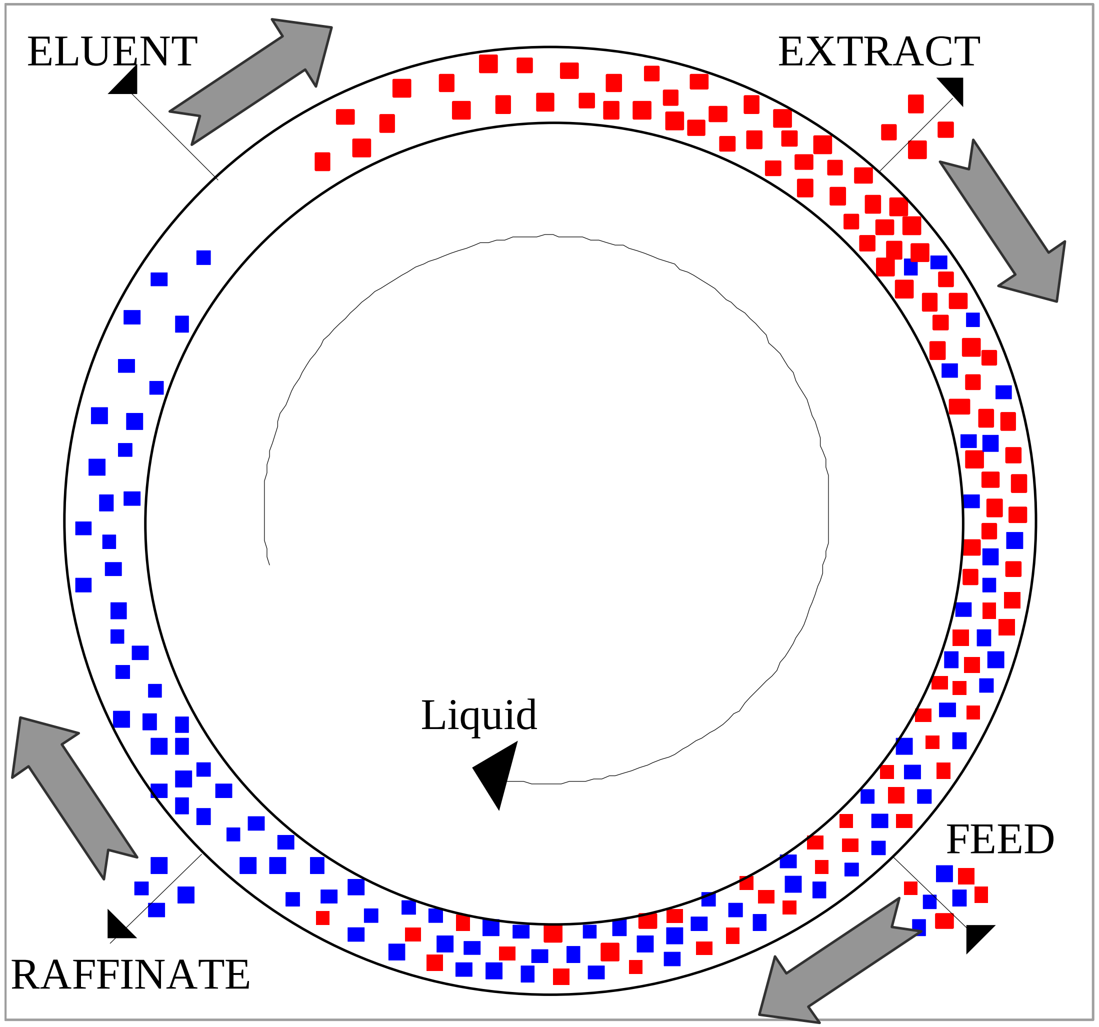


True Moving Bed



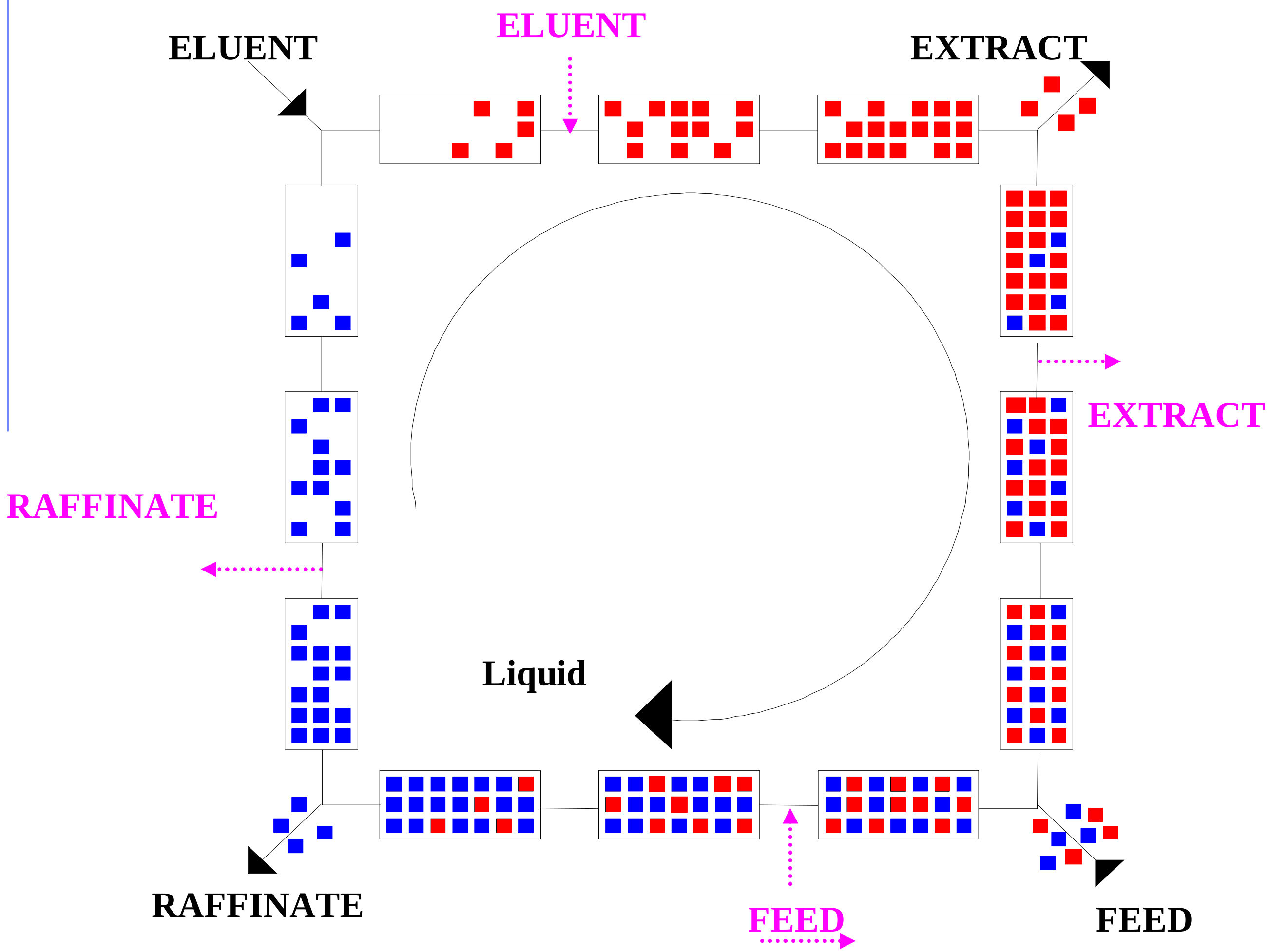
Real counter current between liquid and solid stream

Moving Bed Concept



The solid flow is simulated by a continous displacement of inlets / outlets

Simulated Moving Bed



The solid flow is simulated by a discrete displacement of inlets / outlets

Inlet and outlet flow positions after ΔT
Simulation of the solid phase movement

Chromatographic process modelling

- Fast way to design processes
  - Rapid calculations
  - Numerical optimizations
  - Only small amounts of products required

- Parametric study
  - Estimation of robustness
  - Determination of critical factors

Process simulation

Calculate process productivity for fixed conditions

Physical data :
- isotherms
- pressure drop
- HETP

Obtained from laboratory studies

Operating flow-rates
Column size

Fixed by the user

→ Numerical simulation →

Purity, recovery
Productivity
Eluent consumption

Process Optimization

Physical data :
- isotherms
- pressure drop
- HETP

Numerical optimization

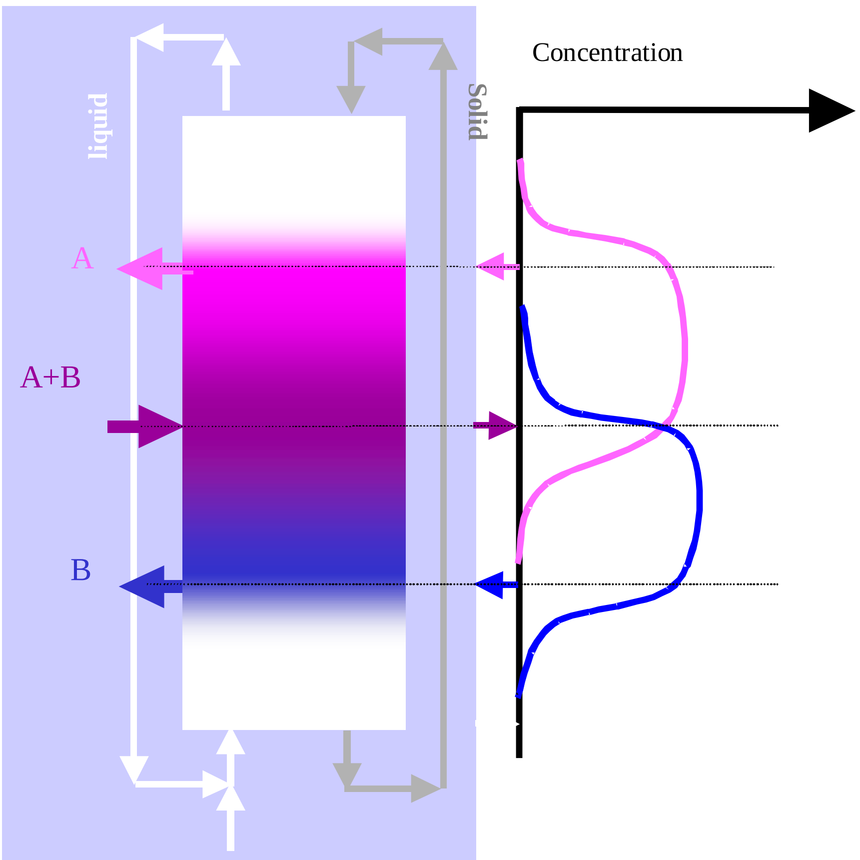
Numerical simulation

Optimal flow-rates
Column size

Productivity
Eluent consumption

The optimization search the operating conditions to get an optimum productivity

Required data for modeling



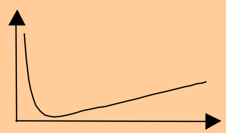
Flow rates and Δt function of

- Adsorption isotherms (retention, selectivity, capacity)

  $C_A^{sol}=f_A(C_A^{liq},C_b^{liq})$ $\quad$ $C_B^{sol}=f_B(C_A^{liq},C_B^{liq})$

- Column efficiency
  Van Deemter

  H=A+Bu+C/u



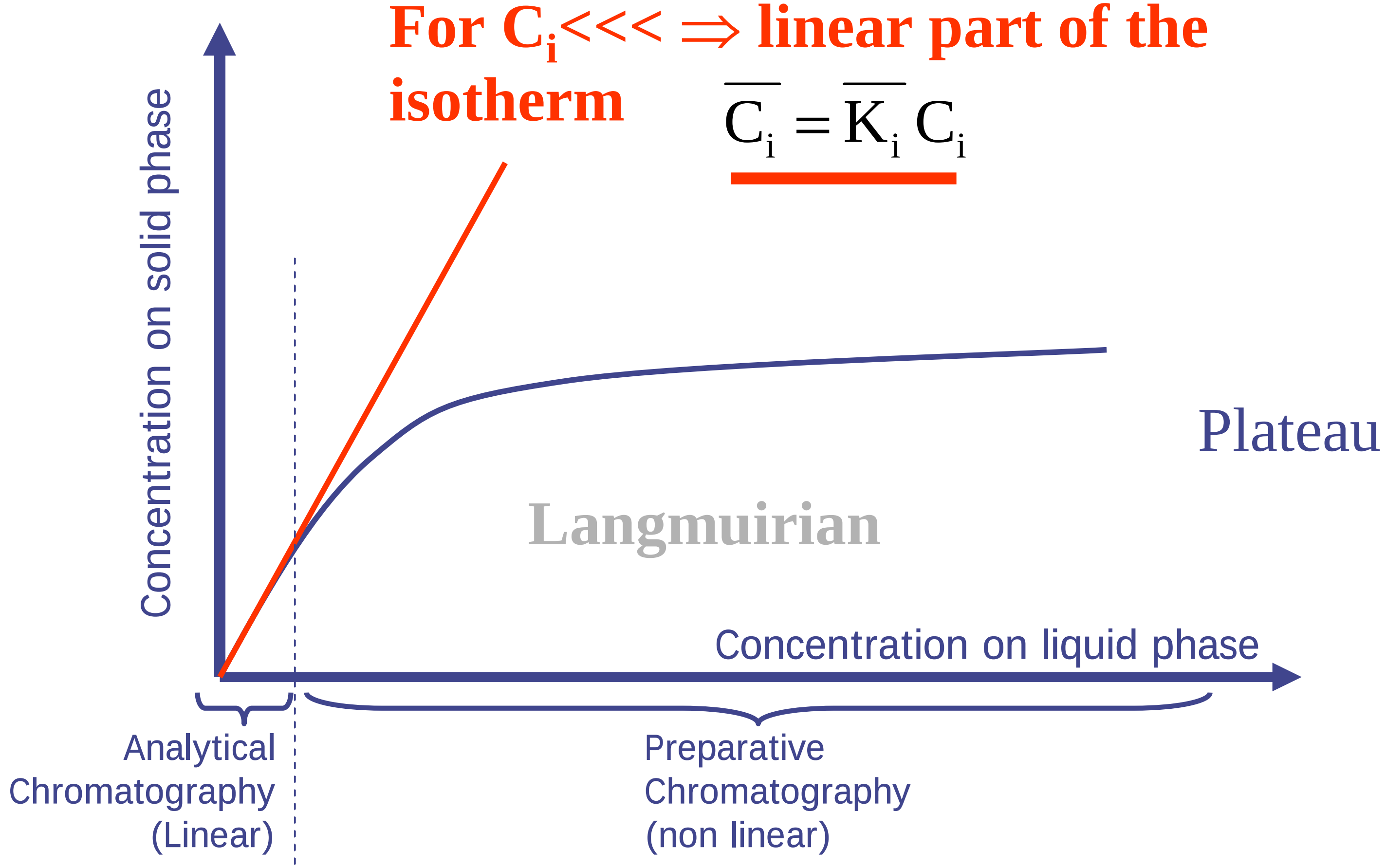
Pressure drop
Kozeny Karman equation

$$\frac{\Delta P}{L}=k\cdot u$$

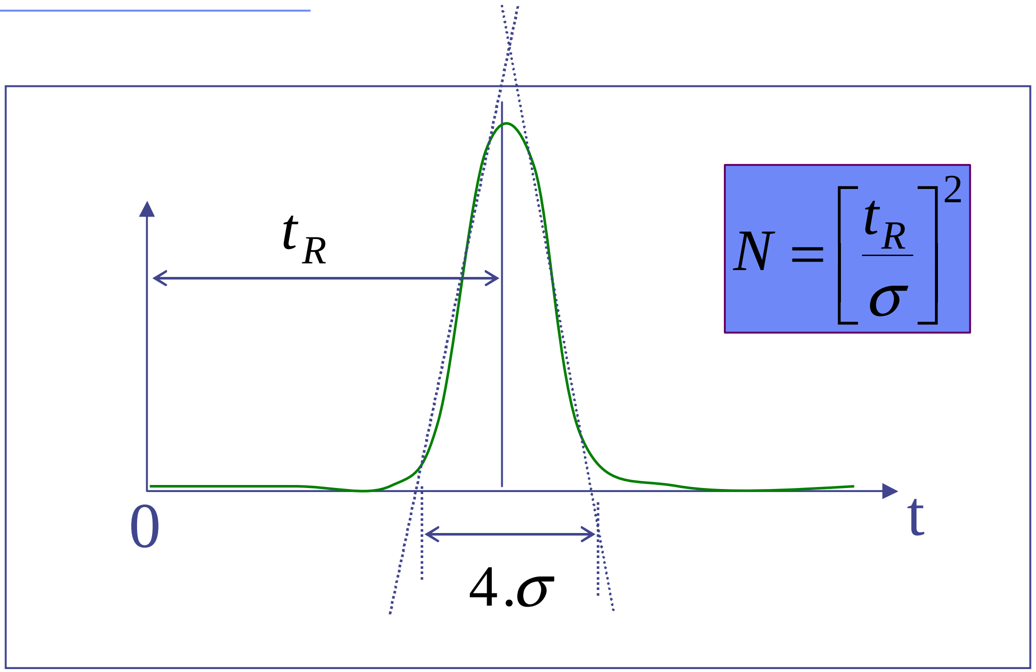
Thermodynamics (Adsorption Isotherm)

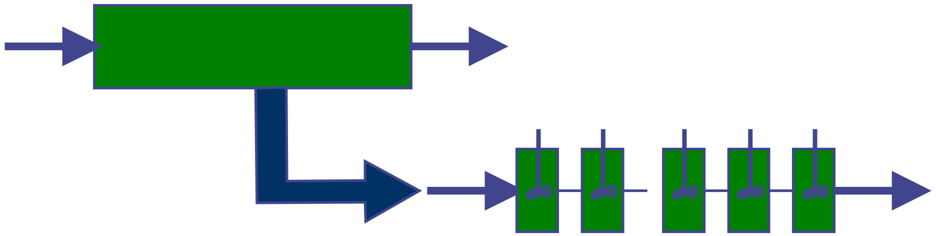
For C_i<<< ⇒ linear part of the isotherm

$$\overline{C_i} = \overline{K_i}\, C_i$$



Column efficiency: plate model





Model N plates (uniform composition)

Column efficiency (N) depends on:

- Liquid velocity (u)
- Column length (L)

Van Deemter model:

$$\frac{L}{N} = A + Bu$$

Pressure drop

The pressure drop (ΔP) over a column filled by monodispersed stationary phase is proportionnal to:

- Column length (L)
- Speed velocity (u)
- 1/(particle diameter)²
- Solvent viscosity

For a fixed eluent and stationary phase: $\frac{\Delta P}{L} = k \cdot u$

Required experiments for modelling

Column efficiency

- 2 Analytical injections at different flowrates

$$\frac{L}{N} = A + Bu$$

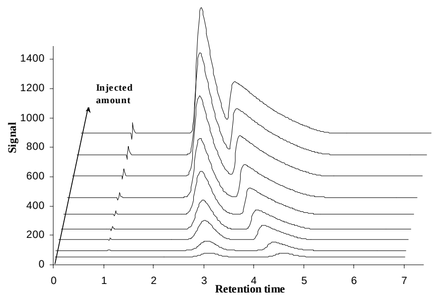
Pressure drop

- 1 Pressure drop measurement

$$\frac{\Delta P}{L} = k \cdot u$$

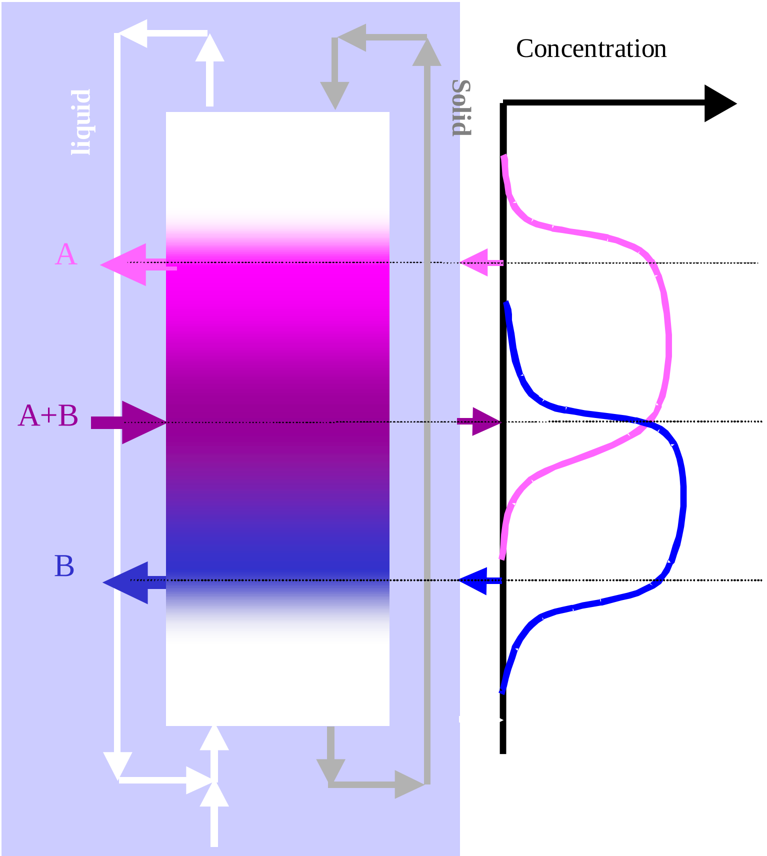
Adsorption isotherm

- Some overloaded injections



$$\overline{C}_i = \lambda_i C_i + \frac{\overline{N}.\tilde{K}_i.C_i}{1 + \sum_{j=1}^{Nesp} \tilde{K}_j.C_j}$$

Calculations of TMB flow rates



Four zones have to be considered

Adsorption of A

Adsorption of B

Desorption of A

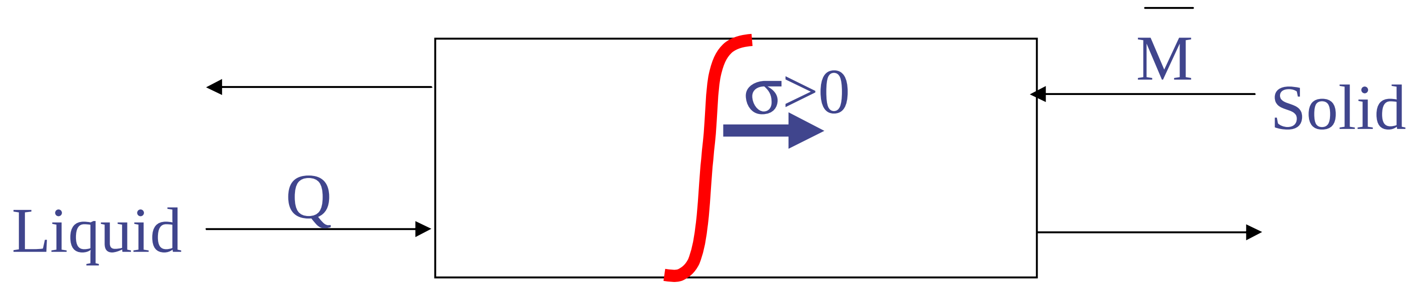
Desorption of B

Each zone have a specific role

Flow rates have to satisfy these constraints

Front Direction in TMB (one zone)

Linear case $\overline{C_i}=\overline{K_i}C_i$



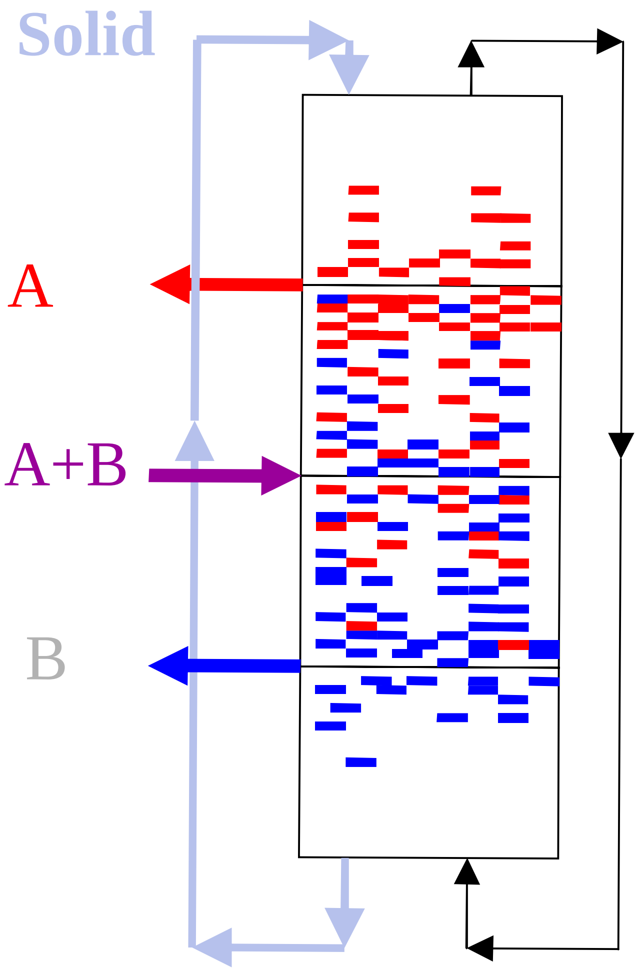
$$\sigma=\frac{\partial z}{\partial t}=\frac{Q-\overline{M}.\overline{K_i}}{\Omega\left(\varepsilon_e+(1-\varepsilon_e).\overline{K_i}\right)}$$

$\sigma>0$ for $\frac{Q}{\overline{M}}>\overline{K_i}$

$\sigma<0$ for $\frac{Q}{\overline{M}}<\overline{K_i}$

TMB Internal flow rates

Linear case $\overline{C}_i = \overline{K}_i C_i$



Zone IV
Adsorption of A

$$q_{IV} = \frac{Q_{IV}}{\overline{M}} \leq \overline{K}_A$$

Zone III
Adsorption of B

$$\left(\overline{K}_A \leq\right) q_{III} = \frac{Q_{III}}{\overline{M}} \leq \overline{K}_B$$

Zone II
Desorption of A

$$\left(\overline{K}_B \geq\right) q_{II} = \frac{Q_{II}}{\overline{M}} \geq \overline{K}_A$$

Zone I
Desorption of B

$$q_I = \frac{Q_I}{\overline{M}} \geq \overline{K}_B$$

TMB flowrates – non linear isotherm Zone I and IV

Zone I :

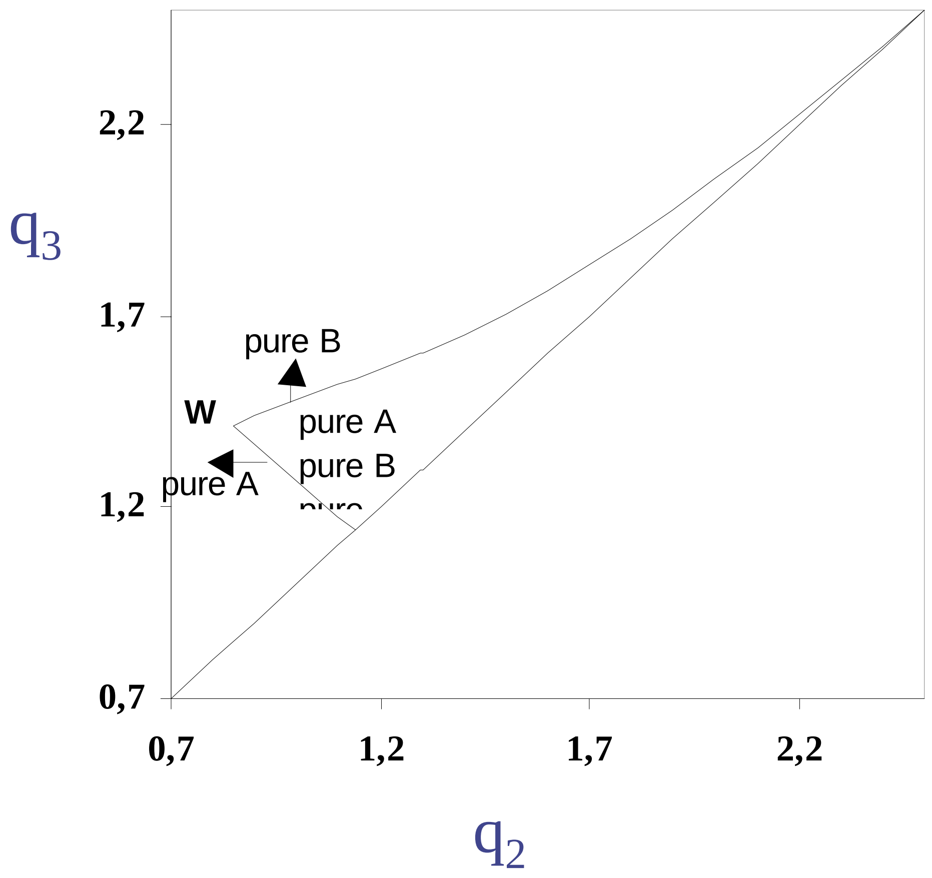
$$q_I \geq \overline{K}_2$$

Zone IV :

$$q_{IV} \leq \frac{1}{2}\left\{\begin{array}{l} \overline{N}\widetilde{K}_1 + q_{III} - \lambda + \widetilde{K}_1 C_A^F (q_{III} - q_{II}) \\ -\sqrt{\left[\overline{N}\widetilde{K}_1 + q_{III} - \lambda + \widetilde{K}_1 C_1^F (q_{III} - q_{II})\right]^2 - 4\overline{N}\widetilde{K}_1 (q_{III} - \lambda)} \end{array}\right\} + \lambda$$

!!!

TMB flowrates – non linear isotherm
Zone II and III

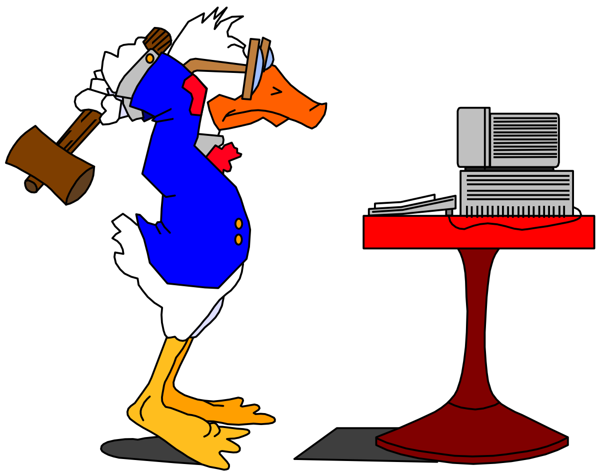


TMB – SMB two equivalent processes

TMB	SMB
Steady state	Periodic steady state
Solid flow-rate $\overline{M}$	Periodic shift of the injection/collection lines $\Delta T = \frac{(1-\varepsilon)V_{col}}{\overline{M}}$
Internal flow-rates $Q_k^{TMB} = q_k.\overline{M}$ k=I, II, III or IV	Internal flow-rates $Q_k^{SMB} = Q_k^{TMB} + \frac{\varepsilon}{1-\varepsilon}\overline{M}$ k=I, II, III or IV
Eluent, extract, feed, raffinate flow-rates $Q_{El}^{TMB}, Q_{Ext}^{TMB}, Q_F^{TMB}, Q_{Raf}^{TMB}$	Eluent, extract, feed, raffinate flow-rates $Q_{El}^{SMB}, Q_{Ext}^{SMB}, Q_F^{SMB}, Q_{Raf}^{SMB}$

Agreement between calculations and experiments

It works !



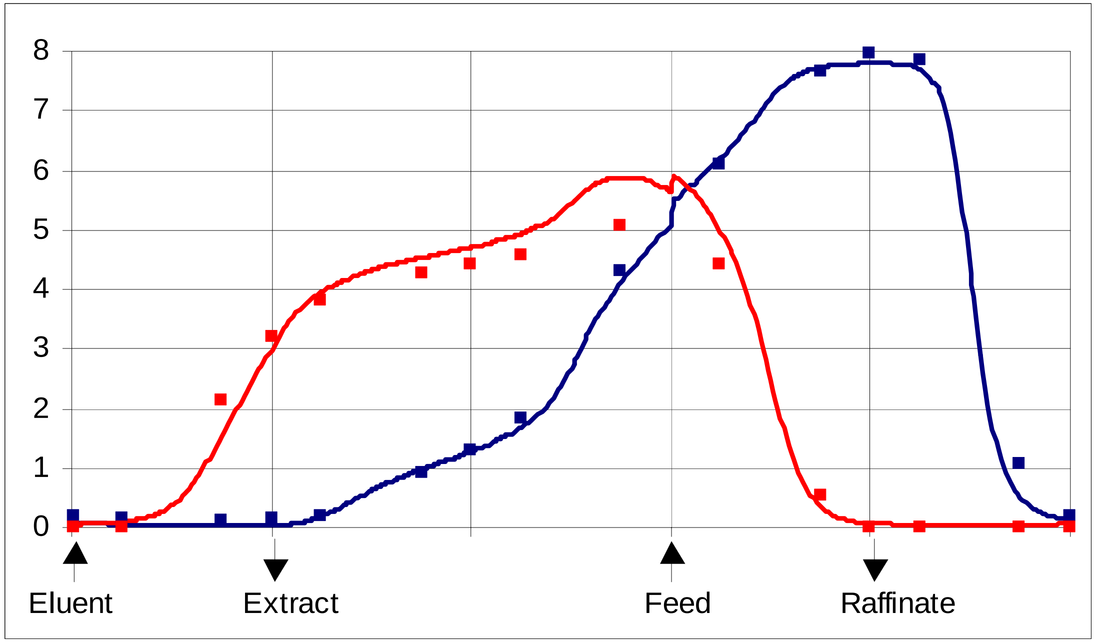
If the input data:

- ***adsorption***
- ***kinetics***
- ***hydrodynamics***

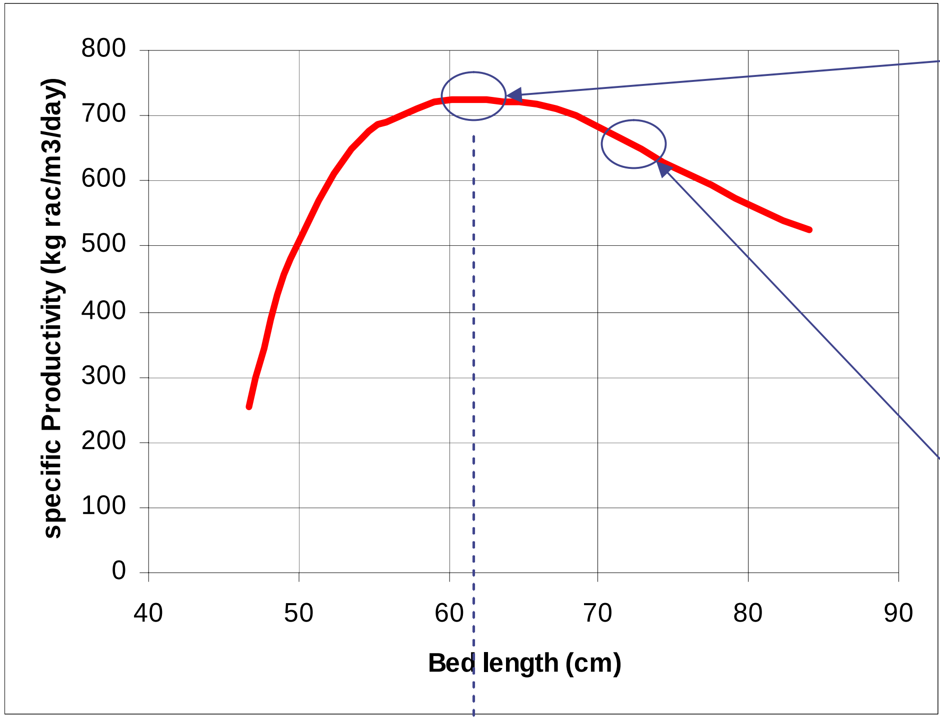
are reliable.

Accuracy of modelling tools

SMB : experimental and simulated internal concentration profiles



Choosing the best conditions



2 effects are taken into account by optimization

Limitation by Col. efficiency

Limitation by Pressure drop

Optimal bed length

Unsecure : bad estimation of column efficiency can involve an important loss of productivity

Secured bed length

Safer : using higher bed length implies a slightly lower but safer productivity