Adaptive Control of **S**imulated **M**oving **B**ed Plants Using Comsol's Simulink Interface

Speaker:

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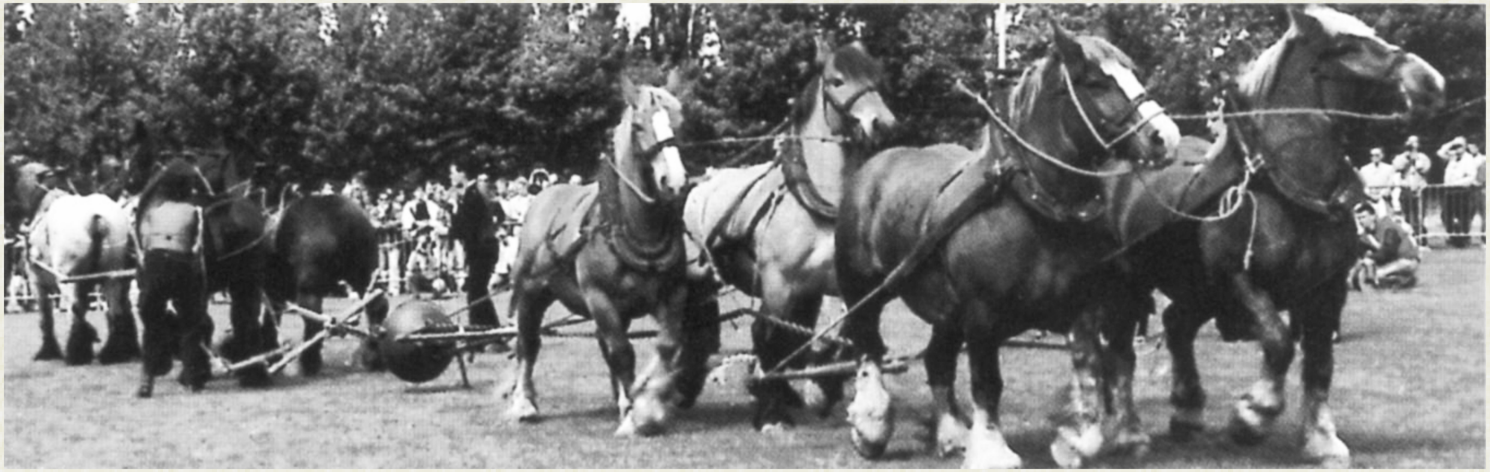
Introduction

Modeling of SMB plants

Control of SMB plants

Conclusions



COMSOL CONFERENCE Hannover 4.-6.Nov. 2008

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Introduction to chromatography

Introduction

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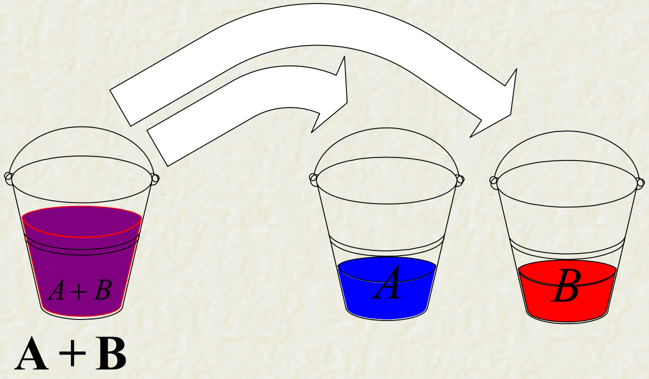
Conclusions

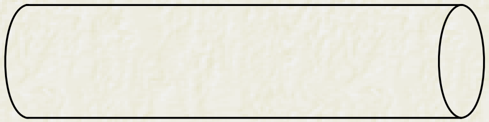
How we can separate a mixture of two components?



One way is to make use of different adsorption affinities of components

Introduction to chromatography

Consider a simple pipe



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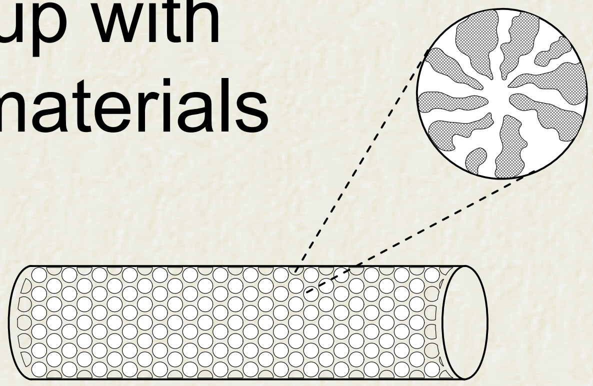
Introduction to chromatography

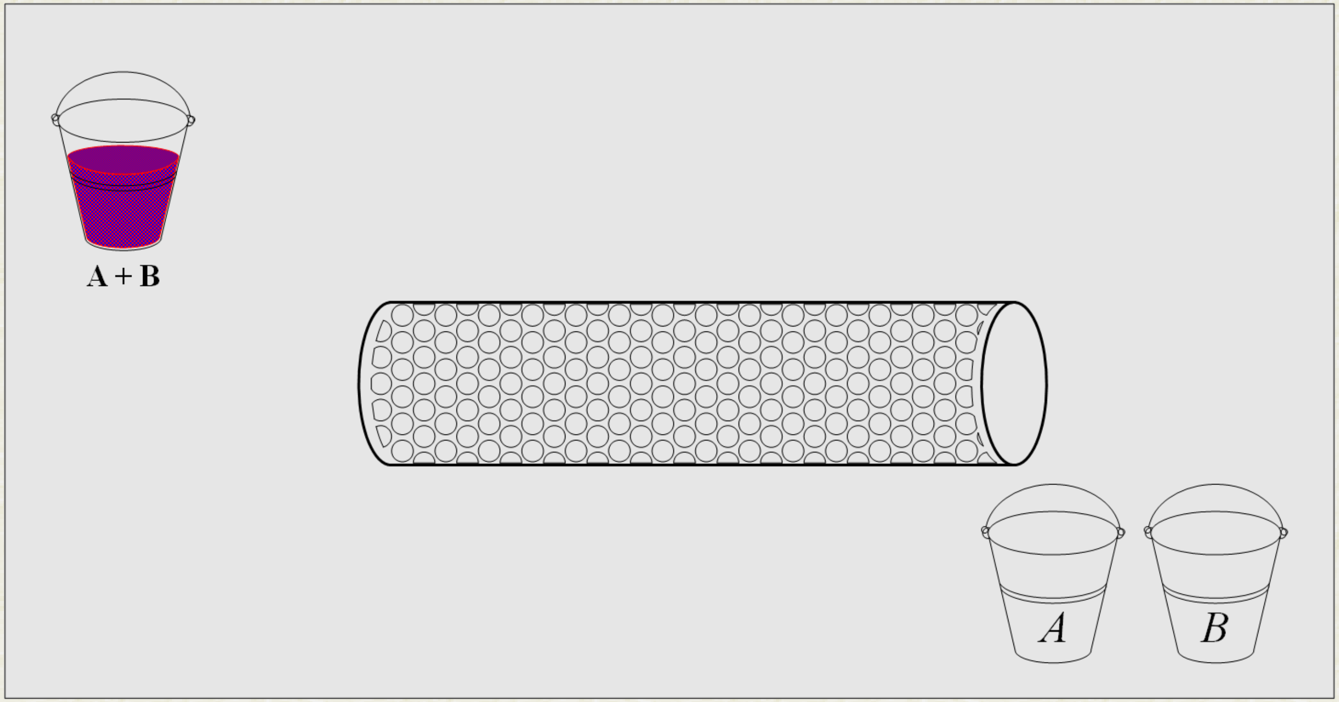
Consider a simple pipe

which is filled up with adsorption materials



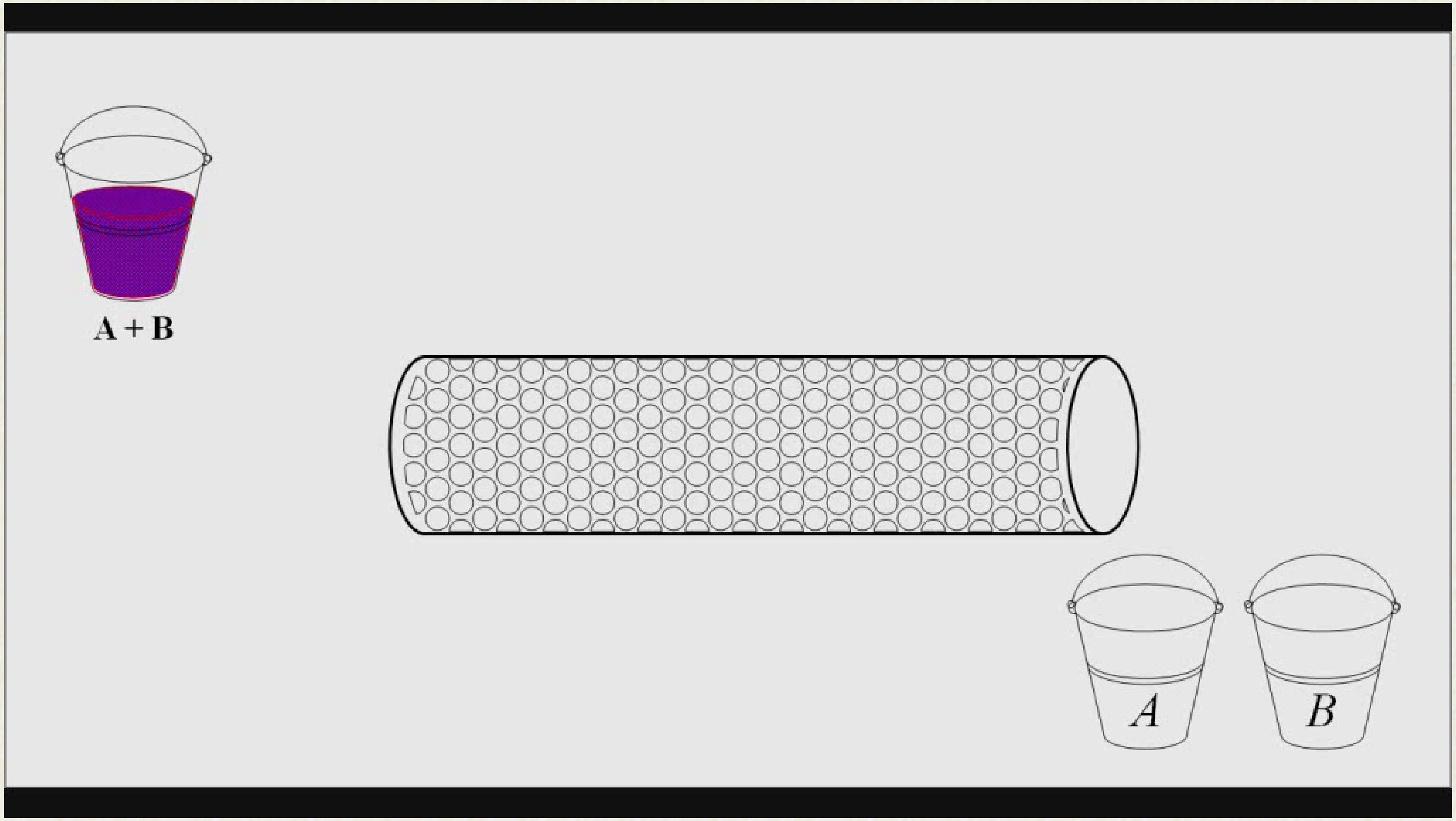
Introduction to chromatography

Now, a bucket with a mixture of two components dissolved in an eluent is pumped through this adsorption column.



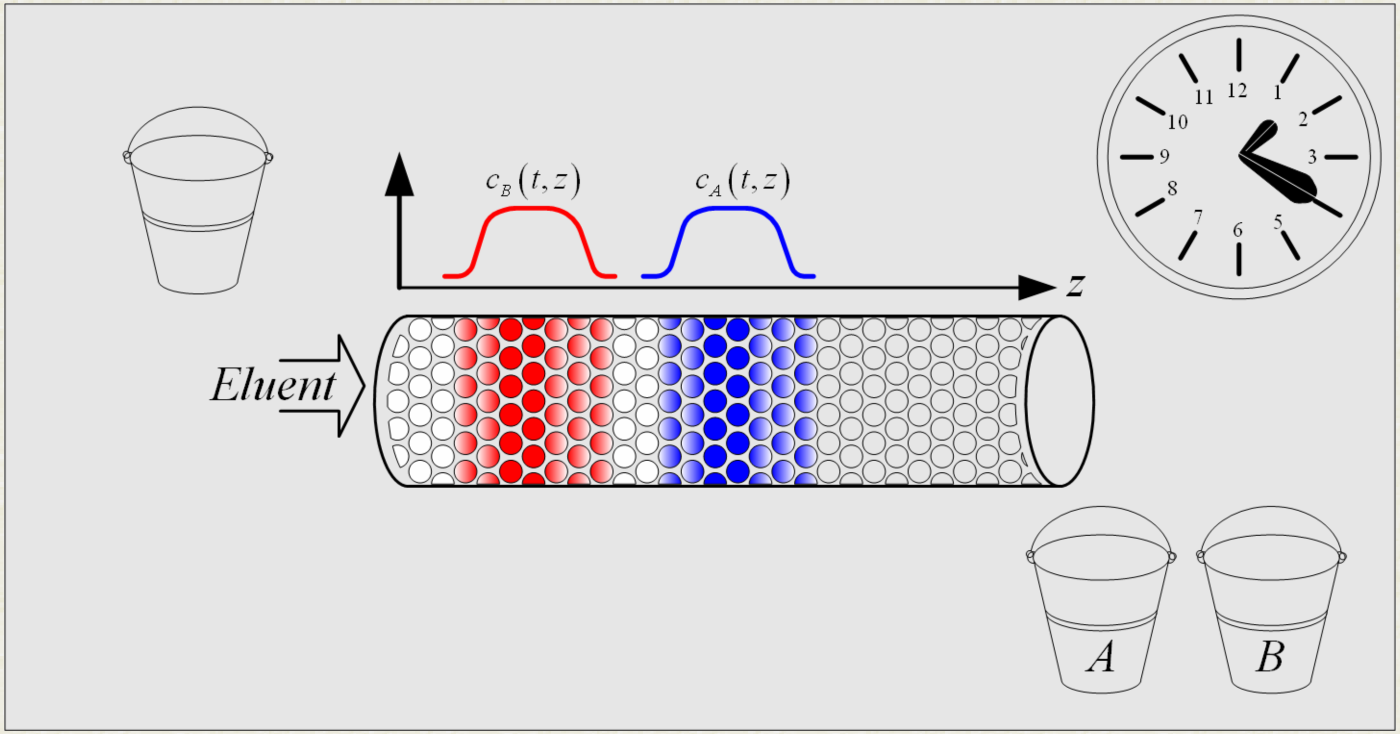
Introduction to chromatography

The more retained component B takes more time to travel through the column as the less retained component A.



Introduction to chromatography

Therefore, chromatography provides a simple method to separate components.



Introduction to simulated moving bed

Introduction

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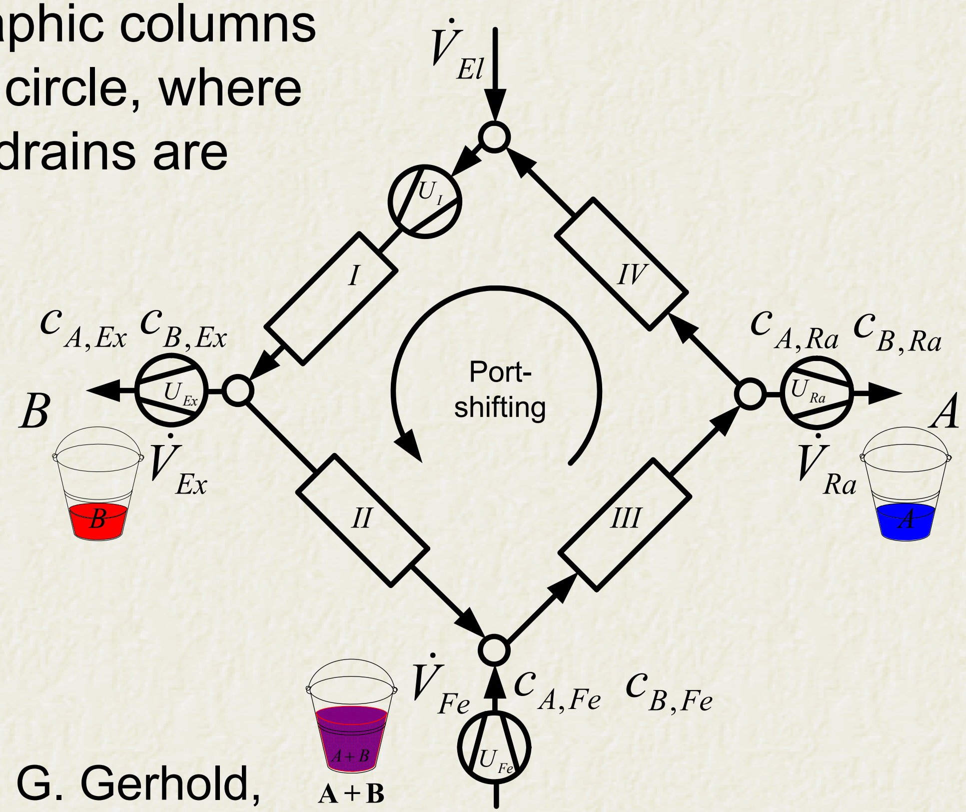
How one can achieve a continuous separation?

Several chromatographic columns are arranged in a circle, where the feedings and drains are shifted cyclically.



Source: D.B. Broughton, G. Gerhold, *US Patent*, 2 985 589 (1961)

Introduction to simulated moving bed

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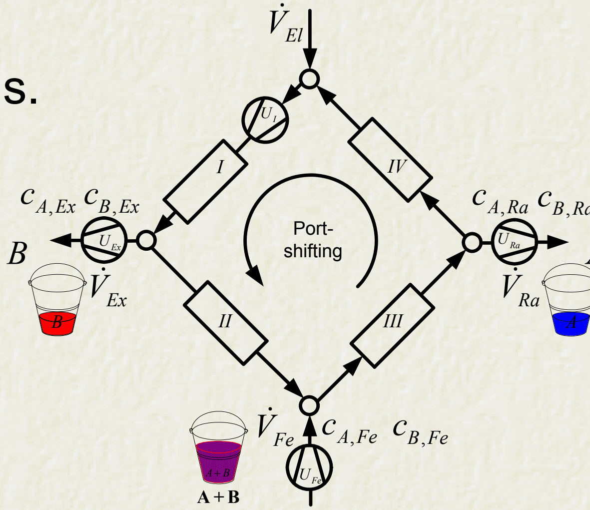
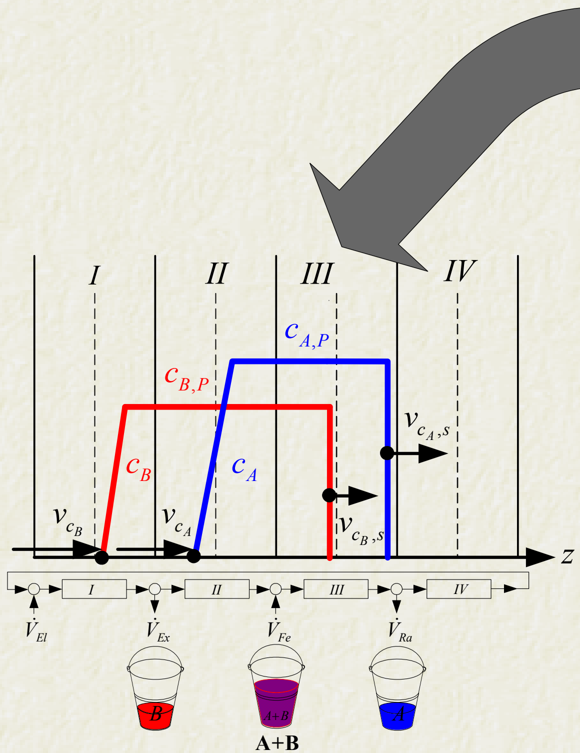
The four zones may be arranged in a plane to plot the associated concentration profile in cyclic-steady-state above the columns.

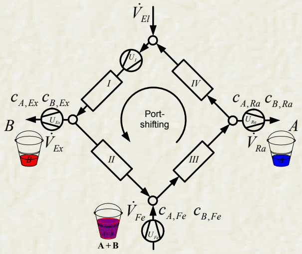


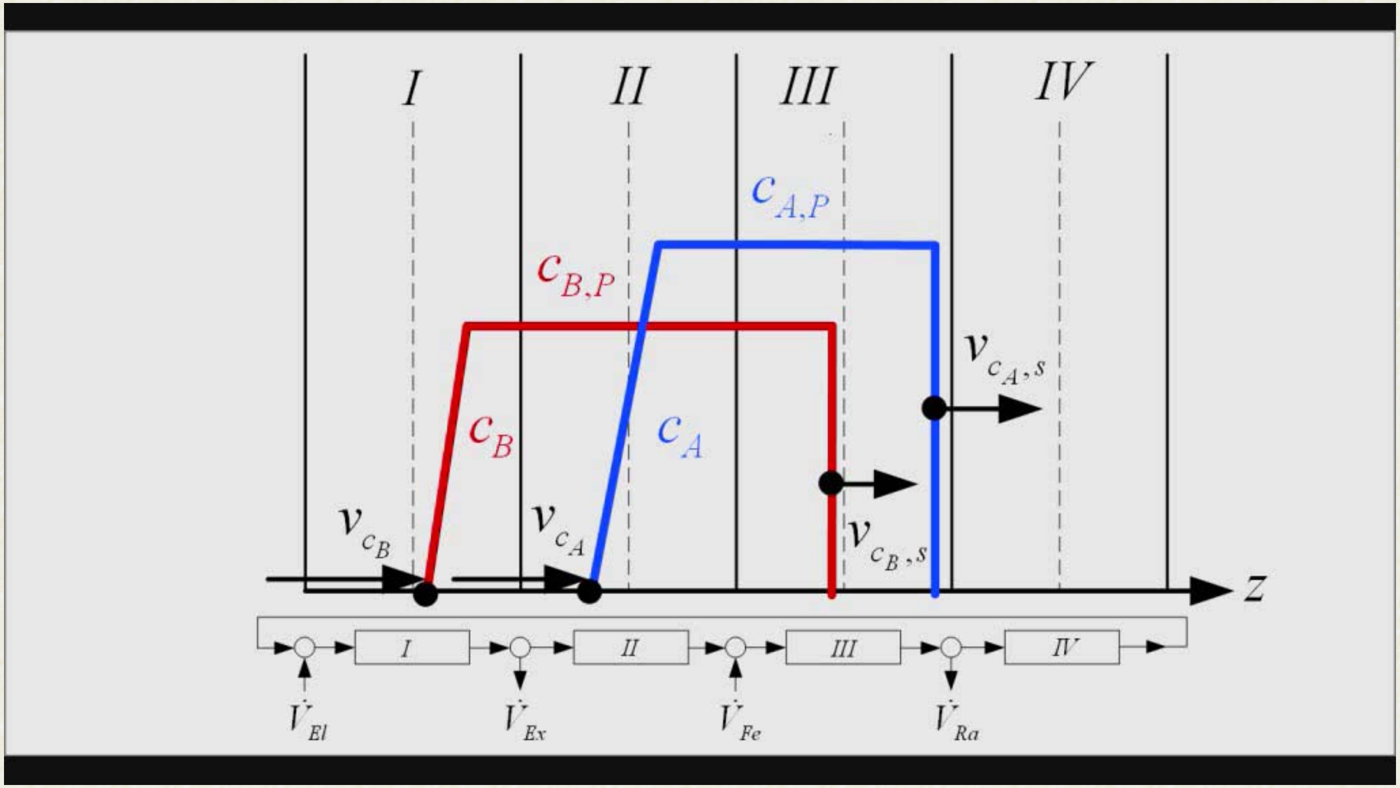


The spatial coordinate is chosen so that this always begins with the first zone

Introduction to simulated moving bed

The four zones may be arranged in a plane to plot the associated concentration profile in cyclic-steady-state above the columns.

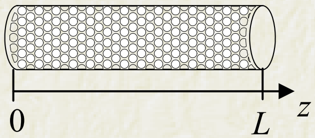




Modeling of a chromatographic column

G. Guiochon, B. Lin, *Modeling for Preparative Chromatography*, Academic Press, San Diego (**2003**)

(fast adsorption)



$$\frac{\partial c_A}{\partial t} + F\frac{\partial q_A(c_A, c_B)}{\partial t} = -v_l \frac{\partial c_A}{\partial z} + D\frac{\partial^2 c_A}{\partial z^2}, \quad F = \frac{1-\varepsilon}{\varepsilon}$$

$$\frac{\partial c_B}{\partial t} + F\frac{\partial q_B(c_A, c_B)}{\partial t} = -v_l \frac{\partial c_B}{\partial z} + D\frac{\partial^2 c_B}{\partial z^2}, \quad v_l = \frac{\dot{V}}{\varepsilon A}$$

left boundary:

$$c_{i,in}(t) = c_i(t,0) - \frac{D\,\varepsilon\,A}{\dot{V}} \frac{\partial c_i(t,z)}{\partial z}\Big|_{z=0} \qquad i = A, B$$

right boundary:

$$\frac{\partial c_i(t,z)}{\partial z}\Big|_{z=L} = 0 \quad i = A, B$$

initial:

$$c_i(0,z) = c_{i,0}(z) \quad i = A, B$$

adsorption behavior

$$q_i = q_i(c_A, c_B) \qquad i = A, B$$

c	fluid concentration
q	adsorbed concentration
$\dot{V}$	volumetric flow rate
ε	void fraction
A	cross section area
D	diffusion

Modeling

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Comsol Implementation

Comsol® Multyphysics Users Guide, Comsol AB, Sweden, http://www.comsol.se (**2005**)

Comsol's pde equation in general form:

$$\mathbf{d_a} \cdot \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{\Gamma} = \mathbf{F}$$

boundary condition in general form:

$$-\mathbf{n} \cdot \mathbf{\Gamma} = \mathbf{G} + \left(\frac{\partial \mathbf{R}}{\partial \mathbf{u}} \right)^T \cdot \boldsymbol{\mu},$$

$$\mathbf{R} = \mathbf{0}$$

$$\mathbf{u} = \begin{pmatrix} c_A & c_B \end{pmatrix}^T,$$

$$\mathbf{d_a} = \begin{pmatrix} 1 + F \cdot \frac{\partial q_A}{\partial c_A} & F \cdot \frac{\partial q_A}{\partial c_B} \\ F \cdot \frac{\partial q_B}{\partial c_A} & 1 + F \cdot \frac{\partial q_B}{\partial c_B} \end{pmatrix},$$

$$\mathbf{\Gamma} = \begin{pmatrix} \frac{\dot{V}}{\varepsilon \cdot A} \cdot c_A - D \cdot \frac{\partial c_A}{\partial z} & \frac{\dot{V}}{\varepsilon \cdot A} \cdot c_B - D \cdot \frac{\partial c_B}{\partial z} \end{pmatrix}^T,$$

$$\mathbf{F} = \begin{pmatrix} 0 & 0 \end{pmatrix}^T.$$

$$\mathbf{G}_{|z=0} = \begin{pmatrix} \frac{\dot{V}}{\varepsilon \cdot A} \cdot c_{A,in} & \frac{\dot{V}}{\varepsilon \cdot A} \cdot c_{B,in} \end{pmatrix}^T,$$

$$\mathbf{G}_{|z=L} = \begin{pmatrix} -\frac{\dot{V}}{\varepsilon \cdot A} \cdot c_A & -\frac{\dot{V}}{\varepsilon \cdot A} \cdot c_B \end{pmatrix}^T,$$

$$\mathbf{R}_{\substack{|z=0 \\ |z=L}} = \begin{pmatrix} 0 & 0 \end{pmatrix}^T.$$

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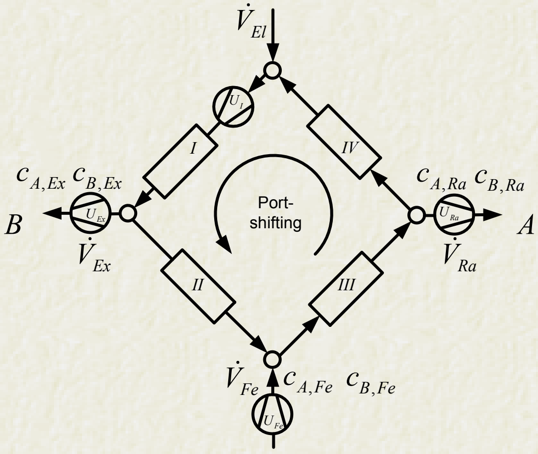
Coupling of columns



External flow- rates: $0 = \dot{V}_{El} + \dot{V}_{Fe} - \dot{V}_{Ex} - \dot{V}_{Ra}$

Eluent feed: $\dot{V}_I = \dot{V}_{IV} + \dot{V}_{El}$ $\quad c_{i,in,I} \cdot \dot{V}_I = c_{i,out,IV} \cdot \dot{V}_{IV}$ $\quad i = A,B$

Extract- drain: $\dot{V}_{II} = \dot{V}_I - \dot{V}_{Ex}$ $\quad c_{i,in,II} = c_{i,out,I} = c_{i,Ex}$ $\quad i = A,B$

Feed: $\dot{V}_{III} = \dot{V}_{II} + \dot{V}_{Fe}$ $\quad c_{i,in,III} \cdot \dot{V}_{III} = c_{i,out,II} \cdot \dot{V}_{II} + c_{i,Fe} \cdot \dot{V}_{Fe}$

Raffinate- drain: $\dot{V}_{IV} = \dot{V}_{III} - \dot{V}_{Ra}$ $\quad c_{i,Ra} = c_{i,in,IV} = c_{i,out,III}$ $\quad i = A,B$

Determining Operating points

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$$\dot{V}_I, \dot{V}_{Ex}, \dot{V}_{Fe}, \dot{V}_{Ra}, T_S \;?$$

Given: $c_{A,Fe}$ $c_{B,Fe}$ $\dot{V}_{Fe}$ $0 \ll \tau_{B,I} \le 1$ $0 \ll \tau_{A,IV} \le 1$

$$c_{B,0} = \frac{1}{K_B} \cdot \frac{H_B - H_A}{\sqrt{H_A \cdot H_B} + H_A} \qquad c_{B,Fe} > c_{B,0}$$

$$c_{A,P} = \frac{H_B - H_A}{2} \cdot \frac{\left(\sqrt{(H_B - H_A)^2 \cdot (1 + K_A \cdot c_{A,Fe})^2 + 4 \cdot H_A \cdot \left(\sqrt{H_B} + \sqrt{H_A}\right)^2 \cdot K_A \cdot K_B \cdot c_{A,Fe} \cdot c_{B,Fe}} - (H_B - H_A) \cdot (1 - K_A \cdot c_{A,Fe})\right)}{K_A \cdot \left(H_A \cdot \left(\sqrt{H_B} + \sqrt{H_A}\right)^2 \cdot K_B \cdot c_{B,Fe} + (H_B - H_A)^2\right)}$$

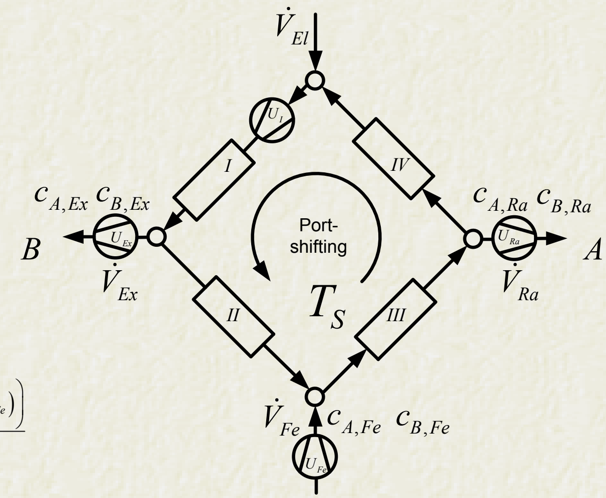
$$c_{B,P} = \frac{H_B - H_A}{K_B} \cdot \frac{\left(\sqrt{H_B} + \sqrt{H_A}\right)^2 \cdot K_B \cdot c_{B,Fe} - (H_B - H_A)}{H_A \cdot \left(\sqrt{H_B} + \sqrt{H_A}\right)^2 \cdot K_B \cdot c_{B,Fe} + (H_B - H_A)^2}$$

$$\dot{V}_I = \frac{\left(\sqrt{H_B} + \sqrt{H_A}\right)^2 \cdot \left[F \cdot \left(H_B - H_A \cdot (1 - \tau_{B,I})\right) + \tau_{B,I}\right]}{F \cdot \tau_{B,I} \cdot (H_B - H_A)^2} \cdot K_B \cdot c_{B,Fe} \cdot \dot{V}_{Fe}$$

$$\dot{V}_{Ex} = \frac{\left(\sqrt{H_B} + \sqrt{H_A}\right)^2}{\tau_{B,I} \cdot (H_B - H_A)} \cdot K_B \cdot c_{B,Fe} \cdot \dot{V}_{Fe}$$

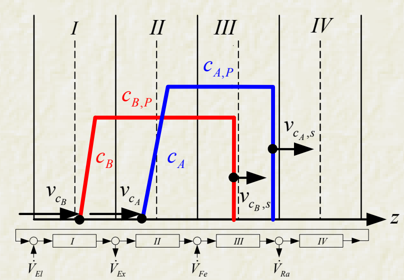
$$\dot{V}_{Ra} = \frac{c_{A,Fe}}{\tau_{A,IV} \cdot c_{A,P}} \cdot \dot{V}_{Fe}$$

$$T_S = \frac{F}{1+F} \cdot \frac{A \cdot L}{\dot{V}_{Fe}} \cdot \frac{(H_B - H_A)^2}{\left(\sqrt{H_B} + \sqrt{H_A}\right)^2 \cdot K_B \cdot c_{B,Fe}}$$



adsorption behavior

$$q_i = \frac{H_i \cdot c_i}{1 + K_i \cdot c_i}$$



M. Fütterer, *Chem. Eng. Tech.*, **2009**, *32*
http://dx.doi.org/10.1002/ceat.200800397

Control of SMB Plants

Why control?

1. robust operation in presence of disturbances

2. minimize running costs

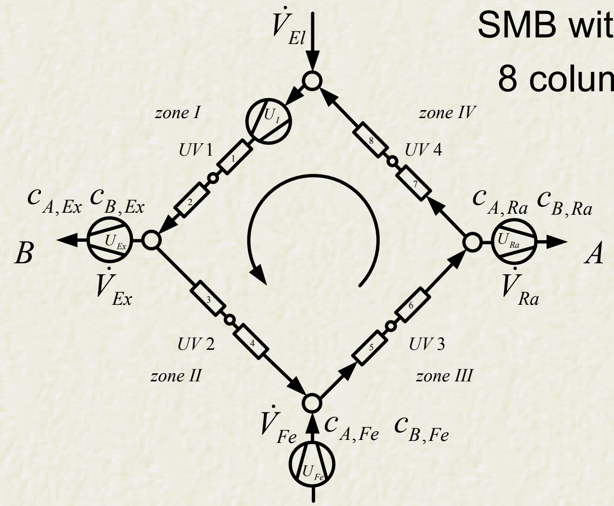
   e.g. reducing eluent consumption

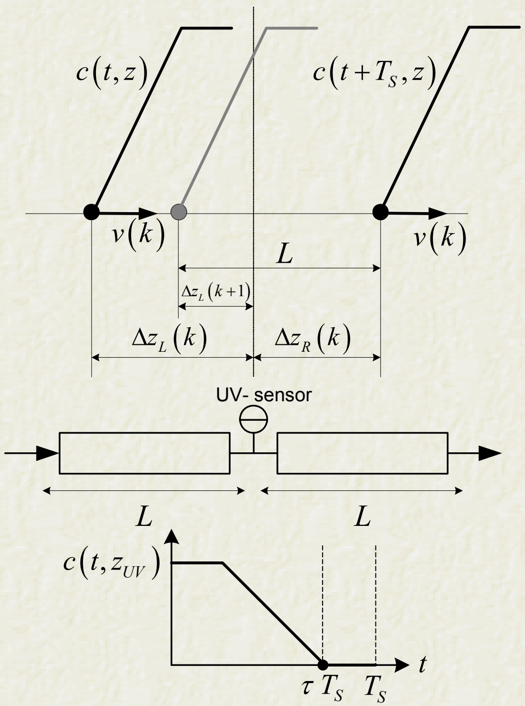
Control of SMB Plants for complete separation

Model the essential dynamic

- UV- sensor mounted between two columns of one zone
- keep all controls fixed during one switching time
- model only the foot point movement.

SMB with 8 columns





$$\Delta z_L(k) = v(k)\tau(k)T_S(k), \quad \tau \in [0,1]$$

$$\Delta z_R(k) = v(k)\left(1-\tau(k)\right)T_S(k)$$

$$\Delta z_L(k+1) = L - \Delta z_R(k)$$

$$v(k+1)\tau(k+1)T_S(k+1) = L - v(k)\left(1-\tau(k)\right)T_S(k)$$

$$\tau(k+1) = \frac{L - v(k)\left(1-\tau(k)\right)T_S(k)}{v(k+1)T_S(k+1)}$$

M. Fütterer, *Chem. Eng. Tech.*, **2008**, *31 (10)*, 1438.
http://dx.doi.org/10.1002/ceat.200800277

Control of SMB Plants for complete separation

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Rename the variables to make it nice for control peoples.

model equations:

$$u_i(k) = \dot{V}_i(k) \quad i = 1,2,3,4 \quad u_5(k) = T_S(k) \qquad v_i(k) = \frac{L}{\theta_i} \cdot \dot{V}_i(k) \quad \theta_i = \hat{u}_i^* = \dot{V}_i^* \cdot T_S^*$$

$$\hat{u}_i(k) = u_i(k) u_5(k) \quad y_i(k) = \tau_i(k-1) \qquad i = 1,2,3,4$$

$$y_i(k+1) = \frac{\theta_i - \hat{u}_i(k-1)(1 - y_i(k))}{\hat{u}_i(k)}$$

Use a P- controller with ideal open loop control:

$$\hat{u}_i(k) = \hat{\theta}_i - 0.25 \cdot \left(y_{i,ref} - y_i(k)\right) \cdot \hat{\theta}_i \qquad i = 1,2,3,4$$

Use a parameter estimator for model parameters:

$$\hat{\theta}_i(k) = \hat{\theta}_i(k-1) + (1 - a_\theta) \cdot \hat{u}_i(k-1) \cdot \left(y_i(k) - \hat{y}_i(k)\right) \qquad |a_\theta| < 1 \qquad i = 1,2,3,4$$

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M. Fütterer, *Chem. Eng. Tech.*, **2008**, *31 (10)*, 1438.
http://dx.doi.org/10.1002/ceat.200800277

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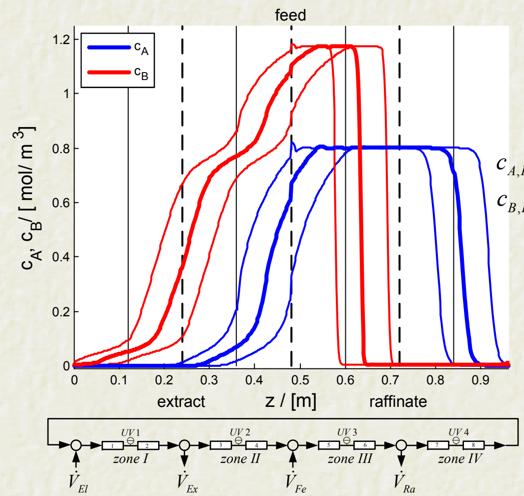
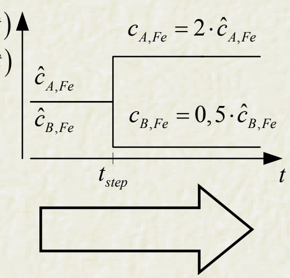
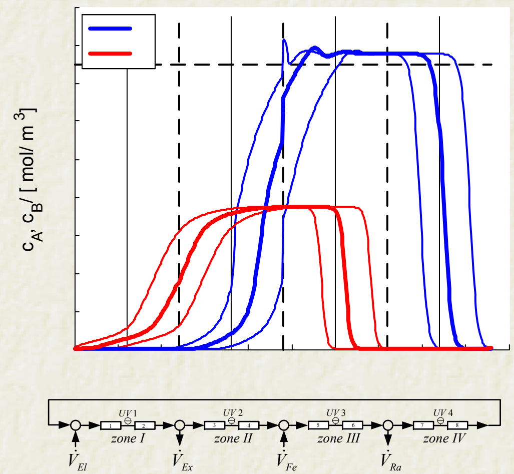
Simulation Results

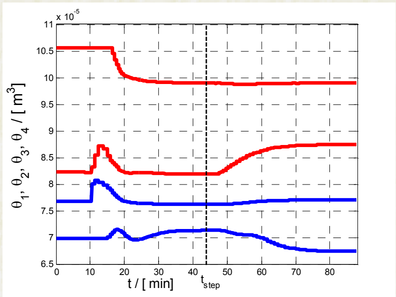
$$q_i(c_i) = \frac{H_i \, c_i}{1 + K_i \, c_i} \qquad i = A, B$$

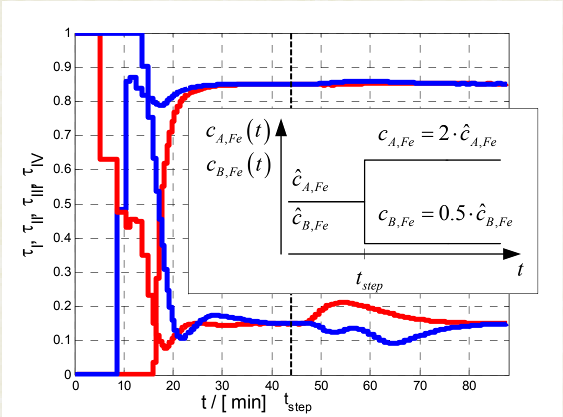


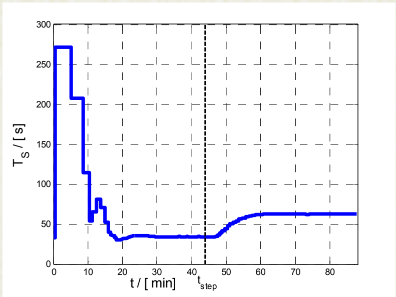
a counter step disturbance











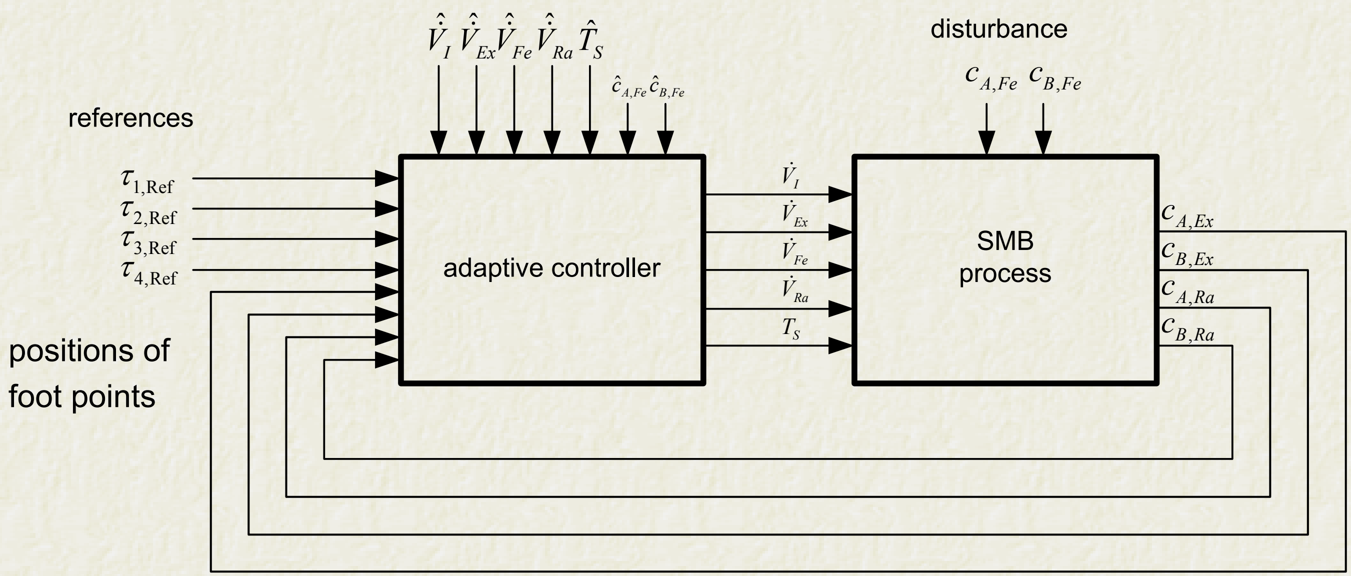
M. Fütterer, *Proc. of the European COMSOL Conf. 2008*
http://www.comsol.se/academic/papers

Control of SMB Plants for complete separation

Control concept with minor a-priori knowledge.

More knowledge is not necessary than for operation in open loop!

Plug and Play solution



Conclusions

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An adaptive control concept of SMB plants was successfully implemented and tested using Comsol® Multiphysics and Matlab® Simulink®.

Comsol is a powerful tool to model complex dynamic systems described by partial differential equations.

Comsol's interface to Matlab Simulink provides control designers a simple way to design and test control loop's in familiar Simulink environment.

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End of Presentation

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- Details can be found at Comsol's conference CD.
- The full simulation example will be made public for everyone.

Thank You