NC STATE UNIVERSITY

Reducing the Complexity of Separation Dynamics using the Computational Analysis through Finite Volume Schemes in Multi-Component Gradient Elution Chromatography.

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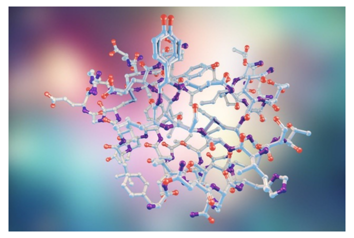
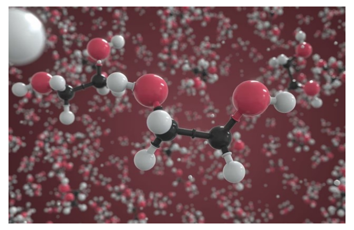
Why Chromatographic Technologies Require?

- **World of Chromatographic Science:**

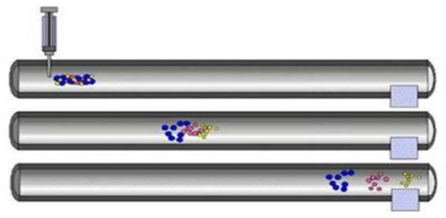
Chromatography: separation technique and high purity and productivity



Evaluating HPLC

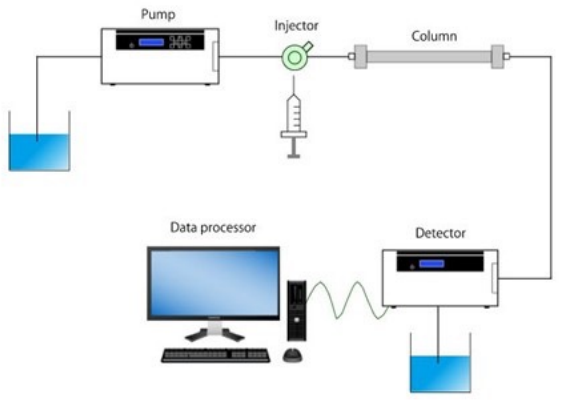


Separation of PEO

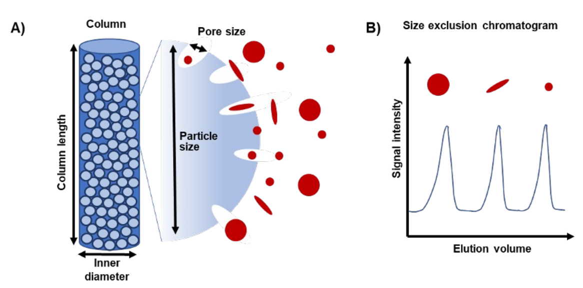


Movement of components

- **EXPERIMENTAL SYSTEM:**



Experimental process



2 Nobel Prizes!

What is Application?

- Pharmaceutical Company: Identify amount of chemicals in new product.
- Environmental Agency: Determine the level of pollutants in water supply.
- Biological application: Separate and identify amino acids, carbohydrates, fatty acids and other natural substances that are the parts of any mixture.
- Law Enforcement: Comparing crime scene samples to suspect samples. Manufacturing Plant: To purify a chemical that needed to make new product.

Mathematical Model:

- **Non-linear LKM Model :**

$$\frac{\partial c_i}{\partial t} + u\frac{\partial c_i}{\partial z} = D_{z,i}\frac{\partial^2 c_i}{\partial z^2} - F\frac{\partial q_i}{\partial t},\quad \frac{\partial q_i}{\partial t} = k_{m,i}(\phi)(q_i^*(\phi(t,z)) - q_i),\quad i = 1,\cdots,N_c$$

$$c_i(z,0) = q_i(z,0) = 0,\quad \text{and}\quad c_i(0,t)\begin{cases} c_{i,inj}, & \text{if}\quad 0 < t < t_{inj} \\ 0, & \text{if}\quad t > t_{inj}\end{cases},\quad \frac{\partial c_i(L,t)}{\partial z} = 0$$

- **Transport Model:**

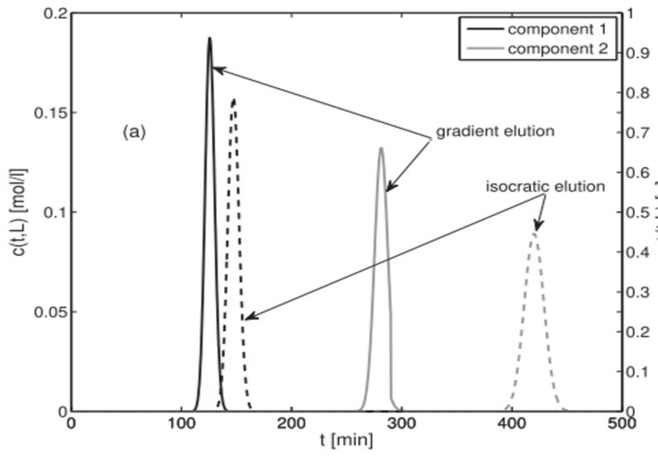
A transport model is used to describe gradient elution in liquid chromatography. The ideal model is:

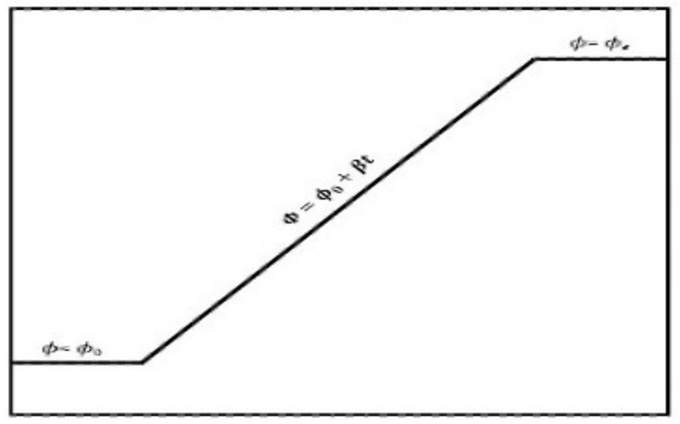
$$a\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial z} = 0, \phi(0,z) = \phi_0,\ z\epsilon[0,L]\ and\ \phi(t,0) = \begin{cases} \phi_0 & if\quad t < t_s \\ \phi(t-t_s) & if\quad t_s \le t \le t_e \\ \phi_e & if\quad t > t_e\end{cases}$$

Types of Elution:

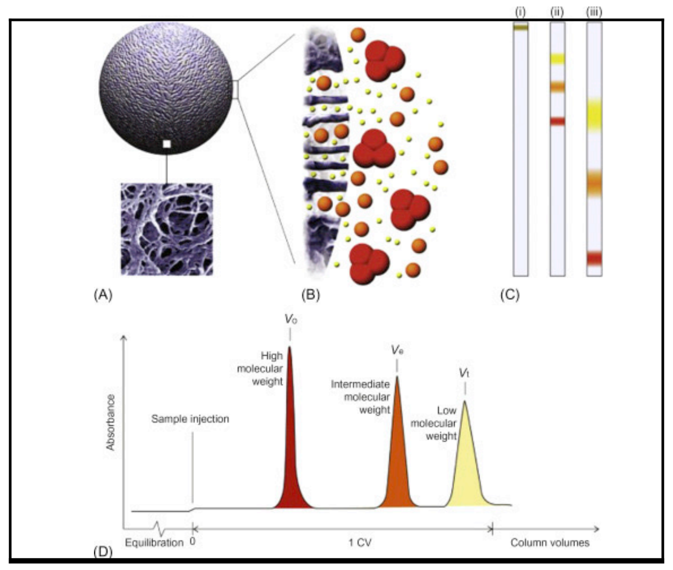
Gradient Elution: Mobile phase composition that changing steadily during process of chromatographic run.
Isocratic Elution: Mobile phase composition that is not changing during the process of chromatographic run.

Parameters and Computer Simulation:



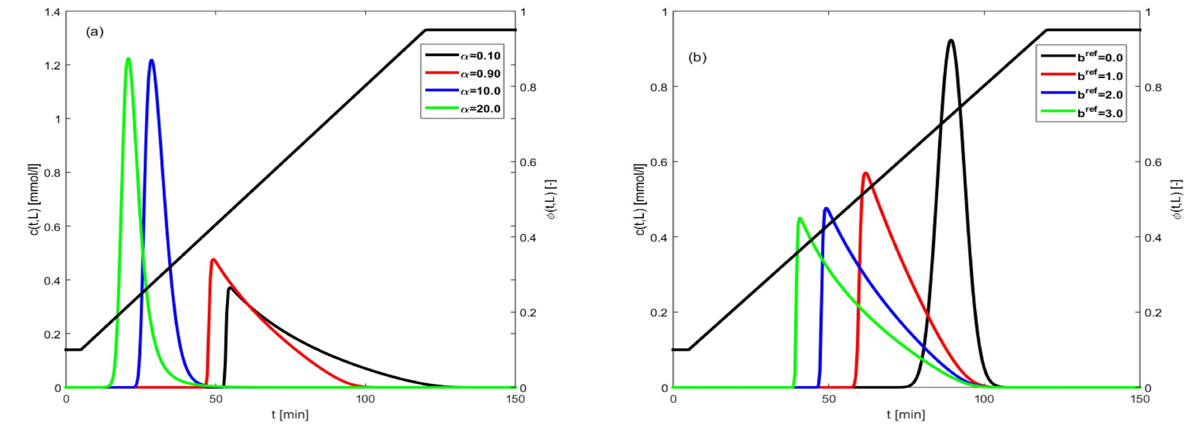


Symbol	Quantity	Value
L	Column Length	$10\ cm$
u	Interstitial velocity	$1.0\frac{cm}{\text{min}}$
k_{Hr}	Henry's constant	7
α	Solvent strength	0.90
b^{bref}	Nonlinearity coefficient	2
c_{inj}	Injected concentration	$10min^{-}$
k_L	Mass transfer coefficient	$1\frac{mol}{l}$

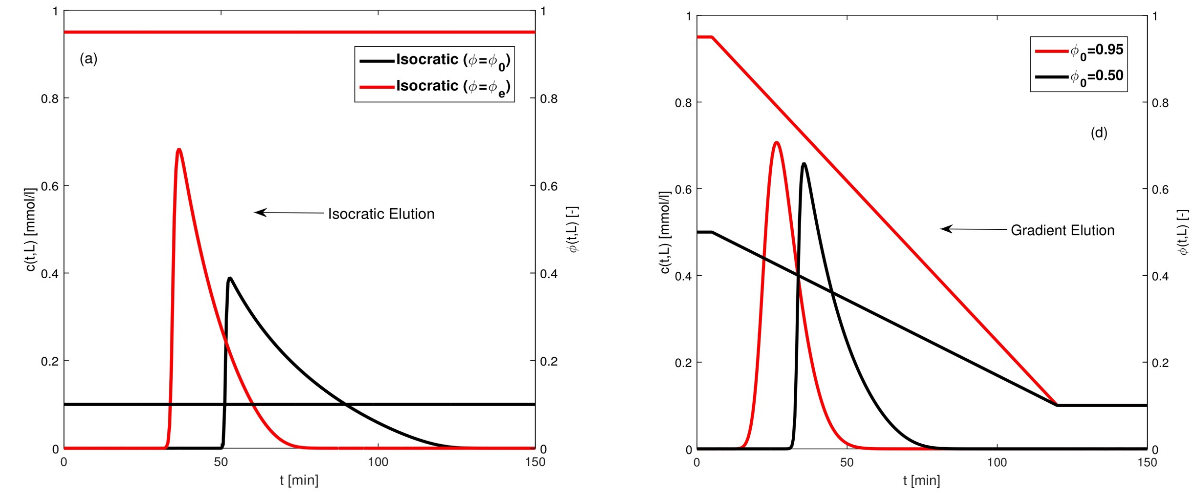


RESULTS OF SIMULATION & EXPERIMENTS:

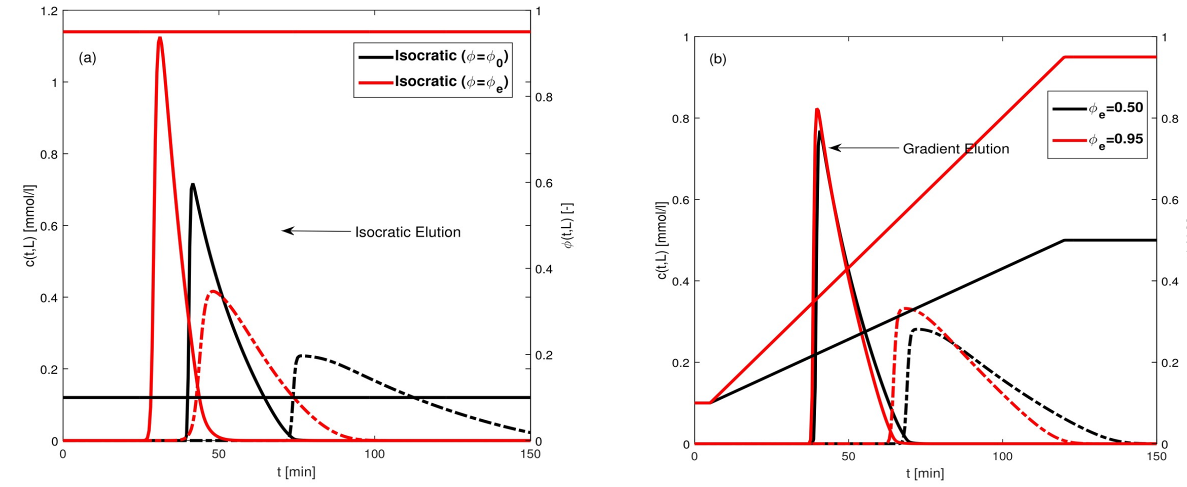
- **One component profiles:**



- **One component elution profiles:**



- **Two component elution profiles:**



SUMMARY AND OUTLOOK:

- Each type of gradient elution affect the adsorption isotherms uniquely.
- Elution technique improves retention and the cycle times, selectivity.

Reference:

[1] Qamar, S., Rehman, N., Carta, G., Seidel-Morgenstern, A. (2020). Analysis of gradient elution chromatography using the transport model. Chem. Eng. Sci. 115809.
[2] N. Rehman; Abid, M.,;S. Qamar,"Numerical approximation of nonlinear and the nonequilibrium model of gradient elution chromatography"-Journal of Liquid Chromatography & and Related T.