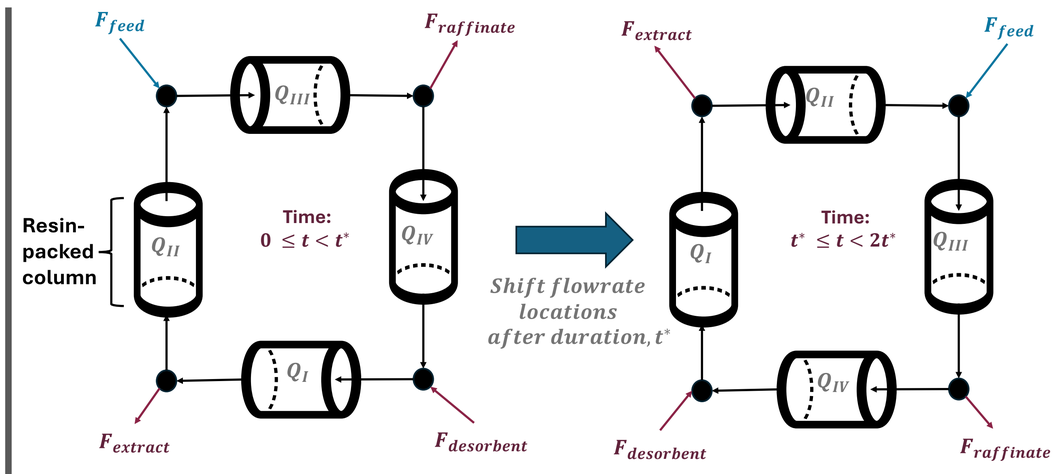
1. Introduction

Simulated Moving Bed chromatography (SMB) is an advanced multi-column chromatographic technique used as a continuous mode of solid-liquid separation. SMB has been greatly adopted in multiple industries (e.g. sugar, pharmaceuticals) due to its proven ability to result in enhanced purity and yield.

Objectives:

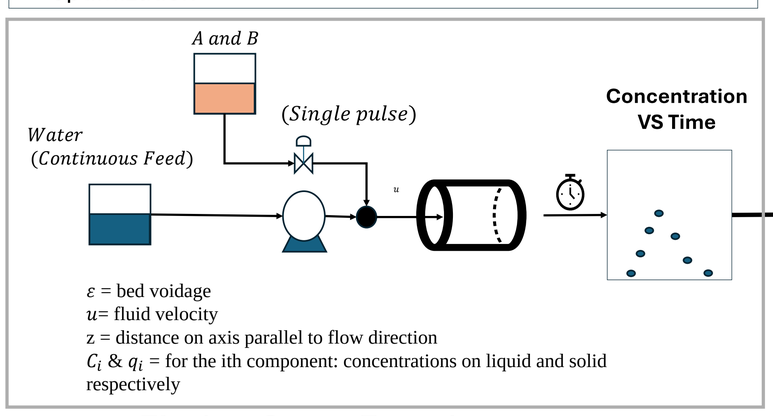
- ❑ Develop a SMB mechanistic model to determine optimal operating conditions for separating:
  (i) borate from hydrochloric acid (HCl) and
  (ii) fructooligosaccharides (FOS).
- ❑ Perform non-linear regression on experimental data to estimate SMB model parameters.
- ❑ Optimization routines focused on maximizing the purities of desired components in raffinate and/or extract streams.



KEY INDEPENDAENT VARIABLES (KIV)	***KEY DEPENDAENT VARIABLES (KDV)***
Flowrates in nth column: Q_i $(for\ i = I, II, III, or\ IV)$	• Raffinate and Extract **Purities** and **Recoveries** and • Productivity (Solvent usage)
Indexing time interval: t^*	

2. Methods

Rationale
The principle of chromatography is the separation of a component A from B based on respective "speeds" of travel through the column. Speed of travel is captured in the isotherm (H) and dispersion (D) and mass transfer kinetic terms (kfp). Once these are measured, possible flowrate recommendations can be estimated from SMB optimization



Elution Curve Experiments

Phase 1: Regression

Column Model

$$\frac{\partial C_i}{\partial t} = D\frac{\partial^2 C_i}{\partial z^2} - \left(\frac{u}{\varepsilon}\right)\cdot\frac{\partial C_i}{\partial z} - \left(\frac{1-\varepsilon}{\varepsilon}\right)\cdot\frac{\partial q_i}{\partial t}$$

$$\frac{\partial q_i}{\partial t} = k_{fp}(q_i^* - q_i)$$

$$q_i^* = f(C_i) = H \cdot C_i$$

Model

Data

NL-Regression
Learn/Estimate Dynamic parameters: D, k_{fp}, H

Fit

D, k_{fp}, H

Phase 2: Optimization

SMB Model

(Column Model × Multiple Columns) + Time Dependent Boundary Conditions

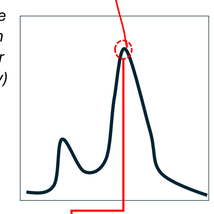
Inputs: $Q_I, Q_{II}, Q_{III}, Q_{IV}, t^*, D, k_{fp}, H$

Outputs (for Objective Function): Purity &/or Recovery

Model

Optimization Routine
Learn/Estimate the combination of input parameters that Parameters that maximize Purity &/or Recovery

Objective Function (Purity or Recovery)

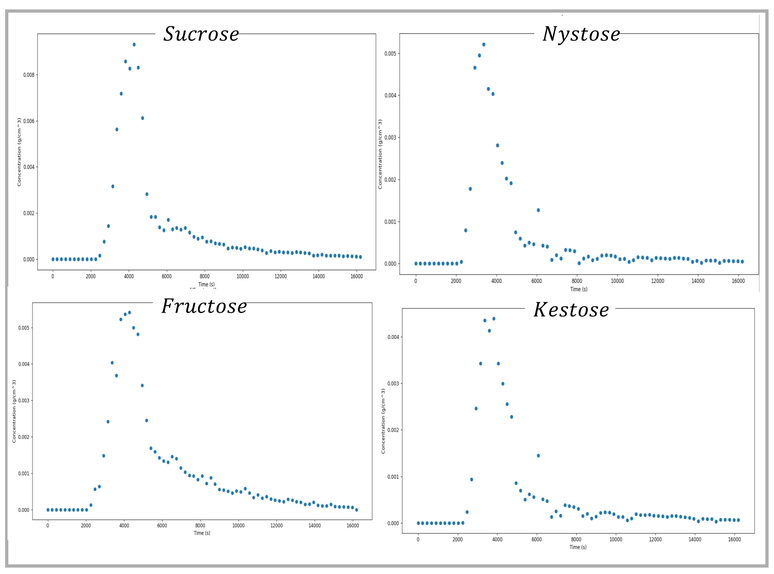


Global Maximum i.e. highest possible purity and recovery

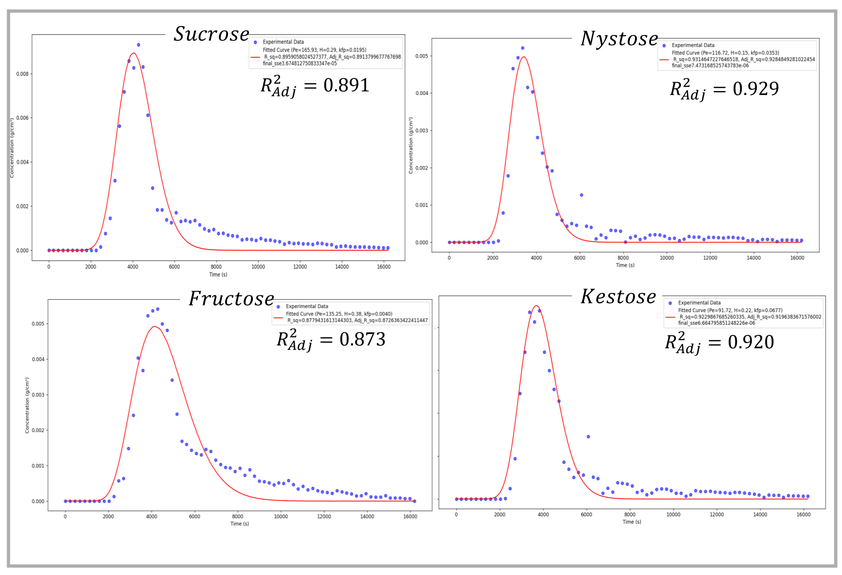
$[Q_I, Q_{II}, Q_{III}, Q_{IV}, t^*]$

*Operating Parameters that give **highest** purity/recovery*

3. Results



Experimental Data



NL-Regression Results

Optimization Results – coming soon!

*However, here are literature results **reproduced** by the developed SMB model:*

Model Results
[Glucose, Fructose]
Feed/Initial Purity: [50, 50] %
Extract Purity: [81.12, 18.87] %, Literature: [85.21, ...]%
Raffinate Purity: [8.24, 91.75] %, Literature: [....., 93.27]%

Stellenbosch UNIVERSITY IYUNIVESITHI UNIVERSITEIT

Machine Learning Group