Instruction of One-Column Analogue for Reproducing the Fully Simulation

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Contents

1 Theoretical basis of the One-Column Analogue

In this part, the periodical four-section process is reproduced by a single-column setup with a recycle lag of $(N-1)t_s$ time units, where the N is the number of columns and t_s is the switching interval, hence the name one-column analogue. The ideal one-column analogue process is theoretically indistinguishable from the equivalent SMB, except for the discontinuous use of the inlets/outlets. And we are not going to discuss how this process can be implemented in practice, since some external tanks/tubes for the discontinuous inlets/outlets are required. It has the advantages of simplicity, only one column would be packed, and less time consuming. This is important for industrial simulation, especially when the optimization is taken into consideration. One-column analogue would decrease the computational efforts tremendous.

For brevity of presentation, the same cases with the previous part are employed. It is the separation of glucose and fructose. The adsorption equilibrium is described by a linear isotherm model.

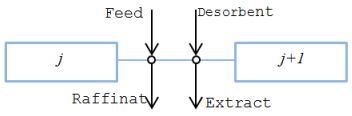
We do not start with mathematical basis of the SMB process again, since it was involved in the former part which is focused on the fundamentals. As known, the cyclic operation of the SMB process is achieved by moving the inlet and outlet ports one column downstream (in the direction of fluid flow) every t_s time units. The working principle of the SMB is illustrated in Fig.1. And due to previous work from our group, we do not track the internal composition profile (the immediate concentration) in each column of process, but instead we follow the outlet concentration of each column. In the one-column analogue, the concentration tracking from the outlets is still adopted, but it has $(N-1)t_s$ lag instead of t_s lag in fully simulation. The following part is the proof:

Proof. Assuming the loop is already under cyclic steady state (CSS), and i represents component while j represents the column index. Once the CSS is reached, the periodic profile, at fixed position z, occurred in each Nt_s time units, is identical.

$$c_{i,j}(z, t + Nt_s) = c_{i,j}(z, t) \tag{1}$$

In other words, the concentration profiles at the beginning and at the end of the cycle must be identical.

And also column j can be viewed as the delayed column $j+1$ with lag t_s.



$$c_{i,j-1}(z, t) = c_{i,j}(z, t + t_s) \tag{2}$$

The alternative explanation for this equation is that the concentration profile at the start and at the end of a switching period are identical, apart from a shift of exactly one column.

According to the equation (1) and equation (2), we can have that,

$$c_{i,j-1}^{out}(z,t) = c_{i,j-1}^{out}(z,t-Nt_s) = c_{i,j}^{out}(z,t-Nt_s+t_s) \tag{3}$$
$$c_{i,j-1}^{out}(z,t) = c_{i,j}^{out}(z,t-(N-1)t_s) \tag{4}$$
$$c_{i,j}^{in}(z,t) = c_{i,j}^{out}(z,t-(N-1)t_s) \tag{5}$$

As seen from the equation (5), the inlet concentration of column j is not the outlet concentration of previous column $j-1$ any more, instead it is the outlet profile of column j, $(N-1)t_s$ time units before in one-column analogue. In this case, only one specific but random column would be selected, so the subscript j can be dropped.

□

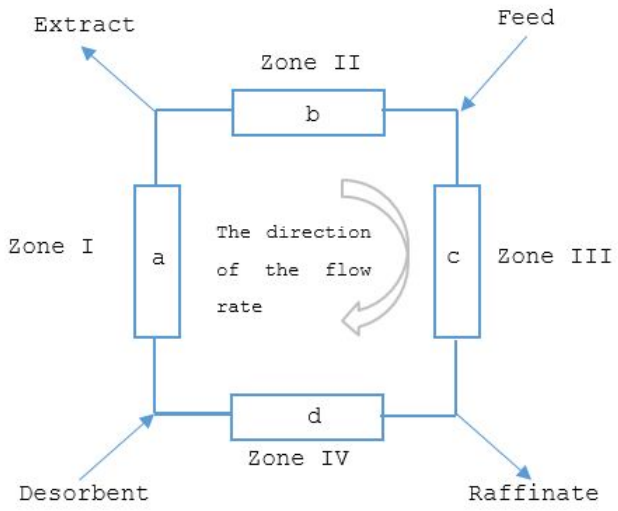


Fig. 1: Scheme of a simulated moving bed

Thus, the mass balance of each node in the fully simulation is then replaced with:

$$\begin{cases} Q_{III}c_{i,j}^{in}(t) = Q_{II}c_{i,j}^{out}(t-(N-1)t_s)) + (Q_{III}-Q_{II})c_F & \text{(Feed node)} \\ Q_{I}c_{i,j}^{in}(t) = Q_{IV}c_{i,j}^{out}(t-(N-1)t_s)) + (Q_{I}-Q_{IV})c_E & \text{(Desorbent node)} \\ c_{i,j}^{in}(t) = c_{i,j}^{out}(t-(N-1)t_s) & \text{others} \end{cases} \tag{6}$$

The following figures (2 and 3) will help to understand the recycle lag $(N-1)t_s$. Fig.2 and Fig.3 compare the complete cycle of the four-zone SMB with

that of the equivalent one-column analogue. It is seen that the one-column analogue is achieved by selecting an arbitrary column (dashed area) of the SMB unit and following its operation over a complete cycle.

Until now, we still need the initial conditions for start-up. The simplest way to carry out a simulation run is to start with a clean column ans assume that, for the $t < 0$, the inlet concentration profile is $c_{i,j}^{in}(t < 0) = 0$.

2 Comparison between Fully Simulation and One-Column Analogue

This comparison focus on the computational time, see the Fig.4.

The computational time increases drastically in the fully simulation, from 159 second in the four-column case to 997 second in the eight-column case; while in the one-column analogue situation, the time consumption only increase a little bit, from 96 second to 105 second. This will be particularly useful in the optimization of column configuration, flow rate, and switch time, since each optimization step require the evaluation of the objective function.

3 Performance Index

The most frequently adopted performance index are productivity and purity in the extract port and raffinate port respectively.

The purity of desired component 1 (the more retained component) in the extract port:

$$\text{Purity}_{ext} = \frac{\int_0^{t_s} c_1^{ext}(t)\frac{Q(t)}{\varepsilon A}\,dt}{\sum_i^{Ncomp}\int_0^{t_s} c_i^{ext}(t)\frac{Q(t)}{\varepsilon A}\,dt} \tag{7}$$

$$= \frac{\int_0^{t_s} c_1^{ext}(t)\,dt}{\sum_i^{Ncomp}\int_0^{t_s} c_i^{ext}(t)\,dt} \tag{8}$$

The purity of component 2 (the less retained component) in the raffinate port:

$$\text{Purity}_{raf} = \frac{\int_0^{t_s} c_2^{raf}(t)\frac{Q(t)}{\varepsilon A}\,dt}{\sum_i^{Ncomp}\int_0^{t_s} c_i^{ext}(t)\frac{Q(t)}{\varepsilon A}\,dt} \tag{9}$$

$$= \frac{\int_0^{t_s} c_2^{raf}(t)\,dt}{\sum_i^{Ncomp}\int_0^{t_s} c_i^{ext}(t)\,dt} \tag{10}$$

Where A is the cross-section area of the column.

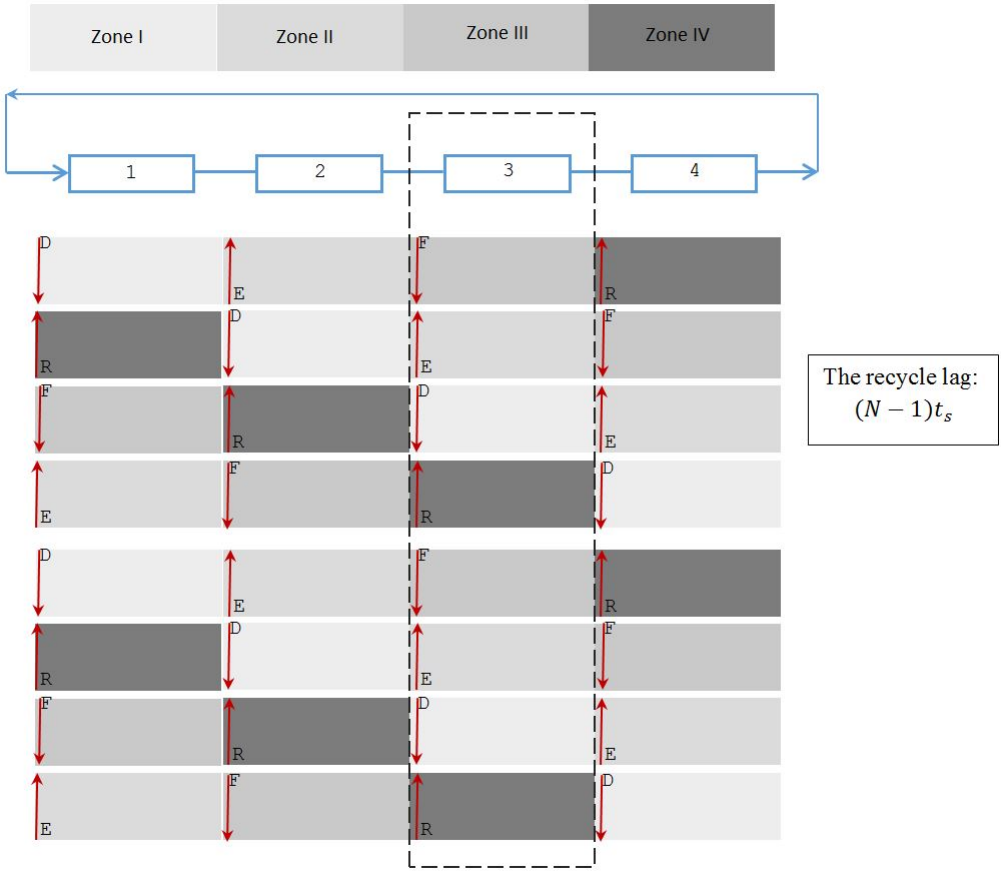


Fig. 2: Schematic diagram showing the sequence of port switching for two cycles of a four-column SMB. The dashed rectangular denotes the selected column for one-column analogue simulation.

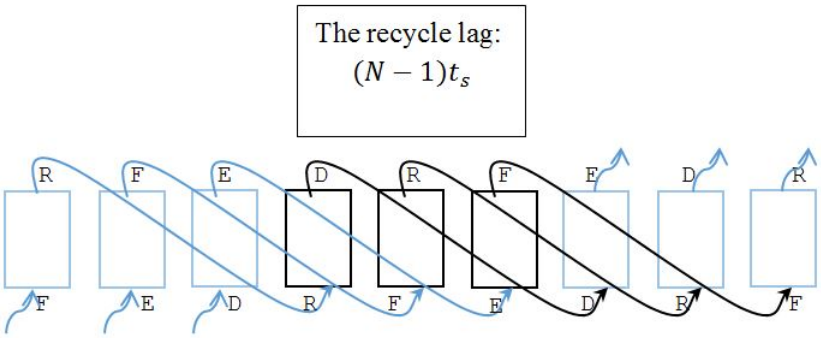


Fig. 3: The analogous one-column process of the selected column. $c_{i,j}^{in}(t) = c_{i,j}^{out}(t-(N-1)t_s)$, without the efforts of inlet ports. Until now, we still need the initial conditions for start-up. The simplest way to carry out a simulation run is to start with a clean column ans assume that, for the $t<0$, the inlet concentration profile is $c_{i,j}^{in}(t<0)=0$.

In regard to the productivity, it is the sum of both extract and raffinate ports:

$$\text{Product} = \frac{\phi Q_E \int_0^{t_s} c_1^{ext}(t)\,dt + \phi Q_R \int_0^{t_s} c_2^{raf}(t)\,dt}{V_{col}(1-\varepsilon)} \tag{11}$$

where ϕ is the factor to transform the unit from mol to g.

4 Optimization

It is well-known in the literature that the performance of SMB system can be dramatically improved by changing the operating conditions such as flow rates and switching time and so one. Moreover, numerous SMB configurations can be created by changing the relative positions of feed and desorbent inlets or the extract, raffinate and the intermediate outlet stream outlets. In this paper, such position changing was not taken into consideration.

Once the SMB configuration is given for a target mixture in the four-zone SMB and the model parameters are estimated through experiments, operating variables (e.g. recycle (Q_{cy}), which is referred to the flow rate between desorbent port and extract port, feed (Q_F), desorbent (Q_D), extract (Q_E) flow rate, and the column length (L_c), switching time (t_s)) should be adjusted to obtain desirable process performance (e.g. purity, productivity, desorbent consumption). In my case, the optimized operating variables are:

$$\boldsymbol{\theta} = \{L_c, t_s, Q_{cy}, Q_F, Q_D, Q_E\} \tag{12}$$

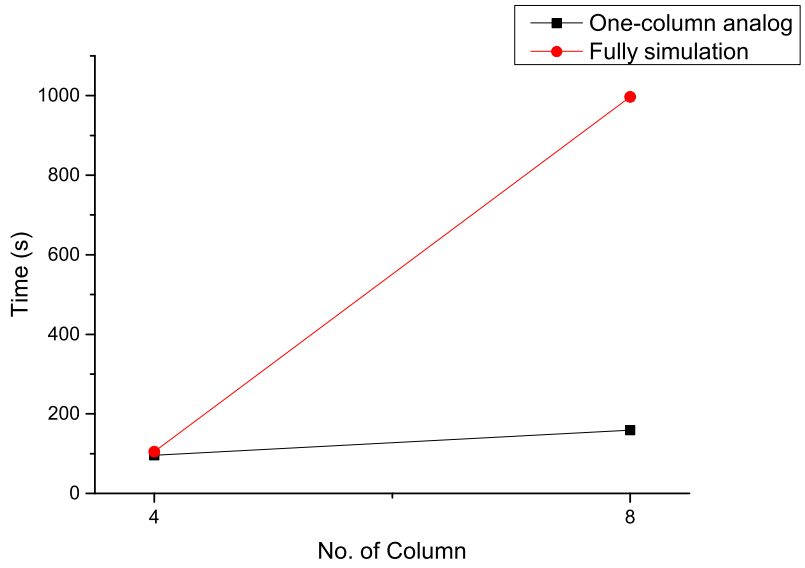


Fig. 4: The comparison of time consumption between Fully simulation and One-column analogue. The computational time increases drastically in the fully simulation, from 159 second in the four-column case to 997 second in the eight-column case; while in the one-column analogue situation, the time consumption only increase a little bit, from 96 second to 105 second.

The multi-objective optimization could be adopted to obtain the Pareto front. So far, the multi-objective optimization problem is converted into the following single-objective optimization problems by the ε-constraint method. The resulting optimization method is referred to as the throughput maximization problem in this study. An optimal solution to this problem will a Pareto point of the multi-objective optimization problem.

$$\max_{\boldsymbol{\theta}} \quad \text{Product} = \frac{\phi Q_E \int_0^{t_s} c_1^{ext}(t)\,dt + \phi Q_R \int_0^{t_s} c_2^{raf}(t)\,dt}{V_{col}(1-\varepsilon)} \tag{13}$$

$$s.t. \quad \begin{cases} Q_F - Q_E = Q_R - Q_D & \\ \text{Purity}_{ext} > 99\% & \\ \text{Purity}_{raf} > 99\% & \\ Q_l < Q_i < Q_u & i = \text{I,II,III,IV} \\ Q_D < Q_{D,lim} & \text{optional; desorbent consumption} \end{cases} \tag{14}$$

The equality is used to ensure the conservation of the flow rate in the loop. You can assign the desired purity limitation on the withdrawn ports by using the purity inequalities. There is also boundary limitation on the flow rates. The last inequality is optional, in some occasion, we need maximum consumption on the desorbent.

4.1 Optimization Methods

There are *four* different algorithms are integrated into the code, range from deterministic algorithm (fmincon) to heuristic algorithms (e.g. DE, PSO), range from optimization algorithms to Bayesian Inference (MADE). The objective function in this demonstration is the Productivity, combining with the penalty function to deal with the inequalities.

4.1.1 fmincon

This is a subroutine from the MATLAB, which belong to the filed of deterministic algorithm.

4.1.2 Differential Evolution (DE)

DE optimizes a problem by maintaining a population of candidate solutions and creating new candidate solutions by combing existing ones according to its mathematical formula, and then keeping whichever candidate solution has the best score or fitness on the optimization problem at hand.

4.1.3 Particle Swarm Optimization (PSO)

PSO optimizes a problem by having a population of candidates (particles), and moving these particles around in the search space according to mathematical formula ovet the particle's position and velocity. Each particle's movement is

influenced by its own local best-known position but, is also guided toward the best-known positions in the search space, which are updated as better positions are found by other particles.

4.1.4 Metropolis Adjusted Differential Evolution (MADE)

MADE optimizes a problem by combining the prominent features of Metropolis Hastings algorithm and Differential Evolution algorithm. In the upper level, each chain is accepted with the Metropolis probability, while in the lower level, chains have an evolution with resort to heuristic method, Differential Evolution algorithm.

Since the uncertainties in isotherm parameters, pump and calibration and so on, it is reasonable to adopt the algorithm based on the Bayesian Inference which provide the confidential interval of parameters rather than single values.

4.2 Results

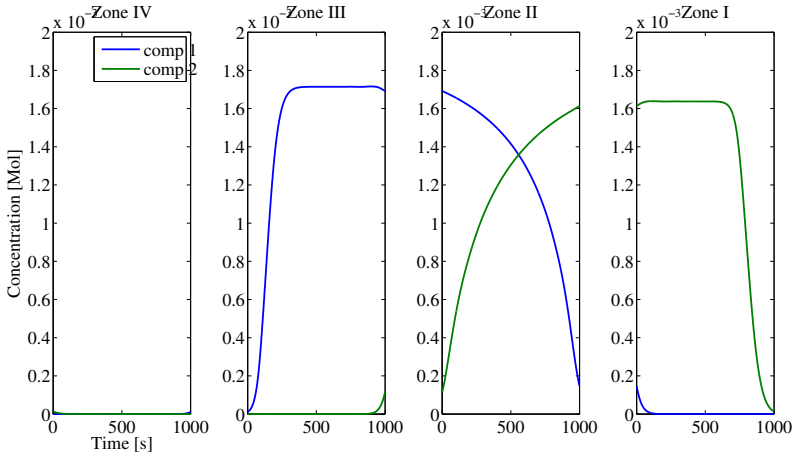
The case study from the paper the paper *Numerical method for accelerated calculation of cyclic steady state of ModiCon-SMB-process* were used again.

Tab. 1: Parameters of *Case 1* for the numerical tests

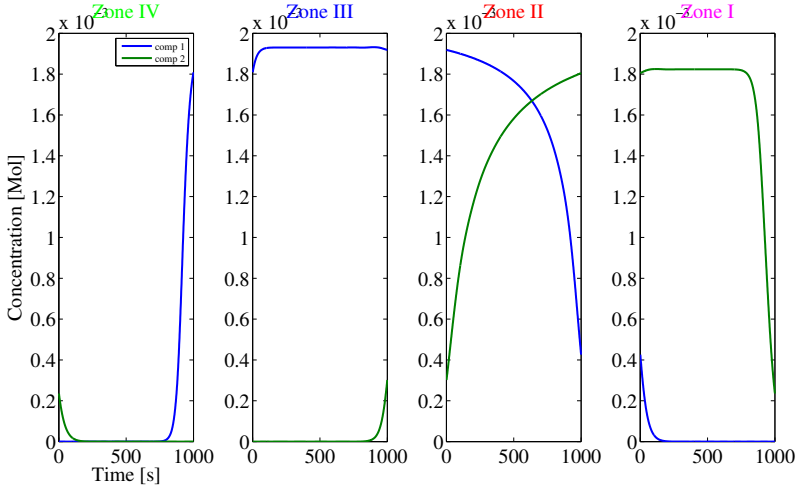
Number of columns	4
Dispersion coefficient	$u \times 10^{-24} \quad m$
Porosity	0.83
Column diameter	$0.02\ m$
Column length	optimized
Switching time	optimized
Linear isotherms	$a_1 = 5.72, a_2 = 7.7$
Concentration of feed	$0.55 \quad g/l$
Cyclic flow rate	optimized
Feed flow rate	optimized
Raffinate flow rate	calculated
Desorbent flow rate	optimized
Extract flow rate	optimized

The original value of parameter $\boldsymbol{\theta} = \{L_c, t_s, Q_{cy}, Q_F, Q_D, Q_E\}$ is $\{0.25m, 180s, 9.62 \times 10^{-7}, 0.98 \times 10^{-7}, 1.96 \times 10^{-7}, 1.54 \times 10^{-7} cm^3/s\}$; Purity of extract ports is 99.63%; Purity of raffinate ports is 99.75%; Productivity is $9.49\, g/t_s$.

After the optimization, the parameter $\boldsymbol{\theta} = \{0.268m, 212.4s, 8.54 \times 10^{-7}, 1.09 \times 10^{-7}, 0.788 \times 10^{-7}, 1.31 \times 10^{-7} cm^3/s\}$; Purity of extract ports is 98.97%; Purity of raffinate ports is 99.43%. Both purity are little less than the original one, but they are still in high quality; Productivity is $12.01\, g/t_S$ which is much higher than the original one.



(a) The originally axial profile. $\boldsymbol{\theta} = \{0.25m, 180s, 9.62 \times 10^{-7}, 0.98 \times 10^{-7}, 1.96 \times 10^{-7}, 1.54 \times 10^{-7} cm^3/s\}$. And the $\text{Purity}_{ext} = 99.63\%$ while the $\text{Purity}_{raf} = 99.75\%$; The productivity in this case $9.49\, g/t_s$



(b) The optimized axial profile. $\boldsymbol{\theta} = \{0.268m, 212.4s, 8.54 \times 10^{-7}, 1.09 \times 10^{-7}, 0.788 \times 10^{-7}, 1.31 \times 10^{-7} cm^3/s\}$. And the $\text{Purity}_{ext} = 98.97\%$ while the $\text{Purity}_{raf} = 99.43\%$; The productivity in this case $12.01\, g/t_s$

Fig. 5: The comparison of the original concentration profile and the optimized one. The upper one is the original one, while the lower one is the optimized one. $\boldsymbol{\theta} = \{L_c, t_s, Q_{cy}, Q_F, Q_D, Q_E\}$. As seen from above figures, the optimized configuration obtained *more* productivity, with the almost *same* purity, what's more, with *lower* consumption of desorbent.

5 Summary

The one-column analogue to reproduce the fully SMB simulation has been implemented successfully. It is identical to the N column SMB simulation. The prominent feature is the computational time. Four different type of optimization algorithms are also available to obtain the desirable SMB process (The code is going to available in our GitHub).