Instruction of the One-Column Analog Approach

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1 Introduction

1.1 One-column analog approach

As known, the cyclic operation of the SMB process (no matter the standard_SMB or the one-column analog approach here) is achieved by moving the inlet and outlet ports one column downstream (in the direction of fluid flow) every t_s time units. And due to technical problems, we can not track the internal composition profile (the immediate concentration) in each column during processing, instead we only detect the concentration profile at the end of each column. In the one-column analog, such tracking manner is still adopted.

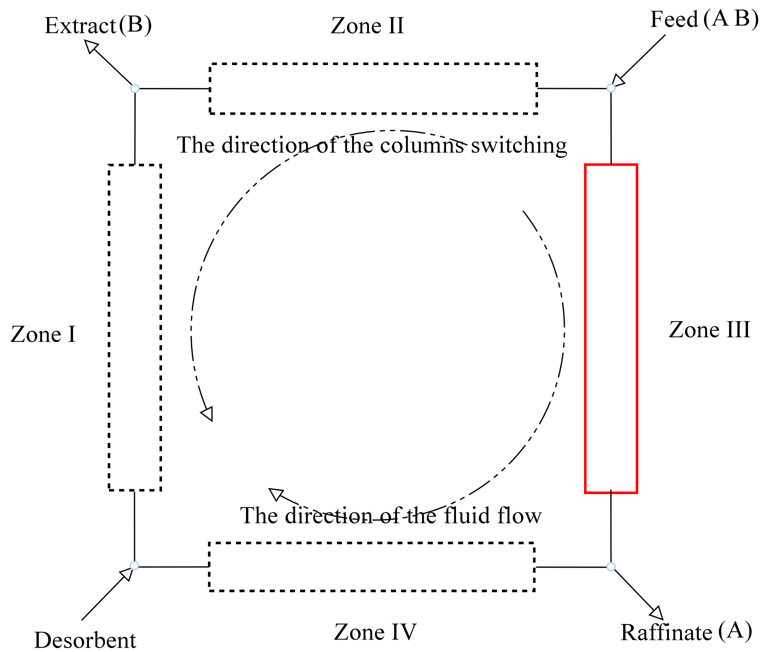


Figure 1: The schematic of the simulated moving bed chromatographic processes with one-column analog approach. For demonstration, the four-zone scheme is used, but it also has ability to deal with the ternarys separation with five-zone scheme.

Some mathematical basis will be omitted in this documentation, as they are totally consistent with the standard_SMB approach. For more information, please see the *doc.pdf* in the *doc* directory of the master branch.

These are the research conditions of the one-column analog method. [2] introduced that the periodic state of the SMB process can be reproduced by a simpler, more flexible, single-column chromatography process (hence the name, one-column analog). The proposed analog is a quite attractive alternative to the traditional SMB processes, especially on the point of simulation. The analog was developed by studying one selected column in a SMB unit through a complete cycle and then, replacing the remaining columns with tanks to provide the necessary recycle streams. These allow for recycling in a manner that mimics the SMB process. The chosen column can be an arbitrary designated one in the SMB unit. The more theory of the one-column analog approach was detailed in [2, 1, 4, 5]. The most prominent advantages of one-column analog are that it will be more stable than the standard_SMB approach, and it reduces the computational burden dramatically. In the subsequent works, they performed both the start-up and shutdown analyses to the analog [1]. Inspired by those works, [4] developed a single-column SMB analog with plug flow devices to implement the appropriate recycle pattern. They also proved the analog process is indistinguishable from the equivalent SMB process with the recycle lag, $(N-1)t_s$ time units (where N is the number of columns and t_s is the switching time). The practical implementation was also discussed in their corresponding works [3], as well as the combination of the variable feed concentration (PowerFeed), modulation of flow rates (ModiCon), and asynchronous shift of inlet/outlet ports schemes (Varicol) [5].

1.2 Recycle Lag

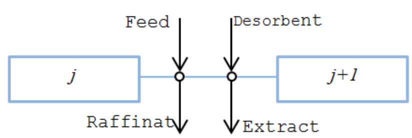
In one-column analog, the periodical SMB process is reproduced by a single-column setup with a recycle lag of $(N-1)t_s$. In other words, the ideal one-column analog process is theoretically indistinguishable from the equivalent standard SMB processes, except for the discontinuous use of the inlets/outlets.

Proof. Assuming the SMB process is already under the cyclic steady state (CSS), and i represents component while j represents the column index, the profiles at fixed position z periodically occur in each Nt_s time units.

$$c_i^{out,j}(z, t+Nt_s) = c_i^{out,j}(z,t) \tag{1}$$

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

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



$$c_i^{out,j-1}(z,t) = c_i^{out,j}(z, t+t_s) \tag{2}$$

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 Eqn.(1) and Eqn.(2), that holds,

$$c_i^{out,j-1}(z,t) = c_i^{out,j-1}(z, t-Nt_s) = c_i^{out,j}(z, t-Nt_s+t_s) \tag{3}$$

$$c_i^{out,j-1}(z,t) = c_i^{out,j}(z, t-(N-1)t_s) \tag{4}$$

$$c_i^{in,j}(z,t) = c_i^{out,j}(z, t-(N-1)t_s) \tag{5}$$

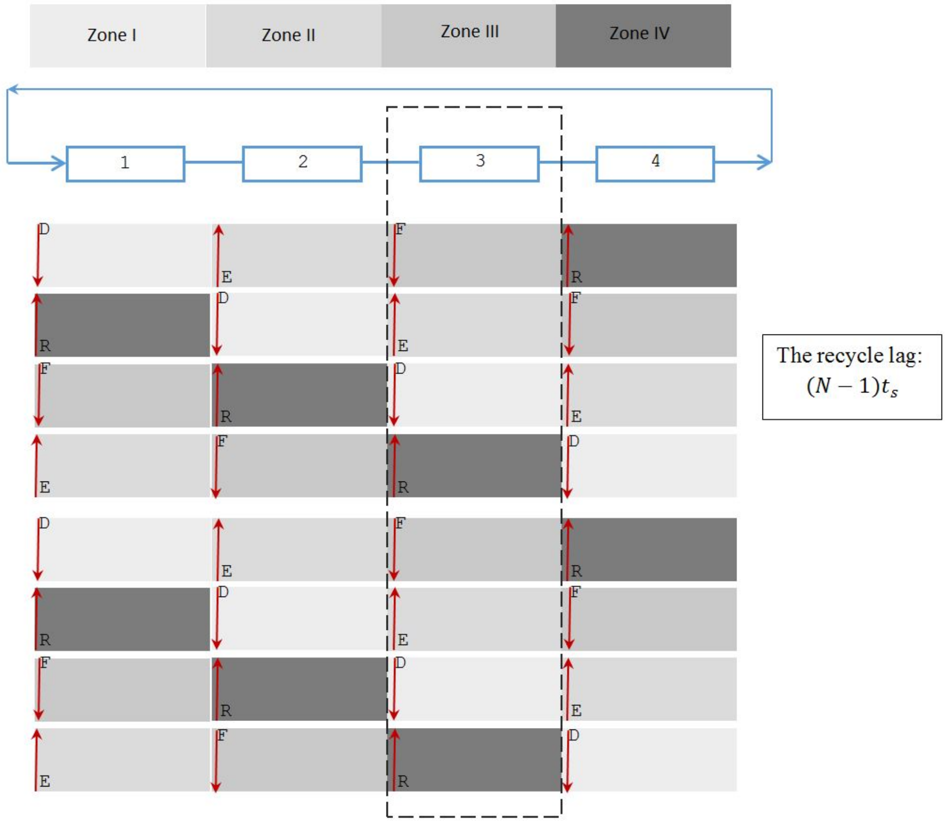


Figure 2: The schematic diagram of the indistinguishable one-column analog process, showing the sequence of port switching in two cycles of a four-column case for binary separation scenario. The dashed rectangular denotes the selected column for one-column analog simulation. The varying degree of gray is used to represent different zones. In the dashed rectangular, we can see that the sequence of column simulation is from zone III to zone II to zone I to zone IV.

As seen from above equations, 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 analog. In this case, only one specific but arbitrary column would be selected, so the subscript j can be dropped.

□

The following Fig.(2) and Fig.(4) will help to understand the recycle lag $(N-1)t_s$.

And we are not going to discuss how one-column analog 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 simulations, notably when the optimization is taken into consideration as one-column analog would decrease the computational efforts tremendous.

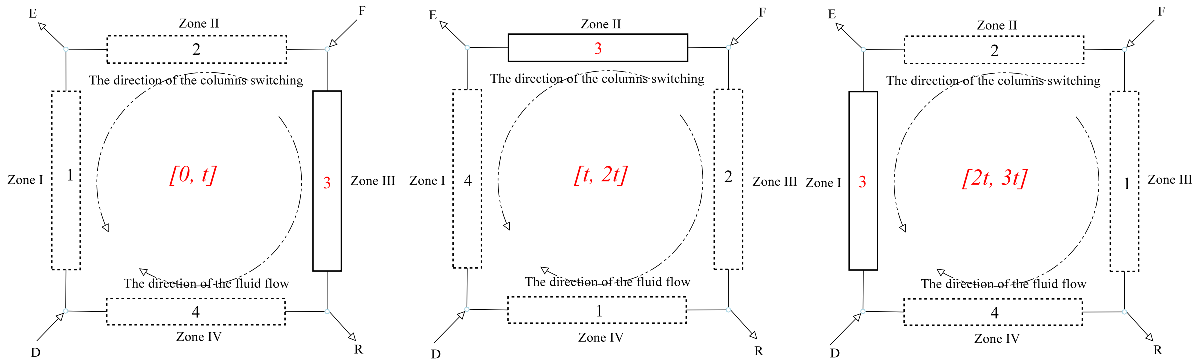


Figure 3: The recycle pattern of the one-column analog approach

1.3 Node Balance

Thus, the mass balance of each node in the standard_SMB approach is then replaced with

$$\begin{cases} Q_{\mathrm{III}} c_i^{in,j}(t) = Q_{\mathrm{II}} c_i^{out,j}(t-(N-1)t_s)) + (Q_{\mathrm{III}} - Q_{\mathrm{II}}) c_F & F \\ Q_{\mathrm{I}} c_i^{in,j}(t) = Q_{\mathrm{IV}} c_i^{out,j}(t-(N-1)t_s)) & D \\ c_i^{in,j}(t) = c_i^{out,j}(t-(N-1)t_s) & Others \end{cases} \tag{6}$$

in the binary situation or the following in the ternary situation

$$\begin{cases} Q_{\mathrm{IV}} c_i^{in,j}(t) = Q_{\mathrm{III}} c_i^{out,j}(t-(N-1)t_s)) + (Q_{\mathrm{IV}} - Q_{\mathrm{III}}) c_F & F \\ Q_{\mathrm{I}} c_i^{in,j}(t) = Q_{\mathrm{V}} c_i^{out,j}(t-(N-1)t_s)) & D \\ c_i^{in,j}(t) = c_i^{out,j}(t-(N-1)t_s) & Others \end{cases} \tag{7}$$

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 $c_i^{out,j}(t < 0) = 0$.

1.4 Recycle Pattern

As there is on adjacent columns any more in this variant as there is only one column packed. So what is the inlet concentration profile of each column? Let's have an insight into the recycle pattern of the one-column analog approach.

Recalling that the simulation sequence in the standard_SMB approach is clockwise, however in this approach it is counter-clockwise. Assuming that each column, including the tanks, are sticked with Arabic numbers permanently, the simulation sequence here is the column 3 in zone III, column 3 in zone II, column 3 in zone I, and lastly column 3 in zone IV.

When the column 3 is in the zone III of first switch interval, the simulation is implemented with the inlet concentration profile and the empty column state. The inlet concentration profile is the combination of the feed inlet and the assumed empty outlet profile of "previous" column. And then the outlet profile and the column state is stored. Please correspond to

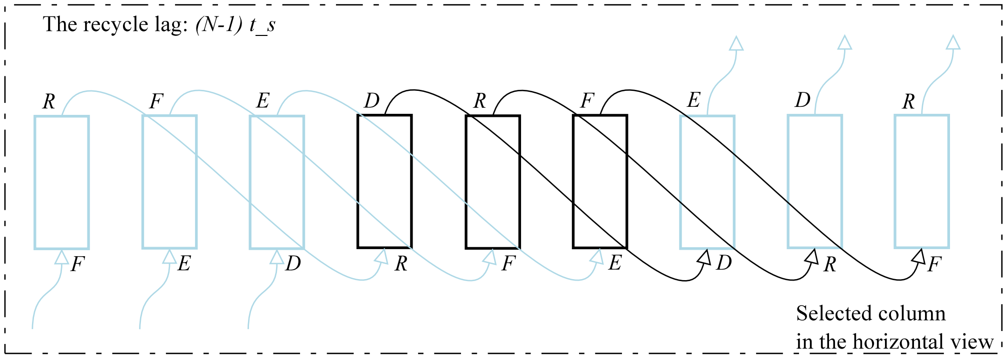


Figure 4: The schematic diagram of the indistinguishable one-column analog, showing the inlets and outlets transfer process in two cycles of a four-column case for binary separation. For the selected column in the above figure, the inlets of the column in the first black position is from the outlets of the column in the first blue position, $c_i^{in,j}(t) = c_i^{out,j}(t-(N-1)t_s)$

the first blue column in Fig.(4). Subsequently, the column 3 is switched to the position, zone II, of second switch interval. The simulation is implemented and data is stored. Similarly, the column 3 in zone I of third switch interval. Please correspond to the second and third blue column in Fig.(4).

Now, the critical point comes. When the column is switch to the zone IV of fourth switch interval, the inlet profile is known. Because under CSS, the outlet of column 3 in zone III is the ingredient composition of the inlet profile of the column 3 in zone IV. It is from the outlet profile that is $(N-1)t_s = 3t_s$ time units before in this demonstration. Please correspond to the first dark column in Fig.(4).

1.5 Time Comparison

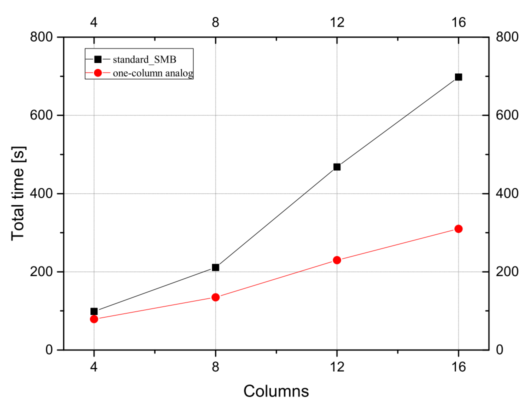


Figure 5: The overall time comparison of the standard_SMB approach and the one-column analog approach under different column amount

As seen from the comparison figure, along with the increasing of the column amount the computational time increases dramatically in the standard_SMB situation. But it is not so obvious in the one-column analog approach.

2 Summary

The one-column analog to reproduce the standard_SMB simulation has been implemented successfully. It is identical to the N column SMB simulation. The prominent feature is the computational time.

3 References

References

[1] Nadia Abunasser and Phillip C Wankat. One-column chromatograph with recycle analogous to simulated moving bed adsorbers: analysis and applications. *Industrial & engineering chemistry research*, 43(17):5291–5299, 2004.

[2] Nadia Abunasser, Phillip C Wankat, Y-S Kim, and Yoon Mo Koo. One-column chromatograph with recycle analogous to a four-zone simulated moving bed. *Industrial & engineering chemistry research*, 42(21):5268–5279, 2003.

[3] João Araújo, Rui Rodrigues, Ricardo Silva, and José Mota. Single-column simulated moving-bed process with recycle lag: Analysis and applications. *Adsorption Science & Technology*, 25(9):647–659, 2007.

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[5] Rui CR Rodrigues, João MM Araújo, Mário FJ Eusébio, and José PB Mota. Experimental assessment of simulated moving bed and varicol processes using a single-column setup. *Journal of Chromatography A*, 1142(1):69–80, 2007.