Instruction of the Operator-splitting Approach

Qiaole HE

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1 Introduction

As known, the cyclic operation of the SMB process (no matter the standard_SMB approach or the one-column analog approach) is achieved by moving the inlet and outlet ports one column downstream (in the direction of fluid flow) each t_s time interval. 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. Thus the simulation sequence in both standard_SMB and one-column analog approach is sequential, although clockwise in standard_SMB while counter-clockwise in one-column analog, namely, zone I $\rightarrow$ zone II $\rightarrow$ zone III $\rightarrow$ zone IV in the standard_SMB while zone III $\rightarrow$ zone II $\rightarrow$ zone I $\rightarrow$ zone IV in the one-column analg, see Fig.(1). Additionally, the effects of the starting simulation point has been covered in the instruction of the standard_SMB approach. So there is no redundant introduction here again.

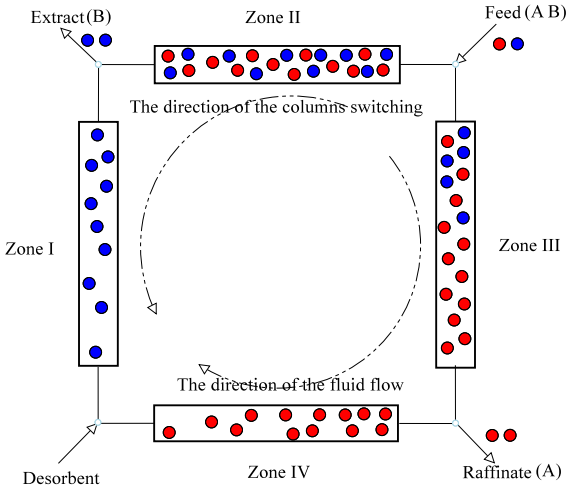


Figure 1: The schematic of the four-zone simulated moving bed chromatographic process. In the approaches of standard_SMB and one-column analog, the simulation order is sequential, namely one column by one column no matter clockwise or counter-clockwise due to the concentration tracking manner in the chromatographic field.

However, the actually simulation sequence in reality should be simultaneous, like which is presented in Fig.(2).

It does not matter what the simulation sequence is, if only the cyclic steady state (CSS) is concerned in the simulations. Since both standard_SMB approach and one-column analog approach converge to the same CSS, though, via the different convergence dynamics (hereafter, I will just call the convergence dynamics the trajectory). However, if the actual trajectories, rather than the CSS, are concerned, neither standard_SMB approach or one-column analog approach can afford any more extra information. We need to resort to new approaches. The operator-splitting technique is used to overcome the sequential simulation order in both standard_SMB approach and the one-column analog approach.

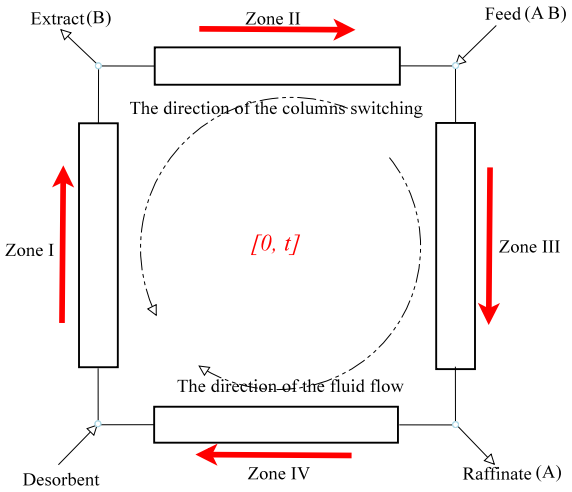


Figure 2: The intended simulation sequence in simulated moving bed chromatographic processes. The columns in a SMB unit should be calculated simultaneously rather than sequentially.

Moreover, some mathematical basis is also 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.

1.1 Idea

Operator splitting is a kind of mathematical terminology. By utilizing splitting of the simulations of columns in a SMB unit into several time sections, we could approach the real flow pattern as what has presented in Fig.(2). The definition of the time section is t_s/n, where n is the amount of time sections. There is a brief demonstration in Fig.(3). For simplicity, the amount of three is used. In considering simulations of one switch time interval, the simulations of all red time sections are implemented sequentially rather than the whole columns. Subsequently, the green time sections and blue time sections. Although the columns are still sequentially calculated, the really simultaneous flow pattern is able to be reproduced if the amount of time sections is big enough.

1.2 Recycle

Honestly, it is a bit confusing in Fig.(3). Let us explain it more explicitly, see Fig.(4).

Assuming the simulations start from the desorbent node, the outlet of the column in zone I within first time section interval $(t_s/3)$ can be calculated given the inlet profile. In other words, the red piece of the column in zone I is pushed out to the first interval chromatogram. Then we switch to simulate the column in zone II with the given inlet profile from the simulation the column in zone I. Similarly, the red piece in zone II is pushed out

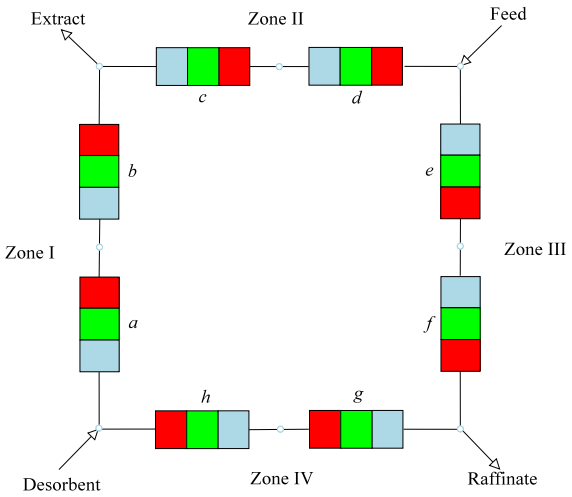


Figure 3: The illustration figure of the underlying idea of the operator-splitting approach. In this demonstration, there are three pieces of time sections ($n = 3$). The simulation of each time section takes up $t_s/3$.

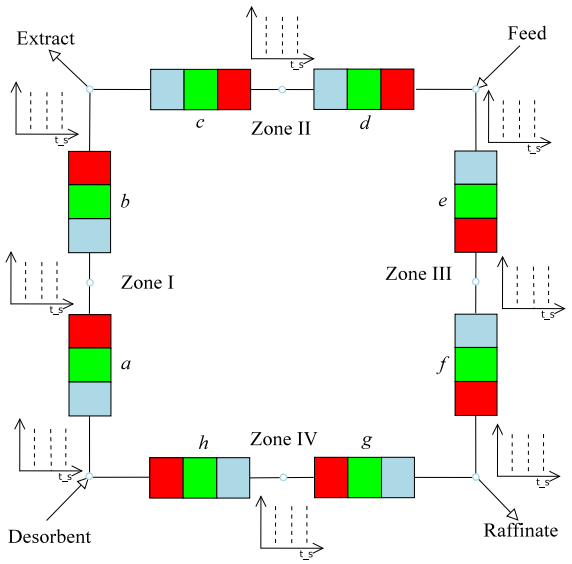
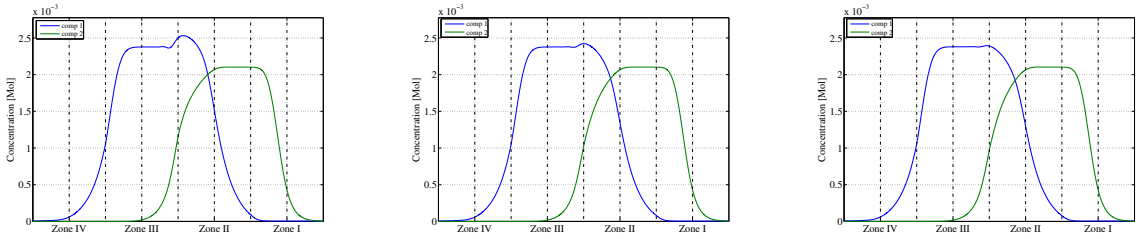


Figure 4: The schematic of the operator-splitting approach.

to the first interval chromatogram. After all the red pieces are pushed out, the simulations of first time section have been accomplished.

Now there is a critical point that in the pushing-out of the green pieces of the column in zone I, what is the inlet profile? If the outlet profile stored in the zone IV chromatogram is adopted as the inlet profile, some errors rather than noise are introduced into the simulations (this will be illustrated later). Again, the green and blue pieces could be pushed out with given inlet profiles, and being stored in respectively chromatograms.

The introduced errors can be eliminated by increasing the amount of the time sections in this variant. In Fig.(5(a)) there is 20 time sections in each column, while 50 time sections in Fig.(5(b)), 100 in Fig.(5(c)). The introduced errors could be eliminated by increasing the amount drastically, correspondingly the price of the computational time what is the major disadvantage.



(a) $n = 20$ (b) $n = 50$ (c) $n = 100$

Figure 5: The influence of the amount of time sections on the final concentration profile under cyclic steady state. As seen in the figures with 20 pieces of time sections, there is a small peak at the plateau of the component 1, which can be attributed to the errors introduced by using setting the outlet of column in zone IV as the inlet of the column in zone I. By increasing the amount n, the peak becomes smaller and smaller, and can be neglected when $n = 100$.

1.3 Node Balance

In the operator-splitting approach, the switching implementation is entirely same with the standard_SMB approach, moving the inlet/outlet ports one column downstream every t_s time unit, rather than each time section. As in simulations of each time section, the SMB unit is kept static. However, the mass conservation of concentration profile differs with the standard_SMB approach. The mass balance of each node in the operator-splitting approach is thus

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

in the binary situation or the following in the ternary situation

$$\begin{cases} Q_{\mathrm{IV}} c_i^{in,j+1}(t+(m-1)\frac{t_s}{n}) = Q_{\mathrm{III}} c_i^{out,j}(t+(m-1)\frac{t_s}{n})) + Q_F c_F \, F \\ Q_{\mathrm{I}} c_i^{in,j+1}(t+(m-1)\frac{t_s}{n}) = Q_{\mathrm{V}} c_i^{out,j}(t+(m-1)\frac{t_s}{n})) & D \\ c_i^{in,j+1}(t+(m-1)\frac{t_s}{n}) = c_i^{out,j}(t+(m-1)\frac{t_s}{n}) & Others \end{cases} \tag{2}$$

where n is the amount of time sections of each column while $m \in [1, n]$ is the current time section index during one switching time simulation, and $t \in [0, t_s/n]$.

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

I am now going to introduce another proposal to eliminate the introduced error which lead to a new variant, advanced operator-splitting approach, using an approximation of the real inlet profile at the end of each time section. Note that the source code of this variant could be found in the *operator-splitting* branch of the GitHub repository and former variant in the *Dynamic_SMB* branch.

1.4 Advanced operator-splitting

Based on the operator-splitting approach, another sophisticated operator-splitting approach will be developed. By the way, this variant would be the official operator-splitting, and the former is treated as a reference.

The underlying idea here is that the very first column (or the starting simulation point) is always be simulated twice, and with some tricks to obtain both the true column state and the true outlet profile.

The attention is paid to the very first column, say, column in the zone I, during one switch time processing, see Fig.(6). At the very beginning, as there is no knowledge regarding the inlet profile of the column in one time section. Without losing the generality, the empty concentration profile is assumed. After one time section simulations, the actual inlet profile of the very first column is known which is gained from the outlet of the column in zone IV.

It is worth mentioning that the column state after the simulation of the very first column within first time section is not reserved, instead only the outlet profile from such simulation is preserved, see the part of Fig.(7) with *assumed inlet profile*. Because with the assumed inlet profile (also incorrect), the column is contaminated with the incorrect inlets. As seen from the Fig.(7), the original column state consists of both true $S1$ and $S2$ parts. With injecting the assumed inlet profile of t_s/n time units, the approximately $S1$ state is pushed out and replaced with $S2$ and *wrong* parts. However, the concentration pushed out is correct. So only the outlet concentration of the simulation within one time section is stored rather the column state.

After one loop time section simulations, the true outlet profile of the column in zone IV is known, as shown in Fig.(6). If the cyclic steady state is arrived, this is the actual inlet profile of the column in zone I in next t_s switch interval. Then using the non-preserved column state and the "actual" column inlet profile, the column state that has not been reserved is

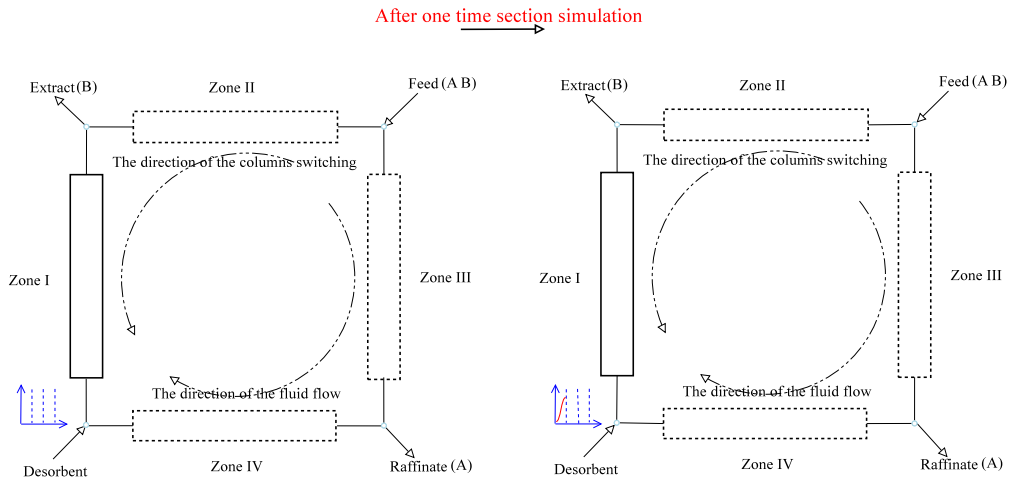


Figure 6: The flow pattern of the operator-splitting. The attention is paid to the very first column during the simulations. At the very beginning, the empty concentration profile is assumed without losing the generality. After one time section simulations, the actual inlet profile of the very first column is abstracted from the outlet of the column in zone IV.

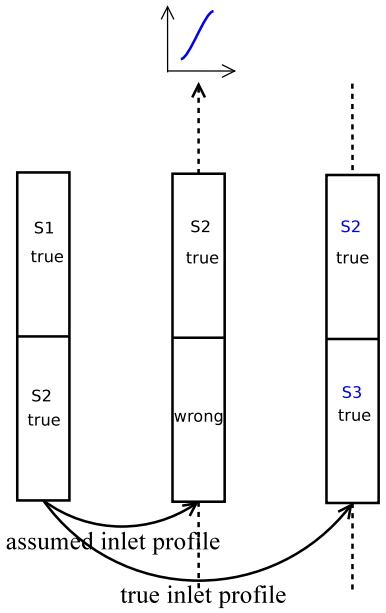


Figure 7: The schematic of the twice computing of the advanced operator-splitting approach, in which S denotes the state of the column, *true* signifies that the part column state is correct, while *wrong* means incorrect.

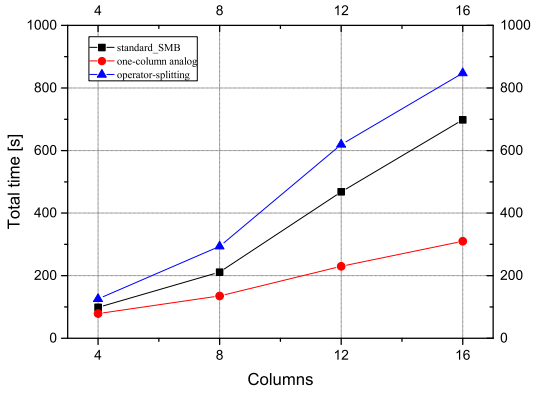


Figure 8: The overall time comparison of the standard_SMB approach, the one-column analog approach, and the operator-splitting approach under different column amount

updated, see the part of Fig.(7) with *true inlet profile*. The originally true column state, $S1$ and $S2$, is updated with also true $S2$ and $S3$ column state. It is the so-called saying that simulating the very first column twice in each time section.

Similarly, in the simulations of the second time section, it still starts with the assumed empty inlet profile and correct column state (only after twice computing of the very first column), and at the end of the second time section, the very first column is updated with the true column state as mentioned before.

There is a vital constraint that must be held in those twice-computing of the very first column. It indicates that the washing time using the actual inlet profile to update the actual column state should be less than half retention time of the column.

$$\frac{t_s}{n} \leq \frac{t_r}{2} \tag{3}$$

$$n \geq \frac{2t_s\overline{u}_{int}}{L} \tag{4}$$

$$\tag{5}$$

where $\overline{u}_{int}$ is the average of interstitial velocities, and L is the column length.

Afterwards, we can have the inequality for restricting the minimal number of the time section amount. There is no need to have a huge amount number in this variant, as it is time-consuming. It suffices to just satisfy above inequality.

1.5 Time Comparison

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

2 Summary

In this documentation, the fundamentals of the operator-splitting approaches are presented. The operator-splitting approaches are aimed to obtain the true convergence dynamics of SMB chromatographic processes. As neither standard_SMB and one-column analog approach are able to afford such information, while they can only offer the information regarding the cyclic steady state, although, one-column analog speeds up the convergence.