

Article

Discrete Dynamic System Modeling for Simulated Moving Bed Processes

Chao-Fan Xie ¹, Hong Zhang ² and Rey-Chue Hwang ^{3,*}

¹ Department of Big Data and Artificial Intelligence, Fujian Polytechnic Normal University, Fuzhou 350300, China; xiecf@fpnu.edu.cn

² Key Laboratory of Nondestructive Testing, Fujian Polytechnic Normal University, Fuzhou 350300, China; zhangh@fpnu.edu.cn

³ Department of Electrical Engineering, I-Shou University, Kaohsiung 84001, Taiwan

* Correspondence: rchwang@isu.edu.tw, Tel.: +886-0928722593

Abstract: Although the simulated moving bed (SMB) process boasts advantages such as high productivity and low consumption, the cost of obtaining optimized parameters through practical experiments to control the separation process can be enormous due to its complex nonlinear characteristics. Consequently, the successful transformation of the SMB separation process into a mathematical dynamic model for computer simulation would greatly reduce the research costs associated with experimental studies. In this study, the Crank–Nicolson method was employed to discretize and dynamize the SMB process, enabling the simulation of processes under both linear and Langmuir isotherms. The results of the simulation experiments demonstrated the feasibility and high efficiency of this approach, thereby establishing a solid foundation for further advancements in online control strategies.

Keywords: Crank–Nicolson; discretize; control

MSC: 37M05

Citation: Xie, C.-F.; Zhang, H.; Hwang, R.-C. Discrete Dynamic System Modeling for Simulated Moving Bed Processes. *Mathematics* **2024**, *12*, 1520. <https://doi.org/10.3390/math12101520>

Academic Editor: Nicolae Dumitru and Adrian Sorin Rosca

Received: 29 March 2024

Revised: 3 May 2024

Accepted: 9 May 2024

Published: 13 May 2024



Copyright: © 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

1. Introduction

The SMB process is recognized as one of the cleanest manufacturing technologies in the chemical industry. The SMB process is illustrated in Figure 1. Achieving improved performance in the SMB process often requires laborious experiments to obtain accurate physical parameters of the moving bed. Due to the high costs involved, researchers tend to simulate the SMB process using mathematical models. Currently, researchers mainly employ two types of mathematical models for the SMB process. One type is the equilibrium diffusion model, where the adsorbent rapidly reaches equilibrium with the components and the eluent. In this case, the transfer process between the mobile and solid phases can be neglected, resulting in a simplified mathematical model [1–3]. This model is used, for example, in the separation of xylose and fructose in sugar products. The other type of model considers the transfer processes between the solid and mobile phases. It considers factors such as internal diffusion between particles in the solid phase and the concentrations of the components in the stagnant layer within the pores. This model is relatively complex, but it provides a more comprehensive and realistic representation of the separation process, aligning with actual production activities [4,5]. This type of model is called the general rate model.

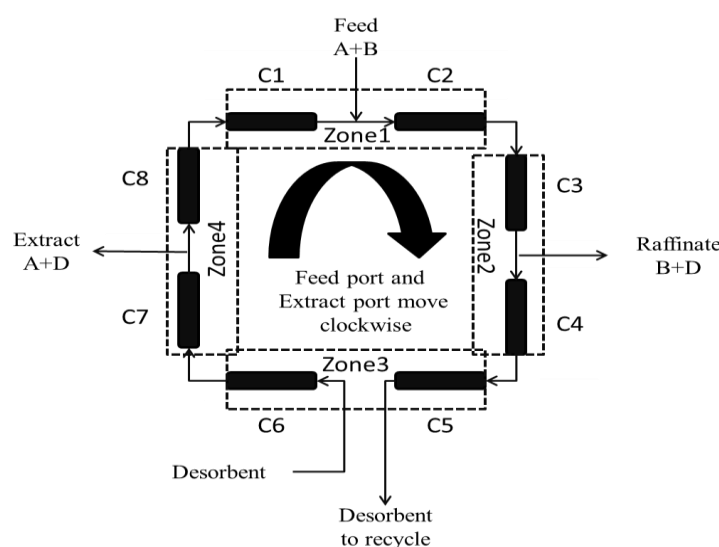


Figure 1. Simulated moving bed operation process.

Regardless of the model type, the mathematical formulation consists of a set of partial differential equations. Due to the complex nonlinear nature of these equations, analytic solutions are generally not obtainable. As a result, many scholars currently employ finite element methods to provide numerical solutions for these models. The mathematical model reported in the literature investigates the behavior of separation processes within multiple columns, each possessing significant advantages in terms of accuracy and computational time, and each employing a linear driving force (LDF) model. Its predictive capabilities have been confirmed to be in line with several prior studies [6–9]. The model comprises cumulative, convective, and axial dispersion equations based on mass balance equations for the mobile phase and solid phase, respectively [10].

To control the simulated moving bed process of binaphthol enantiomers separations, Nogueira et al. proposed a nominally stable MPC controller, also known as infinite horizon model predictive control (IHMPC) [11]. Natarajan and Lee proposed the use of repetitive model predictive control (RMPC) for the SMB process, specifically applied to the chromatographic separation of a phenylalanine–tryptophan mixture [12]. Carlos and Alain introduced a novel approach to controlling the separation process of SMB chromatography [13]. S. Mun et al. proposed an optimization-based separation control method to enhance product purity and economic efficiency [14]. María-Sonia et al. investigated the general dynamic optimization (open-loop optimal control) of SMB chromatographic separation processes [15]. The control processes discussed above are specific to solutes and lack portability. Furthermore, they heavily rely on finite element methods for process optimization, which presents challenges for real-time online control due to significant computational requirements.

Woo Sung Lee and Chang Ha Lee developed mathematical dynamic models and data-driven machine learning methods using limited experimental parameters and real industrial data to evaluate the performance of SMB systems [16]. Marrocos et al. proposed a deep artificial intelligence structure with a nonlinear output error (NOE) architecture and a nonlinear autoregressive with exogenous inputs (NARX) predictor for online soft sensing, providing key information regarding the main characteristics of simulated moving bed chromatography devices [17]. Hoon et al. employed a data-driven Deep Q Network, a model-free reinforcement learning method, to train a control strategy for SMB processes which approaches optimality [18]. More relevant studies can be found in the references [19–25]. Although using machine learning and deep learning approaches to treat the SMB system as a black box can help bypass the complexities of the underlying mechanism, this approach may become highly susceptible to disturbances or

perturbations in the separation parameters, leading to the potential occurrence of ill-conditioned characteristics and the subsequent failure of the separation process.

Overall, these studies are aimed at specific industrial equipment and materials which are to be separated. Conducting experiments based on physical machines is relatively costly, and the developed controllers lack universal applicability. With changes in environmental parameters, the results can easily lead to separation failures. To improve the performance of SMB processes, accurate physical parameters of the moving bed need to be obtained through tedious experiments. However, the physical parameters obtained from experiments may not fully represent the actual operation of the SMB system. The parameters of the entire SMB process may change due to the connection between pipelines or the long-term use of solid phases, causing discrepancies between the physical performance and experimental parameters. These reasons can lead to insufficient operating conditions for the SMB, resulting in unsatisfactory chromatographic separation. Generally, SMB systems exhibit variability during operation. Through identifying the real-time concentration of substances online and immediately correcting the operating conditions of the SMB, the optimal control of the SMB can be achieved. To quickly correct the operating conditions of the SMB, an efficient computational process is required. In this paper, to enhance the efficiency of online control, the system's dynamics are discretized using the Crank–Nicolson method. The discretization of the continuous processes has emerged as a fundamental technique, ultimately leading to significant improvements in control efficiency.

2. SMB Mathematical Model

2.1. Linear Isotherm Model

The traditional SMB dynamic mathematical model is derived from referencing the TMB mathematical model. The meanings of the parameters are presented in Table 1.

Table 1. Parameters of the SMB system.

Parameter	Nomenclature	Parameter	Nomenclature
$x(\text{cm})$	Axial distance	$Q(\text{cm}^3 \text{min}^{-1})$	Volume flow rate
$k(\text{gL}^{-1})$	Comprehensive mass transfer constant	$t(\text{second})$	Time
$v^*(\text{cm min}^{-1})$	Effect velocity of body	$D(\text{cm}^2 \text{min}^{-1})$	Effective dispersion coefficient
$u_s(\text{cm min}^{-1})$	Solid flow rate	ε	Bulk void fraction
$C(\text{gL}^{-1})$	Mobile phase concentration	i	Material index: A or B
$q(\text{gL}^{-1})$	Solid phase concentration	j	Column number: 1, 2, 3, 4, 5, 6, 7, 8
$q^*(\text{gL}^{-1})$	Solid phase concentration at equilibrium between the solid phase and mobile phase		

Here is an overview of the SMB dynamic model mentioned. For the TMB, the mass balance of the bulk phase is provided using the following:

$$\frac{\partial C_{ij}}{\partial t} = D_i \frac{\partial^2 C_{ij}}{\partial x^2} - v_j^{TMB} \frac{\partial C_{ij}}{\partial x} - \frac{1-\varepsilon}{\varepsilon} k_i (q_{ij}^* - q_{ij}) \quad (1)$$

$$\frac{\partial q_{ij}}{\partial t} = \frac{\partial}{\partial x} u_s q_{ij} + k_i (q_{ij}^* - q_{ij}) \quad (2)$$

v_j^{TMB} is the velocity of TMB system. According to the principle of kinematic synthesis, the relationship between the flow velocities of the mobile phase in the SMB system and the TMB system can be expressed using Equation (3).

$$v_j^{SMB} = v_j^{TMB} + u_s \quad (3)$$

As the solid phase is implemented via column switching which controlled by the switching time T_θ , the equivalent flow velocity of the solid phase can be expressed as Equation (4).

$$u_s = \frac{L}{T_\theta} \quad (4)$$

L is the length of the column; by substituting it into Equation (2), the mathematical model of the SMB system can be obtained as follows:

$$\frac{\partial C_{ij}}{\partial t} = D_i \frac{\partial^2 C_{ij}}{\partial x^2} - v_j^{SMB} \frac{\partial C_{ij}}{\partial x} - \frac{1-\varepsilon}{\varepsilon} k_i (q_{ij}^* - q_{ij}) \quad (5)$$

$$\frac{\partial q_{ij}}{\partial t} = k_i (q_{ij}^* - q_{ij}) \quad (6)$$

v_j^{SMB} is denoted as v_j^* ; by substituting Equation (6) into Equation (5), we obtain Equation (7).

$$\frac{\partial C_{ij}}{\partial t} = D_i \frac{\partial^2 C_{ij}}{\partial x^2} - v_j^* \frac{\partial C_{ij}}{\partial x} - \frac{1-\varepsilon}{\varepsilon} \frac{\partial q_{ij}}{\partial t} \quad (7)$$

The adsorption equilibrium for both enantiomers is represented by linear isotherms.

$$q_{ij} = H_i C_{ij} \quad (8)$$

Set

$$E = \frac{1-\varepsilon}{\varepsilon} \quad (9)$$

By substituting Equations (8) and (9) into Equation (7), it can be obtained as

$$(1+EH_i) \frac{\partial C_{ij}}{\partial t} = D_i \frac{\partial^2 C_{ij}}{\partial x^2} - v_j^* \frac{\partial C_{ij}}{\partial x} \quad (10)$$

2.2. Using the Crank–Nicolson Method to Numerate Partial Differential Equations

The Crank–Nicolson method employs central differencing in the spatial domain and the trapezoidal rule in the temporal domain, ensuring second-order convergence in the temporal domain. For example, for a one-dimensional partial differential equation,

$$\frac{\partial u}{\partial t} = F(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}) \quad (11)$$

Let Δx and Δt denote the spatial and temporal step sizes, respectively, and denote $u(i\Delta x, j\Delta t) = u_i^j$, then the discretized formula for the Crank–Nicolson method is as follows [26]:

$$\frac{u_i^{j+1} - u_i^j}{\Delta t} = \frac{1}{2} (F_i^{j+1}(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}) + F_i^j(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2})) \quad (12)$$

In order to better understand the discretization process of the SMB system, let us consider the following simple example:

Example 1. $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$, with a boundary condition is as follows:

Initial Conditions:

$$\begin{aligned} (t = 0) : u(x, 0) &= 0, x \in [0, 10] \\ u(0, t) &= 100, t \geq 0 \\ u(10, t) &= 50, t \geq 0 \end{aligned}$$

In comparison with Equation (1), where $F(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}) = \frac{\partial^2 u}{\partial x^2}$, according to the Crank–Nicolson method, the left-hand side of the equation is rewritten as follows: $\frac{u_i^{j+1} - u_i^j}{\Delta t}$, where the superscript j represents the j -th time point, and the subscript i represents the i -th spatial point. Therefore, the right-hand side of the equation $\frac{\partial^2 u}{\partial x^2}$ needs to be discretized at the time points $j + 1$ and j . Here is the central difference formula for discretizing $\frac{\partial^2 u}{\partial x^2}$. Since it is discretizing the spatial domain, we will omit the time domain subscript below. According to the Taylor expansion formula,

$$u_{i+1} = u_i + \Delta x \frac{\partial u}{\partial x} \Big|_i + \frac{\Delta x^2}{2} \frac{\partial^2 u}{\partial x^2} \Big|_i + \frac{\Delta x^3}{3!} \frac{\partial^3 u}{\partial x^3} \Big|_i + o(\Delta x^4) \quad (13)$$

$$u_{i-1} = u_i - \Delta x \frac{\partial u}{\partial x} \Big|_i + \frac{\Delta x^2}{2} \frac{\partial^2 u}{\partial x^2} \Big|_i - \frac{\Delta x^3}{3!} \frac{\partial^3 u}{\partial x^3} \Big|_i + o(\Delta x^4) \quad (14)$$

Adding the two equations yields results in the following:

$$u_{i+1} + u_{i-1} = 2u_i + \Delta x^2 \frac{\partial^2 u}{\partial x^2} \Big|_i + o(\Delta x^4) \quad (15)$$

By moving terms around, we can obtain the central differencing formula for $\frac{\partial^2 u}{\partial x^2}$ discretization as follows:

$$\frac{\partial^2 u}{\partial x^2} \Big|_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} \quad (16)$$

According to Equations (12) and (16), the discretized formula for the right-hand side of Example 1's equation is as follows:

$$\frac{1}{2}(F_i^{j+1}(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}) + F_i^j(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2})) = \frac{1}{2}(\frac{\partial^2 u}{\partial x^2}|_i^{j+1} + \frac{\partial^2 u}{\partial x^2}|_i^j) \quad (17)$$

By substituting Equation (16) into Equation (17), we obtain the following:

$$\frac{1}{2}(\frac{\partial^2 u}{\partial x^2}|_i^{j+1} + \frac{\partial^2 u}{\partial x^2}|_i^j) = \frac{((u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}) + (u_{i+1}^j - 2u_i^j + u_{i-1}^j))}{2\Delta x^2} \quad (18)$$

Then, the discretized equation for Example 1 can be obtained as follows:

$$\frac{u_i^{j+1} - u_i^j}{\Delta t} = \frac{((u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}) + (u_{i+1}^j - 2u_i^j + u_{i-1}^j))}{2\Delta x^2} \quad (19)$$

To establish iterative computational expressions, based on Equation (19), move the terms at time point j to the right-hand side of the equation and the terms at time point $j + 1$ to the left-hand side of the equation, then we obtain the following:

$$-\frac{\Delta t}{2\Delta x^2}u_{i+1}^{j+1} + (1 + \frac{\Delta t}{\Delta x^2})u_i^{j+1} - \frac{\Delta t}{2\Delta x^2}u_{i-1}^{j+1} = \frac{\Delta t}{2\Delta x^2}u_{i+1}^j + (1 - \frac{\Delta t}{\Delta x^2})u_i^j + \frac{\Delta t}{2\Delta x^2}u_{i-1}^j \quad (20)$$

Let $r = \frac{\Delta t}{2\Delta x^2}$, then Equation (20) can be written as follows:

$$-ru_{i+1}^{j+1} + (1 + 2r)u_i^{j+1} - ru_{i-1}^{j+1} = ru_{i+1}^j + (1 - 2r)u_i^j + ru_{i-1}^j \quad (21)$$

Assumption $\Delta x = 2$ and the interval $([0, 10])$ is divided into five equal parts (resulting in six endpoints), according to the given boundary condition (b) and Equation (21); we can then derive the following:

$$-ru_3^{j+1} + (1 + 2r)u_2^{j+1} - ru_1^{j+1} = ru_3^j + (1 - 2r)u_2^j + ru_1^j \quad (22)$$

where, according to the given boundary condition (b) $u_1^j = 100, u_1^{j+1} = 100$, substituting into Equation (22), we obtain

$$-ru_3^{j+1} + (1 + 2r)u_2^{j+1} = ru_3^j + (1 - 2r)u_2^j + 200r \quad (23)$$

Similarly, according to the given boundary condition (c) and Equation (21), we obtain

$$-ru_6^{j+1} + (1 + 2r)u_5^{j+1} - ru_4^{j+1} = ru_6^j + (1 - 2r)u_5^j + ru_4^j \quad (24)$$

where, according to the given boundary condition (c) $u_6^j = 50, u_6^{j+1} = 50$, substituting into Equation (24), we obtain

$$(1 + 2r)u_5^{j+1} - ru_4^{j+1} = (1 - 2r)u_5^j + ru_4^j + 100r \quad (25)$$

According to Equations (21), (23), and (25), set the matrix as follows:

$$A = \begin{bmatrix} 1 + 2r & -r & 0 & 0 \\ -r & 1 + 2r & -r & 0 \\ 0 & -r & 1 + 2r & -r \\ 0 & 0 & -r & 1 + 2r \end{bmatrix}, \quad B = \begin{bmatrix} 1 - 2r & r & 0 & 0 \\ r & 1 - 2r & r & 0 \\ 0 & r & 1 - 2r & r \\ 0 & 0 & r & 1 - 2r \end{bmatrix}$$

$$w = [200r, 0, 0, 100r]^T$$

Then, based on Equations (21), (23), and (25), the matrix obtained for Example 1 can be represented as follows in the discrete iterative equation:

$$\begin{aligned} & \begin{bmatrix} 1+2r & -r & 0 & 0 \\ -r & 1+2r & -r & 0 \\ 0 & -r & 1+2r & -r \\ 0 & 0 & -r & 1+2r \end{bmatrix} \begin{bmatrix} u_2^{j+1} \\ u_3^{j+1} \\ u_4^{j+1} \\ u_5^{j+1} \end{bmatrix} \\ &= \begin{bmatrix} 1-2r & r & 0 & 0 \\ r & 1-2r & r & 0 \\ 0 & r & 1-2r & r \\ 0 & 0 & r & 1-2r \end{bmatrix} \begin{bmatrix} u_2^j \\ u_3^j \\ u_4^j \\ u_5^j \end{bmatrix} + \begin{bmatrix} 200r \\ 0 \\ 0 \\ 100r \end{bmatrix} \end{aligned} \quad (26)$$

Letting $U^j = [u_2^j, u_3^j, u_4^j, u_5^j]^T$, then the final simplification is

$$AU^{j+1} = BU^j + w \quad (27)$$

For the spatial distribution U , originally divided into five intervals with seven points, the imposition of the boundary conditions (b) and (c) reduces two degrees of freedom, leaving four variables. This allows the unknown variables to be solved precisely by the linear equation set (23). Further iterative computations can then be carried out continuously based on boundary condition (a).

If the PDE equation contains a term involving $\frac{\partial u}{\partial x}$ on the right-hand side, then it needs to be discretized as well. According to the Taylor series expansion, we know the following:

$$u_{i+1} = u_i + \Delta x \frac{\partial u}{\partial x} \Big|_i + \frac{\Delta x^2}{2} \frac{\partial^2 u}{\partial x^2} \Big|_i + o(\Delta x^3) \quad (28)$$

$$u_{i-1} = u_i - \Delta x \frac{\partial u}{\partial x} \Big|_i + \frac{\Delta x^2}{2} \frac{\partial^2 u}{\partial x^2} \Big|_i + o(\Delta x^3) \quad (29)$$

By subtracting the two equations, we obtain

$$u_{i+1} - u_{i-1} = 2\Delta x \frac{\partial u}{\partial x} \Big|_i + o(\Delta x^3) \quad (30)$$

Then, rearranging the terms, we obtain

$$\frac{\partial u}{\partial x} \Big|_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} \quad (31)$$

The use of the diffusion equation for modeling substance diffusion in a simulated moving bed system should be critically examined and validated through numerical simulations for effective control.

In comparison with Equations (10) and (11), it can be observed that

$$(1 + EH_i) \frac{\partial C_{ij}}{\partial t} = F(C_{ij}, x, t, \frac{\partial C_{ij}}{\partial x}, \frac{\partial^2 C_{ij}}{\partial x^2}) \quad (32)$$

$$F(C_{ij}, x, t, \frac{\partial C_{ij}}{\partial x}, \frac{\partial^2 C_{ij}}{\partial x^2}) = D_i \frac{\partial^2 C_{ij}}{\partial x^2} - v_j^* \frac{\partial C_{ij}}{\partial x} \quad (33)$$

In comparison with Example 1, it can be observed that the form of Equation (33) now includes a first-order partial derivative in the spatial domain. Since the indices i, j have already been used to denote the substance category and column number, we select l, k as indices for the spatial and temporal domains. Consequently, the left-hand side of Equation (32) can be written as $(1 + EH_i) \frac{C_{ij,l}^{k+1} - C_{ij,l}^k}{\Delta t}$. The discretization formula for the right-hand side of Equation (33) is as follows:

$$\begin{aligned} & \frac{1}{2} (F_l^{k+1}(C_{ij}, x, t, \frac{\partial C_{ij}}{\partial x}, \frac{\partial^2 C_{ij}}{\partial x^2}) + F_l^k(C_{ij}, x, t, \frac{\partial C_{ij}}{\partial x}, \frac{\partial^2 C_{ij}}{\partial x^2})) \\ &= \frac{1}{2} D_i (\frac{\partial^2 C_{ij}}{\partial x^2} |_l^{k+1} + \frac{\partial^2 C_{ij}}{\partial x^2} |_l^k) - \frac{1}{2} v_j^* (\frac{\partial C_{ij}}{\partial x} |_l^{k+1} + \frac{\partial C_{ij}}{\partial x} |_l^k) \end{aligned} \quad (34)$$

According to Equation (16), we can see that

$$\frac{1}{2} D_i (\frac{\partial^2 C_{ij}}{\partial x^2} |_l^{k+1} + \frac{\partial^2 C_{ij}}{\partial x^2} |_l^k) = D_i \frac{((C_{ij,l-1}^{k+1} - 2C_{ij,l}^{k+1} + C_{ij,l+1}^{k+1}) + (C_{ij,l-1}^k - 2C_{ij,l}^k + C_{ij,l+1}^k))}{2\Delta x^2} \quad (35)$$

According to Equation (31), we can obtain

$$\frac{1}{2} v_j^* (\frac{\partial C_{ij}}{\partial x} |_l^{k+1} + \frac{\partial C_{ij}}{\partial x} |_l^k) = v_j^* \frac{((C_{ij,l+1}^{k+1} - C_{ij,l-1}^{k+1}) + (C_{ij,l+1}^k - C_{ij,l-1}^k))}{4\Delta x} \quad (36)$$

The expression for the right-hand side of Equation (32) can be obtained through substituting Equations (35) and (36) into it as follows:

$$\begin{aligned} (1 + EH_i) \frac{C_{ij,l}^{k+1} - C_{ij,l}^k}{\Delta t} &= D_i \frac{((C_{ij,l-1}^{k+1} - 2C_{ij,l}^{k+1} + C_{ij,l+1}^{k+1}) + (C_{ij,l-1}^k - 2C_{ij,l}^k + C_{ij,l+1}^k))}{2\Delta x^2} - \\ & v_j^* \frac{((C_{ij,l+1}^{k+1} - C_{ij,l-1}^{k+1}) + (C_{ij,l+1}^k - C_{ij,l-1}^k))}{4\Delta x} \end{aligned} \quad (37)$$

In order to establish an iterative calculation equation, according to Equation (37), the term of time point $K + 1$ is moved to the left of the equation, and the term of time point K is moved to the right of the equation to obtain

$$\begin{aligned} & (1 + EH_i + \frac{D_i \Delta t}{\Delta x^2}) C_{ij,l}^{k+1} - (\frac{v_j^* \Delta t}{4\Delta x} + \frac{D_i \Delta t}{2\Delta x^2}) C_{ij,l-1}^{k+1} + (\frac{v_j^* \Delta t}{4\Delta x} - \frac{D_i \Delta t}{2\Delta x^2}) C_{ij,l+1}^{k+1} \\ &= (\frac{v_j^* \Delta t}{4\Delta x} + \frac{D_i \Delta t}{2\Delta x^2}) C_{ij,l-1}^k + (1 + EH_i - \frac{D_i \Delta t}{\Delta x^2}) C_{ij,l}^k + (\frac{D_i \Delta t}{2\Delta x^2} - \frac{v_j^* \Delta t}{4\Delta x}) C_{ij,l+1}^k \end{aligned} \quad (38)$$

2.3. Boundary Numerate Condition

The boundary conditions are as follows:

Initial conditions:

$$C_{ij}(x, 0) = C_{0ij} \quad (39)$$

Pipe column space end:

$$\frac{\partial C_{ij}(x,t)}{\partial x} \Big|_{x=L_{end}} = 0 \quad (40)$$

Pipe column space head:

$$D_i \frac{\partial C_{ij}(x,t)}{\partial x} \Big|_{x=L_0} = v_i^* [C_{ij}(L_0, t) - \bar{C}_{ij}^{sect}(t)] \quad (41)$$

C_{0ij} represents the initial concentration distribution inside the columns at $t = 0$. The boundaries represented by $x = L_{end}$ and $x = L_0$, respectively, represent the conditions of the fixed values, which are the conditions that the end and initial positions of the pipe column must satisfy, corresponding to $u(0, t)$ and $u(10, t)$ in Example 1. The $\bar{C}_{ij}^{sect}(t)$ term is related to the region in which it is located, as Equation (41) describes the concentration variation at the head of the pipeline, and the head of each region depends on the flow rate at the entrance of that region, material concentration, the concentration at the end of the previous pipe column, and the flow rate of the region in contact with the entrance. Therefore, this term can be divided into three cases, as shown in the following formulas [1]:

$$\bar{C}_{ij}^I(t) = \frac{Q_{IV} C_{ij-1}(l_{n-1}, t)}{Q_I}, \text{Section I, 1}^{st} \text{ column} \quad (42)$$

$$\bar{C}_{ij}^{III}(t) = \frac{Q_{II} C_{ij-1}(l_{n-1}, t) + Q_f C_{fi}}{Q_{III}}, \text{Section III, 1}^{st} \text{ column} \quad (43)$$

$$\bar{C}_{ij}^{sect}(t) = C_{ij-1}(l_{n-1}, t), \text{other} \quad (44)$$

C_{fi} is the concentration of the material imported into the column, and Q is the flow rate in each section. The flow rates between the nodes of the pipe columns are constrained by the corresponding outlets and inlets of each column, and the relationship is as follows:

$$\begin{aligned} Q_I > Q_{IV}, Q_I > Q_{II}, Q_{III} > Q_{IV}, Q_{III} > Q_{IV} \\ Q_I - Q_{IV} = Q_d, Q_I - Q_{II} = Q_x, Q_{III} - Q_{IV} = Q_r, Q_{III} - Q_{II} = Q_f \end{aligned} \quad (45)$$

Q_d , Q_x , Q_r , and Q_f represent the flow rates of the wash liquid inlet, extract outlet, residual outlet, and feed inlet; Q_I , Q_{II} , Q_{III} , and Q_{IV} represent the flow rates of the four regions, respectively.

Similarly, we need to eliminate the variables of two degrees of freedom through Equations (40) and (41), which can be transformed into an algebraic linear system of equations. Assuming that each pipe column is divided into $n + 1$ components, Equation (40) can be obtained from Equation (12) as follows:

$$0 = \frac{\partial C_{ij}(x,t)}{\partial x} \Big|_{x=L_{end}} = \frac{1}{2} \left(\frac{\partial C_{ij}}{\partial x} \Big|_n^{k+1} + \frac{\partial C_{ij}}{\partial x} \Big|_n^k \right) = \frac{((C_{ij,n+1}^{k+1} - C_{ij,n-1}^{k+1}) + (C_{ij,n+1}^k - C_{ij,n-1}^k))}{4\Delta x} \quad (46)$$

Moving the term of spatial point $n + 1$ to the left of the equation and the term of spatial point n to the right of the equation yields the following:

$$C_{ij,n+1}^k + C_{ij,n+1}^{k+1} = C_{ij,n-1}^k + C_{ij,n-1}^{k+1} \quad (47)$$

Taking the spatial point $j = n$ in Equation (38), it can be obtained that

$$\begin{aligned}
& (1 + EH_i + \frac{D_i \Delta t}{\Delta x^2}) C_{ij,n}^{k+1} - (\frac{v_j^* \Delta t}{4\Delta x} + \frac{D_i \Delta t}{2\Delta x^2}) C_{ij,n-1}^{k+1} + (\frac{v_j^* \Delta t}{4\Delta x} - \frac{D_i \Delta t}{2\Delta x^2}) C_{ij,n+1}^{k+1} \\
& = (\frac{v_j^* \Delta t}{4\Delta x} + \frac{D_i \Delta t}{2\Delta x^2}) C_{ij,n-1}^k + (1 + EH_i - \frac{D_i \Delta t}{\Delta x^2}) C_{ij,n}^k + (\frac{D_i \Delta t}{2\Delta x^2} - \frac{v_j^* \Delta t}{4\Delta x}) C_{ij,n+1}^k
\end{aligned} \quad (48)$$

By substituting Equation (47) into Equation (48) to eliminate $C_{ij,n+1}^k, C_{ij,n+1}^{k+1}$, which means eliminating spatial point $n+1$, the following equation can be obtained:

$$\begin{aligned}
& (1 + EH_i + \frac{D_i \Delta t}{\Delta x^2}) C_{ij,n}^{k+1} - (\frac{v_j^* \Delta t}{4\Delta x} + \frac{D_i \Delta t}{2\Delta x^2}) C_{ij,n-1}^{k+1} + (\frac{v_j^* \Delta t}{4\Delta x} - \frac{D_i \Delta t}{2\Delta x^2}) C_{ij,n-1}^{k+1} \\
& = (\frac{v_j^* \Delta t}{4\Delta x} + \frac{D_i \Delta t}{2\Delta x^2}) C_{ij,n-1}^k + (1 + EH_i - \frac{D_i \Delta t}{\Delta x^2}) C_{ij,n}^k + (\frac{D_i \Delta t}{2\Delta x^2} - \frac{v_j^* \Delta t}{4\Delta x}) C_{ij,n-1}^k
\end{aligned} \quad (49)$$

Merging similar items can lead to

$$-\frac{D_i \Delta t}{\Delta x^2} C_{ij,n-1}^{k+1} + (1 + EH_i + \frac{D_i \Delta t}{\Delta x^2}) C_{ij,n}^{k+1} = \frac{D_i \Delta t}{\Delta x^2} C_{ij,n-1}^k + (1 + EH_i - \frac{D_i \Delta t}{\Delta x^2}) C_{ij,n}^k \quad (50)$$

Equation (51) can be obtained from Equation (41) as follows:

$$\begin{aligned}
& \frac{v_j^*}{D_i} [C_{ij,1}^k - \bar{C}_{ij}^{\text{sect}}(k)] = \frac{\partial C_{ij}(x,t)}{\partial x} \Big|_{x=L_0} = \frac{1}{2} (\frac{\partial C_{ij}}{\partial x} \Big|_1^{k+1} + \frac{\partial C_{ij}}{\partial x} \Big|_1^k) = \\
& \frac{((C_{ij,2}^{k+1} - C_{ij,0}^{k+1}) + (C_{ij,2}^k - C_{ij,0}^k))}{4h}
\end{aligned} \quad (51)$$

Moving the term of point 0 in space to the left of the equation and moving the other terms to the right of the equation yields

$$C_{ij,2}^{k+1} + C_{ij,2}^k - \frac{4hv_j^*}{D_i} (C_{ij,1}^k - \bar{C}_{ij}^{\text{sect}}(k)) = C_{ij,0}^{k+1} + C_{ij,0}^k \quad (52)$$

By taking the spatial point $j=1$ in Equation (38), it can be obtained that

$$\begin{aligned}
& (1 + FH_i + \frac{D_i s}{h^2}) C_{ij,1}^{k+1} - (\frac{v_j^* s}{4h} + \frac{D_i s}{2h^2}) C_{ij,0}^{k+1} + (\frac{v_j^* s}{4h} - \frac{D_i s}{2h^2}) C_{ij,2}^{k+1} \\
& = (\frac{v_j^* s}{4h} + \frac{D_i s}{2h^2}) C_{ij,0}^k + (1 + FH_i - \frac{D_i s}{h^2}) C_{ij,1}^k + (\frac{D_i s}{2h^2} - \frac{v_j^* s}{4h}) C_{ij,2}^k
\end{aligned} \quad (53)$$

By substituting Equation (52) into Equation (53) to eliminate $C_{ij,0}^k, C_{ij,0}^{k+1}$, which means eliminating spatial point 0, the following equation can be obtained:

$$\begin{aligned}
& (1 + EH_i + \frac{D_i \Delta t}{\Delta x^2}) C_{ij,1}^{k+1} + (\frac{v_j^* \Delta t}{4\Delta x} - \frac{D_i \Delta t}{2\Delta x^2}) C_{ij,2}^{k+1} - (\frac{v_j^* \Delta t}{4\Delta x} + \frac{D_i \Delta t}{2\Delta x^2}) C_{ij,2}^{k+1} = \\
& - (\frac{v_j^* \Delta t}{4\Delta x} + \frac{D_i \Delta t}{2\Delta x^2}) \frac{4\Delta x v_j^*}{D_i} (C_{ij,1}^k - \bar{C}_{ij}^{\text{sect}}(k)) + (1 + EH_i - \frac{D_i \Delta t}{\Delta x^2}) C_{ij,1}^k + \\
& (\frac{D_i \Delta t}{2\Delta x^2} - \frac{v_j^* \Delta t}{4\Delta x}) C_{ij,2}^k + (\frac{v_j^* \Delta t}{4\Delta x} + \frac{D_i \Delta t}{2\Delta x^2}) C_{ij,2}^{k+1}
\end{aligned} \quad (54)$$

Merging similar items can lead to

$$\begin{aligned}
 (1 + EH_i + \frac{D_i \Delta t}{\Delta x^2}) C_{ij,1}^{k+1} - \frac{D_i \Delta t}{\Delta x^2} C_{ij,2}^{k+1} &= (\frac{v_j^{*2} \Delta t}{D_i} + \frac{2v_j^* \Delta t}{\Delta x}) \bar{C}_{ij}^{\text{sect}}(k) + \\
 (1 + EH_i - \frac{D_i \Delta t}{\Delta x^2} - \frac{v_j^{*2} \Delta t}{D_i} - \frac{2v_j^* \Delta t}{\Delta x}) C_{ij,1}^k &+ \frac{D_i \Delta t}{\Delta x^2} C_{ij,2}^k
 \end{aligned} \quad (55)$$

To simplify symbols, let

$$m = \frac{v_j^* \Delta t}{4\Delta x} \quad (56)$$

$$p = \frac{D_i \Delta t}{2\Delta x^2} \quad (57)$$

Then

$$v_j^* = \frac{4m\Delta x}{\Delta t} \quad (58)$$

$$D_i = \frac{2\Delta x^2 p}{\Delta t} \quad (59)$$

Substituting Equations (58) and (59) into Equation (55) yields

$$\begin{aligned}
 (1 + EH_i + 2p) C_{ij,1}^{k+1} - 2p C_{ij,2}^{k+1} &= (\frac{16m^2 \Delta x^2}{\Delta t^2} \frac{\Delta t \Delta t}{2\Delta x^2 p} + \frac{8m\Delta x \Delta t}{\Delta t \Delta x}) \bar{C}_{ij}^{\text{sect}}(k) + \\
 (1 + EH_i - 2p - \frac{16m^2 \Delta x^2}{\Delta t^2} \frac{\Delta t \Delta t}{2\Delta x^2 p} - \frac{8m\Delta x \Delta t}{\Delta t \Delta x}) C_{ij,1}^k &+ 2p C_{ij,2}^k
 \end{aligned} \quad (60)$$

Simplify the equation at the initial position of a spatial point as follows:

$$\begin{aligned}
 (1 + EH_i + 2p) C_{ij,1}^{k+1} - 2p C_{ij,2}^{k+1} &= \frac{8m(m+p)}{p} \bar{C}_{ij}^{\text{sect}}(k) + \\
 (1 + EH_i - 2p - \frac{8m(m+p)}{p}) C_{ij,1}^k &+ 2p C_{ij,2}^k
 \end{aligned} \quad (61)$$

Substituting Equations (58) and (59) into Equation (38) yields the equation for the middle position of a spatial point as follows:

$$\begin{aligned}
 (1 + EH_i + 2p) C_{ij,l}^{k+1} - (m+p) C_{ij,l-1}^{k+1} + (m-p) C_{ij,l+1}^{k+1} \\
 = (m+p) C_{ij,l-1}^k + (1 + EH_i - 2p) C_{ij,l}^k + (p-m) C_{ij,l+1}^k
 \end{aligned} \quad (62)$$

Substituting Equations (58) and (59) into Equation (50) yields the equation for the end position of a spatial point as follows:

$$-2p C_{ij,n-1}^{k+1} + (1 + EH_i + 2p) C_{ij,n}^{k+1} = 2p C_{ij,n-1}^k + (1 + EH_i - 2p) C_{ij,n}^k \quad (63)$$

According to Equations (61)–(63), denote the matrix

$$A = \begin{bmatrix} 1+EH_i+2p & -2p & 0 & \cdots & 0 \\ -(m+p) & 1+EH_i+2p & (m-p) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & -(m+p) & 1+EH_i+2p & (m-p) \\ 0 & \cdots & 0 & -2p & 1+EH_i+2p \end{bmatrix}_{n \times n} \quad (64)$$

$$B = \begin{bmatrix} 1+EH_i-2p-\frac{8m(m+p)}{p} & 2p & 0 & \cdots & 0 \\ (m+p) & 1+EH_i-2p & -(m-p) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & (m+p) & 1+EH_i-2p & -(m-p) \\ 0 & \cdots & 0 & 2p & 1+EH_i-2p \end{bmatrix}_{n \times n} \quad (65)$$

Set

$$C_{ij}^k = [C_{ij,1}^k, C_{ij,2}^k, \dots, C_{ij,n}^k]^T_{1 \times n} \quad (66)$$

$$w(k) = \left(\frac{8m(m+p)}{p} \bar{C}_{ij}^{\text{sect}}(k) \quad 0 \quad \cdots \quad 0 \quad 0 \right)^T_{1 \times n} \quad (67)$$

The final iterative matrix equation incorporating Equations (61)–(63) can be unified as follows:

$$AC_{ij}^{k+1} = BC_{ij}^k + w(k) \quad (68)$$

2.4. Langmuir Isotherm Model

For nonlinear adsorption isotherms, the commonly seen one is the Langmuir isotherm, which can be represented using the following equation:

$$q_{ij} = \frac{GK_i C_i}{1 + K_1 C_1 + K_2 C_2} \quad (69)$$

$K_i, i=1, 2$ are coefficients of material A and B, and G is the adsorption constant. To ensure that the Langmuir isotherm equation does not affect the linearity of the iterative calculations, a temporal grid shift is introduced during the discretization of the isotherm curve. However, to ensure sufficient accuracy, a significantly small-time increment must be chosen. As a result, the increased computational burden is limited to the temporal dimension, while the resulting iterative equation remains linear.

Equation (69) yields

$$\frac{\partial q_{ij}}{\partial t} = \frac{q_{ij}^k - q_{ij}^{k-1}}{\Delta t} = \left[\frac{GK_i C_{ij,l}^k}{1 + \sum_{i=1}^2 K_i C_{ij,l}^k} - \frac{GK_i C_{ij,l}^{k-1}}{1 + \sum_{i=1}^2 K_i C_{ij,l}^{k-1}} \right] / \Delta t \quad (70)$$

The discretization of other equations follows the same linear approach. Substituting Equation (70) into Equation (10) yields

$$(1+2p)C_{ij,l}^{k+1} - (m+p)C_{ij,l-1}^{k+1} + (m-p)C_{ij,l+1}^{k+1} = (m+p)C_{ij,l-1}^k + (1-2p)C_{ij,l}^k + (p-m)C_{ij,l+1}^k - \left[\frac{GK_i C_{ij,l}^k}{1 + \sum_{i=1}^2 K_i C_{ij,l}^k} - \frac{GK_i C_{ij,l}^{k-1}}{1 + \sum_{i=1}^2 K_i C_{ij,l}^{k-1}} \right] \quad (71)$$

Similarly, the boundary condition at the end of the pipe column in the fixed value condition is discretized as

$$(1+2p)C_{ij,l}^{k+1} - (m+p)C_{ij,l-1}^{k+1} + (m-p)C_{ij,l+1}^{k+1} = (m+p)C_{ij,l-1}^k + (1-2p)C_{ij,l}^k + (p-m)C_{ij,l+1}^k - \left[\frac{GK_i C_{ij,l}^k}{1 + \sum_{i=1}^2 K_i C_{ij,l}^k} - \frac{GK_i C_{ij,l}^{k-1}}{1 + \sum_{i=1}^2 K_i C_{ij,l}^{k-1}} \right] \quad (72)$$

The boundary condition at the end of the pipe column in the fixed value condition is discretized as

$$(1+2p)C_{ij,n}^{k+1} - (m+p)C_{ij,n-1}^{k+1} + (m-p)C_{ij,n+1}^{k+1} = (m+p)C_{ij,n-1}^k + (1-2p)C_{ij,n}^k + (p-m)C_{ij,n+1}^k - \left[\frac{GK_i C_{ij,n}^k}{1 + \sum_{i=1}^2 K_i C_{ij,n}^k} - \frac{GK_i C_{ij,n}^{k-1}}{1 + \sum_{i=1}^2 K_i C_{ij,n}^{k-1}} \right] \quad (73)$$

By combining terms of the same category, we can obtain the following equation:

$$(1+2p)C_{ij,n}^{k+1} - 2pC_{ij,n-1}^{k+1} = 2pC_{ij,n-1}^k + (1-2p)C_{ij,n}^k - \left[\frac{GK_i C_{ij,n}^k}{1 + \sum_{i=1}^2 K_i C_{ij,n}^k} - \frac{GK_i C_{ij,n}^{k-1}}{1 + \sum_{i=1}^2 K_i C_{ij,n}^{k-1}} \right] \quad (74)$$

The boundary condition at the head of the pipe column in the fixed value condition is discretized as

$$(1+2p)C_{ij,1}^{k+1} - 2pC_{ij,2}^{k+1} = \frac{8m(m+p)}{p} C_{ij}^{\text{sect}}(k) + (1-2p - \frac{8m(m+p)}{p}) C_{ij,1}^k + 2pC_{ij,2}^k - \left[\frac{GK_i C_{ij,1}^k}{1 + \sum_{i=1}^2 K_i C_{ij,1}^k} - \frac{GK_i C_{ij,1}^{k-1}}{1 + \sum_{i=1}^2 K_i C_{ij,1}^{k-1}} \right] \quad (75)$$

Set

$$O_{ij,l}^k = FGK_i \left[\frac{GK_i C_{ij,l}^k}{1 + \sum_{i=1}^2 K_i C_{ij,l}^k} - \frac{GK_i C_{ij,l}^{k-1}}{1 + \sum_{i=1}^2 K_i C_{ij,l}^{k-1}} \right] \quad (76)$$

According to Equations (73)–(75), the nonlinear isothermal line matrix can be defined as A_{non} and B_{non} as follows:

$$A_{non} = \begin{bmatrix} 1+2p & -2p & 0 & \cdots & 0 \\ -(m+p) & 1+2p & (m-p) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & -(m+p) & 1+2p & (m-p) \\ 0 & \cdots & 0 & -2p & 1+2p \end{bmatrix}_{n \times n} \quad (77)$$

$$B_{non} = \begin{bmatrix} 1-2p - \frac{8m(m+p)}{p} & 2p & 0 & \cdots & 0 \\ (m+p) & 1-2p & -(m-p) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & (m+p) & 1-2p & -(m-p) \\ 0 & \cdots & 0 & 2p & 1-2p \end{bmatrix}_{n \times n} \quad (78)$$

$$w(k) = \left(\frac{8m(m+p)}{p} \bar{C}_{ij}^{\text{sect}}(k) \ 0 \ \cdots \ 0 \ 0 \right)_{1 \times n}^T \quad (79)$$

$$O_{ij}^k = (O_{ij,1}^k, O_{ij,2}^k, \dots, O_{ij,n}^k)_{1 \times n}^T \quad (80)$$

Finally, Equations (73)–(75) can be unified into the following matrix iteration equations:

$$A_{non} C_{ij}^{k+1} = B_{non} C_{ij}^k + w(k) + O_{ij}^k \quad (81)$$

3. Discrete Simulation

In the simulation system, we use a 2-2-2-2 packing column structure, meaning each area has two columns. The initial parameters of the system are set as shown in Table 2, in which we refer to the parameter settings of the material in reference [1] and ensure that the inequality conditions (45) between the corresponding regional flow rates are met. The time step is set to $\Delta t = 0.1$ seconds, and there are 50 spatial points for each column, so

$$\Delta t = \frac{L}{50} = 0.5 \text{ cm.}$$

Table 2. The standard parameters for the separation.

Parameter	Value	Parameter	Value
$L(\text{cm})$	25	$C_{f,i}(\text{gL}^{-1})$	5
$d(\text{cm})$	0.46	$\theta(\text{min})$	3
H_A	0.001	$Q_I(\text{cm}^3 \text{min}^{-1})$	6.75
H_B	0.45	$Q_{II}(\text{cm}^3 \text{min}^{-1})$	6.6
$D_A(\text{cm}^2 \text{min}^{-1})$	0.2	$Q_{III}(\text{cm}^3 \text{min}^{-1})$	7
$D_B(\text{cm}^2 \text{min}^{-1})$	1.265	$Q_{IV}(\text{cm}^3 \text{min}^{-1})$	2
ε	0.8	spatial number	50

The experiment was conducted using MATLAB R2016a software on a PC equipped with an Intel Core i7-3770K 3.53 GHz processor and 16 GB RAM. The experimental data

generated had a size of 70 MB. Figure 2 shows the separation process of SMB without any control conditions.

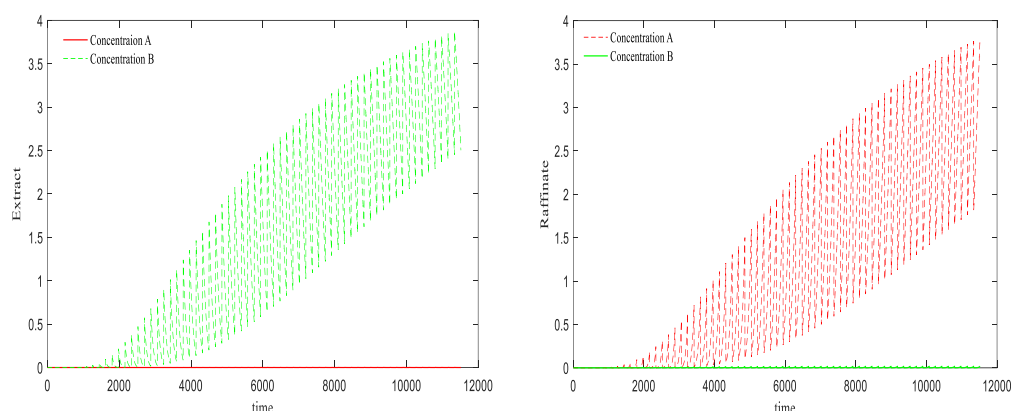


Figure 2. Concentration of the SMB process on the extract and raffinate.

From Figures 2 and 3, it can be observed that the simulation results obtained using the Crank–Nicolson finite difference method are almost the same as those obtained using the finite element method [27]. However, the Crank–Nicolson method only requires ordinary numerical calculations, making it much more efficient than the finite element method. This has important implications for achieving online real-time control or optimization. Similarly, for the analog (discrete) SMB system under the Langmuir isotherm, similar conclusions can be drawn. The main parameter settings are shown in Table 3.

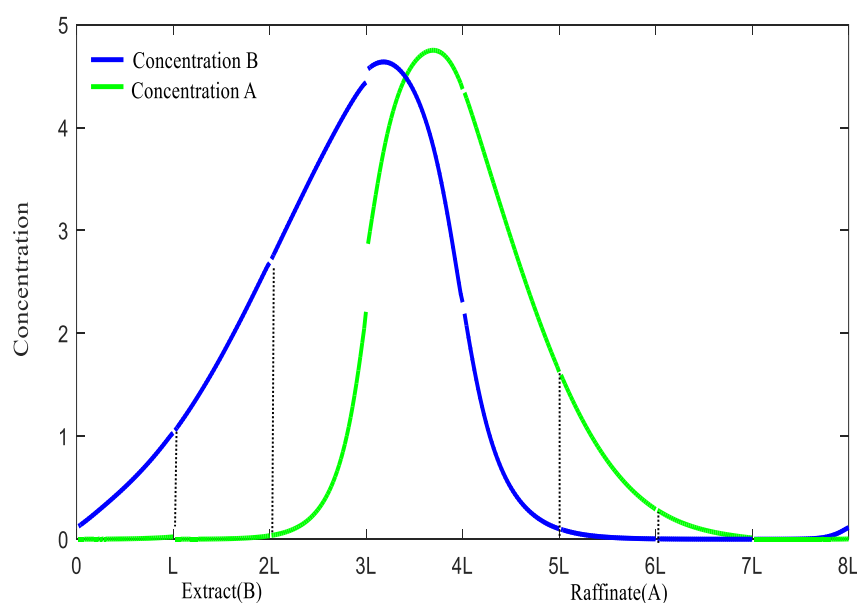


Figure 3. Axial concentration variation curve under linear isotherms.

Table 3. The initial parameters of Langmuir isotherm separation.

Parameter	Value	Parameter	Value
$L(\text{cm})$	23	$C_{f,i}(\text{gL}^{-1})$	4
$d(\text{cm})$	1.1	$T_\theta(\text{min})$	3
$K_A(\text{gL}^{-1})$	0.05	$Q_I(\text{cm}^3 \text{min}^{-1})$	6.03
$K_B(\text{gL}^{-1})$	0.45	$Q_{II}(\text{cm}^3 \text{min}^{-1})$	5.3
$D_A(\text{cm}^2 \text{min}^{-1})$	0.2	$Q_{III}(\text{cm}^3 \text{min}^{-1})$	5.45

$D_B (\text{cm}^2 \text{min}^{-1})$	1.265	$Q_{IV} (\text{cm}^3 \text{min}^{-1})$	3.529
ε	0.8	$G (\text{gL}^{-1})$	1
$\Delta x (\text{cm})$	0.23	$\Delta t (\text{s})$	0.01

From Figures 4 and 5, it can be observed that the Crank–Nicolson method can also provide results under isothermal conditions, and the iterative process converges. The efficient computational efficiency of the finite difference method provides a good platform for further studying the control of SMB systems under Langmuir conditions. Similarly, it is of great significance for the real-time control research of SMB systems.

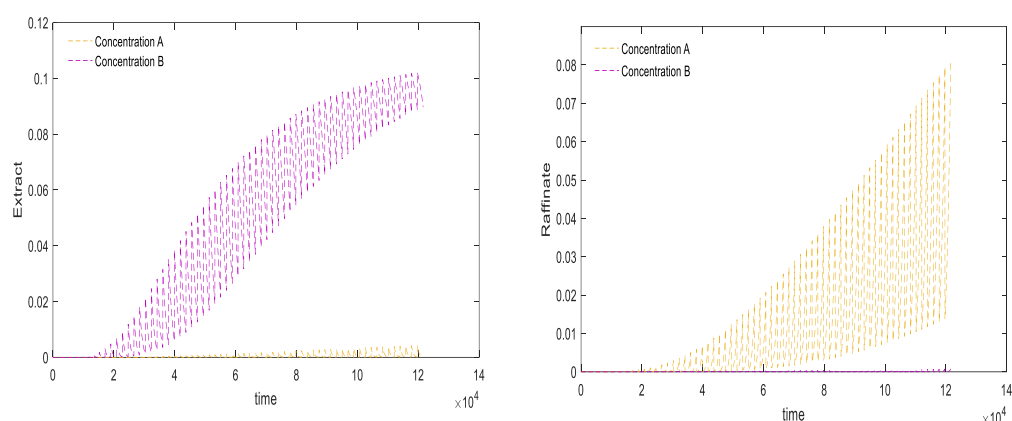


Figure 4. Concentration of the SMB process on the extract and raffinate under Langmuir isotherms.

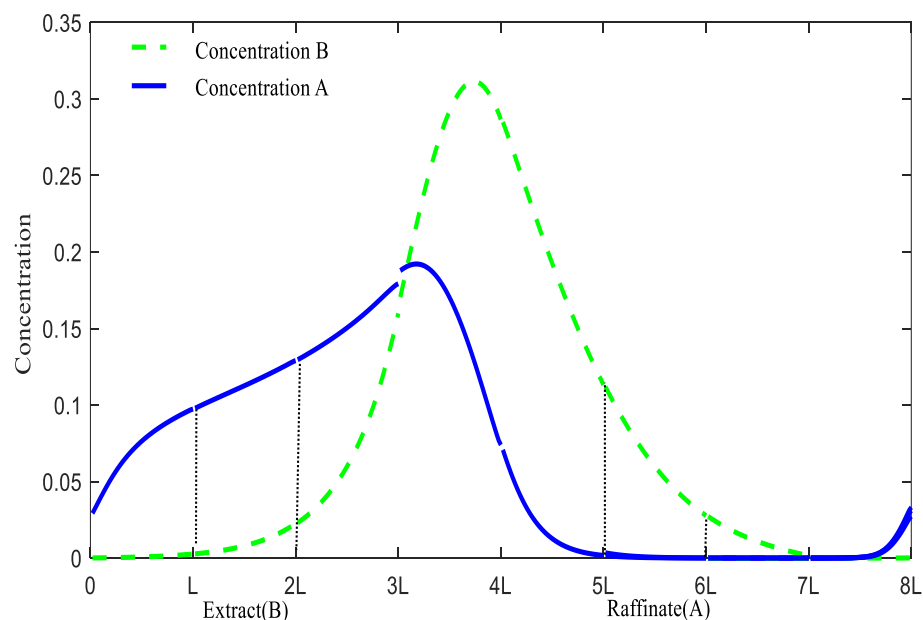


Figure 5. Axial concentration variation curve under Langmuir isotherm.

4. Controller Simulation

4.1. Controller Designer

The error, first-order difference, and second-order difference are selected as input variables, making it three-dimensional. The system has three independent single neuron self-adaptation proportional summation derivative (PSD) or proportion integration

differentiation (PID) controllers, which act on zone I, II, and III, respectively. The equation is as follows:

$$e_1 = \text{desired } B - C_{E,B} \quad (82)$$

$$e_2 = \text{desired } A - C_{R,A} \quad (83)$$

$$e_3 = e_1 + e_2 \quad (84)$$

$$\Delta e_1 = e_1(k) - e_1(k-1) \quad (85)$$

$$\Delta e_2 = e_2(k) - e_2(k-1) \quad (86)$$

$$\Delta e_3 = \Delta e_1 + \Delta e_2 \quad (87)$$

$$\Delta^2 e_1 = \Delta e_1(t) - \Delta e_1(t-1) \quad (88)$$

$$\Delta^2 e_2 = \Delta e_2(t) - \Delta e_2(t-1) \quad (89)$$

$$\Delta^2 e_3 = \Delta e_3(t) - \Delta e_3(t-1) \quad (90)$$

where e_1 , Δe_1 , and $\Delta^2 e_1$ are the inputs of the zone I controller; e_2 , Δe_2 , and $\Delta^2 e_2$ are the inputs of the zone II controller; and e_3 , Δe_3 , and $\Delta^2 e_3$ are the inputs of the zone III controller. $C_{E,B}$ is the B material purity of the extract port, and $C_{R,A}$ is the A material purity of the raffinate port. In order to better understand the trend of change, a periodic average processing of the data is performed; one cycle moving average smoothing equations are defined as follows:

$$\bar{C}_{E,B,t} = \frac{\int_{t-T}^t C_{E,B,t} dt}{T} \quad (91)$$

$$\bar{C}_{R,A,t} = \frac{\int_{t-T}^t C_{R,A,t} dt}{T} \quad (92)$$

$\bar{C}_{E,B,t}$ is the B material purity of the extract port of average periodic, and $\bar{C}_{R,A,t}$ is the A material purity of the raffinate port of average periodic.

The control structure of the PSD single neuron controller in the SMB system is shown in Figure 6.

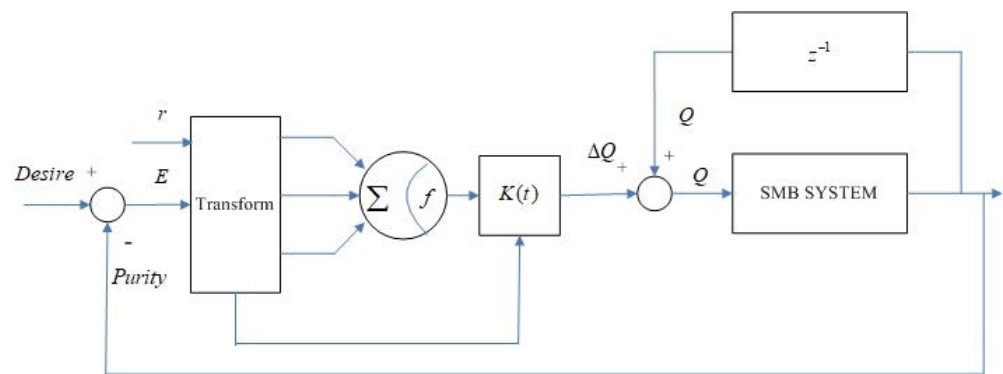


Figure 6. PSD controller for the SMB.

The output of the single neuron is defined using

$$\Delta u(t) = w_1(t)x_1(t) + w_2(t)x_2(t) + w_3(t)x_3(t) \quad (93)$$

$x_i(t) (i = 1, 2, 3)$ are neuron input signals; they represent $x_1(t) = e(t)$, $x_2(t) = \Delta e(t)$, $x_3(t) = \Delta^2 e(t)$, respectively. Since the following equation is universal to the three controllers, the subscripts of the error, first-order error, and second-order error are omitted. $w_i(t) (i = 1, 2, 3)$ is the weighting coefficient corresponding to the inputs in neuron learning. The weights of the neurons that learn and evolve in the process of neural iteration, $w_i(t)$, are proportional to the progressive signal $r_i(t)$ and are slow to attenuation at the same time. The learning rules are as follows [28]:

$$w_i(t+1) = (1-m)w_i(t) + d_i r_i(t), m, d > 0 \quad (94)$$

$$\Delta u(t) = w_1(t)x_1(t) + w_2(t)x_2(t) + w_3(t)x_3(t) \quad (95)$$

d_i is learning rate.

$$r_i(t) = e(t)u(t)[e(t) + \Delta e(t)] \quad (96)$$

$u(t)$ is the output value of the neuron at time t .

In practical application, m is set to 0. To ensure the convergence and robustness of the learning algorithm, a single neuron PSD control law is constructed using a normalized learning algorithm.

$$\Delta u'(t) = K(t)[w_1'(t)x_1(t) + w_2'(t)x_2(t) + w_3'(t)x_3(t)] \quad (97)$$

$\Delta u'(t)$ is the final output of the gain device $K(t)$, $w_i'(t)$ is the result of $w_i(t)$ after normalization, and the equation is as follows:

$$w_i'(t) = w_i(t) / \sum_{i=1}^3 |w_i(t)|, (i = 1, 2, 3) \quad (98)$$

According to Equation (94), the weight of the next moment after learning is as follows:

$$w_1(t+1) = w_1(t) + d_l e(t)u(t)[e(t) + \Delta e(t)] \quad (99)$$

$$w_2(t+1) = w_2(t) + d_p e(t)u(t)[e(t) + \Delta e(t)] \quad (100)$$

$$w_3(t+1) = w_3(t) + d_D e(t) u(t) [e(t) + \Delta e(t)] \quad (101)$$

The learning rules for the gain $K(t)$ are as follows:

If $\text{sgn}[e(t)] = \text{sgn}[e(t-1)]$ ($\text{sgn}(x)$ is symbolic function), then

$$K(t) = K(t-1) + CK(t-1)/Tv(t-1) \quad (102)$$

$$Tv(t) = Tv(t-1) + L^* \text{sgn}(|\Delta e(t)| - Tv(t-1)|\Delta^2 e(t)|) \quad (103)$$

Otherwise, set

$$K(t) = 0.75K(t-1) \quad (104)$$

$$Tv(t) = Tv(t-1) + L^* \text{sgn}(|\Delta e(t)| - Tv(t-1)|\Delta^2 e(t)|) \quad (105)$$

where $Tv(t)$ represents the ratio of the error to the second-order error difference, and the initial parameter of $Tv(t)$ is set to 1. According to the experience, the corresponding parameter setting range is as follows: $0.05 \leq L^* \leq 0.1, 0.025 \leq C \leq 0.05$.

The flow rate of zone I, II, and III is selected as the control variable, and the PSD single neuron control and PID parameter values are set as shown in Tables 4 and 5.

Table 4. PSD Control parameters.

Parameter	Value	Parameter	Value
d_p	15	C	0.06
d_I	7	L	0.05
d_D	7	W_0	1 (matrix)

Table 5. PID control parameter setting.

Region	K_p	K_d	K_i
I	0.015	0.003	0.95
II	0.001	0.002	0.95
III	0.01	0.0025	0.95

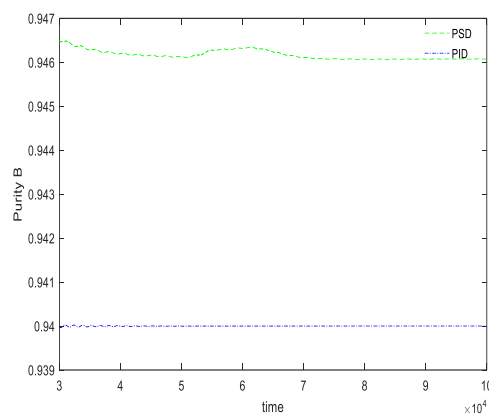
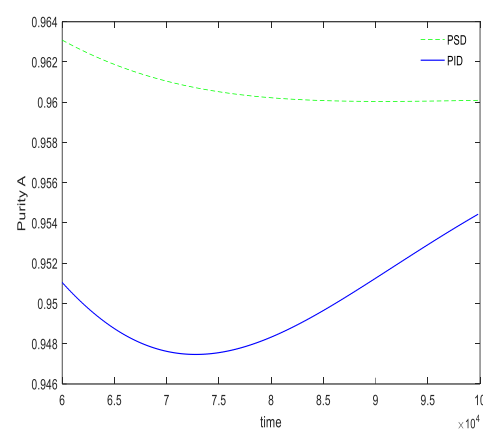
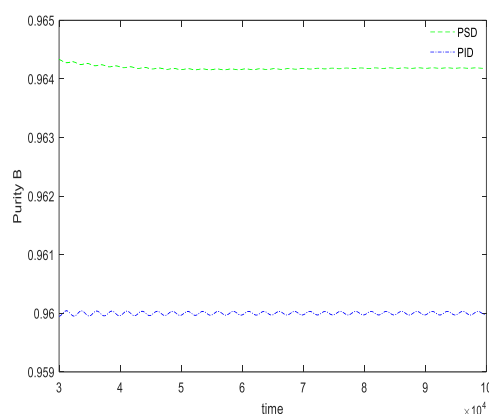
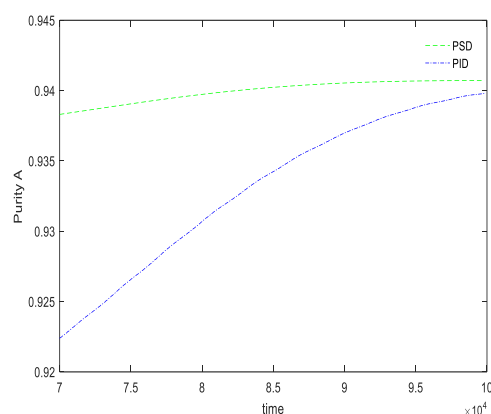
4.2. Experiment Results

In this section, we conducted purity control experiments on the SMB system using an adaptive single-neuron controller and compared it with a PID controller. The results of the control are shown in Figures 7–9. Figure (a) represents the purity of the extract outlet, while Figure (b) represents the purity of the raffinate outlet. The three figures represent the control effectiveness under different switching times and control objectives. The effects of the variations in the adsorbent parameters, feed concentration, and switching time on the controller performance were observed. Each set of experiments was further divided into two trials, with control setpoints for the purity of component B set at 92% and 96% and those for the purity of component A set at 93% and 97%.

In the first set of experiments with a switching time of 180 s, the control results showed that both for the extracted B component at the outlet and the raffinate A component at the outlet, the PID control exhibited smaller steady-state errors. However, overall, the PID control exhibited higher fluctuations, while the PSD control demonstrated better stability, as evident from Figures 7–9 and Table 6.

Table 6. Experimental results of three groups.

Group \ Controller	Target	PSD	PID
Group 1 Material A	96%	96.01%	95.5%
Group 1 Material B	94%	94.61%	94%
Group 2 Material A	94%	94.07%	93.98%
Group 2 Material B	96%	96.42%	96%
Group 3 Material A	93%	92.8%	92.83%
Group 3 Material B	95%	95.52%	95%

**(a)** Extract (Material B)**(b)** Raffinate (Material A)**Figure 7.** Group 1 control results (desired B = 94%, desired A = 96%, switch time = 180 s).**(a)** Extract (Material B)**(b)** Raffinate (Material A)**Figure 8.** Group 2 control results (desired B = 96%, desired A = 94%, Switch time = 180 s).

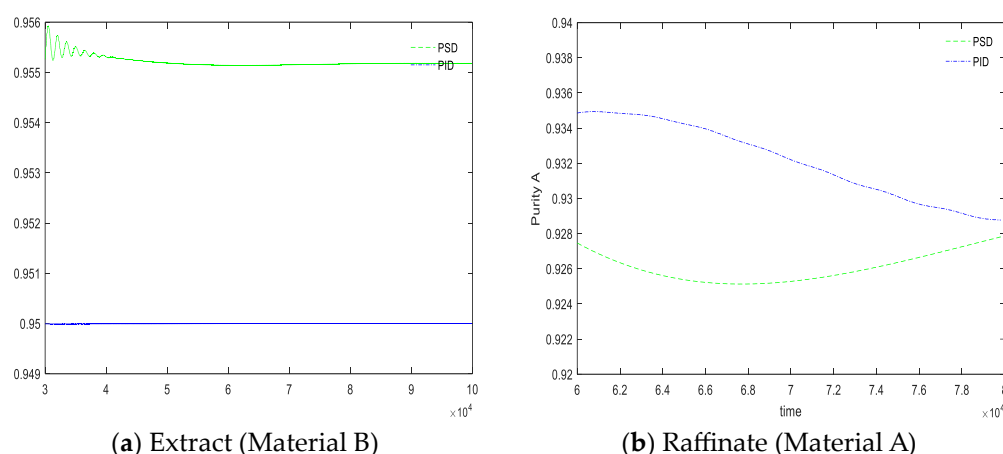


Figure 9. Group 3 control results (desired B = 95%, desired A = 93%, switch time = 178 s).

Figure 10 illustrates the impact of changes in the adsorbent parameters on the control performance of the two controllers. Figure 10a depicts the purity variation of material B at the extract outlet, while Figure 10b shows the purity variation of material A at the raffinate outlet. It can be observed that, under variations in the adsorbent parameters, both controllers maintained stable purity control for component B. However, for component A, the PID control exhibited significant fluctuations, whereas the PSD control showed relatively stable performance.

Figure 11 illustrates the impact of changes in the feed concentration at the material inlet on the control performance of the two controllers. Figure 11a depicts the purity variation of material B at the extract outlet, while Figure 11b shows the purity variation of material A at the raffinate outlet. It can be observed that, when the feed concentration varied for a target purity control of component B at 92%, the PID controller exhibited a Z-shaped oscillation in the control results. The fluctuations in the purity of raffinate component A were also slightly larger when compared to the PSD controller.

Figure 12 demonstrates the impact of changes in the switching time on the control performance of the two controllers. Figure 12a depicts the purity variation of material B at the extract outlet, while Figure 12b illustrates the purity variation of material A at the raffinate outlet. It can be observed that, under variations in the switching time, when the purity of component B was set at 92%, the control results of the PID controller showed deviations and did not converge to a steady state. The purity of component A exhibited significant fluctuations. However, the PSD control remained stable in this scenario.

Overall, we can not only observe the performance of a controller in a discrete dynamic process, but we can also compare the robustness and adaptability of different controllers.

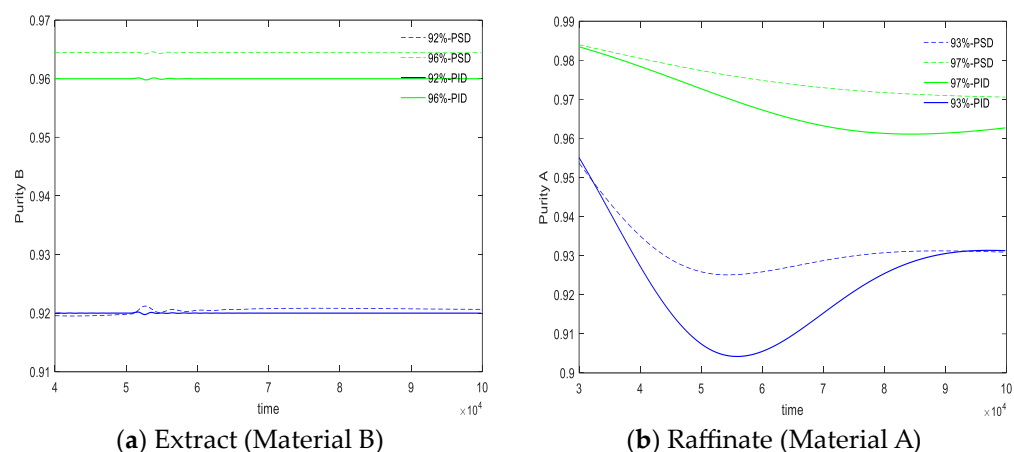


Figure 10. Comparison of two controllers under the disturbance of adsorbent parameters $H_A = 0.01 \rightarrow 0.03$.

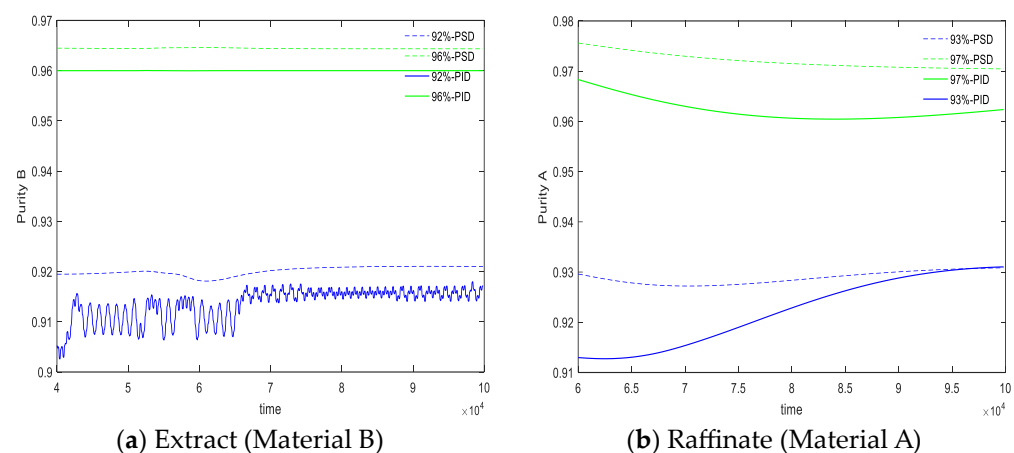


Figure 11. Comparison of two controllers under the disturbance of feed port concentration $C_f = 4.5 \rightarrow 5.2$.

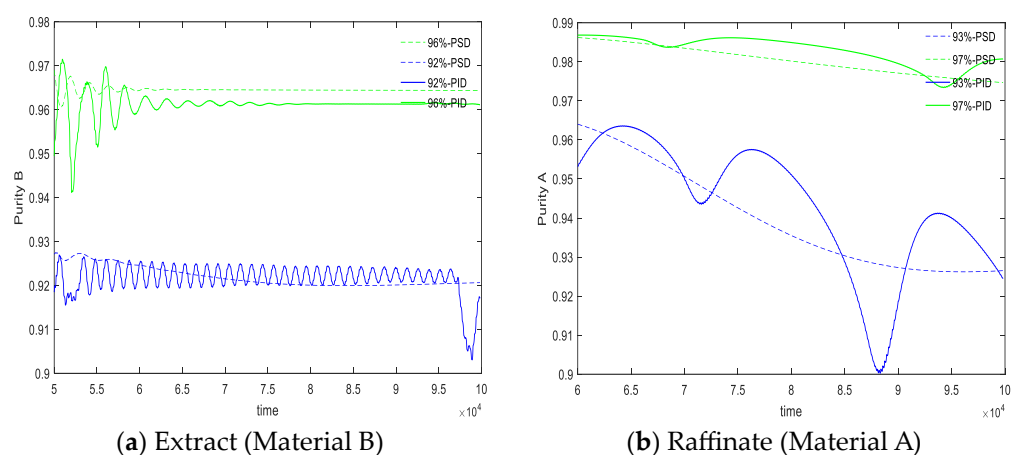


Figure 12. Comparison of two controllers under the disturbance of switch time $C_f = 4.5 \rightarrow 5.2$.

5. Conclusions

In order to enhance the efficiency of online control in SMB systems, it is necessary to abandon models based on the finite element method in computational aspects, and to instead establish dynamic models based on finite difference methods. Although the finite

element method offers higher computational accuracy, it falls short in terms of response computation, rendering it unsuitable for online control. Closed-loop feedback controllers established on the basis of finite difference methods will enable more open and flexible control. In the present study, we discretized the SMB process using the Crank–Nicolson method and performed a computer-based simulation of the entire process. Our research findings demonstrate that the discretized process effectively replicates the dynamic development of separation processes. The application of discretization techniques lays a solid groundwork for the efficient and reliable control of separation processes, which holds significant implications for the advancement of manufacturing.

Subsequent investigations can focus on integrating controllers within the discretized process, enabling efficient computational algorithms that facilitate real-time control. This paper explores the case of the PSD controller when used to control a SMB in comparison to the PID controller. We have successfully compared the strengths and weaknesses of these two controllers in the control process. If the controllers demonstrate effective performance, it will pave the way for industrial-scale applications.

Author Contributions: Conceptualization, R.-C.H. and C.-F.X.; methodology, C.-F.X.; software, C.-F.X.; validation, R.-C.H. and C.-F.X.; formal analysis, R.-C.H.; resources, R.-C.H.; data curation, C.-F.X. and H.Z.; writing—original draft preparation, C.-F.X.; writing—review and editing, R.-C.H.; visualization, H.Z. and C.-F.X.; supervision, R.-C.H.; project administration, R.-C.H. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the National Natural Science Foundation of China under Grant 62071123, 61601125), by Natural Science Foundation of Fujian Province of China (number: 2023J011117), by the Fujian Province Education Hall Youth Project (number: JAT220258), by the Fujian Natural Science Foundation Project (number: 2019J01887).

Data Availability Statement: To request the corresponding research paper data for experimental simulation, please submit your application via the following email address: liurangzhu@163.com.

Conflicts of Interest: The authors declare no conflicts of interest.

References

1. Neto, A.S.A.; Secchi, A.R.; Souza, M.B.; Barreto, A.G. Nonlinear model predictive control applied to the separation of praziquantel in simulated moving bed chromatography. *J. Chromatogr. A* **2016**, *1470*, 42–49.
2. Li, S.; Wei, D.; Wang, J.S.; Yan, Z.; Wang, S.Y. Predictive control method of simulated moving bed chromatographic separation process based on piecewise affine. *Int. J. Appl. Math.* **2020**, *50*, 1–12.
3. Heinonen, J.; Sanlaville, Q.; Niskakoski, H.; Sainio, T. Effect of separation material particle size on pressure drop and process efficiency in continuous chromatographic separation of glucose and fructose. *Sep. Purif. Technol.* **2018**, *193*, 317–326.
4. Suvarov, P.; Kienle, A.; Nobre, C.; Weireld, G.D.; Wouwer, A.V. Cycle to cycle adaptive control of simulated moving bed chromatographic separation processes. *J. Process Control* **2014**, *24*, 357–367.
5. Kim, K.M.; Han, K.W.; Kim, S.I.; Bae, Y.S. Simulated moving bed with a product column for improving the separation performance. *J. Ind. Eng. Chem.* **2020**, *88*, 328–338.
6. Choi, J.H.; Kang, M.S.; Lee, C.G.; Wang, N.H.L.; Mun, S. Design of simulated moving bed for separation of fumaric acid with a little fronting phenomenon. *J. Chromatogr. A* **2017**, *1491*, 75–86.
7. Hasan, M.M.F.; First, E.L.; Floudas, C.A. Discovery of novel zeolites and multizeolite processes for p-Xylene separation using simulated moving bed (SMB) chromatography. *Chem. Eng. Sci.* **2016**, *159*, 3–17.
8. Yao, C.; Tang, S.; Yao, H.M.; Tade, M.O. Continuous prediction technique for fast determination of cyclic steady state in simulated moving bed process. *Comput. Chem. Eng.* **2013**, *58*, 298–304.
9. Yazdian Kashani, S.; Farhadi, F. Simulation of Separation of a Racemic Mixture of Ibuprofen by Supercritical Fluid Chromatography in Simulated Moving Bed. *J. Chem. Pet. Eng.* **2017**, *51*, 123–133.
10. Leipnitz, M.; Biselli, A.; Merfeld, M.; Scholl, N.; Jupke, A. Model-based selection of the degree of cross-linking of cation exchanger resins for an optimized separation of monosaccharides. *J. Chromatogr. A* **2020**, *1610*, 460565–460576.
11. Nogueira, I.B.; Martins, M.A.; Rodrigues, A.E.; Loureiro, J.M.; Ribeiro, A.M. Novel Switch Stabilizing Model Predictive Control Strategy Applied in the Control of a Simulated Moving Bed for the Separation of Bi-Naphthol Enantiomers. *Ind. Eng. Chem. Res.* **2020**, *59*, 1979–1988.
12. Natarajan, S.; Lee, J.H. Repetitive model predictive control applied to a simulated moving bed chromatography system. *Comput. Chem. Eng.* **2000**, *24*, 1127–1133.

13. Carlos, V.; Alain, V.W. Combination of multi-model predictive control and the wave theory for the control of simulated moving bed plants. *J. Chem. Eng. Sci.* **2011**, *66*, 632–641.
14. Mun, S.; Wang, N.H.L. Improvement of the performances of a tandem simulated moving bed chromatography by controlling the yield level of a key product of the first simulated moving bed unit. *J. Chromatogr. A* **2017**, *1488*, 104–112.
15. Garcá, M.-S.G.; Balsa-Canto, E.; Banga, J.R. Dynamic Optimization of a Simulated Moving Bed (SMB) Chromatographic Separation Process. *Ind. Eng. Chem. Res.* **2006**, *45*, 9033–9041.
16. Lee, W.-S.; Lee, C.-H. Dynamic modeling and machine learning of commercial-scale simulated moving bed chromatography for application to multi-component normal paraffin separation NSTL. *Sep. Purif. Technol.* **2022**, *288*, 2–17.
17. Marrocos, H.; Iwakiri, I.G.I.; Martins, M.A.F.; Rodrigues, A.E.; Loureiro, J.M.; Ribeiro, A.M.; Nogueira, I.B.R. A long short-term memory based Quasi-Virtual Analyzer for dynamic real-time soft sensing of a Simulated Moving Bed unit. *Appl. Soft Comput.* **2022**, *116*, 108318.
18. Hoon, O.T.; Woo, K.J.; Hwan, S.S.; Hosoo, K.; Kyungmoo, L.; Min, L.J. Automatic control of simulated moving bed process with deep Q-network. *J. Chromatogr. A* **2021**, *1647*, 462073.
19. Reinaldo, C.S.; Gomes, B.A.; Resende, S.A. Optimal performance comparison of the simulated moving bed process variants based on the modulation of the length of zones and the feed concentration. *J. Chromatogr. A* **2021**, *1651*, 462280.
20. Supelano, R.C.; Barreto, A.G., Jr.; Neto, A.S.A.; Secchi, A.R. One-step optimization strategy in the simulated moving bed process with asynchronous movement of ports: A VariCol case study. *J. Chromatogr. A* **2020**, *1634*, 1672–1718.
21. de Sá Gomes, F.M. Advances in Simulated Moving Bed: New Operating Modes; New Design Methodologies; and Product (FlexSMB-LSRE®) Development. Ph.D. Thesis, FEUP, Porto, Portugal, 2009.
22. Klatt, K.U.; Hanisch, F.; Dunnebier, G. Mode-based control of a simulated moving bed chromatographic process for the separation of fructose and glucose. *J. Process Control* **2002**, *12*, 203–219.
23. Lee, J.W.; Seidel-Morgenstern, A. Model Predictive Control of Simulated Moving Bed Chromatography for Binary and Pseudo-binary Separations: Simulation Study. *IFAC-Pap.* **2018**, *51*, 530–535.
24. Yang, Y.; Chen, X.; Zhang, N. Optimizing control of adsorption separation processes based on the improved moving asymptotes algorithm. *Adsorpt. Sci. Technol.* **2018**, *36*, 1716–1733.
25. Xie, C.-F.; Hwang, R.-C. Purity Control Based on Type-II Fuzzy Controller for Simulated Moving Bed. *Processes* **2022**, *10*, 2437–2456.
26. Crank, J.; Nicolson, P. A Practical method for numerical evaluation of solutions of partial differential equations for the heat conduction type. *Proc. Phil* **1947**, *43*, 50–67.
27. Chen, I.C.; Huang, H.C.; Shen, C.Y.; Hwang, R.C. Identification of Simulated Moving Bed Dynamic System by Neural Network. *Sens. Mater.* **2012**, *33*, 615–623.
28. Marsik, J.; Strejc, V. Application of identification-free algorithms for adaptive control. *Automatica* **1989**, *25*, 273–277.

Disclaimer/Publisher's Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.