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Standing wave design and optimization of a simulated moving bed chromatography for separation of xylobiose and xylose under the constraints on product concentration and pressure drop

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ABSTRACT

The feasibility of a simulated moving bed (SMB) technology for the continuous separation of high-purity xylobiose (X2) from the output of a β-xylosidase X1→X2 reaction has recently been confirmed. To ensure high economical efficiency of the X2 production method based on the use of xylose (X1) as a starting material, it is essential to accomplish the comprehensive optimization of the X2-separation SMB process in such a way that its X2 productivity can be maximized while maintaining the X2 product concentration from the SMB as high as possible in consideration of a subsequent lyophilization step. To address this issue, a suitable SMB optimization tool for the aforementioned task was prepared based on standing wave design theory. The prepared tool was then used to optimize the SMB operation parameters, column configuration, total column number, adsorbent particle size, and X2 yield while meeting the constraints on X2 purity, X2 product concentration, and pressure drop. The results showed that the use of a larger particle size caused the productivity to be limited by the constraint on X2 product concentration, and a maximum productivity was attained by choosing the particle size such that the effect of the X2-concentration limiting factor could be balanced with that of pressure-drop limiting factor. If the target level of X2 product concentration was elevated, higher productivity could be achieved by decreasing particle size, raising the level of X2 yield, and increasing the column number in the zones containing the front and rear of X2 solute band.

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1. Introduction

Xylobiose (X2) is one of well-known rare sugars that are highly useful from an industrial perspective. This sugar was reported to play a remarkable prebiotic role in bifidobacterium proliferation, which has led it to achieve recognition as a highly valuable sugar in food and health industries [1–4].

Since X2 is a kind of disaccharide with two xylose (X1) monomers, it can be produced from X1 via a proper enzymatic reaction [4–6]. However, such X1 → X2 reaction does not go to completion, which causes the necessity for the development of an economically-efficient downstream process for separating a product component (X2) from an unreactant component (X1). This task has been performed in a recent research [4], where a simulated moving bed (SMB) process was applied to the continuous separation of X2 and X1 that resulted from a β-xylosidase X1 → X2 reaction.

It is widely accepted that the use of an SMB process and its separation principle, which is depicted in Fig. 1, is fairly advantageous for achieving a sufficiently high productivity and economical efficiency for a large-scale or an industrial application [7–10]. However, such merit of an SMB process can be ensured only when its operation parameters, column configuration, and adsorbent particle size are comprehensively optimized to attain the following two conditions [11,12]. First, the key performance factor affecting the economical efficiency of SMB should be maximized. Secondly, all the requirements on product specification and process stability that are specific to a given SMB separation task should be satisfied.

In case of the aforementioned X2-separation SMB, its experimental validation was completed previously [4] but its comprehensive optimization has not been attempted so far. To promote the commercialization of the X2 production from the β-xylosidase

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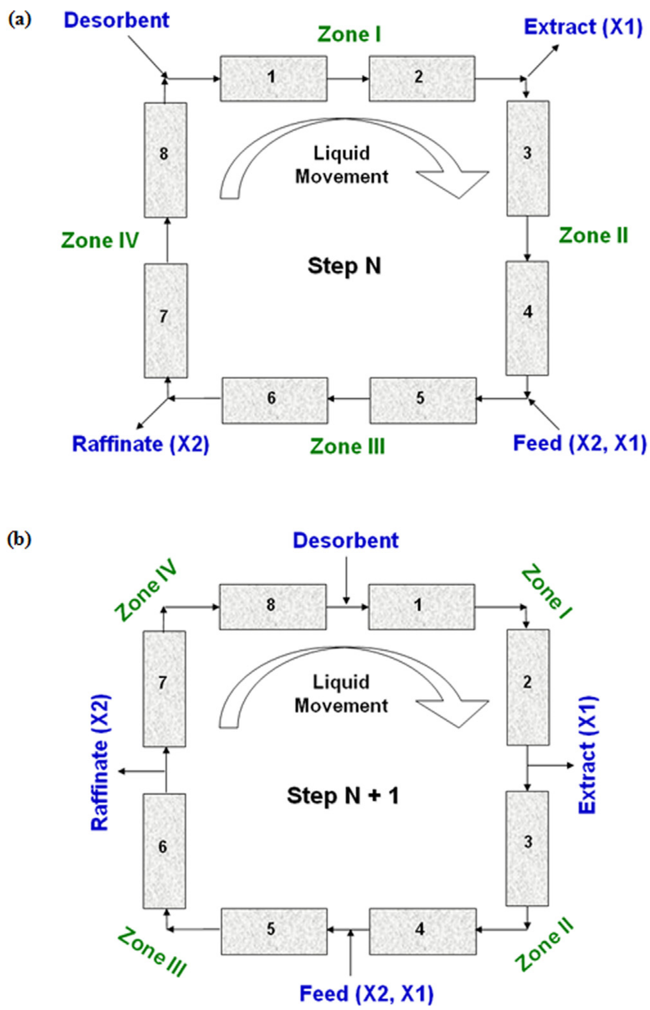

Fig. 1. Schematic diagram of a four-zone SMB process for binary separation. (a) N^{th} Step, (b) $(N+1)^{th}$ step. X2: xylobiose (fast-migrating component), X1: xylose (slow-migrating component).

X1 → X2 reaction, it is essential to investigate the comprehensive optimization of the X2-separation SMB process.

The goal of this study is to accomplish the aforementioned task. In this task, productivity will be taken as a key performance factor to be maximized because it is the most influential factor for the economical efficiency of SMB. During such optimization, the following issues will be taken into account. First, X2 purity should be maintained at a desired level for a successful application in food and pharmaceutical industries. Secondly, the SMB pressure drop should be kept below a commonly acceptable level in bioproduct industries. In addition to such two issues, there is one additional important issue to be considered in relation to the fact that the X2 product solution from a X2-separation process should undergo a subsequent lyophilization step, whose efficiency is largely affected by the level of its feed concentration, i.e. the level of the product concentration from the preceding separation process. This implies that the concentration of X2 in a product stream from the X2-separation SMB process can be an important issue as its productivity and purity of X2 in the stage of the process optimization. To address this issue, a target level of X2 product concentration will be set in the SMB optimization of this study. In order words, the X2-separation SMB optimization will be carried out such that the X2 productivity can be maximized while meeting the constraint on X2 product concentration as well as those on X2 purity and pressure drop.

To facilitate the aforementioned work, a standing wave design (SWD) method [13–15] will be used to prepare a comprehensive SMB optimization tool. The prepared tool will then be utilized to optimize the SMB operation parameters (zone flow rates and switching time), column configuration, total column number, adsorbent particle size, and X2 yield in such a way that the highest X2 productivity can be achieved under given constraints on X2 product concentration, X2 purity, and unit pressure drop. On the basis of the optimization results, we will conduct a deep analysis into the effect of a target X2-product concentration level on the performance of the X2-separation SMB. During such analysis, it will also be investigated how adsorbent particle size and column configuration will influence the SMB performance. Furthermore, we will clarify how the impact of X2 yield on the SMB productivity will be varied depending on the extent of the target level of X2 product concentration. Given that the performance of a X2-separaton step plays an important role in the X2 production based on the β-xylosidase reaction [4], it is highly expected that the results of this study will be of help to the economically-efficient production of X2 at a lower cost and higher purity.

2. Theory

2.1. Standing wave design (SWD) method for a binary-separation SMB process

One of the vital issues for a successful development of an SMB process is to determine its operation parameters (zone flow rates and switching time) in such a way that the key concentration waves of all solutes in feed can be well confined within their respective zones, thereby ensuring high purities and high yields [13–15]. For a binary-separation SMB, it is necessary to confine four concentration waves within their respective zones because each solute band creates two concentration waves (advancing and trailing waves), which are located in the front and rear parts of the solute band. It is thus a general trend to use a four-zone SMB process mode, if a target separation task belongs to the category of a binary or a pseudo-binary separation [13].

As for the optimal design of a four-zone SMB for binary separation, there are several methods available in the literature. Among them, the use of a detailed model and a robust optimization algorithm in combination has been a general method [7–11,16,17]. To pursue computational efficiency in the optimal design of an SMB, one can also utilize the standing wave design (SWD) method, which was known to be highly efficient in determining the optimal SMB operation parameters that can lead to the highest feed flow rate and the lowest desorbent consumption while maintaining a target level in product purity and yield [13–15].

The main principle of the SWD is that the optimal state of SMB can be attained by maintaining a so-called "standing-wave condition", in which all key concentration waves are made standing in their respective zones on the time-averaged sense [13]. To achieve such a standing-wave condition, the migration velocity of a key concentration wave in each zone should be matched with the port movement velocity through a proper modulation of SMB operation parameters. This action can be facilitated by utilizing the SWD equations, which enables the computationally-efficient determination of the operation parameters leading to the standing-wave condition [13].

The SWD equations have been derived previously for a four-zone SMB with linear isotherms, including size-exclusion systems [13,14]. Their mathematical expression is presented below regarding a size-exclusion system under an ideal (or an equilibrium)

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