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Establishment of a nanofiltration rejection sequence and calculated rejections of available monosaccharides

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ABSTRACT

To evaluate the feasibility of mixed monosaccharide separation by nanofiltration (NF), a commercial membrane, Desal-5 DK1812, was selected to filter six monosaccharides, including glucose, fructose, mannose, sorbose, arabinose, and xylose. The experiments were performed under the same conditions in single batch of full cycle mode, and the sequence of monosaccharide nanofiltration rejections was obtained. Differences in NF rejections (R_{obs}) were analyzed by comparing the molecular structures of the monosaccharides, after which computational molecular sizes (r_s) were calculated by a mathematical formula correlated with the 3D structures of the molecules. The Donnan steric pore model was used to obtain the rejections (R_{cal}) of the monosaccharides as a function of r_s. Concentration polarization was also taken into account to calculate R_{real}. The results showed that the r_s values of fructose, glucose, mannose, sorbose, arabinose, and xylose were 0.3235, 0.3156, 0.3113, 0.3012, 0.2748, and 0.2677 nm, respectively, and that their R_{cal} agreed well with their R_{real}. Therefore, differences in R_{obs} were mainly due to differences in the molecular structures of the monosaccharides, and calculating r_s using molecular structural parameters is reasonable. The results indicated the extreme importance of amplifying rejection differences by regulating computational molecular sizes when separating mixed monosaccharides by NF.

1. Introduction

Nanofiltration (NF) is a pressure-driven separation technology that combines the features of reverse osmosis and ultrafiltration [1]. NF is applied widely in the water treatment, food, fermentation, and pharmaceutical industries. Monosaccharides, including trioses, tetroses, pentoses, and hexoses, present three to six carbon atoms and exist as chains or ring structures [2]. Many monosaccharides are important ingredients in food and pharmaceuticals [3,4]; hence, separating and purifying monosaccharides are important undertakings [5]. The separation of some monosaccharides may be achieved by chromatography [6]. However, the performance cost of this technique is relatively higher than that of other separation methods, and selecting an appropriate stationary phase is usually difficult. Most columns present a number of problems, particularly in terms of column stability, lifetime, and separation reproducibility [7]. NF technology presents the advantages of lower energy consumption, sustainable processing, simple operation, and relatively easy scale-up over other filtration procedures [8,9]. From the traditional perspective, membrane filtration requires a tenfold difference in molar mass or a threefold difference in hydrodynamic radius to be able to separate components from one another effectively [10]. Sjöman et al. [11] studied the feasibility of separating xylose from glucose by NF, and investigated the influences of operating pressure, concentration, mass ratio of xylose to glucose, and several other factors on the separation effect. Zhou et al. [12] studied the effects of operating parameters, such as pH, temperature, pressure, and feed concentration, with a synthetic xylose-glucose-acetic acid model solution and successfully separated acetic acid from a monosaccharide solution. Kim et al. [13] obtained galactose from the acid hydrolysate of agarose by NF. Given these positive results, NF may be applied to separate and purify monosaccharides. Researchers generally focus on the separation process, including the separation effects of

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Nomenclature

C_p	permeate concentration (g m^{-3})
C_m	concentration of solution on the surface of the membrane (g m^{-3})
C_b	concentration of solution in the feed (g m^{-3})
R_{real}	real rejection
R_{obs}	observed rejection
R_{cal}	calculated rejection
k	mass transfer coefficient (m s^{-1})
δ	boundary layer of thickness (m)
d_c	hydrodynamic diameter (m)
Re	Reynolds number
Sc	Schmid number
σ	reflection coefficient
Ps	solute permeability coefficient (m s^{-1})
J_s	solute flux (g m^{-2} s^{-1})
D_p	hindered diffusivity (m^2 s^{-1})
J_v	permeate flux (m s^{-1})
K_c	hindrance factors for convection
K_d	hindrance factors for diffusion
D	diffusivity in bulk solution (m^2 s^{-1})
C_i	solute concentration at inlet of the pore (g m^{-3})
Φ	steric partition factor
C_f	feed concentration (g m^{-3})
C_o	solute concentration at outlet of the pore (g m^{-3})
Pe	peclet number
Δx	membrane thickness (m)
Ak	porosity of the membrane
$K^{-1}(\lambda)$	enhanced drag coefficient
$G(\lambda)$	lag coefficient
λ	ratio of solute radius to effective pore radius
r_s	solute radius (nm)
r_p	effective pore radius (nm)
Jw	water flux (m s^{-1})
Δp	trans-membrane pressure (Pa)
u	viscosity of water or solution (Pa s)
W	molecular width (nm)
H	molecular height (nm)
L	molecular length (nm)
M_w	molecular mass (g/mol)
K	boltzmann constant (J K^{-1})
T	absolute temperature (K)
Vp	volume of permeation (m^3)
t	time (h)
A_m	the effective area (m^2)
NF	nanofiltration
DSPM	donnan steric pore model
MWCO	molecular weight cut-offs
Mw	molecular weight

physical parameters, such as pH, operating pressure, temperature, and feed concentration. Thus, the separation mechanism has seldom been investigated during the separation of monosaccharides via NF.

Optimizing the empirical operation to study the separation mechanism of NF and predict the rejection of solutes are important tasks [14–16]. Several theoretical and mathematical models have been used to describe the separation mechanism of NF, including steric hindrance pore, concentration polarization, and Donnan steric pore model (DSPM) [17]. The permeate of neutral solutes is controlled by the sieving effect, and differences in separation mostly involve molecular sizes and diffusivities [11]. Thus, the process of NF must characterize the effective size of solute molecules. As for neutral solutes, the effective size of the solute can be affected by the presence of surrounding species, such as ions. Bouchoux et al. [18] and Bouranene et al. [19] found that the rejection of neutral solutes is lesser in mixed-solute solutions with salt than in single solutions. The phenomenon is due to the decrease in hydrodynamic radius of the neutral solute (i.e., solute effective size) in the presence of ions. Thus, selecting the most appropriate quantity to characterize solute size is a controversial issue in NF modeling. Stokes radius is a common parameter used to represent the effective solute size, which is derived by assuming that the solute is spherical. The drawback of the Stokes radius as the effective solute size, however, is that it completely ignores differences in molecular space structure. Differences in the rejection of solutes with the same molecular weight, especially among isomers, have been reported. Hua et al. [20] found significant rejection differences between xylose and arabinose. Another approach used to characterize the effective size of a solute molecule is through its space structure; such an approach is based on the hypothesis that a solute molecule is non-spherical and that its molecular shape exerts some effect on the transfer process. Van der Bruggen et al. [1] studied the influence of molecular size on the rejection of organic molecules by NF and compared different parameters for the molecule, including molecular weight, Stokes radius, equivalent molar diameter, and the diameter obtained by energy minimization calculations. The shapes of non-spherical molecules have been approximated by several simple geometric shapes. Kiso et al. [14] described the shape of organic molecules as approaching that of a rectangular parallelepiped. The effective size of a solute molecule, especially a non-spherical one, is an important parameter that may explain differences in rejections, particularly among isomers.

In the present study, six commercially available monosaccharides, including four hexoses (i.e., glucose, fructose, mannose, and sorbose) and two pentoses (i.e., xylose and arabinose), were selected. The aim of this study is to establish the rejection sequence of commercially available monosaccharides. Moreover, it seeks to explore the mechanisms behind the observed rejection differences to support the potential application of NF to the separation and purification of monosaccharides.

2. Theoretical background

2.1. Concentration polarization and Donnan steric pore model

A part or all of the solute trapped by a membrane stays on the membrane surface. Therefore, the real rejection (R_{real}) of the membrane is defined by the membrane concentration and the permeation concentration, which is calculated as follows:

$$R_{real} = 1 - \frac{C_p}{C_m} \quad (1)$$

However, measuring the solute concentration on the membrane surface during the experimental process can be difficult. Thus, separation can be evaluated by the observed rejection, which is calculated using Eq. (2) as follows:

$$R_{obs} = 1 - \frac{C_p}{C_b} \quad (2)$$