Dynamic simulation of the integrated bioreactor

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Abstract The article reports numerical simulation for the system combining selective adsorption of fructose and an enzyme reaction to produce higher fructose syrup. A procedure for the dynamic simulation of the process in the frame of equations for mass transfer in fixed bed, is obtained by making a solute material balance. A fixed bed model incorporating axial dispersion and a linear driving force for mass transfer was successfully used to estimate optimum operating conditions (switch times and fluid flow rates).

List of symbols

- \( C \): concentration, mol dm\(^{-3}\)
- \( d \): diameter, m
- \( Dz \): axial dispersion coefficient, m\(^2\)s\(^{-1}\)
- \( k \): overall mass transfer rate constant, min\(^{-1}\)
- \( K \): adsorption equilibrium constant, -
- \( Km \): Michaelis constant, mol m\(^{-3}\)
- \( L \): length of adsorbent bed, cm
- \( q \): concentration in the stationary phase, mol dm\(^{-3}\)
- \( Q \): volumetric flow rate, m\(^3\)s\(^{-1}\)
- \( r \): reaction rate
- \( Re \): Reynold’s number
- \( t \): time, s
- \( u \): interstitial velocity, cm min\(^{-1}\)
- \( v \): superficial velocity, cm min\(^{-1}\)
- \( V_{max} \): maximum reaction rate, mol m\(^{-3}\)s\(^{-1}\)
- \( z \): axial distance, m
- \( RV \): rotary valve
- \( x \): mole fraction

Greek letters

- \( \varepsilon \): voidage, -
- \( \rho \): density, kg m\(^{-3}\)
- \( \mu \): viscosity, Pas

Subscript

- \( G \): glucose
- \( F \): fructose
- \( r \): reactor
- \( a \): adsorber
- \( 0 \): stage of inlet
- \( p \): particle
- \( el \): eluent

1 Introduction

A mathematical model based on unsteady mass balances is used in the study of dynamic behaviour of the process including a catalyst system for the isomerisation of glucose to fructose and separation of glucose and fructose. The isomerisation of glucose catalyzed by Sweetzym S was performed in a fixed bed reactor [4, 5]. The adsorption of glucose and fructose on Lewatit TSW 40 Ca\(^{2+}\) resin was performed simultaneously in counter current adsorption of the packed bed column [6]. The process combining adsorption and enzyme reaction for producing high fructose syrup was reported earlier [1, 2, 3].

In this study we employ column switching procedure to obtain higher fructose concentration. A mathematical model of the integrated bioreactor is presented to calculate concentration profiles of glucose and fructose and numerical simulation of process. The data which are needed for dynamic simulation were determined experimentally.

2 Mathematical model

In formulating the mathematical model of a fixed bed, we assume uniform packing, uniform velocity distribution, isothermal behaviour and constant physical properties.

A mathematical model based on fundamental mass balances for calculating the concentration profiles of glucose and fructose in the system is presented.

Mass balance equations for concentrations of glucose and fructose in the bioreactor, Eqs (1) and (2):

\[
\frac{\partial C_G}{\partial t} = -v_r \frac{\partial C_G}{\partial z} - (1 - \varepsilon_r) \frac{V_{max}^G K_m^G c_G - V_{max}^G K_m^F c_F}{K_m^G K_m^F + K_m^G c_G + K_m^F c_F} + Dz \frac{\partial^2 C_G}{\partial z^2},
\]

(1)

\[
\frac{\partial C_F}{\partial t} = -v_r \frac{\partial C_F}{\partial z} - (1 - \varepsilon_r) \frac{V_{max}^G K_m^G c_G - V_{max}^G K_m^F c_F}{K_m^G K_m^F + K_m^G c_G + K_m^F c_F} + Dz \frac{\partial^2 C_F}{\partial z^2},
\]

(2)
Mass balances equations for the concentration of glucose or fructose in adsorption columns Eqs. (3) to (6):

\[
\frac{\partial c_G}{\partial t} = Dz \frac{\partial^2 c_G}{\partial z^2} - v_a \frac{\partial c_G}{\partial z} \left( 1 - \frac{c_G}{q_a} \right), \quad (3)
\]

\[
\frac{\partial c_F}{\partial t} = Dz \frac{\partial^2 c_F}{\partial z^2} - v_a \frac{\partial c_F}{\partial z} \left( 1 - \frac{c_F}{q_a} \right), \quad (4)
\]

\[
\frac{\partial q_G}{\partial t} = k_G (K_{cG} c_G - q_G), \quad (5)
\]

\[
\frac{\partial q_F}{\partial t} = k_F (K_{cF} c_F - q_F). \quad (6)
\]

Boundary conditions:

\[
z = 0, \quad c_z = c_0 - \frac{Dz}{v} \left( \frac{dc}{dz} \right) \bigg|_{z=0},
\]

\[
z = L, \quad \left( \frac{dc}{dz} \right) \bigg|_{z=L} = 0.
\]

The mathematical model for calculating the concentration profile and dynamic simulation of glucose and fructose was developed for the system presented in Fig. 1.

3 Principle of operation

Figure 1 illustrates a schematic diagram of a theoretical system for the simulation of a bioprocess. The system operates with two adsorption columns connected through switch valves with bioreactor for isomerisation of glucose. The inversion of glucose to fructose has been obtained in bioreactor while an equilibrated mixture of glucose and fructose is introduced in adsorption column 1. The components of the mixtures can be divided into two groups. The first one includes the strongly adsorbable component collected in the extract stream, whereas the second includes a weak adsorbable component collected in the raffinate stream. In this case fructose which has a larger equilibrium constant elutes last in the extract stream, while glucose elutes first in the raffinate stream. Glucose from raffinate stream can be recycled to the reactor. The adsorbent particles are regenerated by desorption of fructose which elutes in the extract stream. At the same time equilibrated mixtures of glucose and fructose could be introduced into adsorption column 2. The inlet and outlet points of feed and eluent are switched on and off at intervals through a fixed adsorbent bed. The column-switching procedure is very important to obtain higher fructose concentration. The eluent, extract, feed and raffinate points are changed at different switch times. At zero time the feed is introduced into adsorption column 1, and eluent is introduced into adsorption column 2. The adsorption column 2 receives the feed at the end of a predetermined period while column 1 elutes mixture of fructose and glucose. This period is called switch time 1 ($t_1$). At the same time raffinate and extract point interchange positions. The next switch time is the time of delay interchanged positions of raffinate and extract point, and this is called switch time 2 ($t_2$).

4 Experimental

Different characteristics such as particle size distribution, void fraction and kinetic parameters of enzyme reaction, adsorption equilibrium constant, overall mass transfer coefficient in adsorption system were determined by pulse response experiment using the moment analysis technique and by batch experiments. More about this was reported earlier [4–10].

4.1 Kinetic parameters of immobilized glucose isomerase

The enzymatic isomerisation of glucose and fructose is a reversible reaction. One of the few well known mechanisms is given by:

\[
G + E \xrightarrow{k_i} GE \xrightarrow{k_1} EG \xrightarrow{k_1} F + E. \quad (7)
\]

The reaction rate is expressed by Michealis-Menten kinetics valid for this reaction:

\[
-r_G = r_F = \frac{V_{max}^G K_m^G c_G}{K_m^G + K_m^G c_G} - \frac{V_{max}^F K_m^F c_F}{K_m^F + K_m^F c_F}, \quad (8)
\]

The Michaelis Menten constants $K_m$ and $V_{max}$ were determined by using a fixed bed reactor packed with Sweetzym S. A jacketed glass column with an inner diameter of 0.015 m and height of 0.25 m was used as enzyme column reactor.

The data required for the simulation of bioreactor are summarized in Table 1.

| Table 1. Summary of data for simulation of bioreactor |
|-----------------|-----------------|-----------------|
| $K_m^G$, mol m$^{-3}$ | 498              | 472              |
| $K_m^F$, mol m$^{-3}$ | 3.719            | 3.01             |
| $V_{max}^G$, mol m$^{-3}$ s$^{-1}$ | 1600             | 7.07$\times$10$^{-4}$ |
| Length of reactor, L, m | 0.25             | 0.015            |
| Diameter of reactor, d_r, m | 3.33             | 0.439            |
| Particle diameter, d_p, m | 0.534            | 1.1445           |
| Porosity of bed, - | 7.00             |                  |

The data for the simulation of bioreactor are summarized in Table 1.