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Research Article

Development of Computational Fluid Dynamic Model for the Production Process of Date Sugars: Chromatographic Separation Process

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Abstract

In this study, chromatographic separation process of date sugars is modeled using a commercial computational fluids dynamics (CFD) code FLUENT 6.3.23 (Fluent Inc., USA). A three phases CFD model was developed using an Eulerian–Eulerian approach to calculate the date volume fraction transferred during time from sugar phase to resine phase. The separation process was studied as function of three sugar concentration *(20, 35 and 50%), three* date syrup flow rate *(2,7 and 12*ml/min*) and three* temperature*(25, 47.5 and 70°C). The results revealed that the numerical data were in good agreement with the experimental data indicating the R^2 of 0.97.*

Keywords:*CFD model, Chromatographic process, date sugars.*

1. Introduction

The high fructose syrup (HFS) is widely used as nutritional sweetener (soft drinks, deserts, jams, dairy products) because of its high quality characteristics such as sweetness, flavor enhancement, stability, high osmotic pressure and crystallization control (Zhang, *et al*, 2004).

In most of the commercial methods, the high fructose syrup is produced from corn (HFCS). However, high Fructose syrup can be produced from date using a chromatographic separation process. Al Eid and al. (2006) produced fructose from date syrup using chromatographic process as function of temperature, flow rate and concentration of date syrup. Also Khosravanipour Mostafazadeh *et al*. (2011) studied the chromatographic separation process of fructose from date syrup in a range of operating conditions such as temperature and initial sugar concentration. They demonstrate that the using of chromatographic systems for the separation of sugars like fructose and glucose are very impressive and feasible methods. A Fructose and glucose separation can be implemented on a continuous process. A purified fraction or recovered as continuous stream operating of a chromatography systems required the calculation of numerous technical parameters such as flow rate, switch period and concentration. All of which can be determined by process modeling and simulation. The scientific Methodology realize on test on small quantity followed by calculations, simulations, optimizations and pilot validation resulting in considerable development in time saving.

Computational fluid dynamics (CFD) and modeling technology is becoming an increasingly useful tool in the analysis of highly complex biotechnologie process such as fluid flow in chromatographic process such as SMB. CFDis a tool that can be used to investigate a parameter affected sugar separation process. CFD allows us to study the hydrodynamics characteristics thereby enhancing our understanding of this topic. It involves obtaining the numerical solution of the equations for the conservation of mass, momentum and energy of the flow through geometry of interest. Additional equations reflecting the nature of the problem may also be needed. CFD is able to predict the fluid flow and the associated species concentration, heat transfer characteristics, chemical reaction rates and other pertinent quantities expected in operation of production of sugar (Trigui, *et al*, 2015).

The main objective of this study was to create a CFD model to predict the performance of the continuous production process of high fructose date syrup (HFDS), determining the optimal conditions of production and finally validate the results on a pilot production unit.

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2. Materials and methods

2.1 Experimental setup

The experimental device of production of sugar from date is presented in figure 1. It is composed by four columns connected in series. Each column measure 1000 mm in length and 25 mm in inside diameter and was packed with resin. The column had a specific inlet and outlet stream, which could be rotated by a four port valve system to either introduce (Feed F or Eluent El) or remove (Extract E or Raffinate R) the stream. Each inlet and outlet streams were pumped by means of rotary piston dispensing pump (ISMATEC REGLO-CPF Digital pump, Wertheim-Mondfeld, Germany).

The Eluent was desionized water and the separation columns were packed with the resin Dowex Monosphere99/Ca320 (Dowex) made of polystyrene containing a strong cation exchange gel matrix with $Ca2+$. The resin had a particle size of 300-350 µm, an exchange capacity of over 150 Cmol+/Kg and a heat tolerance of up to 120° C. The polystyrene cation-exchange resin complex preferentially adsorbs fructose by means of its calcium ions (Kurup, *et al*, 2005). The chromatographic separation process is achieved by the $Ca2+$ ions forming a weak complex with fructose, which results in the preferential retardation of fructose while glucose is carried away by the mobile phase (Al Eid, 2006). The strongly adsorbed component (fructose) was collected in the Extract stream, whereas a weaker adsorbed component (glucose) was collected in the Raffinate stream (Matijašević and Vasić -Rački, 2000).

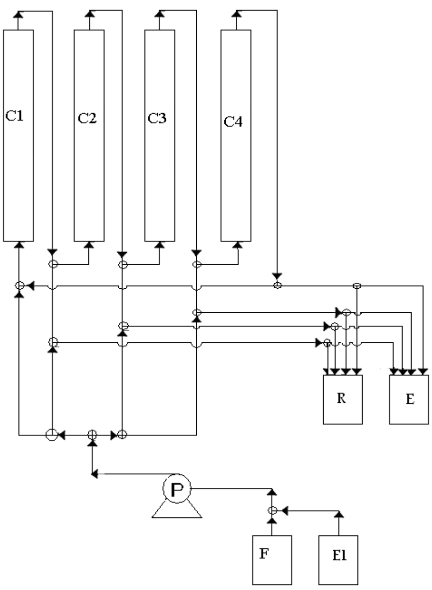

Fig. 1 The SMB system used for fructose separation, where C1, C2, C3 and C4 are the experimental columns measuring 1 m in length and 25 mm in inside diameter, F is the Feed (date syrup), El is the Eluent (distilled water), E is the extract (liquid with the separated fructose), R is the Raffinate (liquid with residual sugars such as glucose), and P is the pump.

2.2 Statistical analysis

Box-Behnken was selected as experimental design for this study. Sugar concentration of date syrup, feed flow rate and temperature were considered as significant variables in the separation step. The low, middle, and high levels of each variable designated as -, 0, and + are given in Table 1 and experimental design is tabulated in Table 2.

The ANOVA procedure was used to identify the significant parameters. To select the best values for any particular experiment in a Box-Bhenken design, sets of linear and quadratic combinations giving the best estimators were considered. Statistical significance was set at ($p < 0.05$) and tested using the Statistica software (StatSoftInc, Tulsa, Oklahoma, USA) for Windows software, Version 7.

Table 1 Process Factors and their levels used to study separation process of sugar from date

Factor \ Levels	-	0	+
Sugar concentration (%)	20	35	50
Date syrup flow rate (ml/min)	2	7	12
Temperature (°C)	25	47.5	70

The industrial statistics and six sigma for Box-Behnken experimental design was performed to predict the effect on sugar concentration of the operational parameters including their interactions, using the statistical software package Statistica (StatSoft Inc, Tulsa, Oklahoma, USA) for Windows software, Version 7.

The predictive regression model was based on the following equation:

$$E[Y/\chi_1,\chi_2,\chi_3] = \beta_0 + \beta_1\chi_1 + \beta_1'\chi_1^2 + \beta_2\chi_2 + \beta_2'\chi_2^2 + \beta_3\chi_3 + \beta_3'\chi_3^2 + \beta_{12}\chi_1\chi_2 + \beta_{13}\chi_1\chi_3 + \beta_{23}\chi_2\chi_3 \quad (1)$$

where Y is the outcome of interest; β_0 is the intercept; β_1, β_2, β_3 are the linear coefficients; β_1',β_2',β_3' are the quadratic coefficients; β_{12}, β_{13}, β_{23}, are the interaction coefficients;χ_1; χ_2 and $\chi_3$are the operational parameters.

Table 2 The design of experiments of separation process

Runs	Sugar concentration (%)	Date syrup flow rate (ml/min)	Temperature (°C)
1	20	7	70
2	50	12	47.5
3	35	7	47.5
4	20	7	25
5	35	7	47.5
6	35	12	25
7	35	2	25

8	35	2	70
9	20	12	47.5
10	35	12	70
11	35	7	47.5
12	50	7	70
13	50	7	25
14	20	2	47.5
15	50	2	47.5

2.3 Analytical procedure

All analysis of sugar content of different sample of date was performed by HPLC assay. The sample of date syrup which rich in carbohydrates was analyzed by injection in a chromatographic ion-exchange column equipped with a refractive index detector. The analysis parameters were:

- Column: SUPEL COSIL LC-NH2, 25cm x 4.6mm I.D., 5μm particles.
- Mobile phase : acetonitrile : water (75 : 25)
- Flow rate: 1ml/min.
- Injection: 10μl, 150μg each sugar.

3. CFD modeling

3.1 Description of the model

The Euler-Euler multiphase approach is used to models the separation of the mixture of glucose and fructose obtained.

The chromatographic separation process of sugar from date syrup viewed as transport through porous media. Three phases are present such as the sugars phase, the water phase which is represents the mobile phase and the resin phase represents the stationary phase. The species model is used to calculate the chemical activities of glucose and fructose in the various phases. For the associated species model, the sugar phase is to be a mixture of glucose and fructose, the resin phase is assumed to be a mixture of calcium and fructose and the water phase is assumed to be a mixture of water and fructose.

For the separation model developed, two steps were required:

- Modeling the interaction of the sugar phase and the resin phase which result that the mass fraction of fructose stopped and only the mass fraction of glucose will be recovered at the outlet of the separation column.
- Modeling the interaction of the water phase and the resin phase. The mass fraction of fructose adsorbed in the resin phase diffuse in the water phase and will be recovered at the outlet of the separation column.

3.2 Governing equations

3.2.1 Conservation of Mass

The description of multiphase flows as interpenetrating continua incorporates the concept of phase volume fraction α_q.

The volume fraction of each phase is calculated from a continuity equation:

The volume fraction of each phase is calculated from a continuity equation:

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q\right) + \nabla\left(\alpha_q \rho_q \overrightarrow{v_q}\right) = \sum_{p=1}^{n}\left(\dot{m}_{pq} - \dot{m}_{qp}\right) + S_q \quad (2)$$

Where $\overrightarrow{v_q}$ is the velocity of phase q and $\dot{m}_{pq}$characterizes the mass transfer from the $p^{th}$to q^{th}phase, and $\dot{m}_{qp}$characterizes the mass transfer from phase q to phase p, and $S_q$is the source terme.

3.2.2 Conservation ofMomentum

The governing model is obtained by mass balance on a chromatography column, which is shown by the following partial differential equation:

$$\frac{\partial C_f}{\partial t} = D_{ax}\frac{\partial^2 C_f}{\partial z^2} - \frac{v}{\varepsilon}\frac{\partial C_f}{\partial z} - \frac{(1-\varepsilon)}{\varepsilon}\frac{\partial \bar{q}_f}{\partial t} \quad (3)$$

Derivatives of variants ($C_i$and $\bar{q}_i$) with respect to the independent parameters (t and z) are presented in the set of partial differential equations.

The sugar concentration on the solid phase is also proportionate with the mass transfer coefficient according to the linear driving force approximation (LDF) model:

$$\frac{\partial \bar{q}_f}{\partial t} = kp_f\left(q_f^* - \bar{q}_f\right) \quad (4)$$

The adsorption equilibrium isotherm is represented by the q_f^*as a function of C_f. In this case, the linear equilibrium isotherm is as follows:

$$q_f^* = K_f C_f \quad (5)$$

where K_f is dimensionless equilibrium constant. By solving the model using the Danckwertz boundary conditions, the concentration of component f in the fluid phase is determined as a function of time and the column length. Boundary and initial conditions are given by Danckwertz equations:

$$C_f = C_{0f} + \frac{\varepsilon D_{ax}}{v}\frac{\partial C_f}{\partial z} \quad @\, z = 0 \quad (6)$$

$$\frac{\partial C_f}{\partial z} = 0 \; @\, z = l \quad (7)$$

$$t = 0 \quad C_f = 0 \quad (8)$$

$$t = 0 \quad \bar{q}_f = 0 \quad (9)$$

3.2.3 Conservation of Energy

The conservation of energy described by the following equation:

$$\frac{\partial}{\partial t}(\alpha_s \rho_s h_s) + \nabla.(\alpha_s \rho_s \vec{u}_s h_s) = -\alpha_s \frac{\partial w_s}{\partial t} + \bar{\bar{\tau}}_s : \nabla.\vec{u}_s - \nabla.\vec{s}_s + S_s + \sum_{w=1}^{n}\left(Q_{ws} + \dot{m}_{ws} h_{ws} - \dot{m}_{sw} h_{sw}\right) \quad (10)$$

Where $h_s$is the specific enthalpy of the sugar phase (s),$\vec{s}_s$ is the heat flux, S_s is a source term that includes sources of enthalpy,Q_{ws} is the intensity of heat exchange between the sugar and water phases, and h_{sw} is the interphase enthalpy

3.3 Phase interaction

The species transport equation for a volumetric reaction is described below:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla\left(\rho\vec{\vartheta}Y_i\right) = -\nabla\vec{J_\imath} + R_i + S_i \quad (11)$$

Where Y_i is the predicted local mass fraction of each species, $\vec{J_\imath}$ is the diffusion flux of species i, R_i is the net rate of production of species i by chemical reaction and S_i is the rate of creation by addition from the dispersed phase plus any user-defined sources.

The diffusion flux of species i written as:

$$\vec{J_\imath} = -\rho D_{i,m}\nabla Y_i \quad (12)$$

Where $D_{i,m}$ is the diffusion coefficient for species i in the mixture.

The net rate of production of species i by chemical reaction is written as:

$$R_i = M_{\omega,i}\sum_{r=1}^{N_R}\widehat{R_{\imath,r}} \quad (13)$$

Where $M_{\omega,i}$ is the molecular weight of species i and $\widehat{R_{\imath,r}}$ is the Arrhenius molar rate of creation/destruction of species i in reaction r.

3.4 Initial and boundary conditions

The column includes one fluid zone representing the region where the resin is located. At the entrance, the date syrup injects only in the axial direction. A velocity inlet boundary condition is given. The pressure is set to 5 bars. At the outlet, a pressure outlet boundary condition is given. On the wall, a no slip boundary condition is assumed.

The initials conditions for the various phase's properties are given in Table 3.

Table 3 The initials conditions of the CFD model

Parameters	Separation step		Elution step	
	Date syrup	Resin	Deionised water	Resi n
u_x	6.73; 23.67; 40.81	0	6.73; 23.67; 40.81	0
u_y	0	0	0	0
Y_w	0.5; 0.65; 0.8	-	1	-
Y_F	0.1; 0.175; 0.25	0	0	-
Y_G	0.1; 0.175; 0.25	0	0	-
T_i	298°K			

3.5 Numerical method

CFD simulations were conducted based on the above mathematical analysis. A two dimensional model was developed. By using Gambit 2.2.30 software, a quadratic map grid of 9168 cells was employed to resolve the species mass fraction, velocity, temperature and pressure gradients in the boundary layer and within the food, induced by the heating, diffusion, volumetric reaction and direction of flow. The Fluent 6.3 software was used to resolve these equations. The residuals were kept to 1.10-3 for all variables and the time step was kept small to 10^{-3}s to ensure stability. Execution time for t=300s elapsed time was approximately 60s on a Pentium 4 with two processor element, 3.02GHz and 1 GB RAM machine running windows XP professional.

3.6 Validation

The procedures for the current study were validated by comparing the variation of volume fraction at the outlet of the column of various conditions with the experimental results (Fig 3).

4. Results and discussions

4.1 Separation process

A process for separation of fructose and glucose from date syrup was carried out by means f chromatographic process. Based on the experimental design, 15 experimental runs were performed. Table 4 presents the fructose concentration for each experimental separation run.

In this experiment and as illustrated in table 5, all experimental test parameters namely sugar concentration, flow rate and temperature and the interaction between sugar concentration and temperature were found significantly affect the fructose concentration ($p<0.05$).

Table 4 High fructose date syrup produced as function of concentration, flow rate and temperature

Runs	Sugar concentration (%)	Date syrup flow rate (ml/min)	Temperature (°C)	Fructose concentration (%)
1	20	7	70	59.86
2	50	12	47.5	67.04
3	35	7	47.5	61.40
4	20	7	25	56.30
5	35	7	47.5	61.40
6	35	12	25	62.17
7	35	2	25	62.36
8	35	2	70	62.57
9	20	12	47.5	59.51
10	35	12	70	62.93
11	35	7	47.5	61.40
12	50	7	70	64.89
13	50	7	25	67.49
14	20	2	47.5	59.53
15	50	2	47.5	67.64

Figures 2a (1,2 and 3) show the fructose concentration plotted as function of sugar concentration and flow rate at the temperature 25, 47.5 and 70°C respectively. The three figures show the clear effect of the sugar concentration on the separation process. The fructose % increase with the increase of sugar concentration. This effect is confirmed in figures 1c which we see a most difference between the fructose concentration obtained with increasing sugar concentration and with the same flow rate and same temperature.

Figures 2b (1, 2 and 3) illustrate the fructose concentration plotted as function of temperature and sugar concentration. The high fructose concentration is obtained with the high temperature in lower sugar concentration.

The effect of temperature is clear in lower sugar concentration but it is dominated in higher level. This deduction is true for all flow rates.

The flow rate has an effect on the separation process (p=0.016) but the impact viewed lowest compared as the two other parameters. Referenced to figures 2c, the high fructose concentration can obtained with minimum or maximum flow rate but not with medium flow rate.

The higher separation performance is obtained with date syrup concentrated at 50% (run 2, run 13 and run 15) which we obtained a fructose concentration higher than 67%. The optimum of separation is obtained in condition 15 with sugar concentration 50%, flow rate 2ml/min and temperature 47.5°C

Table 5 Statistical analysis for the separation process

Factor	Sum of squares	Df	Mean Square	F	p
Concentration	129.418	2	64.709	2694.533	0.000
Flow rate	5.353	2	2.676	111.458	0.000
Temperature	0.498	2	0.249	10.370	0.016
Concentration * Flow rate	0.084	1	0.084	3.502	0.120
Concentration * Temperature	9.486	1	9.486	395.020	0.000
Flow rate * Temperature	0.075	1	0.075	3.149	0.136
Error	0.120	5	0.024		
Total SS	144.694	14			

*Note: R^2 = 0.999; adjusted R^2 = 0.997. The effect was tested using the industrial statistics and six sigma, Box-Behnken experimental design.

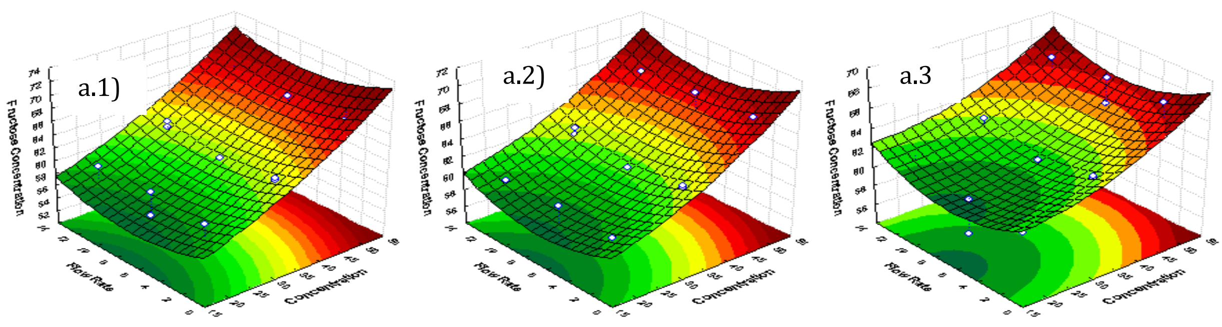

Fig.2a. Evolution of Fructose production as function of concentration and flow rate at temperature: a.1) 25°C, a.2) 47.5°C and a.3) 70°C

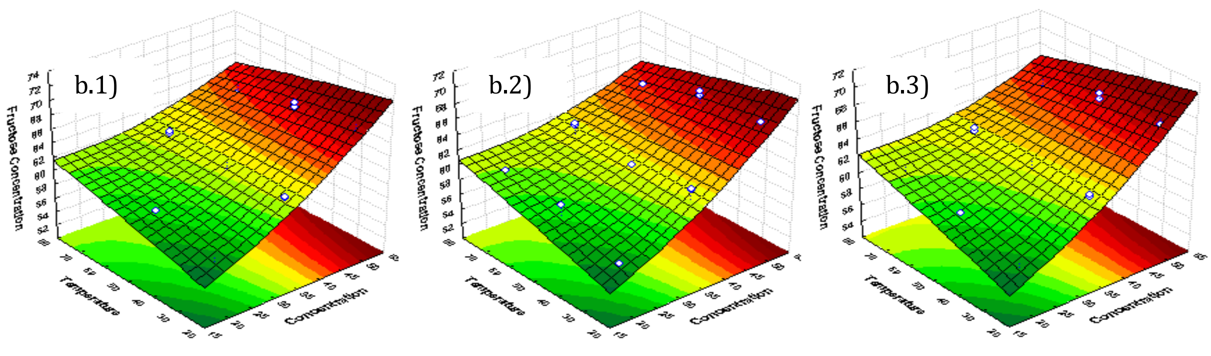

Fig.2b. Evolution of Fructose production as function of concentration and temperature for the flow rate: b.1) 2ml/min, b.2) 7ml/min and b.3) 12ml/min

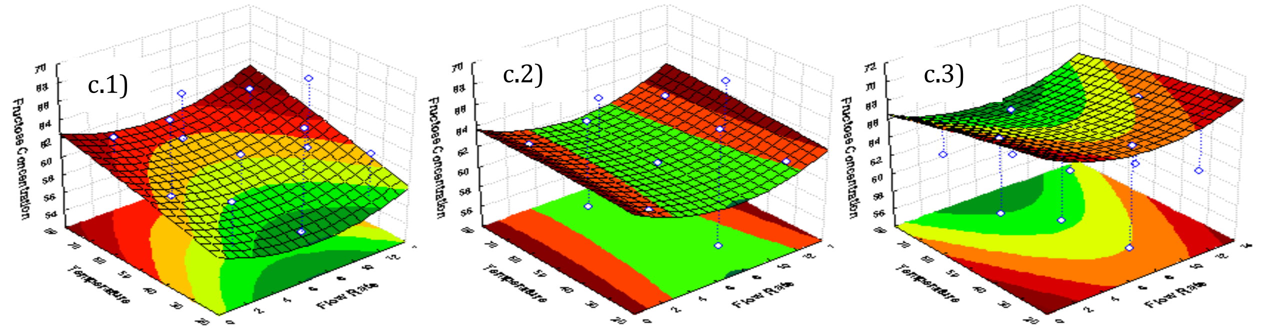

Fig.2c. Evolution of Fructose production as function of flow rate and temperature for the concentration: c.1) 20%, c.2) 35% and c.3) 50%.

4.2 Validation

The comparison between the experimental and predicted date volume fraction of separation process, for 15 runs, is shown in Fig.3. It can be seen that the simulation data is in excellent agreement with the experimental data. The correlation coefficient for the predicted and experimental date also showed a good agreement for the volume fraction (R^2=0.967). This suggests that the separation process of sugar from date can be accurately predicted by the CFD model.

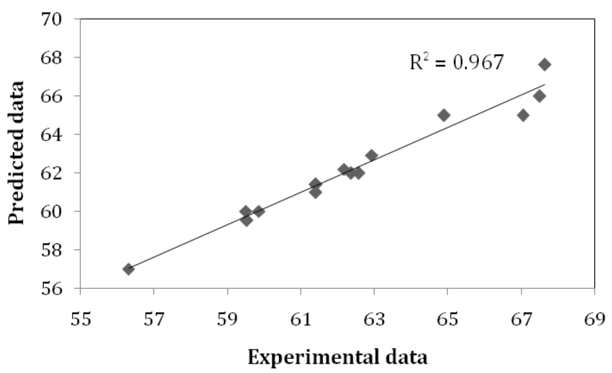

Fig.3 Correlation of experimental versus predicted data

Conclusion

The Euler-Euler multiphase approach is used to models the separation of the mixture of glucose and fructose obtained. The model predicted the performance of chromatographic separation process of date sugars as the function of as function of the sugar concentration, the date syrup flow rate and the temperature.

The numerical results werecompared with the experimental data indicated a good agreement. The optimal condition of separationwas obtained with date syrup concentrated at 50% (run 2, run 13 and run 15) which we obtained a fructose concentration higher than 67%. The optimum of separation is obtained in condition 15 with sugar concentration 50%, flow rate 2ml/min and temperature 47.5°C.

References

A.Khosravanipour Mostafazadeh, M.Sarshar, S.Javadian, M.R.Zarefard, Z.AmirifardHaghighi, (2011). Separation of fructose and glucose from date syrup using resin chromatographic method: Experimental data and mathematical modeling. *Separation and Purification Technology*, 79, 72-78.

A.S.Kurup, H.J.Subramani, K.Hidajat, A.K.Ray, (2005).Optimal design and operationof SMB bioreactor for sucrose inversion.*Chemical Engineering Journal*, 108, 19-33.

Lj.Matijašević, D.Vasić-Rački, (2000).Separation of glucose/fructose mixtures: counter-current adsorption system. *Biochemical Engineering Journal*, 2, 101-106

M.Trigui, K.Gabsi, W.Zneti, S.Barrington, A.N.Helal, (2015). Finite Element Model to Predict the Bioconversion Rate of Glucose to Fructose using Escherichia coli K12 for Sugar Production from Date. *International Journal of Food Engineering*, 11, 105-113.

S.M.Al-Eid, (2006).Chromatographic separation of fructose from date syrup.*International Journal of Food Sciences and Nutrition*, 57, 83-96.

Y.Zhang, K.Hidajat, A.Ray, (2004). Optimal design and operationof SMB bioreactor: production of high fructose syrup by isomerization of glucose. *Biochemical Engineering Journal* , 111-121.