KMUTNB Int J Appl Sci Technol, Vol. 11, No. 1, pp. 53–61, 2018

Research Article

Plant-wide Process Simulation of Ethanol Production from Empty Fruit Bunch

Darunwan Chuenbubpar and Thongchai Rohitatisha Srinophakhun*
Department of Chemical Engineering, Faculty of Engineering Kasetsart University, Bangkok, Thailand

Panuwat Tohsakul
Chemical Engineering Practice School, King Mongkut's University of Technology Thonburi, Bangkok, Thailand

* Corresponding author. E-mail: fengtcs@ku.ac.th

DOI: 10.14416/j.ijast.2017.12.007
Received: 3 March 2017; Accepted: 9 May 2017;

Abstract
Lignocellulosic biomass exhibits itself as an alternative material for ethanol production. Ethanol can be synthesized from cellulose and hemicellulose obtained from an empty fruit bunch. Aspen simulation is used for process design and its capacity. Hot Compressed Water pretreatment (HCW) is the first step to improving ethanol production. The optimal conditions of HCW are 190°C and 15 minute with a cellulose content of 56.56%. Ethanol is converted from lignocellulosic derivative via hydrolysis and fermentation processes. The extractive distillation system is proposed to purify. There are two different operating conditions (reflux ratio, feed stage, and distillate to feed ratio) at the solvent to feed ratio (S/F) of about 0.51. Ethanol of 10,000 kg could be produced from 48,000 kg of EFB with product purity greater than 99.5 wt%.

Keywords: Lignocellulosic ethanol, Empty fruit bunch, Ethanol production simulation, Aspen plus

1 Introduction

At present, the problem of global warming is widely accepted worldwide. Many countries have expressed their concerns and tried to grapple with this problem. Various factors such as carbon monoxide released from the vehicle engine, as well as operations of industry, are considered. Clean and renewable energy sources are essential. Therefore, daily life potential alternative energy resources are produced from biomass, for instance, bioethanol [1]. Bioethanol was commercially produced by the fermentation process. Usually, it can be produced by sugar fermentation from starch-based feedstock such as corn, cassava, and sugarcane [2].

Empty Fruit Bunch (EFB) of the oil palm showed potential as raw material for lignocellulosic bioethanol production. The main compositions of EFB feedstock are 46.77% of cellulose, 17.92% of hemicellulose, 4.15% of lignin based on a dry basis [3]. The bioethanol production process contains four sections: pretreatment, hydrolysis, fermentation, and purification. [4]. Cellulosic biomass was converted to bioethanol via hydrolysis followed by fermentation. Hydrolysis converts complex polysaccharides into simple form sugar. Fermentation then converted sugar into bioethanol with yeast or bacteria. Carbon dioxide was a by-product of fermentation [5]. Then, the fermented broth was taken through the distillation unit in order to purify the ethanol according to a desirable specification.

This article studied the feasibility of bioethanol production from EFB. The commercial software Aspen plus simulation was used to simulate and integrate ethanol plants, including pretreatment, fermentation, hydrolysis and purification. Moreover, the Aspen Custom Modeler (ACM) was also used to create a

Please cite this article as: D. Chuenbubpar, T. R. Srinophakhun, and P. Tohsakul, "Plant-wide process simulation of ethanol production from Empty Fruit Bunch ," *KMUTNB Int J Appl Sci Technol*, vol. 11, no. 1, pp. 53–61, Jan.–Mar. 2018.

new unit of operation. This new unit of operation was exported to Aspen Plus for the whole process. Finally, the ethanol from the azeotropic mixture was improved with the control strategy in Aspen Plus dynamic for separation section at the suitable controller gain.

2 Methodology

2.1 *Ethanol process*

This study will cover the ethanol production at 10,000 kg/day in the simulation viewpoint.

2.1.1 Pretreatment

Hot compressed water pretreatment was used to pretreat the lignocellulosic material before hydrolysis and fermentation. The EFB was used as the main raw material. It would be dried in the sun in order to eliminate the moisture, and then the particle size of it was reduced. The ratio between the EFB (g) and water (mL) was 1:10 and heat in the glycerol bath was 190°C and 15 minute. The experimental information that obtained from Mahidol University the laboratory is shown in Table 1.

Table 1: The composition of an Empty Fruit Bunch (EFB) after hot compressed water as the pretreatment

T	***t***	**Composition (Dry wt%)**					
		C6	**C5**	**Lignin**	**Ash**	**Others**	**%SR**
190	5	51.59	13.81	13.86	1.19	19.53	63.25
	10	56.57	10.28	14.02	1.23	17.90	66.92
	15	57.52	12.24	14.47	1.62	14.15	57.35
200	5	51.97	13.18	11.30	0.99	22.56	58.81
	10	57.14	13.49	13.83	1.44	14.11	60.44
	15	57.72	18.92	12.82	1.33	9.87	56.89

In order to model the specific unit operation, the mathematical model plays a major role. Two variables, temperature and time, were used to formulate the function of outcomes (Solid Recovery, Cellulose, Hemicellulose, lignin, and Ash). The mathematical models after pretreatment are shown in the equations (1)–(5).

$$\%SR = 188.5 - 0.678\times T - 2.70\times t - 0.0460\times t^2 + 0.0199\times T\times t \quad (1)$$

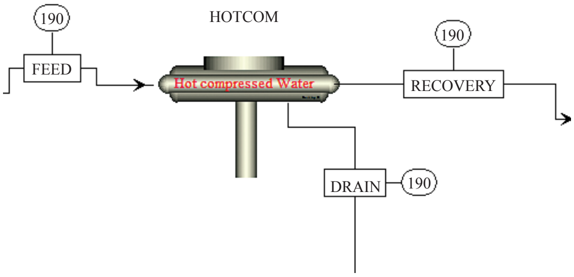


Figure 1: HCW pretreatment unit.

$$C5 = 32.0 + 0.0794\times T + 1.786\times t - 0.02310\times t^2 - 0.00419\times T\times t \quad (2)$$

$$C6 = 63.05 - 0.2397\times T - 7.820\times t + 0.026523\times t^2 + 0.03656\times T\times t \quad (3)$$

$$Lignin = 53.6 - 0.217\times T - 0.61\times t - 0.00810\times t^2 + 0.0046\times T\times t \quad (4)$$

$$Ash = 1.55 - 0.0032\times T + 0.121\times t - 0.00053\times t^2 - 0.00044\times T\times t \quad (5)$$

These equations were implemented to model and simulate for HCW at the operating condition of 190 to 200°C within 5 to 25 minute. Hence, HCW pretreatment will be modeled in Aspen Custom Modeler (ACM) for specific unit operation as shown in Figure 1. These equations were implemented to model and simulate for HCW at the operating condition of 190 to 200°C within 5 to 25 minute. Hence, HCW pretreatment will be modelled in Aspen Custom Modeler (ACM) for a specific unit operation as shown in Figure 1.

The specific unit operation of HCW pretreatment to the main simulation (Aspen Plus) can be worked and formulated within the entire system including fermentation and distillation.

2.1.2 Hydrolysis

The hydrolysis using acid was a widely used process for producing ethanol from biomass. Therefore, in this study, diluted sulfuric was used to hydrolyze the biomass to liquid hydrolysates at high temperature. The hydrolysis process converts cellulosic in biomass into sugar to be fermented into the ethanol [6]. For acidic reaction, it was divided into two parts: diluted and concentrated acid hydrolysis. Diluted acid hydrolysis

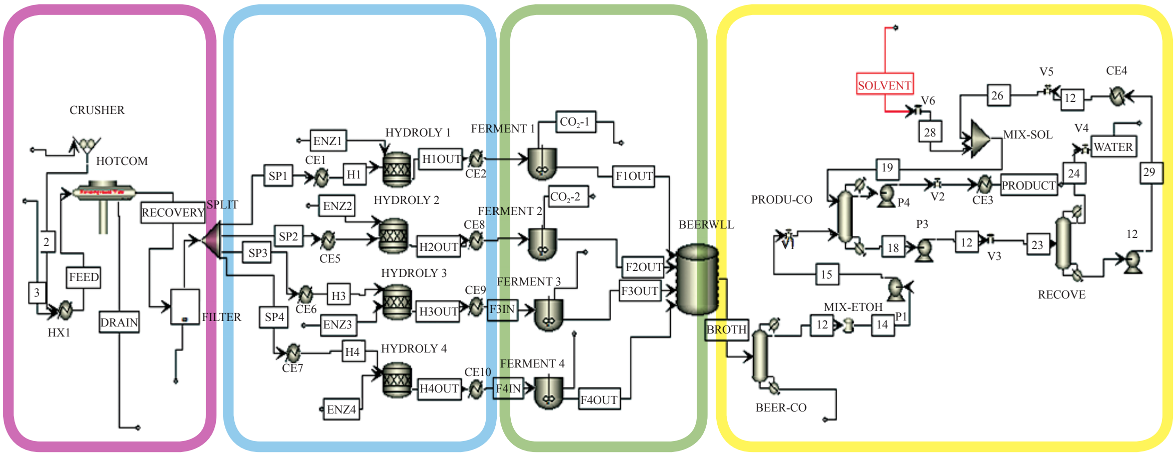


Figure 2: Ethanol process flowsheet in Aspen Plus.

(1–3%) requires a high temperature above 200°C to break cellulose crystal which is suitable considering the environment [7]. The fractional conversion during the hydrolysis process is shown in Table 2.

Table 2: Hydrolysis reaction

Reactions	Reactant	Fractional Conversion
Cellulose (CISolid) + Water → Glucose	Cellulose	0.9
2Cellulose (CISolid) + Water → Cellubiose	Cellulose	0.012
Hemicellulose (CISolid) + Water → xylose	Hemicellulose	0.9
Cellubiose + Water → Glucose	Cellubiose	1

2.1.3 Fermentation

After the pretreatment and hydrolysis, fermentation was the essential unit in order to ferment sugar to alcohol, lactic and other products. S*accharomyces cerevisiae* has been widely used in the industrial yeast in alcohol production. *S. Cerevisiae* had been utilized for corn base and sugar base [8]. The fermentation operates under an anaerobic condition at a temperature of about 32–35°C and pH around 4.2–4.5 [9]. The main reaction takes place in this section shown in Table 3. Carbon dioxide is a by-product. The overall efficiency of fermentable sugars to ethanol is about 95% of yeast. This is the highest conversion of fermentation [10].

Table 3: Fermentation reaction

Reaction	Reactant	Fractional Conversion
Glucose → 2 Ethanol + 2 CO_2	Glucose	0.95
3 Xylose → 5 Ethanol + 5 CO_2	Xylose	0.85

2.2 *Process simulation*

The entire ethanol production process is performed in Aspen Plus. The simulation utilized NRTL with Henry's law for the thermodynamic model because the ethanol and water were of a non-ideal liquid phase and had azeotropic behavior. Carbon dioxide was the light gas occurring during fermentation. The aim of this section is to design and simulate ethanol production. Sensitivity analysis is proposed to study the effect of the main operation, Reflux Ratio (RR), and distillate to feed ratio (D/F) in ethanol purification section. The ethanol process was divided into 4 sections: pretreatment, hydrolysis, fermentation and purification.

2.2.1 Process description

The completed flowsheet of ethanol production from EFB was shown in Figure 2. Firstly, raw material (stream-1) with long size passes was put into the crusher in order to reduce the particle size to 2 mm before pretreatment [11]. Then it went on to the pretreatment section in order to break the cell wall before enzymatic hydrolysis. The pretreatment unit was built in ACM.

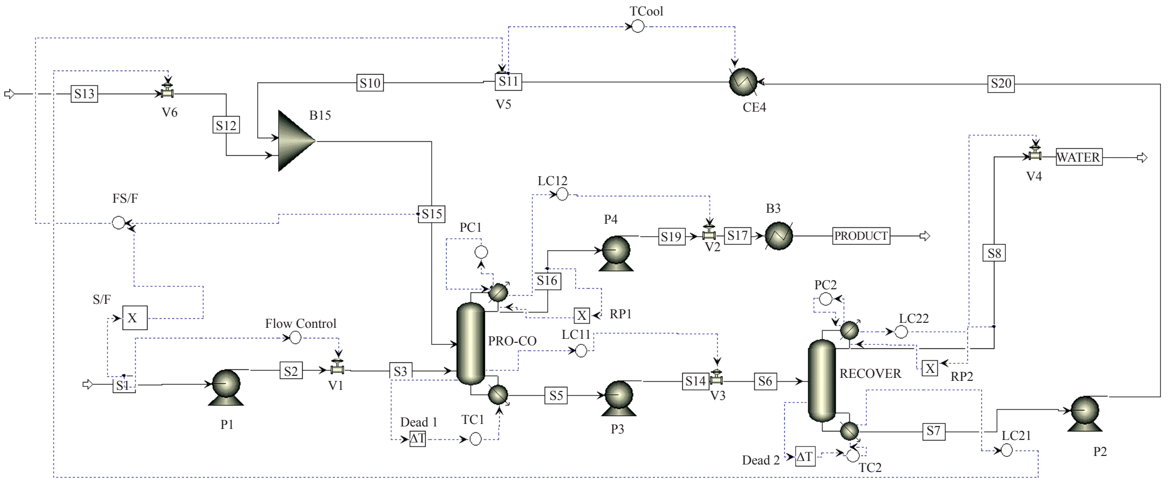


Figure 3: Extractive distillation control in Aspen Plus Dynamic.

The pretreated raw material (stream-5) was put into the hydrolysis unit in parallel to convert cellulose and hemicellulose to glucose and xylose by an enzyme. The simple sugar streams (H1OUT, H2OUT, H3OUT, and H4OUT) were fermented to ethanol stream (F1OUT, F2OUT, F3OUT, and F4OUT).

Moreover, carbon dioxide streams (CO_2-1, CO_2-2, CO_2-3, and CO_2-4) were a by-product during fermentation and vented out of the system. In the fermentation process, the commercial yeast used was *S. cerevisiae*. The fermentation broth would be sent to the storage tank (Beer Well) and then it was transferred to the first distillation column (BEER-CO) in order to purify ethanol up to 90 wt% near the azeotropic point before it is sent to the extractive distillation column (PRODU-CO). Stream 12 mostly contained ethanol and water; therefore, it exhibited the azeotrope behavior and could not get ethanol purity more than 99 wt%. The extractive distillation technique was used to achieve the product specification. Ethylene glycol was widely used as a third component for breaking the azeotrope of the mixture. The mixture (stream-16) was fed to PRODUCT-CO, while the solvent (stream-19) was fed on the top. Ethanol went to the top of the column; water and solvent went to the bottom of the column then recovery column (RECOVE) in order to recover the solvent back to the system and also had makeup solvent in stream-solvent. Some purified ethanol at 99.5 wt% was produced as the ethanol fuel grade.

2.2.2 Control design of ethanol purification

There was the azeotropic point between ethanol and water; the extractive distillation system was proposed to purify the ethanol more than 99.5 wt%, whereas ethylene glycol was used as a solvent for breaking the azeotropic point [12]. The steady-state design was performed in Aspen Plus and then exported to a pressure-driven simulation in Aspen Plus Dynamic (APD). Before exporting to APD, sizing of equipment, such as the size of reflux drum, diameter of column, and sump, was defined. The liquid holdup provides 10 minutes in reflux drum and base level. Extractive distillation control systems were illustrated in Figure 3. The control structure was more important for extractive distillation to maintain the product specification. The solvent to feed ratio was essential to maintain the product specification. The control structure of extractive distillation is as follows [12]:

- Extractive and Recovery have a reflux drum; therefore, its reflux drum level was controlled by the distillate flow rate of the column.
- Feed Flow rate to extractive distillation was controlled by manipulating the valve.
- The pressure along the column was controlled by heat removal duties in the condenser.
- The liquid sump level in the extractive column was controlled by the bottom flow rate.
- The base level for recovery column was controlled by manipulating the makeup flow rate, as

suggested by Grassi [13] and Luyben [14].

- The solvent flow rate in the extractive column was proportional to feed flow rate, and the ratio was controlled by manipulating the bottom flow rate of the recovery column.
- Reflux ratio for both columns will be held constant.
- The reboiler duties of both columns were used to control the temperature in a particular stage of each column for control of the composition.

To conclude, there are 2 controller types with the control tuning shown in Table 4.

Table 4: Tuning parameter of controller

Controller Name	Purpose	Controller Type	K_c	τ_1	Action
PC1, PC2	Control column pressure	PI	20	12	Reverse
LC12, LC22	Control reflux drum level	P	2	9999	Direct
LC11	Control base level of extractive column	P	10	9999	Direct
LC21	Control base level of recover column	P	10	9999	Reverse
Flow Control	Control flow rate of feed	PI	0.3	0.5	Reverse
F-S/F	Control solvent to feed ratio	PI	1.6	2.4	Reverse

3 Results and Discussions

3.1 *The optimal condition of hot compressed water pretreatment*

In order to find the optimal condition which impacts to the percentage of cellulose content after pretreatment, the mathematical model is used and the optimal condition is proposed. Feed flow rate is assumed to be 100 kg of raw material. The result of cellulose showed in Figure 4.

The optimal temperature and time are 190°C and 15 minute in the red area as shown in Figure 4. The highest cellulose content was obtained under this condition. The higher cellulose content after pretreatment is high; the higher sugar in hydrolysis process can be produced. This will affect the productivity of ethanol.

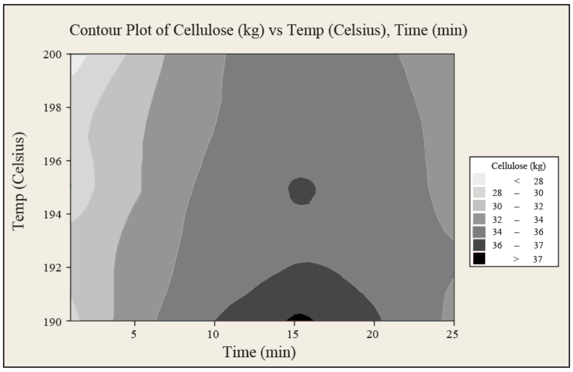


Figure 4: Cellulose content after hot compressed water pretreatment.

3.2 *Ethanol simulation*

3.2.1 Pretreatment

The optimal conditions are 190°C and 15 minute. The total flow rate of raw material is 1,978 kg/h. The composition of the raw material is concluded in Table 5. The result shows that approximately 1,296.754 kg/h of raw material is recovered in the recovery stream along with 56.736% of cellulose. Pretreated EFB is sent to the hydrolysis section.

Table 5: The composition of Empty fruit bunch

	Mass Flow kg/h		
	Feed	**Drain**	**Recovery**
ETHANOL	0	0	0
CO_2	0	0	0
CELLULOS	949.6403	232.3046	717.3357
XYLAN	542.0863	409.627	132.4593
LIGNIN	221.5827	42.26081	179.3219
ACETI-01	0	0	0
GLUCOSE	0	0	0
CELLO-01	0	0	0
WATER	0	0	0
XYLOS-01	0	0	0
ASH	27.7018	9.309168	18.39263
SOLSLD	0	0	0
EXTRAC	237.4101	40.49444	196.9156
ENZYME	0	0	0
FURFURAL	0	0	0

Table 5: (Continued) The composition of Empty fruit bunch

Mass Flow kg/h			
	Feed	**Drain**	**Recovery**
5-HMF	0	0	0
ETHYGLY	0	0	0
Mass Frac			
ETHANOL	0	0	0
CO_2	0	0	0
CELLULOS	0.479999	0.316493	0.5764394
XYLAN	0.2739995	0.558078	0.1064422
LIGNIN	0.1119998	0.0575763	0.1441002
ACETI-01	0	0	0
GLUCOSE	0	0	0
CELLO-01	0	0	0
WATER	0	0	0
XYLOS-01	0	0	0
ASH	0.0140019	0.0126828	0.01478
SOLSLD	0	0	0
EXTRAC	0.1199998	0.0551698	0.1582382
ENZYME	0	0	0
FURFURAL	0	0	0
5-HMF	0	0	0
ETHYGLY	0	0	0
Total Flow kmol/h	22.65747	6.8172	15.84027
Total Flow kg/h	1978.421	733.9961	1244.425
Total Flow l/min	21.49192	5.681	13.20022

3.2.2 Hydrolysis and Fermentation

The suitable temperature in hydrolysis and fermentation are 50 and 30°C. Pretreated hemicellulose and cellulose (stream-H1, H2, H3, and H4) are fed to the hydrolysis reactor at 184 kg/h and 34 kg/h in each stream. Glucose and xylose are produced at 658 kg/h and 143 kg/h as a result. Glucose and xylose are sent to the fermenter to produce ethanol. Fermenter can produce ethanol at 418 kg/h. A large amount of vapor product was produced at about 400 kg/h, mostly containing CO_2, and vented out of the system. Both hydrolysis and fermentation are a batch operation. Therefore, about 48,000 kg of empty fruit bunch can produce ethanol of 10,000 kg per batch. The process simulation contains four hydrolysis reactors and fermenters. Both units operate on a parallel train in Figure 5. The duration of hydrolysis and fermentation is about 6 day. The product will be stored in beer well and sent to purification to purify the product continuously.

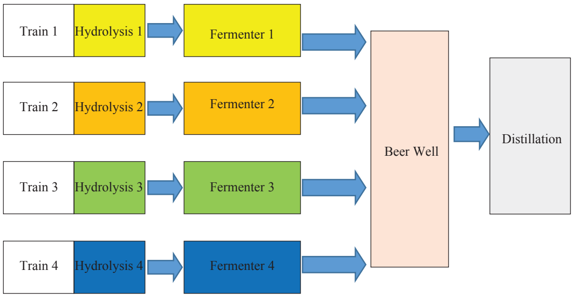


Figure 5: Sequences of hydrolysis and fermentation.

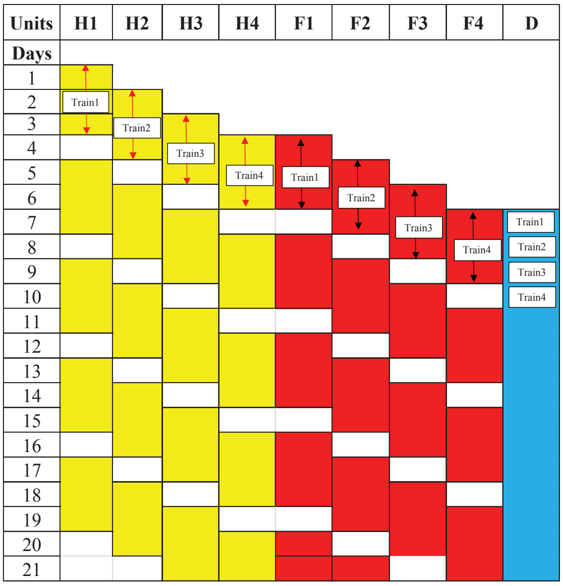


Figure 6: Gantt chart for hydrolysis and fermentation.

As shown in Figure 6, H, F, and D represent hydrolysis, fermentation, and distillation. Gantt chart of ethanol starts (train1) from day 1 and finishes on day 6. Hydrolysis needs 3 more days and one day for cleanup and setup for a new batch. Other trains are the same. Fermentation broth from train1 is purified in the purification section on day 7. From Gantt chart, distillation will operate continuously from day 6.

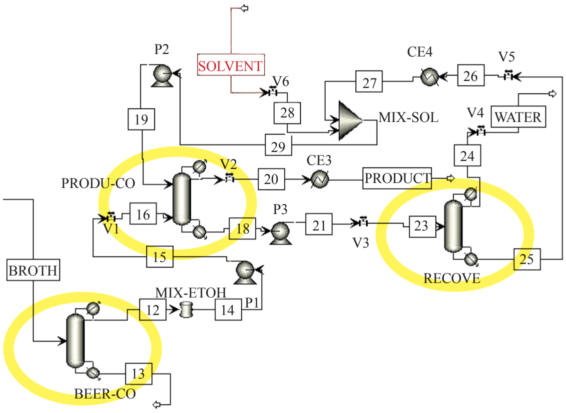


Figure 7: Purification section.

3.2.3 Purification Section

Figure 7 represents the purification section. Fermentation broth (Stream-Broth) is fed in BEER-CO at stage 10; distillate flow rate from BEER-CO is passed through the extractive distillation column (PRODU-CO). Feed stage of the mixture (stream- 16) is at 15, but the solvent is fed at stage 4. The temperature of the solvent is 25°C, and the solvent to feed ratio (S/F) is 0.51. S/F is sensitive once the extractive distillation is performed in APD. This column gives high purification of ethanol more than 99.5 wt% at the top of the column; water and solvent go to the bottom of the column.

In order to investigate the effect of solvent and feed stage on ethanol purification, a sensitivity analysis tool is used to determine the effect of the feed stage. Feed and solvent stages are shown in Figures 8 and 9.

Finally, from process simulation, it was found that about 48,000 kg of EFB can produce 10,000 kg of ethanol with 99.5 wt%. The energy consumption in purification has to be concerned because the main equipment in this section is extractive distillation column; reboiler heat duty consumes a lot of energy. Therefore, sensitivity analysis is needed to find the main operation that obtains the low energy consumption, but the product specification of ethanol is higher at 99.5 wt%. The contour plot between Reflux Ratio (RR) and Distillate to feed ratio (D/F) of three columns are shown in Figure 10.

The lowest of energy consumption in Figure 10(a) and (b) are in the red area and Figure 10(c) is in the blue area. The contour plot expresses that RR and D/F are the operations that directly affect the energy consumption. However, the product specification must be maintained at the suitable RR and D/F.

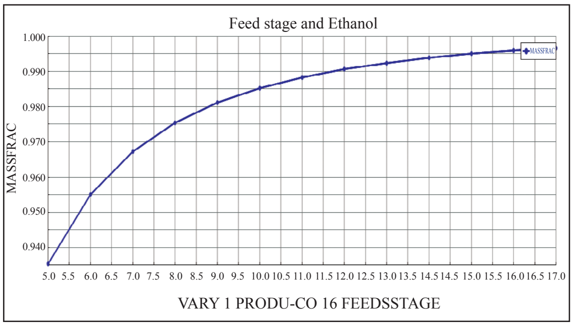


Figure 8: Feed stage and ethanol mass fraction in extractive column.

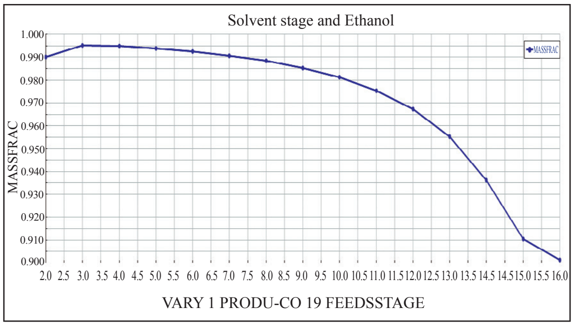
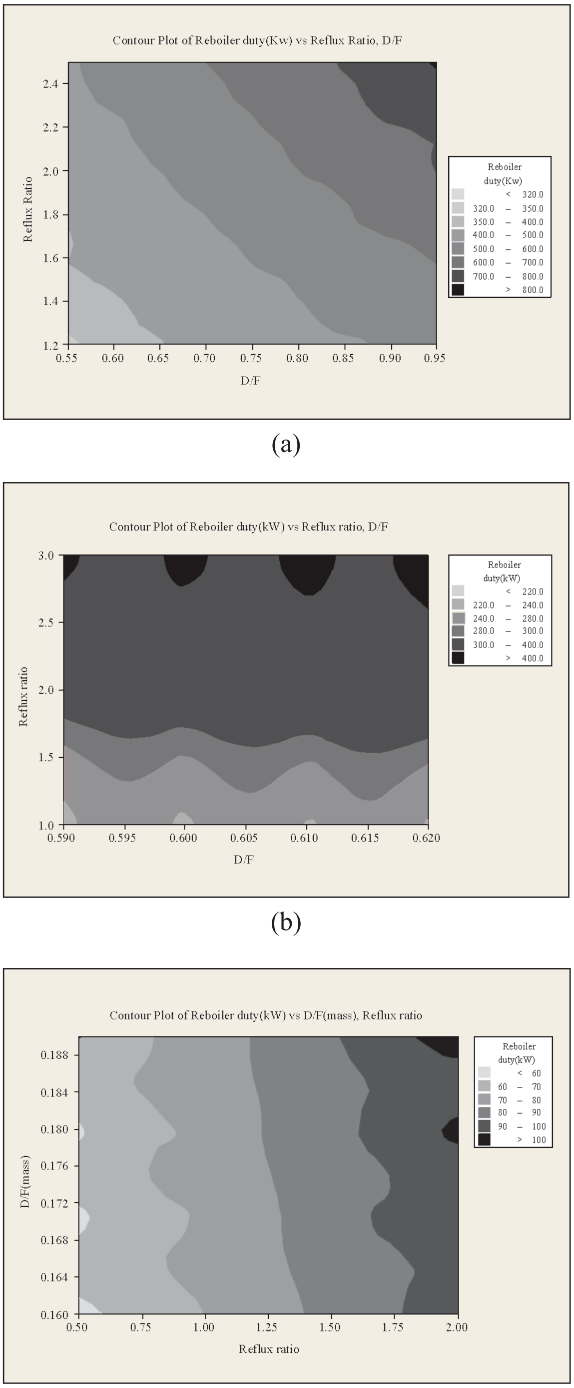


Figure 9: Solvent stage and ethanol mass fraction in extractive column.

4 Conclusions

The article presents process simulation and control of ethanol production from palm waste using Aspen suit v.8.8. Aspen pretreatment model is created from the experimental data and its mathematical model is formulated. The optimal conditions of HCW are 190°C and 15 minute. The train of hydrolysis and fermentation can be divided into 4 sets to suit the continuous distillation section. The simulation found that ethanol of 10,000 kg could be produced from 48,000 kg of EFB. In terms of extractive distillation control, tray temperature control is more important in order to hold the composition profile of the product. Disturbances are introduced to test the performance. The feed composition and feed flow rate are changed at 3 hour. Controller can reject disturbances and the ethanol specification over 99.5 wt%.



(a)

(b)

(c)

Figure 10: The contour plot between reflux ratio (RR) and distillate of (a) Beer column, (b) Extractive column, (c) Recovery column.

Acknowledgments

Funding for this work was provided jointly by the NRCT (The office of the National Research Council of Thailand), in collaboration with NSFC (The National Natural Science Foundation of China) under the topic of Renewable Energy, and Kasetsart University.

References

[1] H. Jeon, K. E. Kang, J. D. Jeong, G. Gong, J. W. Choi, H. Abimanyu, and G. W. Choi, “Production of anhydrous ethanol using oil palm empty fruit bunch in a pilot plant,” *Biomass and Bioenergy*, vol. 67, pp. 99–107, 2014.

[2] M. Balat, H. Balat, and C. Oz, “Progress in bioethanol processing,” *Progress in Energy and Combustion Science*, vol. 34, pp. 551–573, 2008.

[3] D. Piarpuzan, J. A. Quintero, and C. A. Cardona, “Empty fruit bunches from oil palm as potential raw material for fuel ethanol production,” *Biomass and Bioenergy*, vol. 35, no. 64–60, pp. 1130–1137, 2011.

[4] A. Limayem and S. Ricke, “Lignocellulosic biomass for bioethanol production: Current perspectives, potential issues and future prospects,” *Progress in Energy and Combustion Science*, vol. 38, pp. 449–467, 2012.

[5] C. Cheng, K. Hani, and S. Ismail, “Production of bioethanol from oil palm empty fruit bunch,” in *Proceedings 1st International Conference on Sustainable Materials 2007(ICoSM2007)*, 2007, pp. 69–72.

[6] B. Joseph and T. Ronald, “Fermentable sugars by chemical hydrolysis of biomass,” *Proceedings of the National Academy of Sciences*, vol. 107, pp. 4516–4521, 2010.

[7] Q. Xiang, Y. Lee, P. Pettersson, and R. Torget, “Heterogeneous aspects of acid hydrolysis of α-cellulose,” *Applied Biochemistry and Biotechnology*, vol. 105–108, pp. 504–514, 2003.

[8] M. Graeme and G. Graham, “*Saccharomyces cerevisiae* in the production of fermented beverages,” *Beverages*, vol. 2, pp. 1–12, 2016.

[9] D. Keelsall, K. Jcques, and T. Lyons, “Understanding yeast fundamentals,” in *The Alcohol Textbook*, 4th ed. Nottingham: Nottingham University Press, 2003, pp. 94–99.

[10] R. Wooley, M. Ruth, J. Sheehan, and K. Ibsen, "Lignocellulosic biomass to ethanol process design and economics utilizing co-current dilute acid prehydrolysis and enzymatic hydrolysis current and futuristic scenarios," National Renewable Energy Laboratory, Colorado, Tech. Rep. TP-510-32438, Jun. 2002.

[11] H. Meehnian, A. K. Jana, and M. M. Jana, "Effect of particle size, moisture content, and supplements on selective pretreatment of cotton stalks by *Daedalea flavida* and enzymatic saccharification," *3 Biotech*, vol. 6, pp. 235(1–13), 2016.

[12] I. D. Gil, J. M. Gómez, and G. Rodríguez, "Control of an extractive distillation process to dehydrate ethanol using glycerol as entrainer," *Computers and Chemical Engineering*, vol. 39, pp.129–142, Apr. 2012.

[13] V. G. Grassi, "Process design and control of extractive distillation," in *Practical Distillation Control*, New York: Van Nostand Reinhold press, 1993, pp. 370–404.

[14] W. L. Luyben, "Comparison of extractive distillation and pressure-swing distillation," *Industrial and Engineering Chemistry*, vol. 47, no. 8, 2008.