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Original Article

Process simulation of ethanol production from oil palm trunk

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Abstract

Oil palm trunk (OPT) is lignocellulosic biomass and renewable waste obtained from palm oil production, and it can be used to produce ethanol. In this study, the ethanol plant was analyzed using Aspen Plus software for process simulation and modeling, based on of 60,000 kg of OPT, while the model inputs were based on data recently obtained in the laboratory. Various pretreatments of OPT are used such as steam explosion, hot water, alkaline hydrogen peroxide, and simultaneous saccharification and fermentation (SSF). All these pretreatments are used to increase the cellulose content and efficiency of getting fermentable sugars from cellulose for conversion to ethanol. The cellulose content was 73.96% by dry wt after treatment, from 38.67% in the original OPT. For the SSF step in a laboratory, treated OPT was used to ferment ethanol for about 60 h, producing an ethanol yield of 0.469 g EtOH g^{-1} cellulose. This information was used to simulate the SSF unit. Ethanol was purified by extractive distillation using ethylene glycol as a solvent. The simulation of the distillation column comprised 15 stages, the distillate for feeding had mass ratio 0.65, and the reflux mass ratio was 1.4, potentially producing 9,531 kg of ethanol.

Keywords: oil palm trunk, steam explosion, extractive distillation, Aspen Plus, ethanol simulation

1. Introduction

Bioethanol is a form of renewable clean energy for solving global environmental problems (Bungay, 2004; Gavrilescu & Chisti, 2005; Hamelinck, Hooijdonk, & Faaij, 2005). It can be produced by fermentation using micro organisms. *Saccharomyces cerevisiae* (*S. cerevisiae*) is a commonly used microorganism in fermentation. Although bioethanol can be produced using sugar from starch and sugar-based feedstock (e.g., cassava and sugarcane) (Balat, Balat, & Öz, 2008) such processes are of limited benefit because these feedstocks are sources of human food. Lignocellulosic materials are interesting feedstocks because of their low cost and them not have food applications, like rice straw (Yoswathana, Phuriphipat, Treyawutthiwat, & Eshtiaghi, 2010), sugarcane bagasse (Wong, & Sanggari, 2014), oil palm residue, or corn stover (Banerjee *et al.*, 2012).

Palm residue is agro-industrial waste from the palm oil industry. Such waste is a renewable resource for the production of bioethanol. In the global market, Thailand is among the top three producers of palm oil. Most of Thailand's palm oil is produced in the southern peninsular part of the country. The palm oil extraction generates a lot of waste in the forms of fiber, fruit bunch shells, oil palm trunk (OPT), and an empty fruit bunches. OPT is an interesting waste composed mainly of cellulose, hemicellulose, and lignin (Akmar, & Kennedy, 2001). Cellulose is the main component for conversion to sugar by hydrolysis in a bioethanol process.

Bioethanol production from lignocellulosic materials comprises four sections: pretreatment, hydrolysis of recovered cellulose into sugars, fermentation of sugars to ethanol, and purification of ethanol (Limayem & Ricke, 2012). First, OPT can be pretreated by steam explosion (SE), hot water treatment (Lu *et al.*, 2013), or treatment with

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alkaline hydrogen peroxide (AHP). SE is a technique for increasing the potential of cellulose using high-pressure saturated steam (160–260 °C for pressure range 0.69–4.83 MPa). As the pressure is swiftly reduced there is explosive decompression of materials (Khunrong, Punsuvon, Vaithanomsat, & Pomchaitaward, 2010). Recently, Songprom (2011) studied the composition of OPT from SE pretreatment at alternative temperatures (200 and 210 °C) for some time periods (2, 4, and 6 mins). The experimental data revealed that the optimum conditions at 210 °C for 4 mins produced 58.83% of cellulose, 4.03% of pentosan, and 27.12% of lignin. After that, the treated OPT was used for fermentation, producing an ethanol concentration of 16.42 g/l. Hot water treatment can effectively remove monosaccharides, oligosaccharides, toxic substances, and acids. The optimum is at 80 °C and 30 mins. Hot water pretreatment is introduced because of it solubilizing hemicellulose. At the same time, the use of AHP to produce a hydrogen peroxide decomposition reaction can reduce the solid lignin content. Cao, Sun, Liu, Yin, and Wu (2012) studied ethanol production using sweet sorghum bagasse and compared five pretreatments: (1) diluted NaOH solution; (2) a high concentration NaOH solution; (3) diluted NaOH solution and H_2O_2; (4) alkaline peroxide; and (5) autoclaving. The experimental data revealed that the diluted NaOH solution and H_2O_2 pretreatment was the most suitable for sweet sorghum bagasse pretreatment.

Aspen Tech is a process simulation software package used in chemical engineering. Aspen Plus is the main application used to simulate the overall ethanol plant, consisting of pretreatment, hydrolysis, fermentation, and purification. The Aspen Custom Modeler (ACM) can be used to create a unit operation that does not already exist in Aspen Plus. The new units are then exported to Aspen Plus for assembly with others. Recently, Chuenbubpar, Srinophakhun, and Tohsakul (2018) studied the plant-wide process simulation of ethanol production using EFB pretreatment with hot compressed water (HCW) to create a mathematical model from the experimental data. The ACM was used to develop an HCW-unit for export into Aspen Plus. Both hydrolysis and fermentation can be represented by these standard reaction operations in Aspen Plus. From purification the industry provides ethanol concentrations exceeding 99%. Extractive distillation is the dehydration of ethanol using ethylene glycol as a solvent to break up the azeotrope mixture in the distillation column (Lee & Pahl, 1985). Also, a molecular sieve using the adsorption phenomenon can catch water molecules, while it cannot catch ethanol molecules (Onuki, 2006). Kaewklam (2018) studied ethanol production using EFB. This article compared two pretreatments: HCW and SE using Aspen as well as purification, extractive distillation, and molecular sieves. Four models were studied: 1) hot compressed water (HCW) with extractive distillation; 2) hot compressed water (HCW) with molecular sieves distillation; 3) steam explosion with extractive distillation; and 4) steam explosion with molecular sieve distillation. The results suggest that EFB-treated with SE and purified by extractive distillation can produce the most ethanol.

This paper studies the potential for producing ethanol by simulations using Aspen Plus and creates models of the various operating units using the Aspen Custom Modeler (ACM). Information from the Faculty of Agro-Industry, Kasetsart University was used to create a simulation model, including three alternative pretreatment methods (SE, hot water, and AHP) and simultaneous saccharification and fermentation (SSF). Extractive distillation was the purification step used by the sensitivity analysis tool in Aspen Plus to find the optimal operating point for producing ethanol.

2. Materials and Methods

2.1 Feedstock, microorganism, and culture mediums

The oil palm trunk (OPT) was supplied by local farmers in the Plai Phraya District of Krabi. Commercial enzymes Cellic® Ctec2 were purchased from Novozymes. Enzyme activity was analyzed as 178.5 filter paper units (FPU) following the protocols of NERL. Standard sugars (glucose, xylose, arabinose, and cellobiose) for the calibration of high-performance liquid chromatography (HPLC) were purchased from Sigma-Aldrich, while standard ethanol was purchased from DaeJung Chemicals & Metals. The Liquor Distillery Organization provided the yeast, namely *S. cerevisiae* Sc90. Two-loops of cells from a YPD-agar plate were inoculated into the liquid YPD medium (glucose 20 g L^{-1}, yeast extract 10 g L^{-1}, and peptone 20 g L^{-1}) in a flask, during the preparation stage. The inoculated flasks were incubated at 30 ˚C on a rotary shaker (150 rpm) for 18 hours. The culture was then transferred to the fermentation medium.

2.2 Experimental description

Overall the ethanol production in the laboratory comprised three pretreatment methods of OPT and subsequent SSF (hydrolysis and fermentation). The OPT was sun-dried and chopped by a wood chipper into pieces measuring 20×20×5 mm^3. Prior to use, mashed OPT samples were dried in an oven at 105 °C for 24 hours. The samples were divided into two sections, the first of which was used to find the dry weight. Then 150 g of OPT was added to a 2.5 L SE reactor to study the effects of two variables: temperature (200–220 °C) and time (3–5 mins) at a pressure of 19 kg_f/cm^2. The valve was opened to achieve a rapid pressure drop. In the next method, hot water pretreatment was used to remove the hemicellulose in the solids using a liquid ratio of 1:8 and operating at 80 ºC for 30 mins. In the last method, the AHP pretreatment was used with fixed ratio between the pretreated OPT and H_2O_2 solution, namely 1:10 (g dry wt: mL). Three variables were studied: the concentration of H_2O_2 (1, 3, and 5 % w/w), temperature (50, 70, and 90 °C), and time (30, 60, and 90 mins). Following pretreatment, the composition of raw material and residual solids was measured.

Treated OPT solids were subjected to SSF in a 500 mL Erlenmeyer flask containing 300 mL, with 10% (w/v) of treated OPT and YP medium (10 g L^{-1} yeast extract and 20 g L^{-1} peptone). The medium was adjusted to pH 4.8 using a 50 mM sodium citrate buffer, followed by sterilization at 121 ˚C for 15 mins. A 10% starter culture was then simultaneously added to the Erlenmeyer flask with 10 FPU g^{-1} of the enzyme Cellic Ctec 2 . The SSF process was conducted at 40 ˚C for 72 hours at 150 rpm on a rotary shaker.

2.3 Process simulation

2.3.1 Physical property method

The entire ethanol production process was simulated using Aspen Plus V8.8. The physical property method consists of a set of equations to predict the properties of the chemical system during the process. The simulation used NRTL and Henry's law for the thermodynamic model since the ethanol-water system is not ideal, having azeotropic behavior. Sensitivity analysis was used to examine the effects of the main operational variables, including the reflux ratio (RR) and distillate to feed ratio (D/F) during the ethanol recovery process. The pretreatment, SSF, and downstream recovery operations were simulated.

2.3.2 Process description

The complete flowsheet for ethanol production from the OPT is shown in Figure 1. This flowsheet was used in simulations containing data obtained from laboratory experiments. An OPT processing batch of 60,000 kg was used in the simulations.

Firstly, OPT biomass (stream-OPT) with an initial composition of 38.67% cellulose, 11.60% hemicellulose, 30.22% lignin, and 1.62% ash was fed into a multiple roll crusher (CRUSHER) in which the particle size could be reduced to a range of 1–10 mm before pretreatment. The pretreatment unit consisted of three steps and was created in the ACM. The first step (SE-PRET) of pretreatment involved SE. Next, the SE-treated OPT solids (stream-REC-SE) passed through a hot water unit (HOT-PRET), where they made contact with the hot feed water in the stream-HOT-H2O. Finally, the hot-treated OPT solids were subjected to the AHP unit (AHP-PRET), making contact with the fed hydrogen peroxide solution in the stream-H2O2-SOL. Following completion of pretreatment, the treated OPT solids (stream-RECV-AHP) passed through the batch SSF unit (SSF) to convert cellulose into glucose and ferment the glucose into ethanol in a single step.

The waste products (hemicellulose, lignin, ash, and others) were vented out of the process (stream-SOLIDWAS). The main product (stream-IN-P05); the aqueous broth containing ethanol was sent to the first distillation column (BEER-CO) prior to further processing in the extractive distillation column (PRODU-CO). This extractive distillation column employed a solvent (stream-solvent) to split the ethanol-water azeotrope, namely ethylene glycol. Ethanol was recovered as the top product of the column (stream-EtOH), while water and solvent were recovered as the bottom product (stream-IN-P08). The final column (SEP-SOL) represents the solvent recovered for recycling.

3. Results and Discussion

3.1 Steam explosion pretreatment

The chemical compositions of SE treated and untreated OPT are shown in Table 1. According to the results, the untreated OPT consists of 38.67% cellulose, 11.60% hemicellulose, and 30.22% lignin, while the treated OPT using SE at 200–220 ºC for 3–5 mins had a significant increase in cellulose content. The optimal temperature and time were 210 °C and 4 mins. This condition provided the

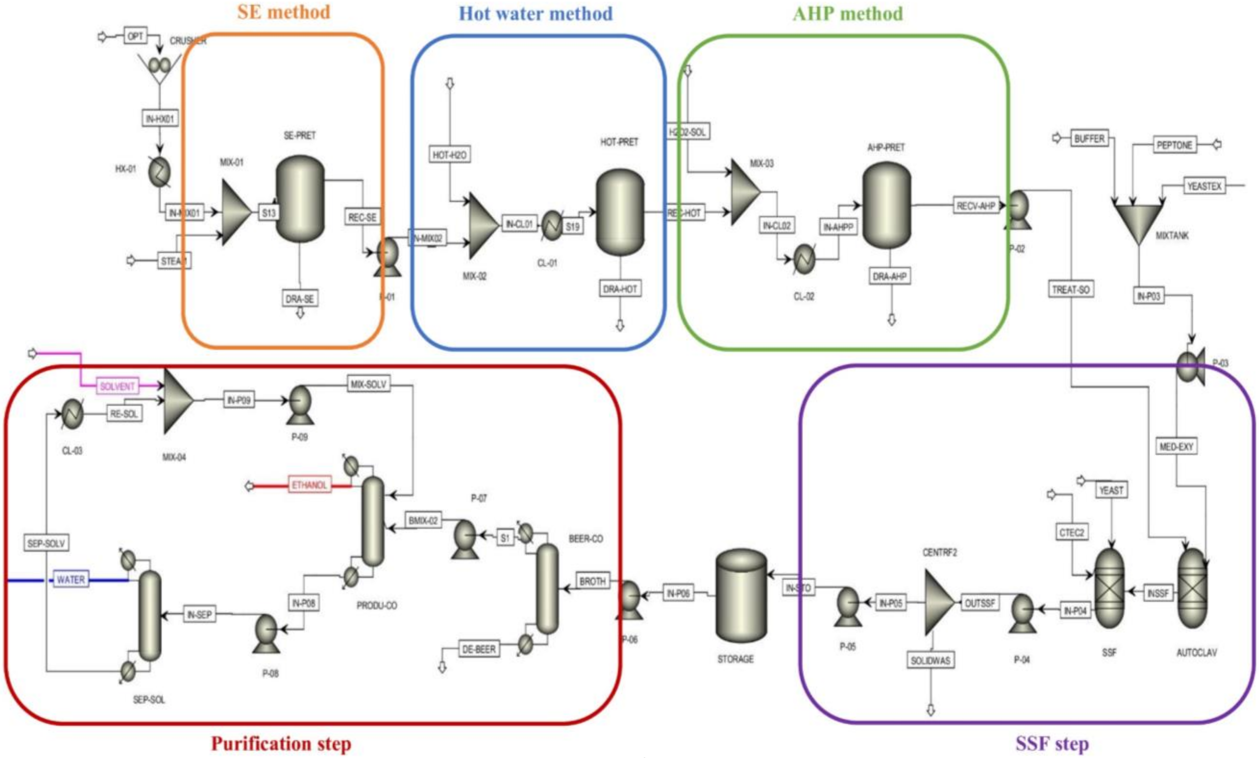

Figure 1. Ethanol process flowsheet in Aspen Plus

Table 1. Chemical compositions of solid untreated OPT and of OPT treated using steam explosion and hot water pretreatment

Temp (°C)	Time (min)	Composition (dry wt%)					Solid yield (%)
		Cellulose	Hemicellulose	Lignin	Ash	Other	
Untreated OPT		38.67	11.60	30.22	1.62	17.89	100.00
Steam explosion pretreatment at 200-220 °C for 3-5 min							
200	3	54.01	11.40	25.71	0.60	8.28	93.55
200	4	56.23	8.06	26.92	1.16	7.63	92.30
200	5	57.20	5.78	27.91	0.56	8.55	90.65
210	3	57.72	6.43	26.73	0.37	8.76	89.16
210	4	58.60	4.16	26.89	0.33	10.01	89.90
210	5	58.24	2.95	26.83	0.03	11.94	90.24
220	3	58.14	1.46	27.76	0.13	12.51	84.77
220	4	58.09	0.26	26.87	3.16	14.65	87.50
220	5	57.93	0.12	25.76	3.03	16.05	89.83
Hot water pretreatment at 70-90 °C for 15, 30 and 45 min							
70	15	58.72	9.33	20.68	0.89	10.37	N/A
70	30	58.94	11.06	18.64	0.33	11.02	N/A
70	45	59.14	9.44	20.38	0.93	10.11	N/A
80	15	59.39	8.81	20.54	1.13	10.13	N/A
80	30	61.76	8.12	18.32	1.33	10.47	68.34
80	45	59.83	9.33	18.31	0.97	11.56	N/A
90	15	58.94	10.82	18.27	1.36	10.61	N/A
90	30	59.39	12.02	16.14	2.33	10.12	N/A
90	45	61.08	12.16	11.37	2.20	13.19	N/A

* Not Available

most cellulose at 58.60% dry wt% (based on solid yield), while the hemicellulose content decreased from 11.60 to 4.16% dry wt with lignin decreasing from 30.22 to 26.89% dry wt, consistent with the results in an earlier report (Songprom, 2011). The SE pretreatment degrades hemi celluloses and lignin, thus making the cellulose more accessible to subsequent enzymatic attack and increasing the efficacy of enzymatic hydrolysis (Sun & Cheng, 2002).

Response surface analysis using the Minitab program was used to identify mathematical relationships between the composition and processing conditions (temperature T (°C) and time t (min), as shown in Table 2. These equations were used to calculate the outcomes (percentages of solid yield, cellulose, hemicellulose, lignin, and ash), modeled using the Aspen Custom Modeler (ACM) for the specific unit operation.

3.2 Hot water pretreatment

SE-treated OPT (210 °C and 4 mins) was used to study the effects of two variables (temperature and time). The chemical composition of hot water treated OPT samples is shown in Table 1. The results indicate that the optimal conditions, namely 80 °C and 30 min, provided the lowest hemicellulose of 8.12% dry wt. The aim of the method was to remove other components occurring during the SE process and reduce hemicellulose by decomposition in hot water. The advantage of this method is that it causes no loss of structure, meaning the amount of solids does not decrease. The solid yield was 68.34% when measured at 80 °C and 30 min.

The experimental results were examined using response surface analysis in the Minitab program to identify the mathematical relationships of composition to the processing temperature (T, °C) and time (t, min), as shown in Table 3. These equations were used to calculate the outcomes (solid yield, cellulose, hemicellulose, lignin, and ash) in the Aspen Custom Modeler (ACM).

Table 2. The model equations for OPT after SE pretreatment at $200 \leq T \leq 220$ (°C) and $3 \leq t \leq 5$(min)

Composition (%)	Model equation
Solid yield	$302.1 - 1.036\times T - 39.65\times t - 0.2\times t^2 + 0.199T\times t$
Cellulose	$-598 + 5.72\times T + 21.9\times t - 0.01253\times T^2 - 0.433\times t^2 - 0.085\times T\times t$
Hemicellulose	$191.4 - 0.818\times T - 28.44\times t + 0.53\times t^2 + 0.107\times T\times t$
Lignin	$-60.481 + 0.39944\times T + 22.9769\times t + 0.000043\times T^2 - 0.10965\times t^2 - 0.105\times T\times t$
Ash	$8.1 - 0.0363\times T - 0.9258\times t + 0.00425\times T\times t$
Other	$562 - 0.528\times T - 15.56\times t + 0.01253\times T^2 + 0.013\times t^2 + 0.079\times T\times t$

Table 3. The OPT model equations after hot water pretreatment at $70 \leq T \leq 90$ (°C) and $15 \leq t \leq 45$(min)

Composition (%)	Modeling equation
Cellulose	$-0.3 + 1.49\times T - 0.059\times t - 0.00958\times T^2 - 0.00228\times t^2 + 0.00287\times T\times t$
Hemicellulose	$136.06 - 3.26\times T - 0.031\times t + 0.02052\times T^2 - 0.00186\times t^2 + 0.00205\times T\times t$
Lignin	$2.07 + 0.1995\times T + 0.5927\times t + 0.00005\times T^2 - 0.00049\times t^2 - 0.007\times T\times t$
Ash	$11.83 - 0.3\times T - 0.08\times t + 0.002\times T^2 + 0.001\times T\times t$
Other	$31.1 - 0.399\times T - 0.462\times t + 0.00185\times T^2 + 0.00204\times t^2 + 0.00477\times T\times t$

3.3 Alkaline hydrogen peroxide (AHP) pretreatment

The AHP pretreatment was operatee at a fixed ratio between hot water treated OPT (80 °C and 30 mins) and the H_2O_2 solution, which was 1:10 (g dry wt: mL). The chemical composition of AHP-treated OPT samples is shown in Table 4 on studying the effects of three variables: the concentration of H_2O_2 (1, 3 and 5 % w/w), temperature (50, 70 and 90 °C), and time (30, 60, and 90 mins). In the laboratory, the antioxidant properties of lignin aliquots from OPT were studied after pretreatment; the solids must contain the least amount of lignin following pretreatment. The evidence reveals that the optimal condition was at 3 % w/w of H_2O_2, 70 °C and 30 mins, producing the lowest dry weight percentage of lignin. The AHP effectively removed the lignin at a moderate temperature, and it dissolved well in the alkaline solution (Banerjee *et al.*, 2012). However, the solid yield was stationary at 82.00% when measured at the optimal condition because this method causes no loss of structure.

The response surface models express the effects of the process variables (temperature T (°C), time t (min), and concentration of H_2O_2 (C_{H2O2}, %w/w)) on the outcomes as shown in Table 5. These equations were used to calculate the outcomes (cellulose, hemicellulose, lignin, ash, and others) in the Aspen Custom Modeler (ACM).

3.4 SSF section

From the experimental data on SSF, the incubation temperature was 40°C throughout and the enzyme (10 FPU Cellic Ctec2 g^{-1}-substrate) and yeast (10% w/v) were added together at the beginning of the process. The treated OPT at 10 %w/v (after all pretreatments) is the substrate of this section containing 73.96 % cellulose, 12.90% hemicellulose, and 11.68% lignin after the optimal AHP.

Table 4. The composition of hot water-treated OPT (at 80 °C and 30 mins) and treated OPT after AHP pretreatment

Temp (°C)	Time (min)	C_{H2O2} (%)	Composition (dry wt%)				
			Cellulose	Hemicellulose	Lignin	Ash	Other
Hot water-treated			61.76	8.12	18.32	1.33	10.47
50	30	1	66.56	11.05	18.02	0.89	3.48
50	30	3	67.61	11.02	17.96	0.81	2.60
50	30	5	69.77	9.93	17.11	0.77	2.42
50	60	1	67.86	5.80	19.22	1.12	6.00
50	60	3	64.92	10.73	17.51	1.11	5.73
50	60	5	63.39	9.57	15.71	1.11	10.22
50	90	1	62.54	3.64	19.11	1.08	13.63
50	90	3	64.38	9.17	18.91	1.11	6.43
50	90	5	67.23	9.88	18.31	0.91	3.67
70	30	1	69.83	12.85	16.11	0.96	0.25
70	30	3	73.96	12.90	11.68	0.95	0.51
70	30	5	73.66	12.45	12.11	0.94	0.84
70	60	1	69.91	12.24	17.75	0.90	0.20
70	60	3	66.24	11.62	17.21	0.91	4.02
70	60	5	70.74	7.27	17.12	0.90	3.97
70	90	1	65.60	10.05	16.87	1.07	6.41
70	90	3	68.18	9.91	16.66	1.05	4.20
70	90	5	68.74	4.80	16.32	1.02	9.12
90	30	1	64.37	10.83	19.21	1.02	4.57
90	30	3	69.59	4.21	19.65	1.01	5.54
90	30	5	70.13	8.65	19.54	0.94	0.74
90	60	1	63.33	9.90	19.63	1.09	6.05
90	60	3	70.22	7.57	19.00	1.08	2.13
90	60	5	70.41	5.70	18.87	1.08	3.94
90	90	1	64.48	10.01	18.44	1.10	5.97
90	90	3	67.14	7.73	18.09	1.04	6.00
90	90	5	70.17	8.61	17.89	1.01	2.32

Table 5. The model equations for pretreated OPT using AHP pretreatment at $1 \leq C_{H2O2} \leq 5$ (%w/w), $50 \leq T \leq 90$ (°C), and $30 \leq t \leq 90$(min)

Component (%)	Model equation
Cellulose	$45.9 + (0.851 \times T) - (0.199 \times t) - (0.96 \times C_{H2O2}) - (0.00689 \times T^2) + (0.000611 \times t^2) - (0.08 \times C_{H2O2}^2) + (0.00104 \times T \times t) + (0.0315 \times T \times C_{H2O2})$
Hemicellulose	$7.1 + (0.325 \times T) - (0.151 \times t) - (0.46 \times C_{H2O2}) - (0.00277 \times T^2) + (0.00081 \times t^2) + (0.191 \times C_{H2O2}^2) + (0.00069 \times T \times t) - (0.0119 \times T \times C_{H2O2})$
Lignin	$43.94 - (0.898 \times T) + (0.1607 \times t) - (1.46 \times C_{H2O2}) + (0.00683 \times T^2) - (0.000706 \times t^2) + (0.051 \times C_{H2O2}^2) - (0.001 \times T \times t) + (0.00883 \times T \times C_{H2O2})$
Ash	$1.402 - (0.0244 \times T) + (0.013 \times t) - (0.0153 \times C_{H2O2}) + (0.000192 \times T^2) - (0.0042 \times C_{H2O2}^2) + (0.000417 \times T \times C_{H2O2})$

From the results, the glucose concentration rose rapidly initially to peak at 6 h (Figure 2). This was because there was insufficient yeast to consume the glucose. As glucose became available, the yeast population grew, and the concentration of glucose rapidly declined to a low level. Subsequently, the glucose concentration remained low as a consequence of ongoing consumption by the yeast.

The maximum ethanol concentration (33.11 g L^{-1}) was observed at 60 h. At 72 h, the ethanol productivity was 0.44 g L^{-1}·h^{-1} while the ethanol yield was 0.442 g EtOH g^{-1} dry cellulose.

The SSF was simulated in Aspen Plus as an RYield (nonstoichiometric) reactor unit. This reactor used the ethanol yield at 60 hours to produce the maximum ethanol from pretreated OPT. The suitable condition for SSF was 40 °C with an ethanol yield of 0.469 g EtOH g^{-1} dry cellulose. Pretreated OPT (stream-RECV-AHP) of 30,227.27 kg was fed into the fermentation reactor. Enzymes, yeast, and medium in amounts 1,693.41, 34,459.15, and 9,068.2 kg, respectively, were fed into the fermentation reactor. The solid waste was then vented out of the system (steam-SOLIDWAS). Due to the constraints of Aspen Plus, steady-state simulation was used, although the actual fermentation was conducted as a batch operation. The fermentation broth was sent to a storage tank (STORAGE) before further processing in the downstream recovery section.

Around 60,000 kg of OPT produced 10,134.57 kg of ethanol per batch. The process simulation contained four fermenters, operated in parallel. The duration of fermentation was about three days. The fermentation broth was stored in a beer well before being sent to the purification section. The purification process required one day for each fermenter batch.

3.5 Purification section

The ethanol purification section in Figure 1 consisted of three distillation columns. The first column (BEER-CO) was an atmospheric distillation column that simply boiled the ethanol-water mixture, with the boiling point of water (100 °C) being higher than that of the ethanol (78.3 °C) (Limayem & Ricke, 2012). This column had 13 stages, feed input (Stream-Broth) at stage 2, pressure 1 bar, a feed molar ratio (D/F) of 0.1, and a reflux molar ratio (RR) of 1.5. Most of the ethanol is distilled at the top of the tower with a concentration of 79.59% wt and unfermented glucose and xylose are in the bottom product (Stream-DE-BEER).

The ethanol flow from BEER-CO was passed to the extractive distillation column (PRODU-CO), with ethylene glycol as the solvent. This column purified to more than 95% wt of ethanol at the top of the column (Stream-ETHANOL), while the bottom product was a mixture of water and solvent (Stream-IN-P08). This column had 15 stages, a distillate to feed mass ratio (D/F) of 0.65, and a reflux mass ratio (R/R) of 1.4. Sensitivity analysis was used to investigate the effects of the feed and solvent stage on ethanol purification.

The effects of feed stage for broth feeding (fixed stage of solvent as 7) shown in Figure 3 (A) gave the feed stage for broth feeding as 11. Regarding the effect of the solvent stage (fixed stage of feed from Figure 3 (A) as 11), the appropriate solvent stage is 3 to obtain ethanol purity exceeding 96.50 wt%, shown in Figure 3 (B). The makeup solvent flow was 1,440 kg (stream-SOLVENT), and the temperature was 25 °C.

The mixture stream (stream-IN-SEP) was fed into the last column (SEP-SOL) and the solvent needs to be recovered back into the system (Stream-SEP-SOLV). The recycled stream was mixed with makeup solvent and returned to the extractive column.

The configuration and operating conditions of each column in the purification section are shown in Table 6. These conditions will produce 60,000 kg of ethanol from OPT.

The results were in good agreement with previous reports on the use of distillation with mixed glycerol for separating ethanol and water. As in earlier work (Gil, Gracia, & Rodriguez, 2013), the distillation process was stimulated using a distillation column (RadFrac), consisting of two columns (extractive and solvent recovery).

3.6 Overall mass balance

Table 7 shows the overall mass balance from process simulation. The OPT material loss in the pretreatment step was inevitable, and 49.62% (29,772 from 60,000 kg) of OPT solids were removed from the raw OPT during the pretreatment steps (SE, hot water, and AHP). The cellulose loss was much lower, and its recovery was as high as 93.13% (21,608.88 from 23,202.00 kg). The mass recoveries of hemicelluloses and lignin were only 39.46 and 30.89%, respectively.

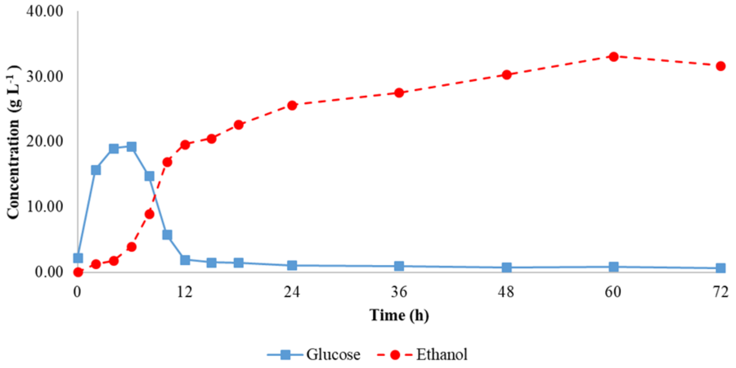

Figure 2. Concentration of glucose and ethanol from SSF at 40 °C. The substrate was pretreated OPT solids

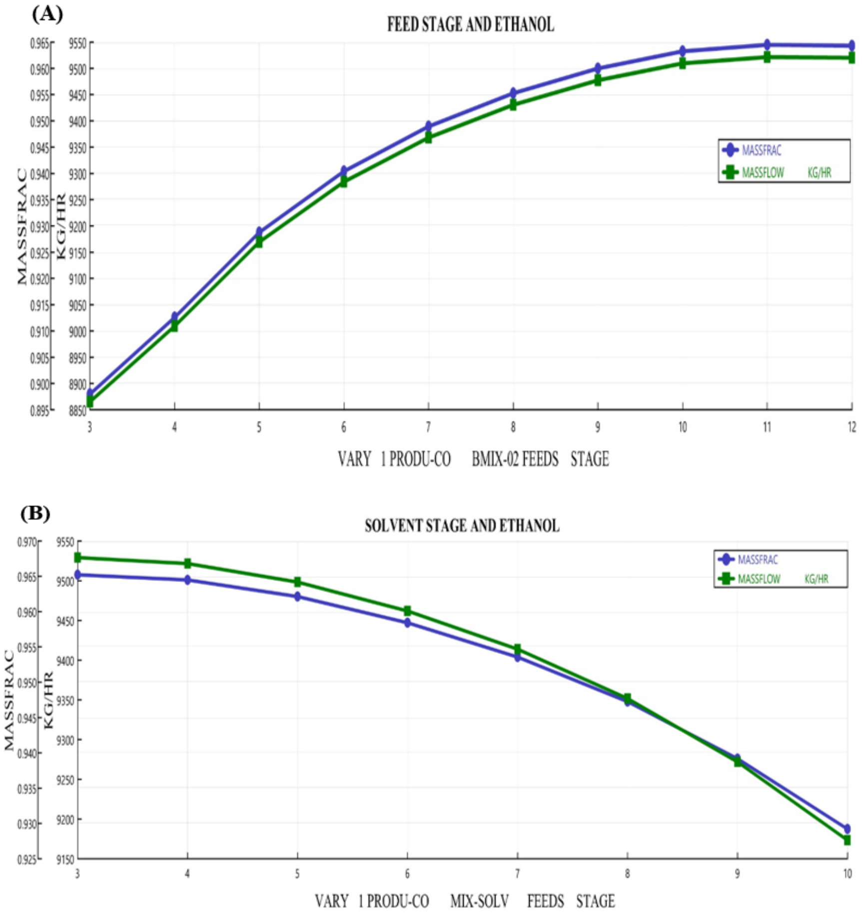

Figure 3. Sensitivity analysis (A) feed stage and (B) solvent stage, mass fraction, and mass flow of ethanol in the extractive distillation column

Table 6. Operating conditions and configuration of each column in the purification section

Unit	Equipment	Model in Aspen Plus	Operating condition and configuration	
BEER-CO	Distillation Column	RadFrac	Number of stages	13
			Condenser	Total
			Reflux ratio (mole)	1.5
			Distillate to feed ratio (D/F, mole)	0.1
			Feed stage	2
			Top/Bottom pressure (bar)	1
PRODU-CO	Distillation Column	RadFrac	Number of stages	15
			Condenser	Total
			Reflux ratio (mass)	1.4
			Distillate to feed ratio (D/F, mass)	0.65
			Feed stage (solvent)	3
			Feed stage (Mixed feed)	11
			Condenser pressure (bar)	1.4
			Stage 2 pressure (bar)	1.41
			Column pressure drop (bar)	0.2
SEP-SOL	Distillation Column	RadFrac	Number of stages	10
			Condenser	Total
			Reflux ratio (mole)	1.5
			Distillate to feed ratio (D/F, mass)	0.4
			Feed stage	4
			Condenser pressure (bar)	1.5
			Stage 2 pressure (bar)	1.51
			Column pressure drop (bar)	0.2

Table 7. Overall mass balance of ethanol simulation using Aspen Plus

Component	Stream									
	OPT	STEAM	HOT-H2O	H2O2-SOL	TREAT-SO	BUFFER, PEPTONE & YEASTEX	YEAST & CTEC2	BROTH	SOLVENT	ETHANOL
Mass Flow kg										
Ethanol	0	0	0	0	0	0	0	10,134.57	0	9531.04
Cellulose	23,202.00	0	0	0	21,608.88	0	0	0	0	0
Hemicellulose	9,012.00	0	0	0	3,556.25	0	0	0	0	0
Lignin	14,256.00	0	0	0	4,402.88	0	0	0	0	0
Water	0	6,676.00	431,520.00	368,625.96	0	0	0	304,702.89	0	341.02
Ash	972.00	0	0	0	310.94	0	0	0	0	0
Other	12,558.00	0	0	0	348.38	0	0	0	0	0
Cellic Ctec2	0	0	0	0	0	0	1,693.41	0	0	0
Ethylene glycol	0	0	0	0	0	0	0	0	1,440.00	0
Hydrogen peroxide	0	0	0	1,105.88	0	0	0	0	0	0
Buffer	0	0	0	0	0	302,273.39	0	0	0	0
Yeast extract	0	0	0	0	0	3,022.73	0	0	0	0
Peptone	0	0	0	0		6,045.47	0	0	0	0
S. cerevisiae Sc90	0	0	0	0	0	0	34,459.15	0	0	0

The SSF step produced 9,531.04 kg ethanol. The ethanol yield based on kg of cellulose was 0.469 g g^{-1}. The purification step produced more than 96.5% wt purity ethanol.

4. Conclusions

Ethanol is a potentially promising renewable energy source and can be used in transport fuel applications as well as for feedstock in the production of diverse chemicals. Starch and sugar based feedstocks for producing ethanol are limited and, therefore, lignocellulosic materials are of interest since they are available in abundance and are inexpensive alternatives.

This article presents the results of simulated ethanol production using the lignocellulosic biomass of the oil palm trunk. Experimental data from the laboratories of the Faculty of Agro-Industry, Kasetsart University, were used as the basis for simulating the OPT pretreatment steps. The mathematical models of pretreatment steps were formulated using the Aspen Custom Modeler (ACM). The optimal conditions of SE pretreatment were 210 °C and 4 mins, while the optimal hot water pretreatment required 30 min at 80 °C. The optimal AHP pretreatment used 3% w/w of H_2O_2 at 70 °C for a duration of 30 min. This custom model was used together with the built-in models in Aspen Plus. The non-random two liquid (NRTL) thermodynamic method was used. For the SSF step, the process was operated at 40 °C for 60 hours using the Cellic Ctec2 enzyme and *S. cerevisiae* Sc90 yeast. This step was modeled as a yield reactor with an ethanol yield of 0.469 g EtOH g^{-1} dry cellulose. The recovery process employed extractive distillation with ethylene glycol as the solvent. Based on the simulation results, 9,531.04 kg of ethanol could be produced from 60,000 kg of OPT with a product purity greater than 96.5% wt. in a process that took three days.

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