

PRODUCTION OF FUEL GRADE ETHANOL FROM CELLULOSE USING ASPEN PLUS- SIMULATION

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ABSTRACT: Energy demand is supposed to increase by about 50% after 10 years because of the increasing demand globally. Petroleum oil is the main energy resource, being depleted rapidly in Pakistan and worldwide. This situation will rouse to emphasize on the need for substitute and renewable resources satisfy the regularly developing need for vitality. Fuel ethanol is a liquid fuel that contains 99.99% ethanol. Making of ethanol from corn feedstock and sugar is often considered as contending with nourishment generation and consumption and increasing food and biofuel costs. That's why the production of ethanol from cellulose-based biomass is in much attraction because using inedible biomass as a feedstock for ethanol production limits rivalry with the sustenance business. Furthermore, cellulosic ethanol guarantees lesser carbon emissions than gasoline and bio-ethanol. The main objective of our project is to give a prototype production of cellulosic ethanol on Aspen plus using agricultural wastes as raw material (mainly, rice husk and corn stover) easily available in Pakistan at the cheapest price. The basic aim is to produce economical and eco-friendly ethanol. The simulation begins with pretreatment process of biomass followed by enzymatic hydrolysis of cellulose, Simultaneous Saccharification and Fermentation (SSF) process, conventional distillation and finally leading to molecular sieves technique to obtain 99.9% pure ethanol with lesser energy requirements as well as optimized temperature and pressure (TP) conditions. The project's outcomes indicate that cellulosic ethanol is indeed the most reliable source of energy leading us towards sustainable development.

Keywords: Aspen HYSYS; Bio-fuel; Ethanol; Cellulose; Economical.

1. INTRODUCTION

In 1819, Henri Braconnot, the French scientist, was the first to find that cellulose could be hydrolyzed into sugars by treatment with sulfuric acid. These days, ethanol can be produced either by conventional methods using corn or molasses or by using cellulosic material. The methods of pretreatment and fermentation may vary depending on the requirement of grade and purity of ethanol. The main problem is to give a prototype production of cellulosic ethanol as second generation fuel on Aspen plus using agricultural wastes as raw materials that are easily available in Pakistan at cheapest price and to produce economical and eco-friendly ethanol by reducing CO₂ and Greenhouse gas emissions and promoting SSF technique for fermentation process and replacing molecular sieve dehydration technique with azeotropic distillation process to achieve 99.99% pure ethanol [1, 2].

Cellulosic ethanol lies in second generation fuel type. Second generation bio-fuels are produced by changing unsuitable vegetation for human feasting into ethanol. First generation bio-fuels are produced by edible feedstock such as corn, sugarcane. We can use almost all non-edible plant parts to produce ethanol, which in result has a reduced impact on the food chain than the first generation biofuels. Though the rate conversion of crude materials to the definite item is much lower for cellulosic ethanol than for the original biofuels and with enhancements in the assembling innovation, the eventual fate of cellulosic ethanol will not be just as a fuel added substance, but rather it will be utilized as a petroleum substitution [3, 4].

Ethanol can't be gotten through simple refining from an ethanol-water blend given an azeotrope. Various strategies are accessible for this reason. The most widely used method is azeotropic distillation utilizing n-pentane or benzene as entrainer. This procedure is preferred over Separate Hydrolysis and Fermentation (SHF) process to achieve many advantages like it lessens the accumulation of the hindering sugars inside the reactor, increases the yield and the saccharification rates. Reduces the capital

cost, area required and, the retention time at the same time, lowering the labour cost [5].

Cellulosic feedstocks offer numerous benefits over starch and sugar-based feedstocks. They found copiously and can be utilized to create cellulosic biofuels required by the Renewable Fuel Standards (RFS). They are either squander items or deliberately developed vitality yields reaped from minimal grounds not reasonable for different harvests. Less non-renewable energy source vitality is required to develop, gather, and convert them to ethanol. Thus, this project encourages the use of cellulosic sources like switchgrass, woodchips and forest residues, which are the energy crops rather than sugar and starch-based feedstock and will eventually decrease food and biofuel prices. Cellulosic ethanol is not only greener than gasoline, but it is also greener than alternative biofuels. Greenhouse gas emissions from cellulosic ethanol are observed to be around 86 percent not as much as oil sources [6, 7].

Inhibition of cellulose movement by the discharged sugars, mostly cellobiose and glucose, is the primary disadvantage of the fermentation procedure. However, saccharification and fermentation (SSF) will reduce the amassing of the repressing sugars inside the reactor and increment the yield and the saccharification rates altogether. Furthermore, it will also reduce the capital cost, area required and, the retention time at the same time, lowering the labour cost.

Molecular sieves can likewise effectively process ethanol-containing contaminants, which would cause quick irritated in an azeotropic refining framework. Although ethanol, an appropriately designed sieve can dehydrate a wide range of different synthetic concoctions, in this way, giving included flexibility in future working alternatives.

The states of the technologies present for the fuel grade ethanol production were studied preceding to performing this investigation. A few sources were investigated that managed the production of cellulosic ethanol. Furthermore, these explored the sensitivities of parameters to the base required offering cost of ethanol to the fermentation, enzyme loadings and distillation techniques.

Energy utilization examination of coordinated flowsheets for production of fuel ethanol from lignocellulosic biomass-2006, investigate the production of fuel-grade ethanol from cellulosic sources was created [8, 9].

The production of ethanol is also research in 2018. The primary difference is the choice of feedstock; however, it also provided beneficial insight into the conversion of fructose to ethanol. In the presence of *Saccharomyces cerevisiae* (a species of yeast) fructose converts to ethanol along with glucose hence increasing the overall yield of the desired product [10].

2. METHODOLOGY

Cellulosic ethanol is created from lignocellulosic biomass in three main phases; pretreatment, hydrolysis and fermentation.

Pretreatment basically includes the utilization of physical procedures (size decrease, steaming or boiling, popping and ultrasonication), chemical procedures (acids, bases, solvents and salts), physicochemical procedures (fluid hot water and ammonium fibre blast or AFEX) and natural procedures (white- rot/brown microorganisms) and a few different blends may likewise use to fractionate the lignocellulose into its parts. Such combinations of pretreatment bring about the disturbance of the lignin seal to build chemical access to holocellulose, decrease of cellulose crystallinity and increment in the surface zone and porosity of pretreated substrates, bringing about expanded hydrolysis rate. The primary motivation behind the pretreatment procedure is to evacuate lignin and hemicellulose to diminish the crystallinity of cellulose and increment the porosity of the lignocellulosic materials however much as could be expected [11].

Enzymatic hydrolysis of cellulose and hemicellulose can be done by profoundly explicit cellulase and hemicellulase compounds, for example, glycosylhydrolases. This enzymatic gathering incorporates as a minimum of 15

protein families and some sub-families. Enzymatic hydrolysis of cellulose comprises of the cellulase adsorption onto the outside of the cellulose, the biodegradation of cellulose to fermentable sugars, and desorption of the cellulose [12, 13].

Ethanol fermentation is an organic procedure wherein particles, for example, glucose, fructose, and sucrose are changed over into cellular energy and in this manner, produce ethanol and carbon dioxide as metabolic waste items. In this procedure, pretreated lignocelluloses are hydrolyzed to glucose and therefore matured to ethanol. It is an anaerobic process because conversion is performed by yeast in the absence of oxygen. Bioconversion or biocatalysis is the utilization of organisms or compounds to change one material into another. The procedure is settled for certain sugars, for example, glucose from cornstarch, presently a developing industry. Figure 1 demonstrates the procedure stream for SHF.

The major advantage of this separate enzymatic hydrolysis and fermentation strategy is that it is conceivable to complete the cellulose hydrolysis and fermentation at their ideal conditions. The ideal temperature for cellulase is more often than not somewhere in the range of 45 and 50°C, contingent upon the cellulose-delivering microorganism. Thus, the ideal temperature for a large portion of the ethanol-creating microorganisms is somewhere in the range of 30 and 37°C [13].

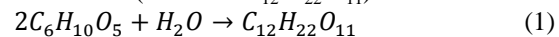
2.1. Process Selection

The simulation begins with the pretreatment process of biomass followed by enzymatic hydrolysis of cellulose and finally leading to simultaneous saccharification and fermentation (SSF) process using yeast to obtain ethanol. The results show the production of 99.98% pure ethanol with least CO₂ emissions, overall attractive yield with lesser energy requirements as well as optimized Temperature and Pressure (TP) conditions [14-16].

hydrolyzation. The feed of our process is Cellulose, hence only the steps that result in the conversion of Cellulose to ethanol as a product will be discussed. The process is divided into enzymatic hydrolysis, simultaneous saccharification and fermentation (SSF), separation of carbon dioxide, fractional distillation and molecular sieves dehydration.

2.2.1. Enzymatic Hydrolysis

There are two kinds of hydrogen bonds in cellulose particles: those that structure between the C₃OH gathering and the oxygen in the pyranose ring inside a similar molecule and those that structure between the C₆OH group of one molecule and the oxygen of the glucosidic obligation of another molecule. Presence of these hydrogen bonds gives cellulose a very firmly packed crystallite structure. Cellulase (an enzyme used for this step) has a structure that attacks the terminal bonds and is effective in degrading it. Hence, Cellulose is broken down to Cellobiose (Sucrose- C₁₂ H₂₂ O₁₁).



In our process, a slurry containing 200 tons/day of cellulose and 20 tons/day of water is pumped to the reactor (R-101), operating at 25°C and 1atm. The temperature is maintained in the reactor to avoid the degradation of product/enzyme. The quantity of enzyme Cellulase used is 0.06 wt.% of the feed to the reactor. A product with 80% of the cellulose content broken down to Sucrose is obtained. This then becomes the feed to the next reactor.

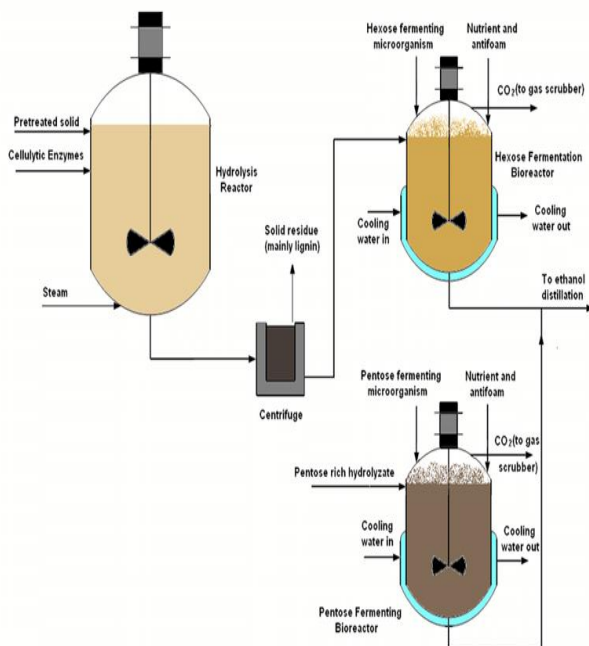


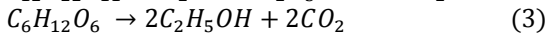
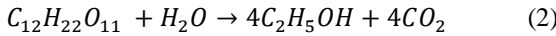
Fig. 1. Process flow of Separate Hydrolysis and Fermentation (SHF)

2.2. Process Description

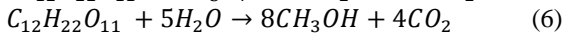
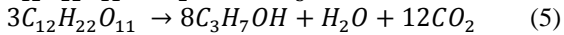
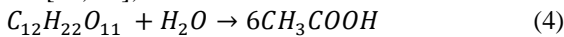
A substantial amount of energy present in the 'Energy Crops' can be converted to Ethanol because of the amount of cellulose present in it. To generate fermentable sugars from cellulose, it must first go through the process of

2.2.2. Simultaneous Saccharification and Fermentation (SSF)

The utilization of Simultaneous Saccharification and Fermentation (SSF), for the change of sucrose to ethanol, brings about a very economical process. In this procedure, the stages are almost the same in the different hydrolysis and fermentation framework, except that both are performed in the equivalent bioreactor. Therefore, the presence of yeast together with the cellulolytic protein complex decreases the collection of the hindering sugars inside the reactor, thus expanding the yield and the saccharification rates. Another benefit of this methodology is that a solitary bioreactor is utilized for the whole procedure, like this lessening the speculation costs. Because of the generally similar procedure conditions in the arrangement of dextrose, and ethanol fermentation, the alternative of doing these two-steps together in one vessel exists. This not only reduces the cost of installing another reactor but also reduces the processing time of fermentation. The main reaction that takes place in our SSF reactor (R-102) is [17]:



The reaction that shows the conversion of Sucrose to Ethanol and CO₂ has a conversion extent of sucrose is 25% in the presence of a single enzyme *Saccharomyces cerevisiae* or simply ‘yeast’. Because the high concentration of ethanol is toxic to the enzyme, it is kept between the ranges of 8 wt.% to 12 wt.% and the conversion of glucose to ethanol is also very low, that is, 40 wt.%. The quantity of enzyme used is 0.06 wt.% of the feed to the reactor. The operating conditions of the reactor are 30°C and 1 atm. However, many side reactions also take place with very little sucrose conversion percentage, which are [18, 19];



The side reactions take place with very little sucrose conversion percentages that are; 5%, 0.1%, 0.01% and 5%, respectively.

2.2.3. Separation of CO₂

This step is necessary to remove the gases particularly CO₂ from the Ethanol Broth that will move to the distillation columns for percentage increase in the purity. The product obtained from the reactor (R-102) contains 10.6wt% of Carbon dioxide and 10.2wt% of ethanol. A flash separator is used, operating at 30°C and 1 atm to remove 95.4wt% of Carbon dioxide from the Ethanol Broth. This overhead of the separator is sent to a fractionation column where CO₂ washing is done to obtain 99.9 wt.% of pure CO₂.

2.2.4. Fractional Distillation

Two fractional distillation columns are installed to increase the purity of ethanol to nearly 95mol%. In the first column (C-102), the reflux ratio is set to 4 and steam at 5atm and 320°C is fed to the column, the Ethanol Broth (10.2 wt% ethanol) entering the column is nearly at 60°C. In the first column, the task is to achieve 92 wt.% concentration of ethanol, resulting in a distillate flowrate of 24.230 tons/day. In the second column (C-101), also called the rectification column (because of the formation of rectified spirit in the distillate), the distillate has a concentration of 95 wt.% of ethanol. Further purity of ethanol cannot be achieved through fractional distillation because of the formation of the azeotrope.

2.2.5. Molecular Sieves Dehydration

For the refining of ethanol for accomplishing fuel grade, the most widely recognized methods for breaking the azeotrope is to utilize the molecular sieves dehydration innovation. An ethanol-water framework is containing 95 wt. % of ethanol is kept running over a molecular sieve which adsorbs water from the blend. The concentration rises above 96% and can be additionally refined. The sieve is warmed to evacuate the water and is reused. The Molecular Sieve beds are made of zeolite with a successful pore size opening of about 3Å. The water molecules are absorbed by the sieve beds, resulting in a pure stream of Ethanol with a concentration of 99.9wt%. Figure 2 shows the schematic view of the overall process for the production of ethanol.

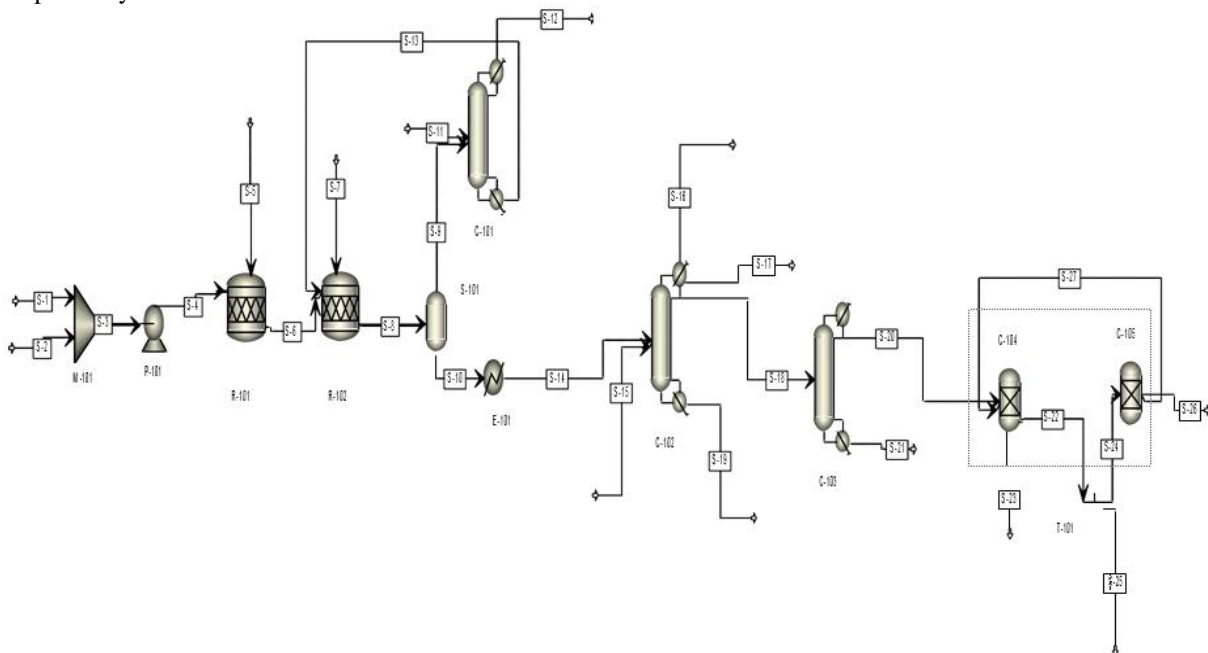


Fig. 2. Process flow of production of ethanol3.

3. RESULT & DISSCUSION

The simulation covers the pretreatment process of biomass followed by enzymatic hydrolysis of cellulose, SSF process, conventional distillation and finally leading to molecular sieves technique to obtain 99.9% pure ethanol with lesser energy requirements as well as optimized Temperature and Pressure (TP) conditions. Table 1 presented the constituents used in the simulation.

Table 1. Components used in simulation

Component abbreviation	Type	Component name	Formula	
Water	Conventional	Water	H ₂ O	
Carbo-01		Carbon-Dioxide	CO ₂	
Ethan-01		Ethanol	C ₂ H ₆ O ₂	
Metha-01		Methanol	CH ₄ O	
Aceti-01		Acetic-Acid	C ₂ H ₄ O ₂₋₁	
Cellulose		Cellulose	C ₆ H ₁₀ O ₅	
1-Pro-01		1-Propanol	C ₃ H ₈ O ₁	
Dexter-01		Dextrose	C ₆ H ₁₂ O ₆	
Sucro-01		Sucrose	C ₁₂ H ₂₂ O ₁₁	
Cellular		Nonconventional		
Yeast				

A property set is a collection of thermodynamic, transport, and other properties that can use in physical property tables and analysis. Aspen Plus and Aspen properties have several built-in property sets that are sufficient for many applications. To select the property package; check the polarity of the components [20]. If polar, the check if it's electrolyte or not. Then select standard electrolyte system otherwise check if system is ideal or not. If system is real chosen standard methods such as Peng Robinson. If system is pseudocereal, the pressure of system shall be checked and properties then will be selected accordingly. For a non-electrolyte system, if pressure is less than 10bar availability of interaction parameters and phases involved in the system. Thus, in this research, the Base Method NRTL, and referenced methods: Peng Robinson and UNIFAC are used [20, 21].

3.1. Material Balance

Chemical composition of lignocellulosic feedstocks is a key factor influencing the effectiveness of biofuel generation during transformation forms. The chemical composition of lignocellulosic feedstocks is profoundly factor on account of hereditary and natural impacts and their interactions. The chemical composition of corn stover, switchgrass and wheat straw is similar when reaped to maximize the lignocellulosic component [22]. The raw materials that will be utilized to create cellulosic ethanol are rice husk and wheat straw as shown in Figure 3. Table 2 shows the total availability of cellulose from raw materials.

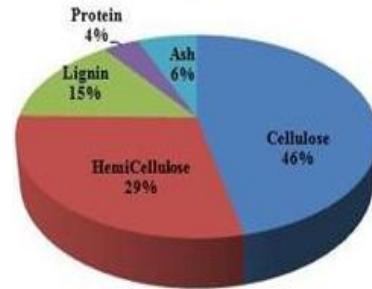
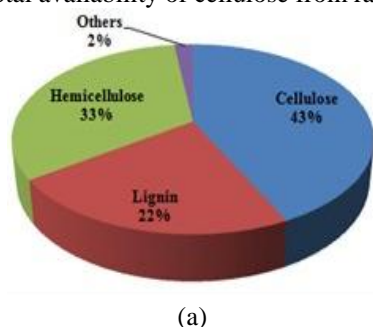


Fig. 3. Chemical composition of (a) Rice husk (b) Wheat straw

Table 2: Total availability of cellulose from raw materials

Raw Materials	Biomass tons/day	Cellulose %	Cellulose tons/day
Rice husk	200	0.427	85.4
Wheat straw	250	0.46	115
Total availability	450	0.887	200

Balance on Mixer Tank (M-101)

Stoichiometric calculations of Figure 4 Mixer M-101 and the balance is given in Table 3.

S-1=Cellulose fed to the Mixer = 200tons/day; S-2=Water fed to the Mixer = 30 tons/day; S-3=Cellulose slurry. Applying Balance on both sides to get;

Mass in + Generation - Consumption=Mass out + Accumulation

S-1 + S-2 = S-3

200 + 30 = 230 tons/day

S-3 = 230 tons/day

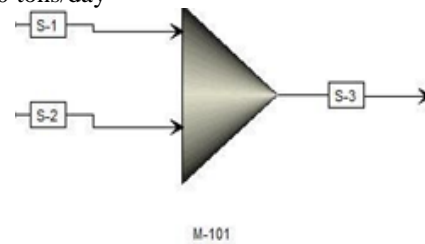


Fig. 4. Simulation results on Mixer M-101

Table 3. The balance on Mixer M-101

Total	S-1	S-2	S-3
Temperature °C	25	25	25
Pressure atm	1	1	1
Vapor fraction	0	0	0
Mole flow kmol/day	1118.998	1012.164	2131.161
Mass flow tons/day	200	20.1	220.1

Balance on Reactor (R-101)

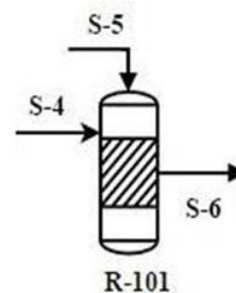


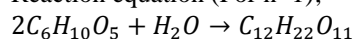
Fig. 5. From cellulose to sucrose

From Figure 5 cellulose to sucrose stoichiometric calculations and the balance on reactor is given in Table 4.

S-4 = Feed to Reactor containing slurry of water and cellulose = 211 tons/day; S-5 = Cellulase;

S-6 = Product from R-101 containing Sucrose and unreacted cellulose and water along with cellulose as shown in Figure 6.

Reaction equation (For n=1);



Applying Balance on both sides;
 Mass in + Generation - Consumption=Mass out + Accumulation
 $S-4 + S-5 = S-6$
 Since; $S-5 = 0.06\%$
 $S-4 = 0.06 \times 211 = 0.127$ tons/day
 Conversion of cellulose=80%
 Mol. wt. of Cellulose =324 kg/kgmol; Mol. wt. of Sucrose =342 kg/kgmol; Molecular weight of water =18 kg/kgmol
 Balance equation gives result: $230 + 0.127 = 230.127$ tons/day.
 $S-6 = 230.127$ tons/day
 where; Sucrose = 169 tons/day; Unreacted Cellulose = 40 tons/day; Water = 40 tons/day and Cellulase = 0.127 tons/day.

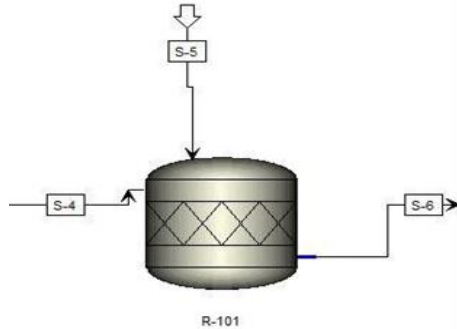


Fig. 6. Simulation results on Reactor R-101
Table 4. Balance on Reactor R-101

Total	S-4	S-5	S-6
Temperature °C	25	25	25
Pressure atm	1	1.2	1
Vapor fraction	0	0	0
Mole flow kmol/day	2131.161		1235.963
Mass flow tons/day	220.1	0.127	220.1

Balance on Reactor (R-102)

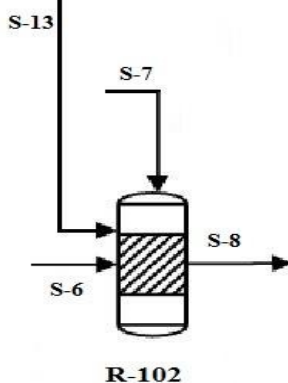


Fig. 7. From sucrose to ethanol

S-6 = Reactor R-101 outlet; S-7 = Enzyme (Baker's yeast) inlet S-8 = Reactor outlet; S-13 = Recycle stream from distillation column C-101

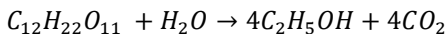


Figure 7 shows the stoichiometric relations and the balance on reactor R-102 is given in Table 5.

For S-7, the required a supply of enzyme (yeast); the quantity to be used is 0.06 wt. % of the feed; required supply of enzyme = 0.128 tons/day

Stream S-5 (Outlet of Reactor R-101) tons/day

The mass flowrate of sucrose	168.9
The mass flowrate of water	11.1
Unreacted cellulose	40
Total stream inlet	220.00

Stream S-13(Bottom product of CO₂ Tower)

Mass Flowrate of Water	7.200
Mass Flowrate of CO ₂	2.783

Mass Flowrate of Ethanol	0.857
Mass Flowrate of Methanol	0.001
Mass Flowrate of Acetic Acid	0.056
Mass Flowrate of Cellulose	0.001
Mass Flowrate of Propanol	0.001
Mass Flowrate of Glucose	0
Mass Flowrate of Sucrose	0
Total Stream Inlet	10.899
Total Reactor Inlet	230.899

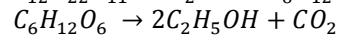
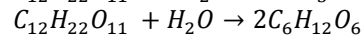
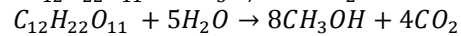
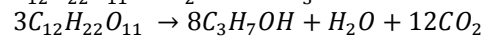
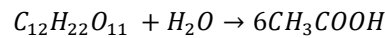
Applying Balance on both sides to get;

Mass in + Generation - Consumption=Mass out + Accumulation

$$S-6 + S-7 + S-13 = S-8$$

Conversion of sucrose=25%; Mol. wt. of Sucrose=342 kg/kgmol, Molecular weight of Ethanol=46 kg/kgmol; Molecular weight of CO₂=44 kg/kgmol
 Required supply of water=3 tons/day; Production of Ethanol=22.7 tons/day; Production of CO₂=21.73 tons/day

Side Reactions:



Parameter

Parameter	tons/day
Quantity of acetic acid produced	8.88
Quantity of methnaol produced	0.012
Quantity of propanol produced	0.079
Quantity of glucose produced	8.889
Quantity of CO ₂	4.43
Quantity of water produced	0.02969
Quantity of ethanol produced	1.82

Reactor Outlet

Ethanol produced	23.57
CO ₂ produced	24.51
Unreacted sucrose	109.6
Unreacted cellulose	40
Acetic acid produced	8.936
Methanol produced	0.013
Propanol produced	0.080
Glucose produced	8.89
Water produced	15.31

Total Reactor Outlet

230.91

Figure 8 shows the simulation results on Reactor R-102.

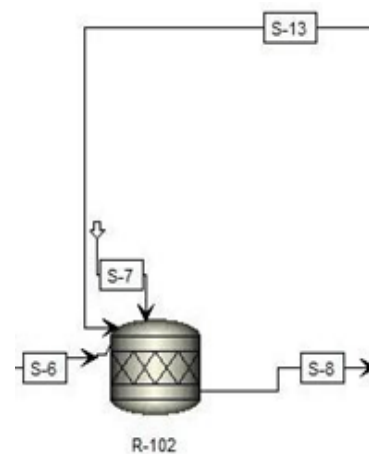


Fig. 8. Simulation results on Reactor R-102

Table 5. The balance on Reactor R-102

Total	S-6	S-7	S-13	S-8
Temperature °C	25		-45.8926	30
Pressure atm	1	1.2	1	1
Vapour fraction	0		5.47E-07	0.207512
Mole flow kmol/day	1235.96	0	437.6762	2437.512
Mass flow tons/day	220.1	0	10.89736	230.9974

Balance on Separator (S-101)

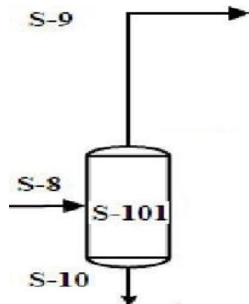


Fig. 9. Balance on Separator (S-101)

Figure 9 represent the balance on separator (S-101) from stoichiometric relations:

S-8 = Separator inlet stream; S-9 = Overheads containing Lighter components; S-10 = Bottom product containing heavier components

Inlet Stream (S-8)	tons/day
Mass flowrate of water	15.2989
Mass flowrate of carbon dioxide	24.5923
Mass flowrate of ethanol	23.587
Mass flowrate of methanol	0.01335
Mass flowrate of acetic acid	8.94459
Mass flowrate of cellulose	40.0006
Mass flowrate of propanol	0.07997
Mass flowrate of glucose	8.88886
Mass flowrate of sucrose	109.592
Total stream inlet = S-8	230.997
Overheads (Stream S-9)	
Mass flowrate of water	0.200
Mass flowrate of carbon dioxide	23.188
Mass flowrate of ethanol	0.857
Mass flowrate of methanol	0.001
Mass flowrate of acetic acid	0.056
Mass flowrate of cellulose	0.001
Mass flowrate of propanol	0.001
Mass flowrate of glucose	0.000
Mass flowrate of sucrose	0.000
Mass flowrate of overheads	24.30
Bottoms (Stream S-10)	
Mass flowrate of water	15.0989
Mass flowrate of carbon dioxide	1.40387
Mass flowrate of ethanol	22.7302
Mass flowrate of methanol	0.01265
Mass flowrate of acetic acid	8.88886
Mass flowrate of cellulose	40
Mass flowrate of propanol	0.07907
Mass flowrate of glucose	8.88886
Mass flowrate of sucrose	109.592

Mass flowrate of bottoms 206.694

Figure 10 presents the simulation results on Separator (S-101) and the balance on Separator S-101 is shown in Table 6.

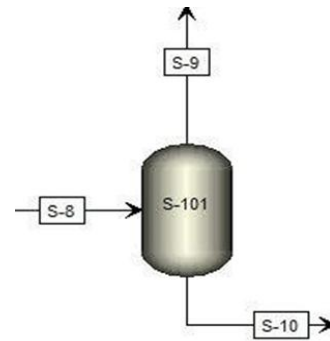


Fig. 10. Simulation results on Separator (S-101)

Table 6. The balance on Separator S-101

Total	S-8	S-9	S-10
Temperature °C	30	30	30
Pressure atm	1	1	1
Vapor fraction	0.207512	1	0.00E+00
Mole flow kmol/day	2437.512	505.812	1931.7
Mass flow tons/day	230.9974	24.30317	206.6942

Balance on Column (C-101)

Figure 11 portrays the balance on Column (C-101) from stoichiometric relations.

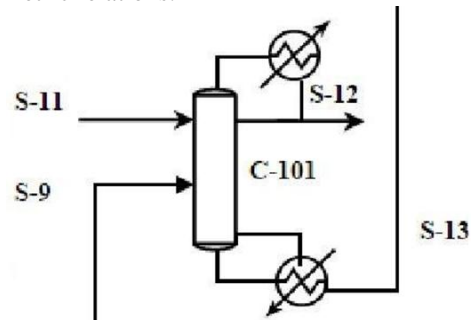


Fig. 11. Balance on Column (C-101)

S-9 = Bottoms from separator; S-10 = Steam inlet; S-12 = Distillate Product; S-13 = Bottom product

Balance on Condensor

Vapor Outlet	tons/day	(wt. %)
Mass flowrate of ethanol	0.917	3.42
Mass flowrate of CO ₂	25.867	96.56
Mass flowrate of unreacted sucrose	0	0
Mass flowrate of acetic acid	traces	traces
Mass flowrate of water	0.005	0.02
Flowrate of unreacted cellulose	0	0
Mass Flowrate of Vapors	26.79	
Water outlet		
Mass flowrate of ethanol	0	
Mass flowrate of unreacted sucrose	0	
Mass flowrate of acetic acid	0	
Mass flowrate of water	24.217	
Distillate		
Mass flowrate of ethanol	67.992	95.45
Mass flowrate of CO ₂	2.837	3.98
Mass flowrate of unreacted sucrose	0	0

Mass flowrate of acetic acid	0.008	0.01
Mass flowrate of water	0.397	0.56
Mass flowrate of unreacted cellulose	0	0
Mass flowrate of distillate	71.234	

Balance on Reboiler

Bottoms

Mass flowrate of ethanol	0	0
Mass flowrate of CO ₂	0	0
Mass flowrate of unreacted sucrose	32	33
Mass flowrate of acetic acid	5.192	5
Mass flowrate of water	26.102	27
Mass flowrate of unreacted cellulose	34	35
Mass flowrate of bottoms	97.294	

Figure 12 presents the simulation results on Column C-101 and the balance on Column C-101 is shown in Table 7.

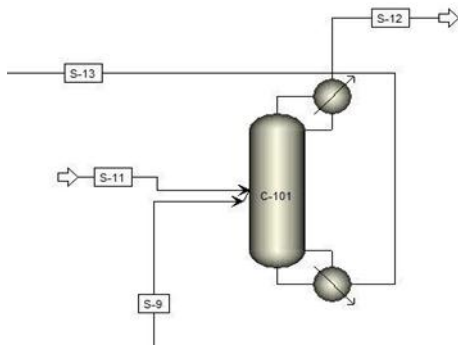


Fig. 12. Simulation results on Column C-101

Table 7. The balance on Column C-101

Total	S-9	S-11	S-12	S-13
Temperature °C	30	25	-82.8444	-45.8926
Pressure atm	1	1	1	1
Vapor fraction	1	0	1.00E+00	5.47E-07
Mole flow kmol/day	505.81	352.49	420.6302	437.6762
Mass flow tons/day	24.303	7	20.40582	10.89736

The balance on Column (C-102)

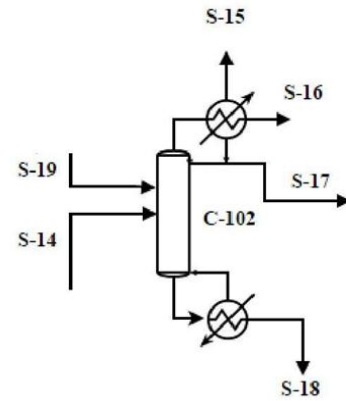


Fig. 13. Balance on Column (C-102)

Figure 13 shows the balance on Column (C-102) from stoichiometric relations:

Column inlets: Feed (Stream S-19) = 206.694 tons/day; Mass Fraction of Ethanol=0.11

Column specifications: Total number of stages=35; Stream (S-19) inlet at 17 and Stream (S-14) inlet at 35

Distillation Column Calculations

Assuming a reflux ratio of $R_d=4$, $R_d=L/D$ and $L=4D$

The distillate required must contain 92.5 wt.% (91.6mol%) of ethanol. The condenser used for C-102 is a partial vapour-liquid condenser, with two liquid outlets, one vapour outlet and 1 reflux.

From simulation results;

Stream (S-15): $V=1.427$ tons/day

Stream (S-16): $W=38.486$ tons/day

Stream (S-17): $D=24.32$ tons/day

Stream (S-18): $B=168.917$ tons/day

The amount of distillate sent back to the column is $L=97.28$ tons/day

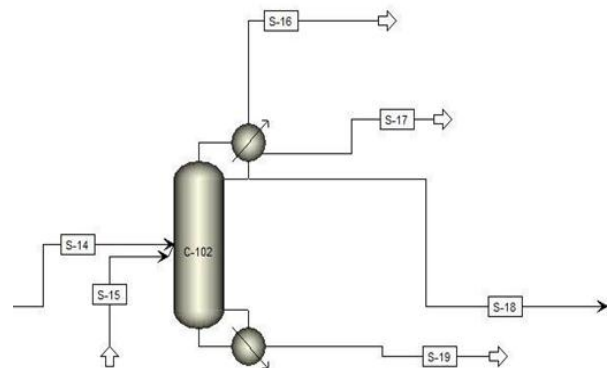


Fig. 14. Simulation results on Column (C-102)

Figure 14 presents the simulation results on Column C-102 and the balance on Column C-102 is shown in Table 8.

Table 8. Balance on Column C-102

Total	S-15	S-14	S-16	S-17	S-18	S-19
Temperature °C	320	60	40	40	40	159.31
Pressure atm	5	1.5	1	1	1	1.5
Vapor fraction	1	0.0050	1.00E+00	0.00E+00	0	0
Mole flow kmol/day	1332.2	1931.7	29.276	1938.01	483.20	813.40
Mass flow tons/day	26.455	206.69	1.4269	38.485	24.319	168.91

Balance on Column (C-103)

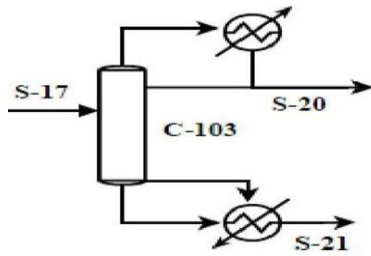


Fig. 15. Balance on Column (C-103)

Figure 15 shows the balance on Column (C-102) from stoichiometric relations.

Column inlets; Feed (Stream S-17) = 24.32 tons/day
Mass fraction of ethanol=0.925

Column specifications; Total number of stages=30
Stream (S-19) inlet at 15

Assuming a reflux ratio of $R_d=4$; $R_d=L/D$ and $L=4D$. The distillate required must contain 95wt% (93.5 mol%) of Ethanol

From simulation results; Stream S-20: $D=23.68$ tons/day and Stream S-21: $B=0.64$ tons/day. Figure 16 shows the simulation results on Column C-103 and the balance on Column C-103 is shown in Table 9.

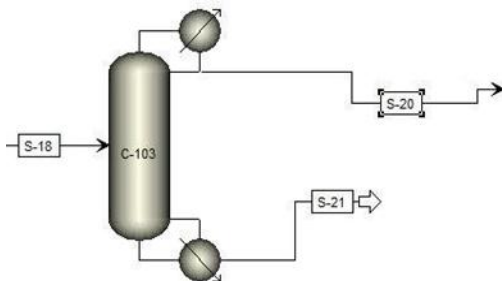


Fig. 16. Simulation results on Column C-103

Table 9. Balance on Column C-103

Total	S-18	S-20	S-21
Temperature °C	40	54.9687	131.73425
Pressure atm	1	1.5	1.5
Vapor fraction	0	0	0.00E+00
Mole flow kmol/day	483.208	473.543	9.66415235
Mass flow tons/day	24.3194	23.6797	0.63973411

The balance on Column (C-104)

Figure 17 displays the balance on Column (C-104) and the stoichiometric calculations from Column C-104 is shown in Table 10.

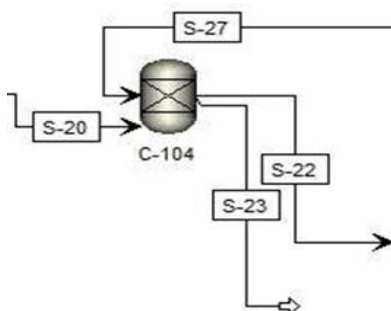


Fig. 17. Balance on Column (C-104)

Table 10. The balance on Column C-104

Total	S-20	S-27	S-22	S-23
Temperature °C	54.9687	54.9641	54.9641	54.964
Pressure atm	1.5	1.5	1.5	1.5
Vapor fraction	0	0	0.00E+00	0.1534
Mole flow kmol/day	473.543	78.7667	520.576	31.733
Mass flow tons/day	23.6797	3.99993	26.4351	1.2444

Balance on Column (C-105)

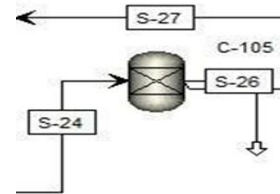


Fig. 18. Balance on Column (C-105)

Figure 18 presents the balance on Column (C-105) and the stoichiometric calculations from Column C-105 is shown in Table 11.

Table 11. Balance on Column C-105

Total	S-24	S-26	S-27
Temperature °C	54.9641	54.9641	54.9641078
Pressure atm	1.5	1.5	1.5
Vapor fraction	0	0	0.00E+00
Mole flow kmol/day	98.463	19.6963	78.7667172
Mass flow tons/day	5	1.00007	3.99992722

3.2. Energy Balance

Energy balance equation is given by:

$$Q - W_s = \Delta H + \Delta E_k + \Delta E_p \tag{7}$$

where; Q =Amount of heat added or removed, W_s =Work done, ΔE_k = Change in Kinetic Energy, ΔE_p = Change in Potential Energy and ΔH = Change in Enthalpy
Neglecting W_s , ΔE_k and ΔE_p

$$Q = m\Delta H \tag{8}$$

Balance on Reactor R-101 (From Cellulose to Sucrose)

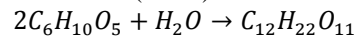
Mass flowrate of cellulose=200 ton/day; Mass flowrate of water=20 ton/day; Feed flowrate to the reactor=220 ton/day; Feed flowrate to the reactor=2.5463 kg/s

Inlet Temperature (T_o) =25°C /298.15K

Outlet Temperature (T) =25°C /298.15K

Reference Temperature (TR) =25°C /298.15K

Difference ($T-TR$) =0°C /0K



Conversion of Cellulose (X) 80%.

Specific heat of cellulose=1.4 kJ/kg.K; Specific heat of water=4.184 kJ/kg.K; Specific heat of sucrose=1.257 kJ/kg.K

Enthalpies at Reference Temperature

H (Cellulose) =44.85 kJ/kg; H (Water) =15833.3 kJ/kg; H (Sucrose) =5090.94 kJ/kg

Enthalpy of Reaction at the temperature 'T' is given as:

$$\Delta H_{rx}(T) = \Delta H_{rx}(TR) + \Delta C_p(T-TR) \tag{9}$$

Now,

$$\Delta H_{rx}(TR) = H_r(\text{Sucrose}) - 2[H_r(\text{Cellulose})] - H_r(\text{Water})$$

$$\Delta H_{rx}(TR) = -10832 \text{ kJ/kg}$$

$$\Delta C_p = C_p(\text{Sucrose}) - 2C_p(\text{Cellulose}) - C_p(\text{Water})$$

$$\Delta C_p = -5.727 \text{ kJ/kg.K}$$

Hence;

$$\Delta H_{rx}(T) = -10832 \text{ kJ/kg}$$

$$Q = 2206.52 \text{ kW} = 2.20652 \text{ MW}$$

Hence the calculated results from simulation are as given in Table 12.

Table 12. Enthalpies on Reactor R-101 (From Cellulose to Sucrose)

Total	Units MW
Enthalpy In	-17.555842
Enthalpy Out	-15.151501
Relative Difference	-0.13695
Net Heat Duty	2.40434031

The simulation result of stream R-101 is shown in Table 13.

Balance on Reactor R-102 (From Sucrose to Ethanol)

Mass flowrate of sucrose=169 ton/day; Mass flowrate of cellulose=40 ton/day; Mass flowrate of water=11.1 ton/day;

Feed flowrate to the reactor=220.1 ton/day; Feed flowrate to the reactor=2.54745 kg/s
 Inlet Temperature (To) =25°C/298.15K
 Outlet Temperature (T) =30°C/ 303.15K
 Reference Temperature (TR) =25°C /298.15K
 Difference (T-TR) =5°C /5K

Enthalpies at Reference Temperature

H (Ethanol) =6030 kJ/kg

H (Water) =15833.3 kJ/kg

H (Sucrose) =5090.94 kJ/kg

H (CO₂) =8943.18 kJ/kg

Enthalpy of Reaction at the temperature 'T' is given as:

$$\Delta H_{rx}(T) = \Delta H_x(TR) + \Delta C_p (T-TR)$$

Now, $\Delta H_{rx}(TR) = 4H(\text{Ethanol}) + 4 H(\text{CO}_2) - H(\text{Sucrose}) - H(\text{Water})$

$$\Delta H_{rx}(TR) = -38968 \text{ kJ/kg}$$

$$\Delta C_p = 4C_p (\text{Ethanol}) + 4 C_p(\text{CO}_2) - C_p(\text{Sucrose}) - C_p (\text{Water})$$

$$\Delta C_p = 7.702 \text{ kJ/kg.K}$$

Hence;

$$\Delta H_{rx}(T) = 38930 \text{ kJ/kg}$$

Required Heat Duty is given as:

$$Q = m \cdot \Delta H_{rx}(T) \cdot X \tag{10}$$

$$Q = 247.93 \text{ kW} = 0.2479 \text{ MW}$$

Hence the calculated results from simulation are given in Table 14.

Table 14. Balance on Reactor R-102 (From Sucrose to Ethanol)

Total	Units MW
Enthalpy In	-16.719036
Enthalpy Out	-17.325152
Relative Difference	0.03498473
Net Heat Duty	-0.6061176

The simulation result of stream R-102 is shown in Table 15.

3.3. Fermenter Sizing

The sizing of the fermenter is done to calculate the total volume required per day of processing and to find out the number of reactors to be attached in parallel to divide the flow per reactor and to have a continuous operation. The result of fermenter sizing will tell us the required diameter and height of each reactor installed [17, 22].

Total mass flowrate to be handled by the fermenter = 230.997 tons/day

Total feeding time of the fermenter = 6 hours = 0.25 day

Total processing time of the fermenter = 48 hours = 2 day

Downtime of the fermenter = 4 hours = 0.17 day

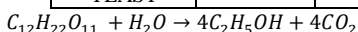
Total time required = 58 hours = 2.42 days

From the simulation results, the mass fractions of the components along with their respective densities at the operating temperature of the Fermenter are given in Table 16.

Table 15. Stream result of R-102

Production of Cellulosic Ethanol					
Stream ID		S-6	S-7	S-13	S-8
Temperature	°C	25.0		-45.9	30.0
Pressure	atm	1.000	1.200	1.000	1.000
Vapor Frac		0.000		<0.001	0.208
Mole Flow	kmol/day	1235.963	0.000	437.676	2437.512
Mass Flow	tons/day	220.100	0.000	10.897	230.997
Volume Flow	m ³ /day	143.526	0.000	8.960	12731.94
Enthalpy	MMkcal/hr	-13.015		-1.335	-14.871
Mass Flow	tons/day				
WATER		11.211		7.200	15.299
CARBO-01				2.783	24.592
ETHAN-01				0.857	23.587
METHA-01				0.001	0.013
ACETI-01				0.056	8.945
CELLULOS		40.000		0.001	40.001
1 -PRO-01				0.001	0.080
DEXTR-0 1				trace	8.889
SUCRO-01		168.889		trace	109.592
Mass Frac.					
WATER		0.051		0.661	0.066
CARBO-01				0.255	0.106
ETHAN-01				0.079	0.102
METHA-01				64PPM	58PPM
ACETI-01				0.005	0.039

Table 13. Stream result of R-101				
Production of Cellulosic Ethanol				
Stream ID	Unit	S-4	S-5	S-6
Temperature	°C	25.0		25.0
Pressure	atm	1.000	1.200	1.000
Vapor Frac		0.000		0.000
Mole Flow	kmol/day	2131.161	0.000	1235.96
Mass Flow	tons/day	220.100	0.000	220.100
Volume Flow	m ³ /day	170.753	0.000	143.526
Enthalpy	MMkcal/hr	-15.082		-13.015
Mass Flow	tons/day			
WATER		20.100		11.211
CARBO-M				
ETHAN-01				
METHA-01				
ACETI-01				
CELLULOS		200.000		40.000
1-PRO-01				
DEXTR-01				
SUCRO-01				168.889
Mass Frac.				
WATER		0.091		0.051
CARBO-01				
ETHAN-01				
METHA-01				
ACETI-01				
CELLULOS		0.909		0.182
1-PRO-01				
DEXTR-01				
SUCRO-01				0.767
Mole Flow	kmol/day			
WATER		1012.164		564.565
CARBO-01				
ETHAN-01				
METHA-01				
ACETI-01				
CELLULOS		1118.997		223.799
1-PRO-01				
DEXTR-01				
SUCRO-01				447.599
Mole Frac				
WATER		0.475		0.457
CARBO-01				
ETHAN-01				
METHA-01				
ACETI-01				
CELLULOS		0.525		0.181
1-PRO-01				
DEXTR-01				
SUCRO-01				0.362
Mass Flow	tons/day	220.100	0.127	220.227
Enthalpy	MMkcal/hr	-15.082	-0.013	-13.028
Temperature	°C		25.0	25.0
Pressure	atm	1.000	1.200	1.000
Vapor Frac.			0.000	0.000
Mass Flow	tons/day	0.000	0.127	0.127
Enthalpy	MMkcal/hr		-0.013	-0.013
Mass Flow	tons/day			
CELLULAS			0.127	0.127
YEAST				
Mass Frac.				
CELLULAS			1.000	1.000
YEAST				



Conversion of Sucrose (X) 25%

Specific heat of sucrose=1.257 kJ/kg.k; Specific heat of water=4.181 kJ/kg.k; Specific heat of ethanol=2.426 kJ/kg.k; Specific heat of CO₂=0.859 kJ/kg.k

CELLULOS		0.182		51PPM	0.173
1-PRO-01				82PPM	346PPM
DEXTR-0 1				trace	0.038
SUCRO-01		0.767		15PPB	0.474
Mole Flow	kmol/day				
WATER		564.565		362.566	770.396
CARBO-01				57.359	506.927
ETHAN-01				16.873	464.472
METHA-01				0.020	0.378
ACETI-01				0.842	135.121
CELLULOS		223.799		0.003	223.803
1-PRO-01				0.014	1.207
DEXTR-0 1				trace	44.760
SUCRO-01		447.599		trace	290.447
Mole Frac					
WATER		0.457		0.828	0.316
CARBO-01				0.131	0.208
ETHAN-01				0.039	0.191
METHA-01				45PPM	155PPM
ACETI-01				0.002	0.055
CELLULOS		0.181		7PPM	0.092
1-PRO-01				31PPM	495PPM
DEXTR-01				trace	0.018
SUCRO-01		0.362		trace	0.119
Mass Flow	tons/day	220.227	0.127	10.897	231.251
Enthalpy	MMkcal/hr	-13.028	-0.013	-1.335	-14.897
Temperature	°C	25.0	25.0		30.0
Pressure	atm	1.000	1.200		1.000
Vapor Frac		0.000	0.000		0.000
Mass Flow	tons/day	0.127	0.127	0.000	0.254
Enthalpy	MMkcal/hr	-0.013	-0.013		-0.026
Mass Flow	tons/day				
CELLULAS		0.127			0.127
YEAST			0.127		0.127
Mass Frac					
CELLULAS		1.000			0.500
YEAST			1.000		0.500

Acetic acid	0.0019	1.05	2.02E-03
Cellulose	7.0501E-06	1.5	1.06E-05
Propanol	3.10E-05	803	0.02
Dextrose	4.6426E-15	1.54	7.15E-15
Sucrose	9.6432E-10	1.59	1.53E-09
$\Sigma x \cdot \rho$			855.57

Density of the mixture = 855.57 kg/m³

Volumetric flowrate = $\dot{m}/\rho(\text{mixture})$

Volumetric flowrate = 270.0 m³/day

The total volume to be handled by a fermenter for 58 hours (2.42 days).

Volume = 652 m³ = 700 m³ (approximately)

Assuming 2 reactors; volume per reactor = 350 m³

Calculation for diameter and height

$$V = \frac{\pi}{4}(d^2h) \tag{11}$$

where; d = 6 m and h = 18 m.

3.4. The Behaviour of Ethanol-Water system

The Vapor Liquid Equilibrium (VLE) Curve of Ethanol-Water system is shown in Figure 19. It can be seen that the atmospheric distillation of this mixture is possible only to a certain extent. The maximum purity that can be attained by atmospheric distillation is 95wt% because as soon as the composition reaches 95.63wt% (4.37 wt% of water) azeotrope is formed. Ethanol-water mixture forms a positive azeotrope. Ethanol boils at 78.4°C and water at 100°C. However the boiling point of azeotrope is 78.2°C, which is lower than both of its constituents. Generally, a positive azeotrope bubbles at a lower temperature than some other proportion of its constituents. For ethanol/water, 78.2°C is the base temperature of the blend can boil at the atmospheric pressure. Positive azeotropes are also known as called least boiling blends or boiling azeotropes [3, 17].

Figure 20 represents a direct relation between volume and temperature. This behaviour is observed in the distillation column, whereas the temperature rises the volume of ethanol increases.

TTable 16. Simulation results, the mass fractions of the components

Component	Mole Fraction	Density	Mole Fraction * Density
	x	ρ	$x \cdot \rho$
Water	0.8284	995.7	824.83
CO ₂	0.1311	1.98	0.26
Ethanol	0.0386	789	30.42
Methanol	4.50E-05	792	0.04

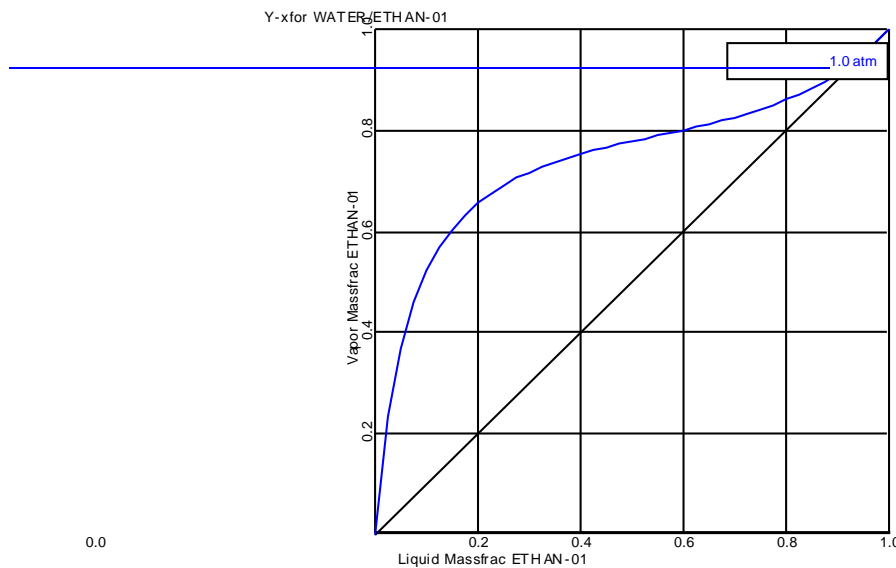


Fig. 19. Vapor Liquid Equilibrium (VLE) curve for Ethanol-Water System

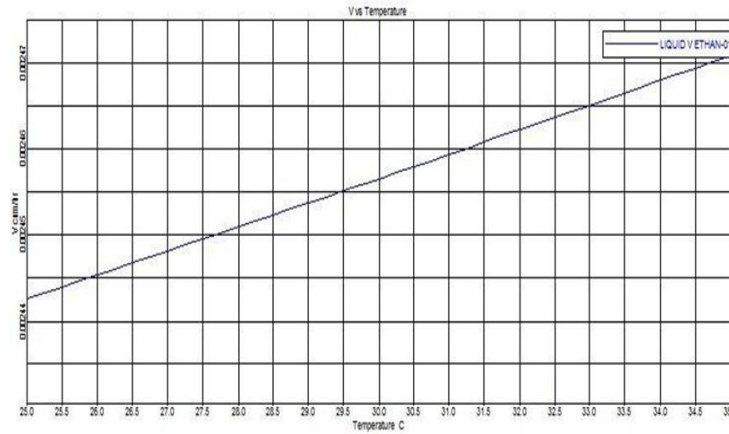


Fig. 20. Temperature versus Volume Curve

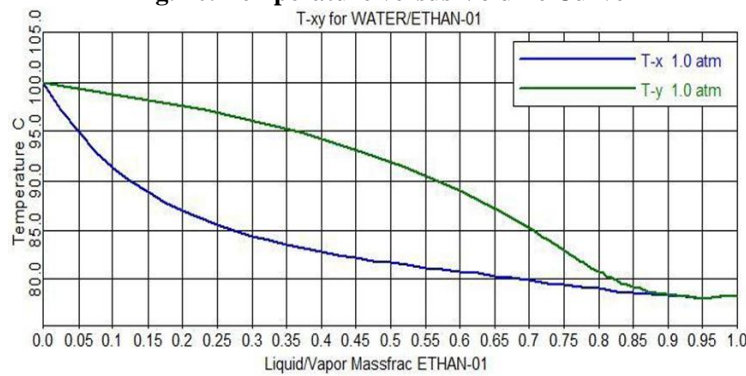


Fig. 21. Temperature versus Liquid/Vapour mole fraction of Ethanol-Water System

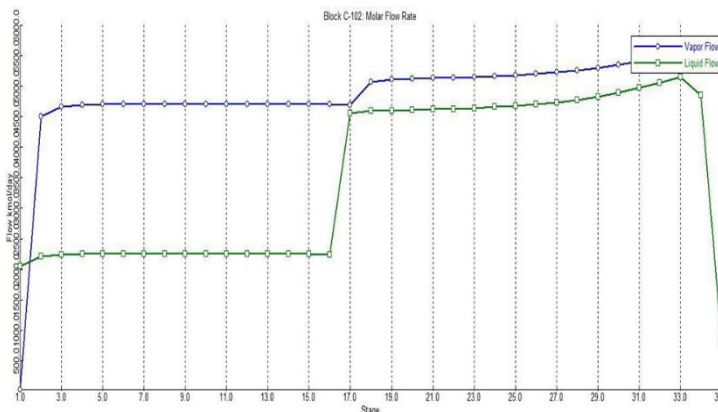


Fig. 22. Stage versus Mole Flow Curve

Figure 21 is plotted using the NRTL property system. The lower bend plots the bubble point of the binary blend as a component of the composition. The upper bend is the dew point. For a given temperature and composition, this graph reveals the nature and creation of each period of the blend that is available [2, 4].

Figure 22 shows the relation of the liquid and vapour flow with the number of stages. It shows that the dilute Ethanol feed is introduced from the 17th stage where it comes in contact with steam coming at very high temperature and immediately starts to change the phase. This then moves to the condenser where the steam is drawn off as condensate and ethanol mixture as distillate [7, 17].

4. CONCLUSION

The research aim was to minimize the energy consumption of an ethanol production facility along with minimization of the Green House Gas Emissions. To achieve this goal, the Saccharification and Fermentation reactions were carried out parallel in one reactor, which eventually

minimized the energy consumption, also a recycle stream of water is introduced to keep the reaction feed diluted, reducing the burden on raw water supply. Furthermore, to ensure eco-friendly production, molecular sieves dehydration technology was preferred over azeotropic distillation. Hence this study has shown that cellulosic ethanol is indeed the most reliable source of energy leading us towards sustainable development. Some recommendations are suggested to make this plant more cost-effective so that it can be operated on more feasible conditions. Perform this study at different SSF solids loadings to evaluate the exchange off of increased fermentation yields with improved distillation energy demand.

5. ACKNOWLEDGEMENT

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