Techno economic and energy analysis of 2,5 dimethylfuran (dmf) production process from rice straw

S.M.S.P. Samarasekara, K.L.C.Y. Liyanage, N.H. Hewage and Dr. S.A.D.T. Subasinghe*
Department of Chemical and Process Engineering, University of Moratuwa, Moratuwa, Sri Lanka
*Corresponding e-mail: thusharas@uom.lk

ABSTRACT - The objective of this research was to perform a process simulation for the production of DMF from rice straw and to analyze the process engineering aspects such as equipment type and catalysts to be used for the production of DMF from HMF. Furthermore, an economic analysis and an energy analysis were carried out for the plant. Eventually, energy indicators were calculated to showcase the economic feasibility of the plant.

Key words: HMF; 2,5-DMF; Aspen Plus

INTRODUCTION

In the present world, ethanol has become the most commonly used biofuel type due to its fuel properties. 2,5-dimethylfuran is another type of biofuel developed to meet the energy requirements. Better properties of DMF has accelerated the research field to find the best routes and enhance the fuel properties of this biofuel. Nhien and the team investigated the design and assessment of hybrid purification processes through a systematic solvent screening for the production of Levulinic Acid from Lignocellulosic biomass using Aspen plus (Nhien *et al.*, 2016). 67% yield was obtained by taking three minutes as the residence time and NaCl as the chemical compound (Wang et al., 2013). In another, fructose was used as the raw material in similar types of reactors. Here the reactions of fructose to HMF and HMF to DMF were carried out at 453K, 1350kPa and 492K, 1650kPa respectively. The respective conversions achieved are 75% and 100% (Rodrigues & Guirardello, 2014). Kazi et al. modelled a plant to produce HMF and DMF from pure fructose and ended up with a capital investment of $188.58 million for 300 metrics tons/day fructose based on 2000 metric tons/day in ligno-cellulosic biorefinery (Gawade et al., 2016).

METHODOLOGY

Development of the process flow diagram

Biomass can either be sourced from energy crops or from waste; rice straw. For this model, rice straw was selected as the raw material due to low moisture content when compared to food waste and due to no additional cost for the its production. Model was developed from processing of rice straw to the purification of produced 2,5-DMF.

Table 1. Process equipment and uses

Process Equipment	Use
Hammer Mill	As a pretreatment process to reduce the size of rice straw.
Mixer I	For the mixing of Rice Straw with HCl.
CSTR	For the production of HMF using hydrolysis
Filter	Separation of lignin
Distillation Column I	Separation of HMF
Separator	Separation of HMF from Levulinic Acid
Mixer II	To mix HMF with H_2
PFTR	Production of DMF
Flash Separator	For the Final Separation

Economic Analysis and Energy Analysis

Aspen process economic and energy analyzer V10 version was used to perform the analysis for the DMF manufacturing plant. The plant size was defined by its feed rate of rice straw which was available at a fixed cost of $15/kg. DMF was the main product whereas Levulinic acid and Furfural were the byproducts of the bio refinery. The plant was operated in a continuous mode for 8000 hours per year. The economic life was assumed to be 20 years. 40% tax was applied to the profits. The methodology can be divided into main sub-sections.

Setting up the Template

The template corresponded to different locations around the world and different unit sets. US-Metric unit set was selected and operating life of the plant, length of plant startup, start of basic engineering were used by Aspen Process Economics Analyzer (APEA) in costing calculations. Currency type was also given.

Feed and Product Stream Prices

Prices of feed and product stream were obtained from market. The price of chemicals may vary with factors, such as season, location, producer, policy, etc.

Utility Association

Under utilities folder, utility types were added and defined and they were later associated with given blocks.

Chemical Process Costing

Initially, a new project was introduced to Aspen Process Economics Analyzer(APEA) followed by entering ‘Metric’ as the units of measure. Simulator data was loaded to APEA and mapping and sizing of each and every equipment was completed. Finally, the project was evaluated followed by fixing of geometrical design related errors. The summary along with the cash flow analysis and the capital cost report were obtained at the end.

RESULTS AND DISCUSSION

DMF Production

Input flow rates for HMF production section were 25506.4 kg/hr, 19410.7kg/hr, 11839.40 kg/hr, 107.542 kg/hr, 19464.6 kg/hr of lignin, cellulose, hemi cellulose, HCl and water.

Table 2. Product flow rate from CSTR

Material	Flow Rate (kg/hr)	Mass (%)
Water	22552.36	0.2955
Lignin	25506.38	0.3342
Cellulose	6463.77	0.0847
Hemicellulose	3682.06	0.0482
Formic acid	2572.58	0.0337
HMF	3020.98	0.0396
Furfural	5932.69	0.0777
Levulinic acid	6490.29	0.0850
HCl	107.54	0.0014

The conversion of cellulose and hemicellulose is around 70%. Large amounts of water formation by cellulose dehydration lowered the HMF selectivity to 4%. Levulinic acid, formic acid and furfural were the valuable by-products that can be separated and marketed. Product stream was admitted to the purification section. Purified HMF stream, pure and recycled hydrogen gases were introduced to the DMF production section. The HMF feed stream consisted of 3017.96kg/hr HMF, furfural, Levulinic acid and a trace amount of formic acid. Total hydrogen feed rate was 1724.11kg/hr. Recycled:92.5%.

Table 3. Product flow rates of PFR

Material	Flow Rate (kg/hr)	Mass (%)
Water	793.87	0.15
DMF	2180.59	0.413
Formic acid	Trace	Trace
HMF	321.38	0.061
Furfural	60.35	0.012
Levulinic acid	322.98	0.061
Hydrogen	1594.58	0.302

Product flowrate composition of DMF from PFR is shown in Table 3. For the considered conversion of 89%, plug flow reactor configuration was 5m length and 1.1m diameter. Hydrogen conversion was low, but additional hydrogen feeding enhanced the reaction and reduced the reactor size.

Economic Analysis

Table 4. Plant cost parameters

Parameter	Value
Raw material cost	1.79E+08 $/yr
Utility cost	2.86E+06 $/yr
Operating cost	1.98E+08 $/yr
Capital cost	1.43E+07

NPV of the plant positively increased from the second year and the profitability index was 2.49 and IRR was 71.9%

Energy Analysis

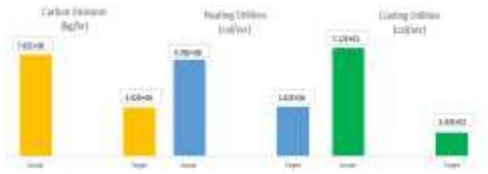

Figure 1. Plant utility consumption and emissions

Target values of utility and emission indicate the possible energy recovery options. Steam is highly consumed in feed preheating and recycled hydrogen heating sections. All carbon emissions are due to fuel combustion in steam and grid electricity generation.

Discussion

In this model, there is the possibility to optimize the DMF yield and PFR size by minimizing the hydrogen flow rate. DMF production plants produce valuable byproducts, but ethanol plants generate only electricity from waste heat. Fermentation in ethanol plants leads to direct carbon emission. In this plant carbon emission in reaction steps in zero. According to these parameters and analyzed economic indicators a DMF plant is beneficial and feasible in various aspects.

References

Nhien, L. C. *et al.* (2016) 'Design and Assessment of Hybrid Purification Processes through a Systematic Solvent Screening for the Production of Levulinic Acid from Lignocellulosic Biomass', *Industrial & Engineering Chemistry Research*, 55(18), pp. 5180–5189. doi: 10.1021/acs.iecr.5b04519.

Wang, Y. et al. (2013) 'Efficient production of the liquid fuel 2,5-dimethylfuran from 5-hydroxymethylfurfural over Ru/Co3O4 catalyst', Applied Catalysis B: Environmental. Elsevier B.V., 146, pp. 244–248. doi: 10.1016/j.apcatb.2013.04.026.

Rodrigues, F. A., & Guirardello, R. (2014). Simulation and Techno-Economic Evaluation of Large Scale 2.5-Dimethylfuran Production from Fructose. Chemical Engineering Transactions, 37, 475–480. https://doi.org/10.3303/CET1437080

Gawade, A.B., Tiwari, M.S., Yadav, G.D., & Accepted, J. (2016). Biobased green process: Selective hydrogenation of 5-Biobased green process : Selective hydrogenation of 5-hydroxymethylfurfural (HMF) to 2, 5-dimethyl furan, 0-49. https://doi.org/10.1021/acssuschemeng.6b00426