TECHNO-ECONOMIC AND ENVIRONMENTAL ASSESSMENT FOR A POLYGENERATION AND LOW EMISSION BIO-DME PRODUCTION FROM RICE STRAW IN VIETNAM

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At



Graphical abstract

Abstract

The conversion of rice straw into energy such as dimethyl ether (DME) plays a significant role in driving and improving energy conversion efficiency due to its abundance and ecofriendliness". Not only is an alternative for fossil fuels, rice straw-derived DME also affects the agriculture-based value chains. In this study, an upgrading DME production process was developed by HYSYS simulation for lower carbon dioxide (CO_2) emission and then figured out its feasibility through techno-economic and environmental analysis. Technically, the modelled process generates around 2.3 ton/h of DME with a purity of 99.96% and an energy conversion efficiency (η DME) of 75%. Otherwise, the additional presence of an off-gas absorber and CHP plant in the process reduced 84% of GHG emissions compared to the conventional process (0.21 kg CO2-eq/kg DME compared to 1.36 kg CO₂-eq/kg DME, specifically). The CO₂ capture also creates more products for this process and increases carbon efficiency to 94.6% with no CO content in fuel gas leaving the CHP section. The unit production cost (UPC) is estimated at 1,143 USD per ton of DME. These results created a net new positive contribution to commercial DME production, directing the majority of economic activity toward green and sustainable technology.

Keywords: dimethyl ether, DME, biomass gasification, carbon capture, HYSYS.

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1.0 INTRODUCTION

Biofuels have attracted consideration in recent years due to their critical potential in bridging the developing crevice between vitality supply and demand [1]. The use of liquid biofuels to replace gasoline, diesel and jet fuels has been emphasized in the Kyoto Protocols and the Paris Agreement [2]. Especially, the production of dimethyl ether (DME) from biomass has recently become a widespread concern owing to its green prospects prominence due to its ability to replace fossil fuels and reduce greenhouse gas (GHG) emissions [3]. The world DME market size was estimated to reach 8755.18 million USD in 2028, although the value in 2020 is only 4001.89 million, which indicates that the DME's global demand is anticipated to expand in the future [4].

Vietnam is one of the world's leading rice exporters, with annually 45 million tons of paddies being produced; in parallel; approximately 53.3 million tons of rice straw are released into the field each year [5]. Instead of burning rice straw to recover heat, the conversion of rice straw into DME is a viable

alternative approach [3], intending to develop the bio-natural field in Vietnam. Based on the environmental and energy policies in many countries, promoting the diversification of biofuel sources has become a necessary issue. Additionally, the cetane number of DME is greater than that of DO with 55-60and 40 – 45, respectively [6], implying it could be used in place of DO as a cleaner and more efficient fuel. Otherwise, the individual combustion of DME used for diesel engines and as a cooking fuel produces low CO_x, NO_x, and SO_x and especially soot-free emissions [7]. Combustion of the LPG/DME mixture shows a 30-80% reduction in CO₂ emissions and 5-15% of NO_x generated, compared with LPG [6]. Silalertruksa et al. [3] demonstrated that production and utilization of straw-based DME as alternative option for DO in transport could respectively reduce 14 - 70% of GHG. That number for LPG blends application was determined at 2 - 66% GHG, compared to single use of LPG at similar efficiency. As a result, the synthesis and use of bio-derived DME (e.g., from rice straw) could play an important role in global warming mitigation and enhances national energy security as well as international

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stability by reducing risks associated with over-reliance on fossil fuel imports.

The conversion of DME from rice straw includes 04 major stages: biomass gasification to synthesis gas, water-gas shift (WGS) reaction, DME synthesis, and purification. Biomass gasification technologies play an essential role in producing syngas. For instance, gasification of rice straw in a fluidized-bed unit resulted in a 61% hot gas efficiency and a 52% refrigerant gas efficiency [8]. Studies on rice straw gasification have shown promising initial results for bio-energy production, especially DME [9]. In the gasification section, the main priority is to increase the reactants as much as possible to synthesize DME (CO and H₂), while H₂ formation corresponds to an increase in CO₂ via the WGS reaction [10]. Consequently, the avoidance of CO₂ formation by gasification operating parameter variation becomes technically unfeasible. Parvez et al. [11] proposed and simulated the synthesis of DME from rice straw based on CO₂ enhanced gasification with about 1.31 kg CO₂-eg/kg DME generated, the GHG emissions from this process are higher than those compared with the works of Lecksiwilai et al. [12] (1.24 kg CO₂-eq/kg DME) and Silalertruksa et al. [3] (0.66 kg CO₂-eq/kg DME), which demonstrates that the recycling of CO₂ to the gasification stage affects the gasification is also not a viable proposition. Clausen et al. [13] designed a low CO₂ DME plant using wood pellets as raw material, integrating a biomassbased DME production process with a commercial process for acid gas removal (AGR) and a power production plant. The AGR system takes care of CO₂ capture in both the WGS outlet and the off-gas stream, and sends out the feed stream for DME synthesis and the combustible gas stream for power generation using Rankine cycle, respectively. The emission source is just the flue gas leaving the power plant with an estimated GHG emission of about 0.4 kg CO₂/kg DME [13]. Not only reducing emission, but this design also captured and stored the pure CO₂, which could be considered for commercial purposes; produced an amount of electricity for local equipment demand and even selling purposes; and completely removed H₂S causing the deactivation of catalysts [14]. Carbon capture associated with combined heat and power plant (CHP), as a result, can lighten the burden upon the environment and bring the bio-DME production process techno-economic benefits to a certain extent.

In addition to upgrading processes, studies comparing changes in feedstock between biomass and coal for DME production with the goal of reducing GHG were investigated. Lecksiwilai et al. [12] made a comparison between five types of agricultural waste: rice straw, palm empty fruit bunches, cassava rhizomes, sugarcane tops and leaves, and corn stalks concerning GHG emissions from bio-DME production. The results indicate that the potential for fossil-derived DME replacement is found from rice straw, sugarcane tops and leaves and maize stem since their life cycle GHG emissions are much lower than that of the coal-based DME. In particular, the GHG emissions from DME production from rice straw are estimated at 1.24 kg CO₂-eg/kg DME, while the figure for coal-DME is 3.9 – 5.5 kg CO₂-eq/kg DME [12]. It is clear that the importance DME derived from rice straw has significant potential to replace DME produced from fossil resources. According to the findings, establishing a technology to produce DME from rice straw using a combination of carbon capture and combined heat and power plant (CHP), could be reduced the burden on the environment and bring about economic - technical benefits for the bio-DME process.

In this study, a DME production upgrading process that reduces CO₂ emissions from rice straw is modelled and simulated using Aspen HYSYS software. The process incorporates the AGR cluster for CO₂ and H₂S capture, which is coupled to the CHP plant for generating electricity, as well as the upgraded ASU section for oxygen (O₂) agent and liquid nitrogen (LN₂) synthesis. The aim is to enhance the existing DME manufacturing method from rice straw and safeguard the environment by utilizing process byproducts such as ash, CO₂ and LN₂ to reduce the price of DME. In addition, this work redesign of the heat exchanger network in the proposed process to minimize utility usage, thus resulting in reducing the operating costs. Furthermore, a comprehensive technical, environmental and economic evaluation of the proposed production process to determine the unit production cost of the DME, or the minimum price of DME in the other words, and the emission level which is specified in terms of CO₂-equivalent emitted per mass of ether produced. This design is expected to provide a breakthrough, environment-friendly solution for the biofuel production industry in general and DME in particular, towards a sustainable economy and energy safety.

2.0 METHODOLOGY

2.1. Feedstock Characterization

Rice straw fed into this process is assumed to be densified into bales with a density of 450 kg/m³ [9] and modelled using the average chemical formula method [15], where the biomass feedstock is set as a hypothetical solid component in Aspen HYSYS under the formula $C_{5.586}H_{7.432}O_{4.032}N_{0.134}S_{0.035}$. Its detailed composition analyses are shown in Table 1.

Table 1 Design parameters and assumptions for the simulation of the low emission DME production process from rice straw

Parameters	Descriptions	Reference
Feedstock	Rice straw bales: density of 450 kg/m ³ Composition (% wt.): 38.61% C, 4.28% H, 37.16% O, 1.08% N, 0.65% S, 12,64% Ash, 5.58% Moisture LHV = 14.4 MJ/kg	[16]
Pretreatment	Moisture removal by drying: 100% Power consumptions for milling: 0.29% thermal input	[13]
CFB gasifier	Operating temperature: 900° , 10 bar Steam agent temperature: $800^{\circ}C$ O_2 agent temperature: $600^{\circ}C$ Cyclone separation efficiency: 85% Carbon conversion of char: 96% Carbon loss: 2% N_2 and S only form NH ₃ and H ₂ S, respectively No tar formation	[10], [15]

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[17]

Plug flow fixed-bed reactor containing catalyst Catalyst: Fe₂O₃/Cr₂O₃/CuO Operating conditions: 400°C, 10 bar

Acid	gas	Absorption column to capture acid gas	[15], [18]			
recovery		from syngas: 10bar				
system		Absorption column to capture CO ₂ from off-gas: 9.5 bar H ₂ S recovery: 100%				
		CO ₂ recovery for two absorbers: 90% Monoethanolamine (MEA): 30% wt.				
DME		Plug flow fixed-bed multi-tube reactor with	[15], [19]			
synthesis		integrated steam generation Catalyst: CuO – ZnO – Al2O3/γ - Al2O3 Operating conditions: 260°C, 50 bar Conversion of CO: 64%				
Air		O2 purity: 99.9%	[13]			
separatior unit	1	Electricity consumption: 1 MWe/(kg-O ₂ /s)				
CHP plant		Gas turbine, HRSG and steam turbine Turbine inlet temperature (TIT): 1377°C η _{isentropic} , turbines = 0.9	[20]			
DME purificatio	n	DME purity: 99.96% Operating pressure: 9.5 – 10 bar				
Heat exchanger	s	ΔT _{min} : 10°C				
Pumps a compresso	and ors	Nisentropic, pumps: 0.9 Nisentropic, compressors: 0.9	[20]			

2.2. Method

Both thermodynamic models, Both Peng – Robinson (P-R) and Non – Random Two–Liquid (NRTL), are applied to estimate properties of involved components as well as to model the subprocesses of the proposed DME production process efficiently.

2.3. Process Description And Design Parameters

Figure 1a illustrates block flow diagram (BFD) of the proposed process. Within pretreatment section, rice straw is imported from domestic suppliers under shape of round bales and roughly washed to remove dust. De-densification of those straw rolls into fiber, and feedstock drying and milling are conducted afterwards. The simulation of this section based on 02 assumptions: drying efficiency of 100% moisture content, and power consumption for milling being equivalent to 0.29% feedstock's thermal input [13].

Dry straw is then gasified in a circulating fluidized bed (CFB) gasifier, where thermo-chemical conversion turns it into synthesis gas (syngas) using two gasifying mediums: pure oxygen (O_2) and steam. This equipment operates at 900°C and

10 bar [15]. For simplification of CFB gasifier model, some assumptions were adopted as shown in Table 1, mainly on neglected formation of tar and several complex substances except ammonia (NH_3) and hydrosulfide (H_2S) [10].

Pure oxygen is self-produced from an air separation unit (ASU), modified for both purposes of oxygen (99.9% wt. purity) and liquid nitrogen production. This unit is illustrated in Figure 1b. where LNG replaces N_2 as refrigerant to participate in heat transfer.

Being cooled to 400°C after leaving gasifier, the produced syngas enters a water-gas shift (WGS) reactor to adjust its internal ratio of H_2 /CO, via the following reactions:

 $CO + H_2O \leftrightarrow CO_2 + H_2$ (1) $CH_4 + H_2O \leftrightarrow CO + 3H_2$ (2)

Whereas (1) is major reaction, (2) is side reaction. Target H_2/CO ratio that facilitates direct DME synthesis was 1, obtained from previous research [21]. The ratio adjustment stage takes place in a plug flow fixed-bed reactor containing $Fe_2O_3/Cr_2O_3/CuO$ as catalyst [17] under operating conditions 400°C and 10 bar. Outlet synthesis gas is cooled to 30°C and dehydrated in a flash separator. Condensed water is utilized as gasifying medium by evaporation in a boiler.

For acid gas recovery (AGR) system, two absorption columns and one stripper are responsible for contaminant removal and recovery (i.e., CO_2 and H_2S). The absorption solvent chosen is monoethanolamide (MEA) solution with industrial concentration of 30 wt.% [18]. Separation efficiency of CO_2 and H_2S were assumed to be 90% and 100%, respectively [15]. Recovered acid gas (mainly CO_2 composition) is stored for commercial purposes, while the dry acid gas free syngas are compressed to 50 bar for DME production.

The single-step DME synthesis is carried out in a plug flow fixed-bed reactor catalyzed by CuO – ZnO – Al2O3/ γ – Al2O3 with integrated steam generation [19]. A plug flow reactor (PFR) model is utilized to simulate the DME synthesis reactor, in which the temperature is maintained at 260°C by an energy stream representing high-pressure steam (HP steam) generator. Three following reaction equations Eqs. (1), Eqs. (2), and Eqs. (3) describe the main reactions taking place in such a reactor, with the kinetic parameters obtained from previous work [19]:

$CO_2 + 3 H_2O \leftrightarrow CH_3OH + H_2O$	(3)
$CO + 2 H_2O \leftrightarrow CH_3OH$	(4)
$2 CH_3OH \leftrightarrow CH_3OCH_3 + H_2O$	(5)

Temperature of the product gas is decreased to 30°C in a cooler and even lowered to -30°C afterwards. At this temperature, DME condenses into liquid phase while other unreacted components remain in vapor phase; therefore, a flash separator is used for two phase split. 95% of vapor at the top of separator is recycled to DME synthesis stage, and AGR system receive the remaining 5%.



Figure 1 (a) Block flow diagram of DME production process from rice straw; and (b) modified air separation unit

The purification section of DME takes place in three distillation processes: off-gas separation (contaminant CO, CO2, CH₄, etc.), DME separation from methanol-water solution, and methanol separation from water for reactant recycling scope, in three respective distillation columns.

Off-gas from purification and 5% purge gas are absorbed in AGR section, releasing combustible gases towards combined heat and power (CHP) section. There, a typical CHP process is applied with fuel gas combustion, first-step power generation by gas turbine, and second-step power generation by heat recovery steam generator (HRSG) and steam turbine, respectively. Some operating conditions assumed were turbine inlet temperature (TIT) of 1377°C and isentropic efficiency of considered turbines of 90% [20]. Exhaust gas is eventually discharged to the environment.

2.4. Techno-Economic And Environmental Analysis Model

For technical analysis, the carbon flow analysis demonstrates carbon element efficiency in outlet streams of each section. Moreover, DME efficiency shows how chemical energy in biomass feedstock is converted to chemical energy stored in DME products [13], expressed by Eqs. (4) [15].

$$\eta_{DME} = \frac{M_{DME} \times LHV_{DME}}{M_{ricestraw} \times LHV_{ricestraw}}$$
(4)

where M_{DME} is the mass flow rate of DME product (kg/h), and $M_{ricestraw}$ is the mass flow rate of dry ash-free (daf) basis rice straw feedstock (kg/h). LHV_{DME} and LHV_{rice straw} are the lower heating value of dimethyl ether and rice straw (kJ/kg), respectively.

For environmental assessment, the CO_2 -equivalent emission is considered and determined by dividing annual CO_2 -equivalent emission by the yearly mass capacity of DME. This parameter, additionally, indicates the emission potential of CO_2 itself and other greenhouse gases multiplied with their corresponding Global Warming Potential (GWP) [22]. Specifically, the GWP of CO_2 and CH_4 are 1 and 28 according to the IPCC Fifth Assessment Report (AR5), respectively [22]. $\label{eq:table_to_$

Economic parameters	Value	Reference	
Location	Vietnam		
Annual operating hours (h/y)	8000	[23]	
Interest rate (%)	6	[24]	
Plantlife (y)	20	[25]	
Steam agent production	Self-produced		
Price of byproducts	Value	Reference	
CO ₂ credit (USD/ton)	20.66	[23]	
Liquefied N ₂ (USD/L)	0.8	[26]	
LP steam (USD/ton)	10.5	[24]	
Ash (USD/ton)	120	[27]	

The evaluation adopts the economic assumptions shown in Table 2 and Table 3. Around 40 USD/ton of rice straw bales price is considered [28]. The electricity is used to be supplied from the grid, while the heat and refrigeration are used to be supplied from natural gas [24]. The price of DME synthesis catalysts is 24.86 USD/kg, and the time to replace them with new catalysts is considered about 3 years [29].

The unit production cost (UPC) of the main product is computed based on total capital investment cost (TCI), total operating cost (TOC), and sales revenue of byproducts (SRB). These constituent costs are estimated using purchased equipment cost (PEC) and ratio factors for solid – fluid processing with their relationship shown in Eq. (5) [30].

$$TCI = \left(\sum_{i=1}^{n} RF_i + 1\right) \times PEC \quad (5)$$

where RF_i represents ratio factors for direct cost, indirect cost, and working capital; and PEC refers to delivered purchased equipment cost, assumed to be 10% overestimated based on process equipment cost.

The equipment costs are estimated using six-tenth factor rule (Eq. (6)) according to reference costs [30].

$$C_2 = C_1 \times \frac{CEPCI_2}{CEPCI_1} \times \left(\frac{S_2}{S_1}\right)^N$$
(6)

where C_1 and C_2 are the base cost and the estimated cost, respectively. CEPCl₁ and CEPCl₂ are the chemical engineering plant cost indices for the base year and the estimated year, respectively. S_1 and S_2 are the size or capacity of the base and estimated equipment, respectively, and N is the size exponent [30]. In this work, the parameters used to calculate unavailable costs in APEA are shown in Table 3.

Eq. (7) expresses the formula to calculate the annualized capital cost (ACI), with interest rate at r % over r years of plant life [24]:

$$ACI = TCI \times \frac{i \times (1+i)^r}{(1+i)^r - 1} \tag{7}$$

To calculate TOC, the mass and energy flow data from the simulation are obtained. The chief parameter for calculating the TOC is the number of operators expressed by Eq. (8), according to Okolie et al. [31].

$$N_{OL} = \sqrt{31.7P^2 + 0.23N_{NP} + 6.29}$$
(8)

where N_{NP} represents the number of non-particulate processing steps including heating, mixing, cooling and compression. P is the number of solid handling steps. The salary for each worker is 40,000 \$/y [32]. Based on Eq. (8), it is estimated that 53 workers are needed for the process operation. A ratio estimation approach to determine the TOC which uses the assumptions mentioned in Table 4 is adopted. Since operating labor cost accounts for 0 – 10% of total production cost (TPC), the number of operators reach the requirement of 53 people [30].

Item	Benchmark	Base CEPCI	Base size	Base cost (MUSD)	Exponent factor	Reference
Gasification island	Input chemical energy	603.1/2018	798.5 MW	169.50	0.7	[13], [33]
Biomass dryer	Moisture flow rate	521.9/2009	0.42 t/h	10.80	0.65	[30], [34]
Baghouse filter	Inlet volume flow rate	390.4/2002	15.6 m³/s	0.07	0.68	[30], [35]
Gas turbine	Electricity output	525.4/2007	266 MW	73.20	0.75	[13]
Steam turbine	Electricity output	525.4/2007	100 MW	105.54	0.67	[36]
HRSG	HRSG duty	567.5/2017	527.92 MW	33.16	0.7	[36]
Combustor	Inlet air flow rate	541.7/2016	59.4 kg/s	0.55	0.67	[36]
ASU	O ₂ flow rate	525.4/2007	2202 kg/s	82.70	0.5	[13]
Steam boiler	Boiler duty	525.7/2007	355 MW	52.00	1	[13]

Table 3 Input data for purchased equipment cost estimation

Item		Assumption	Reference	
1.	Raw material	Rice straw bale price: 40 USD/ton	[28]	
2.	Utilities	Electricity price: 0.098 USD/ kW,	[23]	
		HP steam price: 14.5 USD/ton,	[24]	
		Cooling water price: 0.273 USD/ton,	[23]	
		Refrigeration utility price: 8.53 USD/GJ	[24]	
3.	Operating & maintenance			
3.1.	Operating labour	53 labours needed,	[31], [32]	
		40000 USD/labour/year		
3.2.	Supervisory & clerical labour	15% of (3.1)	[37]	
3.3.	Maintenance & repairs	5% of FCI	[37]	
3.4.	Operating supplies	15% of (3.3)	[37]	
3.5.	Laboratory charges	15% of (3.1)	[37]	
4.	Patent & royalties	1% of TPC	[37]	
5.	Catalysts & solvents			
5.1.	Catalysts	DME synthesis catalyst price: 24.86 USD/kg,	[29]	
		Replacing time: 3 years		
5.2.	Solvents	MEA 30% wt.,	[18], [24]	
		Pure MEA price: 0.97 USD/kg		
6.	Depreciation	Straightforward method, expressed by Eqs. (7)	[24]	
7.	Local taxes & insurance	1% of FCI	[37]	
8.	Plant overhead costs	20% of [(3.1) + (3.2) + (3.3)]	[37]	
9.	General expenses			
9.1.	Administration	15% of (3.1)	[37]	
9.2.	Distribution & marketing	1% of TPC	[37]	
9.3.	Research & development	1% of TPC	[37]	
10.	Total operating cost (TOC)	(1) + (2) + (3) + (4) + (5) + (7) + (8) + (9)		
11.	Total production cost (TPC)	(6) + (10)		

Table 4 Summary of economic assumptions for total operating cost estimation and total production cost

3.0 RESULTS AND DISCUSSION

3.1. Process efficiencies

3.1.1. Process Simulation Results

The process flow diagram (PFD) of the proposed process from the Aspen HYSYS simulation is represented in Figure 2, and the process parameters of the main streams in the flowsheet is shown in Table S1. From obtained results, the annual capacity of DME produced was approximately 18,456 tons with a purity of 99.96%.

The raw rice straw was fed to the pre-treatment section at a flow rate of 7.532 ton/h (81.7 kmol/h), including 43.4 kmol/h, 23.3 kmol/h and 15 kmol/h of dry ash-free basis biomass, moisture content and ash content, respectively [15]. In this section, 71.5 kWe was required for the milling stage operation, and the drying and feeding one consumed the amount of power of 247.8 kWe. Regarding the next section, the H₂/CO ratio in syngas product was 0.995 with steam and oxygen used as agents for gasification (1982 kg/h and 2412 kg/h, respectively). The ASU which was responsible for the supply of 99.9% purity oxygen used approximately 970 kW electricity (including 670 kWe for air separation, 45.7 kWe for LN₂ pressurization, and 255.7 kWe for pure O₂ compressing) and 1.06 GJ/h refrigeration utility and generated 63520 ton-LN₂/y. On the other hand, with a flow rate of around 110 kmol/h, equaling to the steam agent needed for the gasification section

(stream 4), and a pressure of 10 bar, the condensed waterstream following the condenser E-104 was utilized to generate steam at 800° C in the boiler E-108 to provide to the gasifier.

100% H₂S and 90% CO₂ in stream 12 were removed after entering the AGR section (stream 16), requiring around 356.9 kmol/h MEA dissolved in a 30% wt. solution with water at 65°C (stream 17). Moreover, the AGR section was the most energyconsuming section since its use in refrigeration utility accounted for 97.4% of total refrigeration demand (around 143.8 GJ/h), and the HP steam produced by utilization of released heat from heat exchangers and reactors (6229 kW) met just 13.3% of the thermal energy demand of the reboiler of the stripper, leading to the fact that the remaining HP steam required for such equipment (around 40.5 MW) had to be purchased. In the DME synthesis section, E-111 represented the refrigerator provided 2 GJ/h refrigeration utility to drop the temperature of the stream 23 from 30°C to -30°C for the purpose of condensing 97.5% DME into the liquid phase. To gain the desired purity of the product (stream 28), the number of trays of the off-gas column, DME column, and methanol column was 9, 10, and 12, respectively. Finally, the CHP plant used thermal energy released from the combustion of stream 32 to produce electricity using gas turbine K-102 (496.7 kWe) and steam turbine K-103 (159.4 kWe), and supply this resource to P-100, K-100, and the miller. The flue gas (stream 34) at 81°C was emitted to the environment [38].



Figure 2 Process flow diagram and main parameters of streams in the proposed process

3.1.2. Heat Integration Results

The heat integration design is also illustrated in Figure2. Instead of being cooled smoothly from 400°C to 30°C using utilities, the temperature of the product stream of the WGS reactor sequentially dropped to 280°C, 187.3°C, 117.8°C, and 114.9°C prior to 30°C through coolers (E-101 and E-102) and heat exchangers (E-103, E-107, and E-112 against off-gas stream, DME reactor inlet stream, and off-gas column bottom stream, respectively). Similarly, the DME reactor outlet stream entered E-113 in which it was cooled to 238°C and continued to be sent to coolers E-109 and E-110 with an outlet temperature of 30°C. Two – third of reboilers were substituted with heat exchangers (E-112 and E-113) allowing heat transfer between process streams and column bottom streams. High-pressure steam which was generated not only by heat transferred from hightemperature process streams but also by heat released from isothermal reactors, furthermore, was supplied to the AGR section to reduce the utility used for heating; however, lowpressure steam was produced in the way that is as same as the aforementioned one was considered to become a commercial product. Figure 3 indicates the performance of the HEN design for the DME production process from rice straw, where the reduction in the use of hot utility, cold utility, and electricity are 22.5%, 51.8%, and 32.7%, respectively.



Figure 3. Energy consumption of utilities before and after heat integration

3.2. Techno-Economic Analysis

3.2.1. Carbon Flow Analysis

The carbon flow analysis of the proposed process is shown in Figure 4. As can be seen in such diagram, five outlet streams contain carbon elements and are arranged from the highest to the lowest carbon content: acid gas recovered by the AGR system (53.3%), DME product (41.3%), flue gas after power production (4.6%), carbon removed from baghouse filter

(0.6%), carbon loss in gasification (0.1%), and wastewater from methanol tower (less than 0.1%). The last three streams represent the loss for their carbon contents are unable to be utilized. Besides, the amount of captured CO_2 was for selling purposes and thereby, being considered a commercial product.

Compared to the DME production process from rice straw without a CHP plant and off-gas absorption column, the carbon efficiency rises by approximately 21.7% with 94.6% achieved by the proposed process, implying that the latter may restrict the waste of carbon rather than the former.



Figure 4 Carbon flow diagram and carbon efficiency of the suggested process

Table 5 DME efficiency calculated in this work

Parameters	Value	Reference
Daf basis rice straw capacity (ton/h)	6.16	[15]
LHV of feedstock (MJ/kg)	14.4	[16]
DME capacity (ton/h)	2.307	
LHV of DME (MJ/kg)	28.8	[15]
DME efficiency (%)	75	

Based on the hourly capacity of DME (approximately 2307 kg DME/h) obtained from the simulation, it is calculated that this work archives DME efficiency of 75% as shown in Table 5, meaning produced DME is likely to provide a lower amount of thermal energy (LHV) than that of biomass feedstock when being completely combusted, with 75% specifically.

3.2.2. Environmental Evaluation

Environmental impact assessment is conducted based on Table 6. The proposed design sends out 0.21 kg CO_2 -eq over 1 kg DME produced, while the figure for conventional process and CO_2 -enhanced process was 1.36 and 1.31, respectively. Due to the presence of two units AGR and CHP, the amounts of greenhouse gases released considerably reduce by 85% and 84%, contributing to global low emission scope. Moreover,

emitted off-gas in two above cases contains toxic gas (CO 4% wt.) and another GHG (CH₄), so the proposed design also converts these gases into CO₂ prior to being recovered by AGR. Therefore, there is no CO and CH₄ contents in the flue gas leaving CHP plant, prevents releasing toxic gas CO, mitigating the risk of CH₄ emission (GWP_{CH4} = $28 \times \text{GWP}_{\text{CO2}}$) and increasing Heating Value Of The Gas Stream Fed To CHP Plant.

 $\label{eq:table_to_compared} \ensuremath{\mathsf{Table}}\xspace \ensuremath{\mathsf{6}}\xspace \ensuremath{\mathsf{CO}_2}\xspace \ensuremath{\mathsf{equivalent}}\xspace \ensuremath{\mathsf{compared}}\xspace \ensuremath$

Processes	CO2-eq emission (CO2/kg DME)	kg
Conventional process [11]	1.36	
CO ₂ -enhanced process [11]	1.31	
This work	0.21	

3.2.3. Estimate Of Purchased Equipment Cost (PEC)

The spending on purchasing pieces of equipment is shown in Figure 5. Based on the pie chart, the total cost spent on equipment is 59.2 MUSD with the two most cost-intensive sections involving the ASU section and the gasification section. Specifically, the capital investment in the former section

accounts for 34% of total purchased process equipment cost (20.2 MUSD) while the latter one is 4% smaller than that of the ASU section with around 18.1 MUSD. Following those with 12.8 MUSD (accounting for 22%), the acid gas recovery system is the third most expensive section, where the stripper which separates acid gases from the rich solvent stream is noticeable since purchasing cost for this equipment occupies 36.5% of the total investment in AGR section. Besides, the cost of the CHP section is around twice lower than which of the AGR system. The others including DME synthesis, pretreatment, WGS, and DME purification are the least cost-intensive section with 1.7 MUSD, 1.2 MUSD, 0.6 MUSD, and 0.4 MUSD, respectively.



Figure 5 Breakdown of purchased equipment cost

3.2.4. Economic Analysis

Table 7 summarizes the constituent costs contributing to the unit production cost (UPC). Firstly, approximately 302.1 MUSD is required as total capital investment (TCI) for the proposed process. Its dominant contributor accounting for 83.8% is fixed capital investment (FCI) with 253.3 MUSD and working capital cost (WCC) occupies the remaining percentage. The FCI is composed of direct cost (171.2 MUSD) and indirect cost (82 MUSD). Among of those, the delivered equipment cost is estimated at 65.1 MUSD (10% overcalculation of purchased process equipment cost) and plays a role as the base cost for the estimate of other constituent costs of both direct and indirect cost. The second major expense mentioned in such table, total operating cost (TOC), is an annual basis cost including the variable operating cost (VOC) and fixed operating cost (FOC) with 37.6 MUSD/y and 24.2 MUSD/y, respectively. In terms of the VOC, the yearly largest cost is for utility supply occupying almost two-fifth of the TOC, followed by those for MEA operating in ARG section (8.5 MUSD/y), rice straw as raw materials (2.4 MUSD/y) and catalyst replacement for DME synthesis reactor (1.6 MUSD/y). On the other hand, operating and maintenance cost (16 MUSD/y), patent and royalty cost (0.9 MUSD/y), local taxes and insurance cost (2.3 MUSD/y), and plant overhead cost and general expenses (5.1 MUSD/y) compose the FOC. Based on Eqs. (6), it is calculated that 26.3 MUSD per year must be paid for process plant operation and amortization involving linear depreciation and debt payment, known as ACI. The sum of TOC and ACI is total production cost (TPC), composed of sales revenue of by-products (64.7 MUSD/y) and annual production cost of DME (10.3 MUSD/y). As a result, this work computes the unit production cost (UPC) at 555 USD/ton DME - in other words, 1 ton of DME with the purity of 99.96% produced in the proposed process is priced at least 555 USD. Compared to current DME price in 3 other regional markets such as North America (920 USD/ton), Europe (1060 USD/ton) or Northeast Asia (550 USD/ton) [39], this price is quite competitive. However, what should be remembered is that the price of DME calculated in this work is estimated at the break-even point, meaning that there will be no profit if it is commercialized. Therefore, further evaluations on economic performance of this process should be conducted in future in order to secure the profit; and some cost-driven parameters should be addressed to decrease product's price, which is discussed in the below sensitivity analysis.

Table 7 Cost breakdown of DME production process from rice straw

Item	Value	%
1. Total capital investment (TCI) [MUSD]	302.1	100
1.1. Fixed capital investment (FCI)	253.3	83.8
1.1.1. Direct cost	171.2	56.7
Purchased equipment cost (delivered)	65.1	21.6
Purchased equipment installation	25.4	8.4
Instrumentation & controls	11.7	3.9
Piping	10.4	3.4
Electrical systems	6.5	2.2
Buildings (including services)	16.3	5.4
Yard improvement	9.8	3.2
Service facilities	26.0	8.6
1.1.2. Indirect cost	82.0	27.2
Engineering & supervision	20.8	6.9
Construction expenses	22.1	7.3
Legal expenses	2.6	0.9
Contractor's fee	12.4	4.1
Contingency	24.1	8.0
1.2. Working capital cost	48.8	16.2
2. Total operating cost (TOC) [MUSD/y]	61.9	100
2.1. Variable operating cost (VOC)	37.6	60.8
Raw materials	2.4	3.9
Utilities (HP steam, electricity, cooling water and		40.7
refrigeration)		
Catalyst replacement	1.6	2.6
MEA make-up	0	0
MEA operating	8.5	13.7
2.2. Fixed operating cost (FOC)	24.2	39.2
2.2.1. Operating & maintenance	16.0	25.9
Operating labor	2.1	3.4
Supervisory & clerical labor	0.3	0.5
Maintenance & repairs	11.5	18.6
Operating supplies	1.7	2.8
Laboratory charges	0.3	0.5
2.2.2. Patent & royalty	0.9	1.4
2.2.3. Local taxes & insurance	2.3	3.7
2.2.4. Plant overhead & general expenses	5.1	8.2
Plant overhead cost	3.1	4.9
General expenses	2.0	3.3
3. Annualized capital investment (ACI)	26.3	
4. Total production cost (TPC) [MUSD/y]	75.0	
Annual sales revenue of byproducts	64.7	86.3
Annual production cost of DME		13.7
Unit production cost (UPC) [\$/ton-DME]		

3.2.5 Sensitivity Analysis

As the variation of both TOC and ACI, which leads to the change in the value of the UPC of DME, depends on economic parameters, a sensitivity analysis is carried out to investigate to what extent these cost drivers affect the minimum price of main product in this process. Figure 6a illustrates the results of this investigation where plant life and annual interest rate attract special attention as the dominant cost-drivers. For number of operating years, the longer it lasts, the lower UPC is obtained (approximately 408 USD/ton-DME with 24 years). Likewise, DME minimum price drops to an approximate value compared to the aforementioned one with 411 USD/ton if the interest rate is 4.8%. HP steam price and refrigeration utility price are as sensitive as each other with around 0.2% of the difference between their sensitivities. Another notable one which changes the UPC of DME rapidly is MEA solvent's price, varying it to 457 USD/ton (at lower bound) or 704 USD/ton (at upper bound). The rest of parameters influence the DME minimum price at the least level with around \pm 3.9% variation on this value.



Figure 6 Influences of economic parameters on the UPC of product: (a) Sensitivity analysis results; Influence of plant life (b) and interest rate (c) on DME unit production cost

Deeper investigations on the two major cost-driven parameters were carried out, with results shown in Figure 6b and Figure 6c. As for plant life, a longer operation time up to 40 years can decrease almost 3.5 times (around 170 USD/ton). However, long time of operation in this design case, e.g., 40 years, may produce some drawbacks on each individual unit due to high temperature and pressure of the process, leading to huge costs to be spent in the future for unexpected repairs, maintenance, or even replacement. This unfortunately makes the process uneconomical. Consequently, prolonging the plant life is potentially an option to reduce minimum price of DME, but the number of years should be chosen around 25 - 30 years at longest. On the other hand, the interest rate of banks affecting the amortization can lower the UPC to around 200 USD/ton. The calculation was based on the assumption that entire the capital investment (TCI) was a loan, and therefore the annual interest is also included in the depreciation, which elevates the UPC. For this reason, there are two options for the scope of reducing UPC: (1) the interest is decreased; and (2) the investor should have their own finance to a certain extent.

4.0 CONCLUSION

This process is successfully simulated on Aspen HYSYS and generates around 18,456 tons of DME 99.96% annually from 60,256 tons/y raw rice straw bale. Also, liquid nitrogen (LN2), captured CO_2 , and ash after gasification are considered as byproducts with yearly capacity of 63,520 tons/y, 45,826 tons/y, and 6,868 tons/y, respectively. After heat integration, the use of heating, cooling, and electricity utility decreases 22.5%, 51.8%, and 32.7% as compared to preliminary design, leading to the reduction in the operating cost.

For technical analysis, the carbon efficiency of proposed process acchives 94.6% based on the AGR system, where CO₂ captured by such section accounts for 53.3% of carbon element efficiency. Moreover, the chemical energy (LHV) converted from rice straw to product (nDME) is calculated at around 75%. In terms of environmental performance, once 1 kg DME is produced via this process, 0.21 kg CO₂ is emitted to the environment with no CO content in exhaust gas, gaining approximately 84% of reduction in CO₂-equivalent emission as compared to conventional process. Finally, the economic analysis indicates that the minimum price of DME 99.96% in this research is estimated at 555 USD/ton with plant life and interest rate playing the roles as cost-drivers in this project. Though the calculated price is relatively high compared to which of current market, DME produced by the pathway utilizing agricultural residue can be considered as a perspective option in further future because of the increase in forecasted DME demand in future and the exhaustion of traditional feedstocks for DME production (coal, natural gas...).

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Conflicts of Interest

The author(s) declare(s) that there is no conflict of interest regarding the publication of this paper

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