

# Dimethyl ether production from rice straw: process modelling and simulation

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## History

- Received: 27-5-2022
- Accepted: 11-01-2023
- Published: 31-01-2023

## DOI :

<https://doi.org/10.32508/stdjet.v5i4.1014>



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## ABSTRACT

Climate change has been a worldwide concern for recently centuries, and exploitation as well as use of fossil fuels dominantly contribute towards the environmental degradation. Several types of alternative energy resources have been taken into account and evaluated in order to find out viable options for the future, and dimethyl ether (DME) is one of those that are worth serious consideration. In this research, a continuous DME production process was developed and simulated using Aspen HYSYS<sup>TM</sup>. Rice straw, the most popular type of biomass in Vietnam, was chosen to be feedstock for the fuel production. The proposed process consists of five major sections: rice straw pretreatment and gasification for synthesis gas (syngas) generation using a circulating fluidized bed gasifier (CFBG); water-gas shift reaction (WGSR) for H<sub>2</sub>/CO ratio adjustment in syngas; gas cleaning stage where H<sub>2</sub>O, H<sub>2</sub>S and CO<sub>2</sub> are removed; DME synthesis via direct production pathway; and DME purification for separation of main product and recycling of methanol. The simulation results indicated a production capacity of approximately 2,307 kg of DME per hour and chemical energy conversion efficiency ( $\eta_{DME}$ ) from biomass into DME of 75%. In addition to that finding, an investigation into the gasifier's operating parameters was conducted for the purpose of maximizing amount of DME generated. From investigation data obtained, the operating temperature of CFBG, steam to biomass (S/B) ratio, and equivalence ratio (ER) that fulfilled such an aim were concluded to be 900°C, 0.27, and 0.32, respectively. This work offers a novel option for utilization of massive availability of agricultural residues in Vietnam by turning it into a type of promising fuel, and therefore lessen environmental burden as well as may develop Vietnam's energy market.

**Key words:** Dimethyl ether, process modeling, simulation, rice straw

## INTRODUCTION

Energy transition to renewable energy usage has become a widespread concern due to global warming and the depletion of fossil fuel resources. Among several sources of energy taken into account, dimethyl ether (DME) is a viable option regarding its potential to substitute diesel oil (DO) and liquefied petroleum gas (LPG). In 2020, the world's DME market size was 4001.89 MUSD, and the long-term forecast reveals this metric will reach 8755.18 MUSD in at least next 8 years<sup>1</sup>. As a result, the DME demand in Asia Pacific is likely to increase during such a period as this area accounted for approximately 80% of DME market size of the globe [1]. Currently, 65% of globally produced DME is blended with liquefied petroleum gas (LPG) for residential and industrial purposes<sup>2</sup> based on its liquefaction at 0.54 MPa and 20°C, which is similar to that of LPG<sup>3</sup>. The combustion of LPG/DME blends shows a reduction of 30 – 80% in CO<sub>2</sub> emission and 5 – 15% in NO<sub>x</sub> produced, as compared with LPG burning<sup>2</sup>. Moreover, in addition to the low emission of greenhouse gases (GHGs), the amount of generated

soot and sulfur causing several adverse impacts on human health is proved to be zero<sup>4</sup>, and the cetane number of DME is 55 – 60<sup>3</sup>. These outweigh the properties of diesel oil (DO) in terms of toxic waste generation and combustion efficiency. The aforementioned outstanding properties of DME bring its promisingly potential to substitute LPG and DO as a clean and effective type of fuel.

Technically, synthesis gas plays a role as the major intermediate material for DME production, meaning the primary sources of feedstocks, such as natural gas (NG), coal, or biomass waste, should be considered for processing<sup>5</sup>. Among those, biomass waste has been considered to be converted into available bio-fuels, especially DME, because of their relatively low prices and abundant availability<sup>5</sup>. Specifically, rice straw, a type of residue left on rice paddy fields after harvesting, contributes to a massive capacity of agricultural residues in Southwest Asia countries whose appropriate climate is for rice cultivation and harvesting. For instance, in Vietnam, one of the world's leading rice exporters, about 45 million tons of rice paddies are produced; in parallel, approximately 53.3 mil-

**Cite this article :** Huynh V Q, Duong Y H P, Le T M, Le D T, Tran V T. **Dimethyl ether production from rice straw: process modelling and simulation.** *Sci. Tech. Dev. J. – Engineering and Technology*; 5(S1):1651-1660.

lion tons of straw are released into the fields yearly<sup>6</sup>. The standard treatment measure for rice straw is to burn out for heat recovery, which not only obtains poor energy efficiency but also places a burden on the environment due to pollutants produced. According to previous work by Silalertruksa et al.<sup>5</sup>, the use of rice straw-based DME decreased around 2 – 66% (as an LPG supplement for household application) and 14 – 70% (as the fuel for diesel engines) of GHG emissions in comparison with LPG at the same performance and the existing diesel fuel for transport, respectively<sup>5</sup>. Therefore, the conversion pathway that turns rice straw into DME is worth considering, providing a sustainable approach for agricultural residue utilization and global warming reduction.

Overall, the DME production process from rice straw consists of two major stages: feedstock gasification and DME synthesis from rice straw-derived syngas<sup>7</sup>. Regarding the DME synthesis section, the single-step method, where DME is directly formed from syngas within one reactor, has been recently prioritized rather than the two-step one using methanol as the intermediate feedstock between rice straw and DME<sup>3</sup>. Specifically, the direct route is catalyzed over a bifunctional catalyst CuO – ZnO – Al<sub>2</sub>O<sub>3</sub>/γ – Al<sub>2</sub>O<sub>3</sub> at 260°C and 50 bar<sup>8</sup>. It is proved that the H<sub>2</sub>/CO ratio in syngas feed critically affects synthesis performance. Ogawa et al.<sup>9</sup> originally developed the single-step DME synthesis process, namely JFE technology. This technology showed that the ratio of H<sub>2</sub> to CO should be adjusted at 1 in a slurry bed reactor, gaining the DME yield as much as 90% with an extremely small amount of water produced<sup>9</sup> as compared to the findings of Song et al.<sup>10</sup> with H<sub>2</sub>/CO = 1.5 and DME yield of around 50% in a fixed bed reactor using computer-based – experimental methodology<sup>10</sup>. As a result, to achieve a high DME yield, the amount of the two most necessary reactants that participate in the synthesis stage (CO and H<sub>2</sub>) has to be maximized by the prior section, the gasification stage. Several research on the investigation of the effects of biomass types, gasifier configurations and gasifying agent options, which meet process requirements, were conducted. The circulating fluidized bed gasifier type was proved to fulfill the expectations for biomass gasification based on the following reasons: suitable for various biomass types, even a mixture of biomass and municipal solid waste; easier to be controlled compared to entrained bed gasifier, with the operating temperature of 800 – 1000°C; and higher char conversion compared to traditional fluidized bed type owing to solid circulation<sup>11</sup>. By way of illustration, Mirmoshtaghi et al.<sup>12</sup> conducted research on circulating

fluidized bed gasifier operating parameters optimization via general algorithm (GA) by MATLAB R2015b, which obtained the results fulfilling the aims of low tar yield and high carbon conversion (S/B = 0.37 and ER = 0.6)<sup>12</sup>. Those findings satisfy such output requirements for syngas leaving the gasifier in the biomass-based DME production process using two combined gasifying agents: steam and air (or pure oxygen or sometimes CO<sub>2</sub>)<sup>7</sup>. The gasification performance of steam/air as mediums is fundamentally less than that of steam/O<sub>2</sub> mediums due to the participation of inert components (i.e., N<sub>2</sub>, Ar...) occupying large proportions in air<sup>13</sup>; nevertheless, the optimal operating conditions of the rice straw gasification process for DME synthesis are still yet to be specified.

This research, therefore, aims to accomplish the following objectives: (1) modeling and simulating the DME production process from rice straw; (2) investigating the influence of gasification operating parameters on the produced syngas composition, thereby determining the most appropriate conditions for produced DME maximization. Such a design is expected to offer a beneficial and sustainable solution for DME production in agriculture-based countries where rice straw is the major crop.

## MATERIALS AND METHODS

The below steps were carried out to set up the database for physicochemical property calculation and simulation of models involved in this research.

### Chemical component list creation

Most of the chemical components involved in this work, excluding rice straw and ash, are represented under pure component type, whose databases are available in HYSYS Databank (O<sub>2</sub>, H<sub>2</sub>O, CO, CO<sub>2</sub>, DME...). On the other hand, the hypothetical solid component type is chosen to simulate both ash and rice straw components due to their unavailability in HYSYS Databank. Significantly, the feedstock component is modeled through the average chemical formula method proposed by Heryadi et al.<sup>8</sup>, with rice straw composition analyses shown in Table 1. This average formula is estimated at C<sub>5.586</sub> H<sub>7.432</sub> O<sub>4.032</sub> N<sub>0.134</sub> S<sub>0.035</sub>.

### Choice for thermodynamic models

An appropriate thermodynamic model for the estimate of physicochemical properties of components is essential, enabling Aspen HYSYS to establish boundary conditions for the equipment modules used in the simulation. Based on the attributes of the chemical

**Table 1: Detail analyses of rice straw composition**

Category	Analysis parameters	Value	Reference
(MJ/kg)	Lower heating value (LHV)	14.4	14
Proximate analysis (% wt. raw basis)	Volatile matters	65.23	
	Fixed carbon	16.55	
	Ash	12.64	
	Moisture	5.58	
Ultimate analysis (% wt. raw basis)	C	38.61	
	H	4.28	
	O	37.16	
	N	1.08	
	S	0.65	

components involved, two fluid packages were chosen and simultaneously adopted. Chief among these is the Peng – Robinson model (P – R), which provides the accuracy calculation for hydrocarbons and gas phase components at high temperature and high pressure. The other one, Non – Random Two – Liquid model (NRTL), plays a role as the appropriate model to perform a three-component system of methanol – water – DME separation due to its binary coefficient database, thus ensuring high accuracy in distillation process calculation.

### Establishment of reaction sets

Three sets of reactions were prepared: the decomposition of rice straw into constituent elements, water-gas shift reactions (WGSR) for H<sub>2</sub>/CO ratio adjustment, and direct synthesis of DME. The first one is a conversion type representing the pyrolysis stage in the gasifier<sup>15</sup>, where the hypothetical solid component C<sub>5.586</sub> H<sub>7.432</sub> O<sub>4.032</sub> N<sub>0.134</sub> S<sub>0.035</sub> (rice straw) is broken down into C, H<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub>, and S. The WGSR set consists of two reactions (WGS as the primary reaction and steam methane reforming – SMR as side reaction) whereas the direct synthesis of DME includes three reactions. Both are categorized as heterogeneous catalyst types, with adopted kinetic parameters obtained from the previous work of Amran et al.<sup>16</sup> and Song et al.<sup>10</sup>.

### Process design and assumptions

A rice straw-derived DME production process includes six sections, as shown in Figure 1. Among

those, the gasification and DME synthesis blocks are significant sections. Before being fed to the gasification section, the feedstock is milled and dried to remove its external moisture in the pretreatment stage. The gasifier chosen for turning rice straw into a gas product is a circulating fluidized bed type (CFBG). Furthermore, several assumptions were imposed to simplify the gasifier model because of the complication of the gasification process<sup>15</sup>. Gasifying agents used are a combination of steam and pure oxygen. Whereas the gas drying and cleaning section purifies the input syngas stream to the synthesis section, the purification and recycle block is responsible for separating high purity DME from contaminants and unreacted components recycling such as methanol and syngas. Significantly, the raw DME stream is cooled to a negative temperature (-30°C) for reactants recovery, and DME presence restriction in syngas recycled may reverse the synthesis reaction equilibrium<sup>17</sup>. Finally, DME is synthesized within one fixed bed reactor proposed by Song et al.<sup>10</sup>, and DME conversion is assumed to be 64%<sup>8</sup>. Table 2 summarizes the design parameters and assumptions for the corresponding sections.

### Case study and optimization of operating parameters

This work's investigation aims to maximize the amount of DME produced. Various enterprises have commercialized the DME synthesis technology, for example, JFE Group (Japan), Haldor – Topsoe (Denmark), and Air Products and Chemicals (United

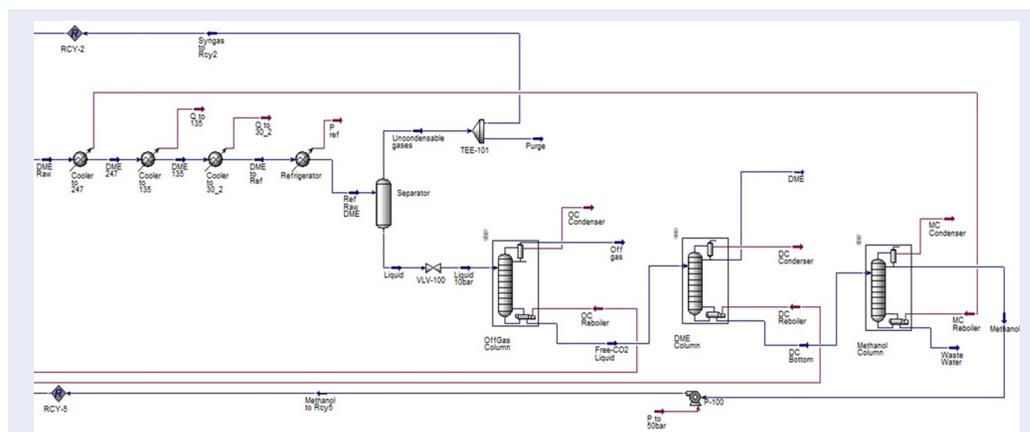


Figure 1: Block flow diagram of the DME production process from rice straw

Table 2: Design parameters and assumptions for the DME production process from rice straw

Section	Parameters and assumptions	Reference
Pretreatment	Drying efficiency = 100%	15
Gasification	Operating conditions: 900 <sup>o</sup> , 10 bar Cyclone separation efficiency = 85% Carbon conversion of char = 96% Carbon loss = 2% N <sub>2</sub> and S only form NH <sub>3</sub> and H <sub>2</sub> S, respectively No tar formation Autothermal operating status	12,15
Water gas shift	Operating conditions: 400oC, 10 bar	8
Gas drying & cleaning	H <sub>2</sub> S removal efficiency = 100% CO <sub>2</sub> removal efficiency = 90% Monoethanolamine (MEA) as absorption solvent	8,18
DME synthesis	Plug flow fixed-bed multi-tube reactor Catalyst: CuO – ZnO – Al <sub>2</sub> O <sub>3</sub> /γ - Al <sub>2</sub> O <sub>3</sub> Operating conditions: 260oC, 50 bar Conversion of CO = 64%	8,10
Purification & recycle	Purge ratio = 5% Distillation operating pressure: 9.5 – 10 bar	8

States) ... Therefore, instead of the case studies into DME synthesis stage operating parameter optimization, the amount of gasifying agent used for rice straw gasification as well as the operating temperature of CFBG should be optimized. For these reasons, this work investigated the effects of the operating temperature of CFBG, S/B ratio, and ER on the output syngas composition, recognizing the patterns and determining points that satisfy the requirements.

## RESULTS AND DISCUSSION

### Process simulation results

The complete process flow diagram (PFD) of the DME production process from rice straw simulated on the Aspen HYSYS environment is separated and presented as follows. Figure 2 demonstrates the three first sections: pretreatment, gasification, and water gas shift. Furthermore, this PFD also includes a heat exchanger network recommended by the Aspen Energy Analyzer (AEA) design for reduction of utility use (heat and cooling utilities).

As no equipment module represents a biomass dryer on Aspen HYSYS, a component splitter block was utilized to separate the H<sub>2</sub>O component from the raw

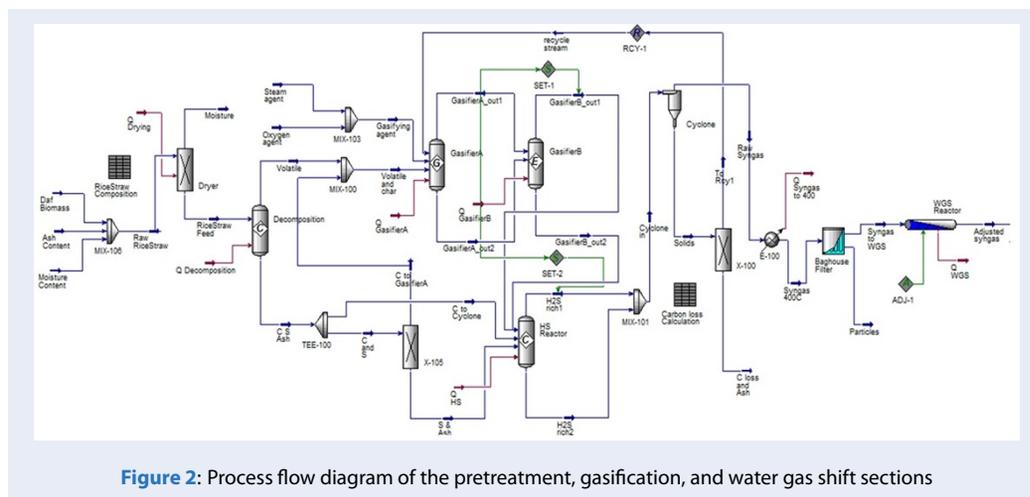


Figure 2: Process flow diagram of the pretreatment, gasification, and water gas shift sections

rice straw. The system of unit operations that starts from the decomposition conversion reactor and ends at X-100 describes the CFBG, followed by a baghouse filter model to remove flying particles left from syngas entirely. In the WGS section, the WGS reaction and SMR reaction occur in a plug flow reactor (PFR) model, and ADJ-1 is used to maintain the output H<sub>2</sub>/CO ratio at 1, with reactor volume as the independent variable and H<sub>2</sub>/CO as the dependent variable.

The PFD of the gas drying & cleaning and the DME synthesis sections are shown in Figure 3, where the H<sub>2</sub>O and acid gases (H<sub>2</sub>S, CO<sub>2</sub>) are removed through the flash separator and the MEA scrubbing system at 30°C, respectively. The 50-bar outlet dry syngas is mixed with recycled streams prior to entering the synthesis section. It is noticeable that although there are two PFRs used in this stage, these reactors fundamentally represent one fixed-bed reactor. The DME Segment 2 illustrates the high-pressure steam (HP steam) generator, utilizing the exothermic DME synthesis stage for the other section.

Figure 4 demonstrates the last section, purification and recycling. The refrigerator brings the raw DME stream's temperature to -30°C, facilitating the mostly total condensation of DME, CO<sub>2</sub>, and water. Three distillation towers undertake the separation of remaining gas components, high purity DME, and methanol for recycling, respectively. In addition, the reboilers of those columns are designed to receive thermal energy from high-temperature process streams and HP steam produced by the DME synthesis reactor.

### Process specifications

In terms of product quality, the pure DME stream that leaves the distillation column reaches a purity of 99.96%, higher than the empty fruit bunch (EFB) based DME with 99.6%<sup>8</sup>. On the other hand, the hourly production capacity of the proposed process is approximately 2.307 tons DME/h, leading to the calculated DME efficiency of 75%, according to Eqs. (1). This parameter reflexes the chemical energy conversion efficiency from feedstocks to products; specifically, the thermal energy stored in DME produced accounts for 75% of the initial rice straw. Also, compared to the  $\eta_{DME} = 73\%$  of the conversion of EFB to DME<sup>8</sup>, rice straw-derived DME is likely to be better.

$$\eta_{DME} = \frac{M_{DME} \times LHV_{DME}}{M_{ricestraw} \times LHV_{ricestraw}} \quad (1)$$

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. Other critical specifications for the involved unit operations are listed in Table 3.

### Influence of operating conditions on outlet syngas composition

The investigations focus on the impacts of three gasification operating parameters: gasifier temperature, steam to biomass ratio, and equivalence ratio. While the S/B ratio represents the relationships between biomass fed to the gasifier and the amount of steam agent used, ER stands for the proportion of actual oxygen agent used for gasification to stoichiometry oxygen for the total combustion of feedstock. These parameters were set to vary from 600 – 1400°C (iteration

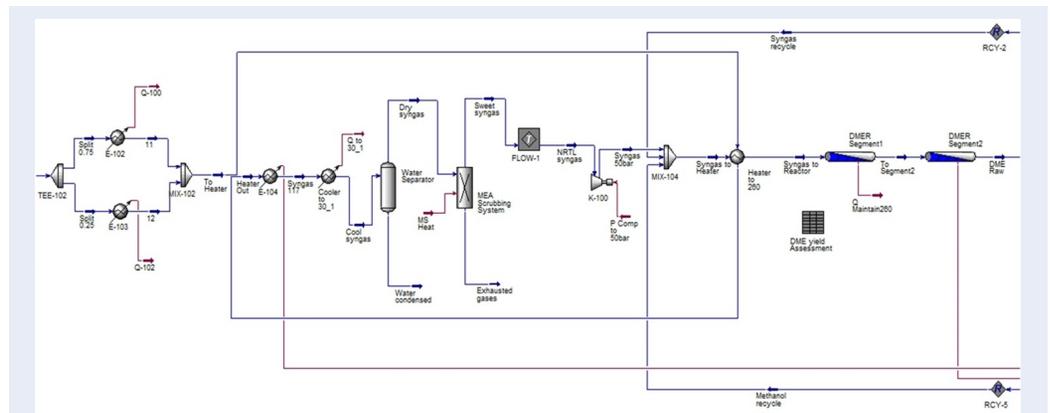


Figure 3: Process flow diagram of the gas drying and cleaning and DME single-step synthesis sections

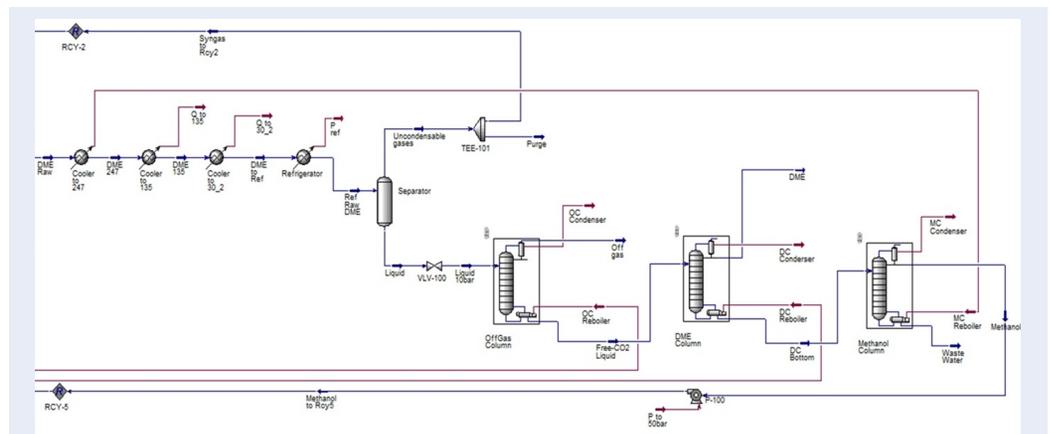


Figure 4: Process flow diagram of the purification and recycling section

= 100°C), 0 – 1 (iteration = 0.1), and 0 – 1 (iteration = 0.1) in respect of gasifier temperature, S/B, and ER, respectively. Figure 5 and Figure 6 show the results of the investigations conducted.

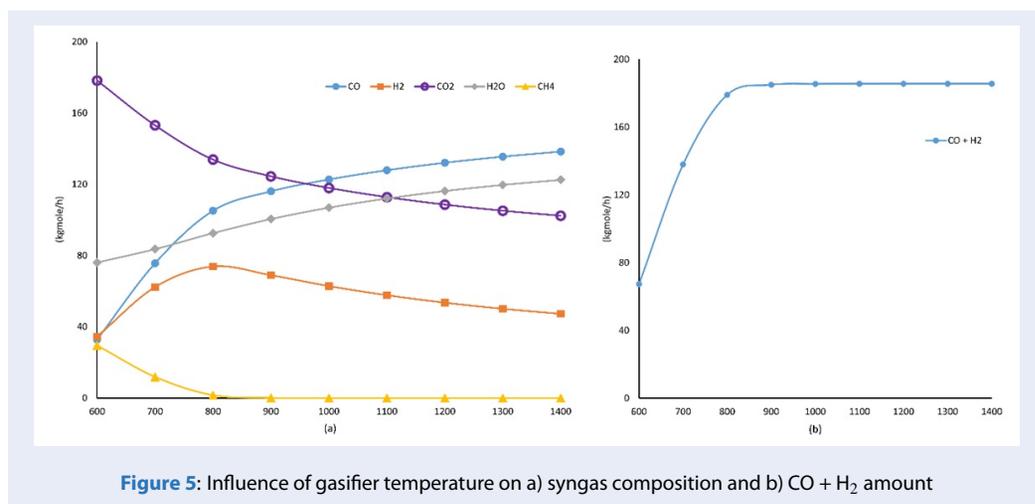
In Figure 5 (a), according to the increasing temperature tendency, the amount of CO<sub>2</sub> decreases steadily while the significantly rising trend of CO is witnessed. However, the other component that takes part in DME synthesis, H<sub>2</sub>, increases when the temperature reaches 800°C and afterward drops slightly. The opposite tendencies of CO and H<sub>2</sub> curves prevent the decision on optimal temperature that maximizes the production of DME. Consequently, the total amount of precursors for DME synthesis was considered, and its result is described in Figure 5 (b): total molar flow rate of (CO + H<sub>2</sub>) grows dramatically by 900°C before unnoticeably rising after that. This reveals that 900°C is capable of optimal operating temperature for the CFBG used in this work. Furthermore, the amount

of CH<sub>4</sub> becomes insignificant at 800°C and more extensive as this component forms CO<sub>2</sub> and even CO; therefore, the higher operating temperature encourages the complete conversion of CH<sub>4</sub> into the dominant component of syngas.

Figure 6 (a) and Figure 6 (b) show the results of two case studies of how syngas composition changes based on the variation of S/B ratio and ER, respectively. The chief similarity between these charts is that the CO<sub>2</sub> and H<sub>2</sub>O generated a rise when the judged variables increased. Another resemblance lies in the CH<sub>4</sub> amount, which is almost trivial and tends to decline; therefore, this component can be ignored. The behaviors of the CO curve and H<sub>2</sub> curve are different in the S/B scenario, whereas the downward trend is observed from both curves in the ER scenario. For S/B variation scenario, simulation results illustrate the similar increased tendencies between (CO + H<sub>2</sub>) produced and H<sub>2</sub>/CO ratio (CO + H<sub>2</sub>) produced and

**Table 3: Key specifications of the DME production process from rice straw**

Item	Function	Specification
DME production capacity	-	2.307 tons/h
DME purity	-	99.96%
DME efficiency	-	$\eta_{DME} = 75\%$
WGS Reactor	Plug flow reactor	D = 0.062 m, L = 2 m, n = 1 tube
Baghouse Filter	Baghouse filter	$A_{cell} = 14.2 \text{ m}^2$ , $A_{bag} = 1.48 \text{ m}^2$
Water Separator	Gas-liquid separator	D = 0.762 m, H = 2.7 m
DME Reactor	Plug flow reactor	D = 1.73 m, L = 10 m, n = 10 tubes
Recycling Separator	Gas-liquid separator	D = 0.61 m, H = 3.35 m
Off-gas Column	Distillation column	9 stages, feed at 1 <sup>st</sup> tray RR = 0.5 P = 950 – 1000 kPa
DME Column	Distillation column	10 stages, feed at 4 <sup>th</sup> tray RR = 0.8 P = 950 – 1000 kPa
Methanol Column	Distillation column	12 stages, feed at 5 <sup>th</sup> tray RR = 7 P = 950 – 1000 kPa



H<sub>2</sub>/CO ratio; nevertheless, they simultaneously reduce in case of ER.

**Decision on S/B ratio and ER**

Fundamentally, gasifiers operate in autothermal or exothermal conditions<sup>13</sup>. The presence of O<sub>2</sub> as gasifying agent provides the process with heat radiated by oxidation reactions, raising the operating temperature of gasifiers. As a result, the total heat balance of the CFBG model simulated in Aspen HYSYS must be equal to 0 (representing autothermal) or smaller

than 0 (representing exothermic). At a specific value of S/B ratio, a minimum amount of O<sub>2</sub> where the heat balance becomes 0 was specified, summarized in Figure 7 (a) – in other words, the O<sub>2</sub> flow rates supplied to CFBG must be higher than the minimum value determined, at the corresponding steam flowrate. Moreover, Figure 7 (b) shows the amount of DME produced against the increased oxygen agent: the larger O<sub>2</sub> is used, the less DME generates. This leads to the point that at a constant value of the S/B ratio, its minimum value of O<sub>2</sub> brings the highest production rate.

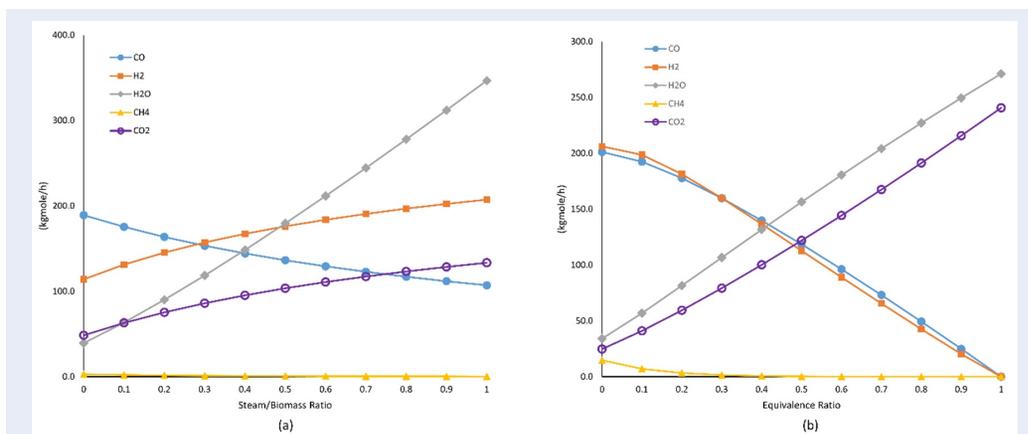


Figure 6: The variation in syngas composition, depending on: a) steam/biomass ratio; and b) equivalence ratio

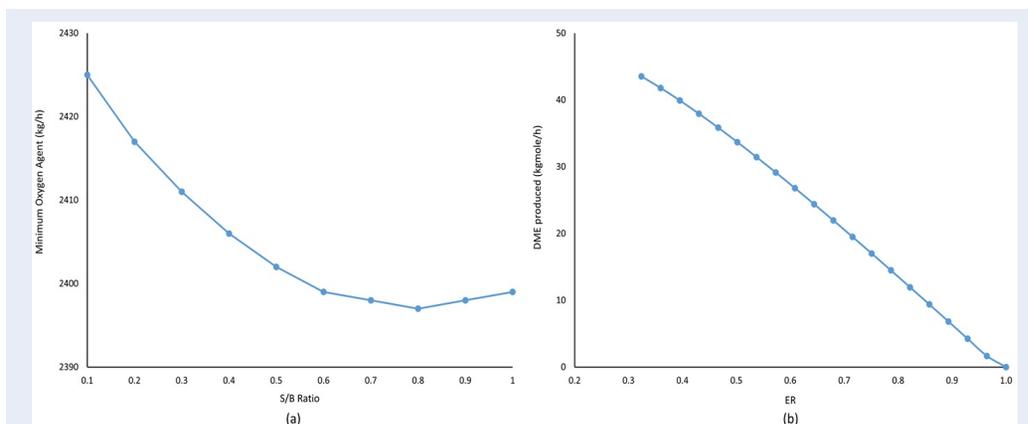


Figure 7: (a) Minimum values of O<sub>2</sub> at respective S/B ratios (a); and (b) impact of ER on DME produced amount

From the aforementioned evaluations, DME production yield was afterward investigated by having gasifying agent flow rate varied from 10 – 110 kmol/h to determine corresponding minimum O<sub>2</sub> amount as above proofs. Eventually, those parameters which yields the highest amount of DME produced are 110 kmol/h steam and 2412 kg/h oxygen (S/B = 0.27 and ER = 0.32, respectively). Therefore, these are the values of S/B ratio and ER that maximizes DME production in our investigation.

### CONCLUSION

This research adopted a computational method to design and optimize a production process that converts the dominant type of agricultural residue in Vietnam, rice straw, into dimethyl ether (DME), a promising alternative fuel. A complete process flowsheet was modeled and simulated on Aspen HYSYS<sup>TM</sup>, and the production capacity was obtained at 2.307 tons

DME/h with 99.96% purity. On the other hand, the DME efficiency achieved 75%, and the results of the CFBG’s operating parameters for maximizing DME produced were also specified: operating temperature of 900°C, S/B ratio = 0.27, and ER = 0.32.

### ACKNOWLEDGMENTS

This research is funded by Ho Chi Minh city University of Technology-VNU-HCM, under grant number To- KTHH-2021-10. We acknowledge the support of time and facilities from Ho Chi Minh City University of Technology (HCMUT), VNU-HCM for this study.

### ABBREVIATION

- EFB: Empty fruit bunch
- DME: Dimethyl ether
- DO: Diesel oil
- LPG: Liquefied petroleum gas

GHGs: Greenhouse gases  
 NG: Natural gas  
 NRTL: Non-random two-liquid  
 WGSR: Water-gas shift reaction  
 CFBG: Circulating fluidized bed gasifier  
 PFD: Process flow diagram  
 AEA: Aspen Energy Analyzer  
 PFR: Plug flow reactor

## COMPETING INTERESTS

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

## CREDIT AUTHOR STATEMENT

**Vinh Q.H.** and **Yen H.P.D.** Conceptualization; Data curation; Roles/Writing - original draft; Writing - review & editing; **Tan M.L.** Conceptualization; Data curation; Roles/Writing - original draft, review & editing. **Duc T.L.** Formal analysis; Investigation; Visualization, review & editing. **Viet T.T.** Funding acquisition; Methodology; Project administration; Resources; Supervision; review & editing. Both **Vinh Q.H** and **Yen H.P.D.** contributed equally and have the right to list their name first in their CV. All authors contributed to the article and approved the submitted version.

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# Mô hình hóa và mô phỏng quy trình sản xuất dimethyl ether từ rơm rạ

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## TÓM TẮT

Biến đổi khí hậu đã và đang là mối quan tâm trên toàn thế giới trong những thế kỷ gần đây, và sự khai thác cũng như sử dụng nhiên liệu hóa thạch là tác nhân góp phần lớn vào sự hủy hoại môi trường. Nhiều nguồn năng lượng thay thế đã được xem xét và đánh giá để tìm ra một phương án khả thi cho tương lai, và dimethyl ether (DME) là một lựa chọn đáng được quan tâm. Trong bài nghiên cứu này, một quy trình sản xuất DME liên tục đã được phát triển và mô phỏng bằng phần mềm Aspen HYSYS™. Rơm rạ, nguồn sinh khối phổ biến nhất tại Việt Nam, được chọn để trở thành nguyên liệu cho quá trình. Quy trình được đề xuất bao gồm năm cụm chính: tiền xử lý rơm rạ và khí hóa tạo khí tổng hợp bằng thiết bị khí hóa tầng sôi tuần hoàn (CFBG); phản ứng water-gas shift (WGSR) cho việc điều chỉnh tỉ lệ H<sub>2</sub>/CO trong khí tổng hợp; cụm làm sạch khí, nơi loại bỏ nước, H<sub>2</sub>S và CO<sub>2</sub> bị loại bỏ; tổng hợp DME bằng phương pháp sản xuất trực tiếp; và cụm làm sạch DME nhằm phân tách sản phẩm chính và hồi lưu methanol. Kết quả mô phỏng cho thấy năng suất sản xuất của quy trình là khoảng 2307 kg mỗi giờ, cùng với hiệu suất chuyển hóa năng lượng hóa học ( $\eta_{DME}$ ) từ sinh khối đạt 75%. Bên cạnh đó, bài báo cũng thực hiện khảo sát ảnh hưởng từ các thông số vận hành của thiết bị CFBG cho mục tiêu tối đa hóa lượng DME sản xuất ra. Từ dữ liệu khảo sát thu được, các giá trị của nhiệt độ vận hành CFBG, tỉ lệ hơi nước trên sinh khối (S/B), và tỉ số đương lượng (ER) thỏa mãn mục tiêu trên lần lượt là 900°C, 0,27, và 0,32. Nghiên cứu này đưa ra một lựa chọn mới cho việc tận dụng nguồn sinh khối thải có trữ lượng cực lớn từ hoạt động nông nghiệp tại Việt Nam bằng cách chuyển hóa nó thành một loại nhiên liệu tiềm năng, từ đó giảm thiểu gánh nặng môi trường cũng như có thể phát triển thị trường năng lượng Việt Nam.

**Từ khóa:** Dimethyl ether, mô hình hóa quy trình, mô phỏng, rơm rạ

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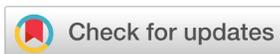
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## Lịch sử

- Ngày nhận: 27-5-2022
- Ngày chấp nhận: 11-01-2023
- Ngày đăng: 31-1-2023

DOI : <https://doi.org/10.32508/stdjet.v5i4.1014>



**Trích dẫn bài báo này:** Vinh H Q, Yến D H P, Tấn L M, Đức L T, Việt T T. **Mô hình hóa và mô phỏng quy trình sản xuất dimethyl ether từ rơm rạ.** *Sci. Tech. Dev. J. - Eng. Tech.*; 2022, 5(S1):1651-1660.