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# Bio-DME production based on conventional and CO<sub>2</sub>-enhanced gasification of biomass: A comparative study on exergy and environmental impacts

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## **Abstract**

In this study, a novel single-step synthesis of dimethyl ether (DME) based on CO<sub>2</sub>-enhanced biomass gasification was proposed and simulated using ASPEN Plus<sup>TM</sup> modelling. The exergetic and environmental evaluation was performed in comparison with a conventional system. It was found that the fuel energy efficiency, plant energy efficiency and plant exergetic efficiency of the CO<sub>2</sub>-enhanced system were better than those of the conventional system. The novel process produced 0.59 kg of DME per kg of gumwood with an overall plant energy efficiency of 65%, which were 28% and 5% higher than those of conventional systems, respectively. The overall exergetic efficiency of the CO<sub>2</sub>-enhanced system was also 7% higher. Exergetic analysis of each individual process unit in both the CO<sub>2</sub>-enhanced system and conventional systems showed that the largest loss occurred at gasification unit. However, the use of CO<sub>2</sub> as gasifying agent resulted in a reduced loss at gasifier by 15%, indicating another advantage of the proposed system. In addition, the LCA analysis showed that the use of CO<sub>2</sub> as gasifying agent could also result in less environmental impacts compared with conventional systems, which subsequently made the CO<sub>2</sub>-enhanced system a promising option for a more environmental friendly synthesis of bio-DME.

**Keywords:** Exergy analysis; Environmental analysis; Bio-DME; CO<sub>2</sub>-enhanced gasification; conventional gasification

## 26 **1 Introduction**

27 Biomass derived dimethyl ether (Bio-DME) is a clean synthetic fuel that has high cetane number  
28 and similar physical properties as LPG [1, 2]. The combustion of bio-DME generates small amount  
29 of NO<sub>x</sub>, almost zero SO<sub>x</sub> and particulate matter. Thus, bio-DME is considered as a sustainable  
30 alternative to diesel and LPG. Compared with commercially available double-step synthesis, the  
31 single-step synthesis is a better option for DME production due to its low investment and low  
32 production costs [3, 4]. Among single-step synthesis technologies developed, JFE technology, a  
33 process adopting H<sub>2</sub>: CO ratio of 1:1 for DME synthesis, was found to be more cost-effective than  
34 other technologies, such as Hardlor Topsoe technology [1, 5].

35 Over the past two decades, the use of CO<sub>2</sub> as a gasifying agent in biomass gasification has drawn  
36 increasing interests [6-8]. One of its unique features in this technology is that the H<sub>2</sub>/CO ratio in  
37 syngas can be adjusted by controlling the amount of CO<sub>2</sub> injected to gasifier, despite the additional  
38 heat need to be supplied into gasifier due to the endothermic nature of reaction involved during  
39 gasification [9-11]. Recent research demonstrated that for DME production based on CO<sub>2</sub>-enhanced  
40 gasification, the water gas shift (WGS) reactor and the energy intensive CO<sub>2</sub> removal process could  
41 be avoided while the production of DME could be enhanced [12]. In addition, the pure CO<sub>2</sub> can be  
42 easily recycled as CO<sub>2</sub> is a major by-product of DME synthesis. However, not much effort has yet  
43 been made to understand the exergy efficiency and environmental impacts of this novel system.

44 Generally, exergy analysis specifies the location, type and magnitude of process irreversibility [13-  
45 15]. It also helps better understand the benefits of energy utilization by providing more useful and  
46 meaningful information than what energy analysis could possible provide. Therefore, exergy  
47 analysis is commonly used to compare the performance of different processes, such as biomass-  
48 gasification and coal-gasification based processes [16-21]. With regard to exergy analysis of bio-  
49 DME production, to date, only a few studies have been reported [22, 23]. Exergy analysis of  
50 double-step bio-DME production using steam as gasification agent was carried out by Zhang et al.

51 [23] to measure the exergy efficiency of the entire system as well as the exergy losses occurred in  
52 each unit of the system. The reasons behind these losses were explored and suggestions to improve  
53 the exergy efficiency of the system were made. Recently, Xiang et al. [22] conducted the exergetic  
54 evaluation of a single-step bio-DME production from biomass where pure DME was obtained as  
55 the final product. The estimation of system exergetic efficiency and the origin of losses were also  
56 identified and quantified. Moreover, the causes of the inefficiencies were investigated and by  
57 optimising various process parameters, the higher exergetic efficiency of the system was achieved.  
58 However, in spite of the great potential of DME production based on CO<sub>2</sub>-enhanced gasification, in  
59 depth assessment of this new route has hardly been explored due to the lack of detailed process  
60 design. To the best of our knowledge, there is not any published research on the exergetic  
61 assessment of bio-DME production using CO<sub>2</sub> as the gasifying agent. In addition, although life  
62 cycle assessment (LCA) is commonly used to evaluate environmental impacts of a product over its  
63 life cycle [16, 24, 25], the application of LCA approach for the environmental assessment of bio-  
64 DME production based on CO<sub>2</sub>-enhanced gasification has not been reported.

65 This study was focused on the simulation of conventional DME synthesis system as well as DME  
66 production based on CO<sub>2</sub>-enhanced gasification of biomass. The goal of this study was to assess the  
67 exergetic and environmental performance of bio-DME production using CO<sub>2</sub> as a gasifying agent.  
68 The comparison of energy, exergetic and environmental analyses between the two processes were  
69 also carried out. In addition, effort was made to show the location, magnitude and causes of the  
70 process unit inefficiencies.

## 71 **2 Process description and design**

### 72 **2.1 Process overview**

73 Fig. 1 shows the simplified process flow diagrams of the single-step DME production based on  
74 conventional and CO<sub>2</sub>-enhanced biomass gasification systems. The configurations have been

75 optimized following the guidelines proposed elsewhere [1, 22, 23, 26, 27]. In these systems,  
76 biomass feedstock is converted to syngas in a fluidised-bed gasifier, which is then conditioned prior  
77 to DME synthesis. The present work was focused on the assessment of the influence of CO<sub>2</sub>  
78 addition on the overall system performance.

79 The gasifiers for the two processes are operated under relatively different conditions. As seen in  
80 Fig. 1, the conventional process uses oxygen and steam as the gasifying agent while the CO<sub>2</sub>-  
81 enhanced process utilises carbon dioxide with steam. For the CO<sub>2</sub>-enhanced biomass gasification  
82 based DME production (CEBG-DME) process, since H<sub>2</sub>/CO ratio can be tuned by selecting proper  
83 CO<sub>2</sub>/biomass ratio and steam/biomass ratio (as shown in Fig. 1b), the WGS and energy intensive  
84 CO<sub>2</sub> separation unit are eliminated. Another beneficial feature of this process is the avoidance of  
85 using of the oxygen separation unit, which could cause significant energy consumption as well as  
86 high capital and operating costs. As CO<sub>2</sub> is one of the main products of the single-step DME  
87 synthesis, in the CEBG-DME system, a portion of the emitted CO<sub>2</sub> is used in the gasifier as the  
88 gasifying agent, which helps reduce net CO<sub>2</sub> emission of the system. However, due to the  
89 endothermic nature of gasification reactions, additional energy is required to maintain a desired  
90 temperature in the gasifier. Since fluidized bed gasifier is used in this study, it was proposed that  
91 heat was introduced into the gasifier using an inert energy carrier. However, during simulation,  
92 electrically-heated gasifier was considered in the current study.

93

## 94 **2.2 Biomass to syngas train**

95 In this study, gumwood was selected as the biomass feedstock because it is widely available in  
96 China as well as in South-East Asian countries. Its properties are listed in Table 1 [28].

97 During gasification, the C, H, and O are transformed to CO, H<sub>2</sub>, CO<sub>2</sub>, and CH<sub>4</sub>, while N and S are  
98 converted to NH<sub>3</sub>, H<sub>2</sub>S and COS, respectively. Since particulates (such as fly ash) that can  
99 potentially foul and/or poison the catalyst in the downstream, prior to DME synthesis, particulate

100 matter is removed using a bag filter. A heat exchanger is used in the HRSG unit to recover waste  
101 heat to produce steam that is used in gasification unit as well as other process units. Part of the  
102 recovered heat is used for electricity generation, which is to meet electricity demand of the entire  
103 plant.

104 In conventional DME synthesis process, the gas product (syngas) is then transported to a WGS unit  
105 to adjust the H<sub>2</sub>/CO molar ratio of 1 to satisfy the requirement for DME synthesis, followed by the  
106 purification prior to synthesis because H<sub>2</sub>S is poisonous to the synthesis catalyst [3, 29] and an  
107 excessive amount of CO<sub>2</sub> will reduce the conversion efficiency of DME synthesis [2, 12]. In the  
108 purification section, a typical chemical absorption process with monoethanolamine (MEA) is  
109 selected to remove H<sub>2</sub>S and CO<sub>2</sub>, which is detailed elsewhere [30, 31].

110 However, for CO<sub>2</sub>-enhanced gasification based DME synthesis (Fig. 1b), the required H<sub>2</sub>/CO molar  
111 ratio and CO<sub>2</sub> concentration in syngas is attained by adjusting gasification operating parameters  
112 such as temperature, CO<sub>2</sub>/biomass ratio and steam/biomass ratio. Consequently, the WGS reaction  
113 unit and energy intensive CO<sub>2</sub> purification unit, the two essential steps for conventional DME  
114 production process (Fig. 1a), are avoided. It is important to note that with the addition of steam in  
115 the gasifier, WGS unit in conventional system can be avoided. However, from the perspective of an  
116 overall plant economics, this approach is not likely to be feasible, as many factors such as type of  
117 gasifier need to be considered. In order to prevent catalyst from being poisoned, only H<sub>2</sub>S removal  
118 unit is installed.

### 119 **2.3 Syngas to DME train**

120 The purified syngas is then fed into the compressor and cooler, and subsequently introduced to the  
121 single-step synthesis reactor. As the single-step DME reaction is exothermic, to maintain an  
122 optimal reaction temperature, certain amount of heat must be removed rapidly from the reaction  
123 system, which can be utilized to generate high-pressure steam. Hence, a slurry reactor was

124 considered in this study due to its easiness in temperature control and uniform temperature  
125 distribution [1, 22]. The product stream from the synthesis reactor is cooled down and flashed so  
126 that the unreacted syngas is separated from the DME-methanol-water mixture. Afterwards, the  
127 majority of the unreacted syngas from the flash separator is recycled to DME synthesis reactor.  
128 This leads to an overall high DME conversion, while the rest of the stream was purged. The DME–  
129 methanol–water mixture contains some residual gas such as CO and CO<sub>2</sub>, hence, it is sent to CO<sub>2</sub>  
130 removal unit to remove the residual gas. It is essential to note that a fraction of emitted CO<sub>2</sub> by the  
131 synthesis reactor is fed to the gasifier as it is used as one of the gasifying agents for the CO<sub>2</sub>-  
132 enhanced biomass gasification. In the meantime, bottom product of the CO<sub>2</sub> removal unit is fed to  
133 the DME distillation unit. Distillate from this unit is taken as DME product. The methanol-water  
134 mixture, the bottom product, is sent to methanol distillation unit to separate water from methanol.  
135 The recovered methanol is also recycled to the DME reactor, whereas bottom product water, which  
136 still contained a very low amount of methanol, requires further purification. A base-case design of  
137 this study is illustrated in Fig. 1, which is for the preliminary assessment of a process design and  
138 has not yet been optimized at this stage.

## 139 **2.4 Key gasification parameters**

140 Apart from operating pressure, temperature and oxidising agent are the two important factors that  
141 dictate the composition of syngas in any gasification processes. Whilst for syngas, H<sub>2</sub>/CO ratio and  
142 the percentage of CO<sub>2</sub> are the two crucial parameters that have significant impacts on its  
143 purification and application. There are other factors commonly used to evaluate gasification  
144 process, such as lower heating value (LHV) of gas product, cold gas efficiency (CGE), and  
145 gasification system efficiency (GSE) [9, 10]. Moreover, for JFE single-step DME synthesis, the  
146 H<sub>2</sub>/CO ratio is also vital, which should be controlled to be 1.

147 In order to design a process for the highly efficient synthesis of DME, it is important to understand  
148 the relationship of these parameters. In this study, the parametric analysis was therefore conducted

149 to optimize the gasification process. The parameters for the gasification process used in this work  
150 are listed in Table 2, in comparison with those for a conventional (O<sub>2</sub>-steam) process. In addition,  
151 for comparison purposes, Table 2 also includes a set of gasification data that were reported by  
152 others under similar conditions [1].

## 153 **3 Methodology**

### 154 **3.1 Process simulation**

155 Simulation of the two DME systems was conducted using Aspen Plus<sup>TM</sup> to establish materials  
156 balance, and to estimate the energy and utility requirements as the inputs for exergy and  
157 environmental analysis. Details of assumptions and modelling procedures have been discussed  
158 elsewhere [9, 12].

159 In this study, a RYield module (yield reactor) integrated with a RGibbs module (chemical and  
160 phase equilibrium by Gibbs free energy minimisation) was employed to simulate gasifier, which  
161 was operated (0.1 MPa). Thus, heat inputs to the gasifier included heat duty of RYield and RGibbs  
162 reactors. The operating conditions of the gasifier for both systems are presented in Table 2.

### 163 **3.2 Model validation**

164 Before thermodynamic evaluation of the studied systems, the CO<sub>2</sub>-enhanced gasification model has  
165 to be validated. In this study, the model developed was validated against data published by other  
166 researchers [10, 21, 32]. As mentioned previously, biomass gasification was modelled using Gibbs  
167 minimisation approach, which has been validated with experimental data [33-35]. Since there is no  
168 relevant data available on CO<sub>2</sub>-enhanced gasification using gumwood as the raw material, in order  
169 to validate the model developed in this work, data of steam gasification of wood and CO<sub>2</sub>  
170 gasification of biomass were extracted from literature and compared with the simulation results  
171 (under the same experimental conditions as adopted in the literature) as shown in Table 3 and Table

172 4, respectively [10, 21]. Based on these comparisons, it can be concluded that the simulation results  
173 are in good agreement with data reported in literature [10, 21, 32]. The deviation was found to be in  
174 a range of 4.1%-8.6%. Therefore, the CO<sub>2</sub>-enhanced gasification model developed in this study is  
175 reliable, and was subsequently used for the prediction of CO<sub>2</sub>-enhanced gasification of gumwood.

176 The product gas from the gasifier was sent to the SSplit (SSEPARAT) module to remove ash, prior  
177 to cooling down to 220 °C. HeatX (HRSG) module was used to recover heat (via steam at 0.5 MPa,  
178 225 °C) from hot syngas. Afterwards, syngas was sent to WGS reactor to adjust its H<sub>2</sub>/CO ratio.  
179 The WGS reactor (0.1 MPa, 220 °C) was modelled with a REquil module. After WGS reactor, the  
180 syngas was cooled down to 60 °C before being directed to syngas purification unit. The removal of  
181 CO<sub>2</sub> and H<sub>2</sub>S by MEA absorption process in syngas purification unit was modelled as a simple  
182 component separator SEP2 module due to the complexity of the system. The energy required for  
183 this system was assumed to be 3 MJ/kg of CO<sub>2</sub> captured by MEA absorption process [10]. The  
184 single-step DME synthesis was operated at 6 MPa and 250 °C. The purified syngas was then  
185 pressurised, cooled down, and introduced into the DME reactor. A REquil module was employed  
186 as the DME reactor to simulate the synthesis process, which is reliable in DME synthesis  
187 simulation [36, 37]. The other operating parameters and DME synthesis reactions simulated in the  
188 present work were adopted from literatures [36-39].

189 Product of the DME reactor was cooled down to -30 °C in MHeatX (X) module and consequently,  
190 non-condensable gases were removed using Flash2 (FLASH) separator module. In order to recycle  
191 the non-condensable gaseous, most of the gas was sent back to DME reactor and the remainder was  
192 purged. After the flash separator, the liquid stream was then sent to the product purification  
193 process. This section is consisted of three units, i.e., CO<sub>2</sub> removal unit (2 MPa), DME distillation  
194 unit (1.52 MPa) and MeOH unit (1.52 MPa) as illustrated in Fig 1. Distillation column was  
195 employed for each of the unit, which was simulated using RadFrac module. The distillation  
196 parameters, such as the number of stages and reflux ratio, were set to achieve high purity (99.9

197 mol%) of DME product. The reaction heat from synthesis reactor was recovered using Heat Stream  
198 option in Aspen Plus<sup>TM</sup> to generate high-pressure steam at 3.5 MPa and 244 °C.

### 199 3.3 Exergy analysis

200 From a thermodynamic point of view, exergy is defined as the maximum amount of work that can  
201 be generated by an energy system as it comes to equilibrium with the reference of environment [15,  
202 17]. It measures both the quality and quantity of energy involved in the conversion within a system.  
203 Therefore, it enables the detection of losses and identifies the opportunities for the improvement of  
204 energy consumption. The objective of exergy analysis is to identify process units with relatively  
205 high inefficiency. In addition, exergy analysis can also be used to compare different process  
206 configurations to find better options.

207 Generally, the exergy balance of individual process unit within energy transformation system can  
208 be expressed as:

$$209 \quad \sum \dot{E}ex_{in} = \sum \dot{E}ex_{out} + \dot{E}ex_{loss} + \dot{E}ex_{des} \quad (1)$$

210 where,  $\sum \dot{E}ex_{in}$  and  $\sum \dot{E}ex_{out}$  denote the sums of exergy rates for inlet flows and outlet flows,  
211 respectively, including the materials streams, thermal stream and work. The  $\dot{E}ex_{loss}$  stands for the  
212 exergy loss rate of the streams that exit the system without further use. Meanwhile,  $\dot{E}ex_{des}$  depicts  
213 the exergy destruction rate, which represents the inefficiencies existed in the system. For simplicity,  
214 these two parts were merged in a term called exergy losses and destructions,  $\dot{E}ex_{L\&D}$ , which is  
215 evaluated as follows:

$$216 \quad \dot{E}ex_{L\&D} = \sum \dot{E}ex_{in} - \sum \dot{E}ex_{out} \quad (2)$$

217 In the present work, exergy of streams, such as biomass, gases, liquid and heat, was calculated  
218 using the concept, which has been explained elsewhere [9, 17, 40, 41]. The considered systems  
219 were decomposed into different functional process units. For each unit, exergy balance was  
220 performed and  $\dot{E}x_{L\&D}$  was calculated.

### 221 **3.4 Energy and exergy efficiencies**

222 The fuel energy efficiency is the fraction of energy stored in the biomass that is converted into  
223 energy of the fuel product, as given in Eq. (3) [27, 42].

$$224 \quad \eta_{Fuel} = \frac{E_{fuel,out}}{E_{biomass,in}} \quad (3)$$

225 where,  $E_{fuel, out}$  is the energy in the fuel produced and  $E_{biomass,in}$  is the energy in the feedstock.

226 As Eq. (3) does not include all inputs and useful outputs of the system, the plant energy efficiency  
227 was also used to evaluate performance of the entire system as shown in Eq. (4).

$$228 \quad \eta_{Plant} = \frac{E_{fuel,out} + Q_{net,out}}{E_{biomass,in} + E_{agent,in} + E_{Q,in} + E_{W,in}} \quad (4)$$

229 where,  $E_{agent,in}$ ,  $E_{Q,in}$ , and  $E_{W,in}$  are the total energy input as gasification agent, thermal energy and the  
230 net work in plant, respectively, whereas  $Q_{net,out}$  represents the total heat output as district heat level.

231 Gasification process efficiency was evaluated using cold gas efficiency (CGE) and gasification  
232 system efficiency (GSE), which are described elsewhere [9].

233 The system exergy efficiency ( $\eta_{ex}$ ) was calculated using Eq. (5) (derived from Eqs. 1 & 4) as the  
234 useful exergy content in outlet flows divided by the exergy content in inlet flows.

235 
$$\eta_{ex} = \frac{Eex_{out}}{Eex_{in}} \quad (5)$$

236 **3.5 Environmental analysis**

237 The goal of environmental analysis was to assess the environmental impacts of CO<sub>2</sub> utilisation in  
238 bio-DME production. Thus, investigation was conducted to compare the two scenarios:  
239 conventional bio-DME production (scenario 1) and CO<sub>2</sub>-enhanced bio-DME production (scenario  
240 2). Energy and exergetic assessment of these two scenarios indicated that using CO<sub>2</sub> as gasification  
241 agent can significantly improve the process performance. Moreover, CO<sub>2</sub> was consumed in CO<sub>2</sub>-  
242 enhanced process. This meant that, the net CO<sub>2</sub> emission in CO<sub>2</sub>-enhanced system was lower than  
243 that of conventional. The environmental impact assessment was performed using the ReCiPe 2008  
244 v.3.14 method from SimaPro 8.0 software package. ReCiPe 2008 encompasses two sets of impact  
245 categories (mid-point level and end-point level) associated with two sets of categorization factors.  
246 Detail explanation of impact categories and qualitative indicator can be found elsewhere [9, 43-45].  
247 In the present work, approximately 1 kg of DME produced from conventional and CO<sub>2</sub>-enhanced  
248 biomass gasification was used as the functional unit for environmental analysis. LCA of individual  
249 input and output streams of the overall system, including full life cycle of components, was  
250 conducted. The input data (*i.e.*, consumption of feedstock, agents and energy as well as emissions)  
251 of this analysis are obtained from Aspen Plus<sup>TM</sup> simulation results. The system boundaries set for  
252 this study are illustrated in Fig. 1. The scope of this study includes the following aspects: (1) supply  
253 of biomass, gasification agents and other utilities to the DME production system; (2) production of  
254 DME via biomass gasification process; (3) heat recovery from the system; and (4) utilisation of  
255 emitted CO<sub>2</sub>. Both CO<sub>2</sub> and CH<sub>4</sub> were considered as the main GHG (greenhouse gases) for the  
256 assessment of environmental impact.

## 257 **4 Results and Discussion**

258 In this study, the energetic comparison between conventional and CO<sub>2</sub>-enhanced bio-DME  
259 production, the biomass consumption per kilogram of DME production, exergy balance of the  
260 entire plant and exergy losses and destructions to each unit were carried out to disclose the energy  
261 saving mechanism. Finally, the environmental impacts caused by these two routes were assessed  
262 using LCA method.

### 263 **4.1 Mass and energy balances**

264 Table 5 presents the overall mass and energy balances for the two DME production routes, i.e.,  
265 conventional and CO<sub>2</sub>-enhanced processes. The energy balances indicated that biomass feedstock  
266 required most of the energy input (37-46%) in the system. It is noted that biomass input with  
267 respect to its mass and energy content and the quality of product DME were equalized in both  
268 cases; thus, results could be compared. It can be seen from Table 5 that CO<sub>2</sub>-enhanced system  
269 produced 0.59 kg DME per kg gumwood with a fuel conversion efficiency (detailed in Eq. 3) of  
270 85.0%, which is 18% higher than the conventional process. This was because of higher amount of  
271 syngas processed in DME synthesis reactor as a results of using CO<sub>2</sub> in the gasifier which reduced  
272 the molar ratio of H<sub>2</sub>/CO by increasing CO fraction in syngas [9]. It was also found that the  
273 addition of CO<sub>2</sub> reduced the percentage of CH<sub>4</sub> in syngas. Hence, this resulted to a lower amount of  
274 purge gas from the synthesis reactor in the CO<sub>2</sub>-enhanced system as DME conversion efficiency is  
275 generally limited by high CH<sub>4</sub> percentage in syngas [37]. The aforementioned phenomena could  
276 also result in a higher DME production rate. An overview of DME system parameters of the  
277 present work and published works is given in Table 6, particularly in terms of comparing the mass  
278 yield and plant energy efficiency of the systems. Clearly, CO<sub>2</sub>-enhanced system produced higher  
279 amount of DME, which led to the greater plant energy efficiency. The present work is  
280 fundamentally differed from the reported work as it uses CO<sub>2</sub> as the gasifying agent. The CO<sub>2</sub>  
281 addition could lead to the increase in CO fraction in syngas which influenced the H<sub>2</sub>/CO ratio and

282 the yield of syngas [9]. For instance, H<sub>2</sub>/CO ratio of 1 was achieved in the CO<sub>2</sub>-enhanced system  
283 while the value was around 0.85 in conventional systems. Moreover, the yield of syngas was also  
284 increased by 20% in the proposed system. In addition to the improved CO<sub>2</sub>-enhanced system  
285 proposed in this work, the studied conventional system has also exhibited a better performance than  
286 the work conducted by previous researchers, as shown in Table 6. The main difference between this  
287 study and reported work [22] was in terms of DME synthesis reactor: equilibrium reactor was used  
288 in this study whilst RStoic reactor was used in the reported work [22]. An important feature of  
289 equilibrium reactor is that the DME synthesis reactor was assumed to have chemical equilibrium  
290 property which resulted in 84% conversion of CO while the RStoic reactor was modelled by  
291 assuming only 64% conversion of CO. Consequently, flow rate of the recycled stream in the  
292 present work was lower which greatly increased the yield of product DME in the synthesis process.  
293 Another potential reason for the high value of yield was that the treated gumwood was considered  
294 as a feedstock in the current work, whereas raw sawdust was used in Ref [24]. Similar study was  
295 also conducted by others [1] with a mass yield around 0.37. This value was 15% larger than that in  
296 [22] but 24% lower compared to the conventional system investigated in the current work. In  
297 contrast, a double-step synthesis route was selected by Zhang et al.,[23] and one-pass conversion of  
298 methanol to DME was about 70-85%. Accordingly, the conventional system obtained the highest  
299 DME yield. Hence, in the present work, the improvement of DME yield in CO<sub>2</sub>-enhanced systems  
300 was mainly contributed by the utilisation of CO<sub>2</sub> in gasifier, which was not considered in the  
301 conventional system, as well as by the employment of equilibrium reactor in synthesis process. As  
302 also shown in Table 6, a similar trend was noticed when plant energy efficiencies were compared  
303 where the highest efficiency was obtained by the CO<sub>2</sub>-enhanced system. Compared to that of  
304 conventional system, however, the increase in plant energy efficiency in the CO<sub>2</sub>-enhanced system  
305 was not as obvious as what was the case in terms of fuel energy efficiency. The reason for such is  
306 further explained in the followings.

307 As shown in Table 5, CO<sub>2</sub>-enhanced DME system had a higher plant energy efficiency (detailed in  
308 Eq. 4) of 65.97%, which was about 5% higher than that of conventional systems. This was mostly  
309 caused by the CO<sub>2</sub>-enhanced system having a larger amount of both DME production and heat  
310 output. The higher heat output was attributed to two sources: more syngas was produced in the  
311 gasifier and the high reaction heat in DME reactor. It can be seen that the demand of total input  
312 energy for gasifying agent and net heat generation in CO<sub>2</sub>-enhanced system were significantly  
313 higher than those of the conventional system. Additionally, the amount of heat required by the  
314 gasifier in CO<sub>2</sub>-enhanced process was 901,969 MJ/h, which was around 45% larger than that of  
315 conventional process. However, this trade-off was worthwhile as the proposed system offered a  
316 more significant increment of the plant outputs, which in this case, were DME production and heat  
317 output. Besides, CO<sub>2</sub>-enhanced system avoided water-gas shift and acid gas cleaning processes,  
318 indicating lower capital costs. Thus, the addition of CO<sub>2</sub> was proven to be beneficial in terms of  
319 feed consumption, fuel production and economical aspects. Another important feature of the  
320 proposed system was that it consumed CO<sub>2</sub>, thus, provided considerable environmental advantages.

321 There are other parameters that might influence the system efficiencies, including the properties of  
322 feedstock, system configurations and operating conditions. However, the analysis presented above  
323 provides first-hand information about DME yield per kg of biomass via CO<sub>2</sub>-enhanced system.

## 324 **4.2 Exergy analysis of DME production processes**

325 Exergetic efficiency of the DME production process can be calculated based on the evaluation of  
326 performance of the entire plant. Moreover, by analysing exergy flows within the plant, efficiencies  
327 of individual process units and their significance to the overall plant performance can be estimated.  
328 Table 7 presents the exergy balance of the two bio-DME routes compared in this study. In both  
329 processes, biomass contributed to the major exergy flow (57-67%) followed by exergy content of  
330 heat flows to the system. With respect to plant outputs, DME represented the highest contributor

331 (83-85%) whereas the additional output such as exergy of steam generated throughout the system  
332 was the second highest.

333 Table 7 also shows a comparison of exergetic efficiency of the bio-DME process between the two  
334 routes. Exergetic efficiency of the conventional plant was found to be 50.8% which was higher than  
335 those reported by others [22, 23]. Meanwhile, 85% of the total exergy output was contributed by  
336 DME. An important aspect of the current conventional system is that it generates more DME per  
337 unit mass of biomass than those of the previous work [22, 23], which increased the net production  
338 rate. This basically contributed to the higher exergetic efficiency of the current system.  
339 Furthermore, various variables including process operating conditions and biomass properties, such  
340 as moisture content, usually affect plant exergetic efficiency. Previous research stated that chemical  
341 exergy of biomass decreased with the increase of its moisture content [46]. The biomass used in  
342 this work contained 2.1 wt% moisture, lower than the values used in reported works which were  
343 13.4 wt% [22] and 7.5 wt% [23]. The aforementioned characteristic also contributed to a higher  
344 exergetic efficiency of the present work. The exergetic efficiency of the calculated system was 10%  
345 lower compared with its energetic efficiency. This deviation was normal as biomass underwent  
346 gasification process at a high temperature, which typically had a higher inefficiency associated with  
347 the related chemical reactions [17]. The difference arisen was caused by: (i) energetic performance  
348 which only considers energy loss due to emissions to the environment; (ii) exergetic assessment,  
349 considers both the external exergy losses (caused by system emissions) and the destruction of  
350 internal exergy based on the second law of thermodynamics. Hence, unlike energetic analysis,  
351 exergetic analysis is useful in identifying the causes, locations and magnitudes of process  
352 inefficiencies in order to improve the performance of the entire system [17, 21, 47]. On the other  
353 hand, exergetic efficiency of the CO<sub>2</sub>-enhanced system was 57.3%, almost 7% higher than that of  
354 conventional one. Out of the 100% useful outputs, DME contributed as much as 83.3% while the  
355 rest was the recovered heat from the system. It is worth noting that plant exergetic efficiency and  
356 energetic efficiency of the CO<sub>2</sub>-enhanced system were higher compared with those of conventional

357 systems, which was previously discussed in Section 4.1. It is found that process efficiency was  
358 highly influenced by DME yield, which was also in relation with the exergy content of 30.85 MJ/kg  
359 and the heating value (LHV) of 28.40 MJ/kg for the respective exergetic and energetic evaluations.  
360 In this case, exergy content and heating value had less influence on the efficiencies since the  
361 difference between them was relatively small.

362 Fig. 2 presents the relative exergy losses and destructions (L&D) for each process unit, which was  
363 previously illustrated in Fig. 1.

364 In both routes, the major exergy losses and destructions were associated with gasifier, methanol  
365 tower, CO<sub>2</sub> removal and DME reactor units (38-45%, 7-30%, 3-8% and 4-5%, respectively). These  
366 units are therefore endowed with potential for system improvement. On the other hand, the exergy  
367 L&Ds of other units such as in HRSG, WGS, Cleaner and DME Tower were much smaller. It is  
368 clear from Fig. 2 that gasifier was the critical unit of the system because of it is of the largest value  
369 of exergy losses and destructions. Hence, further analysis of this unit is worthwhile in improving  
370 the overall exergetic performance of the system. Generally, the exergy losses in the biomass  
371 gasification are highly dependent on the heat duty required to achieve chemical equilibrium at the  
372 given gasification temperature [21]. It is interesting to note that gasifier in conventional process  
373 consumed around 55% (619,056 MJ/h) of the total electricity requirement while the value for  
374 gasifier used in CO<sub>2</sub>-enhanced process was around 61% (901,969 MJ/h). In the gasifier, the  
375 decomposition of large molecules into smaller ones at higher temperatures causes large damage of  
376 chemical exergy. Previous studies showed that lower temperatures and higher pressures were  
377 beneficial for exergetic performance of the gasification process [19, 21].

378 Despite the adjustment of operating parameters and/or the use of different types of gasifier could  
379 increase the performance of gasifier, it cannot significantly reduce the total losses due to the  
380 existence of intrinsic energy and material degradation within gasification process. In addition,  
381 adjusting the composition of syngas to improve the process economy also limits the range of

382 operating parameters of the fluidized bed gasifier. It is important to highlight that the main  
383 characteristic of CO<sub>2</sub>-enhanced system is the use of CO<sub>2</sub> recycled from DME distillation unit as  
384 gasification agent. Therefore, the amount of CO<sub>2</sub> or the CO<sub>2</sub>/biomass ratio is crucial to plant  
385 performance, which needs to be optimized. Accordingly, CO<sub>2</sub>/biomass ratio was adjusted in the  
386 present work. However, as the amount of CO<sub>2</sub> addition directly affects CO<sub>2</sub> percentage in syngas  
387 and there is a limitation of CO<sub>2</sub>% in syngas (around 3% maximum), the potential of adjusting  
388 CO<sub>2</sub>/biomass ratio for exergy efficiency improvement is small, which could only lead to a small  
389 increment (1.2%) of exergy efficiency. Since the CO<sub>2</sub>/biomass ratio in gasifier (Table 2) has  
390 already been optimized, no significant impact was observed.

391 Similarly, marginal improvement of process efficiency might be achieved by tuning the  
392 temperature and pressure of gasifier, and also the temperature of the reacting streams. Thus, the  
393 increment of gasification efficiency via controlling the operating parameters is very limited.  
394 Upgrading the biomass feedstock via torrefaction could improve the performance but there is a  
395 compromise for extra energy required in the process that contributes to further exergy, energy and  
396 environmental losses. Other types of irreversibilities, such as fluid dynamic losses and heat losses,  
397 might also lead to a further degradation of the energy.

398 It can be seen from Fig. 2 that the exergy L&D in gasifier of the CO<sub>2</sub>-enhanced system was lower  
399 (by about 15%) compared to that of the conventional system although additional heat exergy and  
400 gasification agent exergy were required. This phenomenon can be explained by the properties of  
401 gas generated in the gasifier. The amount of H<sub>2</sub> and CO in the product gas in CO<sub>2</sub>-enhanced route  
402 was higher (44% and 21%, respectively) while the amount of CO<sub>2</sub> and H<sub>2</sub>O was lower (47% and  
403 28%, respectively) than those of the conventional one. The chemical exergy values of H<sub>2</sub> and CO  
404 are extremely higher (236100 kJ/kmol and 275100 kJ/kmol, respectively) than those of CO<sub>2</sub> and  
405 H<sub>2</sub>O (19870 kJ/kmol and 9500 kJ/kmol, respectively). Accordingly, the rise of total exergy was  
406 noticed to be directly proportional to the increments of H<sub>2</sub> and CO in the product gas. At the same

407 time, the reduction of CO<sub>2</sub> and H<sub>2</sub>O in the product gas led to the decrease of total exergy. Moreover,  
408 as extra heat and gasification agent were needed in CO<sub>2</sub>-enhanced process, the input exergy to the  
409 gasifier was increased, which also resulted in the increase in inefficiencies. Other than H<sub>2</sub> and CO,  
410 the total exergy losses due to extra input exergy and the reduction of exergy values contributed by  
411 CO<sub>2</sub> and H<sub>2</sub>O had less impact to the total exergy. Hence, exergetic efficiency of the CO<sub>2</sub>-enhanced  
412 route was greater than that of the conventional system. Besides, CO<sub>2</sub>-enhanced biomass  
413 gasification-based DME production experienced better performance within HRSG, Syn Cleaner,  
414 CO<sub>2</sub> removal units. However, exergy L&Ds from the Comp and Cool (compression and cooling)  
415 unit in CO<sub>2</sub>-enhanced route were higher than those in the conventional route, as more syngas needs  
416 to be processed. These units are usually standard products of manufacturing industries, therefore,  
417 the potential for further reduction in their exergy losses (*i.e.*, by more efficient equipment) is  
418 associated with high costs [48].

419 In comparison with the gasifier, which involved several reactions and led to low exergetic  
420 efficiency, DME synthesis reactor (DME-R) offered a significantly better performance in both  
421 routes. This was due to the relatively low chemical exergy stream entered to DME-R was  
422 transformed into a product stream that contained a higher chemical exergy. This product stream  
423 was obtained due to the formation of compounds, such as DME, MeOH, which had a high standard  
424 chemical exergy. The exergy losses in DME-R were mainly derived from the intrinsic synthesis  
425 reaction, which is hard to avoid. In this work, the production of DME was analysed based on the  
426 two routes. In DME purification process, the major losses were attributed to the MeOH tower unit  
427 (7-15%) and CO<sub>2</sub> removal unit (3-7%). It was found that conventional route performed better than  
428 CO<sub>2</sub>-enhanced route in terms of irreversibilities in MeOH tower unit.

### 429 **4.3 Environmental analysis**

430 The DME production based on CO<sub>2</sub>-enhanced gasification has shown clear advantages against  
431 conventional gasification in terms of fuel energetic and exergetic evaluation. An assessment of

432 environmental impacts is therefore needed. Accordingly, LCA-based environmental analysis was  
433 conducted to compare the two routes. The environmental impacts caused in mid-points and end-  
434 points categories under the investigated operation parameters are presented in Fig. 3 and Fig. 4,  
435 respectively. It is obvious that CO<sub>2</sub>-enhanced system showed overall less environmental impacts,  
436 indicating a better performance compared with the conventional system although the differences in  
437 various impact categories between the two systems are not notable. This is as the environmental  
438 impacts are affected by many factors which will be detailed in the following paragraphs.

439 As seen in Fig. 3, there were five significant factors being considered in mid-point category where  
440 climate change human health, fossil depletion and climate change ecosystem were the most  
441 significant causes whose values were lower in CO<sub>2</sub>-enhanced system than those in conventional  
442 one. It is worth mentioning that the DME production in CO<sub>2</sub>-enhanced system was 28% higher  
443 although both total energy consumption and heat recovery were higher than those of conventional  
444 system. Accordingly, the consumption of biomass and water per kg DME yield in the CO<sub>2</sub>-  
445 enhanced system were significantly lower (22% and 9%, respectively), which minimized the  
446 energy requirement and therefore reduced environmental impacts. Furthermore, the net CO<sub>2</sub>  
447 emission per kg DME in CO<sub>2</sub>-enhanced system was lower (about 16%) as it was used as an agent in  
448 gasifier. As CO<sub>2</sub> is the key issue in the evaluation of environmental impacts of any processes, hence,  
449 the reduction in CO<sub>2</sub> emission normally has a positive effect on environmental impacts. Similar  
450 result was noticed with respect to particulate matter formation where its impact was moderate. On  
451 the other hand, human toxicity demonstrated an insignificant impact where the values were almost  
452 similar for both systems.

453 Regarding end-points impacts, the CO<sub>2</sub>-enhanced system showed lower environmental impacts  
454 than those of the conventional system as the end-points merge the information obtained from the  
455 mid-points. It can be seen from Fig. 4 that human health combined the three categories of climate  
456 change human health, human toxicity and particulate matter formation from the mid-points;

457 whereas ecosystem and resources stood for climate change ecosystem and fossil depletion,  
458 respectively. From the end-points graph, it is obvious that human health and resources were highly  
459 influenced than the ecosystem itself, which was around 50% lower than the others. In comparison  
460 with conventional system, the CO<sub>2</sub>-enhanced system showed a better environmental performance  
461 by having a high-energy output, less biomass consumption and less CO<sub>2</sub> emission, which  
462 compensated the additional heat and gasifying agent required in the process.

463 Besides, energetic, exergetic and environmental evaluation, an economic assessment is needed to  
464 check the feasibility of the industrial scale bio-DME production based on CO<sub>2</sub>-enhanced  
465 gasification to compete with the current fossil fuel and biomass-based system. In spite of the huge  
466 potential of CO<sub>2</sub> utilization introduced in gasification process for DME system, such advantages  
467 that CO<sub>2</sub> can offer is vital in the assessment of gasifier performance as well as the total costs of  
468 DME production. Due to the increment of DME production in CO<sub>2</sub>-enhanced system, the product  
469 costs are lower compared with those of the conventional system where the operation cost and cost  
470 related to CO<sub>2</sub> emission are essential factors that will justify the utilization of CO<sub>2</sub> for industrial  
471 applications. Furthermore, CO<sub>2</sub>-enhanced based bio-DME production process is expected to  
472 contribute to more efficient, competitive and sustainable clean fuel in near future, in order to fulfil  
473 the recent challenges in more strict environmental regulations regarding low CO<sub>2</sub> emission  
474 combined with the demand of low-cost product for the industries.

## 475 **5 Conclusions**

476 This work adopted thermodynamic and environmental approaches to compare conventional and  
477 CO<sub>2</sub>-enhanced biomass gasification based bio-DME production. Based on thermodynamic  
478 efficiency indexes, *i.e.*, plant energy efficiency and plant exergetic efficiency, the proposed CO<sub>2</sub>-  
479 enhanced system demonstrated better performance than the conventional system. This improved  
480 performance was mainly due to higher DME production and higher heat output. Meanwhile, the  
481 exergetic evaluation in both routes showed that the largest loss occurred at the gasifier unit.

482 However, the addition of CO<sub>2</sub> as a gasifying agent reduced the loss in gasifier unit by 15%. The  
483 environmental analysis showed that the CO<sub>2</sub>-enhanced system offered a more sustainable approach  
484 for bio-DME production. This is another benefit of using CO<sub>2</sub> in gasification compared with the  
485 conventional one. These findings could assist in the development and commercialization of CO<sub>2</sub>-  
486 enhanced bio-DME production.

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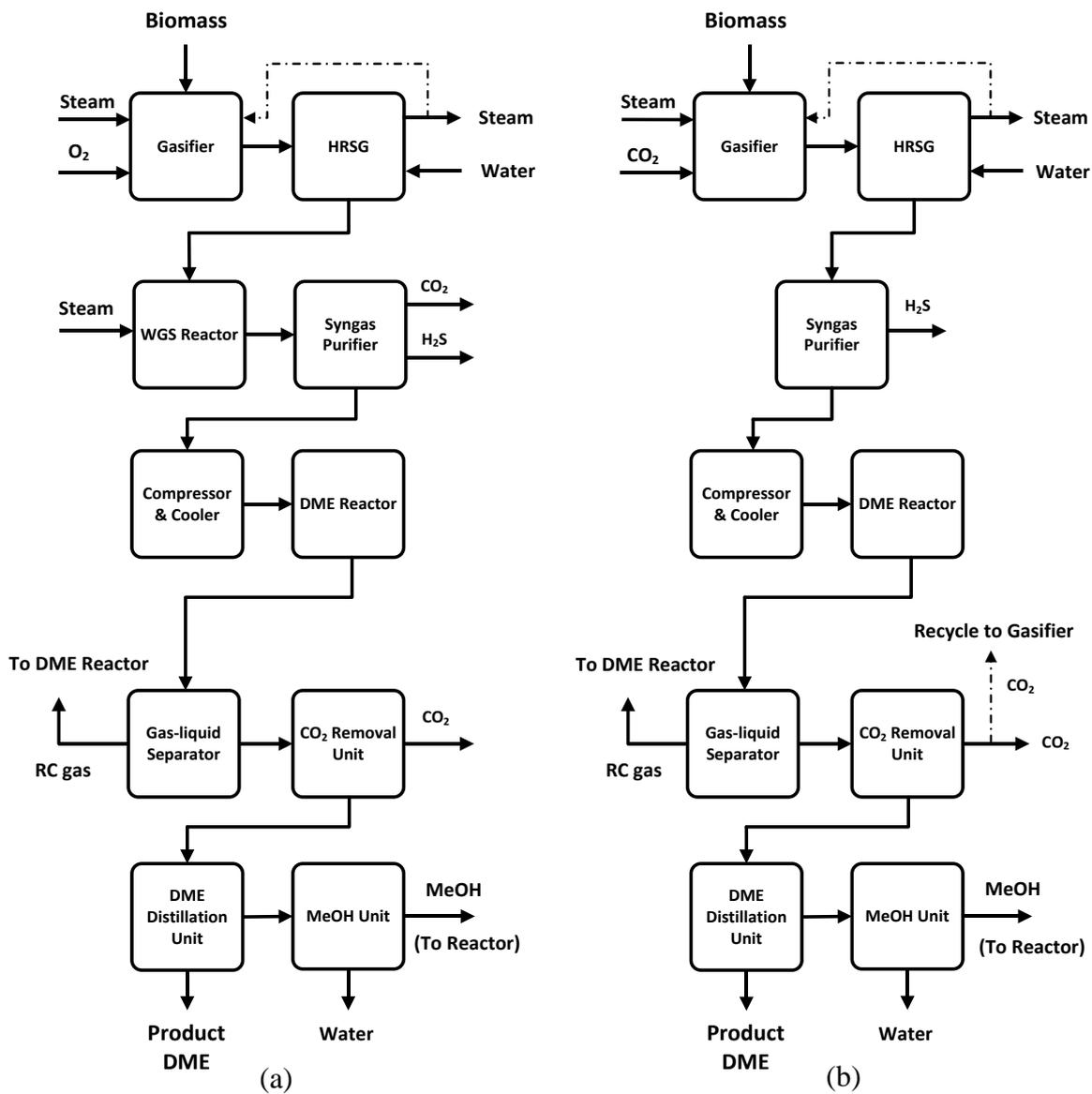
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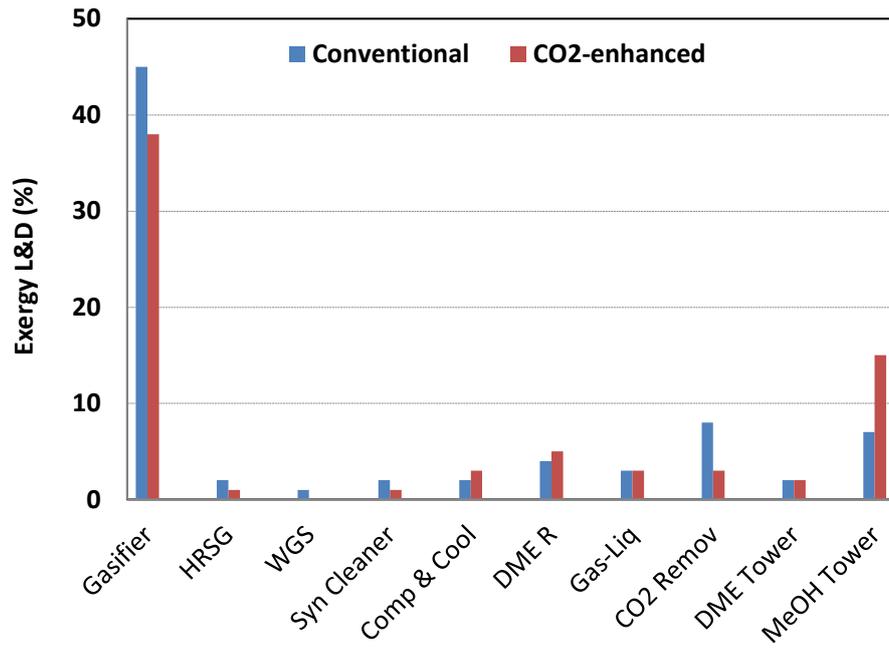


614

615 **Figure 1: Process flow diagram of the single-step DME production based on (a) conventional**  
 616 **and (b) CO<sub>2</sub>-enhanced biomass gasification.**

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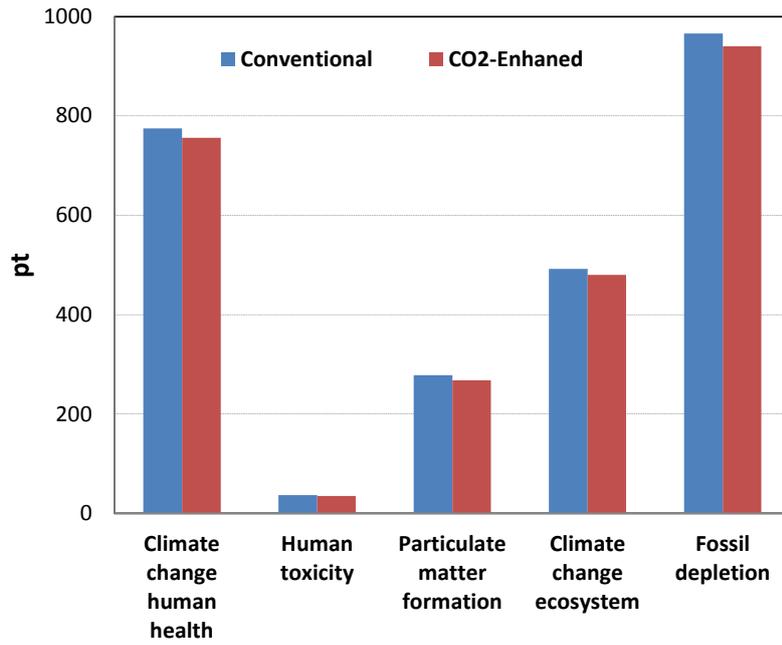
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**Figure 2: Relative exergy losses and destructions of the considered bio-DME systems.**

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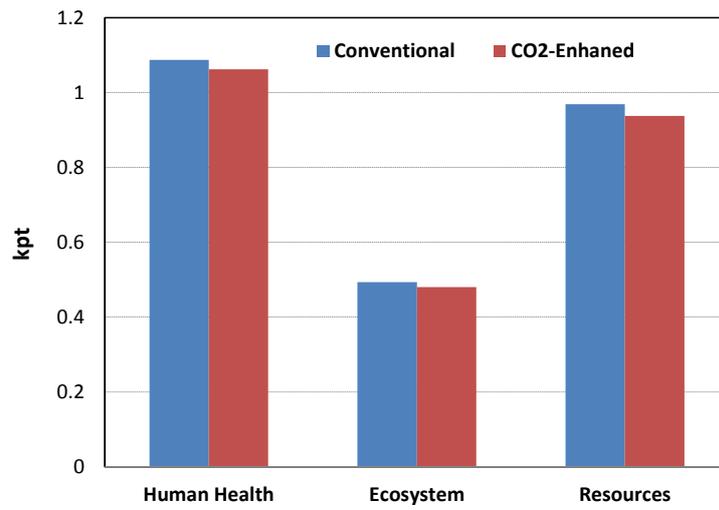
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625 **Figure 3: Environmental impacts (ReCiPe) in different categories (mid-points) – conventional**  
626 **bio-DME system and CO<sub>2</sub>-enhanced bio-DME system**

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630 **Figure 4: Environmental impacts (ReCiPe) caused in the end-points (Human health,**  
631 **Ecosystem and Resources) – conventional bio-DME system and CO<sub>2</sub>-enhanced bio-DME**  
632 **system**  
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**Table 1: Properties of gumwood**

Net calorific value (MJ/kg)	20.0
<b>Proximate analysis (wt %)</b>	
Moisture	2.1
Volatile matter	86.0
Fixed carbon	11.8
Ash	0.1
<b>Ultimate analysis <sup>a,b</sup> (wt %)</b>	
C	47.1
H	6.3
O <sup>c</sup>	43.5
N	2.1
S	1.0
a: dry basis, b: ash free basis, c: by difference	

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**Table 2: Gasification process parameters for the considered bio-DME systems.**

<b>Parameter</b>	<b>Conventional</b>	<b>CO<sub>2</sub>-enhanced</b>	<b>Ju et al. [1]</b>
Temperature (°C)	900	950	850
Pressure (MPa)	0.1	0.1	0.1
Biomass flow rate (kg/h)	50,000	50,000	75,600
O <sub>2</sub> flow rate at 25 °C, 0.1 MPa (kg/h)	15,000	-	unknown
Steam flow rate at 150 °C, 0.5 MPa (kg/h)	2,000	11,500	unknown
CO <sub>2</sub> flow rate at 25 °C, 0.1 MPa (kg/h)	-	9,500	-
Total gasification agent/Biomass	0.34	0.42	0.51
H <sub>2</sub> /CO in syngas	0.85	1.0	1.0
CO <sub>2</sub> mol% in syngas	6.7	2.9	17.0
LHV (MJ/Nm <sup>3</sup> )	10.8	11.2	9.7
CGE (%)	70.5	77.8	74.6
GSE (%)	34.5	32.8	-

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641 **Table 3: Model validation against the gasification of wood (steam/biomass =0.2, P=0.1 MPa).**

Temp (°C)	H <sub>2</sub> (mol. fraction)			CO (mol. fraction)			CO <sub>2</sub> (mol. fraction)		
	Ref [21]	Present work	Error %	Ref [21]	Present work	Error%	Ref [21]	Present work	Error %
750	0.490	0.510	4.2	0.380	0.362	4.7	0.050	0.047	5.6
800	0.500	0.521	4.3	0.430	0.412	4.3	0.020	0.018	7.5
850	0.500	0.529	5.7	0.450	0.427	5.1	0.013	0.012	7.7
900	0.501	0.531	6.0	0.460	0.4247	7.7	0.008	0.008	6.2
950	0.508	0.543	6.9	0.465	0.446	4.1	0.001	0.0005	4.0
1000	0.510	0.552	8.3	0.470	0.449	4.4	0.0001	9.2E-05	8.0

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**Table 4: Model validation against CO<sub>2</sub> gasification of biomass (CH<sub>1.56</sub> O<sub>0.78</sub>, CO<sub>2</sub>/C= 0.5,**

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**P=0.1 MPa).**

Temp (°C)	H <sub>2</sub> (mol. fraction)			CO (mol. fraction)			CO <sub>2</sub> (mol. fraction)		
	Ref [10]	Present work	Error%	Ref [10]	Present work	Error%	Ref [10]	Present work	Error%
800	0.310	0.331	7.0	0.598	0.572	4.4	0.091	0.085	6.3
1000	0.302	0.320	5.8	0.6248	0.592	5.2	0.073	0.067	8.6
1200	0.294	0.307	4.2	0.643	0.611	5.0	0.063	0.058	8.0

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**Table 5: Summary of mass and energy balances for the considered bio-DME systems.**

	<b>Conventional (0.1 MPa, 900 °C)</b>	<b>CO<sub>2</sub>-enhanced (0.1 MPa, 950 °C)</b>
<b>Plant inputs</b>		
Biomass (kg/h)	50,000	50000
Biomass (MJ/h)	1,000,000	1,000,000
Oxygen (kg/h)	15,000	-
Oxygen (MJ/h)	-	-
Carbon dioxide (kg/h)	-	9,500
Carbon dioxide (MJ/h)	-	84,930
Steam (kg/h)	2,000	11,500
Steam (MJ/h)	26,380	151,685
Water (kg/h)	35,500	42,000
Water (MJ/h)	3,692	4,368
<b>Electricity (MJ/h)</b>	1,119,411	1,459,642
<b>Plant outputs</b>		
Dimethyl ether (kg/h)	23,312	29,941
Dimethyl ether (MJ/h)	662,061	850,324
<b>Heat (MJ/h)</b>	648,720	931,170
<b>Efficiencies</b>		
<b>Fuel energy efficiency (%)</b>	66.21	85.03
<b>Plant energy efficiency (%)</b>	60.98	65.97

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652 **Table 6: Comparison of DME yield and energetic efficiency of different bio-DME systems.**

Author	Gasification system	Biomass feedstock	Gasification agent	DME synthesis	DME yield (kg/kg biomass)	Plant energy efficiency (%)
Xiang et al. [22]	Entrained flow (1000 °C)	Raw sawdust	Steam, O <sub>2</sub>	Single-step	0.32	55.2
Zhang et al.[23]	Fluidized bed (880 °C)	Wood pellets	Steam	Double-step	0.34	51.3
Ju et al.[1]	Fluidized bed (850 °C)	Wood	Steam, O <sub>2</sub>	Single-step	0.37	52.7
Present work	Fluidized bed (900 °C)	Gum wood	Steam, O <sub>2</sub>	Single-step	0.46	60.98
	Fluidized bed (950 °C)	Gum wood	Steam, CO <sub>2</sub>	Single-step	0.59	65.97

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**Table 7: Summary of exergy flow rate of the considered bio-DME systems.**

	<b>Conventional (0.1 MPa, 900 °C)</b>	<b>CO<sub>2</sub>-enhanced (0.1 MPa, 950 °C)</b>
<b>Plant inputs</b>		
Biomass (MJ/h)	1,056,557	1,056,557
Oxygen (MJ/h)	1,845	-
Carbon dioxide (MJ/h)	-	4,283
Steam (MJ/h)	1,259	7,240
Water (MJ/h)	1,775	1,500
<b>Electricity (MJ/h)</b>	<b>516,953</b>	<b>753,869</b>
<b>Plant outputs</b>		
<b>Product</b>		
Dimethyl ether (MJ/h)	719,545	923,637
<b>Outputs</b>		
Carbon dioxide (MJ/h)	27,778	47,791
Water (MJ/h)	637	430
Purge (MJ/h)	11,873	13,468
<b>Heat</b>		
Heat (MJ/h)	81,861	122,886
<b>Efficiencies</b>		
<b>Exergetic efficiency (%)</b>	<b>50.8</b>	<b>57.3</b>

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