



## Research paper

## Process simulation of single-step dimethyl ether production via biomass gasification

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## ABSTRACT

In this study, we simulated the single-step process of dimethyl ether (DME) synthesis via biomass gasification using ASPEN Plus™. The whole process comprised four parts: gasification, water gas shift reaction, gas purification, and single-step DME synthesis. We analyzed the influence of the oxygen/biomass and steam/biomass ratios on biomass gasification and synthesis performance. The syngas H<sub>2</sub>/CO ratio after water gas shift process was modulated to 1, and the syngas was then purified to remove H<sub>2</sub>S and CO<sub>2</sub>, using the Rectisol process. Syngas still contained trace amounts of H<sub>2</sub>S and about 3% CO<sub>2</sub> after purification, which satisfied the synthesis demands. However, the high level of cold energy consumption was a problem during the purification process. The DME yield in this study was 0.37, assuming that the DME selectivity was 0.91 and that CO was totally converted. We performed environmental and economic analyses, and propose the development of a poly-generation process based on economic considerations.

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## 1. Introduction

Increasing attention has recently been focused on the use of bioenergy, because of the huge energy demand and the depletion of fossil fuel supplies. Biomass is abundant and renewable, and could therefore play a key role in future energy supplies. Its inherent nearly carbon-neutral property has the crucial advantage of minimizing CO<sub>2</sub> emissions, which could mitigate global warming. It has been predicted that the energetic use of biomass will increase in the future by a factor of 2–3 (Bandi and Specht, 2006), and it is expected to significantly contribute to a quarter of the world total energy consumption by 2050 (Komiya et al., 2001).

Liquid and gaseous fuels based on biomass are promising options as substitutes for petroleum and natural gas (Kumabe et al., 2008). Dimethyl ether (DME) is one such fuel. It is a colorless, non-toxic fuel and is the simplest ether that can be produced from carbonaceous feedstock, including biomass (Bandi and Specht, 2006). DME shows a better performance than many other diesel fuels (Arcoumanis et al., 2008; Fukunaga et al., 2008).

DME production has traditionally been based on natural gas auto-reformation or coal gasification. Two-step DME synthesis is the main process used, which includes separate steps of methanol synthesis and methanol dehydration. Recently, however, single-step DME synthesis has been developed (Lewnard et al., 1990; Brown et al., 1991; Lee et al., 1992; Ogawa et al., 2003; Moradi et al., 2008a,b,c), which combines methanol synthesis and methanol dehydration in one reactor. Compared with two-step synthesis, the single-step process has overcome the equilibrium limitations posed by methanol synthesis (Marchionna et al.,

2008) and can obtain a higher conversion efficiency. The production costs for the single-step process are now 20% lower than for the two-step process (Fukunaga et al., 2008). The initial investment is also smaller for single-step DME synthesis, compared with two-step synthesis (Tan et al., 2005), which makes it more attractive.

Previous studies have focused on the development of bifunctional catalysts and slurry reactors (Lewnard et al., 1990; Brown et al., 1991; Lee et al., 1992; Ogawa et al., 2003; Moradi et al., 2008a,b,c). Bifunctional catalysts are generally used in single-step DME synthesis; better interaction of synthesis catalyst and dehydration catalyst make the combination of methanol synthesis and dehydration in one reactor practical. Control of reaction temperature is easier in slurry DME production reactors because of the liquid phase solvent (Lewnard et al., 1990; Brown et al., 1991; Lee et al., 1992). This process has recently been further developed in Japan, where a 100-t/day DME synthesis project based on JFE (2007) technology was recently put in operation. Single-step DME synthesis technology has been improved and process simulation is an important means of predicting DME process performance in order to facilitate the further development, especially of biomass-based DME production. This study simulated the process of DME synthesis via biomass gasification. Environmental and economic analyses were also performed. Based on economic considerations, a poly-generation system that generated DME, steam and electricity was also proposed.

## 2. Materials and methods

## 2.1. Materials

The biomass used in the simulation was a dried woody biomass with a moisture content of 11%. Its basic properties are listed in Table 1.

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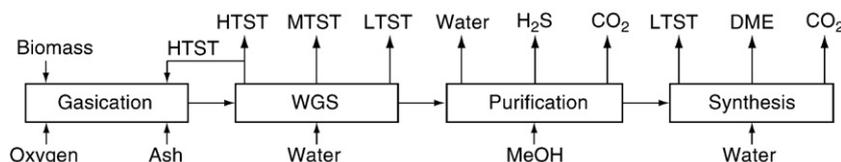
**Table 1**  
Basic properties of the material.

Ultimate analysis (dry basis, wt.%)							M	Ash	HHV
C	H	O	N	S	Cl	(wt.%)	(dry basis, wt.%)	(dry basis, wt.%)	
50.88	6.04	41.90	0.17	0.09	0.00	11.00	0.92	20.29	

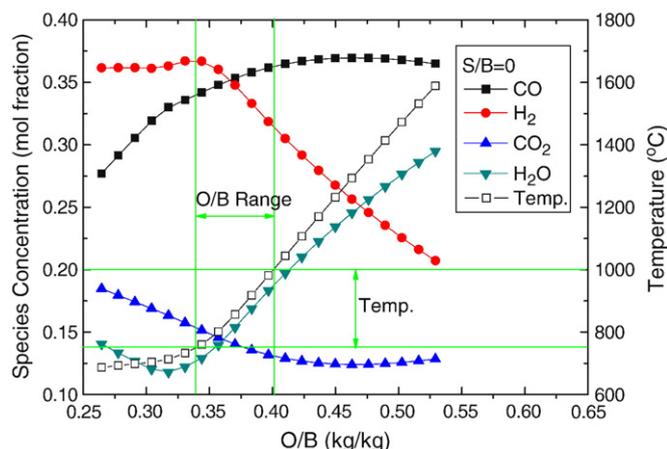
## 2.2. Process description of DME synthesis via biomass gasification

ASPEN Plus™ (Aspen Technology Inc., USA) was used for the process simulation. ASPEN Plus™ is a software developed for design, steady state simulation and optimization of real plant behaviors (Kanniche et al., 2005; Shim et al., 2007; Nikoo and Mahinpey, 2008). The process of single-step DME synthesis via biomass gasification is shown in Fig. 1. It is composed of four parts: gasification, water gas shift (WGS) reaction, gas purification, and single-step DME synthesis. During the gasification stage, an oxygen and steam blown gasifier was simulated. Biomass material is initially gasified in the gasifier, and the C, H, and O contents of the biomass are transformed to CO, H<sub>2</sub>, CO<sub>2</sub>, and CH<sub>4</sub>, while N and S are converted to N<sub>2</sub> and H<sub>2</sub>S, respectively. The gas product is then transported to a WGS reactor in order to modulate the H<sub>2</sub>/CO molar ratio to the required value. The WGS reaction stage also includes a heat recovery steam generation system to produce steam. The modulated gas must be purified before transfer to the synthesis reactor, as H<sub>2</sub>S will poison the synthesis catalyst (Koizumi et al., 2004; Fukunaga et al., 2008), and CO<sub>2</sub> would reduce the conversion efficiency of DME synthesis. A typical physical adsorption process, the Rectisol process (Hochgesand, 1970; Weiss, 1988), is used to remove the H<sub>2</sub>S and CO<sub>2</sub> at low temperature. After purification, the syngas is preheated and pressurized in the DME synthesis reactor.

During the gasification process, 75.60 metric tons h<sup>-1</sup> biomass was fed into the DME synthesis system. The oxygen input varied from 20–40 tons/h, corresponding to an oxygen to biomass ratio (O/B) range of 0.265–0.370. The temperature and pressure of steam purged in the gasifier was 540 °C and 10 MPa, respectively, and the steam mass rate varied from 0–22.68 metric tons h<sup>-1</sup>, corresponding to a steam to biomass mass ratio (S/B) in the range of 0–0.3. The gasifier was operated at 0.17 MPa and the temperature was adjusted by varying the oxygen and steam mass rates. Several studies have used the Gibbs free energy minimization approach for simulating gasifier performance (Li et al., 2001; Ptasinski et al., 2002; Zhu, 2004). In this study, the RGibbs module, which is based on the Gibbs free energy minimization approach, was used to calculate the gasification temperature and component species concentrations. In the WGS reaction process, a medium temperature WGS reaction was used and the CO conversion efficiency was set at 70%, according to previous studies (Chen and Ying, 2005; Wang et al., 2008). The RStoic module was introduced to simulate the WGS process. The WGS reaction temperature was adjusted by water injection (215 °C, 4 MPa). During the purification process, -50 °C methanol was used for acid gas adsorption. A Rfrac module without a reboiler or condenser was used to simulate the absorption tower. The synthesis stage operated at 250 °C and 5 MPa (Ogawa et al., 2003; Ren et al., 2006), and the RStoic module was used to simulate the synthesis process.



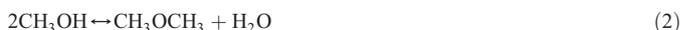
**Fig. 1.** Diagram of single-step DME production via biomass gasification. HTST: high temperature steam (540 °C, 10 MPa); MTST: medium temperature steam (450 °C, 4 MPa); LTST: low temperature steam (152 °C, 0.4 MPa); WGS: water gas shift process.



**Fig. 2.** Gasification performance variations for different O/B when S/B=0.

## 2.3. Single-step DME synthesis reaction analysis

Single-step DME synthesis consisted of several competing reaction pathways:



If reaction (3) does not participate in the reaction, the total DME synthesis can be represented by combining reactions (1) and (2), as follows:



If reaction (3) does occur, the total DME synthesis reaction can be expressed as:



There are two main, typical single-step DME synthesis technologies, Hardlor Topsoe and JFE. The Hardlor process adopts a H<sub>2</sub>/CO ratio of 2, which is favorable for reaction (4), while the JFE technology adopts a H<sub>2</sub>/CO ratio of 1, and reaction (5) mainly occurs. The results of previous studies suggest that reaction (5) is more profitable (Peng, 2002; Marchionna et al., 2008). In this study, a H<sub>2</sub>/CO ratio of 1 was simulated, based on JFE technology.

## 2.4. Related indices

Several parameters were calculated to evaluate gasification performance, including product lower heating value (LHV), gas yield and cold gas efficiency.

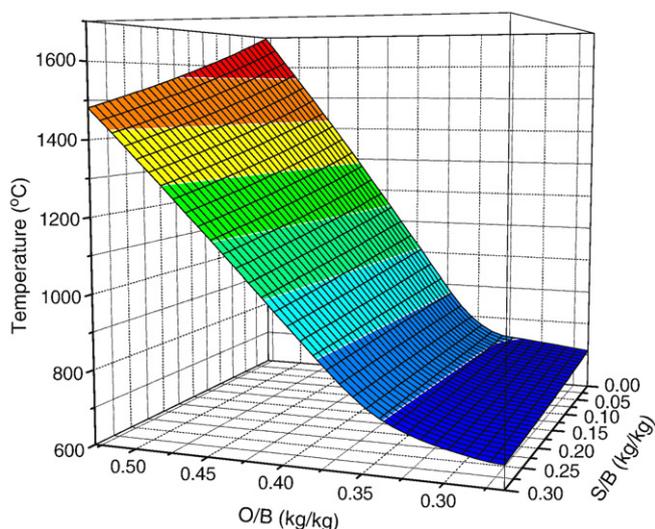


Fig. 3. Gasification temperature variations at different S/B and O/B.

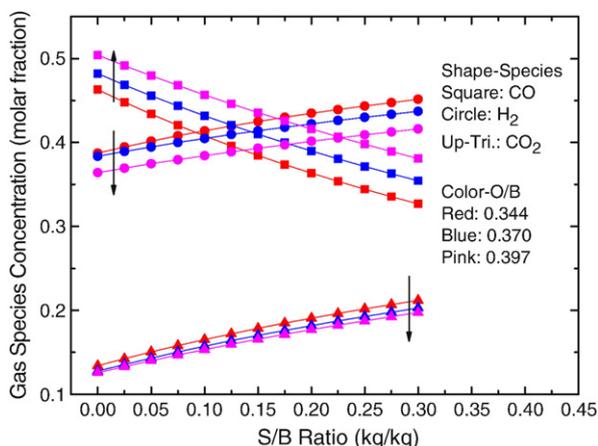


Fig. 4. Gas species concentration variations at different S/B and O/B.

Gas LHV (MJ/Nm<sup>3</sup>) can be expressed as follows:

$$Q_{LHV} = 12.636 \times CO\% + 10.806 \times H_2\% + 35.786 \times CH_4\%$$

where CO%, H<sub>2</sub>% and CH<sub>4</sub>% represents the dry volumetric percentage of CO, H<sub>2</sub> and CH<sub>4</sub> in fuel gas, respectively.

The dry gas yield, Y<sub>GAS</sub> (Nm<sup>3</sup>/kg), is expressed as follows:

$$Y_{GAS} = \frac{N_{Gas}}{M_{biomass}} \times 22.4.$$

N<sub>gas</sub> represents the molar flow (kmol/kg) in the fuel gas. It is assumed that the fuel gas consists only of CO, CO<sub>2</sub>, H<sub>2</sub>, O<sub>2</sub>, CH<sub>4</sub>, H<sub>2</sub>S and N<sub>2</sub> in the dry gas yield calculation.

Cold gas efficiency is calculated by the following equation:

$$Eff. = \frac{Q_{LHV} \times Y_{Gas}}{Q_{biomass,LHV} \times (1 - Moisture\%)} \times 22.4.$$

Moisture is the percent moisture in the material.

DME yield (kg/kg) is defined as follows:

$$Y_{DME} = \frac{m_{DME}}{m_{Biomass}} \times 100\%$$

where m<sub>DME</sub> represents the DME production mass rate and m<sub>Biomass</sub> is the biomass feed mass rate.

### 3. Results and discussion

#### 3.1. Gasification performance

Gasification temperature is a key parameter for determining gasification performance. Gasification performances at various O/B without steam addition are shown in Fig. 2. Temperature increased with increasing values of O/B, and two apparent temperature ranges of 680–710 °C and >710 °C were evident. However, biomass gasification in industrial fluidized bed gasifiers operates in the range of 750–1000 °C, and the corresponding O/B range is 0.33–0.40. In this temperature range, steam and CO increase while H<sub>2</sub> and CO<sub>2</sub> decrease with increasing O/B, which leads to a reduction in H<sub>2</sub>/CO. This may be because more H<sub>2</sub> is consumed at higher O/B, with the consequent production of more H<sub>2</sub>O. An H<sub>2</sub>/CO of 1 is required for DME synthesis using JFE technology, and a lower O/B favors a higher H<sub>2</sub>/CO. However, a lower O/B also causes a lower temperature, which is unfavorable for the gasification reaction rate. In this case, a moderate temperature around 850 °C was adopted, and an O/B of 0.37, while various values of S/B from 0 to 0.15 were selected.

Variations in gasification temperature with S/B and O/B are shown in Fig. 3. Gasification temperature decreased with increasing S/B because of the lower temperature steam (at 540 °C) endothermic effect and intensification of the WGS reaction. The gas species distribution at different O/B and S/B is shown in Fig. 4. The increase in S/B at different O/B resulted in sharp decreases in CO and increases in H<sub>2</sub> and CO<sub>2</sub> concentrations. Higher O/B at the same S/B increased the gasification temperature, which benefited the Boudouard and water gas reactions. The H<sub>2</sub>/CO ratio of 1 could be reached by adjusting the S/B and O/B (Fig. 4). The calculated S/B, O/B and other relevant data when H<sub>2</sub>/CO = 1 is listed in Table 2. The product gas LHV, gas yield and cold gas efficiency under different gasification conditions were also calculated. The results are shown in Figs. 5 and 6. As S/B increased at the same O/B, the gas yield increased while the LHV and the cold gas efficiency decreased. When O/B was increased at the same S/B, the LHV increased while the gas yield cold gas efficiency decreased.

#### 3.2. WGS process simulation

The WGS reaction is the main industrial H<sub>2</sub> generation technology (Fan et al., 2008; Zhang et al., 2008). There are two main types of WGS reactions according to the catalyst operation temperature: medium (or high) temperature WGS reactions and low temperature WGS reactions (Perna, 2008; Zhang et al., 2008). In this study, the medium temperature with a sulfur-resistant shift catalyst was adopted and the

Table 2  
S/B and O/B ratios when H<sub>2</sub>/CO = 1.

O/B	S/B	Temperature (°C)	Gas species molar fraction					LHV (MJ/Nm <sup>3</sup> )	Y <sub>GAS</sub>	Efficiency (%)	H <sub>2</sub> /CO
			CO	H <sub>2</sub>	CO <sub>2</sub>	CH <sub>4</sub>	H <sub>2</sub> S				
0.370	0.143	856.00	0.41	0.41	0.17	0.00054	0.0024	9.68	1.44	74.62	1

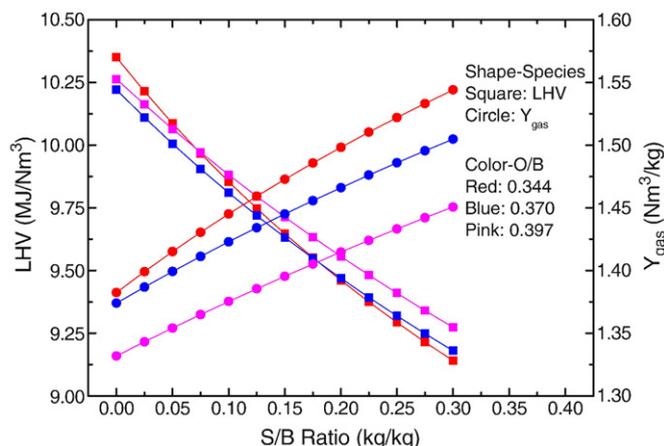


Fig. 5. Gas LHV and gas yield variations at different S/B and O/B.

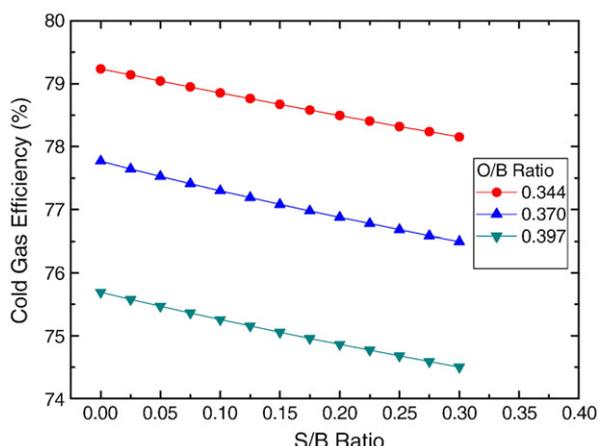


Fig. 6. Cold gas efficiency variations at different S/B and O/B.

operating temperature was set at 440 °C. The RStoic module was used to simulate the WGS reactor. Water or steam acted as both the reactant and the temperature controller. In the simplified process, gas was divided in two ways, one entering the shift reactor and the other not, and the specified  $H_2/CO$  ratio could thus be reached by adjusting the shifted gas ratio. The shifted gas and the unshifted gas then combined and underwent the purification process.

A heat recovery steam generator system (HRSG) was included in this system. Three types of steam were generated: high (HTST), medium (MTST) and low temperature steam (LTST). Table 3 shows

**Table 3**  
Heat recovery during the WGS process and power generation estimation.

O/B	S/B	HTST	Gas. <sup>a</sup>	Net. <sup>b</sup>	MTST	LTST	Elec. <sup>c</sup>	Syngas Steam <sup>d</sup>
		tons h <sup>-1</sup>		MW				
0.370	0.000	18.82	0	18.82	6.36	7.23	6.92	8.43
0.370	0.025	19.22	1.89	17.33	6.52	7.4	6.53	9.79
0.370	0.050	19.71	3.78	15.93	6.68	7.55	6.16	11.17
0.370	0.075	19.97	5.67	14.3	6.84	7.78	5.73	12.56
0.370	0.100	20.32	7.56	12.76	7.01	7.98	5.32	13.96
0.370	0.125	20.66	9.45	11.21	7.17	8.2	4.91	15.37
0.370	0.143	20.89	10.83	10.06	7.28	7.76	4.60	15.41

<sup>a</sup> Gas.: steam consumption during the gasification stage as gasification reactant.

<sup>b</sup> Net: net HTST production during single-step DME synthesis process via biomass gasification.

<sup>c</sup> Elec.: electricity production was estimated based on the net power generation efficiency of 30% and 25% when net HTST and MTST acted as the working media, respectively.

<sup>d</sup> Syngas Steam: total mass amount of steam in syngas.

the results of heat recovery steam generation in this process. The steam production and corresponding electricity generation were calculated when  $H_2/CO = 1$ , and attainment of  $H_2/CO = 1$  by adjustment of the O/B and S/B in the gasifier is shown in Table 2. Increasing S/B slightly increased the total HTST, MTST and LTST, because of the increasing steam concentration in the product gas. However, the HTST net production decreased because of the increased steam returned to the gasifier. Lower S/B decreased the steam concentration in the syngas, which could reduce the load of the purification process and reduce the energy loss. On the other hand, a lower S/B reduced  $H_2/CO$  which would increase the load of the WGS reactor and catalyst consumption. The optimal choice thus needs to be a compromise for the whole process performance. In the present study, the WGS reactor load was not the main determinant of the process. A lower S/B was preferred and an S/B equal to 0.00 was selected, though the biomass had an actual moisture content of 11%, so the true S/B was about 0.124. A lower S/B leads to more HTST production, which could be used to produce electricity needed for the DME production process, though less MTST and LTST were produced. The electricity that could be produced from HTST and MTST decreased with increasing S/B. The LTST and the steam from the steam turbine could be used in the DME production process, such as during the DME refinery stage, etc.

### 3.3. Gas purification process

The purpose of gas purification is to remove  $H_2S$  and partial  $CO_2$ .  $H_2S$  is fatal to the DME synthesis catalyst and directly influences catalysis performance and the synthesis reaction (Quinn et al., 2004). In single-step DME production technology,  $H_2S$  should be almost totally removed before the synthesis process to protect the synthesis catalysis from sulfuration.  $CO_2$  should be partially removed, taking into account the required equilibrium and purification load.  $CO_2$  concentration is critical to the conversion efficiency, and a  $CO_2$  concentration of about 3% is acceptable for JFE technology. There are several methods for removing acid gas, which can be generally divided into physical adsorption and chemical adsorption methods, according to the adsorption mechanism (Kanniche et al., 2005). The Rectisol washing process (Hochgesand, 1970; Weiss, 1988), which is a typical physical adsorption process, has been shown to be efficient and to lower energy consumption (Hochgesand, 1970; Weiss, 1988; Kanniche et al., 2005), compared with other known methods. The Rectisol washing process was developed based on differential species solubilities.  $H_2S$  and  $CO_2$  are more soluble in low temperature methanol, compared with  $CO$  and  $H_2$ . The Rectisol process has been widely used in the syngas purification process. In this study, a simplified Rectisol process was built and simulated. The PSRK (short

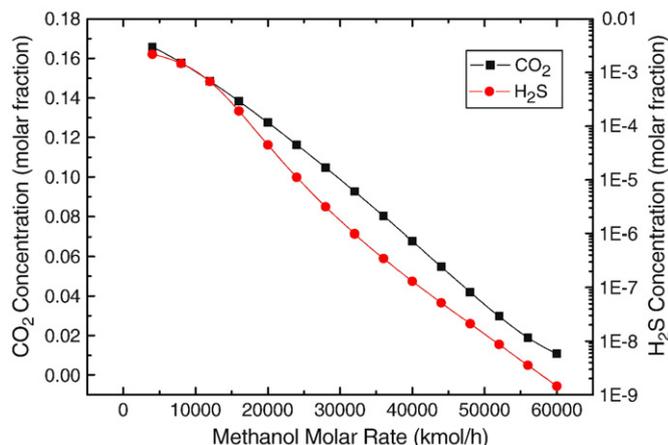


Fig. 7. Variations in  $CO_2$  and  $H_2S$  concentrations with increasing methanol during the Rectisol process.

**Table 4**  
Cold energy consumption and resource recovery during the purification process.

Cold energy consumption	kW	−6715.93
Electricity consumption during refrigeration (refrigeration coefficient = 1.05)	kW	6396.12
Sulfur recovery (assumed recovery rate was 0.85)	tons h <sup>−1</sup>	0.06
CO <sub>2</sub> recovery	tons h <sup>−1</sup>	30.71

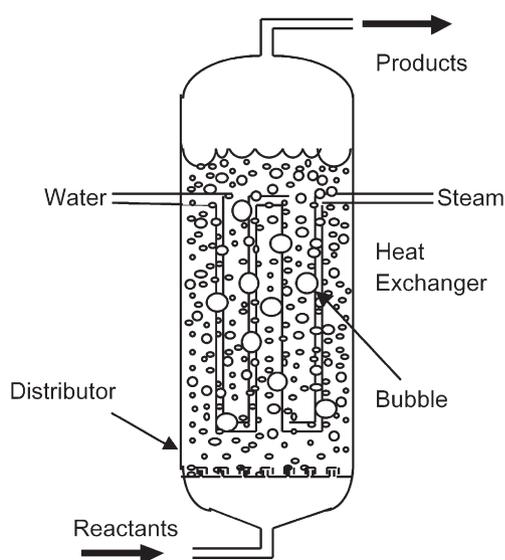
for Predictive Soave-Redlich-Kwong) property method was used, based on the Soave-Redlich-Kwong state equation, and was shown to be efficient for simulation of the Rectisol process (Chang et al., 1983).

Cold energy consumption is a problem during the purification process. The removal of H<sub>2</sub>S and CO<sub>2</sub> need massive amounts of low temperature methanol. H<sub>2</sub>S is more soluble than CO<sub>2</sub> and is more easily absorbed by methanol. As shown in Fig. 7, the CO<sub>2</sub> concentrations in the purified gas can be reduced to 3% at a methanol molar rate of 52,000 kmol h<sup>−1</sup>, and the H<sub>2</sub>S concentration is <0.1 ppm. Resource recovery was also an issue; the H<sub>2</sub>S and CO<sub>2</sub> absorbed by the methanol could be easily separated and re-used. Separation of H<sub>2</sub>S could produce sulfur and sulfuric acid. The CO and H<sub>2</sub> absorbed by the methanol were added to the purified gas. The cold energy consumption and resource recovery data is listed in Table 4. The absorbed methanol, after H<sub>2</sub>S and CO<sub>2</sub> adsorption, was cooled to undergo further absorption, with only a slight loss of volume. The electricity consumption during the cooling process was very high, but slightly less than the required amount could be generated during the HRSG process in the WGS stage.

#### 3.4. DME synthesis process

The development of a DME bifunctional synthesis catalyst is a key to single-step DME synthesis (Hu et al., 2005). The catalyst significantly influences the synthesis reaction performance but its effect is difficult to determine during long-term synthesis operations. The catalyst effect was neglected during the total recycling of unreacted CO and H<sub>2</sub> in the simulated process.

DME synthesis from syngas is an exothermic reaction. The heat generated during the reaction should be entrained out of the reactor by cool medium to maintain the appropriate temperature. The slurry reactor has better temperature control, because of the large heat capacity of the liquid phase solute. Fig. 8 shows a diagram of a JFE slurry reactor. Water is purged into the heat exchanger in the reactor



**Fig. 8.** Diagram of a JFE single-step synthesis slurry reactor (Kanniche et al., 2005).

**Table 5**  
Simulation results of DME synthesis process.

Biomass mass rate	tons h <sup>−1</sup>	75.60
DME production	tons h <sup>−1</sup>	28.14
Methanol production	tons h <sup>−1</sup>	3.86
CO <sub>2</sub>	tons h <sup>−1</sup>	34.87
LTST (152 °C, 0.4 MPa)	tons h <sup>−1</sup>	65.35
YDME	–	0.37

**Table 6**  
Comparison of pollutant emission between DME production and utilization, and direct biomass combustion.

	DME production and utilization	Biomass direct combustion
CO <sub>2</sub> (kg/MJ)	0.067	0.092
SO <sub>2</sub> (kg/MJ)	Trace	$8.87 \times 10^{-5}$

to remove heat from the reactor. The heat recovered by the water generated low pressure and low temperature steam. A DME selectivity of 0.91 and methanol selectivity of 0.09 were assumed (Ogawa et al., 2003), with total CO and H<sub>2</sub> conversion. The simulation results are shown in Table 5.

#### 3.5. Environmental evaluation and process optimization

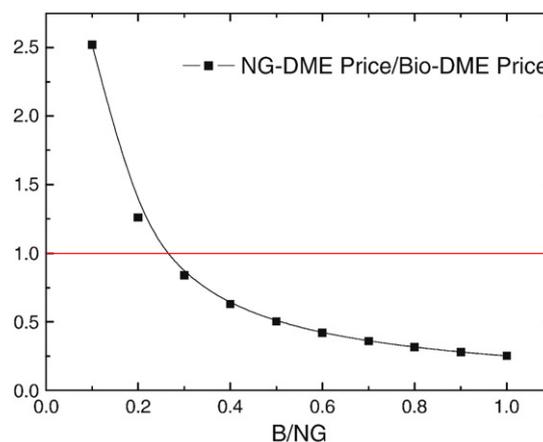
##### 3.5.1. Environmental analysis

Conventional environmental analyses were performed from the viewpoint of pollutant emissions, mainly CO<sub>2</sub> and SO<sub>2</sub>. Total CO<sub>2</sub> and H<sub>2</sub>S emission were compared between DME direct synthesis and utilization, and direct biomass combustion, based on heat equivalence. It is assumed that S was totally transformed to SO<sub>2</sub> and the heat equivalence was based on fuel LHV value. The results are shown in Table 6.

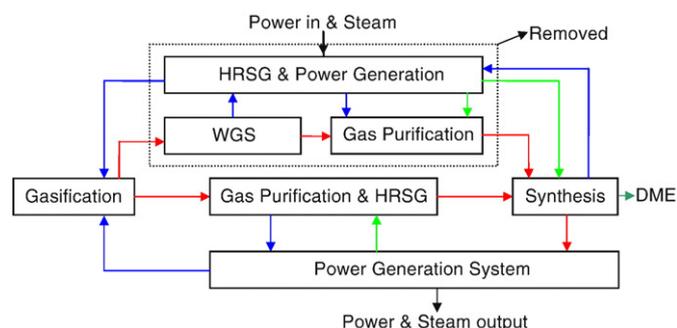
DME synthesis via biomass gasification not only increased the fuel energy density but also reduced CO<sub>2</sub> and SO<sub>2</sub> emissions. Because H<sub>2</sub>S was almost totally removed in the purification process, only trace SO<sub>2</sub> emissions were produced by DME utilization, while direct biomass combustion can produce  $8.87 \times 10^{-5}$  kg/MJ SO<sub>2</sub> emission. DME synthesis via biomass gasification also significantly reduced CO<sub>2</sub> emissions by 26.7%, compared with direct biomass combustion.

##### 3.5.2. Economic analysis

The sensitive key factors for the economic feasibility of the plant are: raw material price, plant capacity, DME price and capital cost (Kumabe et al., 2008). The material price is an important determinant of the DME production cost, and is easier to determine than the other factors. Production cost sensitivity was analyzed by changing the



**Fig. 9.** NG-DME price/biomass-DME price ratio variations with changes in biomass/natural gas price ratios.



**Fig. 10.** Single-step DME synthesis via biomass gasification process optimization. Blue line: steam; red line: syngas gas; green line: electricity. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

biomass to natural gas price ratio (B/NG) to compare DME production from biomass and natural gas. Generally, for JFE natural gas-based DME production, 1 kg natural gas could produce 1.31 kg DME (Ogawa et al., 2003), while 1 kg biomass could produce 0.37 kg DME in this study. As shown in Fig. 9, increasing the B/NG decreased the NG–DME to biomass–DME price ratio, without considering other factors affecting DME price. DME production via biomass gasification will be at an advantage when the biomass/NG price ratio is  $<0.257$ , when only raw material costs are considered.

### 3.5.3. Process optimization

Single-step DME synthesis has great environmental and economic significance, but the high conversion rate is associated with high energy consumption (Hamelinck et al., 2004; Gao et al., 2004; Yamashita and Barreto, 2005). A poly-generation system, able to simultaneously produce power, chemical products, and clean synthetic fuels through gasification of fossil fuels and renewable biomass, is a promising future prospect that is attracting increasing interest. In direct single-step DME synthesis, total conversion of syngas is also not the optimal choice. In this study, we developed an optimized poly-generation process (Fig. 10). The WGS reaction process could be removed to simplify the process by changing the S/B and O/B in the gasifier to change the  $H_2/CO$  ratio. The gas purification process could be simplified by using a sulfur-resistant DME synthesis catalyst (Koizumi et al., 2004). Using the JFE technology, the single pass CO conversion rate at  $H_2/CO = 1$  could reach 70% (Ogawa et al., 2003). If a single pass CO conversion rate of 50% could be achieved to synthesize DME without a WGS, the unreacted syngas could be transported to the power generation system to produce electricity. In this case, the calculated DME yield could reach 0.23, and the electricity production could reach 39.67 MW (the assumed net efficiency in the electricity production was 30%).

## 4. Conclusions

We analyzed single-step DME synthesis via biomass gasification in depth using ASPEN Plus™ simulation. The main conclusions were as follows:

- (1) O/B and S/B greatly influenced the gasification performance and synthesis products. The optimal O/B and S/B were 0.370 and 0.00, respectively.
- (2) A WGS process HRSG system could produce steam and electricity, which were almost adequate to satisfy the power requirements of the purification refrigeration stage.
- (3) The Rectisol process was used during the purification process. High cold energy consumption was a problem in the purification process.

- (4) The DME yield in this study was 0.37, assuming a DME selectivity of 0.91 and total CO and  $H_2$  conversion.
- (5) DME synthesis and utilization had environmental advantages over direct biomass combustion.  $CO_2$  emission could be reduced by about 27.6%, and  $SO_2$  emission was almost absent. From the economical aspect, DME from biomass could be more economical than NG when the biomass/NG price ratio was  $<0.257$ , without considering other factors affecting DME production costs.
- (6) A poly-generation process should be adopted, considering the large energy demand of total conversion of syngas. In the optimized poly-generation system, the WGS reactor could be removed and the purification process could be simplified, based on the development of a sulfur-resistant DME synthesis catalyst. The DME yield could reach 0.23 and the net electricity production could reach 39.67 MW in an optimized poly-generation process.

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