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Simulation of DME synthesis from coal syngas by kinetics model

Hyun Min Shim*, Seung Jong Lee, Young Don Yoo**, Yong Seung Yun**, and Hyung Taek Kim*,†**

*Division of Energy Systems Research, Ajou University, Suwon 443-749, Korea
**Institute for Advanced Engineering, Wonchun-dong, Suwon 443-749, Korea

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Abstract−DME (Dimethyl Ether) has emerged as a clean alternative fuel for diesel. There are largely two methods for DME synthesis. A direct method of DME synthesis has been recently developed that has a more compact process than the indirect method. However, the direct method of DME synthesis has not yet been optimized at the face of its performance: yield and production rate of DME. In this study it is developed a simulation model through a kinetics model of the ASPEN plus simulator, performed to detect operating characteristics of DME direct synthesis. An overall DME synthesis process is referenced by experimental data of 3 ton/day (TPD) coal gasification pilot plant located at IAE in Korea. Supplying condition of DME synthesis model is equivalently set to 80 N/m^3 of syngas which is derived from a coal gasification plant. In the simulation it is assumed that the overall DME synthesis process proceeds with steady-state, vapor-solid reaction with DME catalyst. The physical properties of reactants are governed by Soave-Redlich-Kwong (SRK) EOS in this model. A reaction model of DME synthesis is considered that is applied with the LHHW (Langmuir-Hinshelwood Hougen Watson) equation as an adsorption-desorption model on the surface of the DME catalyst. After adjusting the kinetics of the DME synthesis reaction among reactants with experimental data, the kinetics of the governing reactions inner DME reactor are modified and coupled with the entire DME synthesis reaction. For validating simulation results of the DME synthesis model, the obtained simulation results are compared with experimental results: conversion ratio, DME yield and DME production rate. Then, a sensitivity analysis is performed by effects of operating variables such as pressure, temperature of the reactor, void fraction of catalyst and H_2/CO ratio of supplied syngas with modified model. According to simulation results, optimum operating conditions of DME reactor are obtained in the range of 265-275 °C and 60 kg/cm^2. And DME production rate has a maximum value in the range of 1-1.5 of H_2/CO ratio in the syngas composition.

Key words: DME Synthesis, Coal Syngas, Kinetics, ASPEN Plus

INTRODUCTION

The economic situation of fossil fuels will experience a remarkable change in the near future with the introduction of hydrogen fuel. Especially, transportation fuel is gradually changing into high hydrogen content fuel with increasing oil prices and crises facing climate change on the earth. Fossil fuel technologies are gradually claiming to be cleaner and more effective. So gasification has become a technical issue as a representative clean coal technology. It can convert these fuels into a higher quality, cleaner and more flexible energy carrier, avoiding the disadvantages of their direct use. The syngas is able to generate marketable products such as chemicals (45%), Fischer-Tropsch liquids (28%), power (19%) and gaseous fuel (8%) in the overall syngas product distribution in the 2007 survey of the International Gasification Council. Gasification facilities consume various carbon-based feedstocks, including coal, petroleum, pet coke and biomass. From the 2007 survey, coal has increased its leading position as the predominant gasifier feedstock, now accounting for 55% of syngas capacity generated from all feedstocks, compared to 49% in 2004 [1].

In the current change of the energy paradigm, DME has been suggested recently as a clean alternative fuel for diesel. DME is a well-known alternative fuel for diesel engines due to its relatively good cetane number (55-60) and low emission of CO, NO_x and particulates in the exhaust gas. Moreover, DME can substitute with LPG in the domestic energy sector, because it has the similar characteristics for distribution and utilization in rural areas [1]. Besides its easy storage for transportation, its volatile nature facilitates its use as a hydrogen source for the fuel cells by means of catalytic reforming. DME can be produced from syngas which is obtained from various energy sources such as natural gas, waste, biomass and coal. The DME manufacturing methods are largely divided into two methods: the direct method (one step process) is simultaneously converted to DME by hybrid catalyst mixed methanol with dehydration catalyst; and the indirect method (two steps process) is first converted to methanol and followed by methanol dehydration to DME.

The DME synthesis reaction model is applied for the kinetics model of the direct (one step) DME synthesis reaction in this study. Process optimum parameters are proposed and compared with experimental data. The evaluated results will be able to be utilized for designing and operating a commercial DME synthesis plant.

1. Chemical Reaction for DME Synthesis

The syngas from gasification mainly contains carbon monoxide (CO) and hydrogen (H_2). Overall DME synthesis reactions consist of 3-step reactions: methanol synthesis, dehydration and water gas shift (WGS) reaction as following reactions. The formation of methanol is considered by two reaction mechanisms as illustrated in both reaction (1) and (2); reaction (1) is the formation of methanol par-

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[†] To whom correspondence should be addressed.
E-mail: htkim@ajou.ac.kr

ticipating CO and H_2 as major reactants. This reaction emits high reaction enthalpy. While reaction (2) is led to by participating CO_2 and H_2, it has less reaction enthalpy than reaction (1). It is assumed that both reactions can proceed to produce methanol simultaneously in this study.

$$CO+2H_2 \leftrightarrow CH_3OH \qquad -43.4\ \text{kcal/mol-DME} \tag{1}$$

$$CO_2+3H_2 \leftrightarrow CH_3OH+H_2O \qquad -13.5\ \text{kcal/mol-DME} \tag{2}$$

Methanol passes through the following dehydration reaction with DME synthesis catalyst as in reaction (3). DME catalyst is used to $Cu/ZnO/Al_2O_3+\gamma\text{-}Al_2O_3$ in this process. Reaction (4) is shown as a WGS reaction, and it has a role to supply CO_2 and H_2 for DME synthesis.

$$2CH_3OH \leftrightarrow CH_3OCH_3+H_2O \qquad -5.6\ \text{kcal/mol-DME} \tag{3}$$

$$CO+H_2O \leftrightarrow CO_2+H_2 \qquad -9.8\ \text{kcal/mol-DME} \tag{4}$$

By relative reaction rate among reactants, the overall DME reaction shows two mechanisms: reaction (5) and reaction (6) by integrating reactions (1)-(4). The combination of reaction (1) and (3) gives overall reaction (6); the combination of reactions (1), (3) and (4) gives overall reaction (5) [2]. And if reaction (4) proceeds slowly, the overall DME reaction leads to reaction (6) [3].

$$3CO+3H_2 \leftrightarrow CH_3OCH_3+CO_2 \qquad -58.8\ \text{kcal/mol-DME} \tag{5}$$

$$2CO+4H_2 \leftrightarrow CH_3OCH_3+H_2O \qquad -49.0\ \text{kcal/mol-DME} \tag{6}$$

According to DME overall reactions by reaction (5) and (6), the DME reaction heat is exothermal reaction which generates reaction heat highly. If DME reactor temperature is increased by reaction heat of DME synthesis, thermodynamic equilibrium conversion is decreased. And for DME catalyst it is noted that its performance is decreased in the DME synthesis reaction. So its reaction heat is should be cooled DME reactor temperature at the range of 240-280 °C by heat exchanger in the DME synthesis [4].

2. Reaction Kinetics of DME Synthesis

Reaction kinetics of methanol synthesis as a major part in DME synthesis has been studied by many researchers; however it could not be proven with accuracy until now [5-8]. Villa et al. state that methanol synthesis governed by only reaction (1) is preceded by $Cu/ZnO/Al_2O_3+\gamma\text{-}Al_2O_3$ catalyst in industrial conditions. After all, with an increase of CO_2 concentration, the reaction rate of methanol is decreased [5]. Klier et al. state that most methanol production proceeds with reaction (1), which is accelerated at low concentration of CO_2 [6].

Because DME synthesis is governed by catalytic reactions of syngas on the surface of the catalyst, it is applied to the LHHW model for simulating the DME synthesis reaction. It is assumed that each CO and CO_2 is comparatively adsorbed at an active site on the catalyst surface, and each H_2 and H_2O is also comparatively adsorbed at the other [7]. Therefore, it is suggested that methanol production is led by both CO and CO_2 components throughout catalytic reactions under the LHHW model.

For simplifying the DME synthesis reaction, the overall reaction is respectively divided into three sections: methanol synthesis, methanol dehydration and WGS reaction. The reaction rates (r) of methanol synthesis are individually expressed in Eq. (7) led by CO and Eq. (8) led by CO_2. Where, β is defined as fugacity to equilibrium reaction of each component [9,10].

Table 1. Rate constants, adsorption coefficients and equilibrium constants for DME synthesis reaction

Parameters A(i)exp(B(i)/RT)	Reference[a]		Modified	
	A(i)	B(i)	A'(i)	B'(i)
k_1	7,380	–54,307	7,380	–58,464
k_2	5,059	–67,515	5,059	–67,509
k_3	1,062	–43,473	1,062	–43,473
k_4	7.3976	–20,436	7.3976	–10,808
K_{CO}	3.934×10^{-6}	37,373	3.917×10^{-6}	49,884
K_{CO_2}	1.858×10^{-6}	53,795	1.858×10^{-6}	53,795
K_{H_2}	0.6716	–6,476	0.6716	–6,476
K_{CH_3OH}	3.480×10^{-6}	54,689	7.928×10^{-4}	48,221
$\ln K_{f1}, K_{f2}$[b]	$4213/T-5.752\ \ln T-1.707\times10^{-3}T+2.682\times10^{-6}T^2-7.232\times10^{-10}T^3+17.6$			
$\ln K_{f3}$[b]	$4019/T+3.707\ \ln T-2.783\times10^{-3}T+3.8\times10^{-7}T^2-6.561\times10^4/T^3-26.64$			
$\ln K_{f4}$[b]	$2167/T-0.2258\ \ln T-1.037\times10^{-3}T-2.331\times10^{-7}T^2-1.2777$			

[a] Rate constant and adsorption coefficient are provided by Z. G. Nie, H. W. Liu et al. (2005) [9]

[b] Equilibrium constant are provided by Zhang et al. (2001) and Herman et al. (1979) [10]

$$r_{CO}=\frac{k_1 f_{CO} f_{H_2}^2(1-\beta_1)}{(1+K_{CO}f_{CO}+K_{CO_2}f_{CO_2}+K_{H_2}f_{H_2})^3} \qquad \beta_1=\frac{f_{CH_3OH}}{K_{f_1}f_{CO}f_{H_2}^2} \tag{7}$$

$$r_{CO_2}=\frac{k_2 f_{CO_2} f_{H_2}^3(1-\beta_2)}{(1+K_{CO}f_{CO}+K_{CO_2}f_{CO_2}+K_{H_2}f_{H_2})^4} \qquad \beta_2=\frac{f_{CH_3OH}f_{H_2O}}{K_{f_2}f_{CO_2}f_{H_2}^3} \tag{8}$$

The r_{DME} of DME synthesis through methanol dehydration is shown in Eq. (9), and r_{WGS} of WGS reaction is shown in Eq. (10). WGS reaction takes place on Cu cluster among the DME catalyst and it proceeds through two steps: supplying H_2 by adsorption of oxygen in H_2O molecule, and generating CO_2 between CO and adsorptive oxygen [11]. The modified reaction rate constants, adsorption coefficients and equilibrium constants following Eq. (7)-(10) are shown in Table 1.

$$r_{DME}=\frac{k_3 f_{CH_3OH}(1-\beta_3)}{(1+\sqrt{K_{CH_3OH}f_{CH_3OH}})^2} \qquad \beta_3=\frac{f_{DME}f_{H_2O}}{K_{f_3}f_{CH_3OH}^3} \tag{9}$$

$$r_{WGS}=\frac{k_4 f_{H_2O}(1-\beta_4)}{1+K_{CO}f_{CO}+K_{CO_2}f_{CO_2}+\sqrt{K_{H_2}f_{H_2}}} \qquad \beta_4=\frac{f_{CO_2}f_{H_2}}{K_{f_4}f_{CO}f_{H_2O}} \tag{10}$$

METHODOLOGY

1. Governing Theory

For simulating the DME synthesis process model, thermodynamic parameters must be used that can be applied to the fundamental equation of state (EOS). During the simulation study, Soave-Redlich-Kwong (SRK) EOS is utilized for calculating thermodynamic properties in the model. The Redlich Kwong (1949) EOS is widely applied to binary components. It has good accuracy in volumetric and thermal properties between pure components and mixtures, but it tends to lower the accuracy of the VLE (vapor liquid equilibrium) calculation in multi-components. To complement the weak point of RK EOS, Giorgio Soave (1972) suggests appropriate SRK EOS as RK EOS improved through a generalized term of temperature from $a/T^{0.5}$ to a(T) in multi-components. The SRK EOS is shown in Eq. (11) [12].

$$P=\frac{RT}{v-b}-\frac{a(T)}{v(v+b)} \qquad \text{where } a(T)=\{1+m(1-T_r^{0.5})^2 \quad m=0.480+1.574\omega-0.176\omega^2 \tag{11}$$

Graaf et al. state that the chemical equilibrium of the methanol reaction and WGS reaction can be described very well by relationships derived from thermo-chemical data, assuming ideal gas behavior and correcting for non-ideal gas behavior by using the SRK EOS at high pressure condition [13]. DME synthesis reaction is also based on a conventional methanol synthesis reaction under high pressure condition. By the reason of Graaf's study, SRK EOS is selected as the governing equation of state for simulating the DME synthesis reactor.

To simulate catalytic behavior in the DME synthesis reaction, the LHHW model is adopted. Each reaction rate as Eq. (7)-(10) is converted into calculating formation like Eq. (12); then the DME reactor is formatted by the Rplug block with reaction rate controlled by Eq. (7)-(10) in ASPEN plus [14]. Each reaction rate is calculated by referenced kinetics parameters from Table 1.

$$r=\frac{(\text{kinetic factor})\times(\text{driving force expression})}{(\text{adsorption term})} \tag{12}$$

$$\text{where kinetic factor}=k[(T/T_0)^n]\exp[(E/R)(1/T-1/T_0)]$$

$$\text{driving force}=k_1\prod_{i=1}^{N}C_i^{ai}-k_2\prod_{j=1}^{N}C_j^{bj}$$

$$\text{adsorption term}=\left(\sum_{i=1}^{M}K_i\left[\prod_{j=1}^{N}C_j^{nuj}\right]\right)^{\cdots}$$

2. Simulation Methods

During simulation of the DME synthesis process model, several assumptions are established:

(1) Overall process is operated at steady-state with constant input flow rate of syngas.

(2) DME synthesis catalyst is composed of homogeneous catalyst and charged with constant void fraction of catalyst bed in the DME synthesis reactor.

(3) Catalytic poisoning effected by H_2S is neglected.

The input parameters for syngas as feedstock are based on supplying and operating data from 3TPD coal gasification pilot plant. Those supplying conditions are shown in Table 2. Even though these

Table 2. Operating conditions of supplied syngas from 3TPD coal gasification pilot plant

	Components	Real values
Synthesis gas composition (vol%)	CO	47.5
	H_2	16.5
	CO_2	5.5
	N_2	28.5
	H_2O	1.9
	CH_4	0.1
	H_2S	0.001
Input conditions	Total tlow (Nm^3/hr)	80
	Pressure (kg/cm^2)	1
	Temperature (°C)	40

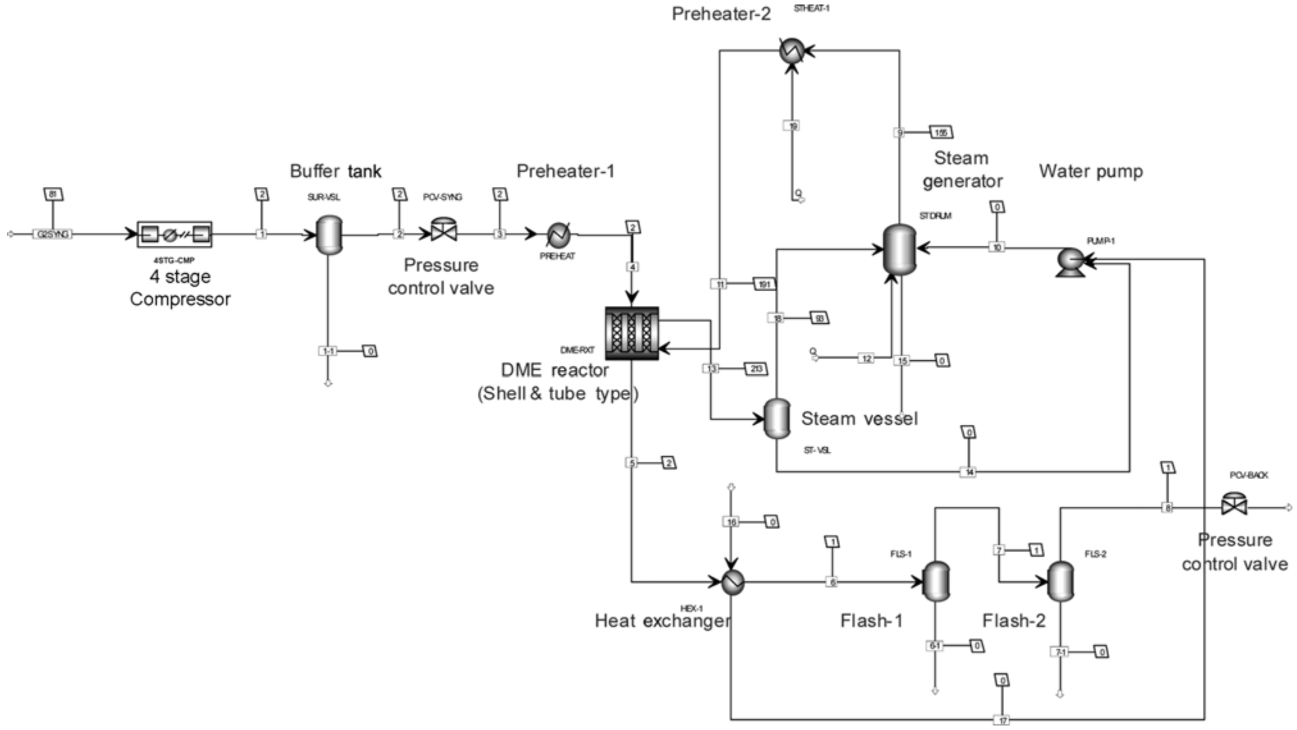

Fig. 1. Process flow diagram of DME synthesis process simulation in ASPEN plus.

Table 3. Comparison of experimental and simulation results with different input conditions

		Case 1			Case 2			Case3		
		Inlet*	Exp*	Sim	Inlet*	Exp*	Sim	Inlet*	Exp*	Sim
Mole fraction dry basis (mol%)	CO	0.378	0.313	0.316	0.374	0.314	0.311	0.377	0.305	0.316
	H_2	0.142	0.029	0.026	0.143	0.028	0.026	0.142	0.015	0.026
	CO_2	0.08	0.146	0.134	0.080	0.151	0.135	0.093	0.158	0.149
	H_2O	-	-	0.003	-	-	0.003	-	-	0.003
	N_2	0.40	0.466	0.473	0.403	0.461	0.477	0.389	0.472	0.458
	MeOH	-	0.002	0.007	-	0.001	0.007	-	0.002	0.007
	DME	-	0.044	0.042	-	0.044	0.043	-	0.048	0.042
X_{H_2} (%)		-	79.6	81.7	-	80.4	81.8	-	89.4	81.7
X_{CO} (%)		-	17.2	16.4	-	16.0	16.8	-	19.1	16.2
Y_{DME} (%)		-	19.2	18.3	-	19.4	18.9	-	20.4	17.9
P_{DME} (kg/hr)		-	5.7	5.5	-	5.3	5.6	-	5.5	5.5

*Experimental data of DME pilot plant connected with 3TPD coal gasification pilot plant, IAE, Korea [15]

parameters are unsteady for actual plant operation, these are also assumed constant factors during the simulation. And unit blocks of DME synthesis process are based on the design and operating parameters of the DME pilot plant.

The model is developed with ASPEN plus as illustrated in Fig. 1. It should be noted that a fixed bed type reactor was chosen to simulate the characteristics of the DME reactor during the study. The DME synthesis process model is composed of the following unit blocks: 4STG-CMP as a 4 stage compressor which can be operated to maximum 90 kg/cm^2; PCV, as control valve which controls pressure; PREHEAT, as pre-heater which raises to 220 °C of syngas temperature; DME-RXT, as fixed bed reactor with shell & tube heat exchanger which is operated to the range of 240-310 °C, 50-70 kg/cm^2; STDRUM, as steam generator has the role of controlling the DME reactor temperature by generating steam; HEX-1, as heat exchanger which cools the product gas after the DME reactor; FLS-1, as separator can separate methanol in the product, and FLS-2 as separator can also separate high purity of DME in the product [15].

After setting a DME synthesis process model, simulation procedures are performed by the following order.

(1) Apply initial kinetics parameters of reference from Table 1 in the DME synthesis reactor model as DME-RXT.

(2) Validate variation between experimental and simulation results.

(3) Modify kinetics parameters of DME synthesis reaction through simulation feedback.

(4) Confirm modified kinetics parameters being approximated to experimental results.

(5) Perform sensitivity analysis for changing operation parameters.

The variables of sensitivity analysis include temperature, pressure, void fraction of catalyst bed and H_2/CO ratio of syngas in the developed DME synthesis process model. In this study the void fraction of the catalyst bed is defined as the fraction of the DME reactor volume not occupied by catalyst.

RESULTS AND DISCUSSION

1. Evaluation of Simulation Results

Before evaluating simulation results, operating parameters such as conversion and yield are defined. These parameters are defined as Eq. (13) and Eq. (14), respectively.

$$\text{conversion} = \frac{\text{molar flow rate of i reacted}}{\text{molar flow rate of i feed}} = \frac{F_{i0} - F_i}{F_{i0}} \tag{13}$$

$$\text{yield} = \frac{\text{exit molar flow rate of product}}{\text{molar flow rate of initial reactant}} = \frac{2F_{DME}}{F_{CO} + F_{CO_2}} \tag{14}$$

Through simulation of the DME synthesis model, we are able to predict the tendency of performance parameters like conversion, DME production rate (P_{DME}) and DME yield (Y_{DME}), which are validated by comparison of experimental and simulation results. These results are indicated in Table 3. Each case of Table 3 represents a different input condition in the DME synthesis pilot plant. P_{DME} is average 5.55 kg/h, and Y_{DME} is average 18.4%. According to each case of conversion and yield in Table 3, relative errors for case 1, 2

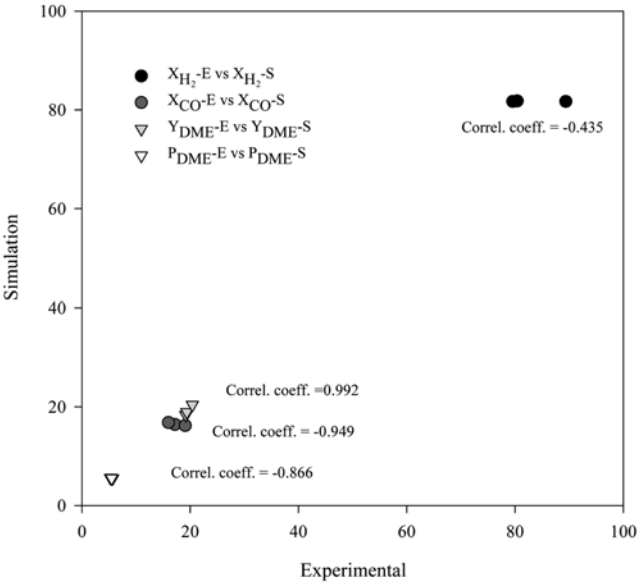

Fig. 2. Comparison of experimental and simulation results of Table 3.

are, respectively, 2.15% of H_2 conversion (X_{H_2}), 4.80% of CO conversion (X_{CO}) and 3.54% of Y_{DME}. On the other hand, case 3 obtained larger relative error than the other cases. In comparing simulation with experimental results from DME synthesis pilot plant, the accuracy of this model has above 95%. Correlation coefficients for three cases of Table 3 are calculated in Fig. 2. According to the result of correlation analysis, the correlation coefficients of X_{CO} (−0.949), Y_{DME} (0.992) and P_{DME} (−0.866) are well consistent except X_{H_2} (−0.435).

2. Sensitivity Analysis

Sensitivity analysis of the developed model is performed by changing operation variables such as temperature, pressure, void fraction of catalyst bed and H_2/CO of syngas. With changing pressure of the DME reactor from 5 to 90 kg/cm^2 with fixed at 280 °C of DME reactor temperature (based on 14.2 mol% H_2, 37.8 mol% CO, 8.0 mol% CO_2), the production rate, conversion and yield profiles for each major product (DME, MeOH, CO_2) are shown in Fig. 3. The production rate of MeOH shows a maximum value around at 30 kg/cm^2. Since MeOH is converted to DME above 30 kg/cm^2, that production rate of DME represents a maximum around over 60 kg/cm^2. Above 60 kg/cm^2, DME production rate does not change largely with increasing pressure. Both CO conversion and DME yield are showing similar tendency by increasing pressure, and CO_2 is also increased similarly from 25 kg/cm^2.

Fig. 4 indicates the same profiles like Fig. 3 with changing DME

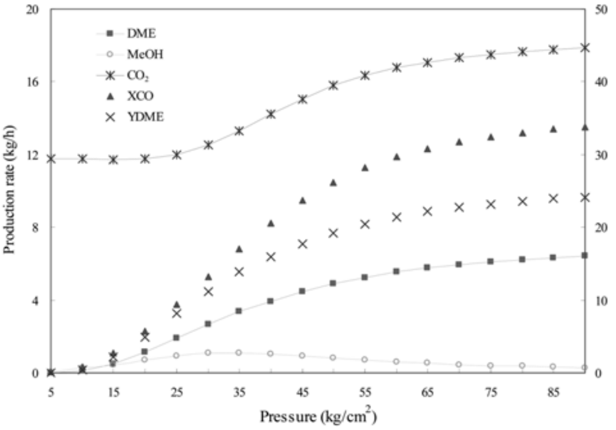

Fig. 3. Production rates, X_{CO} and Y_{DME} profiles dependent on pressure change at 280 °C (14.2 mol% H_2, 37.8 mol% CO, 8.0 mol% CO_2).

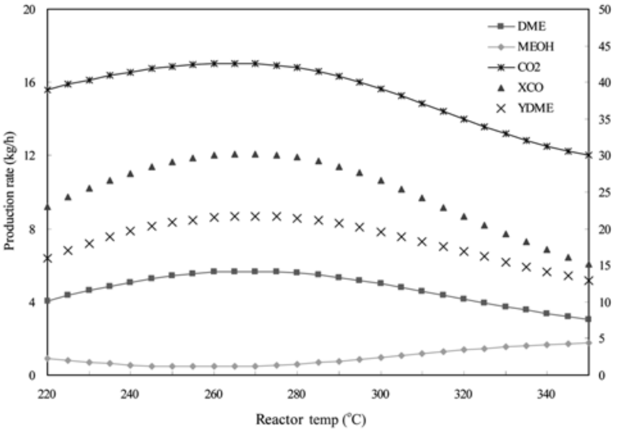

Fig. 4. Production rates, X_{CO} and Y_{DME} profiles dependent on temperature change at 60 kg/cm^2 (14.2 mol% H_2, 37.8 mol% CO, 8.0 mol% CO_2).

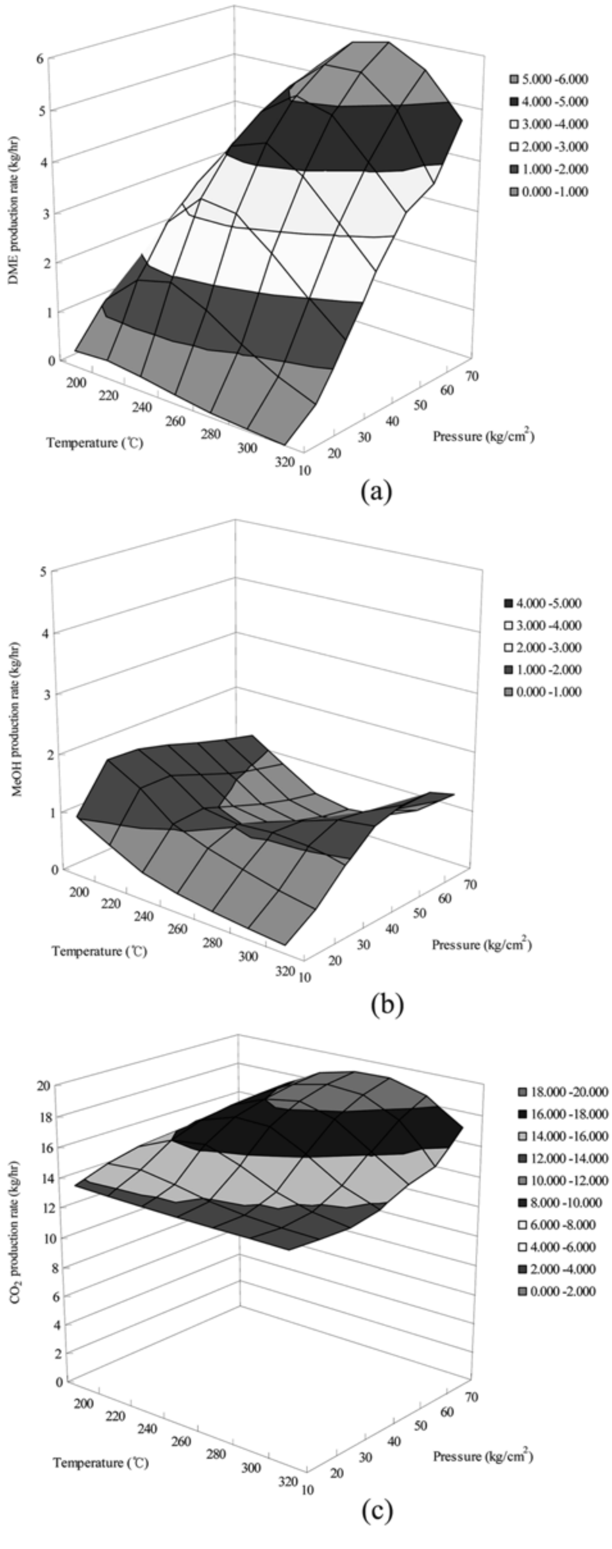

Fig. 5. Production rate of (a) DME, (b) MeOH, (c) CO_2 profiles dependent on pressure and temperature (14.2 mol% H_2, 37.8 mol% CO, 8.0 mol% CO_2).

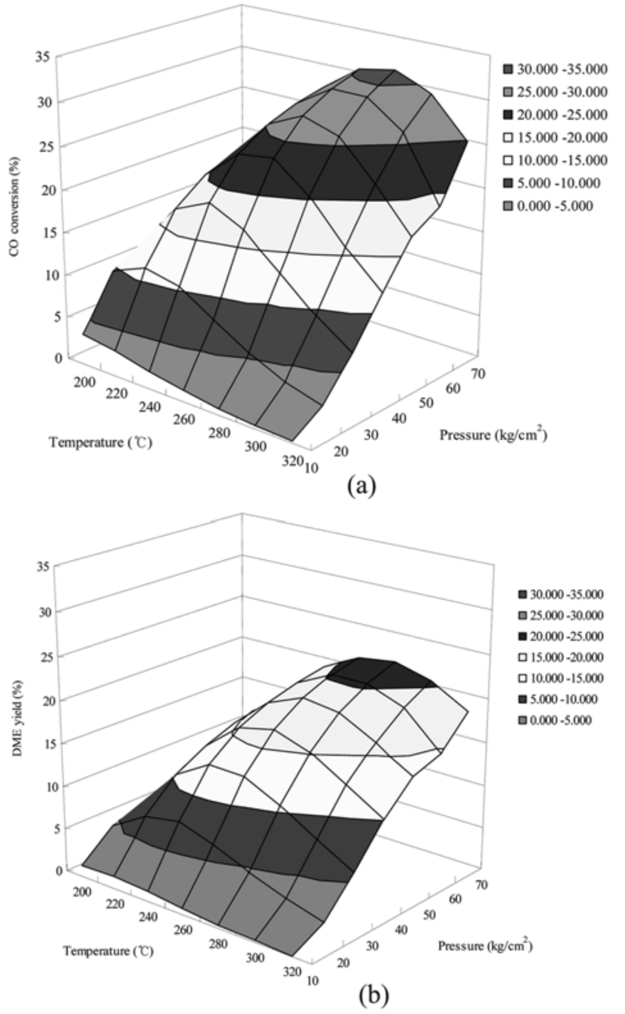

Fig. 6. (a) X_{CO} and (b) Y_{DME} profiles dependent on pressure and temperature (14.2 mol% H_2, 37.8 mol% CO, 8.0 mol% CO_2).

reactor temperature in the range of 220-350 °C at 60 kg/cm². This is since the production rate of DME and CO_2 shows a maximum quantity near 270 °C, while MeOH shows minimum production rate near 260 °C. CO conversion and DME yield are shown convex similarly around 270 °C. So this point can be recognized as the optimum temperature of DME synthesis. Fig. 5(a)-(c) show the production rate of DME, MeOH and CO_2, respectively, with simultaneous changing of pressure and temperature of the DME reactor. And profiles for CO conversion and DME yield are also shown in Fig. 6(a)-(b) under the same conditions.

With changing void fraction of catalyst bed at 280 °C, 60 kg/cm² (based on 14.2 mol% H_2, 37.8 mol% CO, and 8.0 mol% CO_2), the production rate of each product is a constant value over 0.1 of void fraction as shown in Fig. 7. The void fraction of the catalyst bed does not mainly affect the rising temperature of the DME reactor; however, the residence time increases linearly with void fraction, as shown in Fig. 8.

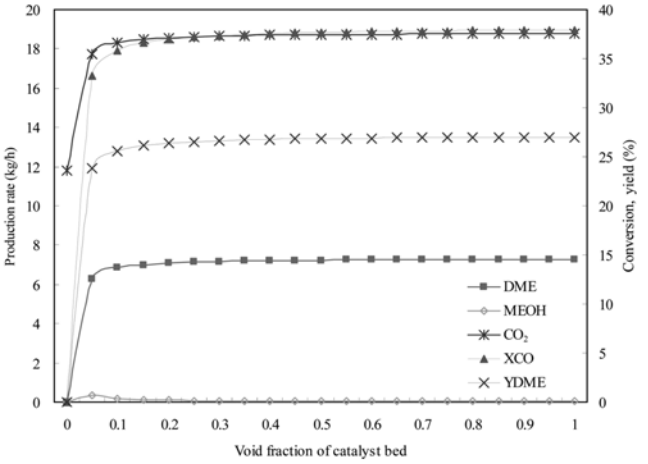

Fig. 7. Production rates, X_{CO} and Y_{DME} profiles dependent on void fraction of catalyst bed at 280 °C, 60 kg/cm² (14.2 mol% H_2, 37.8 mol% CO, 8.0 mol% CO_2).

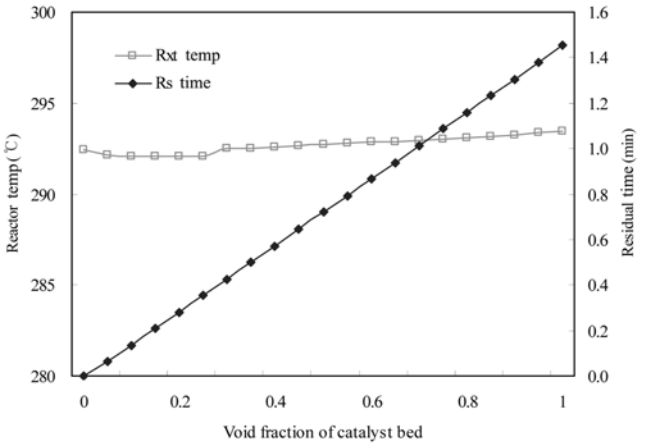

Fig. 8. Residence time and reactor temperature profiles dependent on void fraction of catalyst bed at 280 °C, 60 kg/cm².

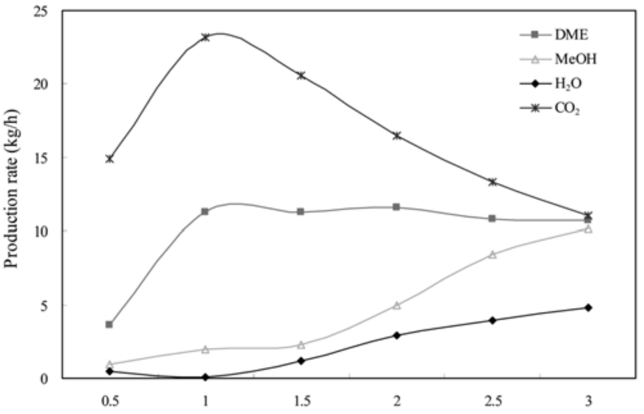

Fig. 9. Production rates (DME, MeOH, H_2O, CO_2) profiles dependent on H_2/CO ratio of syngas at 270 °C, 60 kg/cm².

Fig. 9 indicates production rate profiles for DME, MeOH, H_2O, and CO_2 with changing H_2/CO ratio of syngas at 270 °C, 60 kg/cm². H_2/CO ratio is controlled by the following ratio ($CO : H_2 : N_2 = 1 : X : 3-X$) in the range of 0.5-3.0. Production rate profiles for each product are indicated in Fig. 9. According to this result, the H_2/CO ratio, with which can be obtained maximum DME product, is closed in

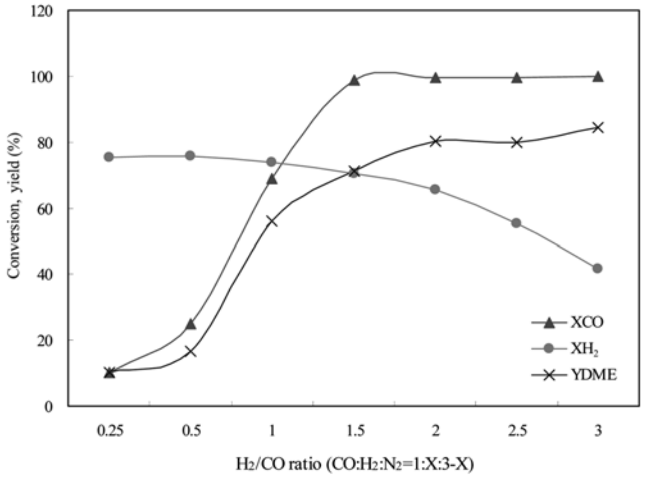

Fig. 10. X_{CO}, X_{H_2} and Y_{DME} profiles dependent on H_2/CO ratio of syngas at 270 °C, 60 kg/cm^2.

the range of 1.0-2.0. When H_2/CO ratio of supplied syngas becomes 1.0, it is certain that the overall DME synthesis reaction is led by reaction (5). And approaching to 2.0 of H_2/CO ratio, the overall DME synthesis reaction is led by reaction (6). But as the H_2/CO ratio goes through over 1.5, the CO conversion approaches to being restricted. Because the CO component which can react with H_2 does not exist anymore, H_2 conversion is relatively decreased. Those results are indicated in Fig. 10. Over 2.0 of H_2/CO ratio, the MeOH production rate is gradually increased to the point close to the DME production rate. And CO_2 production rate shows a maximum quantity at 1.0 of H_2/CO ratio, gradually decreasing after that point. The syngas-to-DME synthesis reaction is fully utilized under CO-rich conditions, but the total productivity is limited by methanol synthesis. The rate-determining step shifts to methanol dehydration, and the DME synthesis becomes poor over 2.0 of H_2/CO ratio [16].

If syngas with 1.0 of H_2/CO ratio is fed to a DME reactor, the product quantity of CO_2 is increased more than three times than initial CO_2. So considered for reduction of CO_2 sub-products in this process, it is better to feed syngas of 2.0 of H_2/CO ratio. Since the methanol product is increased at this operating point, recycling of methanol should be considered for maximizing the DME product. Additionally, for maximizing DME product under the given plant operating conditions, it is required to recycle the separated stream and modify DME process with WGS reactor being available to add H_2.

CONCLUSIONS

This study was able to perform simulation of the DME synthesis reaction from coal syngas by applying a kinetics model under the environment of ASEPN plus. A modified DME synthesis model based on kinetics parameters has approximate operating values through validating by experimental data of a DME synthesis pilot plant. So operating conditions of DME synthesis are able to be predicted by sensitivity analysis of the DME synthesis model for various operating variables. According to sensitivity analysis, optimal operating conditions of DME synthesis from coal syngas are proposed to operate at 60-65 kg/cm^2 of pressure, 265-270 °C of temperature, 0.15-0.35 of void fraction and 1.0-1.5 of H_2/CO ratio. Comparing DME synthesis controlled by reaction (5) with reaction (6) for DME synthesis, its production rate is approximately similar.

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NOMENCLATURE

C_i : concentration of component i [mol/kg]
E : activation energy [kJ/kmol]
EOS : equation of state
F_i : molar flow rate of component i [kmol/h]
K_i : equilibrium constant of component i
N : number of components
M : number of terms in adsorption
P_i : partial pressure of component i [kg/cm^2]
R : gas constant [8.314472 J·K^{-1}·mol^{-1}]
T : temperature [K]
P_{DME} : DME production rate [kg/h]
Y_{DME} : DME yield, dimensionless
X_{CO} : CO conversion
X_{H_2} : H_2 conversion
a, b : parameters in Redlich-Kwong equation
n : temperature exponent
m : adsorption term exponent
nu : exponent for each component
k : reaction rate coefficient
f_i : fugacity of component i
v : specific volume
β : equilibrium degree, dimensionless
r : reaction rate [mol/gcat/s]
ω : acentric factor

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