
SUPPLEMENTARY MATERIAL

Validation of a fixed bed reactor model for dimethyl ether synthesis using pilot-scale plant data

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Table S1. Reaction rate equations, the equilibrium constant of each reaction and kinetic parameters.

Reaction rate equations	$r_{MS} = \frac{k_1(p_{H_2} p_{CO_2})[1 - (1/K_{eqm1})(p_{CH_3OH} p_{H_2O})/(p_{CO_2} p_{H_2}^3)]}{(1 + K_2(p_{H_2O}/p_{H_2}) + \sqrt{K_3 p_{H_2}} + K_4 p_{H_2O})^3} \quad (Eq.1)$	
	$r_{RWGS} = \frac{k_5 p_{CO_2} [1 - K_{eqm2}(p_{CO} p_{H_2O}/p_{CO_2} p_{H_2})]}{1 + K_2(p_{H_2O}/p_{H_2}) + \sqrt{K_3 p_{H_2}} + K_4 p_{H_2O}} \quad (Eq.2)$	
	$r_{MD} = k_6 K_{CH_3OH}^2 \left[\frac{C_{CH_3OH}^2 - (C_{H_2O} C_{DME}/K_{eqm3})}{(1 + 2\sqrt{K_{CH_3OH} C_{CH_3OH}} + K_{H_2O} C_{H_2O})^4} \right] \quad (Eq.3)$	
The equilibrium constant	$\text{Log}_{10} K_{eqm1} = \frac{3066}{T} - 10.592 \quad (Eq.4)$	
	$\text{Log}_{10} \frac{1}{K_{eqm2}} = -\frac{2073}{T} + 2.029 \quad (Eq.5)$	
	$\text{Log}_{10} K_{eqm3} = \frac{10194}{T} - 13.91 \quad (Eq.6)$	
Kinetic parameters and equilibrium constants		A(i)
	k_1	1.65
	K_2	3610
	K_3	0.37
	K_4	7.14×10^{-11}
	k_5	1.09×10^{10}
	K_{ch3oh}	0.00079
	k_6	3.7×10^{10}
	K_{H2O}	0.084
		B(i)
		36696
		0
		17197
		124119
		-94765
		70500
		-105000
		41100
	$parameter = A_{(i)} \cdot e^{\frac{B_{(i)}}{RT}}$	

Table S2. The heat and mass transport property.

The heat transfer coefficient on the surface of the catalyst	$N_{nu} = \frac{h_p d_p}{k_g} = 2 + 0.6 N_{Re sph}^{0.5} N_{Pr}^{1/3} \quad (Eq.7)$	
	$N_{Re sph} = \frac{d_p v \rho}{\mu} \quad (Eq.8)$	
	$N_{Pr} = \frac{c_p g \mu}{k_g} \quad (Eq.9)$	
The heat transfer between the surface of the catalyst and the reaction fluid	$\sum_i r_i \Delta H_{r g cat} = h_p A_p (T_p - T_f) \quad (Eq.10)$	
Tube side heat transfer coefficient	$h_i = \left(\frac{1}{\frac{1}{h_r + 2\lambda_{effw}^0/d_p + a_w c_p g \rho g v} + \frac{1}{h_{packet}}} \right) \quad (Eq.11)$	
	$h_{packet} = 1.13 \left(\frac{\lambda_{eff}^0 \rho_p (1 - \varepsilon_{mf}) C_{ps}}{\tau_t} \right)^{0.5}$	
	$\lambda_{effw}^0 = \varepsilon_w \lambda_g + (1 - \varepsilon_w) \lambda_s \left(\frac{1}{\varphi_w (\lambda_s/\lambda_g) + 1/3} \right)$	
	$\lambda_e^0 = \varepsilon_{mf} \lambda_g + (1 - \varepsilon_{mf}) \lambda_s \left(\frac{1}{\varphi_b (\lambda_s/\lambda_g) + 2/3} \right)$	
	$a_w = 0.05, h_r(\text{radiation}) = 0 \quad (Eq.12)$	
The diffusion rate and mass transfer coefficient equation	$W_{Ar.i} = m_{ci} (C_{A0.i} - C_{As.i})$	
	$N_{Sh} = \frac{m_{ci} d_p}{D_{i,j}} = 1.17 N_0 0.585 Sc^{1/3} Re$	
	$N_{Re} = \frac{d_p v \rho}{\mu}$	

	$N_{Sc} = \frac{\mu}{\rho D_{i,j}} \quad (Eq.13)$
The effectiveness factor	$\eta_{MS/WGS/MD} = \frac{4\pi R_p^2 D_{eff,j} (-\frac{dc}{dr})_{r=R}}{\frac{4}{3}\pi R_p^3 r_{MS/WGS/MD}} \quad (Eq.14)$
Pressure drop	$\frac{\Delta p}{L} = \frac{150\mu_a(1-\varepsilon)^2 u_0}{\varepsilon^3 d_p^2} + \frac{1.75(1-\varepsilon)\rho u_0^2}{\varepsilon^3 d_p} \quad (Eq.15)$

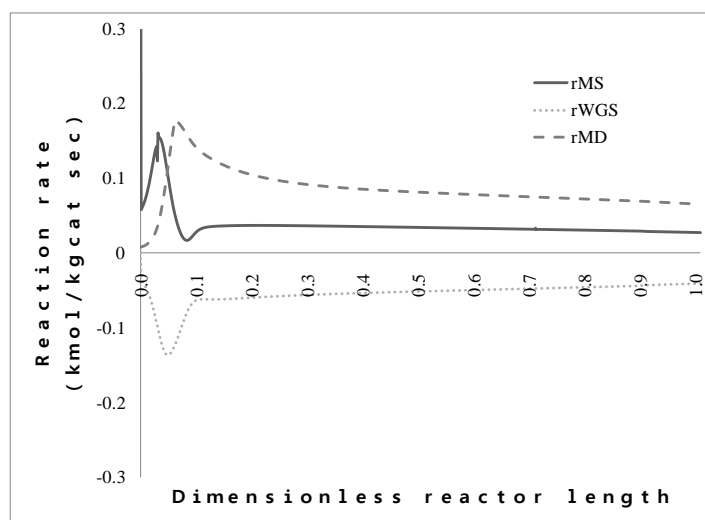


Figure S1. Simulated reaction rates along the reactor length (data set 1).

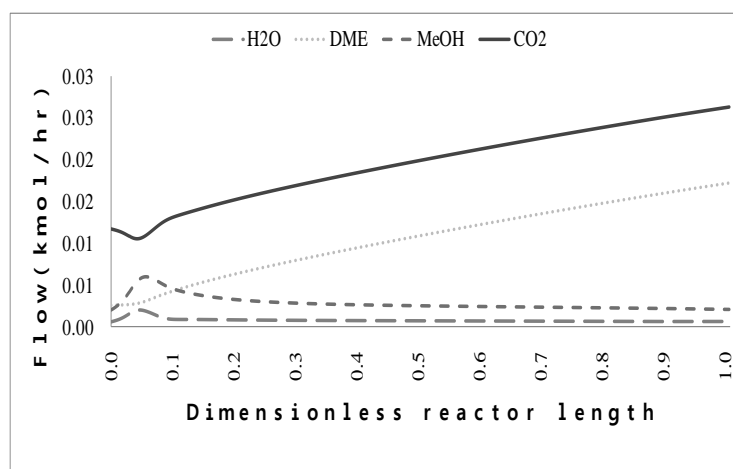


Figure S2. Simulated mole flow rate along the reactor length (data set 1).

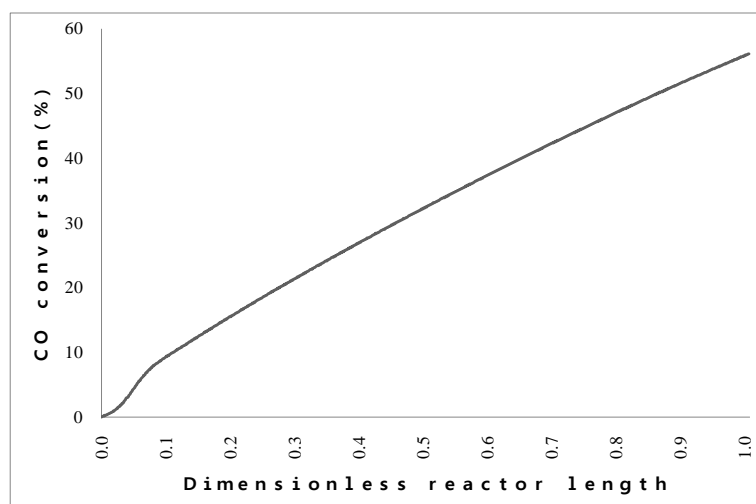


Figure S3. Simulated CO conversion along the reactor length (data set 1).

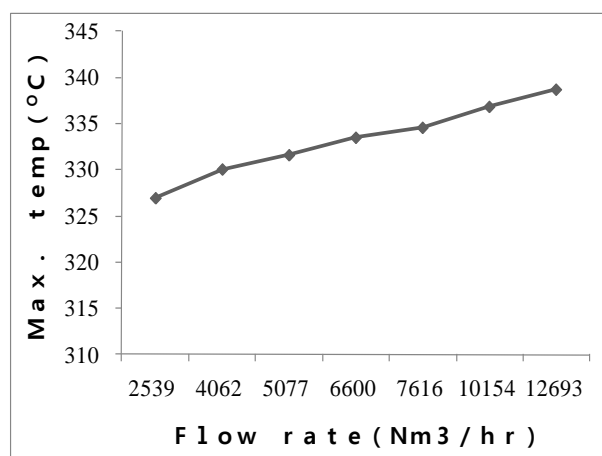
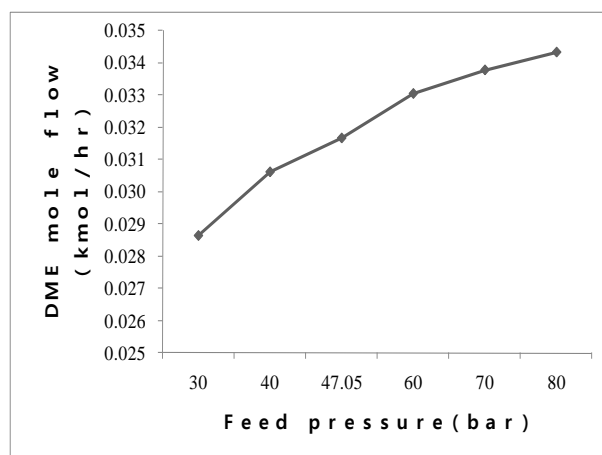
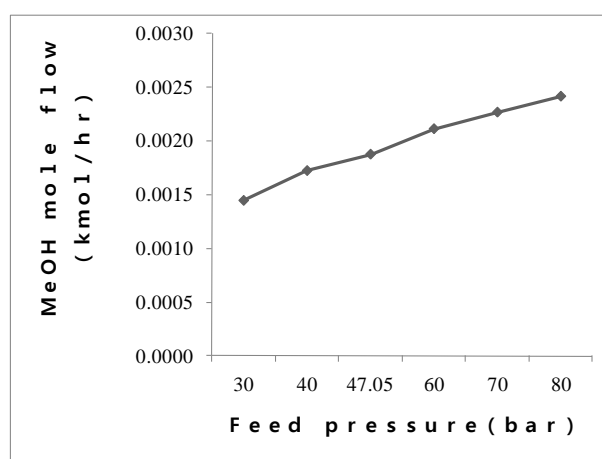


Figure S4. Influence of the flow rate on the maximum temperature in the reactor.



(a)



(b)

Figure S5. Influence of the feed pressure on (a) DME and (b) methanol mole flow at the outlet of the reactor.

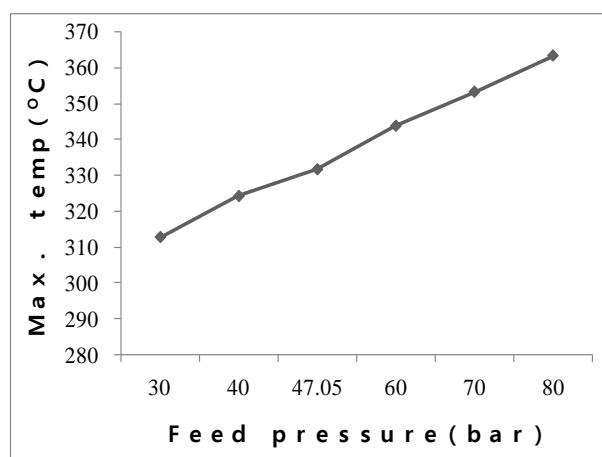


Figure S6. Influence of the feed pressure on the maximum temperature in the reactor.

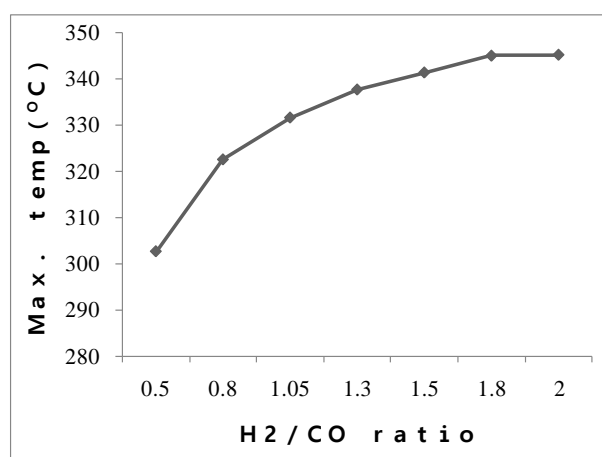


Figure S7. Influence of the H₂ to CO ratio on the maximum temperature in the reactor.

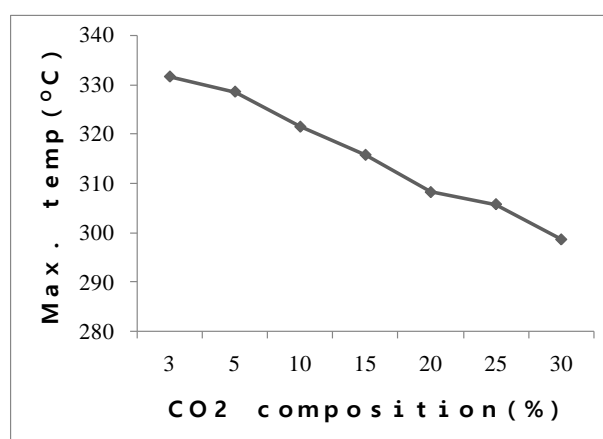


Figure S8. Influence of CO₂ mole fraction on the maximum temperature in the reactor.

Nomenclature

A_p	Surface area of the catalyst, m^2
$C_{A0,i}$	Concentration of component i in reactants fluid, $kmol\ m^{-3}$
$C_{AS,i}$	Concentration of component i on the catalyst surface, $kmol\ m^{-3}$
C_{pg}, C_{pfluid}	Specific heat of fluid, $cal\ mol^{-1}\ K^{-1}$
C_{ps}, C_{pw}	Specific heat of particles at the surface and of cooling water, $cal\ mol^{-1}\ K^{-1}$
$dHr, \Delta Hr$	Heat of reaction, $kJ\ mol^{-1}$
d_p	Particle diameter, m
D_{ij}	Binary diffusivity of gas, $cm^2\ s^{-1}$
$D_{eff,j}$	Effective diffusivity of component i within a catalyst pellet, $m^2\ h^{-1}$
g_{cat1}, g_{cat2}	Mass of the MeOH synthesis catalyst and the MeOH dehydration catalyst, g
h_i, h_o	Film coefficient at a tube inside and outside, $J\ m^{-2}\ h^{-1}\ ^\circ C^{-1}$
h_p	Film coefficient at heat transfer on a catalyst pellet, $J\ m^{-2}\ h^{-1}\ ^\circ C^{-1}$
h_{packet}	Film coefficient in a packet, $J\ m^{-2}\ h^{-1}\ ^\circ C^{-1}$
h_r	Heat transfer coefficient for a radiation, $J\ m^{-2}\ h^{-1}\ ^\circ C^{-1}$
m_{ci}	Mass transfer coefficient of component i , $m\ s^{-1}$
k_i	Reaction rate constants
$K_i, K_{eqm,j}$	Adsorption constant and Equilibrium constant of reaction j
L	Height of the bed, m
N_{nu}	Nusselt number
N_{Pr}	Prandtl number
N_{Re}	Reynolds number
$N_{Re\ sph}$	Particle Reynolds number
N_{Sc}	Schmidt Number
N_{Sh}	Sherwood Number
Δp	Pressure drop, bar
P_i	Partial pressure of component i
r	Radial distance in the catalyst, m
r_i	Reaction rate of i reactions, $mol\ g_{cat}^{-1}\ h^{-1}$
r_{MS}	Reaction rate of the methanol synthesis reaction, $mol\ g_{cat}^{-1}\ h^{-1}$
r_{RWGS}	Reaction rate of the reverse water gas shift reaction, $mol\ g_{cat}^{-1}\ h^{-1}$
r_{WGS}	Reaction rate of the water gas shift reaction, $mol\ g_{cat}^{-1}\ h^{-1}$
r_{MD}	Reaction rate of the methanol dehydration reaction, $mol\ g_{cat}^{-1}\ h^{-1}$
R	Gas constant, $8.314\ J\ mol^{-1}\ K^{-1}$
R_p	Particle radius, m
T_f	Fluid Temperature, K
T_o, T_p	Lagrange multipliers
$W_{Ar,i}$	Diffusion rate of component i $kmol\ m^{-2}s^{-1}$
u_o	Volumetric average fluid velocity, $m\ s^{-1}$

Greek letters

$\lambda_{eff}^0, \lambda_{effw}^0$ Effective thermal conductivity at the fixed bed and the wall region, $J.m^{-2}\ h^{-1}\ ^\circ C^{-1}$

λ_g Fluid thermal conductivity, $J\ m^{-2}\ h^{-1}\ ^\circ C^{-1}$

λ_m, λ_s Heat conductivity of a wall and a particle, $J\ m^{-2}\ h^{-1}\ ^\circ C^{-1}$

\mathcal{E} The void space of the bed

$\mathcal{E}_{mf}, \mathcal{E}_w$ The void fraction at the minimum fluidizing bed and at the wall layer

ϕ_w Ratio of effective thickness of gas film around a contact point to particle diameter for contact between

particle and surface

η_j Effectiveness factor of j reaction

η_{MS} Effectiveness factor of the methanol synthesis reaction

η_{WGS} Effectiveness factor of the water gas shift reaction

μ, μ_a	Dynamic viscosity and absolute viscosity, $\text{kg m}^{-1} \text{s}^{-1}$
ρ, ρ_g	Fluid density, kg m^{-3}
ρ_b	Bulk density of the bed, kg m^{-3}
$\rho_p, \rho_{p1}, \rho_{p2}$	Particle density of hybrid catalyst, MeOH synthesis catalyst and MeOH dehydration catalyst, g m^{-3}
v	Fluid line velocity, m s^{-1}
$\sum v_i$	Diffusion volume, mol cm^{-3}
τ_t	Residence time, h