

Optimal Condition of DME Production through Syngas Hydrogenation in Dual Membrane Reactor

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ARTICLE INFO	ABSTRACT
<p>Article History: Received: 27 November 2022 Revised: 21 January 2023 Accepted: 22 January 2023</p> <p>Article type: Research</p> <p>Keywords: DME, Dual Membrane Reactor, Heterogeneous Modeling, Process Optimization</p>	<p>Typically, supporting the dimethyl ether synthesis reactor by hydrogen and steam permselective membrane modules and optimization of operating conditions are practical solutions to shift the equilibrium conversion of reactions toward dimethyl ether synthesis and CO₂ conversion. In this regard, the aim of this research is to calculate the desired condition of hydrogen and steam Selective membrane reactors to improve dimethyl ether productivity. At first, the mass and energy conservation laws are applied to the membrane supported reactor to develop a heterogeneous model. After model validation, an optimization problem is programmed to calculate the optimal value of manipulated variables considering the limitations and constraints of the problem. Then, the main parameters of conventional and optimized membrane supported reactor including carbon monoxide and carbon dioxide conversion, dimethyl ether productivity, and temperature profiles are presented at steady-state conditions. The results of the simulation prove that dimethyl ether productivity is 0.0211 and 0.0262 mole s⁻¹ in conventional and optimized membrane reactors, respectively. In general, operating at optimal conditions increases DME production by up to 24.2%.</p>

Introduction

Typically, DME as a colorless and organic compound is utilized as the synthetic fuel for compression ignition, refrigerant agent, aerosol spray propellant, and feed to produce dimethyl sulfate and acetic acid [1]. Currently, adopted environmental restrictions by governments and the need for alternative fuels have introduced DME as a synthetic fuel to mix with LPG and Diesel [2- 6]. Direct syngas conversion over a dual site catalyst and methanol dehydration over single site Al₂O₃ catalyst are two common routes of DME production. Due to the lower cost and higher equilibrium conversion, the direct DME production method is more attractive compared to the methanol dehydration method [7].

In this regard, much research have been conducted on DME production through the direct route and process planning to increase production capacity [8]. Vakili and Eslamloueyan designed a process to enhance the equilibrium conversion of syngas to DME [9]. The simulation results proved that the designed reaction system could enhance DME productivity by up to 12%. Lu et al. focused on the direct conversion of synthesis gas to DME in a non ideal reactor

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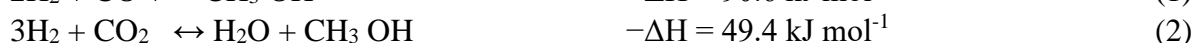
[10]. The main benefits of applied fluidized bed against fixed bed reactor were lower pressure drop, higher carbon monoxide conversion, and higher DME productivity and yield. Papari et al. investigated the operability of slurry bubble column reactors to produce DME from syngas [11]. The considered reactor was modeled considering the two bubbles hydrodynamic flow approach. The results proved that the main benefit of a bubble column reactor is the uniform temperature in the system.

Although the combination of chemical reaction and separation makes the process more complex, it is a suitable technique to decrease operating costs and increase conversion. Iliuta et al. introduced the sorption-enhanced reaction process for syngas conversion to DME by in situ combination of chemical adsorption and reaction [12]. The simulation results showed that decreasing steam concentration in the reactor by chemical adsorption improves DME yield. The regeneration of saturated adsorbent was the critical section of the proposed process. Although supporting conventional reactors with the membrane module makes the process more complex and expensive, it shifts the equilibrium limited reactions toward the desired product. Since the hydrogenation of carbon monoxide and carbon dioxide and methanol dehydration are thermodynamically limited reactions, changing the concentration of components in the reaction zone, operating pressure and temperature could shift the reactions toward the DME production side. Mardanpour et al. simulated the syngas conversion to DME in a membrane supported reactor [13]. The results showed that increasing hydrogen concentration over the catalyst by applying a hydrogen permselective membrane module could enhance DME productivity. Falco et al. developed a Double Recycling Loop configuration to produce DME from carbon dioxide in a membrane supported reactor [14]. In the proposed structure, pure CO₂ was used as the sweep gas to shift CO₂ hydrogenation reaction toward the methanol synthesis. Farsi et al. designed a dual membrane supported configuration to enhance the equilibrium conversion of reactions in the direct DME synthesis route [15]. The results of the simulation proved that supporting the DME reactor by hydrogen and H₂O permselective membrane modules was a useful approach to enhance rate of CO and CO₂ conversion and methanol dehydration reactions.

Although supporting the conventional reactor by membrane improved DME production, finding the optimal condition of a dual membrane supported reactor was a challenge and could enhance DME productivity [15]. In this regard, the aim of current research is to calculate the optimal operating condition of the considered membrane reactor to enhance the DME productivity. Thus, a constrained optimization problem is programmed and the optimal condition of the membrane supported reactor is determined considering the process limitations and bounds.

Reaction Kinetics

In general, the mixture of γ -Al₂O₃ and CuO–ZnO–Al₂O₃ catalysts are applied in the reactor to progress the rate of syngas conversion and methanol dehydration reactions, respectively [16]. The DME synthesis reaction network includes the hydrogenation of carbon monoxide, carbon dioxide, and methanol dehydration reactions. The hydrogenation of carbon monoxide and carbon dioxide to methanol reactions could be listed as:



The methanol dehydration to DME reaction is as:



The rate of carbon monoxide and carbon dioxide hydrogenation to methanol, and methanol dehydration reactions are as follows [17, 18]:

$$r_{\text{CO}} = \frac{k_1 f_{\text{CO}} f_{\text{H}_2}^2 \left(1 - \frac{f_{\text{CH}_3\text{OH}}}{K_{f1} f_{\text{CO}} f_{\text{H}_2}^2}\right)}{\left(1 + K_{\text{CO}_2} f_{\text{CO}_2} + K_{\text{CO}} f_{\text{CO}} + K_{\text{H}_2} f_{\text{H}_2}\right)^3} \quad (4)$$

$$r_{\text{CO}_2} = \frac{k_2 f_{\text{CO}_2} f_{\text{H}_2}^3 \left(1 - \frac{f_{\text{CH}_3\text{OH}} f_{\text{H}_2\text{O}}}{K_{f2} f_{\text{CO}_2} f_{\text{H}_2}^3}\right)}{\left(1 + K_{\text{CO}_2} f_{\text{CO}_2} + K_{\text{CO}} f_{\text{CO}} + K_{\text{H}_2} f_{\text{H}_2}\right)^4} \quad (5)$$

$$r_{\text{DME}} = \frac{k_3 f_{\text{CH}_3\text{OH}} \left(1 - \frac{f_{\text{DME}} f_{\text{H}_2\text{O}}}{K_{f3} f_{\text{CH}_3\text{OH}}^2}\right)}{\left(1 + \sqrt{K_{\text{CH}_3\text{OH}}} f_{\text{CH}_3\text{OH}}\right)^2} \quad (6)$$

Process Modeling

Reactor Modeling

Typically, the considered reactor includes three coaxial tubes that the annulus zone between the inner and middle tubes is packed by the solid catalyst. The inner tube is H₂O permselective membrane and H₂O permeates from the reaction zone toward the inner tube. The middle tube is hydrogen permselective and hydrogen is permeated from a hydrogen-rich stream to the reaction section. Since the carbon monoxide and carbon dioxide hydrogenation and methanol dehydration reactions are exothermic, the heat of reactions is removed by circulating saturated water around the outer tube. Table 1 presents the specifications of feed, and the characteristics of the reactor in the conventional DME synthesis process [19]. The diameter of the water permselective tube, reaction tube, and hydrogen permselective module are 38, 56.2, and 72 mm, respectively [15].

Table 1. Feed specification and characteristics of catalyst in the DME synthesis reactor

	Parameter	Value	Unit
Feed Specification	Composition (mole fraction)		
	Carbon monoxide	17.16	-
	Carbon dioxide	4.09	-
	Dimethyl ether	0.18	-
	Methanol	0.3	-
	Steam	0.02	-
	Hydrogen	43.25	-
	Nitrogen	31.6	-
	Methane	4.4	-
	Feed temperature	493	K
Feed pressure	50	Bar	
Reactor Characteristics	Pipe number	4177	-
	Pipe diameter	Φ38×2	mm
	Feed flow rate	2.04×10 ⁵	Nm ³ h ⁻¹
	Reactor Length	5.8	M
	Shell temperature	513	K
	Wall heat conductivity	48	Wm ⁻¹ K ⁻¹
Catalyst Data	Diameter of catalyst	5	mm
	Bed density	1200	Kg m ⁻³
	Bed porosity	0.455	-

In this section, the considered model for membrane supported and conventional reactors are presented. The considered assumptions are:

- The ideal gas condition is valid.
- Since Pe is sufficiently large, radial dispersion of mass and energy is insignificant.
- Since Re is sufficiently large, the flow pattern in tubes is Plug.
- Since catalyst Bi is adequately small, the lumped body assumption is valid.

Based on the considered simplifications, the balance equations for the gas phase could be explained as:

$$u_g \frac{dC_i}{dz} + k_{gi} a_v (C_i - C_i^s) + \frac{\pi D_w}{A_R} Q_w - \frac{J_H}{A_R} = 0 \quad (7)$$

$$u_g \rho_g C_{pg} \frac{dT}{dz} + h_f a_v (T - T^s) + \frac{\pi D_w}{A_R} U_{rw} (T - T_w) + \frac{\pi D_r}{A_h} U_{rh} (T - T_H) = 0 \quad (8)$$

The governing equations for solid phases could be explained as:

$$\eta_i \rho_B r = k_{gi} a_v (C_i - C_i^s) \quad (9)$$

$$\eta_i \rho_B r (-\Delta H) = h_f a_v (T - T^s) \quad (10)$$

The governing equations for water permselective module are:

$$u_m \frac{dC_w}{dz} - \frac{\pi D_m}{A_m} Q_w = 0 \quad (11)$$

$$u_m \rho_m C_{pm} \frac{dT}{dz} - \frac{\pi D_w}{A_R} U_{rw} (T - T_w) = 0 \quad (12)$$

The governing equations for the hydrogen permselective module are:

$$u_m \frac{dC_H}{dz} + \frac{J_H}{A_m} = 0 \quad (13)$$

$$u_h \rho_h C_{ph} \frac{dT}{dz} - \frac{\pi D_r}{A_h} U_{rh} (T - T_H) + \frac{\pi D_h}{A_h} U (T_H - T_{sh}) = 0 \quad (14)$$

Table 2 presents the applied correlation to calculate the thermal and physical properties of components and transfer resistances.

Table 2. The characteristics of hydrogen and water membrane modules

Parameter	Correlation	Ref.
Specific heat capacity	$c_p = a + bT + cT^2 + dT^3$	
Viscosity	$\mu = \frac{c_1 T^{c_2}}{1 + \frac{c_3}{T} + \frac{c_4}{T^2}}$	(22)
Diffusion mass transfer coefficient	$D_{im} = \frac{1 - y_i}{\sum_{i=j} \frac{y_i}{D_{ij}}}$	(23)
Mass transfer coefficient	$k_{gi} = 1.17 Re^{-0.42} Sc_i^{-0.67} u_g 10^3$	(24)
Overall heat transfer coefficient	$\frac{1}{U} = \frac{1}{h_i} + \frac{A_i \ln(D_o/D_i)}{2\pi L K_w} + \frac{A_i}{A_o} \frac{1}{h_o}$	
Convective heat transfer coefficient	$\frac{h}{c_p \rho \mu} \left(\frac{c_p \mu}{K}\right)^{2/3} = \frac{0.458}{\varepsilon_B} \left(\frac{\rho u d_p}{\mu}\right)^{-0.407}$	(25)

Water Membrane Tube

Since H₂O is produced through CO₂ hydrogenation and methanol dehydration reactions, decreasing the concentration of H₂O in the reaction zone by the applied membrane module could increase equilibrium conversion of both reactions. The H₂O permeation rate through the applied alumina-silica composite membrane could be calculated by [20]:

$$Q_i = \pi_w (P_w^R - P_w^S) \quad (15)$$

Hydrogen Membrane

In general, increasing the concentration of hydrogen could progress the carbon monoxide and carbon dioxide hydrogenation reactions toward the methanol synthesis side and consequently enhances the rate of MeOH dehydration. The rate of hydrogen permeation through Pd-Ag membrane module could be calculated as:

$$J_h = 6.33 \times 10^{-8} \frac{2\pi e^{-\frac{E_p}{RT}}}{\ln(R_o/R_i)} \left(\sqrt{P_h^R} - \sqrt{P_h^S} \right) \quad (16)$$

Process Optimization

Optimization is a practical approach to determine the desired inputs of a system considering limitations and constraints. The main steps in process optimization are process modeling, defining the objective function, and selection of available inputs and bounds. Typically, the goal in DME synthesis plans is to enhance the production capacity without violating constraints and bounds. In this regard, DME productivity has been chosen as the objective function. In addition, inlet syngas pressure, inlet syngas temperature, feed temperature of inlet sweep gas to hydrogen and H₂O permselective sides, and temperature of circulating water have been selected as the decision variables. Thermodynamically, changing operating pressure and temperature change equilibrium constant of reactions and could increase equilibrium conversion of reactions. In addition, increasing temperature causes catalyst deactivation by sintering and coke formation. Although increasing operating pressure shifts the hydrogenation of carbon monoxide and carbon dioxide reactions toward the methanol synthesis side, there is a maximum operating condition based on the reactor design pressure. Besides, the operating pressure affects the rate of hydrogen and H₂O permeation along the applied membrane modules. In this regard, 533K

and 70 bar have been selected as the upper bound of temperature and pressure, respectively. The genetic algorithm method, with 200 generations and 150 populations, is used to calculate the optimal condition of a dual membrane supported reactor [21].

Numerical Solution

The obtained equations in the modeling section provide a set of mixed non-linear differential and algebraic equations. These equations are solved numerically by the Forth Order Runge Kutta method.

Results and Discussions

Model Validation

Since the established mathematical model is utilized in the optimization stage, the precision of optimization results depends on the accuracy of the reactor model. The comparison of the model results and available data points is tabulated in Table 4 at the same feed condition. As seen in Table 3, there is a tolerable error between data points and the results of the simulation, and the model results is valid.

Table 3. Utilized equations to estimate the transfer coefficient, physical and thermal properties

	Hu et al.	Result of Model	Relative Error (%)
DME	0.0491	0.0509	3.66
CO	0.0877	0.0851	-2.9
CO ₂	0.0671	0.0674	0.44
Outlet temperature (K)	516.7	519.8	0.59

Process Optimization

Although the dual membrane configuration is more efficient over the conventional DME reactor, applying the optimal value of manipulated variables on the membrane supported reactor enhances DME productivity considerably. the calculated optimum condition of dual membrane supported reactor is shown in Table 4. Typically, DME productivity in the conventional and optimized membrane supported reactors are 0.0262 and 0.0211 mole s⁻¹, respectively. Applying optimal value of manipulated variables on the system enhances DME productivity up to 24.17%.

Table 4. Comparing simulation results and taken data points from industrial plant

Decision variables	Value
Feed Temperature (K)	515.4
Inlet sweep gas in water side (K)	508.6
Inlet sweep gas in hydrogen side (K)	494.7
Circulating water side (K)	503.3
Feed pressure (Bar)	60.6
DME production rate	0.0262

Increasing operating pressure shifts the methanol synthesis reactions in the direction of CO and CO₂ hydrogenation and enhances the syngas equilibrium conversion. Then, the produced methanol through hydrogenation reactions is dehydrated and converted to DME. On the other hand, increasing the pressure of the reaction zone could reduce the partial pressure difference between the sweep gas and reaction zone and result in lower hydrogen permeation. Thus, there

is an optimum operating pressure to set DME productivity at the highest value. The difference between the calculated optimal pressure and the considered upper bound for pressure proves that the applied pressure constraint is inactive. Thus, the process is safe and fluctuation of feed pressure during the process run time does not make the process risky. Fig. 1 illustrates the DME productivity profile along the conventional and optimized membrane supported reactors. It appears that hydrogen permeation from the hydrogen-rich stream toward the reaction increases the concentration of hydrogen over the catalyst and shifts methanol synthesis reactions toward methanol productivity. In addition, decreasing the concentration of H_2O over the catalyst shifts carbon monoxide and carbon dioxide hydrogenation and DME synthesis reactions toward the completion. Thus, applied membrane modules to increase the concentration of hydrogen and decrease the concentration of H_2O over the catalyst and operating at optimized condition have a positive impact on the reaction network and improves the DME yield.

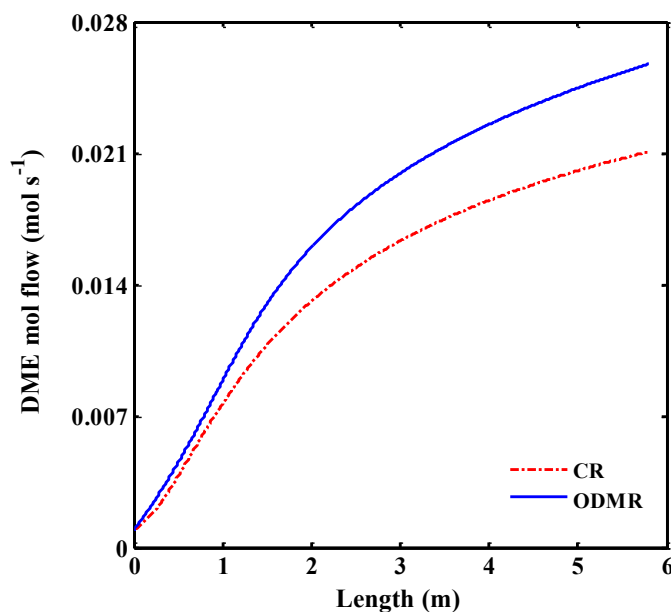


Fig. 1. Flow rate of DME in the conventional and optimized membrane supported reactors

Fig. 2 explains the profile of gas temperature along the conventional and optimized membrane supported reactors. Although increasing operating temperature enhances the rate of methanol synthesis and dehydrogenation reaction, it has a negative impact on the final conversion of exothermic reactions and reduces the equilibrium conversion in those reactions. Theoretically, increasing the reaction rate by applying hot feed and overcoming the equilibrium limitations by reducing the temperature at the second part is the optimal temperature trajectory along the reactor. In this regard, the developed optimal temperature trajectory along the dual membrane reactor enhances the DME productivity. As seen the heat production by the reaction is dominant over the energy transfer at the first half of the reaction zone and temperature increases gradually. Since the concentration of reactants decreases along the reactor, the rate of energy transfer is dominant over the energy production rate in the second part and temperature decreases gradually. Since the hydrogen permselective zone creates an extra heat transfer resistance to remove the heat of the reaction, a higher temperature is developed in the membrane supported reactor against the conventional reactor.

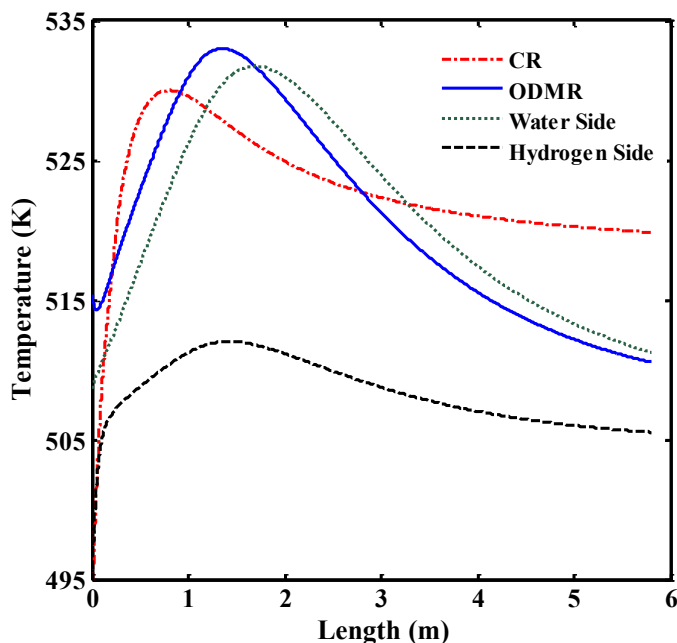


Fig. 2. Profile of temperature in the conventional and optimized dual membrane supported reactors

Fig. 3 presents the carbon monoxide profile in the conventional and optimized membrane supported reactors. In addition, Figs. 4a and b illustrate the carbon dioxide content and rate of carbon dioxide hydrogenation along the conventional and optimized membrane supported reactors. Typically, the applied changes in the system shift the carbon monoxide hydrogenation reaction in the direction of the completion reaction and improve the rate methanol dehydration to DME by increasing methanol concentration in the system. Besides, since equilibrium constant of the CO_2 hydrogenation reaction is small, increasing methanol concentration in the system via progress of CO hydrogenation reaction shifts the hydrogenation of carbon dioxide reaction in the reverse direction. The results of simulation illustrate that the CO_2 productivity are 0.0279 and 0.0247 mole s^{-1} in the conventional and optimized reactors, respectively.

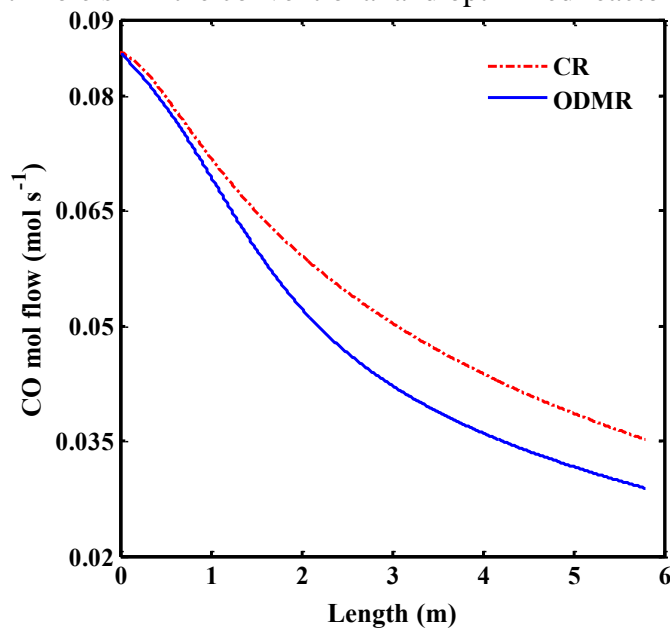


Fig. 3. Flow rate of CO in the conventional and optimized membrane supported reactors

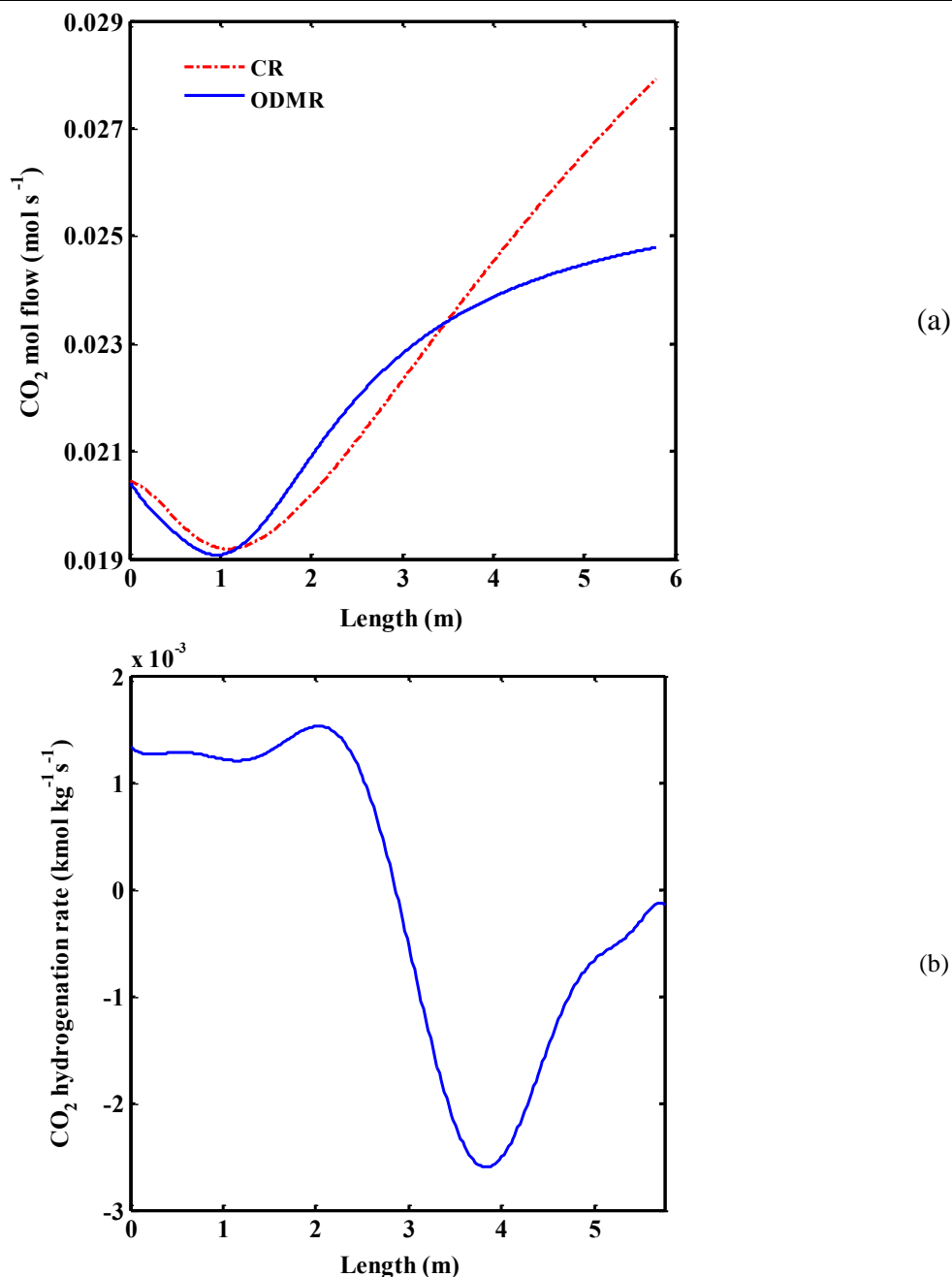


Fig. 4. (a) flow rate of CO₂ and (b) rate of CO₂ hydrogenation along the conventional and optimized dual membrane supported reactors

The hydrogen and H₂O content along the conventional and membrane supported reactors have been presented in Figs. 5 and 6, respectively. Although methanol synthesis reactions decrease hydrogen concentration in the conventional reactor, hydrogen-rich sweep gas act as a hydrogen source for CO and CO₂ hydrogenation reactions, and a part of the consumed hydrogen is supplied by an applied membrane module. The results of the simulation show that the permeation rate of hydrogen dominates over the hydrogen consumption rate and hydrogen concentration increases at the last part of the dual membrane supported reactor. Besides, the steam productivity through CO₂ hydrogenation and methanol dehydration reactions is dominants over the rate of steam permeation and H₂O concentration increases along the optimized membrane supported reactor continuously.

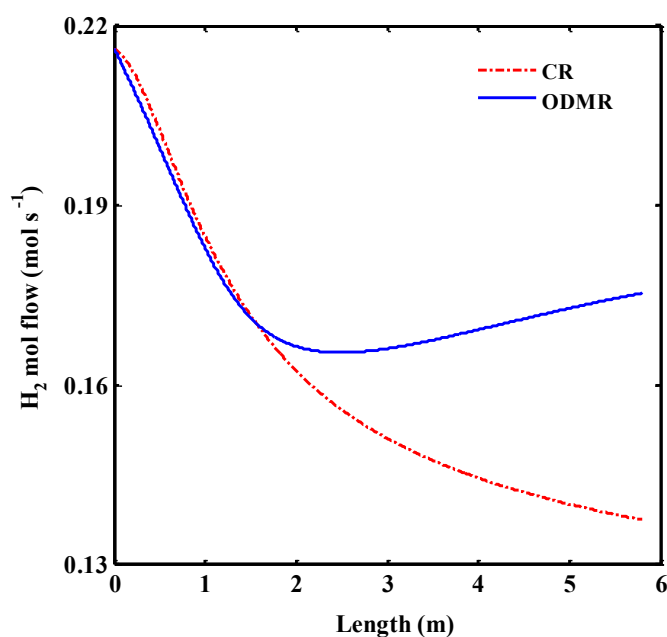


Fig. 5. Flow rate of H₂ in the conventional and optimized membrane supported reactors

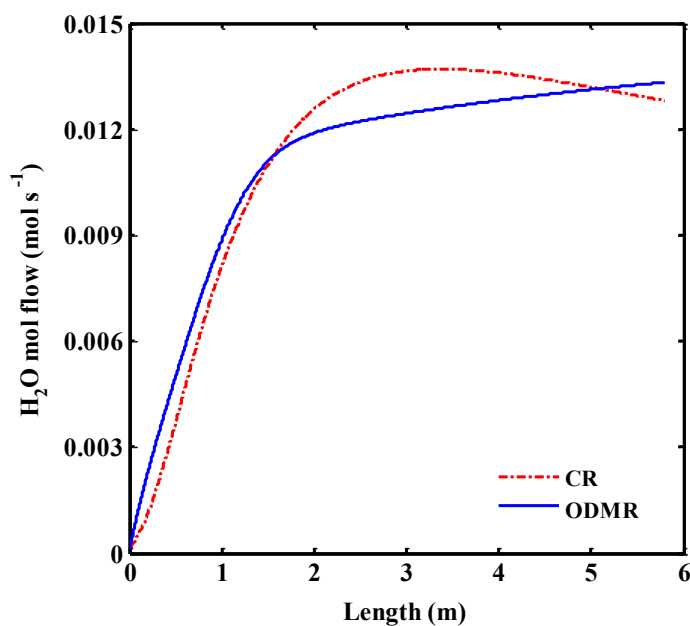


Fig. 6. Flow rate of H₂O in the conventional and optimized membrane supported reactors

Conclusions

In this research, the optimal value of manipulated variables in the hydrogen and steam permselective membrane reactor was determined to set DME productivity at the maximum value. The considered isothermal reactor was mathematically modeled considering internal and external mass and heat diffusion limitations. To optimize the process performance, an optimization problem was programmed considering DME productivity as the objective function, feed pressure, feed temperature, the inlet temperature of sweep gas flow rate and boiling water temperature as decision variables. The Genetic Algorithm method was applied to

handle the programmed optimization problem. The results of the simulation proved that DME production was enhanced up to 24.17% in the optimized membrane supported reactor compared to the conventional process. Besides, carbon dioxide emission was decreased by about 11.5% in the optimal dual membrane reactor. In general, the applied membrane modules enhanced DME productivity, carbon dioxide and carbon monoxide conversion, and enhanced catalyst lifetime by changing the concentration of hydrogen and steam over the applied catalyst.

Nomenclature

A_c	Cross section area (m^2)
a_v	Catalyst specific surface area ($m^2 m^{-3}$)
C_i	Concentration ($mol m^{-3}$)
C_p	Specific heat capacity ($J mol^{-1} K^{-1}$)
D	Diameter (m)
F	Molar flow rate ($mol s^{-1}$)
f_i	Fugacity of component i, (bar)
ΔH	Heat of reaction ($J mol^{-1}$)
h_f	Heat transfer coefficient ($W m^{-2} K^{-1}$)
k	Arrhenius factor of reaction rate ($mol kg^{-1} s^{-1} bar^{-1/2}$)
k_g	Mass transfer coefficient ($m s^{-1}$)
L	Length (m)
P	Pressure (bar)
r_i	rate of reaction ($mol kg^{-1} s^{-1}$)
R	Universal gas constant [$Pa m^3 mol^{-1} K^{-1}$]
T	Temperature (K)
u	Superficial velocity ($m s^{-1}$)
U	Overall heat transfer coefficient ($W m^{-2} K^{-1}$)
z	Axial coordinate (m)

Greek Letters

α_h	Hydrogen flux constant ($mol s^{-1} m^{-1} Pa^{-1/2}$)
μ	Viscosity ($kg m^{-1} s^{-1}$)
ρ	Density ($kg m^{-3}$)
π_w	Steam flux constant, ($mol m^{-2} s^{-1} Pa^{-1}$)
ε	Bed void fraction

Superscripts and Subscripts

g	Gas phase
H	Hydrogen membrane side
m	Water Membrane side
r	Reaction side
s	Catalyst surface
t	Tube side
W	Water vapor membrane side

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