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Full Length Article

Maximization of dimethyl ether production from synthesis gas by obtaining optimum temperature profile and water removal

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HIGHLIGHTS

- The reactor is optimized by applying differential evolution (DE) algorithm as an effective and robust optimization method.
- In case 1, inlet temperature of each segment has been optimized via differential evolution (DE).
- Same approach has been applied in the second case in order to achieve optimum water permeation rate.
- In the third case, the optimum profiles of temperature and water removal have been obtained.
- 1.5%, 55% and 70% enhancement in the dimethyl ether production have been obtained in case 1, case 2, case 3 respectively.

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ABSTRACT

In this study, a novel method optimizing direct dimethyl ether generation from syngas is proposed. A bi-functional catalyst is used containing commercial catalyst for direct DME synthesis ($CuO/ZnO/Al_2O_3$). The length of reactor has been discretized into twenty segments and optimum temperature profile in the inlet of each segment and the amount of water removal from the main stream are calculated. This optimization is done via differential evolution (DE) method, in which the inlet temperature and water removal flux in each segment are considered as the decision variables and mole fraction of dimethyl ether in the reactor outlet is the objective function. Three different cases are considered. In the first case, inlet temperature of each segment has been optimized. Then, flux of water removal is considered. And, finally, a combination of two previous cases is investigated. Obtained results of this novel theoretical study showed that water removal results in more methanol production; and Consequently, dimethyl ether production increased. By applying the proposed optimization methods, 1.5%, 55% and 70% enhancement in the dimethyl ether production have been obtained in comparison with the conventional reactor of direct dimethyl ether production.

1. Introduction

1.1. Dimethyl ether (DME)

Because of excessive demand for energy, deprivation fuel resources and environmental concerns, the global community is seeking new alternative fuels. DME could be considered to be a perspective of future fuel due to its unique characteristics. Its physical properties are similar to those of liquefied petroleum gas (LPG) [1–5]. It burns with the discharge of no sulfur oxides (SO_x), less nitrogen oxides (NO_x) and less carbon monoxide (CO). Also, it could be used as hydrogen source in fuel cells. DME could be used as an intermediate to produce chemicals such as methyl acetate [6].

Basically, there are two routes to synthesize DME: direct synthesis and indirect synthesis. In the indirect method, DME is produced via a two- step process. In the first step, syngas is converted to methanol in the presence of catalyst. Then, methanol is dehydrated over the alumina or zeolite based acidic materials [7]. On the other hand, in the direct method, known as the single step process, the feedstock (syngas) converts directly to DME. In this method, a bifunctional catalyst is used which consist of metallic side for methanol synthesis and acidic side for methanol dehydration. It should be mentioned that all of the reactions take place in one reactor simultaneously and the produced methanol is not separated during the process [8]. Therefore, the direct method is more economical in comparison with the other one.

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Nomenclature

A_c	cross section area (m^2)
a_{sp}	specific surface area of catalyst pellet ($m^2\ m^{-3}$)
C_i	concentration of each component (mol m^{-3})
C_p	specific heat of the gas at constant pressure (J mol^{-1})
D_e	effective diffusivity ($m^2\ s^{-1}$)
d_p	particle diameter (m)
f_i	partial fugacity of component *i* (bar)
F	molar flow rate (mol s^{-1})
h_f	heat transfer coefficient of fluid (W $m^{-2}\ K^{-1}$)
K_{fi}	rate constant for the rate of reaction
K_{eff}	conductivity of fluid phase (W $m^{-1}\ K^{-1}$)
K_{pi}	equilibrium constant based on partial pressure for component *i* in DME synthesis reaction
M_i	molecular weight of component *i* (g mol^{-1})
P	total pressure (bar)
Q	volumetric flow rate ($m^3\ s^{-1}$)
r_1	rate of reaction for hydrogenation of CO (mol kg $cat^{-1}\ s^{-1}$)
r_2	rate of reaction for hydrogenation of CO_2 (mol kg $cat^{-1}\ s^{-1}$)
r_3	rate of reaction for DME (mol kg $cat^{-1}\ s^{-1}$)
R	gas constant (kJ $kmol^{-1}\ K^{-1}$)
T	temperature (K)
T_{ref}	reference temperature (K)
Z	length of reactor coordinate

Acronyms

CR	conventional packed bed reactor
NP	Number of Population
OF	objective function
SC	Schmidt number
Re	Reynolds number

Greek letters

M	viscosity of fluid phase (kg $m^{-1}\ s^{-1}$)
P	density of gas phase (kg m^{-3})
ρ_b	density of catalytic bed (kg m^{-3})
ε	porosity
ΔH_i	heat of reaction ith (kJ kg^{-1})
υ_i	stoichiometric coefficient of component ith in reaction
ϕ_s	sphericity

1.1.1. Experiment studies

In recent years, many studies have been done to investigate various reactor configurations for one-step DME production. Sun et al. studied on a series of bifunctional catalysts CuO/ZnO/ZrO_2/HZSM-5 with different ZrO_2. These catalysts were characterized by surface area, XRD and XPS analysis [9]. Cai et al. studied the effect of Tin addition to catalyst of direct synthesis of DME and concluded that there is an optimized concentration of Tin which the yield of DME generation is the highest [2]. García-Trenco and Martínez considered the effect of different metallic oxides ratios on the CO conversion and DME generation [10]. Raoof et al. conducted an experimental study on a fixed bed reactor of DME production [11]. They investigated the effect of methanol purity on the DME production yield in the indirect synthesis method.

1.1.2. Modeling studies

Hu et al. presented a successfully mathematical model in relation to DME reactor in direct synthesis method [12]. Vakili et al. designed an optimal industrial scale dual-type reactor for direct dimethyl ether production. The results of their study showed that the proposed configuration led to an increase in DME production capacity, which was estimated to be about 60 ton/day in comparison to conventional industrial DME reactor [5]. In other study, Vakili et al. proposed a thermally coupled heat exchanger reactor for direct dimethyl ether (DME) synthesis. In this novel configuration, DME production increases about 600 ton/year [13]. Nasehi et al. simulated an adiabatic fixed bed DME reactor at steady state condition [14]. They used indirect synthesis method in their simulation and showed that obtained results for one dimensional and two dimensional reactors have a little difference. The effect of heat transfer boundary condition on the process was studied by Farsi et al. [15]. They designed and simulated an isothermal reactor and showed that isothermal reactor has a positive effect on the yield of reaction in comparison with adiabatic reactor. Coupling of endothermic and exothermic reaction has been done by Khademi et al. [16]. In their proposed configuration, the exothermic reaction of DME generation was coupled with the endothermic reaction of cyclohexane dehydrogenation. Omata et al. [17] studied DME production from syngas in a temperature gradient reactor to overcome both the equilibrium limitations at high temperatures and low catalyst activity related to low temperatures. Then, they optimized the operating conditions of the reactor for higher CO conversion by combining genetic algorithms and artificial neural networks. Iranshahi et al. [18] suggested a reactor configuration for naphtha reforming process, in which hydrogen and aromatics productions were increased by obtaining optimum temperature profile and hydrogen removal rate. The main advantage of their research compared with other studies about naphtha reforming is the application of the optimum temperature profile and hydrogen removal along the reactors. The length of naphtha reforming reactor has been discretized into twenty segments. In order to find the optimum values of the temperature and hydrogen removal rate, differential evolution (DE) method was used, which is a simple heuristic approach. The inlet optimum values for each segment were found and they were joined on the figures along the reactor. Arabpour et al. [19] also evaluated maximum gasoline production of FischereTropsch synthesis reactions in GTL technology by a discretized approach. In this way, the conventional synthesis reactor has been discretized into some elements. For each element, the inlet temperature, the injected hydrogen and the removed water are considered as decision variables. Then, the optimum amount of these decision variables is defined by using the differential evolution (DE) algorithm as an optimization method.

1.1.3. Objectives

In the present study, the effect of temperature and concentration on the process yield is studied to obtain the maximum production of dimethyl ether. Regarding this, the length of reactor has been discretized into twenty segments. Three cases are considered to obtain the inlet optimum values for each section of reactor. In the first case, temperature has been optimized. Then if second case, water removal has been optimized. And finally, in the third case, combination of optimized temperature and water removal has been investigated. Obtained results compared with the results of Hu et al. [12] to validate the accuracy of the method.

2. Reaction scheme and kinetics

DME synthesis from syngas is an exothermic reaction. In this study, a bi-functional catalyst is used containing commercial