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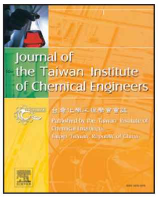

A green industrial scale di-methyl ether reactor with aiming to CO_2 reduction: staging and multi-objective optimization approach

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ABSTRACT

CO_2 and H_2O are two important by-products that affect DME production in the reactor. Besides, CO_2 is an important air pollutant and may have an impact on global climate change. Therefore, this study tries to increase CO_2 conversion along with DME production simultaneously and independently proposing a multi-stage reactor using a multi-objective approach. In this respect, a variety of effective optimization degrees of freedom such as H_2O separation ratio, feed temperature, inter-stage cooling temperature, shell temperatures, number of reactors in series and reactor configurations (adiabatic/non-adiabatic fixed bed reactor; (non-)AFBR) at each stage are optimized to improve overall reactor efficiency. An industrial scale catalytic fixed bed reactor is used and the results of the proposed multi-objective multi-stage case are compared with a single-stage single-objective (base case) and single-stage multi-objective optimization one. The comparative test studies clearly demonstrate superiority of the proposed methodology to give optimal solutions with much less CO_2 productivity and high DME productivity at the end of the staged reactor. Besides, the simulation results of multi-objective optimization introduced more optimum points as a Pareto front compared to the single objective optimization case.

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1. Introduction

DME is known as a suitable intermediate for producing chemicals like light olefins, dimethyl sulfate and methyl acetate [20]. Also, because of its high cetane number about 55–60 it can be used in diesel engines, power generation and other purposes [22,35]. DME is known as an ultra-clean fuel that does not produce pollutants such as hydrocarbons, CO, NO_x and particulates [26]. Meanwhile, DME can be considered as a suitable feedstock for fuel cells because it can be reformed to hydrogen at lower temperatures [37]. It has a boiling point of −25 °C, which is 20 °C higher than liquefied petroleum gas (LPG) and can be liquidized at 0.54 MPa (20 °C). Therefore, no serious problem exists for the storage, transportation and usage of DME [1,24,40].

Modeling and optimization of indirect and direct synthesis of DME have been done in various studies. Khademi et al. [21] performed a steady state heterogeneous model of a thermally coupled reactor for DME synthesis and cyclohexane dehydrogenation. They optimized operating conditions, enhancement of DME and benzene production. A thermally coupled dual-membrane reactor for simultaneous production of hydrogen, DME and naphthalene was modeled by Samimi et al. [31]. In their study, operating conditions were optimized to maximize DME and hydrogen mole fractions. Samimi et al. [32] considered modeling of two stage spherical packed bed reactors and optimized inlet temperature and catalyst distribution to maximize DME production from methanol. Farsi et al. [14] focused on 1D modeling and optimization of a steady state heterogeneous model of two concentric spherical reactors to produce DME from methanol. In that study DME production rate was maximized by staging the reactor. Mentioned studies were focused on indirect synthesis of DME.

Omata et al. [27] studied direct synthesis of DME in a single stage (SS) temperature gradient reactor. They optimized operating conditions of the reactor to improve CO conversion. In order to increase production of DME, Hu et al. [18] optimized structure and operating conditions of the pipe-shell fixed bed reactor. Modeling and optimization of a shell and tube fixed bed reactor was also done by Farsi et al. [15]. They improved DME production by adjusting temperature profile through the reactor. Dynamic modeling and optimization of direct synthesis of DME in the shell and tube reactor was performed by Yasari et al. [39]. Optimum shell temperature was specified in their study in order to increase DME productivity and selectivity and control hot spot in the reactor. Vakili and Eslamloueyan [34] designed and optimized an industrial scale fixed bed reactor for the direct synthesis of DME from syngas. The reactor operating conditions and its internal configuration were optimized to maximize DME production in each tube of a single reactor. Vakili et al. [35] investigated a multifunctional auto-thermal reactor for direct DME synthesis and hydro-

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Nomenclature

A_r	tube cross section area (m^2)
C_i	concentration of the *i*th component (mol/m^3)
$C_{p,g}$	specific heat capacity of gas (J/ kgK)
d_p	equivalent diameter of catalyst particle (mm)
d_{out}	external diameter of tube (mm)
$h_{i,g}$	gas phase heat transfer coefficient, inside of the tube wall (kw/m^2 K)
$h_{o,c}$	gas phase heat transfer coefficient, outside of the tube wall (kw/m^2 K)
$h_{i,s}$	solid phase heat transfer coefficient, inside of the tube wall (kw/m^2 K)
K_i	equilibrium and kinetic constants
K_{MT}	pseudo mass transfer coefficient
K_w, K_s, K_g	conductivity coefficient, gas, pellet, tube wall
Krg, Krs	effective radial conductivity, gas phase, solid phase, respectively (Kw/m K)
L_r	reactor length (m)
P_i	partial pressure of *i*th component (bar)
R_g	gas constant (J/mol K)
R_r, $R_{r,y}$	reactor tube radius, inside, outside, respectively (m)
r_i	reaction rate (mol/skg)
T_C	shell temperature (K)
u_s	gas velocity in the reactor (m/s)
U_{eff}, $U_{overall}$	overall heat transfer coefficient (W/m^2K)
y_i	mole fraction of *i* component
z	reactor dimensionless length
ρ_g	gas density (kg/m^3)
ρ_b	bed density (kg/m^3)
ε	bed porosity
μ_g	gas phase viscosity (kg/ms)
ΔH_i	heat of *i*th reaction (J/mol)

gen production by the cyclohexane dehydrogenation. The effects of parameters such as feed flow rates and the inlet temperatures of exothermic and endothermic sections on the reactor behavior were investigated. Their results showed improvement of DME production in this configuration. Papari et al. [29] developed a 1D mathematical model to simulate and optimize an industrial scale slurry reactor for one step synthesis of DME from CO_2 and synthesis gas. Conversion of CO and DME productivity was optimized by manipulating variables such as concentration of catalyst, superficial gas velocity, pressure, temperature, *etc.* In other work, dynamic simulation and behavior of a commercial scale slurry bubble column reactor for direct synthesis of DME from syngas was also studied by Papari et al. [28]. They investigated effect of operating conditions on CO conversion and DME productivity. Moradi et al. [25] assessed flow behavior of a fixed bed reactor through a three dimensional CFD simulation. Effect of various operating conditions was performed for both adiabatic and isothermal conditions. De Falco et al. [10] evaluated direct production of DME from CO_2-rich feedstock from thermodynamic perspective. They showed role of temperature, pressure, inlet composition of H_2/CO and CO_2/CO and coolant temperature on DME yield. Furthermore, with the thermodynamic approach, the negative effect of water formed on CO_2 conversion was investigated in a simulated pipe-shell reactor. The integration of a highly selective membrane to H_2O for continuous removal of water in the direct synthesis of DME is investigated by De Falco et al. [11]. A 1D, non isothermal model was simulated to evaluate the performance of the reactor. They showed an improvement of 15.4% and 30.2% in CO_x and CO_2 conversion comparing a conventional reactor. Frusteri et al. [17] prepared a bi-functional catalyst (Cu–Zn–Zr/zeolite) in a home-made slurry reactor and evaluated its behavior experimentally in a fixed-bed reactor for DME production from CO_2 hydrogenation. The results indicated superior performance of Cu–Zn–Zr-FER catalyst to reach the highest DME productivity and CO_2 conversion.

All mentioned works, have focused on optimizing operation conditions in order to enhance DME production, but none of them have considered reduction of CO_2 as the feed/by product and air pollutant in an industrial scale reactor. In this respect, in the present study, another important objective beside DME productivity is introduced: reduction of CO_2 productivity (increasing CO_2 conversion) at the end of the reactor path.

Considering increasing conversion of CO_2 in the reactor section is less investigated in the literature [5,10,11,17,30]. Therefore, in order to improve reactor efficiency a multi-objective multi-stage (MOMS) catalytic reactor is proposed and different degrees of freedom (optimization variables) are considered: H_2O and DME separation ratio after each stage, feed temperature, inter-stage temperatures, shell temperatures, number of reactor in series and reactor type at each stage (adiabatic/non-adiabatic). Some studies investigated effect of in-situ water removal in direct synthesis of DME using membrane reactors [11,12,19]. Iliuta et al., [19] discussed benefit and limits of in-situ removal of water in a fixed bed membrane reactor. One of the limitations is dependency of conversion and yields on membrane transport characteristics.

In the current study, it tried to improve reactor performance by optimization of mentioned operating conditions of a staged industrial scale pipe-shell reactor. DME productivity and CO_2 productivity are maximized and minimized respectively and independently as the two main objective functions using a variety of degrees of freedom.

Modeling and optimization procedure are presented in Section 2. In Section 3 the proposed approach is applied and compared with two other cases. Finally, the conclusion is presented in Section 4.

2. Modeling and optimization procedure

2.1. Direct synthesis of DME

There are two common methods for DME production: indirect (two-step) and direct (one-step) approaches. The following reactions are involved in DME production process:

$$CO + 2\ H_2 \Leftrightarrow\ CH_3OH \qquad \Delta H_{25^\circ C} = -90.85\ kJ\ /mol \tag{1}$$

$$CO+\ H_2O \Leftrightarrow CO_2+H_2 \qquad \Delta H_{25^\circ C} = -41.1\ kJ/mol \tag{2}$$

$$CO_2+3\ H_2 \Leftrightarrow CH_3OH+H_2O \qquad \Delta H_{25\ ^\circ C} = -50.1\ kJ\ /mol \tag{3}$$

$$2\ CH_3OH \Leftrightarrow CH_3OCH_3+H_2O \qquad \Delta H_{25\ ^\circ C} = -23.4\ kJ\ /mol \tag{4}$$

Indirect production of DME from methanol is traditionally used and prepares DME from methanol dehydration Eq. 4. Dependency on the methanol price and thermodynamic limitation of methanol synthesis Eqs. 1 and (3) are the two major drawbacks for this method. A high pressure and a huge recycle stream to the reactor require overcoming thermodynamic limitation and having an adequate overall conversion [6]. Companies such as Toyo, Udhe, Lurgi and MGC proposed indirect production of DME from methanol [3].

Producing DME from syngas which is also called direct method is another alternative Eqs. 1–(4). Different companies such as Topsoe, Air products, JFE HO., NKK and Korea Gas Co. established direct synthesis of DME [3]. In this method bi-functional catalysts are used to produce DME from syngas in a single reactor. Methanol

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