



DME synthesis and cyclohexane dehydrogenation reaction in an optimized thermally coupled reactor

M.H. Khademi^a, M. Farsi^a, M.R. Rahimpour^{a,b,*}, A. Jahanmiri^{a,b}

^a Department of Chemical Engineering, School of Chemical and Petroleum Engineering, Shiraz University, Shiraz 71345, Iran

^b Gas Center of Excellence, Shiraz University, Shiraz 71345, Iran

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ABSTRACT

This paper presents a study on optimization of DME synthesis and cyclohexane dehydrogenation in a thermally coupled reactor. A steady-state heterogeneous model has been performed in order to evaluate the optimal operating conditions and enhancement of DME and benzene production. In this work, the catalytic methanol dehydration to DME is coupled with the catalytic dehydrogenation of cyclohexane to benzene in a heat exchanger reactor formed of two fixed beds separated by a wall, where heat is transferred across the surface of tube. The optimization results are compared with corresponding predictions for a conventional (industrial) methanol dehydration adiabatic reactor operated at the same feed conditions. The differential evolution (DE), an exceptionally simple evolution strategy, is applied to optimize thermally recuperative coupled reactor considering DME and benzene mole fractions as the main objectives. The simulation results have been shown that there are optimum values of initial molar flow rate and inlet temperature of exothermic and endothermic sides to maximize the objective function. The results suggest that optimal coupling of these reactions could be feasible and beneficial and improves the thermal efficiency of process. Experimental proof-of-concept is needed to establish the validity and safe operation of the novel reactor.

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1. Introduction

Dimethyl ether (DME) is a colorless gas at the ambient condition and easily liquefied under low pressure. Recently, DME is an attractive topic in academic and industrial research due to global environment pollution and energy supply problem. DME does not produce any particulate matter and toxic gases such as NO_x at burning, when used as a fuel. It can be produced from a variety of feed-stock such as natural gas, crude oil, residual oil, coal, waste products and bio-mass [1]. It is useful for a variety of application such as LPG substitute, transportation fuel, propellant; chemical feedstock and fuel cell [2].

DME production in the conventional process involves a methanol dehydration reaction as an indirect method. Currently, DME synthesizes from syngas as a direct method is developed to produce it at low cost. DME production through direct synthesis from syngas using a dual catalyst system permits both methanol synthesis and dehydration in a single process, with no methanol purification. At present, DME is commercially produced by dehydration of methanol in the adiabatic packed bed reactor using acidic porous catalysts [3].

There are several articles in the literature that discuss modeling of DME catalytic packed bed reactors. Eslamlueyan [4] modeled and simulated DME synthesis in adiabatic fixed bed reactor and shown that difference between one-dimensional and two-dimensional modeling is negligible. Liu et al. [5] modeled and designed a three-phase bubble column reactor for direct synthesis of DME from syngas with considering the influence of inert carrier backmixing on transfer and the influence of catalyst grain sedimentation on reaction. Simulation of fluidized-bed reactor for DME synthesis from syngas has been performed by Lu et al. [6] using plug flow model, which shows the great advantage of fluidized-bed over fixed-bed or slurry reactor. Moradi et al. [7] studied DME synthesis from synthesis gas in slurry reactor experimentally and determined the optimum operating conditions of DME synthesis. Omata et al. [8] studied DME production from syngas in a temperature gradient reactor for overcoming both the equilibrium limit of the reaction at high temperature and low activity of the catalyst at low temperature. Then, they optimized the reactor for higher CO conversion by combined genetic algorithm and neural network.

Multifunctional reactors integrate, in one vessel, one or more transport processes and a reaction system and are widely used in industries as process intensification tools [9,10]. These multifunctional reactors make the process more efficient and compact and result in large savings in the operational and capital costs [11]. A multifunctional reactor can be used, for example, for coupling

* Corresponding author. Tel.: +98 711 2303071; fax: +98 711 6287294.

E-mail address: rahimpour@shirazu.ac.ir (M.R. Rahimpour).

Nomenclature

a_v	Specific surface area of catalyst pellet ($\text{m}^2 \text{m}^{-3}$)
A_c	Cross section area of each tube (m^2)
A_i	Inside area of inner tube (m^2)
A_o	Outside area of inner tube (m^2)
c	Total concentration (mol m^{-3})
C_i	Molar concentration of component i (mol m^{-3})
C_p	Specific heat of the gas at constant pressure (J mol^{-1})
d_p	Particle diameter (m)
D_i	Tube inside diameter (m)
D_{ij}	Binary diffusion coefficient of component i in j ($\text{m}^2 \text{s}^{-1}$)
D_{im}	Diffusion coefficient of component i in the mixture ($\text{m}^2 \text{s}^{-1}$)
D_o	Tube outside diameter (m)
D_{sh}	Shell inside diameter (m)
F	Total molar flow rate (mol s^{-1})
G	Mass velocity ($\text{kg m}^{-2} \text{s}^{-1}$)
h_f	Gas-solid heat transfer coefficient ($\text{W m}^{-2} \text{K}^{-1}$)
h_i	Heat transfer coefficient between fluid phase and reactor wall in exothermic side ($\text{W m}^{-2} \text{K}^{-1}$)
h_o	Heat transfer coefficient between fluid phase and reactor wall in endothermic side ($\text{W m}^{-2} \text{K}^{-1}$)
$\Delta H_{f,i}$	Enthalpy of formation of component i (J mol^{-1})
k	Rate constant of dehydrogenation reaction ($\text{mol m}^{-3} \text{Pa}^{-1} \text{s}^{-1}$)
k_1	Rate constant for the rate of methanol dehydration reaction ($\text{mol}^2 \text{kg}^{-1} \text{s}^{-1} \text{m}^{-3}$)
k_g	Mass transfer coefficient for component i (m s^{-1})
K	Conductivity of fluid phase ($\text{W m}^{-1} \text{K}^{-1}$)
K_B	Adsorption equilibrium constant for benzene (Pa^{-1})
K_{eq}	Reaction equilibrium constant for methanol dehydration reaction (mol m^{-3})
K_i	Adsorption equilibrium constant for component i in methanol dehydration reaction ($\text{m}^3 \text{mol}^{-1}$)
K_p	Equilibrium constant for dehydrogenation reaction (Pa^3)
K_w	Thermal conductivity of reactor wall ($\text{W m}^{-1} \text{K}^{-1}$)
L	Reactor length (m)
M_i	Molecular weight of component i (g mol^{-1})
N	Number of components ($N=3$ for both dehydration and dehydrogenation reaction)
P	Total pressure (for exothermic side: bar; for endothermic side: Pa)
P_i	Partial pressure of component i (Pa)
r_1	Rate of reaction for DME synthesis ($\text{mol kg}^{-1} \text{s}^{-1}$)
r_2	Rate of reaction for dehydrogenation of cyclohexane ($\text{mol m}^{-3} \text{s}^{-1}$)
r_i	Reaction rate of component i (for exothermic reaction: $\text{mol kg}^{-1} \text{s}^{-1}$; for endothermic reaction: $\text{mol m}^{-3} \text{s}^{-1}$)
R	Universal gas constant ($\text{J mol}^{-1} \text{K}^{-1}$)
R_p	Particle radius (m)
Re	Reynolds number
Sc_i	Schmidt number of component i
T	Temperature (K)
u	Superficial velocity of fluid phase (m s^{-1})
u_g	Linear velocity of fluid phase (m s^{-1})
U	Overall heat transfer coefficient between exothermic and endothermic sides ($\text{W m}^{-2} \text{K}^{-1}$)
v_{ci}	Critical volume of component i ($\text{cm}^3 \text{mol}^{-1}$)
y_i	Mole fraction of component i (mol mol^{-1})
z	Axial reactor coordinate (m)

Greek letters

μ	Viscosity of fluid phase ($\text{kg m}^{-1} \text{s}^{-1}$)
ρ	Density of fluid phase (kg m^{-3})
ρ_b	Density of catalytic bed (kg m^{-3})
τ	Tortuosity of catalyst

Superscripts

g	In bulk gas phase
s	At surface catalyst

Subscripts

0	Inlet conditions
B	Benzene
C	Cyclohexane
i	Chemical species
j	Reactor side (1: exothermic side, 2: endothermic side)
k	Reaction number index

exothermic and endothermic reactions. In this type of reactor, an exothermic reaction is used as the heat producing source to drive the endothermic reaction(s). In the last years promising concepts for the recuperative coupling of exothermic and endothermic reactions have been published [12–22]. A distributed mathematical model for thermally coupled membrane reactor that is composed of three sides is developed for methanol and benzene synthesis by Khademi et al. [23]. Methanol synthesis takes place in the exothermic side and supplies the necessary heat for the endothermic dehydrogenation of cyclohexane reaction. Selective permeation of hydrogen through the Pd/Ag membrane is achieved by co-current flow of sweep gas through the permeation side. Also, recently Farsi et al. [24] investigated the effect of various parameters on the performance of a novel recuperative reactor. In this reactor, catalytic DME synthesis reaction is coupled with the catalytic dehydrogenation of cyclohexane to benzene. From these previous studies, coupling of endothermic and exothermic reactions may enable both the concentration and temperature profiles along the reactor to be manipulated, shifting the conversion of thermodynamically limited reactions to higher values, and efficiently using the heat liberated by an exothermic reaction side to provide the endothermic heat requirements of the other reaction side [25].

In the last few years, a Differential Evolution (DE) algorithm for dealing with optimization problems has been proposed. DE algorithm is a stochastic optimization method minimizing an objective function that can model the problem's objectives while incorporating constraints. The algorithm mainly has three advantages; finding the true global minimum regardless of the initial parameter values, fast convergence, and using a few control parameters. Being simple, fast, easy to use, very easily adaptable for integrand discrete optimization, quite effective in nonlinear constraint optimization including penalty functions and useful for optimizing multi-modal search spaces are the other important features of DE algorithm. Recently, Khademi et al. [26] optimized the methanol synthesis reaction and cyclohexane dehydrogenation in a thermally coupled reactor using differential evolution (DE) method. Also, a novel thermally coupled membrane reactor that is composed of three sides is optimized for methanol, benzene and hydrogen productions by Khademi et al. [27] using DE algorithm.

In our previous work [24], a distributed mathematical model for thermally coupled reactor -containing DME synthesis reactions and cyclohexane dehydrogenation- is developed. The effect of various key operating variables on the performance of the reactor is

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