



## A comparative study of two different configurations for exothermic–endothermic heat exchanger reactor

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### ABSTRACT

The coupling of the energy intensive endothermic reaction systems with appropriate exothermic reactions reduces the size of the reactors and can improve the thermal efficiency of processes. One type of a suitable reactor for such a kind of coupling is the heat exchanger reactor. In this study, the catalytic methanol synthesis is coupled with the catalytic dehydrogenation of cyclohexane to benzene in an integrated reactor formed from two fixed beds separated by a wall where heat is transferred across the surface of the tube. A steady-state heterogeneous model of the two fixed beds predicts the performance of the two different configurations of the thermally coupled reactor. The co-current mode is investigated and the simulation results are compared with the corresponding predictions for the industrial methanol fixed bed reactor operating in the same feed conditions. The results of the study reveal that should the exothermic and endothermic reactions be located in the shell side and tube side, respectively, the methanol production rate will increase in comparison with the conventional methanol synthesis reactor as well as the case where the exothermic reaction is located in the tube side and endothermic reaction in the shell side.

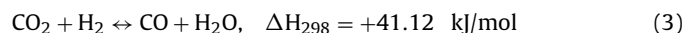
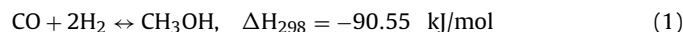
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## 1. Introduction

### 1.1. Methanol

An increase in energy prices and global warming has led to an increased interest in alternative fuels. The viability of alcohol as a fuel is a debatable issue due to the fact that other energy sources are required for production. Methanol has been considered as a fuel because of its physical and chemical characteristics. Methanol has proven to be an attractive automotive fuel [1]. Methanol is an important multipurpose base chemical and a simple molecule which can be obtained from many resources, mostly from natural gas. It has the advantage of being liquid under normal conditions. It can be stored and transported as easily as gasoline, as well as having a higher octane rating than gasoline. This reduces “knock” in the today’s engines and can result in greater fuel efficiency through the proper adjustment of the engine compression ratio and can be used in the conventional combustion engines without requiring any major adjustments. It is a clean-burning fuel as a combustion fuel. It provides extremely low emissions. Methanol can also be used as a solvent or a fuel additive and especially as a building block to produce chemical intermediates such as dimethyl ether

(DME) and methyl *t*-butyl ether [2] and it can be used as a raw material for the production of chemicals such as formaldehyde and acetic acid. Methanol has twice the energy density of liquid hydrogen and can be more conveniently stored and transported [3,4]. Basically, methanol is still produced by catalytic conversion of synthesis gas (CO<sub>2</sub>, CO, H<sub>2</sub> and some inert components such as argon and nitrogen) on a large scale. The methanol synthesis reaction is exothermic and the total moles reduce as the reaction proceeds. In the methanol synthesis, three overall reactions are possible: hydrogenation of carbon monoxide, hydrogenation of carbon dioxide and reverse water–gas shift reaction, which are as follows:



Reactions (1)–(3) are not independent so that one is a linear combination of the other ones. The temperature and pressure of reaction are 495–535 K and 5–8 MPa, respectively [5].

Methanol synthesis process is the second largest present use of hydrogen, after ammonia synthesis and basically consisted of three steps: synthesis gas generation, methanol synthesis and methanol distillation. The main step of methanol process is methanol synthesis. The importance of the methanol has motivated numerous studies whose aim was to improve the production efficiency in

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the methanol synthesis process. To improve the performance of the methanol reactor, a number of configurations have been proposed including conventional dual-type reactor [6,7], fixed-bed with hydrogen perm-selective membrane reactor [1,8], membrane dual-type reactor [9], cascade membrane reactor [10], fluidized-bed reactor [11], fluidized-bed membrane dual-type reactor [12,13] and cascade fluidized-bed reactor [14,15].

### 1.2. Dehydrogenation of cyclohexane

The greatest difficulties in expanding the use of hydrogen energy are safe storage and transport, because hydrogen is a gas under ordinary temperature and pressure and its liquefaction temperature is around 20 K. To overcome this barrier, organic chemical hydrides are among the proposed carriers of hydrogen because of their ease of handling.

The main advantage of using organic chemical hydrides, such as cyclohexane, as a carrier component is from the following points of view:

- (1) Higher hydrogen content (e.g. 7.1 wt% of cyclohexane) which is very attractive compared with metal hydrides (at most 3 wt%)
- (2) More convenient for storage and transportation due to high boiling point (bp = 80.7 °C)
- (3) The dehydrogenated products, benzene and toluene, can be reversibly hydrogenated and reused and those are all liquids at ordinary temperatures
- (4) No CO<sub>2</sub> emission in the dehydrogenation process will be rated highly in terms of environmental issues, whereas the steam reforming process of methanol produces not only hydrogen but also CO<sub>2</sub> [16]. The dehydrogenation of cyclohexane reaction is endothermic and the total moles increase as the reaction proceeds.

However, the separation of hydrogen from other gases remains a major unsolved problem for hydrogen production systems from organic chemical hydrides. The process of separating hydrogen from other gases is generally expensive and energy-intensive.

### 1.3. Defect of the conventional methanol reactor

The methanol conversion in the conventional fixed bed methanol reactor is low due to the equilibrium nature of the reaction. Therefore, most of the synthesis gas must be circulated around the loop and this poses problems in operating costs. As the conversion of the exothermal reaction in the methanol synthesis reactor is equilibrium limited, it is of the utmost importance that the reaction is operated in such a way to drive the equilibrium composition towards the product.

### 1.4. Coupling reactor

Process intensification (PI) is currently one of the most significant trends in the chemical engineering and process technology. It has been paid much attention in the research world [17–20]. It is related to strategies for reduction of emissions as well as consumption of energy and materials. Innovations in the catalytic reactor technologies, which somehow could be the heart of chemical processes, are often the preferred starting point. In this way multifunctional auto-thermal reactor is a novel concept in process intensification.

At present, coupling of endothermic and exothermic reactions would be a promising field of using multifunctional auto-thermal reactors. In this type of the reactors, an exothermic reaction is considered as the heat producing source to drive the endothermic reaction(s) [21,22]. Hunter and McGuire [23] were among the first

to suggest the coupling of endothermic with exothermic reaction by means of indirect heat transfer. They considered heat exchangers where catalytic combustion or other highly exothermic reaction is used as a heat source for an endothermic reaction. An extension of applications of multifunctional auto-thermal reactors for coupling of endothermic and exothermic reactions has been attempted. It can be referred to the merits of the multifunctional auto-thermal reactors, some of which are as follows:

- Production of multiple products
- Establishment of auto-thermal conditions
- Enhancement of productivity (if the reaction is equilibrium)
- Overcoming the thermodynamic limitation on the reactions
- Integrating, in one vessel, one or more transport processes and a reaction system

Multifunctional auto-thermal reactors make the process more efficient and compact and result in large savings in the operational and capital costs [22].

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 to provide the endothermic heat requirements of the other reaction [24]. Itoh and Wu [25] investigated an adiabatic type of palladium membrane reactor for coupling endothermic and exothermic reactions. On one side of membrane, dehydrogenation of cyclohexane takes place in the catalyst packed layer, and on the membrane surface of the other side hydrogen permeated react in situ with oxygen. They simulated a simple mathematical model for analyzing the reaction process. Eigenberger's group studied the process of the methane steam reforming coupled with methane combustion both experimentally and theoretically, mainly in counter-current configuration utilizing a ceramic honeycomb monolith with specially designed reactor heads [26–28]. A mathematical simulation and numerical method based on a two-dimensional model are developed by Fukuhara and Igarashi [29] to analyze the operation of the coupling methanol decomposition and methane combustion. They compared the performance of a wall-type reactor with a fixed-bed reactor in which exothermic and endothermic reactions proceed simultaneously. Ramaswamy et al. [30] analyzed the steady-state and the dynamic behavior of coupling exothermic and endothermic reactions in directly coupled adiabatic packed-bed reactors (DCAR) for the first order reactions using one-dimensional pseudo-homogeneous plug flow model. The effects of symmetric and asymmetric longitudinal vortices on heat and mass transfer and on the mixing process and also flow regimes in coupling reactors have widely been studied [31–33]. A variety of coupling configurations for methanol and benzene synthesis have been studied by Rahimpour et al. [34–37].

### 1.5. Objectives

The main purpose of this study is enhancement of the methanol production in the process of the coupling of the methanol synthesis reaction with the dehydrogenation of cyclohexane to benzene in the thermally coupled reactor. Methanol has a special significance in this study thus the comparison of the methanol generation as a desirable product of the exothermic side of two different configurations is another objective in this study.

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