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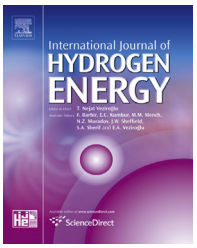

A computational model of hydrogen production by steam reforming of dimethyl ether in a large scale CFB reactor. Part II: Parametric analysis

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ABSTRACT

This study presents a computational parametric analysis of DME steam reforming in a large scale Circulating Fluidized Bed (CFB) reactor. The Computational Fluid Dynamic (CFD) model used, which is based on Eulerian–Eulerian dispersed flow, has been developed and validated in Part I of this study [1]. The effect of the reactor inlet configuration, gas residence time, inlet temperature and steam to DME ratio on the overall reactor performance and products have all been investigated. The results have shown that the use of double sided solid feeding system remarkable improvement in the flow uniformity, but with limited effect on the reactions and products. The temperature has been found to play a dominant role in increasing the DME conversion and the hydrogen yield. According to the parametric analysis, it is recommended to run the CFB reactor at around 300 °C inlet temperature, 5.5 steam to DME molar ratio, 4 s gas residence time and 37,104 ml g_{cat}^{-1} h^{-1} space velocity. At these conditions, the DME conversion and hydrogen molar concentration in the product gas were both found to be around 80%.

Introduction

Hydrogen production through Dimethyl Ether (DME) steam reforming in a fluidized bed is a relatively new process, therefore, there is a need of reliable design and optimization tool in order to take this process into industrial scale application. Improved hydrogen production, enhanced operability of the reactor and increased economic viability of the process can be achieved by optimizing the reactor design and using the appropriate range of operating conditions. In Part I of this study [1], a valid computational model was developed and the prediction of the reactor hydrodynamics (in terms of phases distribution, velocities and residence time) and thermo-chemical performance (in terms of temperature, species distribution and gas composition) were studied at one selected operating condition of temperature = 300 °C, steam to DME molar ratio = 7.6 and a space velocity = 37,104 ml g_{cat}^{-1} h^{-1}. The reported studies on methanol (MeOH) and DME steam catalytic reforming suggest that the ratio of steam to methanol or DME and the reactor temperature are the two most important parameters that influence the degree of chemical conversion

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and hydrogen production in fluidized bed reactors (e.g. Refs. [2,3]).

There are several reported experimental and theoretical studies on parametric analysis of catalytic steam reforming of DME or methanol (e.g. Refs. [3,4]). None of these have looked into the performance of a circulating fluidised bed reactor at a range of operating conditions. This is despite of the great potential of a circulating fluidised bed for industrial scale application compared to fixed or bubbling fluidized bed reactors. It is therefore of interest to shed light on the performance of this type of reactor at a range of operating conditions relevant to industrial scale processing. The parameters that are commonly investigated are the temperature, steam to DME ratio, space velocity and the catalyst type. In a theoretical and experimental study of DME steam reforming (DME-SR) in a micro-reactor [5] it was reported that higher DME conversion and carbon monoxide concentration in the product gas occurs at increasing the reactor wall temperature. A wall temperature of 270 °C was recommended as optimum for the hydrogen production. Another experimental study on DME-SR over a metallic catalyst ($CuO/ZnO/Al_2O_3/Z_rO_2$ + ZSM5) in a fixed bed reactor [6] has shown increased DME conversion and hydrogen yield when increasing the temperature and steam to DME ratio. On the contrary, the increase in the space velocity was reported to decrease both the DME conversion and hydrogen yield but increased the carbon dioxide selectivity [4–6]. A similar experimental and numerical study on a fixed bed reactor has shown the hydrogen production to decrease with increasing the temperature beyond 300 °C [4]. The experimental results at various operating conditions (space velocity of 2420–4615 h^{-1} and temperature of 270–310 °C) have been found to reasonably match the numerical results obtained using a simple one-dimensional heterogeneous model.

Hydrogen production by steam reforming of DME is particularly an attractive option because the process can be carried out at a relatively low temperature compared to the conventional method of natural gas reforming, which takes place around 600 °C. This is in addition to other advantages related to DME properties such as high hydrogen to carbon ratio, non-corrosive, non-carcinogenic, non-toxic nature and increased worldwide mass production from various resources [7]. Hydrogen produced by methanol steam reforming is another alternative option for low temperature processing (200–300 °C) [8], however methanol is more expensive to produce and entails the risk of biological poisoning [4,9]. Recent theoretical studies on DME steam reforming have looked into the potential of making the process thermal efficiency more attractive by utilizing exhaust gas as a source of heat to derive the endothermic DME reforming reaction [10,11]. These studies included the solution of CFD models (mass, energy, momentum and reaction equations) [10] and Aspen plus software [11] to predict the hydrogen yield and process thermal efficiency with respect to varying the DME to steam ratio and heat supply. Both parameters were found to play an important role in the overall reactor performance.

Studies on the types of catalyst (e.g. Refs. [12–14]) are generally in agreement that the DME steam reforming process occurs in two-steps involving the hydrolysis of DME and the steam methanol reformation. These two steps led to the requirement of a bifunctional catalyst to facilitate both reactions [15]. However depending on the catalyst system utilised and reaction parameters some side reactions may occur, which could include water-gas shift reaction and DME decomposition reaction.

In this second part of the study, the computational fluid dynamic (CFD) model developed and validated in part I [1] is used to study the reactor design improvement by altering the feeding points, carry out parametric analysis and identify the optimum operating conditions for increased hydrogen production in a circulating fluidized bed reactors. A simple energy balance is first described to allow estimation of the thermal input required to derive the reaction. This is followed by studying the impact of changing the solid catalyst feeding points on the overall flow hydrodynamics and product quality. In the last section, parametric analysis focused on the effect of steam to DME ratio, reactor temperature and the gas residence time is presented. The study is then concluded with a summary of the optimum conditions recommended for increasing the hydrogen yield.

Computational model and chemical reactions

The DME steam reforming reactions, rate laws and the computational model used to simulate the overall reactor performance and product gas composition have been given in details in Part I of this study [1]. Here, only the main model equations (hydrodynamics, heat transfer and reactions) in addition to the computation method are briefly described.

Conservation of mass:

$$\frac{\partial}{\partial t}(\alpha_i \rho_i) + \nabla\cdot(\alpha_i \rho_i v_i) = S_i \quad i = \text{gas or solid} \tag{1}$$

Gas phase momentum:

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g v_g\right) + \nabla\cdot\left(\alpha_g \rho_g v_g\right) = -\alpha_g \nabla P_g + \nabla\cdot\bar{\bar{\tau}}_g + \alpha_g \rho_g g - \sum_{j=1}^{2} \beta_{s_j}\left(v_g - v_{s_j}\right) \quad j = \text{solid 1 or 2} \tag{2}$$

Solid phase momentum:

$$\frac{\partial}{\partial t}\left(\alpha_{s_i} \rho_{s_i} v_{s_i}\right) + \nabla\cdot\left(\alpha_{s_i} \rho_{s_i} v_{s_i}\right) = -\alpha_{s_i} \nabla P_{s_i} + \nabla\cdot\bar{\bar{\tau}}_{s_i} + \alpha_{s_i} \rho_{s_i} g + \beta_{s_i}\left(v_g - v_{s_i}\right) + \sum_{j=1}^{2} K_{s_{i,j}}\left(v_{s_i} - v_{s_j}\right) \quad j \neq i \tag{3}$$

Granular kinetic energy:

$$\frac{3}{2}\left[\frac{\partial}{\partial t}\left(\rho_{S_i} \alpha_{s_i} \theta_{s_i}\right) + \nabla\cdot\left(\rho_{s_i} \alpha_{s_i} \theta_{s_i} v_{s_i}\right)\right] = \left(-P_{s_i}\bar{\bar{I}} + \bar{\bar{\tau}}_{s_i}\right) : \nabla v_{s_i} + \nabla\cdot\left(k_{s_i} \theta_{s_i} \nabla \Theta_{s_i}\right) - \gamma_{s_i} + \varnothing_{gs_i} \quad j = \text{solid 1 or 2} \tag{4}$$

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