Purification of Hydrogen by Absorption and Examination of Absorption Kinetics and Absorbers Type

Mohammad Taghi Falahati, Farhad Shahraki, Mohammad Reza Sardashti Birjandi

Department of Chemical Engineering, University of Sistan and Baluchestan, Iran

**ABSTRACT**

**Background:** Nowadays, environmental issues and increasingly depleting fossil fuels have shifted attentions to alternative energy sources. Hydrogen is one of such energy sources which can be used in transportation. Various approaches have been proposed for producing and purifying hydrogen. One of these approaches is producing hydrogen through the conversion reaction of methanol and water vapor in the catalyst-bed reactor. Since this process is performed in mild conditions, it has attracted the attentions of various researchers in energy production. **Objective:** In this project, as an essential and significant source of energy, hydrogen is characterized. Then, various methods of producing and purifying hydrogen and their advantages, disadvantages, and costs are discussed. **Method:** The following sections focus on the production of hydrogen through the conversion reaction of methanol and water vapor and discuss the stages of the process, the proposed syntheses, various adopted catalysts, and their production methods. Then, the process is simulated using the experimental data derived from a creditable study. **Results:** The comparison of the simulation results and those of the aforementioned study revealed that they are compatible. After simulation, the influences of various parameters (temperature, the length of the reactor, feed flow rate, and feed percentage composition) on the mole fraction of hydrogen are studied. A final simulation was conducted based on the results and an attempt was made to raise the amount of hydrogen in the product. Finally, the mole fraction of hydrogen was raised from %23 to %60.

© 2014 AENSI Publisher All rights reserved.


**INTRODUCTION**

**Methanol/Water Vapor Reaction in Catalyst-Bed Reactor to Produce Hydrogen:**

Producing hydrogen through the reaction of methanol and water vapor is economic for producing the hydrogen used in various ways including fuel cells. It is a short and effective method for reaching the optimal product:

\[ CH_3OH + H_2O \rightarrow CO_2 + 3H_2 \quad \Delta H = 57 \text{kJ/mol (at 200°C)} \]

This reaction occurs at low temperatures within the range of 200 to 300 °C on the catalyst bed. In addition to hydrogen, carbon dioxide, and nominal amounts of carbon monoxide (less than one percent) are produced as byproducts [9], [12]. Thus, hydrogen is occasionally introduced as the source of liquid hydrogen.

Over the past decade, considerable attention has been paid to this reaction to produce hydrogen for various purposes such as fuel cells. Recently, methanol has been proposed as a good feed for a number of chemical processes [15]. Such applications require catalysts with high activity, selection, and resistance under the reaction conditions [10, 14]. Hence, an essential issue regarding this process is the type of the catalyst, its specifications, and production process. This is discussed in detail in 3-3.

While designing the reactor, it is essential to consider the catalyst bed used in the methanol/water vapor reaction, the synthetics of the reaction in specifying the process, and especially the size of the reactor [16]. Therefore, an essential issue in this process is the investigation of the reaction synthesis, which is discussed in detail in 3-4.

**Keywords:** Hydrogen, Methanol-Water Vapor Reaction, Catalyst-Bed Reactor, Synthetic
Discussion of Catalyst:

The most attractive catalysts for the conversion reaction of methanol include copper-based ones in the presence of zinc oxide [17, 20], to which aluminum oxide is often added [21-27]. Such systems are the result of famous industrial processes for synthesizing methanol and transmitting gas-water in low temperatures. Beginning with these systems, many other catalysts have been proposed in which copper is diffused in a metal oxide matrix such as ZrO₂ [28, 31], CeO₂ [32, 34], MnO₂ [35], or in mixed oxides such as CuO/ZrO₂ [28-31], ZrO₂/Al₂O₃ [37], ZnO/ZrO₂ [10, 11], ZnO/Sm₂O₃ [38] and CeO₂/ZrO₂ [39-40]. Although several systems have been proposed for the conversion reaction of methanol/water vapor, no significant one has been reported. Thus, the Cu/ZnO-based catalyst is still the most attractive one for this reaction [14]. The role of ZnO is well identified as the promoter of the copper-based catalyst and characterized through various mechanisms [37, 42-46]. Aluminum oxide is also introduced as a promoter which raises the active level and heat resistance of copper [47-49]. It can also have a direct role in the absorption and activation of methanol [50].

To date, various technical models including technics associated with wet chemistry such as co-sedimentation of an alkali solution [51, 52], half-liquid and half-jelly processes [54], reverse micro-emulsion technics [55], as well as technics associated with dry chemistry such as chemical vapor sediment [56] and flame synthesis [57] for producing the copper/zinc catalysts required in many applications. Among these methods, co-sedimentation through hydro-carbonate accompanied by calcination for the commercial production of the copper/zinc based catalyst is more useful [58, 59].

The effect of the chemical composition has been investigated in a number of studies, which have given to various results. For the ratio of copper/zinc, it is demonstrated that the values ranging between 0.7 and 4 are optimal values for the reaction of transforming methanol [27, 37, 44, and 48]. On the other hand, a number of scholars have reported that the ratio of copper/zinc does not significantly influence the frequency and choice for the conversion reaction of methanol/water vapor [60].

Yung Fang Lee et al [70] produced the catalyst CuZn(Zr)AlO through the co-sedimentation method acted in the following way:

They used a water solution containing Cu, Zn, Zr, and Al Nitrate for the co-sedimentation at 347 kelvin and PH between 8 and 9, with Na₃CO₃ as the sedimentation factor. After the aging process at 333 kelvin for 3 hours, the sediment was drained, washed with distilled water, dried at 383 kelvin for 12 hours and cooked at 723 kelvin for 6 hours.

They also performed the rests for investigating the catalyst in a catalyst-bed reactor at 483-573 kelvin and under the atmospheric pressure. A 0.2 gram sample of catalyst thinned with quartz sands was placed in a pipe reactor made of rust steel with a 7-millimeter internal diameter. After a certain amount hydrogen flew out at 573 kelvin for 5 hours, water and methanol which had already been mixed at certain a ratio were fed into a heater by a micro feeder. The products were cooled and the gas products including hydrogen, carbon monoxide, carbon dioxide, and methane were directed into a GC equipped with thermal steerable detectors and the TDX column. Liquid products such as water and methanol were detected through a Shang-Fen equipped with an organic 401 support column. The activities of the catalyst was analyzed using the data gathered between 5 to 6 hours the operation of transforming methanol (X(MeOH)), hydrogen selectivity (S(H₂)), carbon dioxide selectivity (S(CO₂)), and hydrogen production (Y(H₂)).

\[
X(\text{MeOH}) = \frac{n(\text{MeOH}, \text{conversion})}{n(\text{MeOH}, \text{input})} \times 100\% \\
S(H₂) = \frac{n(H₂, \text{out})}{3}{n(\text{MeOH}, \text{conversion})} \times 100\% \\
Y(H₂) = X(\text{MeOH}) \times S(H₂) \times 100\% \\
S(CO₂) = \frac{n(\text{CO₂}, \text{out})}{n(\text{CO₂}, \text{out}) + n(\text{CO}, \text{out})} \times 100\% \\
\]

The purpose of Fang Lee et al was to produce a series of catalysts through the co-sedimentation method with proper activity and selectivity in the methanol/vapor reaction.

Simulation and Results:

Simulation Used in Simulation:

In order to simulate the specified process, the synthesis of methanol/vapor reaction introduced by Taser et al (2009) [1] was used. They examined the syntheses of the reaction in the laboratory conditions similar to
those used in industrial applications. The catalysts adopted in that study were the commercial ones including Cu-Zn-Al oxides, which are commonly used in industrial processes which are based on water vapor reactions. The density of the catalyst was $1.111 \text{ g/cm}^3$.

They presented a power velocity equation as:

$$r = k p_m^a p_w^b p_{CO_2}^c p_{H_2}^d$$

Where, $M$ and $W$ stand for methanol and water, respectively.

For the synthesis, we have:

$$k = k_0 \exp\left(-\Delta E_A / RT \right)$$

The degrees of the reaction were fitted to the laboratory data. Table 4-2 represents the specifications of the synthetic equation:

<table>
<thead>
<tr>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
<th>$d$</th>
<th>$k_p$ (mol l/(gh))</th>
<th>$E_A$ (cal/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.351</td>
<td>0</td>
<td>0</td>
<td>5/587*10^8</td>
<td>21667</td>
<td></td>
</tr>
</tbody>
</table>

The synthetic equation has good fit with the laboratory data; the conversion value of methanol predicted by the equation in operational conditions similar to laboratory ones has a 1-percent difference from the value obtained from the experiment.

Validating Simulation Results:

In order to test the validity of the simulation results, the conversion percentage of methanol and the amount of hydrogen produced in the simulated process were compared to the experimental results reported in [1]. Table 4-2 lists the simulation results and the experimental data.

<table>
<thead>
<tr>
<th>Reference</th>
<th>Produced Hydrogen Percentage</th>
<th>Methanol conversion percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Present Project</td>
<td>23</td>
<td>45</td>
</tr>
<tr>
<td>[1]</td>
<td>29</td>
<td>52</td>
</tr>
<tr>
<td>Error</td>
<td>6</td>
<td>7</td>
</tr>
</tbody>
</table>

According to the table, the error between experimental and simulation results is smaller than 7 percent. Therefore, it can be concluded that the simulation has good fit with experimental results. Figure 4-1 shows the conversion of the materials involved in the reaction and the amount of produced materials against the length of the reactor. According to the table, as the methanol/water reaction continues along the reactor, they reduce in amount while hydrogen and carbon dioxide increase. Figure 4-2 shows the changes in temperature against the length of the reactor during the reaction. As the table depicts, the temperature has a falling trend through the reaction. This indicates that the reaction is exothermic and in order to raise the amount of hydrogen, the temperature of the reactor must be raised and temperature fall must be prevented. This is done with the injection of water vapor. In the following sections, temperature changes and their influences on the amount of hydrogen will be discussed.
According to Figure 4-3, which shows the length of time that the materials must stay in the reactor, the time required for the conversions is 11.49 seconds.

4-3 The Influences of Temperature, Feed Percentage Composition, Feed Flow and Reactor Size on the Amount of Yielded Hydrogen:

In this section we examine whether changing the Temperature, Feed Percentage Composition, Feed Flow and Reactor Size can lead to greater amounts of yielded hydrogen. Finally, using the results, the process is simulated under optimal conditions for producing high purity hydrogen. It should be noted that in the following sections only the amount of specified parameters change and others remain unchanged, retaining the values stated in 4-2.

4-3-1 Reactor Size:

As mentioned before, the process is stimulated based on the conditions specified in [1]. The reactor had a length of 12 cm and a diameter of 4 cm. Now, the simulation is conducted with reactors of 10, 20, 40, and 80 cm long and the influence of this change is investigated. Figures 4-4, 4-5, 4-6, and 4-7 show the amount of reacting materials and yielded materials in 10, 20, 40, and 80 cm long reactors, respectively.
The simulation results in this section are listed in Table 3-4.

Table 3-4: The Influence of Changes in Reactor Size on the Conversion Value of Methanol and Yielded Hydrogen.

<table>
<thead>
<tr>
<th>Reactor length (cm)</th>
<th>Methanol Conversion Percentage</th>
<th>Yielded Hydrogen Percentage</th>
<th>Stay Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>41</td>
<td>22</td>
<td>9</td>
</tr>
<tr>
<td>12</td>
<td>45</td>
<td>23</td>
<td>12</td>
</tr>
<tr>
<td>20</td>
<td>45</td>
<td>25</td>
<td>20</td>
</tr>
<tr>
<td>40</td>
<td>48</td>
<td>27</td>
<td>40</td>
</tr>
<tr>
<td>80</td>
<td>52</td>
<td>28.5</td>
<td>83</td>
</tr>
</tbody>
</table>

According to the table, as the length of the reactor increases, the conversion amount of methanol and the amount of yielded hydrogen increases. Although the amount of hydrogen increases, the stay time also increases. For instance, the time required for yielding 37 percent of hydrogen in the 40-cm long reactor is 41 seconds while the hydrogen with 40 percent purity in the 80-cm long reactor is 83 seconds. In other words, for achieving a 3-percent increase in the purity of hydrogen, the stay time grows twice as much. In such cases, it should be considered which one is important: the amount yielded hydrogen or its purity?

It should be noted that as the length of the reactor increases, the costs of making one rise, which is out of this discussion.

4-3-2- Input Feed Flow:
The input feed flow, which was derived from [1] and used in the simulation, was 1.621*10^-6 kmol/s. In this project, the simulation was conducted with 1.621*10^-5, 1.621*10^-7, 1.621*10^-8, 1.621*10^-9 kmol/s flows. The conversion percentage of the materials and the formation of the products in the simulations are demonstrated in Figures 8-4, 9-4, 10-4, and 11-4.

Fig. 4-8: Conversion of Raw Materials and Formation of Products with 1.621*10^-5 kmol/s Flow.

The results of the simulation are listed in Table 4-4. According to the results, as the flow is multiplies by 10, the amount of hydrogen decreases considerably. As flow decreases, methanol conversion and the amount of yielded hydrogen increase; however, stay time will also greatly increases. For instance, as the feed floe
decreases to $1.621 \times 10^{-8}$, the mole fraction of hydrogen increases for 52 percent, but stay time will increase to 21 minutes.

**Fig. 4-9:** Conversion of Raw Materials and Formation of Products with $1.621 \times 10^{-7}$ kmol/s Flow.

**Fig. 4-10:** Conversion of Raw Materials and Formation of Products with $1.621 \times 10^{-8}$ kmol/s Flow.

**Fig. 4-11:** Conversion of Raw Materials and Formation of Products with $1.621 \times 10^{-9}$ kmol/s Flow.

<table>
<thead>
<tr>
<th>Stay Time</th>
<th>Yielded Hydrogen</th>
<th>Methanol Conversion</th>
<th>Feed Flow Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/3</td>
<td>16</td>
<td>31</td>
<td>$1/621 * 10^7$</td>
</tr>
<tr>
<td>12</td>
<td>23</td>
<td>45</td>
<td>$1/621 * 10^8$</td>
</tr>
<tr>
<td>124</td>
<td>29/5</td>
<td>52</td>
<td>$1/621 * 10^9$</td>
</tr>
<tr>
<td>1300</td>
<td>34</td>
<td>62</td>
<td>$1/621 * 10^{10}$</td>
</tr>
<tr>
<td>13560</td>
<td>37/5</td>
<td>69</td>
<td>$1/621 * 10^{11}$</td>
</tr>
</tbody>
</table>

As the feed flow rate decreases to $1.621 \times 10^{-9}$ kmol/s, the percentage of methanol conversion and the mole fraction of hydrogen increases to %69 and %60, respectively. However, stay time increases to 226 minutes. Therefore, as the feed flow rate decreases, stay time increases and if the flow rate decreases considerably, stay time increases.

**4-3-3 Temperature:**

The process was simulated at 250 degrees of Celsius (based on [1]). In this project, the simulation was conducted at the 225, 275, and 300 °C temperatures were used. Figures 12-4, 13-4, and 14-4 demonstrate the amounts of raw material conversions and products formations.

**Fig. 4-12:** Raw Materials Conversion and Yielded Products in Simulation at 225 °C.
The results of the simulation are listed in Table 4-5. According to the table, with temperature rises, methanol conversion and the mole fraction of hydrogen increase considerably. In this case, in contrast to those of changing flow rate and reactor size, the stay time does not raise with the raise in the amount of hydrogen. However, increasing the temperature is a costly process. In short, one approach to increase the amount of yielded hydrogen is to increase temperature.

### Table 4-5: Influence of Temperature Changes on Methanol Conversion and Yielded Hydrogen

<table>
<thead>
<tr>
<th>Stay Time (s)</th>
<th>Yielded Hydrogen Percentage</th>
<th>Methanol Conversion Percentage</th>
<th>Input Feed Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>19/5</td>
<td>38</td>
<td>225</td>
</tr>
<tr>
<td>12</td>
<td>23</td>
<td>45</td>
<td>250</td>
</tr>
<tr>
<td>11</td>
<td>28</td>
<td>52</td>
<td>275</td>
</tr>
<tr>
<td>11</td>
<td>32</td>
<td>59</td>
<td>300</td>
</tr>
</tbody>
</table>

### 4-3-4. Feed Percentage Composition:

In this section the influence of feed percentage composition on methanol conversion percentage and the amount of yielded hydrogen us investigated. The simulations are conducted with feeds containing 3 different mole ratios of water to that of methanol. They include .5, 1.5, and 3. The changes in raw materials and yielded products are presented in Figures 4-15, 4-16, and 4-17.
According to table, as the mole ratio of water to methanol increases, the mole fraction of yielded hydrogen decreases. The highest amount of yielded hydrogen is achieved when the mole ratio is .5.

Table 4-6: Influence of Feed Percentage Composition Changes on Methanol Conversion and Yielded Hydrogen Amounts.

<table>
<thead>
<tr>
<th>Stay Time (s)</th>
<th>Yielded Hydrogen</th>
<th>Methanol Conversion Percentage</th>
<th>Mole Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>28</td>
<td>32</td>
<td>0/5</td>
</tr>
<tr>
<td>12</td>
<td>25</td>
<td>38</td>
<td>1/5</td>
</tr>
<tr>
<td>12</td>
<td>23</td>
<td>45</td>
<td>2/4</td>
</tr>
<tr>
<td>12</td>
<td>22</td>
<td>46</td>
<td>3</td>
</tr>
</tbody>
</table>

4-4 Final Simulation Using Results Achieved in 3-4:

In this section, the results achieved in section 3-4 are used to simulate the process so that the mole fraction of hydrogen increases. In other words, the investigations on the influences of various parameters on the improvement of this process revealed the influence each parameter has on increasing the mole fraction of hydrogen. Therefore, according to these pieces of information, the parameters are optimized and simulated in a process with good output.

In section 4-3-1, it was indicated that greater sizes of the reactor considerably increase the mole fraction of hydrogen (see Table 4-3). By raising the length of the reactor to 80cm, the mole fraction of hydrogen reached %40, with 83 seconds of stay time. Therefore, in the final simulation, the length of the reactor is raised.

Section 4-3-2 revealed that cutting the feed flow rate plays a significant role in reaching greater mole fractions of hydrogen (see table 4-4). Since stay time increases as the flow rate decreases, in the final simulation the flow rate will be $1.621*10^{-8}$.

The investigations conducted in 4-3-3 demonstrated that higher temperatures increase the mole fraction of hydrogen (see table 4-5). In the simulations, a temperature of 300 degrees of Celsius led to good results. Therefore, in the final simulation, the temperature of the input feed will be 300 degrees.

In section 4-3-4, it was found that by decreasing the mole ratio of water to methanol, the mole fraction of hydrogen in the final product increases (see table 4-6). A ratio as small as 0.5 yielded better results; therefore, this ratio will be used in the final simulation.

The final simulation was conducted with the previously specified characteristics. Table 4-7 shows the reactor specifications and the operational conditions.

Table 4-7: Reactor Specifications and Operational Conditions in Final Stimulation.

<table>
<thead>
<tr>
<th>Reactor Length</th>
<th>Feed Flow</th>
<th>Temperature</th>
<th>Mole Ratio of Water and Methanol</th>
</tr>
</thead>
<tbody>
<tr>
<td>80 cm</td>
<td>$1.621*10^{-8}$</td>
<td>300 °C</td>
<td>0/5</td>
</tr>
</tbody>
</table>

Figure 4-18 depicts the process of the raw materials conversion against the length of the reactor.

Fig. 4-18: Raw Material Conversion and Products in Final Simulation.
As Table 4-8 shows, the mole fraction of Hydrogen is 0.5. This shows a considerable improvement compared to the previous simulations. In fact, in the final simulation, the dominant output is hydrogen.

4-5 Final Discussion:
In this paper, the methanol/water reaction in the catalyst-bed reactor was simulated to produce hydrogen. In this simulation, the synthesis introduced by Taser et al in 2009 [1] was used. A comparison of the simulation results with those of the experimental study in [1] revealed a good fit. Following that, the influences of various parameters (temperature, reactor size, flow rate, and feed percentage composition) on the amount of yielded hydrogen were examined. In the final simulation, it was attempted that, using the results of the investigations, the amount of yielded hydrogen be increased.

Finally, the amount of hydrogen considerably increased and the dominant product was hydrogen. According to the results in Section 4-3, the amount of yielded hydrogen increases when the reactor length and temperature increase and feed flow rate and water/methanol ratio decrease. Increased reactor length and decreased flow rate lead to increased stay time. Therefore, the issue to be addressed is whether the goal is to produce highly purified hydrogen or produce higher amounts of hydrogen. The former is achieved through decreased flow rate and increased reactor length. For instance, the simulation specified in Table 4-7 with the flow rate of 1.621*10^{-10} k mol/s increases the mole fraction of hydrogen to 0.6. Nevertheless, the stay time greatly increases as well.

Conclusion and Suggestions:
The environmental problems created by the burning and depletion of fossil fuels have led the world to search for new sources of energy which are renewable and clean. Using hydrogen as a clean form of fuel in large scales is not convenient. To our knowledge, renewable energies do not solely pave the way to a world free of fossil fuels since their large-scale production is costly and difficult. Also, the geographical features affect the uses of clean fuels such as the wind and the sun's energy. The proposal of developing nuclear energy (which is not considered as a renewable source of energy but different from fossil fuels) is hated due to its threats such as radioactive rays. However, a majority of countries produce a part of their electricity through nuclear energy. Hydrogen is the most abundant element in the world. It is the main building block of stars including the sun. The light and heat produced by the burning of the sun is actually the result of the process of a nuclear fusion which turns hydrogen into helium. Hydrogen does not abound on the earth as a separate element and in order to extract it from water and fossil fuels, energy must be consumed. Therefore, hydrogen is not a primary source of energy but it is an important secondary energy source. According to what was discussed, hydrogen is one promising future source of energy.

In the molecular form, hydrogen can be produced through various sources and methods. In energy systems, hydrogen is the best alternative to carry energy. It can be produced through any fossil fuel since, according to the definition, they all contain hydrogen. It can also be extracted from water and biological materials. The process of water fission is called electrolyze, which is the oldest electrochemical process.

The methods of producing hydrogen include: the conversion reaction of methane/water vapor, taking hydrogen from the coal, producing biomass through burning biomass, electrolyzing water and producing hydrogen through the conversion reaction of methanol/water vapor. The clean methods of hydrogen production (electrolyze through the wind as the energy source or other clean sources) are costly but the process of gasifying the biomass is not as costly and it is comparable to fossil fuels.

In order to use hydrogen as a fuel in applications such as fuel cells, the produced hydrogen must be purified. The hydrogen purification methods include physical and chemical absorption, partial condensation, purifying through membrane and surface absorption with pressure changes.

If the purity of hydrogen can be heightened at the time of hydrogen production for applications such as fuel cells so that other purification methods are not required, the costs are greatly reduced. In addition to the costs, the process of production can be implemented so that the diffused carbon dioxide is minimized. One method which is capable of doing this approach is the process of producing hydrogen through the conversion reaction of methanol/water vapor in a catalyst-bed reactor. The advantages of this approach include: mild conversion conditions of methanol/water vapor, lack of pre-conversion requirement, lack of serious problems of carbon dioxide formation, and high volume density of the energy of methanol in the room temperature.

In this project, the process of producing hydrogen using the methanol/water vapor reaction was simulated. In this simulation, the synthesis introduced by Taser et al was used. The comparison of experimental results reported in that paper and those of the simulation process showed good fit between them. The mole fraction of

Table 4-8: Briefing of Final Simulation Results.

<table>
<thead>
<tr>
<th>Stay Time</th>
<th>Mole Fraction of Hydrogen</th>
<th>Methanol Conversion Percentage</th>
<th>Final Simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>7000</td>
<td>50</td>
<td>58</td>
<td>Final Simulation</td>
</tr>
</tbody>
</table>

As Table 4-8 shows, the mole fraction of Hydrogen is 0.5. This shows a considerable improvement compared to the previous simulations. In fact, in the final simulation, the dominant output is hydrogen.
produced hydrogen was 0.31. Then, the influences of various parameters (temperature, flow rate, feed percentage composition, and reactor size) on the conversion percentage of methanol and the mole fraction of hydrogen were investigated. According to the results, the final simulation was conducted. The mole fraction of hydrogen in the final simulation increased to %50, which is %27 greater than what was achieved in the simulation based on Taser et al (2009). In the final simulation, attempt was made to prevent stay time from increasing. If this is taken into account, the mole fraction of hydrogen can be raised to %60 by decreasing flow rate and increasing the reactor length.

According to the results, it is suggested that:
1- The results be applied in building a reactor and producing hydrogen with the mole fraction of %60.
2- The methods of reducing carbon dioxide as a byproduct be investigated.
3- The output of the final simulation be used input feed to a dispenser for heightening the purity of hydrogen.
4- The syntheses be used in other studies and the results be compared.
5- The simulated process be economically studied and be compared to other methods in terms of costs.

REFERENCES