

## INVESTIGATING THE CAPABILITY OF ARTIFICIAL NEURAL NETWORK TO MODIFY AND OPTIMIZE AN INDUSTRIAL METHANOL PRODUCTION PROCESS

M. A. Khademi, J. Shariati, M. Bahmani, S. Talati

*Young Researchers and Elite Club, Darab Branch, Islamic Azad University, Darab, Iran*

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### Abstract

In the present study, a great effort is made to improve the performance of a conventional methanol synthesis unit. In the proposed modified scheme, the traditional one single carbon dioxide hydrogenation reactor is replaced with the two jacketed reactors connected in series. Artificial neural network approach is used to model the conventional and modified methanol synthesis processes and the simulation results are validated against the industrial plant data. The effect of reactor inlet pressure and temperature on the methanol production rate is investigated. Sensitivity analyses indicate that increasing the pressure and decreasing temperature can move the process towards increasing the amount of methanol production. So, in the proposed modified scheme, the first reactor effluent enters to the second reactor after passing through a heat exchanger. The obtained results reveal that the modified scheme is an appropriate tool to increase amount of methanol production respect to the conventional one.

**Keywords:** methanol; optimization; artificial neural network; modification.

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## 1. Introduction

Methanol or methyl alcohol can play a critical role as a solvent, gas hydrate inhibitor in the oil and gas processes and as a raw material in the petrochemical industries for production of formaldehyde, methyl *tert*-butyl ether and other solvents [1]. Fielder *et al.* investigated that 27% of the produced methanol in 1996 was used for methyl *tert*-butyl ether synthesis [2]. Methanol is usually produced from different sources like syngas, natural gas, coal, biomass and petroleum.

Conventional methanol synthesis reactor is a vertical shell and tube heat exchanger whose vertical tubes are packed with CuO/ZnO catalyst and surrounded by boiling water [3]. Since the catalyst is highly sensitive to temperature, it can be deactivated due to sintering in the temperatures above than 300°C [4-5].

Graaf *et al.* [6] worked on the modeling of a low-pressure methanol reactor by using commercial CuO/ZnO/Al<sub>2</sub>O<sub>3</sub> catalyst. They used the dusty-gas model for explanation of the internal mass transfer limitations in the methanol synthesis reactor. In 1995, Skrzypek *et al.* [7] worked on the thermodynamic and the kinetic of methanol production reactions. Bussche and Forment [8] developed a model for methanol synthesis reactions based on Cu catalyst in the steady state condition. Methanol synthesis simulation and optimization with a rigorous pseudo-steady state model considering the catalyst deactivation was performed by Lovik *et al.* [9]. Jahanmiri and Eslamloueyan [10] developed a one and two dimensional modeling on the methanol synthesis reactor. The two different developed models were found to have a similar trend. Velardi and Barresi [11] showed that the methanol reactor efficiency can be increased using a multi methanol network with auto-thermal behavior. Rahimpour and Ghader [12] discovered that the amount of methanol production can be raised using Pd/Ag perm-selective membrane in which only hydrogen was assumed to permeate through the membrane layer. Gallucci *et al.* [13] compared the performance of a membrane reactor with a conventional one. Higher CO<sub>2</sub> conversion, methanol

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selectivity and methanol yield were obtained in the membrane concept. Kordabadi and Jahanmiri [14] focused on the modeling and optimization of the methanol synthesis reactor and it was found that the optimal conditions can increase the amount of methanol production rate. Farsi and Jahanmiri [15] modeled and optimized the methanol production process in a dual-membrane reactor. The results of their study showed that the amount of methanol production in this configuration was 13.2% higher than the industrial methanol synthesis reactor

## 2. Methanol production process description

A schematic of the methanol production unit is shown in Figure 1. As illustrated, the feed stream, which mainly contains methane, hydrogen and a trace amount of water, are preheated in the heat exchanger E-1 using the outlet products from the reactor. The reactor effluent are divided into two streams, one of them enters to the heat exchanger E-1 and another goes to E-2. After cooling the reactor outlet streams to 109°C in the two heat exchangers, they are mixed in the mixer M-1. Then, the mixer outlet stream passes through the two next heat exchangers AC-1 and E-3. The heat exchanger E-3 effluent with the operational temperature of 40°C enters a flash drum which separates methanol from unreacted gases. The bottom product of the flash drum is a liquid mixture composed of methanol and unreacted compounds which are finally recycled to the reactor. This process is often carried out in a jacketed reactor whose vertical tubes are packed with Cu/Al<sub>2</sub>O<sub>3</sub> and Zn/Al<sub>2</sub>O<sub>3</sub> catalyst and surrounded by boiling water.

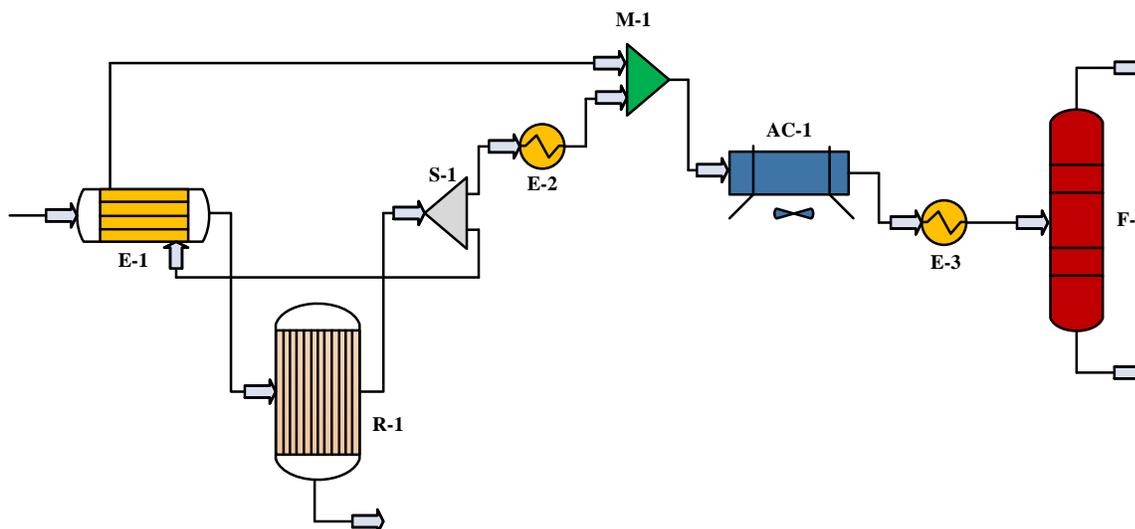
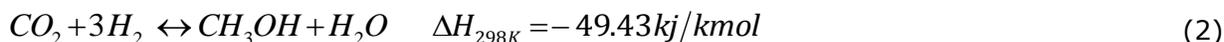
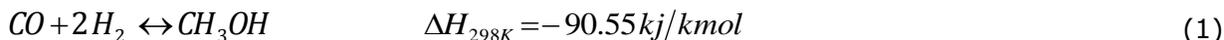
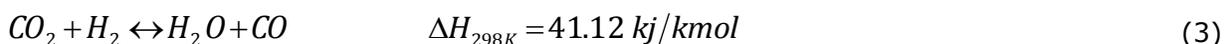


Figure 1. Schematic diagram of the conventional methanol production process

Carbon dioxide hydrogenation reactor, as the main part of the methanol production process is used to convert carbon dioxide and hydrogen to methanol. The main reactions occurred in the reactor are as follows:



Water-gas-shift reaction also takes place in the carbon dioxide hydrogenation reactor simultaneously with the two abovementioned synthesis reactions [16]:



## 3. Artificial neural networks

Deriving reliable and precise analytical correlations for modeling of highly non-linear phenomena are often difficult and sometimes impossible. Artificial intelligence techniques e.g.,

artificial neural networks (ANN), have been successfully applied in the modeling of complex realistic and synthetic processes behavior in areas where precise analytical or semi-experimental correlations are unavailable [17-22].

ANNs, as computationally efficient tools can be trained with experimental information to construct a black-box model which can predict the process performance accurately [23].

These networks are designed in such a way that does not require the exact relations between the independents and dependents variables or assumption about the parametric nature of the related parameters. ANNs can correlate the inputs and outputs of most nonlinear multi-variable phenomena with any complexity or no available relation.

ANNs are composed of a large number of key processing elements namely neurons that are connected together in a specified manner according to the type of the network. Strictly feed-forward structure provides the weighted connections between neurons of the two consecutive layer. Information received from neurons of previous layer or perhaps from an external source is sent to neurons in a next layer. The layers between the input and output layers are called hidden layers. The output of neurons can be expressed mathematically using Equation 4:

$$net_j = f\left(\sum_{r=1}^N w_{jr} x_r + b_j\right) \quad (4)$$

where  $w_{jr}$  refers to the weight from neuron;  $r$  indicates neuron  $j$ ;  $b_j$  and  $net_j$  represent the bias and output of  $j^{th}$  neuron.

As can be concluded from Equation 4, the entry information ( $x_r$ ) of each neuron are weakened or strengthened through their multiplication to weights and then added with the biases coefficients i.e.,  $\sum_{r=1}^N w_{jr} x_r + b_j$ . This summation is often called the net input to neuron  $j$ , and known as  $net_j$ . The biases are activation thresholds added to the multiplication of inputs and their particular weight coefficients. The net output of each neuron passes through a function called activation or transfer function ( $f$ ). Different types of transfer functions such as linear, log-sigmoid, tan-sigmoid, and radial basis have been proposed for artificial neural networks [24].

In this study, the functions defined by Eqs 5 and 6 are used as the transfer functions in the input and output layers, respectively.

$$f(net_j) = \frac{e^{net_j} - e^{-net_j}}{e^{net_j} + e^{-net_j}} \quad (5)$$

$$f(net_j) = \frac{1}{1 + e^{-net_j}} \quad (6)$$

where  $f(net_j)$  denotes the output of the  $j^{th}$  neuron introducing the input of the next neurons or network output.

The correlations indicated by equations 5 and 6 are usually called tan-sigmoid and log-sigmoid transfer functions. These transfer functions compress their inputs into intervals of [-1 1] and [0 1] respectively.

The nonlinearity, continuity and differentiability of these transfer functions allow the network to find complex mappings among the input information. The gradient of the errors are used in optimizing the network parameters i.e., weights and biases.

### 3.1. Training

To reach a proper approximation result for ANN model, the biases and weights of the links between neurons have to be regulated with respect to some objective functions during the training stage.

There are several methods to train and optimize the strengths of the network connections, such as their adjustment explicitly using a priori knowledge about the process. Another training algorithm such as back propagation (BP) and quick propagation are among the most practical learning techniques used if sufficient experimental samples are available. However, back propagation method usually gives out better results in case of chemical engineering systems [25].

Learning process using BP training algorithm involves two phases: During the first phase, the input signals are fed to the input layer and propagated through the hidden and output layers for computation the output of ANN model. Obtained outputs are compared with their corresponding experimental targets, resulting in an error signal. The second phase involves a back flow of errors through the network during which the biases and weights of network would be adjusted so that the output approaches to the observed data. According to gradient descent, the BP modifies and adjusts the network parameters (weights and biases) with respect to the negative gradient of the error function. The most frequently used error function is the mean squared error (MSE) which can be defined by Equation 7. Training continues until the network outputs meet the desired preciseness.

$$MSE = \frac{1}{N} \sum_{i=1}^N (y_i^{\text{exp.}} - y_i^{\text{cal.}})^2 \quad (7)$$

Although back-propagation training algorithm can be applied to networks with any number of layers, it has been proved that only one hidden layer suffices to approximate any function with finitely discontinuities to arbitrary precision, provided the activation functions of the hidden units are non-linear [25-28].

## 4. Results and discussion

The current unit is simulated according to available reaction rates. The simulation results are validated against the three-day experimental data. The effect of reactor inlet temperature and pressure on methanol flow rate in the outlet of the reactor and unit is then presented. Finally, the process is modified to increase the methanol production and decrease the utility consumption.

### 4.1. Simulation and experimental results

By using process simulation, it is possible to investigate the system behavior against process variables. Tables 1 and 2 represent three-day operational conditions and compositional data of the fresh feed stream.

Table 1. Operational conditions as well as composition of feed stream

Day	T (°C)	P (atm)	CO <sub>2</sub> (kmol/hr)	CO (kmol/hr)	H <sub>2</sub> (kmol/hr)	CH <sub>4</sub> (kmol/hr)
1	255.00	61.12	109.00	75.18	3817.25	599.59
2	254.72	61.10	108.71	75.06	3816.92	599.54
3	254.83	61.03	109.20	75.26	3817.35	599.64

Table 2 Operational conditions as well as composition of feed stream

Day	T (°C)	P (atm)	N <sub>2</sub> (kmol/hr)	H <sub>2</sub> O (kmol/hr)	CH <sub>3</sub> OH (kmol/hr)
1	255.00	61.12	220.16	84.34	168.66
2	254.72	61.10	220.16	84.17	168.43
3	254.83	61.03	220.16	84.49	168.52

## 4.2. Effect of reactor inlet temperature

In this stage, the effect of reactor inlet temperature on the methanol production is investigated. Figure 2 illustrates the variation of produced methanol in the reactor and unit outlets respect to temperature at the pressure of 73.03 atm.

It is obvious that increasing the reactor inlet temperature leads to reduction of methanol yield in the reactor and unit outlets. The exothermic reactions occurred in carbon dioxide hydrogenation reactor are responsible for decreasing the rate of the methanol production. According to Le Chatelier's principle, increasing the temperature can shift the equilibrium reactions to the left side (Eqs. 1 and 2), so the methanol production decreases.

## 4.3. Effect of reactor inlet pressure

The effect of reactor inlet pressure on the methanol production is verified and the obtained results are depicted in the Figure 3. This Figure shows the profile of produced methanol in the reactor and unit outlets versus the reactor inlet pressure at temperature of 246°C.

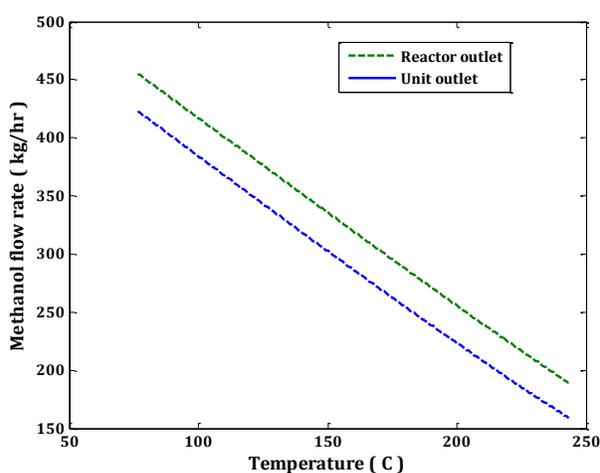


Figure 2. Effect of reactor inlet temperature on the produced methanol at  $P = 73.03$  atm.

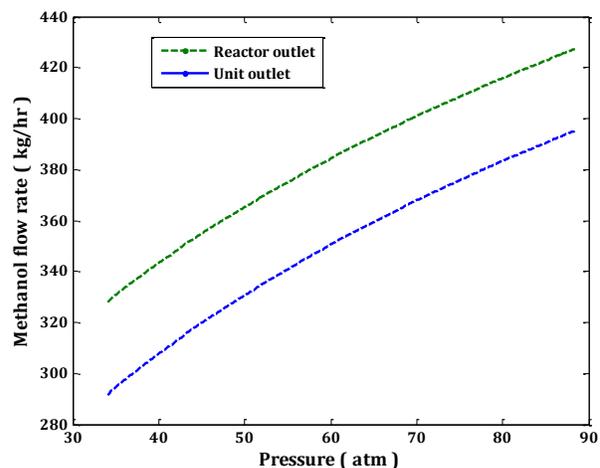


Figure 3. Effect of reactor inlet pressure on the methanol production at  $T = 246$  °C

As illustrated in Figure 4, the methanol flow rate in the reactor and unit outlets increases by increasing the reactor inlet pressure. It can be explained by Le Chatelier's principle which states that any equilibrium reaction moves toward products when the summation of reactants stoichiometric coefficients is higher than the summation of products stoichiometric coefficients.

It can be inferred from the exothermic reactions that decreasing the temperature gives result in higher amounts of methanol production. When the summation of reactants coefficient of methanol synthesis is higher than products one, increasing the reaction zone pressure can increase the methanol production according the Le Chatelier's principle.

## 4.4. Process modification

As previously mentioned, methanol production can be improved by increasing reactor inlet pressure and decreasing its inlet temperature. Although more methanol production can be obtained at lower temperatures, the exothermic reactions of carbon dioxide hydrogenation reactor tend to increase the temperature along the reactor.

In order to reduce undesired products and raise the methanol yield, in this study some modifications are proposed in the conventional methanol synthesis process. A schematic diagram of the modified process is presented in Figure 4.

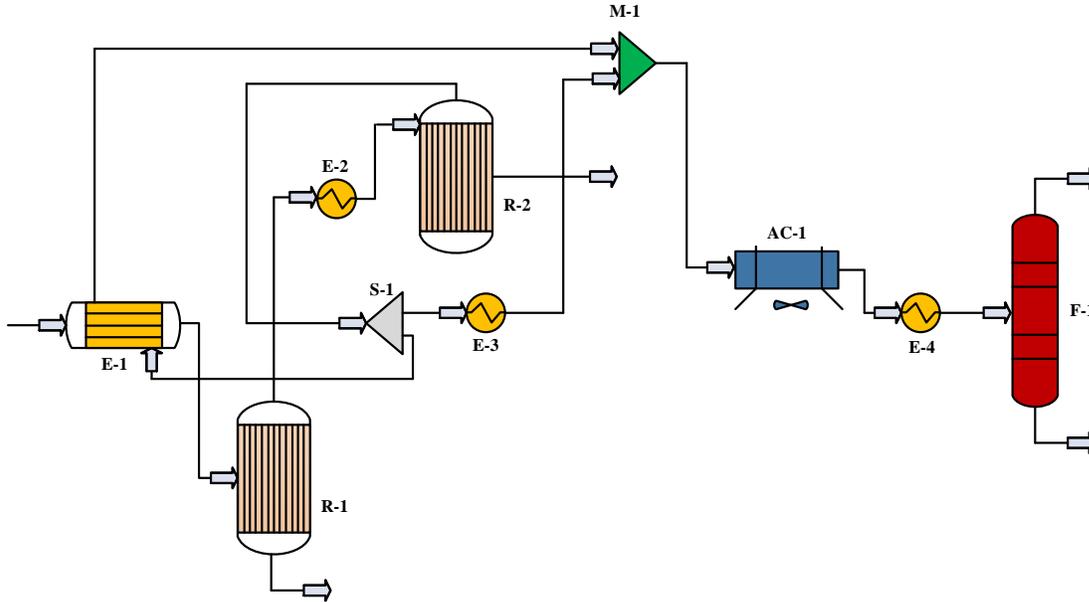


Figure 4. Flow diagram of the modified methanol synthesis process

In this configuration, the traditional one single carbon dioxide hydrogenation reactor is replaced by the two jacketed reactors connected in series. The traditional reactor effluent enters into the second reactor after passing through heat exchanger E-2 located between the two reactors. Heat exchanger E-2 is responsible for reducing the inlet temperature of the reactor R-2. In the second reactor of the proposed scheme, the unreacted gases are allowed to convert to the desired product i.e. methanol.

**4.5. Selection of optimal configuration of ANN**

The optimal configuration of the MLP network is determined by a trial and error procedure through selection the number of hidden layers as well as the number of neurons in each hidden layers. As noted earlier, a MLP network that has only one hidden layer can correlate any types of nonlinear mapping [25-28]. So the applied networks in this research for modeling the conventional and modified methanol production processes have only one hidden layer. The number of neurons in the hidden layer is determined through an optimization procedure which minimizes error indexes. Figure 5 shows the schematic presentation of MLP network used in the present study.

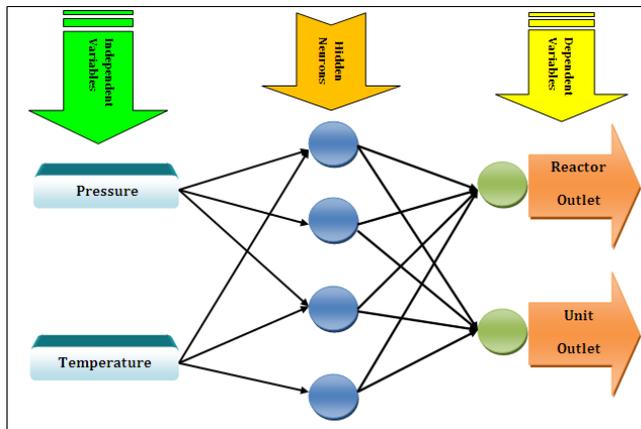


Figure 5. Schematic presentation of the proposed MLP network with single hidden layer

The appropriate number of neurons in the hidden layer depends chiefly on three issues: 1: complexity of correlation between the input and output data, 2: the number of available training and test data, and 3: the severity of noise imposed on the data sets. A few neurons may cause a network unable to reach to the desired error, while a large number of neurons may result in over fitting.

In the present study, the number of neurons in the hidden layer has been evaluated through minimizing MSE and AARD values of the test and training data sets. MSE and AARD can be described by Equations 7 and 8, respectively [29].

$$AARD(\%) = \frac{1}{N} \sum_{i=1}^N \left( \left| \frac{y_i^{exp.} - y_i^{cal.}}{y_i^{exp.}} \right| \right) \times 100 \quad (8)$$

where N is the number of available data sets;  $y_i^{exp.}$  is the  $i^{th}$  experimental target vector (solubility);  $y_i^{cal.}$  is the  $i^{th}$  calculated target value by ANN model and  $\bar{y}$  is the average value of the target.

By using this procedure, the ANN model with one hidden layer consisting of fifteen neurons is found as an optimal structure for conventional methanol production process. Optimal ANN model shows overall AARD = 0.0035 and 0.004 for reactor and unit outlets respectively while MSE = 0.0042 is achieved for both reactor and unit outlets. Results of performed sensitivity error analyses for conventional and modified methanol production are tabulated in Table 3 and Table 4 respectively.

As presented in Table 4, the ANN model with one hidden layer consisting of twelve hidden neurons is found as the optimal structure for modified methanol production process. This optimal model shows overall MSE = 0.0009 and 0.0008 for the reactor and unit outlets respectively, while AARD is found to be 0.0024 for both of them.

Table 3 Performed sensitivity analysis to find the optimal ANN configuration of conventional process

Hidden Neuron	AARD		MSE	
	Reactor Outlet	Unit outlet	Reactor Outlet	Unit outlet
2	0.9289	1.0455	123.05	120.50
4	0.0862	0.0962	0.9783	0.9590
6	0.0345	0.0384	0.3090	0.3147
8	0.0157	0.0166	0.0336	0.0329
10	0.0072	0.0079	0.0149	0.0145
12	0.0061	0.0067	0.0132	0.0125
13	0.0044	0.0048	0.0052	0.0052
14	0.0051	0.0059	0.0065	0.0066
<b>15</b>	<b>0.0035</b>	<b>0.0040</b>	<b>0.0042</b>	<b>0.0042</b>

Table 4 Performed sensitivity analysis to find the optimal ANN configuration of modified process

Hidden Neuron	AARD		MSE	
	Reactor Outlet	Unit outlet	Reactor Outlet	Unit outlet
2	0.2855	0.3266	10.975	11.120
4	0.0360	0.0409	0.2258	0.2316
6	0.0151	0.0167	0.0485	0.0502
8	0.0074	0.0084	0.0140	0.0140
10	0.0032	0.0036	0.0028	0.0028
<b>12</b>	<b>0.0024</b>	<b>0.0024</b>	<b>0.0009</b>	<b>0.0008</b>
14	0.0030	0.0033	0.0020	0.0020
15	0.0025	0.0028	0.0025	0.0025

Tables 5 and 6 represent the comparison between the simulated results and the industrial data from the carbon dioxide hydrogenation reactor.

Table 5 Comparison between the simulated results and industrial plant data

Day	T (°C)	P (atm)	CO <sub>2</sub> (kmol/hr)	CO (kmol/hr)	H <sub>2</sub> (kmol/hr)	CH <sub>4</sub> (kmol/hr)
1	255.00	61.12	109.00	75.18	8408.05	1320.68
2	254.72	61.10	108.71	75.06	8407.32	1320.57
3	254.83	61.03	109.20	75.26	8408.25	1320.79
Simulated	255.28	61.50	103.71	55.78	8287.56	1320.56
Error			4.8%	25.8%	1.4%	0.1%

Table 6. Comparison between the simulated results and industrial plant data

Day	T (°C)	P (atm)	N <sub>2</sub> (kmol/hr)	H <sub>2</sub> O (kmol/hr)	CH <sub>3</sub> OH (kmol/hr)
1	255.00	61.12	220.16	84.34	168.66
2	254.72	61.10	220.16	84.17	168.43
3	254.83	61.03	220.16	84.49	168.52
Simulated	255.28	61.50	219.20	89.45	169.00
Error			0.4%	6.0%	0.3%

The small differences between experimental data and simulation results show that the simulator can predict the unit performance by a good approximation.

#### 4.6. Methanol yield profile versus temperature in the modified and conventional processes

Figures 6 and 7 indicate the profile of methanol production rate of the conventional process and modified one in the unit and reactor outlets respectively. The dashed lines of these Figures represent the amount of produced methanol obtained from the conventional process while the solid lines show its variation in the modified process. It can be inferred from Figures 6 and 7 that although increasing the reactor inlet temperature affects highly on the methanol production in the conventional process, it has a small effect on the one in the modified process.

Figures 6 and 7 clearly show that the amount of produced methanol from modified process is higher than the methanol production from the conventional scheme.

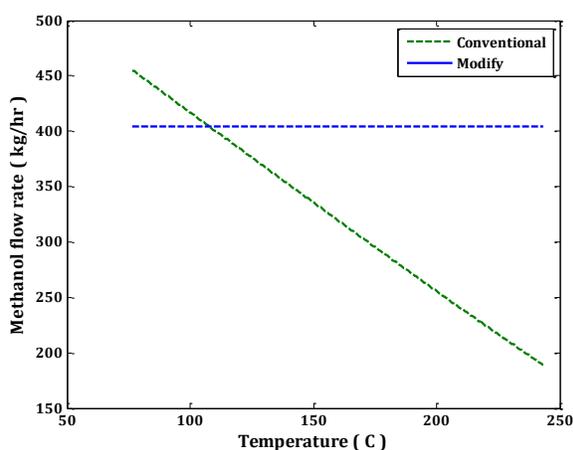


Figure 6. Effect of inlet stream temperature on the produced methanol of reactor outlet at P = 73 atm.

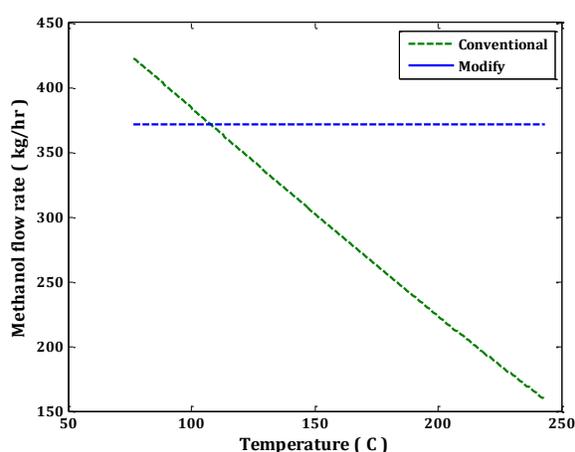


Figure 7. Effect of inlet stream temperature on the methanol yield of unit outlet at P = 73 atm.

#### 4.7. Methanol yield profile versus pressure in the modified and conventional processes

The simulation results of variation of the methanol production in the reactor as well as unit outlets versus ranges of pressures are plotted in Figures 8 and 9 respectively. As clearly shown, the produced methanol of modified scheme is higher than that of conventional process.

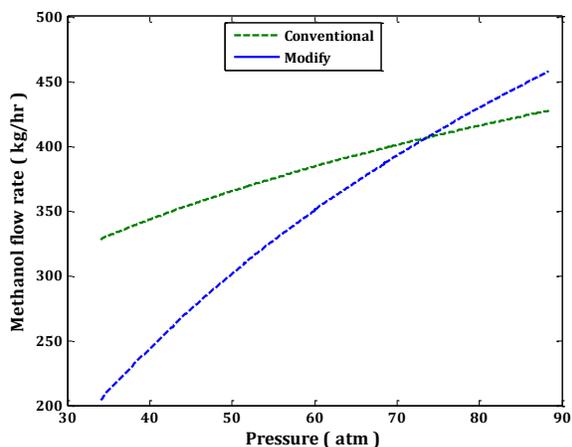


Figure 8. Effect of reaction zone pressure on the methanol flow rate of reactor outlet at  $T = 246^{\circ}\text{C}$

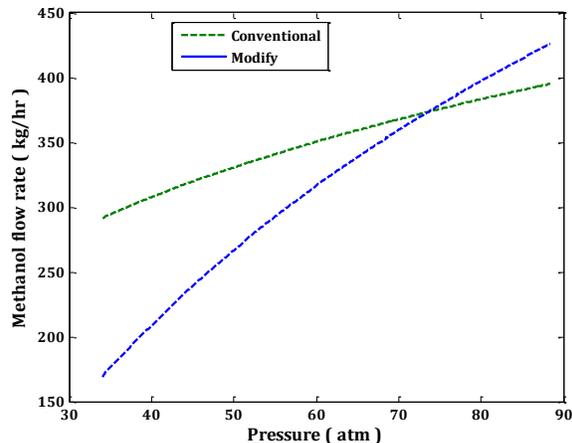


Figure 9. Effect of reactor pressure on the methanol flow rate of the unit outlet at  $T = 246^{\circ}\text{C}$ .

It is obvious that in the presented model, the rate of increasing methanol is very higher than the one in the conventional model.

#### 5. Conclusion

The present work investigates the enhancement of methanol production in a system with two-catalytic reactor instead of traditional one single reactor. In this novel configuration, the effluent of the carbon dioxide hydrogenation reactor is cooled and then sent to the second reactor. The performance of the conventional and modified methanol production units are modeled using artificial neural network. Sensitivity analyses confirm that decreasing the temperature and increasing the pressure, can lead to higher methanol production rate. In comparison between the performances of these two methanol synthesis processes, it was found that the rate of methanol production in the modified scheme is significantly higher than the conventional process.

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\*(Corresponding Author): [m.aminkhademi20@gmail.com](mailto:m.aminkhademi20@gmail.com) (M. A. Khademi)