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Optimization of an Industrial Methanol Reactor Using Aspen Plus Simulator and Design Expert

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ABSTRACT

The chemical conversion of carbon dioxide into methanol has the potential to address two major sustainability issues: the economically viable replacement of fossil energy resources and the avoidance of greenhouse gas emissions. However, the chemical stability of carbon dioxide poses a difficult barrier to its conversion, necessitating extreme reaction conditions, resulting in increased energy input and, subsequently, elevated equipment, operation, and environmental costs. This, in turn, could potentially undermine its promising sustainability as a raw material for the chemical and energy industries. This research aims to optimise methanol production from a methanol reactor by using design of experiment (DOE) in Design Expert and Aspen Plus as a reactor simulator. The optimisation process involved eight parameters: five inlet molar flowrates (CO, CO_2, H_2O, H_2, CH_3OH) and three reactor conditions (inlet temperature, pressure, and temperature profile). The methanol production in Design Expert was optimised using the Box-Behnken method and a quadratic model. This study used the maximum range for each parameter as the actual industrial data and the minimum range to be 50% below it. The validated Aspen-Plus model was used for methanol production simulation. Response surface methodology (RSM) was used to determine the optimal parameters. This simulation required 120 samples. The optimal parameter values from the RSM were 142.2 kmol/hr of inlet CH_3OH, 2250.91 kmol/hr of CO, 1398.3 kmol/hr of CO_2, 15.6973 kmol/hr of H_20, 19053.7 kmol/hr of H_2, 497.883K of reactor inlet temperature, 81.9999 bar of reactor pressure, and 30K for reactor temperature profile with the actual methanol production of 2814.23 kmol/hr. The optimal values were simulated to test the accuracy of the predictive model, and the error was less than 5.2 percent. Overall, the inlet H_2 molar flowrate was reduced in optimised conditions, reducing raw material usage and increasing output.

Keywords: *industrial reactor, methanol, optimisation, Aspen plus, design expert, reactor*

1. INTRODUCTION

Carbon dioxide (CO_2) is the main greenhouse gas contributing to global warming. Substantial amounts of CO_2 are essentially emitted by power plants engaged in the combustion of fossil fuels. As part of ongoing research efforts to reduce CO_2 emissions into the atmosphere,

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converting CO_2 into valuable products, including methanol, stands as a key research. Due to the chemical stabilisation of CO_2, the proposed conversions require the utilisation of extreme reaction conditions [1], which necessitate energy for heating and compression, thereby increasing the capital, process, and environmental costs. Energy consumption is highly dependent on the chosen processing method. Notably, relevant analysis of chemical conversion technologies should transcend the simple evaluation of reactor performance, which frequently relies on conversion and selectivity as the only performance indices.

Methanol (CH_3OH) is typically utilised as a feedstock in petrochemical industries and as a solvent and fuel in other industries. Methanol is usually produced in large quantities from synthesis gas [2][3]. Since 1923, the methanol synthesis process has been commercialised, but the kinetic and reaction mechanisms remain anonymous [4]. Synthesis gas, also known as syngas, is a mixture of fuel gases that are primarily composed of carbon dioxide (CO_2), carbon monoxide (CO), and hydrogen (H_2). Syngas derives its name as an intermediate in producing synthetic natural gas, methanol, and ammonia [5]. In fact, syngas is the primary raw material employed in methanol production. The most prevalent method for producing methanol involves the low-pressure catalytic reaction of syngas. These low-pressure operating conditions permit the conversion of methanol and reduce the by-product yield to greater than 99 percent [9].

In the present study, an ANOVA was developed for the methanol-producing reactor. The selected factors within the factorial design framework include the inlet molar flowrates (CO, CO_2, H_2O, H_2, CH_3OH) and the reactor parameter conditions (inlet temperature, pressure, and temperature profile). Production of methanol was the measured response. Thus, it is possible to identify ways to improve methanol production by reducing the inlet molar flowrates and the significant factors in the selected responses. Additionally, the Box-Behnken Design (BBD) method was employed to determine the optimal operating conditions of the process and a response surface plot for the production of methanol, along with the corresponding mathematical model. Aspen Plus software was used to simulate the reactor and acquire modelling data for the analyses.

2. PROCESS MODELLING

The following reactions (Equation 1- Equation 3) occurred for the production of methanol during the hydrogenation of CO and CO_2 [6]:

$$CO + 2H_2 \leftrightarrow CH_3OH \qquad \Delta H°_{298} = -90.55\ \text{kJmol}^{-1} \tag{1}$$

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \qquad \Delta H°_{298} = -49.43\ \text{kJmol}^{-1} \tag{2}$$

$$CO_2 + H_2 \leftrightarrow CO + H_2O \qquad \Delta H°_{298} = 41.12\ \text{kJmol}^{-1} \tag{3}$$

CO_2 and CO produced from syngas would produce methanol using Equation 1 and Equation 2. CuO or ZnO-based catalysts, renowned as Synetix catalysts, were utilised in the synthesised carbon oxides to produce methanol. The effectiveness of this catalyst type was demonstrated by utilising adiabatic and isothermal reactors. These reactors operated under low temperatures and high-pressure conditions during the exothermic reaction between carbon oxides and methanol. This process was carried out at pressures between 40 and 110 bar and temperatures between 200 and 300 degrees Celsius [6]. The process temperature substantially affected the reactor's production and yield because catalytic reactions are typically highly exothermic. Due

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to its dynamic work behavior and low-pressure control, fixed-bed reactors were considered for methanol synthesis.

Typically, the rate of the chemical process corresponded with the chemical kinetic reaction. A chemical process may consist of a series of one or more single-step processes [2]. This reaction was a simple process, reaction, and step. The elementary reaction consists of a single collision between two molecules, known as a bimolecular step, or the isomerization of such a single reactant molecule, known as an unimolecular step [2]. The kinetic rate equations used in this modelling were derived from the equations adopted by Bussche and Forment and represented by Equation 4, Equation 5 and Equation 6 [7]. Notably, the equations were chosen due to the similar composition of the catalysts (CuO and ZnO) used by Bussche and Forment, which are commercially available.

$$r_{CH3OH} = \frac{k_1 P_{CO2} P_{H2}\left(1-\frac{P_{CH3OH} P_{H2O}}{K_2^{eqn} P_{CO2} P_{H2}}\right)}{\left(1+\frac{k_3 P_{H2O}}{P_{H2}}+\sqrt{k_4 P_{H2}}+k_5 P_{H2O}\right)} \quad (4)$$

$$r_{RWGS} = \frac{k_2 P_{CO2}\left(1-K_3^{eqn}\frac{P_{H2O} P_{CO}}{P_{CO2} P_{H2}}\right)}{\left(1+\frac{k_3 P_{H2O}}{P_{H2}}+\sqrt{k_4 P_{H2}}+k_5 P_{H2O}\right)} \quad (5)$$

The k value was determined by the Arrhenius equation:

$$kj = Aj\ exp\ (Bj/RT) \quad (6)$$

Table 1: Factors of Frequency for Kinetic Equation [7-9]

k1	A	4.39517 x 10^{-13}
	B	36696
k3	A	345.38
	B	-
$\sqrt{k4}$	A	0.499
	B	17197
k5	A	6.62 x 10^{-11}
	B	124119
k2	A	1.22 x 10^{10}
	B	-94765
K_2^{eqn}	$10^{3066/T-10.592}$	
K_3^{eqn}	$10^{-2073/T+2029}$	

Aspen Plus Design Spec. parameter estimation tools were used to determine the value of A for the k1 frequency factor. The value was obtained by minimising the difference between the predicted and desired product streams. Upon achieving convergence during the search iteration process, the estimated value of A for the k1 frequency factor was 4.39517 x 10^{-13} [9].

The reactor block served as the fundamental basis of the methanol production model development. The reaction parameters and conditions of the inlet and the outlet streams between industrial data (the Khark petrochemical methanol plant in Iran) and the previous research's

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data were satisfied, and these data were used as a benchmark and comparison to configure the Aspen Plus simulation model for this study [2]. Fixed bed catalytic reactor was used as the type of reactor (plug flow). Figure 1 and Table 2 illustrate the process setup and specification data.

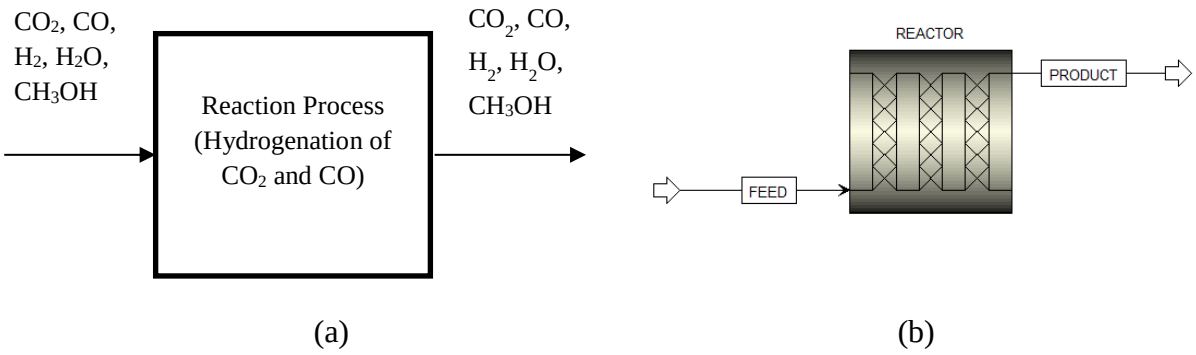

Figure 1: (a) and (b) Methanol model development in a fixed-bed reactor

Table 2: Data from the industry [2]

Parameter	Value
Reactor temperature	498 K
Reactor pressure	82 bar
Inlet CH_3OH molar flowrate	142.2 kmol/hr
Inlet CO molar flowrate	2256.24 kmol/hr
Inlet CO_2 molar flowrate	1398.3 kmol/hr
Inlet H_2O molar flowrate	28.44 kmol/hr
Inlet H_2 molar flowrate	37920 kmol/hr
Reactor length	10 m
Quantity of tubings	5947
Void fraction of bed	0.285 [4]

Based on a review of the relevant literature, the reaction was characterised as a polarity condition and pseudo-reaction type [3]. Due to the nonlinear equation, Aspen Plus opted for the Langmuir-Hinshelwood-Hougen-Watson (LHHW) reaction method [8]. Equation 4 – Equation 6 and Table 1 provide the equations and data for the kinetic reaction, the driving force expression, and the adsorption expression.

The fixed bed catalytic reactor is depicted in Figure 1(b). The following assumptions were made in order to develop the reactor block simulation:

i. Only the vapour at the reactor's outlet was in thermal equilibrium.
ii. Heat mixing was negligible for liquid mixtures.
iii. Tray vapour holdup was negligible.
iv. The chemical reaction of the vapour was completely mixed.
v. The reaction was characterised as adiabatic.

3. RESPONSE SURFACE METHODOLOGY (RSM)

Figure 2 depicts the process flow of the RSM in this research. Eight parameters were selected, which were the inlet molar flowrates (CO, CO_2, H_2O, H_2, CH_3OH), along with the remaining three were reactor conditions (inlet temperature, pressure, and temperature profile) to determine

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the optimum conditions of the reactor for methanol production. The Box-Behnken Design (BBD) method and quadratic model were utilised to introduce additional parameters to the Design Expert (DE). BBD was recommended due to its advantage of requiring fewer experimental runs and less time to conduct all experiments [10]. The parameters and ranges used in the experiment are listed in Table 3. The maximum ranges of the parameters were established based on actual data from the industry (Table 2), assuming that the reactor's design was at its maximum at this point. The minimum ranges were 50% less than the maximum ranges. The mean values were the midpoint between the minimum and maximum ranges.

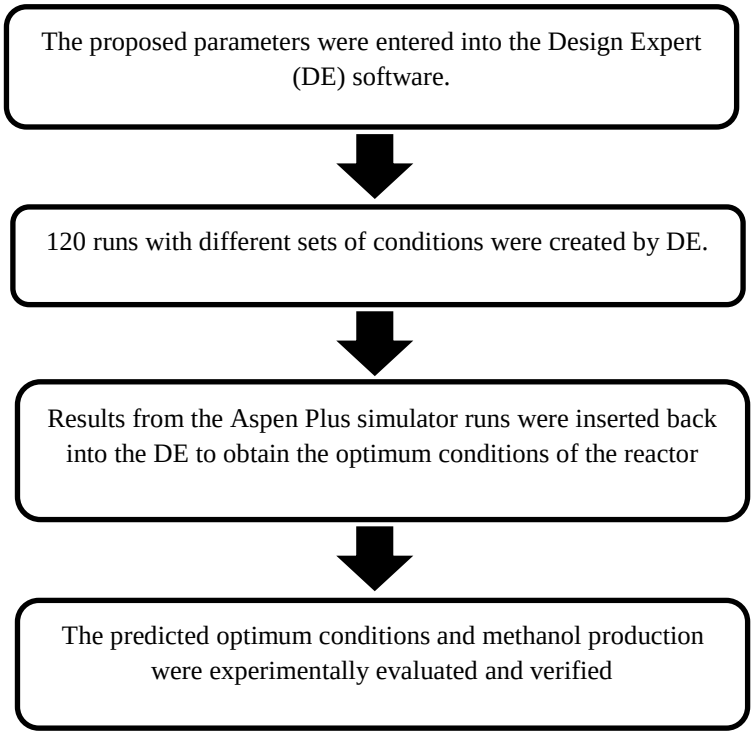

Figure 2: The Process Flow of RSM's Methodology for Reactor-Based Methanol Production.

Table 3: List of factors (terms) and ranges of the experimental parameters

No.	Factor	Name	Units	Minimum	Mean	Maximum
1	A	Inlet CH_3OH molar flowrate	kmol/hr	71.10	106.65	142.20
2	B	Inlet CO molar flowrate	kmol/hr	1128.12	1692.18	2256.24
3	C	Inlet CO_2 molar flowrate	kmol/hr	699.15	1048.72	1398.30
4	D	Inlet H_2O molar flowrate	kmol/hr	14.22	21.33	28.44
5	E	Inlet H_2 molar flowrate	kmol/hr	18960.00	28440.00	37920.00
6	F	Inlet reactor temperature	K	249.00	373.50	498.00
7	G	Reactor pressure	bar	41.00	61.50	82.0
8	H	Reactor Difference Temp. Profile	K	15.00	22.50	30.00

Based on the DE's design, a total of 120 runs of designed experiments were generated, and these involved 120 samples of simulations. The simulations were based on the validated Aspen Plus Simulator from Section 2.0 of this research's Process Modelling. The DE-predicted optimum conditions were experimentally evaluated and verified. After simulating the methanol production using the Aspen Plus, the error between the predicted and experimental optimal conditions of methanol production was calculated and compared. To ensure the model's validity, the difference in error should be less than 10% [11-12].

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4. RESULTS AND DISCUSSION

4.1 The ASPEN Plus model simulation and validation results

Methanol synthesis occurred in the fixed bed catalytic reactor (plug flow model), producing methanol as the primary product, including CO, CO_2, H_2 , and H_2O. Table 4 provides the simulation data for all components in the outlet stream, obtained through Aspen Plus. To validate the model, the Aspen Plus simulation data results were compared to the industrial data and the work done by a researcher who used Artificial Neural Network (ANN) MATLAB to simulate the same process [2]. Table 4 summarises the comparison data.

Table 4: Process Data for Product Stream [9]

Component	Industrial Data (kmol/hr)	Simulation Data (kmol/hr)	% Error
CH_3OH	2775	2762	0.5
CO	399	421	5.5
CO_2	620	614	1.0
H_2	31870	31895	0.1
H_2O	813	813	0.0

Based on the data in Table 4, it can be seen that the Aspen Plus simulation accurately predicted the molar flowrate of the CH_3OH product stream, with an error of only 0.5% when compared to the industrial data. Furthermore, it demonstrates that the maximum error value during simulation with Aspen Plus was less than 5.5%. Consequently, it is concluded that Aspen Plus simulation for such a model could be utilised to simulate the process given any changes to the process parameters.

4.2 RSM Regression, Model Fitting and Significance Analysis

The simulation setup was carried out following the previously described experimental design, where 120 samples were run, and it was determined that the minimum and maximum methanol productions were 70 and 2618 kmol/hr, respectively. Figure 3 depicts the regression line between predicted and actual results. The 120 dots represented a total of one hundred and twenty simulations. The greater the number of points on the regression line, the greater the validity of the results. Table 5 presents the regression score for the molar flowrate of methanol production. The coefficient of determination (R^2) was a guideline for determining the model's adequacy. The closer the R^2 value is to one, the more closely an empirical model matches the actual data [13]. According to Table 5, the model's R^2 is 0.9860, which is close to one. R^2 of 0.9860 indicates that 98.60% of the variance in predicted data is accounted for by actual (simulation) data. Computed values for the predicted and adjusted R^2 are 0.9619 and 0.9777, respectively. The difference between these values is less than 0.2, so they agree reasonably. Measurement of the signal-to-noise ratio was the required precision function, with a preference for a ratio greater than four. As for this experiment, the precise value of 35.0135 indicates an adequate signal.

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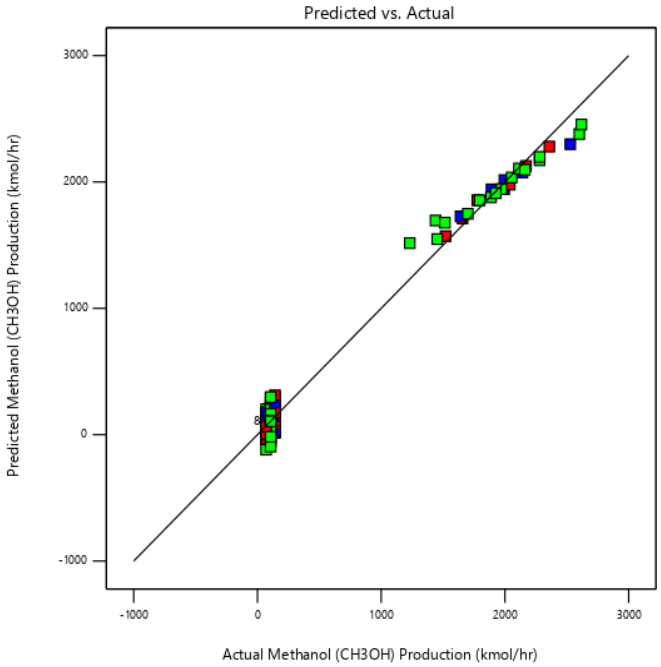

Figure 3: The predicted vs. actual graph of CH_3OH production

Table 5: The Regression Score

Std Dev.	120.01	R^2	0.9860
Mean	537.99	Adjusted R^2	0.9777
C.V. %	22.31	Predicted R^2	0.9619
		Adeq Precision	35.0135

4.3 Development of Regression Model Equation

With the quadratic model, the interactions between the eight parameters in this study were well structured. Table 6 displays the ANOVA results for the production of methanol. The P-values were used to evaluate the significance of every coefficient describing the interaction patterns between independent variables [14]. P-values below 0.05 indicate that model terms are statistically significant, whereas P-values larger than 0.1000 indicate that model terms are not statistically significant [14 - 15].

The Model F-value of 119.64, as shown in Table 6, indicates that the model is significant. There is just a 0.01 percent chance that an F-value of this magnitude could arise from noise. In addition, P-values below 0.05 imply that the model term is statistically significant. Significant model terms include the inlet CH_3OH molar flowrate (A), the inlet CO molar flowrate (B), the inlet reactor temperature (F), the reactor pressure (G), the interaction between the inlet CO molar flowrate and the inlet reactor temperature (BF), the interaction between the inlet reactor temperature and the reactor pressure (FG), the interaction between the inlet reactor temperature and the reactor difference temperature profile (FH), and the interaction between the inlet reactor temperature itself (F^2). Model terms with values exceeding 0.1 are considered insignificant. The terms B, F, BF, and F^2 (P-values < 0.0001) played the most significant role in producing reactor methanol, followed by FG, A, G, and FH. Equation 7 depicts RSM's predicted model:

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Table 6: Analysis of Variance (ANOVA) for the regression model

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	7.581E+07	44	1.723E+06	119.64	< 0.0001	significant
A-Inlet CH_3OH molar flowrate	92542.13	1	92542.13	6.43	0.0133	
B-Inlet CO molar flowrate	5.378E+05	1	5.378E+05	37.35	< 0.0001	
C-Inlet CO_2 molar flowrate	17306.72	1	17306.72	1.20	0.2765	
D-Inlet H_2O molar flowrate	1048.08	1	1048.08	0.0728	0.7881	
E-Inlet H_2 molar flowrate	7947.88	1	7947.88	0.5519	0.4599	
F-Inlet reactor temperature	4.784E+07	1	4.784E+07	3322.05	< 0.0001	
G-Reactor pressure	83506.47	1	83506.47	5.80	0.0185	
H-Reactor diff. temperature profile	42817.65	1	42817.65	2.97	0.0888	
AB	336.03	1	336.03	0.0233	0.8790	
AC	223.93	1	223.93	0.0155	0.9011	
AD	518.26	1	518.26	0.0360	0.8501	
AE	802.81	1	802.81	0.0557	0.8140	
AF	2682.09	1	2682.09	0.1862	0.6673	
AG	9121.64	1	9121.64	0.6334	0.4286	
AH	375.41	1	375.41	0.0261	0.8722	
BC	35.41	1	35.41	0.0025	0.9606	
BD	193.33	1	193.33	0.0134	0.9081	
BE	6127.09	1	6127.09	0.4254	0.5162	
BF	1.004E+06	1	1.004E+06	69.72	< 0.0001	
BG	1770.46	1	1770.46	0.1229	0.7269	
BH	1749.45	1	1749.45	0.1215	0.7284	
CD	686.13	1	686.13	0.0476	0.8278	
CE	2853.51	1	2853.51	0.1981	0.6575	
CF	32259.93	1	32259.93	2.24	0.1387	
CG	3121.96	1	3121.96	0.2168	0.6429	
CH	37.03	1	37.03	0.0026	0.9597	
DE	501.09	1	501.09	0.0348	0.8525	
DF	1922.89	1	1922.89	0.1335	0.7158	
DG	7127.90	1	7127.90	0.4949	0.4839	
DH	764.85	1	764.85	0.0531	0.8184	
EF	14842.93	1	14842.93	1.03	0.3133	
EG	849.82	1	849.82	0.0590	0.8087	
EH	806.53	1	806.53	0.0560	0.8136	
FG	1.557E+05	1	1.557E+05	10.81	0.0015	
FH	79803.26	1	79803.26	5.54	0.0212	
GH	1977.08	1	1977.08	0.1373	0.7120	
A^2	83.22	1	83.22	0.0058	0.9396	
B^2	576.89	1	576.89	0.0401	0.8419	
C^2	69.35	1	69.35	0.0048	0.9449	
D^2	94.61	1	94.61	0.0066	0.9356	
E^2	1770.65	1	1770.65	0.1229	0.7268	
F^2	2.392E+07	1	2.392E+07	1661.07	< 0.0001	

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G^2	12996.08	1	12996.08	0.9024	0.3452
H^2	1381.31	1	1381.31	0.0959	0.7576
Residual	1.080E+06	75	14401.76		
Lack of Fit	1.080E+06	68	15884.30		
Pure Error	0.0000	7	0.0000		
Cor Total	7.689E+07	119			
$R^2 = 0.9860$					

The Model F-value of 119.64, as shown in Table 6, indicates that the model is significant. There is just a 0.01 percent chance that an F-value of this magnitude could arise from noise. In addition, P-values below 0.05 imply that the model term is statistically significant. Significant model terms include the inlet CH_3OH molar flowrate (A), the inlet CO molar flowrate (B), the inlet reactor temperature (F), the reactor pressure (G), the interaction between the inlet CO molar flowrate and the inlet reactor temperature (BF), the interaction between the inlet reactor temperature and the reactor pressure (FG), the interaction between the inlet reactor temperature and the reactor difference temperature profile (FH), and the interaction between the inlet reactor temperature itself (F^2). Model terms with values exceeding 0.1 are considered insignificant. The terms B, F, BF, and F^2 (P-values < 0.0001) played the most significant role in producing reactor methanol, followed by FG, A, G, and FH. Equation 7 depicts RSM's predicted model:

Methanol Production (kmol/hr) = +8615.86016 + 1.49344 (A) - 0.997315 (B) - 0.46627 (C) – 6.56812 (D) + 0.00889* (E) - 46.7164 (F) - 5.5907 (G) - 31.69357 (H) - 0.000209 (A) (B) + 0.000275 (A) (C) + 0.020555 (A) (D) - 0.000019 (A) (E) + 0.00267 (A) (F) - 0.029908 (A) (G) + 0.016584 (A) (H) + 0.0000068877 (B) (C) + 0.000791 (B) (D) - 0.00000334074 (B) (E) + 0.003256 (B) (F) - 0.00083 (B) (G) + 0.002256 (B) (H) - 0.002405 (C) (D) + 0.00000367867 (C) (E) + 0.000942 (C) (F) + 0.001779 (C) (G) - 0.00053 (C) (H) + 0.000076 (D) (E) - 0.011305 (D) (F) + 0.132192 (D) (G) - 0.118361 (D) (H) - 0.000024 (E) (F) - 0.000034 (E) (G) - 0.000091 (E) (H) + 0.035282 (F) (G) + 0.069044 (F) (H) + 0.066 (G) (H) + 0.001364 (A^2) + 0.000014 (B^2) - 0.000013 (C^2) + 0.036363 (D^2) + 0.0000000884853 (E^2) + 0.059633 (F^2) -0.051265 (G^2) + 0.124866 (H^2) (7)

4.4 Process Parameters Studies

The DesignExpert software generates a three-dimensional illustration of the relationship between the responses, parameter range, and type of interaction between the tested parameters. According to the ANOVA regression model in Table 6, there are three significant (P-values < 0.05) interactions between different parameters: FG, FH, and BF. Figure 4 illustrates the relationship between the temperature (F) and pressure (G) at the reactor's inlet and methanol production. Based on Figure 4, the maximum production of methanol through the reactor was attained when both the reactor's inlet temperature and pressure were on the high side. The molar flowrate of methanol production exhibited a gradual increase as the reactor temperature rose until it reached 398 K, at which point it began to increase steeply. In addition, Figure 5 depicts the response surface plot for the relationship between the inlet reactor temperature (F) and the reactor difference temperature profile (H) of the tubing in relation to methanol production. The higher the inlet temperature and the reactor temperature difference profile, the higher the methanol production.

This indicated that the reactor's temperature directly affected the methanol production; consequently, a high temperature demonstrated advantageous for the reaction rate. The

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principle of Le Chatelier [16] states that reversible reactions are self-correcting. Whenever the reactions went out of equilibrium by a change in concentration, temperature, or pressure, the mechanism would spontaneously shift or change to "re-balance" itself. The effect of temperature variation on reaction equilibrium was due to the heat of the reaction. Increasing the temperature of the endothermic reaction was essentially equivalent to adding more reactants to the system. Consequently, in accordance with Le Chatelier's principle, the equilibrium of the reaction would shift to the right. In contrast, lowering the temperature for an endothermic reaction would result in a shift to the left since lowering the temperature corresponds to removing the reactant.

Raising the temperature would favor reaction (Equation 3) and encourage the reaction equilibrium to shift to the right, producing more CO. The increasing concentration of CO, which was a reactant to reaction (Equation 1), would shift reaction (Equation 1) equilibrium to the right and increase the amount of CH_3OH production. Furthermore, the increasing temperature would make the collisions among the reactant molecules generate sufficient energy to achieve a higher reaction than the activation energy. The speed and frequency of collision for reactant molecules increased the reaction rate when the temperature increased. Therefore, it increased the amount of CH_3OH production as well.

Varying pressure or volume would necessitate the production of fewer or more moles of gas to restore equilibrium [16]. When the pressure rises or the volume is lowered in a system, the equilibrium of the reaction is more likely to shift toward the side of the reaction with fewer moles of gas. Similarly, if the pressure lowered or the volume increased, producing more moles of gas would be preferable. Equations 1 and Equation 2 involve reactants that have a greater number of moles than the products. Consequently, increasing the pressure would cause the equilibrium of the reactions to shift to the right, producing a greater amount of methanol.

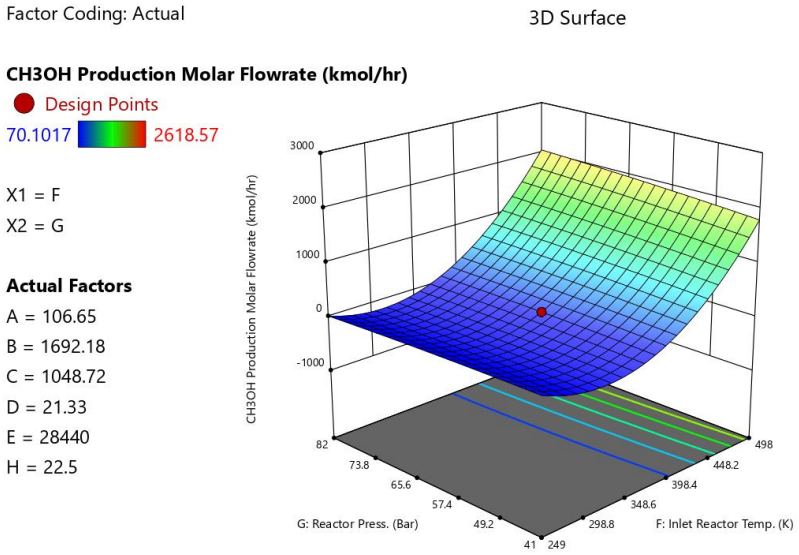

Figure 4: Response surface plot for the effect of inlet reactor temperature and reactor pressure

From the perspective of the ideal gas equation applied to the gas-phase hydrogenation reaction, the pressure was proportional to methanol production. Due to the application of the Henry Law

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in Aspen Plus, it was limited to the execution of the gas phase state, as no supercritical situation existed in the system [8]. The increased concentration of methanol molecules that resulted from increased pressure was only effective until the limit was reached. The higher the pressure, the greater the likelihood that the system will encounter supercritical conditions, producing a small quantity of methanol.

Figure 6 illustrates the effect of inlet CO molar flowrate (B) and inlet reactor temperature (F) on methanol production. Based on Figure 6, it was determined that an increase in the CO molar flowrate at the inlet corresponded to an increase in methanol production. This pattern aligns with the findings in the literature. Carbon monoxide hydrogenation is the primary route to methanol under typical industrial conditions, whereas carbon dioxide is the primary route at lower temperatures and pressures, as determined by previous researchers [17-19].

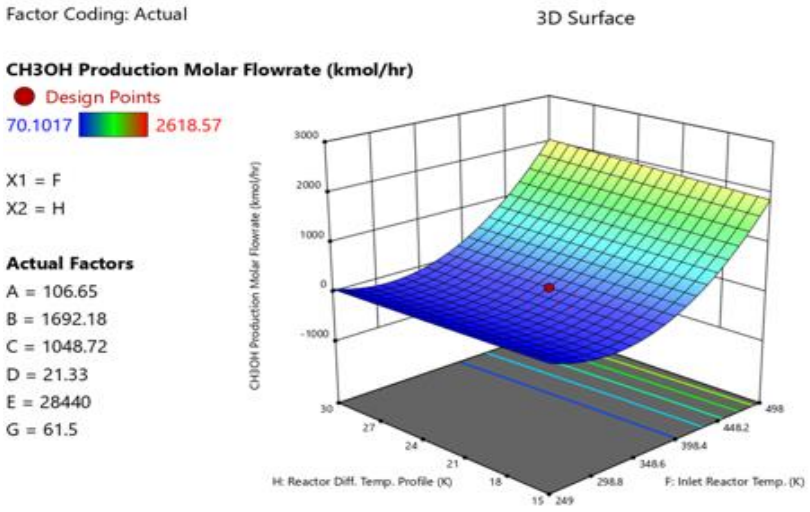

Figure 5: Response surface plot for the effect of inlet reactor temperature and reactor difference temperature profile

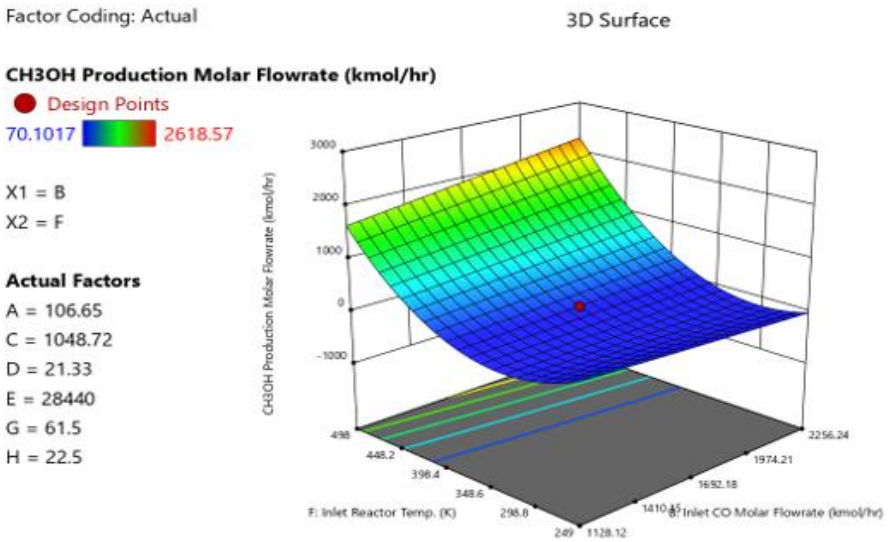

Figure 6: Response surface plot for the effect of inlet CO molar flowrate and inlet reactor temperature

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Similarly, it was discovered that methanol production increased as the reactor's inlet temperature increased. The maximum amount of methanol produced by the reactor was 2,618.57 kmol/hour. Increasing the temperature of the reactor's inlet would cause the reaction (Equation 3) to move to the right because of the endothermic process [16]. Thus, CO_2 would be used up more, resulting in a higher conversion rate at a lower temperature than CO. With the ongoing rise in the reactor's temperature, a larger quantity of CO would be produced and available within the reactor. A high amount of carbon dioxide in the reactor would accelerate the shift of reaction (Equation 1) to the right, producing a greater quantity of methanol, and the conversion of CO to methanol would increase substantially as the reactor temperature rose.

4.5 Optimisation of Reactor Parameters for Methanol Production

The optimal conditions of independent variables with a desirable response goal, methanol production, were identified using numerical optimisation in DE software. Figure 7 depicts the predicted value of inlet molar flowrates (CO, CO_2, H_2O, H_2, CH_3OH) and the three reactor conditions (inlet temperature, pressure, and temperature profile) from methanol production optimisation using RSM.

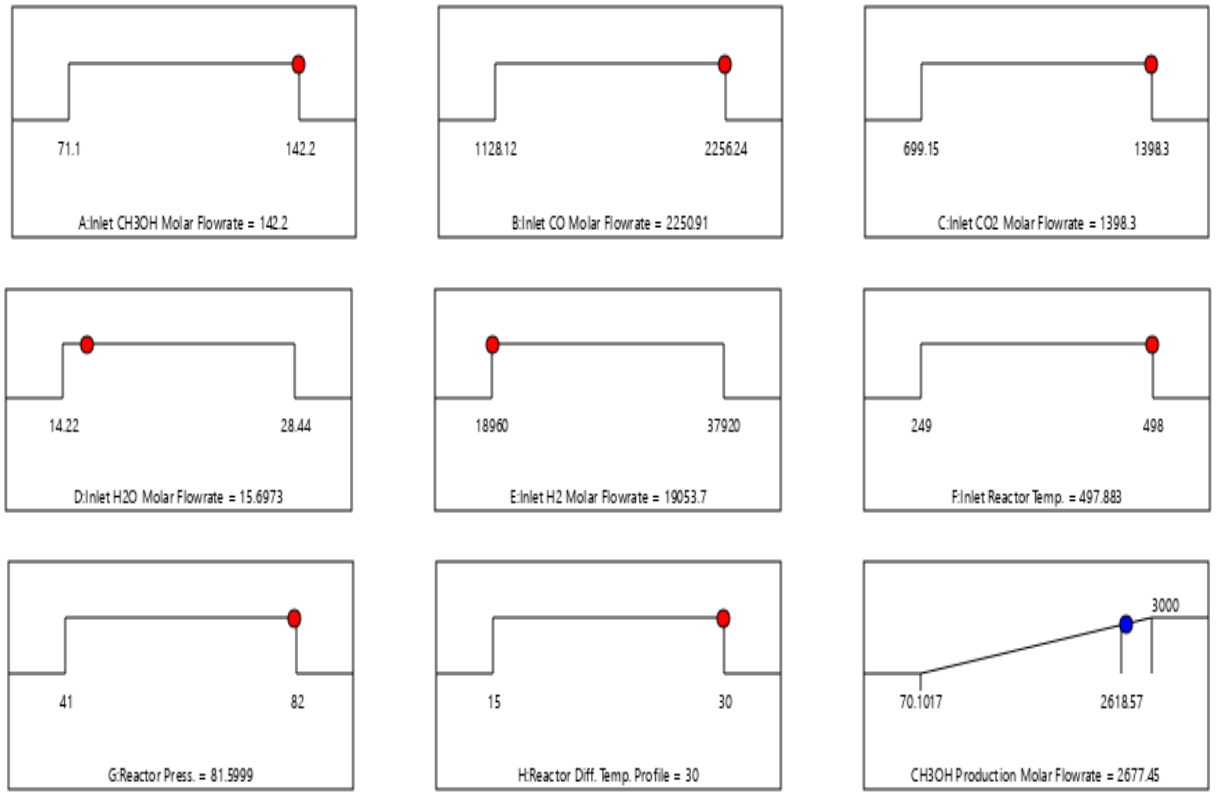

Figure 7: The ramping line (numerical) of the suggested optimum parameters and predicted optimum response (CH_3OH Production Molar Flowrate, which is the methanol production)

A validation run simulation was performed to confirm the optimal prediction's adequacy, yielding a methanol production molar flowrate of 2,814.23 kmol/hr. The error percentage difference was less than 5.2%, demonstrating the model's reliability. Consequently, the proposed model was accurate and satisfactory.

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5. CONCLUSIONS

This study was able to determine the optimal conditions for maximising methanol production from a methanol reactor using Design Expert modelling. Among the eight investigated parameters, inlet CO molar flowrate, inlet reactor temperature, the interaction between the inlet CO molar flowrate and the inlet reactor temperature, and the interaction between the inlet reactor temperature itself were the most important (P-values 0.0001) in methanol production, followed by the interaction between inlet reactor temperature and reactor pressure, inlet CH_3OH molar flowrate, reactor pressure, and interaction between inlet reactor temperature and reactor difference temperature profiling. RSM generated the following optimal conditions: inlet CH_3OH molar flowrate of 142.2 kmol/hr, inlet CO molar flowrate of 2250.91 kmol/hr, inlet CO_2 molar flowrate of 1398.3 kmol/hr, inlet H_2O molar flowrate of 15.6973 kmol/hr, inlet H_2 molar flowrate of 19053.7 kmol/hr, 497.883 K of reactor inlet temperature, 81.9999 bar of reactor pressure, and 30 K for reactor temperature profile. Under these conditions, the predicted methanol production was 2,677.45 kmol/h. The simulation utilised the generated optimal conditions for validation, resulting in an optimal methanol production rate of 2,814.23 kmol/hr, as opposed to 2,775 kmol/hr for the unoptimised rate. Overall, most optimised conditions were reduced, especially the inlet H_2 molar flowrate, which was reduced by 49.8% compared to unoptimised industry conditions. It is also suggested that future optimisation efforts in methanol production should consider the H_2/CO_2 ratio, carbon dioxide conversion, and methanol selectivity in addition to reactor temperature, pressure, and molar flowrate.

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CONFLICT OF INTEREST

The authors declare no conflicts of interest in publishing this paper. Authors have the option to disclose any potential conflicts of interest.

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