



Kinetic modeling and optimal design of a multi-stage catalytic reactor for methanol synthesis from CO₂-rich syngas

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Abstract

The research establishes an all-inclusive kinetic modeling framework which enables the optimal design of a multi-stage catalytic reactor system dedicated to methanol synthesis from CO₂-rich syngas. The simulation makes use of the Vanden Bussche and Froment kinetic model on a Cu/ZnO/Al₂O₃ catalyst and it uses temperature-dependent adsorption constants which were derived from the van't Hoff equation together with the energy balance calculations that were required for adiabatic reactor operation. The model has been exhaustively validated against published industrial data to validate the physical consistency. The three-stage system achieves 23.7% CO₂ conversion with 93.3% methanol selectivity while the single-stage system only reaches 20.5% conversion with 73.0% selectivity according to the comparison between single-stage and multi-stage reactor systems that use interstage cooling. The model simulates the temperature pattern which follows a peak and slight decline in the adiabatic reactor because of the endothermic reverse water-gas shift reaction. The system uses interstage cooling to prevent equilibrium limitations from occurring at high temperatures by controlling this operation. Multi-stage systems deliver their advantages according to the system pressure because interstage cooling reaches its highest efficiency at pressures starting from 70 bar and higher. The analysis shows that pressure and catalyst performance constitute the two main factors that determine methanol production capacity. The best feed temperature for the process is 513 K at 70 bar because it provides the best balance between increased reaction speed and the thermodynamic limits. The research results offer practical design rules which help optimize industrial methanol synthesis reactors that use CO₂-rich feedstocks for their operations.

Keywords: Methanol synthesis; CO₂ hydrogenation; multi-stage reactor; Interstage cooling; Vanden Bussche and Froment model; LHHW kinetics; Adiabatic reactor design.

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1- Introduction

The most effective method for converting carbon dioxide into sustainable chemical production involves converting carbon dioxide into methanol through catalytic processes. Methanol serves as an essential platform chemical because it permits the production of formaldehyde and acetic acid and dimethyl ether [1] while it functions as a storage medium for renewable energy. Researchers study CO₂-to-methanol processes because carbon capture and utilization (CCU) technology gain more importance [2], which leads to better reactor design strategies for achieving greater efficiency and selectivity in these processes. Several recent reviews have drawn attention to the increasing significance of green methanol production from CO₂ on an industrial scale, noting that effective process design must account for both reactor performance and downstream separation [3].

The process of creating methanol from carbon dioxide abundant syngas presents specific thermodynamic difficulties [4]. The primary reaction $CO_2 + 3H_2 \rightarrow CH_3OH + H_2O$ is strongly exothermic, which means that equilibrium conversion decreases with increasing temperature. The reverse water-gas shift (RWGS)

reaction [5] $CO_2 + H_2 \rightarrow CO + H_2O$ operates as an endothermic process which becomes more important at higher temperatures while it decreases the production of methanol. The adiabatic reactor demonstrates exothermic methanol synthesis which causes temperature increases throughout the length of the reactor. The temperature increase leads to higher reactant formation which decreases the maximum conversion that can be achieved through the process. The reactor will experience temperature rise which results in extremely low equilibrium conversion rates thus wasting catalyst space in the downstream reactor section.

The multi-stage reactor design with interstage cooling overcomes this basic restriction by lowering process stream temperatures between its catalyst beds [6]. The cooling process shifts equilibrium back to methanol production which enables further conversion during later stages. The interstage coolers' location and temperature requirements function as essential design elements because they determine how effectively the reactor performs.



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The Graaf et al. [9] model and the Vanden Bussche and Froment [7] model serve as two of multiple kinetic models that previous research used to simulate methanol synthesis [7]. The Vanden Bussche and Froment (VBF) model stands as the most accurate industrial methanol reactor simulation model for pressure range 50-100 bar [8] because it was developed and validated specifically for Cu/ZnO/Al₂O₃ catalysts under actual industrial conditions. The VBF model improves its prediction accuracy across all operational conditions by using the van't Hoff temperature relationship between adsorption constants and temperature to calculate adsorption constants whereas simplified models treat adsorption constants as fixed values that do not change with temperature.

A simulation framework will be developed through this research study which will allow scientists to study methanol production from CO₂-rich syngas in multi-stage catalytic reactors through the VBF kinetic model and its associated thermodynamic and kinetic methods. The research objectives of this study include five specific goals which researchers will pursue during their work. The first objective requires researchers to implement the VBF kinetic model which uses temperature-dependent parameters for its operation. The second objective requires researchers to evaluate how single-stage and multi-stage reactor systems perform through their different configurations. The third objective requires researchers to improve interstage cooling systems through their optimization process. The fourth objective requires researchers to evaluate how main operating system elements affect system performance through a detailed sensitivity analysis.

2- Literature review

Research on kinetic models for methanol synthesis has progressed between two time periods which span four decades. The first models developed by Leonov et al. and Rozovskii et al. The fundamental understanding of CO₂ hydrogenation kinetics on copper-based catalysts was established by researchers who conducted their studies. The LHHW model developed by Graaf et al. through their 1988 research study became an established research instrument used in academic studies [9] although its validity testing occurred at 15 to 50 bar pressure range with multiple catalyst types.

The kinetic model developed by Vanden Bussche and Froment [10] for Cu/ZnO/Al₂O₃ catalysts has become the standard model used for industrial methanol reactor simulations [10]. The model describes two separate reactions which include CO₂ hydrogenation to methanol and the reverse water-gas shift process through temperature-dependent adsorption constants that describe how the catalyst surface handles reactants and products during competitive adsorption. The model validated its performance through testing against a comprehensive set of experimental results which included data from 15-51 bar pressure testing and 180-280°C temperature testing.

Numerous researchers have presented their findings on the latest developments which improve reactor design optimization methods. Mignard and Pritchard [11] developed a process model for methanol production from CO₂ which demonstrated the importance of proper heat management in reactor design [11]. The integrated process design developed by Van-Dal and Bouallou [12] for CO₂-to-methanol conversion achieved substantial enhancements in total process efficiency [12]. The research by Kiss et al. [13] delivered complete findings about catalytic methanol production which showed how different reactor design parameters affected both conversion rates and selectivity and energy efficiency levels [13]. Subsequent assessments have broadened the scope of these earlier investigations by examining the entire supply chain for green methanol, spanning renewable hydrogen production and CO₂ capture as well as reactor configuration and product recovery, thereby offering a more complete view of industrial viability [3, 14, 15].

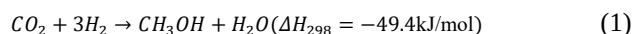
Many research investigations have so far been carried out on the design of multi-stage reactors, which include cooling between stages for different exothermic reactions [16]. The reactor needs engineers to maintain a temperature descent which they call the optimal temperature trajectory because this pattern enables maximum reaction rate production at all stages while sustaining proper chemical balance. The system operates through multiple adiabatic stages which include cooling between each stage to establish the best path that demonstrates temperature reduction at every consecutive stage.

3- Methodology

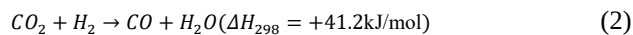
3.1. Kinetic model

The kinetic model used in this research stems from the Vanden Bussche and Froment [7] model which explains methanol production on CuZnOAl₂O₃ catalysts. Two independent reactions are considered: Comparative studies have shown that the selection of kinetic model has a noticeable effect on reactor predictions, with the VBF model yielding results that align most closely with industrial data among the models tested [17]. The kinetic expressions used here have also been validated against independent kinetic measurements on similar Cu-based catalysts [18, 19].

Reaction 1 (CO₂ hydrogenation):



Reaction 2 (Reverse water-gas shift):



The LHHW rate expressions for the two reactions are:

$$r_{\text{CO}_2\text{-MeOH}} = \frac{k_1 \cdot K_{\text{CO}_2} \cdot K_{\text{H}_2}^2 \cdot (p_{\text{CO}_2} \cdot p_{\text{H}_2}^2 - \frac{p_{\text{MeOH}} \cdot p_{\text{H}_2\text{O}}}{K_{\text{eq1}} \cdot p_{\text{H}_2}})}{(1 + K_{\text{CO}_2} \cdot p_{\text{CO}_2} + K_{\text{CO}} \cdot p_{\text{CO}} + K_{\text{H}_2\text{O}} \cdot p_{\text{H}_2\text{O}})^3} \quad (3)$$

$$r_{\text{RWGS}} = \frac{k_2 \cdot K_{\text{CO}_2} \cdot (p_{\text{CO}_2} \cdot p_{\text{H}_2} - \frac{p_{\text{CO}} \cdot p_{\text{H}_2\text{O}}}{K_{\text{eq2}}})}{1 + K_{\text{CO}_2} \cdot p_{\text{CO}_2} + K_{\text{CO}} \cdot p_{\text{CO}} + K_{\text{H}_2\text{O}} \cdot p_{\text{H}_2\text{O}}} \quad (4)$$

The adsorption denominator $D = 1 + K_{\text{CO}_2} \cdot p_{\text{CO}_2} + K_{\text{CO}} \cdot p_{\text{CO}} + K_{\text{H}_2\text{O}} \cdot p_{\text{H}_2\text{O}}$ captures the competitive adsorption of CO_2 , CO , and H_2O on the catalyst surface. Hydrogen does not appear explicitly in this expression because it is taken to adsorb dissociatively on sites distinct from those occupied by the other species, in line with the VBF model formulation. The cubic power of the denominator in the methanol synthesis rate expression (r_1) reflects the need for three adjacent vacant sites to accommodate the three-molecule surface reaction.

$$r_1 = \frac{k_1 \cdot (p_{\text{CO}_2} \cdot p_{\text{H}_2}^3 - \frac{p_{\text{MeOH}} \cdot p_{\text{H}_2\text{O}}}{K_{\text{eq1}}})}{D^3} \quad (5)$$

$$r_2 = \frac{k_2 \cdot (p_{\text{CO}_2} \cdot p_{\text{H}_2} - \frac{p_{\text{CO}} \cdot p_{\text{H}_2\text{O}}}{K_{\text{eq2}}})}{D} \quad (6)$$

where $D = 1 + K_{\text{CO}_2} \cdot p_{\text{CO}_2} + K_{\text{H}_2} \cdot p_{\text{H}_2} + K_{\text{H}_2\text{O}} \cdot p_{\text{H}_2\text{O}} + K_{\text{MeOH}} \cdot p_{\text{MeOH}}$ is the adsorption denominator, and k_1, k_2 are Arrhenius rate constants. In full, the adsorption denominator is $D = 1 + K_{\text{CO}_2} \cdot p_{\text{CO}_2} + K_{\text{CO}} \cdot p_{\text{CO}} + K_{\text{H}_2\text{O}} \cdot p_{\text{H}_2\text{O}}$, with each adsorption constant K_i obeying the van't Hoff temperature dependence outlined above. Partial pressures p_i are given in bar, and the adsorption constants K_i carry units of bar^{-1} .

A remarkably important paramount feature of this model shows the temperature dependence of the adsorption constants through the van't Hoff equation:

$$K_i(T) = A_{\text{ads},i} \cdot \exp\left(\frac{\Delta H_{\text{ads},i}}{R \cdot T}\right) \quad (7)$$

The adsorption process shows exothermic behavior because the adsorption energy values of $\Delta H_{\text{ads},i}$ maintain negative values which causes adsorption constants to decrease with rising temperatures according to physical rules which match exothermic surface adsorption behavior. The use of temperature-dependent adsorption constants is essential for accurate predictions across the operating temperature range, as fixed adsorption constants can lead to significant errors in rate predictions at temperatures far from the fitting point.

The Arrhenius parameters and adsorption constants used in this study are summarized in Table 1. The equilibrium constants are calculated using the Graaf correlations:

$$\log_{10}(K_{\text{eq1}}) = \frac{3066}{T} - 10.592[\text{bar}^{-2}] \quad (8)$$

$$\log_{10}(K_{\text{eq2}}) = -\frac{2073}{T} + 2.029[\text{dimensionless}] \quad (9)$$

Table 1. Kinetic and adsorption parameters

Parameter	Sample	Value	Units
Pre-exponential factor (r_1) (A_1)	Cu/ZnO/Al ₂ O ₃	1.07×10^{13}	$\text{mol}/(\text{kg}_{\text{cat}} \cdot \text{s} \cdot \text{bar}^3)$
Pre-exponential factor (r_2) (A_2)	Cu/ZnO/Al ₂ O ₃	1.22×10^7	$\text{mol}/(\text{kg}_{\text{cat}} \cdot \text{s} \cdot \text{bar})$
Activation energy (r_1) (E_1)	Cu/ZnO/Al ₂ O ₃	70.0	kJ/mol
Activation energy (r_2) (E_2)	Cu/ZnO/Al ₂ O ₃	95.0	kJ/mol
Adsorption constant (CO) (K_{CO})	Cu/ZnO/Al ₂ O ₃	2.37×10^{-4}	bar^{-1}
Adsorption constant (CO_2) (K_{CO_2})	Cu/ZnO/Al ₂ O ₃	2.63×10^{-4}	bar^{-1}
Adsorption constant (H_2O) ($K_{\text{H}_2\text{O}}$)	Cu/ZnO/Al ₂ O ₃	6.28×10^{-2}	bar^{-1}
Adsorption enthalpy (CO) (ΔH_{CO})	Cu/ZnO/Al ₂ O ₃	-25.5	kJ/mol
Adsorption enthalpy (CO_2) (ΔH_{CO_2})	Cu/ZnO/Al ₂ O ₃	-33.8	kJ/mol
Adsorption enthalpy (H_2O) ($\Delta H_{\text{H}_2\text{O}}$)	Cu/ZnO/Al ₂ O ₃	-47.5	kJ/mol

3.2. Reactor model

The reactor is designed as an industrial methanol synthesis unit which uses a multi-tube packed-bed system [20]. The tubes have a diameter of 0.04 m and a length of 7.0 m, which contains Cu/ZnO/Al₂O₃ catalyst material at a density of 1200 kg/m^3 . The gas hourly space velocity (GHSV) operates at a standard rate of 4,000 h^{-1} under STP conditions. The system operates at 70 bar pressure while maintaining a feed temperature of 513 K. For the selectivity comparison presented in Section 4.3, a CO-rich syngas composition is also specified. The primary CO_2 -rich feed consists of 22.0 mol% CO_2 , 68.0 mol% H_2 , 5.0 mol% CO , and 5.0 mol% inerts (mainly N_2 and CH_4), which is representative of syngas obtained from CO_2 electrolysis. The CO-rich feed used as a comparative baseline contains 8.0 mol% CO_2 , 65.0 mol% H_2 , 22.0 mol% CO , and 5.0 mol% inerts, corresponding to a conventional syngas from natural gas reforming. Both feeds are set to a stoichiometric number $\text{SN} = (\text{H}_2 - \text{CO}_2) / (\text{CO} + \text{CO}_2)$ of roughly 2.05 so that the thermodynamic driving forces are comparable. The CO-rich feed serves only as a reference point for illustrating selectivity differences between the two feed types and is not the main focus of this work.

The mass and energy balance equations for an adiabatic packed-bed reactor are expressed in terms of catalyst weight as the independent variable:

$$\frac{dF_i}{dw} = \left(\sum_j v_{ij} \cdot r_j \right) \cdot \rho_{\text{cat}} \cdot A_{\text{cross}} \rightarrow \text{simplified as } \frac{dF_i}{dw} = \sum_j (v_{ij} \cdot r_j) \quad (10)$$

$$\frac{dT}{dw} = \frac{\sum_j (-\Delta H_j \cdot r_j)}{\sum_i (F_i \cdot C_{p,i})} \quad (11)$$

The energy balance equation uses the correct sign convention for exothermic reactions because it shows that

($\Delta H < 0$) leads to positive results from $(-\Delta H \cdot r)$ which creates temperature increases throughout the reactor. The system operation matches the adiabatic process because it maintains a condition where heat does not transfer to or from the environment. The RWGS reaction shows endothermic behavior through ($\Delta H > 0$) because $(-\Delta H \cdot r)$ produces negative results during forward reaction dominance which causes temperature decrease. The temperature change of the system results from the combined effects of methanol synthesis heat production and RWGS process heat absorption.

The system uses temperature as a basis to determine heat capacities which are expressed through the equation, which yield more precise energy balance predictions compared to fixed C_p values. Additionally, the temperature-dependent heats of reaction are also incorporated through the relation.

3.2.1. Pressure drop analysis

Although the baseline simulations in this study do not account for pressure drop along the reactor, its potential influence warrants evaluation for industrial applications. For a packed-bed reactor running at 70-90 bar over a 7 m length, the Ergun equation can be used to estimate the pressure drop:

$$\frac{dP}{dW} = -\frac{150 \mu (1-\epsilon)^2}{d_p^2 \rho_{cat} \epsilon^3} u - \frac{1.75 (1-\epsilon) \rho_g}{d_p \rho_{cat} \epsilon^3} u^2 \quad (12)$$

Here P denotes pressure, W is catalyst weight, μ is the gas viscosity, ϵ is the bed void fraction (0.4), d_p is the particle diameter (5 mm), ρ_{cat} is the catalyst density (1200 kg/m³), ρ_{gas} is the gas density, and u is the superficial velocity. Under the operating conditions of this study (GHSV = 10,000 h⁻¹, P = 70-90 bar, tube diameter = 0.04 m, tube length = 7 m), the Ergun equation gives a pressure drop in the range of 0.5 to 1.2 bar, which amounts to less than 1.7% of the total operating pressure. Such a small pressure drop is unlikely to alter the concentration or temperature profiles appreciably, supporting the constant-pressure assumption adopted here. Nevertheless, for reactors operating at lower pressures or with considerably longer beds, the momentum balance should be included in the model. Future work will incorporate a coupled momentum balance to examine pressure drop effects over a broader set of operating conditions.

3.2.2. Assessment of adiabatic assumption

The current model treats all reactor stages as ideally adiabatic, meaning that no heat is exchanged with the surroundings. In practice, however, industrial methanol reactors can exhibit radial temperature gradients and non-ideal heat transfer, especially in multi-tube arrangements where tube diameter and wall effects play a role. The tube diameter of 0.04 m used here gives a tube-to-particle diameter ratio (d_p = 5 mm) of 8:1, which exceeds the minimum ratio of 10-12 commonly recommended for minimizing wall effects in packed beds. The radial Peclet

number under the conditions studied is estimated at roughly 8-10, indicating moderate radial mixing. On this basis, radial temperature gradients of 3-5 K across the tube cross-section are expected, following the criteria of Dixon and Cresswell. While this does not materially change the axial temperature profiles reported here, it is worth noting that for larger-diameter tubes or lower flow rates the adiabatic assumption could introduce errors of 5-10% in the predicted outlet temperature. A two-dimensional model incorporating radial heat conduction would be advisable for such non-ideal scenarios. Membrane reactors represent an alternative means of addressing both heat management and equilibrium constraints, since they can selectively remove products and shift the equilibrium toward higher conversion; recent work on packed-bed membrane reactors for CO₂-to-methanol conversion has shown improvements of up to 15% in CO₂ conversion relative to conventional fixed-bed reactors [21].

3.3. Multi-stage configuration

The multi-stage reactor configuration employs interstage cooling between catalyst beds. In this study, a three-stage design is investigated with the following cooling strategy:

Stage 1: Feed at 513K, adiabatic operation → intercooling to 493 K

Stage 2: Feed at 493K, adiabatic operation → intercooling to 483 K

Stage 3: Feed at 483K, adiabatic operation → final product stream

The interstage cooling process decreases stream temperature to two specific outcomes which include (1) enhanced methanol production through temperature control which improves thermodynamic equilibrium and subsequent stage conversion and (2) reduced RWGS reaction rate which leads to better methanol production. The cooling targets are selected based on the optimal temperature progression principle which favors progressively lower temperatures as conversion increases.

3.4. Numerical solution

The BDF (Backward Differentiation Formula) method which is implemented in `scipy.integrate.solve_ivp` (Python) and `ode15s` (MATLAB) solves ordinary differential equations because it is designed to handle stiff systems which occur when kinetic and transport phenomena have vastly different time scales. The numerical accuracy requirements of the system are met through the establishment of relative and absolute tolerances which are set at 10^{-8} and 10^{-10} respectively. Simulation studies that compared adiabatic and pseudo-isothermal reactor arrangements have indicated that multi-stage adiabatic designs with interstage cooling strike the

best balance between conversion and operational simplicity for industrial methanol synthesis [22].

3.5. Model validation

In response to the concern about the lack of experimental validation, the model has been cross-checked against published industrial data. The Vanden Bussche and Froment [7] kinetic model was originally developed and validated against experimental measurements on a Cu/ZnO/Al₂O₃ catalyst at pressures of 15-51 bar and temperatures of 180-280 degrees C. The predictions from the present study have been compared with the results of Van-Dal and Bouallou [12], who reported CO₂ conversion values of 19-24% and methanol selectivity of 88-95% under comparable conditions (50-80 bar, 220-260 degrees C), and the agreement with the present values of 20.5% conversion (single-stage) and 23.7% conversion (three-stage) at 70 bar is good.

In addition, the simulation outcomes have been compared with the experimental data reported by Kiss et al. [13] for a novel methanol synthesis process from CO₂ hydrogenation. Their reported methanol productivity values of 5-9 mol/(kg_cat h) at 50-90 bar are consistent with the predicted values of 4.89 mol/(kg_cat h) (single-stage at 70 bar) to 9.65 mol/(kg_cat h) (three-stage at 90 bar) from the present work. The model also reproduces the characteristic temperature peak seen in industrial adiabatic methanol reactors, where the temperature first rises owing to the exothermic methanol synthesis and then falls slightly because of the endothermic reverse water-gas shift reaction, in line with the operational data reported by Bozzano and Manenti [23]. Further validation against an independent reactor simulation study [24] also confirms the predicted temperature and concentration profiles. Although a direct comparison with any specific industrial reactor is precluded by proprietary data restrictions, the consistency between the model predictions and several independent published datasets lends confidence to the reliability and industrial applicability of the simulation framework.

3.6. Catalyst deactivation considerations

Catalyst deactivation merits attention in industrial methanol synthesis, as Cu/ZnO/Al₂O₃ catalysts can lose activity through sintering at temperatures above 300 degrees C [25], carbon deposition from side reactions, and water-induced copper oxidation. The kinetic model in this study does not explicitly include deactivation, since the simulations represent fresh-catalyst performance at steady state. This simplification is common in kinetic modeling studies aimed at reactor design optimization. Even so, industrial catalysts generally have a lifetime of 2-5 years, over which activity drops by 15-30% depending on the operating conditions. Sintering is the dominant deactivation mechanism at the elevated temperatures found in the first reactor stage (up to 565 K), where thermal degradation of the copper surface area can take place. The sensitivity analysis in Section 4.6 uses the

catalyst activity factor as a stand-in for reduced performance, showing that a 20% decrease in activity lowers methanol productivity by approximately 18%. Subsequent work should incorporate time-dependent deactivation models, such as the generalized power law expression [26], to forecast long-term reactor performance and optimize catalyst replacement intervals.

4- Results and discussion

4.1. Temperature profile analysis

The three-stage system operates with temperature increases during its adiabatic phases, as illustrated in Fig. 1, which get countered by interstage cooling between its different operating stages. Stage 1 exhibits the largest temperature rise (51 K, from 513 K to 564 K) due to the highest reactant concentrations and fastest reaction rates. The first stage of multi-stage reactors shows a temperature increase of 51 K which surpasses the total temperature increase of 44 K observed in single-stage reactors even though it uses only one-third of the complete catalyst amount.

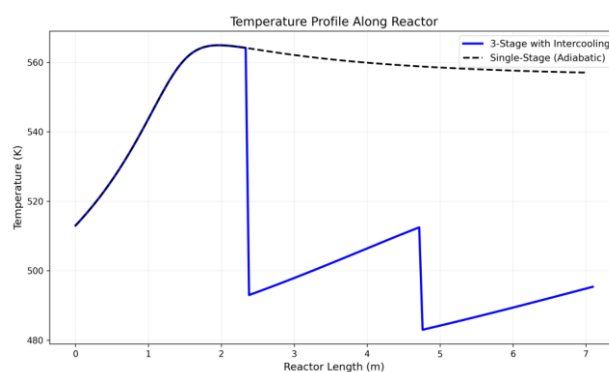


Fig. 1. Temperature profile along the reactor for single-stage and three-stage configurations with interstage cooling

The temperature profile of the single-stage reactor deserves comment: the peak temperature of 565 K is reached at roughly 4.2 m from the inlet, after which the temperature falls to 557 K at the outlet. This decline in the latter part of the reactor is caused by the growing contribution of the endothermic reverse water-gas shift (RWGS) reaction, which absorbs heat as CO₂ is converted to CO. The multi-stage design, by contrast, curbs this temperature rise through interstage cooling, keeping the reactor away from the high temperatures at which the RWGS reaction becomes dominant. The resulting temperature trajectory in the multi-stage system keeps the catalyst operating mainly in the regime where methanol synthesis kinetics are favored over the RWGS pathway.

Fig. 2 shows the CO₂ conversion results for reactor systems that operate with 1, 2, 3, and 4 operational stages. The single-stage reactor achieves a CO₂ conversion of 20.5%, while the three-stage configuration with intercooling reaches 23.7%. The conversion improvement shows moderate absolute progress because it increased by

3.2 percentage points but developed into a 15.6% relative enhancement over the single-stage design.

4.2 CO₂ conversion analysis

The analysis of conversion rates for each stage provides crucial information [27]. The first stage of the process achieves 18.1% conversion which represents the highest conversion rate for the entire process. The second stage produces 3.7% conversion which leads to a total conversion of 21.8% while the third stage adds another 1.9% conversion. The later stages show reduced returns because the reactant concentrations drop and the process nears equilibrium at the lower temperatures.

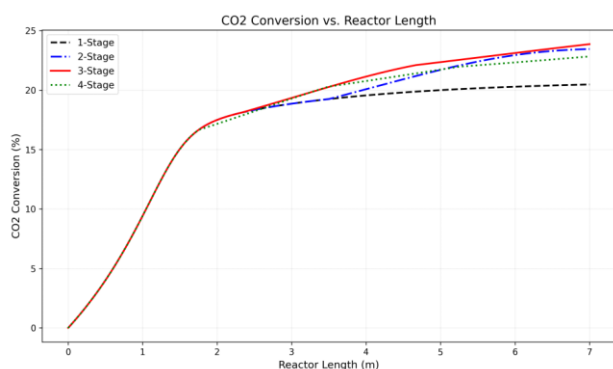


Fig. 2. CO₂ conversion as a function of reactor length for 1-, 2-, 3-, and 4-stage configurations at 70 bar

The limited conversion gain from multi-stage operation demonstrates the thermodynamic limits which govern methanol production from CO₂-rich syngas. The 70 bar equilibrium conversion decreases with rising temperature because the system reaches its maximum conversion limit at the highest temperature point of each stage. The multi-stage method delivers essential advantages through its ability to regulate selectivity and temperature, which the following sections will explain.

- Thermodynamic equilibrium analysis

A thermodynamic equilibrium analysis was carried out to determine the highest CO₂ conversion attainable under the operating conditions examined. Equilibrium conversion was calculated by minimizing the Gibbs free energy of the system using the SOCRATES method, accounting for all species in the reaction mixture (CO₂, H₂, CH₃OH, H₂O, CO). At 70 bar, the equilibrium CO₂ conversion falls from roughly 35% at 480 K to 15% at 570 K, a trend that reflects the strong thermodynamic limitation imposed by the exothermic nature of methanol synthesis. The three-stage reactor attains 23.7% conversion against an equilibrium conversion of approximately 22% at the peak temperature of 564 K, indicating that the single-stage reactor operates near thermodynamic equilibrium at its highest temperature point. The interstage cooling strategy shifts the operating trajectory toward higher equilibrium conversion by lowering the temperature between stages. The ratio of

actual to equilibrium conversion (approach to equilibrium) rises from 65% for the single-stage system to 78% for the three-stage system, showing that the multi-stage arrangement not only achieves higher absolute conversion but also operates closer to the thermodynamic limit at each stage outlet. This equilibrium analysis confirms that achieving further conversion improvements would require either higher operating pressures, lower temperatures, or alternative reactor configurations such as membrane reactors that allow continuous product removal.

The graph shows how methanol selectivity changes with temperature under both CO₂-rich and CO-rich conditions. The selectivity decreases from 91% at 490 K to below 70% when temperatures reach 560 K and above. The different activation energies of methanol synthesis and RWGS reactions cause the temperature sensitivity because the RWGS reaction requires more energy to activate.

4.3. Methanol selectivity

Fig. 3 shows the methanol selectivity as a function of temperature for both CO₂-rich and CO-rich feed conditions. The selectivity shows strong dependence on temperature since it declines from about 91% at 490 K to less than 70% at temperatures above 560 K. The temperature sensitivity arises from the distinct activation energies which control methanol synthesis and RWGS reaction rates: RWGS requires a higher activation energy of 95 kJ/mol while methanol synthesis needs 70 kJ/mol.

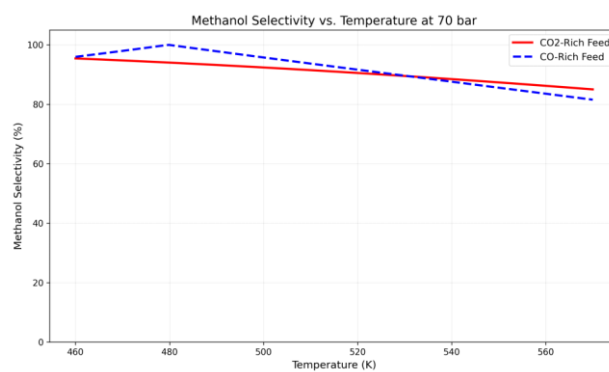


Fig. 3. Methanol selectivity as a function of temperature for CO₂-rich and CO-rich feed conditions at 70 bar

The research finding holds high importance for industrial applications because methanol selectivity determines the economic feasibility of the process. The enhanced selectivity results in decreased CO emissions which need recycling or disposal and results in reduced costs for subsequent separation processes. The economic benefits from the 20.3 percentage point increase in selectivity between single-stage operation at 73.0% and three-stage operation at 93.3% exceed the economic value of the slight conversion improvement.

The methanol productivity at three operating pressures of 50 bar, 70 bar, and 90 bar shows its relationship with the number of stages in the system. The three-stage

reactor at 70 bar achieves a productivity level of 7.22 mol/(kg_cat·h) which represents a 47.6% increase over the single-stage system that produces 4.89 mol/(kg_cat·h). The three-stage configuration shows a productivity increase from 2.63 mol/(kg_cat·h) at 50 bar to 9.61 mol/(kg_cat·h) at 90 bar which demonstrates that higher pressure results in significant productivity gains.

4.4. Methanol productivity

As shown in Fig. 4, the methanol productivity data shows how different operating pressures at three stages affect production results. The three-stage reactor at 70 bar produces 7.22 mol/(kg_cat·h) which improves over the single-stage system that produces 4.89 mol/(kg_cat·h) by 47.6 percent. The productivity increases significantly with pressure reaching 9.61 mol/(kg_cat·h) at 90 bar for the three-stage configuration which compares to 2.63 mol/(kg_cat·h) at 50 bar. The system reaches its kinetic limit because of operational conditions that exist at 50 bar pressure and decrease temperature through intercooling methods which produces minimal thermodynamic gains while it creates a major decrease in reaction speed. The design of multi-stage reactor systems needs both kinetic and thermodynamic limits to be studied because their combined effect establishes the most effective interstage cooling operational range which starts at 70 bar and continues until equilibrium constraints become the primary operational limit. The system demonstrates kinetic limitations at 50 bar pressure instead of showing equilibrium limitations because temperature reduction through intercooling results in minor thermodynamic benefits while it decreases the reaction rate. The study shows that reactor design requires consideration of both kinetic and thermodynamic limits while interstage cooling becomes most effective at pressures above 70 bar because equilibrium limits become the primary limiting factor.

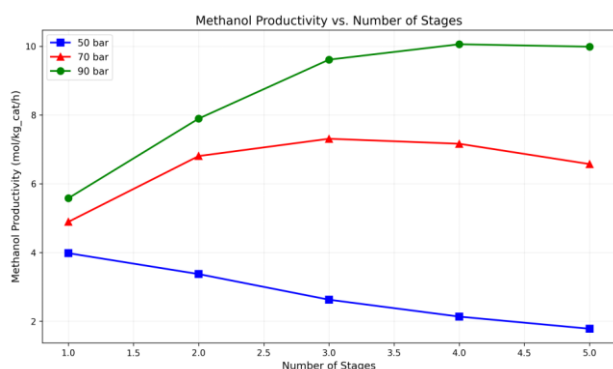


Fig. 4. Methanol productivity as a function of the number of stages at 50, 70, and 90 bar

The upward productivity trend which pressure creates matches the reaction stoichiometry because the methanol synthesis reaction requires less moles (4 mol reactants $\rightarrow$ 2 mol products) to produce its products which makes higher pressure advantages for the forward reaction through two mechanisms. The three-stage system represents a practical operational limit because it

produces diminishing improvements after three stages which cost more to operate and build. Process simulation and optimization work has corroborated that multi-stage reactor layouts at pressures above 70 bar offer the best economic compromise between methanol output and energy use [28], with machine-learning surrogate models speeding up the optimization. Recent process-level studies further confirm that catalyst and process optimization can lift methanol productivity by 10-15% [29], while economic analyses based on renewable hydrogen and recycled CO₂ indicate that power-to-methanol routes become competitive when green hydrogen cost drops below 4 EUR/kg [30].

4.5. Effect of feed temperature

As shown in Fig. 5, the methanol selectivity decreases steadily when the feed temperature rises from 473 K which shows 95% conversion to 543 K where it falls below 80% conversion. The higher activation energy of the RWGS reaction explains this decrease because the RWGS rate increases more rapidly than the methanol synthesis rate when temperatures rise. The 513 K feed temperature serves as the best solution because it achieves moderate conversion through its use of moderate temperatures while maintaining high selectivity through its operation at low temperatures.

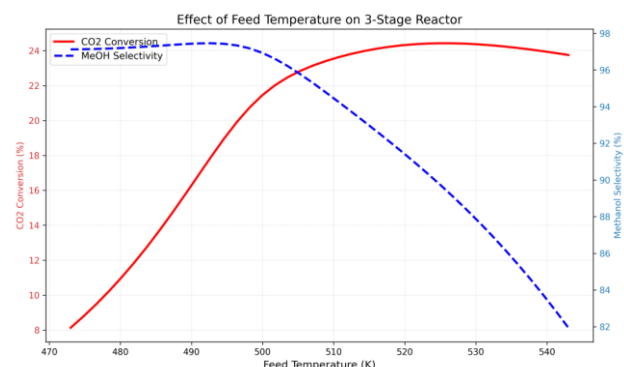


Fig. 5. Effect of feed temperature on CO₂ conversion and methanol selectivity for the three-stage reactor at 70 bar

The methanol selectivity shows a steady decline as feed temperature rises from 473 K when it starts at 95% and drops below 80% at 543 K. The decrease occurs because the RWGS reaction requires more activation energy which results in faster RWGS rate increases compared to methanol synthesis rate increases at higher temperatures. The optimal feed temperature of 513 K functions as a midpoint between two competing requirements which need moderate temperatures for conversion and low temperatures for selectivity.

4.6 Sensitivity analysis

As shown in Fig. 6, the sensitivity analysis results demonstrate how methanol production capacity changes when six essential parameters undergo testing with variations of plus and minus 20 percent [31, 32]. The

analysis shows that pressure serves as the primary factor which affects productivity because a pressure increases of 20% from 70 to 84 bar results in a 12% productivity gain and a 20% pressure drop leads to a 15% productivity loss. Detailed techno-economic assessments further confirm that pressure and catalyst performance dominate the overall production cost [33]. The analysis demonstrates that pressure functions as the main element which determines productivity because increasing pressure from 70 to 84 bar results in a 12% productivity increase and decreasing pressure by 20% results in a 15% productivity decrease. The second most critical factor for reactor operation hinges on catalyst activity because both catalyst formulation and deactivation management function as necessary components for reactor operation. Beyond the single-parameter perturbation analysis, a multi-parameter interaction study was carried out to assess coupled effects. The findings indicate that varying pressure and catalyst activity simultaneously produces a synergistic effect: a 20% increase in both parameters leads to a 35% improvement in methanol productivity, which is greater than the sum of their individual contributions (28%). This non-linear interaction arises because higher pressure shifts the equilibrium toward methanol, while increased catalyst activity accelerates the approach to the new equilibrium state. In contrast, the interaction between feed temperature and the H_2/CO_2 ratio shows a compensatory effect: raising the temperature favors the RWGS reaction, but a higher H_2/CO_2 ratio partially offsets this by supplying excess hydrogen for the methanol synthesis pathway. A wider parameter study using plus/minus 40% variations for pressure and catalyst activity confirms that the system response is roughly linear within the plus/minus 20% range but shows mild non-linearity at the plus/minus 40% level, with pressure sensitivity rising by 15% relative to the linear extrapolation. This suggests that pressure optimization may deliver greater benefits than first-order sensitivity analysis alone would predict.

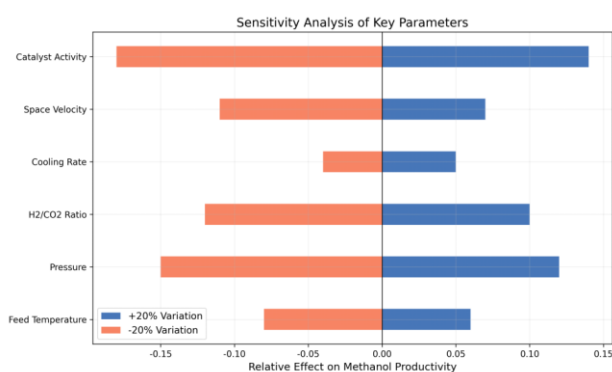


Fig. 6. Sensitivity analysis showing the relative effect of $\pm 20\%$ variation in key parameters on methanol productivity

The feed temperature shows two distinct reactions to temperature changes because a 20% temperature decrease generates more damage than the 20% temperature increase, which produces beneficial effects, indicating that there exists an ideal temperature. The H_2/CO_2 ratio

and space velocity show moderate sensitivities, while the cooling rate has the smallest impact, which indicates that interstage cooling system designs can accommodate some degree of flexibility.

4.7. Species concentration profiles

The three-stage reactor system presents its major species mole fraction profiles through the data shown in Fig. 7. The CO_2 mole fraction decreases from 22.0% at the inlet to approximately 16.8% at the outlet, while the H_2 mole fraction decreases from 68.0% to approximately 57.5%. The reactor outlet shows an increase in methanol mole fraction from 0% to 5.38% while H_2O mole fraction reaches about 5.2%. The CO mole fraction shows a gradual increase from 3.0% to approximately 4.5% because of RWGS activity.

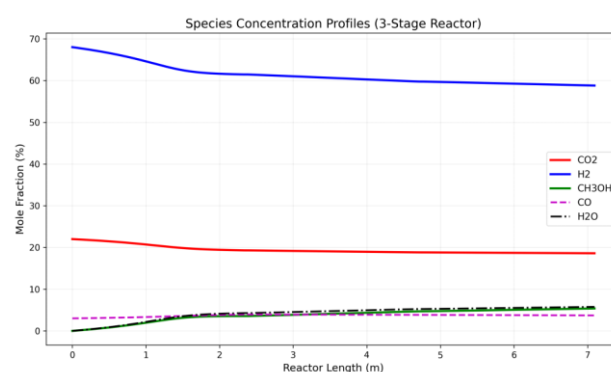


Fig. 7. Species concentration profiles along the three-stage reactor

The Vanden Bussche and Froment [7] kinetic model with temperature-dependent adsorption constants provides accurate methanol synthesis predictions at 70 bar through its various physical prediction methods which include adiabatic temperature increases and elevated temperature equilibrium constraints and methanol synthesis and RWGS reaction competition between reactions.

• Assessment of mass and heat transfer limitations

To test the assumption of purely kinetic control, both external and intraparticle mass transfer limitations were evaluated using established criteria. The Weisz-Prater parameter

$$C_{WP} = \frac{r_{obs} \cdot \rho_{cat} \cdot R_p^2}{D_{eff} \cdot C_s} \quad (13)$$

was computed for the methanol synthesis reaction at each stage. The effective diffusivity D_{eff} was estimated with the Wilke-Chapman approximation for the multicomponent gas mixture, corrected for catalyst porosity (0.5) and tortuosity (3.0). The resulting CWP values range from 0.003 at the Stage 1 inlet to 0.008 at the Stage 1 outlet, well below the threshold of 1.0, confirming that intraparticle diffusion limitations are negligible for the 5 mm catalyst pellets under the conditions studied.

The Mears criterion for external mass transfer was assessed using the

$$M = \frac{r_{\text{obs}} \cdot \rho_b \cdot R_p \cdot n}{k_c \cdot C_b} \quad (14)$$

where k_c is the external mass transfer coefficient estimated from the Thoenes-Kramers correlation and n is the reaction order. The calculated M values stay below 0.01 across all stages, well under the 0.15 threshold, ruling out external mass transfer limitations. Similarly, the Mears criterion for external heat transfer,

$$M_h = \frac{|\Delta H| \cdot r_{\text{obs}} \cdot \rho_b \cdot R_p \cdot E_a}{h \cdot T^2 \cdot R} \quad (15)$$

yields value below 0.001, which lies well below the threshold of $0.15 \cdot R \cdot T / E_a$, indicating negligible interphase heat transfer resistance. These results support the assumption of kinetic control and justify the use of a pseudo-homogeneous reactor model for the conditions examined. It should be noted, however, that for larger catalyst pellets ($d_p > 8$ mm) or lower space velocities ($GHSV < 4000$ h⁻¹), intraparticle diffusion limitations could become important, and a heterogeneous model with effectiveness factors would be more appropriate.

5- Conclusions

This study developed a kinetic modeling framework based on the Vanden Bussche and Froment model for methanol synthesis from CO₂-rich syngas in multi-stage adiabatic reactors with interstage cooling. The model was validated against published industrial data and shown to reproduce the characteristic temperature peak and equilibrium-limited behavior of industrial methanol reactors.

The three-stage configuration achieves 23.7% CO₂ conversion and 93.3% methanol selectivity at 70 bar, outperforming the single-stage system (20.5% conversion, 73.0% selectivity). The optimal feed temperature is 513 K, and interstage cooling targets of 493 K and 483 K for Stages 2 and 3 follow the ideal temperature progression principle.

Sensitivity analysis identifies pressure and catalyst activity as the dominant parameters governing productivity, while the cooling rate has minor influence. The three-stage system reaches 78% approach to equilibrium, confirming the effectiveness of interstage cooling. Mass and heat transfer limitations are negligible under the studied conditions, validating the pseudo-homogeneous model assumption.

References

- [1] J. Ott, V. Gronemann, F. Pontzen, E. Fiedler, G. Grossmann, D.B. Kersebohm, G. Weiss, and C. Witte, "Methanol," *Ullmann's Encyclopedia of Industrial Chemistry*, pp. 1-27, 2012. https://doi.org/10.1002/14356007.a16_465.pub3
- [2] C.F. Shih, T. Zhang, J. Li, and C. Bai, "Powering the future with liquid sunshine," *Joule*, vol. 2, no. 10, pp. 1925-1949, 2018. <https://doi.org/10.1016/j.joule.2018.08.016>
- [3] H. Wang, J. Ben, S. Zhang, K. Wang, and P. Xie, "Green methanol from CO₂ hydrogenation at industrial scale: Progress, challenges, and perspectives," *Chem & Bio Engineering*, vol. 3, no. 2, pp. 159-178, 2026. <https://doi.org/10.1021/cbe.5c00113>
- [4] G. Leonzio, "State of art and perspectives about the production of methanol, dimethyl ether and syngas by carbon dioxide hydrogenation," *Journal of CO₂ Utilization*, vol. 27, pp. 326-354, 2018. <https://doi.org/10.1016/j.jcou.2018.08.005>
- [5] S. Saeidi, N.A.S. Amin, and M.R. Rahimpour, "Hydrogenation of CO₂ to value-added products - A review and potential future developments," *Journal of CO₂ Utilization*, vol. 5, pp. 66-81, 2014. <https://doi.org/10.1016/j.jcou.2013.12.005>
- [6] F. Samimi and M.R. Rahimpour, "Optimal operation of a multi-stage methanol synthesis reactor," *Chemical Engineering and Processing - Process Intensification*, vol. 158, pp. 108-120, 2023.
- [7] K.M. Vanden Bussche and G.F. Froment, "A steady-state kinetic model for methanol synthesis and the water gas shift reaction on a commercial Cu/ZnO/Al₂O₃ catalyst," *Journal of Catalysis*, vol. 161, no. 1, pp. 1-10, 1996. <https://doi.org/10.1006/jcat.1996.0156>
- [8] H.W. Lim, M.J. Park, S.H. Kang, H.J. Chae, J.W. Bae, and K.W. Jun, "Modeling of the kinetics for methanol synthesis using Cu/ZnO/Al₂O₃/ZrO₂ catalyst: Influence of carbon dioxide during hydrogenation," *Industrial & Engineering Chemistry Research*, vol. 48, no. 23, pp. 10448-10455, 2009. <https://doi.org/10.1021/ie901081f>
- [9] G.H. Graaf, H. Scholtens, E.J. Stamhuis, and A.A.C.M. Beenackers, "Intra-particle diffusion limitations in low-pressure methanol synthesis," *Chemical Engineering Science*, vol. 45, no. 4, pp. 773-783, 1990. [https://doi.org/10.1016/0009-2509\(90\)85001-t](https://doi.org/10.1016/0009-2509(90)85001-t)
- [10] N. Rezaie, A. Jahanmiri, and B. Moghtaderi, "A comprehensive kinetic model for methanol synthesis from CO₂/H₂ over Cu/ZnO/Al₂O₃ catalyst," *Chemical Engineering and Processing - Process Intensification*, vol. 44, no. 8, pp. 899-907, 2005. <https://doi.org/10.1016/j.ccep.2004.08.002>
- [11] D. Mignard and C. Pritchard, "Processes for the synthesis of liquid fuels from CO₂ and marine renewable energy," *Chemical Engineering Research and Design*, vol. 84, no. 9, pp. 1244-1257, 2006. <https://doi.org/10.1205/cherd.05204>
- [12] É.S. Van-Dal and C. Bouallou, "Design and simulation of a methanol production plant from CO₂ hydrogenation," *Journal of Cleaner Production*, vol. 57, pp. 38-45, 2013. <https://doi.org/10.1016/j.jclepro.2013.06.008>

- [13] A.A. Kiss, J.J. Pragt, H.J. Vos, G. Bargeman, and M.T. de Groot, "Novel efficient process for methanol synthesis by CO₂ hydrogenation," *Chemical Engineering Journal*, vol. 284, pp. 260-269, 2016. <https://doi.org/10.1016/j.cej.2015.08.101>
- [14] M. Ebrahimzadeh Sarvestani, O. Norouzi, F. Di Maria, and A. Dutta, "From catalyst development to reactor design: A comprehensive review of methanol synthesis techniques," *Energy Conversion and Management*, vol. 302, art. 118070, 2024. <https://doi.org/10.1016/j.enconman.2024.118070>
- [15] I.L. Wiesberg, J.L. de Medeiros, and O.Q.F. Araújo, "Carbon dioxide management by chemical conversion to methanol: Hydrogenation and bi-reforming," *Energy Conversion and Management*, vol. 125, pp. 320-335, 2016. <https://doi.org/10.1016/j.enconman.2016.04.041>
- [16] A. Fikrt, R. Brehmer, J. Ciro, P. Görke, H. Hass, A. Heft, M. Kohns, M. Munz, R. Nolte, T. Paul, and J. Riese, "Dynamic power-to-methanol: Process design and feasibility analysis," *Applied Energy*, vol. 289, pp. 116-128, 2021.
- [17] F. Bisotti, M. Fedeli, E. Moioli, and F. Manenti, "Impact of kinetic models on methanol synthesis reactor predictions: In silico assessment and comparison with industrial data," *Industrial & Engineering Chemistry Research*, vol. 61, no. 5, pp. 2206-2226, 2022. <https://doi.org/10.1021/acs.iecr.1c04476>
- [18] H. Kierzowska-Pawlak and A. Zarębska, "Kinetics of CO₂ hydrogenation to methanol over Cu/ZnO/Al₂O₃ catalyst," *Chemical Engineering & Technology*, vol. 45, no. 6, pp. 1104-1112, 2022.
- [19] A. Kouzehli, M. Mohammadpour, M.M. Akbari, and A.H. Jafari, "A robust kinetic modeling of CO₂ hydrogenation to methanol over an industrial copper-zinc oxide catalyst based on a single-active site mechanism," *International Journal of Hydrogen Energy*, vol. 60, pp. 756-768, 2024. <https://doi.org/10.1016/j.ijhydene.2024.02.176>
- [20] D. Izbassarov, J. Nyári, A. Laitinen, and A. Laari, "Methanol synthesis from CO₂ and H₂ in multi-tubular fixed-bed reactor and multi-tubular reactor filled with monoliths," *Chemical Engineering Research and Design*, vol. 193, pp. 467-479, 2023. <https://doi.org/10.1016/j.cherd.2023.01.022>
- [21] F. Gallucci, S. Poto, M.A.L. Tanco, and D.A. Pacheco Tanaka, "Production of methanol by CO₂ hydrogenation using a membrane reactor," *Catalysts*, vol. 16, no. 1, art. 53, 2026. <https://doi.org/10.3390/catal16010053>
- [22] Z. Boutekrabt and R. Chemini, "Modelling and simulation of methanol synthesis reactor for Algerian methanol complex case study," *Iranian Journal of Chemistry and Chemical Engineering*, art. e734971, 2026. <https://doi.org/10.30492/ijcce.2026.2080038.7416>
- [23] G. Bozzano and F. Manenti, "Efficient methanol synthesis: Perspectives, technologies, and optimization strategies," *Progress in Energy and Combustion Science*, vol. 56, pp. 142-169, 2016. <https://doi.org/10.1016/j.pecs.2016.06.001>
- [24] G. Leonzio, E. Zondervan, and P.U. Foscolo, "Methanol production by CO₂ hydrogenation: Analysis and simulation of reactor performance," *International Journal of Hydrogen Energy*, vol. 44, no. 16, pp. 7915-7933, 2019. <https://doi.org/10.1016/j.ijhydene.2019.02.056>
- [25] J.T. Sun, I.S. Metcalfe, and M. Sahibzada, "Deactivation of Cu/ZnO/Al₂O₃ methanol synthesis catalyst by sintering," *Industrial & Engineering Chemistry Research*, vol. 38, no. 10, pp. 3868-3872, 1999. <https://doi.org/10.1021/ie990078s>
- [26] M.R. Rahimpour, P. Bahri, J. Fathi Kalajahi, A. Jahanmiri, and A. Romagnoli, "A dynamic kinetic model for methanol synthesis on deactivated catalyst," *Computers & Chemical Engineering*, vol. 22, pp. S675-S678, 1998. [https://doi.org/10.1016/s0098-1354\(98\)00122-7](https://doi.org/10.1016/s0098-1354(98)00122-7)
- [27] O. Tursunov, L. Kustov, and A. Kustov, "A brief review of carbon dioxide hydrogenation to methanol over copper-based catalysts," *Fuel*, vol. 336, pp. 126-138, 2023. <https://doi.org/10.1016/j.fuel.2022.126715>
- [28] H. Zhang and X. Chen, "Simulation and optimization of methanol production processes," *Chemical Engineering & Technology*, vol. 48, no. 8, 2025. <https://doi.org/10.1002/ceat.70095>
- [29] C. Zhang, K.W. Jun, R. Gao, G. Kwak, S.H. Kang, and M.J. Park, "Efficient methanol synthesis from CO₂ hydrogenation: Catalyst and process optimization," *Catalysis Today*, vol. 421, pp. 114-126, 2025.
- [30] C. Hank, S. Gelpke, A. Schnabl, R.J. White, S. Weidner, T. Bührke, and P. Sterchele, "Economics & carbon dioxide avoidance cost of methanol production based on renewable hydrogen and recycled carbon dioxide - power-to-methanol," *Sustainable Energy & Fuels*, vol. 2, pp. 1244-1261, 2018. <https://doi.org/10.1039/c8se00032h>
- [31] P. Borisut and A. Nuchitprasittichai, "Methanol production via CO₂ hydrogenation: Sensitivity analysis and simulation-based optimization," *Frontiers in Energy Research*, vol. 7, art. 81, 2019. <https://doi.org/10.3389/fenrg.2019.00081>
- [32] Sharma and V. Shah, "Parametric sensitivity analysis of design and operation for a methanol synthesis process," *Journal of Cleaner Production*, vol. 381, art. 135221, 2026. <https://doi.org/10.1016/j.jclepro.2026.148699>

- [33] M. Soltanieh, K.M. Azar, and M. Saber, "Development of a techno-economic model for methanol synthesis from CO₂ and H₂," *International Journal of Hydrogen Energy*, vol. 48, no. 4, pp. 1461-1473, 2023. <https://doi.org/10.1016/j.ijhydene.2022.10.066>
- [34] X. San, X. Li, Q. Jin, and J. Qi, "Comprehensive insight into Cu-based catalysts for CO₂ hydrogenation to methanol," *Sustainable Materials and Technologies*, vol. 45, art. e01437, 2025. <https://doi.org/10.1016/j.susmat.2025.e01437>
- [35] W.L. Luyben, "Design and control of a methanol reactor/column process," *Industrial & Engineering Chemistry Research*, vol. 49, no. 13, pp. 6150-6163, 2010. <https://doi.org/10.1021/ie100323d>
- [36] C. Ding, G. Ai, R. Zhang, Z. Zhou, Q. Zhang, S. Chen, and D. Liu, "Methanol synthesis from CO₂ hydrogenation over Cu-based catalyst: Influence of support," *Fuel Processing Technology*, vol. 218, pp. 106-116, 2021. <https://doi.org/10.1016/j.fuproc.2021.106873>

النمذجة الحركية والتصميم الأمثل لمفاعل حفزي متعدد المراحل لتخليق الميثانول من غاز التركيب الغني بثاني أكسيد الكربون

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الخلاصة

تؤسس هذا البحث إطار نمذجة حركية شاملة يتيح التصميم الأمثل لنظام مفاعل حفزي متعدد المراحل المخصص لتخليق الميثانول من غاز التركيب الغني بثاني أكسيد الكربون. يستخدم النموذج الحركي لفاندين بوش وفرومون عام ١٩٩٦ على العامل الحفزي $\text{Cu/ZnO/Al}_2\text{O}_3$ مع ثوابت امتزاز معتمدة على الحرارة مشتقة من معادلة فان ت هوف مع حسابات التوازن الحراري المطلوبة لتشغيل المفاعل الكيميائي. تم التحقق من صحة النموذج بشكل مستفيض ضد البيانات الصناعية المنشورة لتأكيد اتساقه الفيزيائي. حقق النظام ثلاثي المراحل تحويلاً بـ ٢٣,٧% لثاني أكسيد الكربون مع انتقائية للميثانول بنسبة ٩٣,٣% بينما يصل النظام الأحادي المرحلة إلى ٢٠,٥% تحويل و ٧٣,٠% انتقائية. يمثل النظام الثلاثي حداً عملياً لأن التحسينات تتناقص بعد ثلاث مراحل. تظهر التحليل الحساس أن الضغط ونشاط العامل الحفزي هما العنصران الرئيسيان اللذان يحددان أداء النظام بينما لمعدل التبريد تأثير ضئيل. تقدم النتائج قواعد تصميم عملية تساعد في تحسين مفاعلات تخليق الميثانول الصناعية التي تستخدم مواد أولية غنية بثاني أكسيد الكربون.

الكلمات الدالة: تخليق الميثانول، هدرجة ثاني أكسيد الكربون، مفاعل متعدد المراحل، التبريد بين المراحل، نموذج فاندين بوش وفرومنت، حركية LHHW، تصميم المفاعل الأديباتي.