

Modeling and Simulation of Membrane Reactor for Carbondioxide Capturing from Flue Gas

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Abstract The increasing concentration of carbon dioxide (CO₂) in industrial flue gas has intensified the need for efficient and energy-conscious carbon capture technologies. Membrane reactors provide an attractive alternative to conventional separation processes by integrating chemical reaction and selective membrane separation within a single process unit. This study presents the steady-state mathematical modelling and simulation of a water–gas shift (WGS) membrane reactor for CO₂ capture from simulated flue gas. The feed mixture consisted of CO, H₂O, CO₂, H₂ and N₂ with mole fractions of 0.244734, 0.491474, 0.056169, 0.190572 and 0.017051, respectively. The model was formulated using component material balances, WGS reaction kinetics, membrane permeation relationships and an energy balance to describe the coupled reaction–separation behaviour of the reactor. The steady-state isothermal simulation predicted a CO conversion of 57.57% and H₂O conversion of 28.24%, demonstrating substantial progress of the WGS reaction. The membrane exhibited highly effective CO₂ separation, achieving a CO₂ recovery of 99.97%, while the CO₂ concentration remaining in the retentate was only 0.19527 mol%. The reported H₂ recovery was 75.64%, with H₂ in the permeate corresponding to 0.33103 mol%, indicating effective retention of hydrogen under the simulated operating conditions. The component profiles showed a progressive decrease in CO and H₂O mole fractions and corresponding increases in CO₂ and H₂ along the reactor, while N₂ exhibited only a slight increase in mole fraction because of its essentially inert behaviour and the reduction in total retentate flow caused by membrane separation. The isothermal energy-balance simulation predicted a slight increase in temperature from 855K at the reactor inlet to 859.96K at the outlet, corresponding to a relatively small temperature rise of 4.96 K. This result indicates that the reactor operates under near-isothermal conditions despite the exothermic nature of the WGS reaction. Model validation against published results showed reasonable agreement, with the predicted CO₂ recovery of 99.97% compared with 97.62% reported in the reference study, while H₂ recovery was 75.64% compared with 77.23%. The results demonstrate that the integration of WGS reaction and selective membrane separation can provide highly effective CO₂ capture while supporting hydrogen production. The developed steady-state model therefore provides a useful computational framework for evaluating membrane-reactor performance and for optimizing operating and membrane parameters for integrated CO₂ capture and hydrogen recovery systems.

Keywords: Membrane Reactor, Steady State, Water–Gas Shift Reaction, Hydrogen Recovery

1.0 Introduction

The continuous increase in carbon dioxide (CO₂) emissions from fossil-fuel combustion, power generation, and industrial activities has intensified the need for efficient carbon capture technologies. Post-combustion capture is particularly important because it can be integrated with existing industrial facilities without major modifications to the primary energy-conversion systems. However, conventional absorption and adsorption processes are associated with high energy consumption, solvent or adsorbent requirements, equipment complexity, and regeneration costs. These limitations have encouraged the development of membrane-based technologies as alternative approaches for CO₂ separation and capture [1, 3]. Membrane technology has attracted considerable interest because of its compact equipment requirements, modularity, continuous operation, and potentially lower energy consumption compared with conventional separation processes. Membrane gas separation has been extensively investigated for industrial applications, particularly for the separation of CO₂ from gas mixtures [2 - 4]. For post-combustion applications,

membrane processes offer the possibility of separating CO₂ directly from flue gas without the phase-change requirements associated with conventional solvent-based systems. [5] demonstrated the potential of membrane technology for post-combustion CO₂ capture and highlighted the importance of membrane permeability, selectivity, pressure ratio, and process configuration. Despite these advantages, CO₂ separation from flue gas remains challenging because flue gas generally contains a relatively low concentration of CO₂ and is dominated by nitrogen. Consequently, membranes must possess sufficient CO₂ permeability and CO₂/N₂ selectivity to achieve effective separation. The development of suitable membrane materials has therefore become an important area of research, with polymeric, inorganic, mixed-matrix, and other advanced membrane materials being investigated for CO₂ separation [6]. Recent studies have further demonstrated the continuing development of membrane materials and configurations for post-combustion CO₂ capture [7-8]. An alternative approach to improving CO₂ capture performance is the integration of membrane separation with chemical reaction. This configuration, commonly referred to as a membrane reactor, combines reaction and separation within a single process unit. The simultaneous occurrence of reaction and selective product removal can improve reactor performance by continuously removing one or more products from the reaction environment. This principle is particularly relevant to the water-gas shift (WGS) reaction, represented by $\text{CO} + \text{H}_2\text{O} \rightleftharpoons \text{CO}_2 + \text{H}_2$. The WGS reaction is important in hydrogen production because it converts carbon monoxide into carbon dioxide while producing additional hydrogen. Its equilibrium-limited nature makes it suitable for integration with membrane separation [9]. In a WGS membrane reactor, selective removal of hydrogen or carbon dioxide can shift the reaction equilibrium toward the products, thereby increasing CO conversion. Mathematical models have therefore been developed to describe the interaction between WGS reaction kinetics and membrane permeation. [10] developed a non-isothermal model for a WGS membrane reactor and demonstrated the importance of thermal behaviour in determining reactor performance. Similarly, [11] developed a model for a CO₂-selective WGS membrane reactor and investigated the effects of operating conditions on reaction and separation performance.

The modelling of membrane reactors is particularly important because reactor performance depends on the simultaneous interaction of chemical kinetics, thermodynamic equilibrium, membrane transport, temperature, pressure, and gas composition. Lotric *et al.* and Mendes *et al.* demonstrated that mathematical modelling could successfully describe the behaviour of a catalytic membrane reactor for the WGS reaction. Their results showed that operating pressure and membrane characteristics significantly influence CO conversion and hydrogen recovery [12, 13]. Merkel *et al.* and Wang *et al.* further demonstrated the importance of considering phenomena occurring at different scales when modelling WGS membrane reactors [14, 15]. Temperature is another important operating parameter because it influences both reaction kinetics and membrane permeation. The WGS reaction is exothermic, and changes in temperature can affect the equilibrium composition as well as the reaction rate. Consequently, the assumption of constant temperature may not always adequately represent actual membrane-reactor behaviour. Non-isothermal modelling has therefore been applied to account for the coupling between reaction, heat transfer, and membrane separation [16, 17]. Such models provide a more comprehensive representation of reactor behaviour than models based solely on reaction kinetics or membrane transport. The influence of membrane characteristics and operating conditions has also been investigated through detailed numerical models. Factors such as membrane area, membrane thickness, feed pressure, permeate pressure, temperature, sweep-gas flow rate, and feed

composition can significantly influence reactor performance [18]. Liu *et al.* demonstrated the potential of WGS membrane reactors for integrated gasification systems with CO₂ capture, while other studies have shown that membrane-assisted WGS can achieve enhanced conversion and hydrogen recovery compared with conventional reactors [19]. Mathematical modelling and simulation provide an effective means of investigating these complex interactions without the extensive experimental resources required for evaluating every possible operating condition. Process models can be used to predict concentration profiles, conversion, recovery, permeate composition, retentate composition, and the influence of operating parameters. Modelling and simulation have therefore become important tools for the design and analysis of membrane-based separation systems [20, 21]. Recent developments have also focused specifically on CO₂-selective membrane reactors. Studies involving ceramic-carbonate dual-phase membranes have demonstrated that selective CO₂ removal can enhance WGS conversion while simultaneously producing a hydrogen-rich stream. Such systems provide an attractive route for combining carbon capture and hydrogen production in a single process configuration. Recent modelling studies have investigated the effects of temperature, feed composition, pressure, gas hourly space velocity, membrane area, and sweep conditions on the performance of these reactors [22, 23]. Although considerable research has been conducted on membrane materials, hydrogen-selective membrane reactors, CO₂ separation, and detailed computational models, there remains a need for practical steady-state models that can clearly describe the coupled reaction–separation behaviour of membrane reactors for CO₂ capture from flue gas. Many existing studies focus on experimental membrane development, highly detailed computational fluid dynamics, catalyst-pellet-scale modelling, or complete process and economic assessments. A relatively simple but sufficiently rigorous steady-state mathematical framework can provide an important basis for evaluating reactor performance and identifying favourable operating conditions. Therefore, this study focuses on the steady-state modelling and simulation of a membrane reactor for CO₂ capture from flue gas. The model incorporates component material balances, WGS reaction kinetics, and selective membrane permeation to describe the behaviour of the reactor under steady-state conditions. The developed model is used to investigate species concentration profiles, CO conversion, H₂O conversion, CO₂ recovery, H₂ recovery, permeate composition, and retentate composition. The effects of important operating conditions on reactor performance are also examined. The study provides a computational framework for understanding the interaction between chemical reaction and membrane separation and contributes to the development of membrane-reactor systems for efficient CO₂ capture and hydrogen recovery.

2.0 Materials and Methods

2.1 Materials

The materials and computational resources used in this study comprised a simulated flue-gas mixture containing CO₂, CO, H₂O, H₂, and N₂; a CO₂-selective membrane; and a suitable catalyst for the water–gas shift reaction. The principal model inputs included feed temperature, pressure, flow rate, composition, membrane area, membrane permeability, membrane selectivity, and WGS kinetic parameters. MATLAB was applied in solving the developed model and simulation of the steady-state membrane-reactor system.

2.2 Methods

The method adopted in this study involved the development and simulation of a steady-state mathematical model of a membrane reactor for CO₂ capture from flue gas. The model was

formulated using component material balances, water–gas shift (WGS) reaction kinetics, and membrane permeation relationships. Relevant operating and membrane parameters were obtained from published literature and used as model inputs. The resulting nonlinear equations were solved numerically using MATLAB to predict the concentration profiles and performance of the reactor. The effects of selected operating conditions on CO₂ recovery, CO conversion, H₂ recovery, and permeate and retentate compositions were subsequently evaluated to assess the effectiveness of the membrane-reactor configuration for CO₂ capture.

2.2.1 Kinetic Model Water Gas Shift Membrane Reaction

The kinetic model of the membrane reactor can be developed as follows:



i. Adsorption



ii. Surface Reaction



iii. Desorption



The water gas shift reaction is a reversible and moderately exothermic reaction. Consequently, temperature has an important influence on both the reaction kinetics and the thermodynamic equilibrium. Lower temperatures favour the equilibrium conversion of carbon monoxide to carbon dioxide and hydrogen, whereas higher temperatures increase the reaction rate. Industrially, the high-temperature water gas shift reaction is commonly operated within approximately 320–450°C using iron-based catalysts, while low-temperature water gas shift operation is generally conducted at lower temperatures using copper-based catalysts. For the present membrane reactor model, the operating conditions must provide a suitable balance between reaction kinetics, thermodynamic equilibrium, catalyst stability and membrane separation. A temperature range of approximately 350–450°C is therefore appropriate for a high-temperature WGS membrane reactor employing an iron-based catalyst. Experimental kinetic studies of commercial Fe-Cr WGS catalysts have been conducted at pressures of about 20 bar and temperatures between 350 and 450 °C, demonstrating the feasibility of these conditions for WGS operation.

2.2.2 Development of Steady State Model Equation

The schematic diagram of a water gas shift membrane reactor is shown in Figure 1

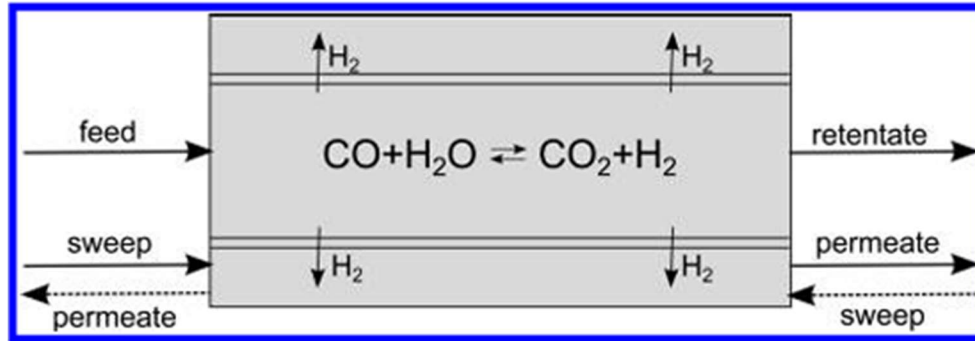


Figure 1: Water Gas Shift Membrane Reactor

Total Mass Balance

The general total and component mass balance expressions are depicted in Equations 6 and 7 respectively

$$\frac{\left(\text{Accumulation of total mass in the Membrane reactor} \right)}{\text{Time}} = \frac{\left(\text{Inflow of total mass into the membrane reactor} \right)}{\text{Time}} - \frac{\left(\text{Outflow of total mass from the membrane reactor} \right)}{\text{Time}} \quad (6)$$

Component Mass Balance

$$\begin{aligned} \frac{\left(\text{Accumulation of component mass in the Membrane reactor} \right)}{\text{Time}} &= \frac{\left(\text{Inflow of component mass into the membrane reactor} \right)}{\text{Time}} - \frac{\left(\text{Outflow of component mass from the membrane reactor} \right)}{\text{Time}} + \\ &\frac{\left(\text{Generation of component mass in the membrane reactor} \right)}{\text{Time}} \end{aligned} \quad (7)$$

For a steady state process and constant cross-sectional area of membrane reactor, Equation (7) becomes

$$\frac{dF}{dz} = -Ar_i \quad (8)$$

Thus for unit cross sectional area of membrane reactor, Equation 8 yields

$$\frac{dF}{dz} = -r_i \quad (9)$$

Equation (9) can be written in terms of CO, H₂O, CO₂, H₂ and N₂ components as

For CO component:

$$\frac{dF_{CO}}{dz} = -r_i \quad (10)$$

For H₂O component

$$\frac{dF_{H_2O}}{dz} = -r_i \quad (11)$$

For CO₂ component;

$$\frac{dF_{CO_2}}{dz} = r_i \quad (12)$$

For H₂ component;

$$\frac{dF_{H_2}}{dz} = r_i - J_{H_2} \quad (13)$$

For N₂ component

$$\frac{dF_{N_2}}{dz} = r_i \quad (14)$$

$$\text{Where } r = k \frac{(P_{CO} P_{H_2O} - (P_{CO_2} P_{H_2}))}{K_{eq}} \quad (15)$$

$$k = e^{\left(\frac{-47400}{RT}\right)} \quad (16)$$

$$K_{eq} = e^{\left(\frac{4577.8}{T} - 4.33\right)} \quad (17)$$

$$J_{H_2} = H_{2perm} \cdot P_{H_2}$$

$$P_i = \frac{F_i}{F_{total}} P \quad (18)$$

Where *i* stands for the components

2.2.3 General Differential Energy Balance (Retentate)

At steady state, the differential energy balance equation with no accumulation yields

$$\frac{d}{dz}(F\bar{h}) = Ua_m(T_s - T) - h_{H_2}(T)J_{H_2}a_m - \Delta H_r(T)rA \quad (19)$$

where *F* is total molar flow, $\bar{h} = \sum_i y_i h_i(T)$ is the mixture molar enthalpy, *U* is the overall heat-transfer coefficient, *a_m* is membrane area per unit length, *T* is the retentate temperature, *T_s* is the shell/permeate or jacket temperature at the membrane, *J_{H₂}* is the hydrogen permeation flux, *r* is the WGS reaction rate per reactor volume, *A* is the reactor cross-sectional area, and $\Delta H_r(T)$ is the reaction enthalpy (negative for exothermic WGS), *r* is the WGS rate (mol·m⁻³·s⁻¹), *A* is the tube cross-section *a_m* is membrane area per unit length, and *T_s* is the shell/permeate (or jacket) temperature at the membrane.

3.0 Results and Discussion

3.1 Flue Gas Characterization

The flue gas characterization results obtained from the study are presented in Table 1. The composition of the major constituents was determined and analyzed to establish the feed conditions

used for the membrane reactor modelling and simulation. The characterized components include CO, H₂O, CO₂, H₂, and N₂ provided the basis for evaluating the reaction and separation behaviour of the reactor.

Table 1: Characterization of Flue Gas

Constituent	Mole Fraction Composition (mol%)	
Carbon monoxide	0.244734	24.4734
Water vapour	0.491474	49.1474
Carbon dioxide	0.056169	5.6169
Hydrogen	0.190572	19.0572
Nitrogen	0.017051	1.7051
Total	1.000000	100.0000

The results showed that water vapour (H₂O) has the highest mole fraction of 0.491474, corresponding to 49.1474 mol% of the feed and carbon monoxide (CO) constitutes the second-largest component with a mole fraction of 0.244734 (24.4734 mol%). The relatively high concentrations of H₂O and CO are important because both species participate directly in the water-gas shift (WGS) reaction. Carbon dioxide (CO₂), which is the target species for capture in the study has a mole fraction of 0.056169 corresponding to 5.6169 mol%, Hydrogen (H₂) has a mole fraction of 0.190572 (19.0572 mol%) and represents a product of the WGS reaction as well as the permeating species through the selective membrane. Nitrogen (N₂) has the lowest mole fraction of 0.017051 (1.7051 mol%) and serves as an inert component in the reactor since it does not participate in the reaction or membrane permeation. Hence, the characterized feed has a total mole fraction of 1.000000, equivalent to 100.0000 mol%, indicating that the reported composition is normalized. These feed compositions were subsequently used as the basis for the modelling and simulation of the membrane reactor and for evaluating its reaction, separation and CO₂-capture performance.

3.2 Steady State Isothermal Membrane Results

The simulation results obtained for the membrane reactor operated isothermally using the water gas shift (WGS) reaction is presented in Table 2 for various parameters such as conversion of CO, H₂O, recovery of H₂ and CO₂, amount of H₂ and CO₂ left in the permeate and retentate respectively.

Table 2: Simulation Results for Steady State Isothermal Membrane Reactor

Parameter	Unit	Value
Conversion of CO	%	57.57
Conversion of H ₂ O	%	28.24
H ₂ Recovery	%	75.64
CO ₂ Recovery	%	99.97
H ₂ in Permeate	mol%	0.33103
CO ₂ in Retentate	mol%	0.19527

The simulation indicates effective coupling of reaction and separation as CO conversion (57.57%) alongside lower H₂O conversion (28.24%) reflects steam-excess operation and forward reaction shifting aided by in-situ CO₂ removal. Separation performance yielded CO₂ recovery of 99.97% with only 0.195 mol% CO₂ remaining in the retentate, yielding an H₂-rich retentate and a high-purity CO₂ permeate. The permeate contains just 0.331 mol% H₂, implying minimal hydrogen loss at the current operating point. The reported H₂ recovery” of 75.64% appears definition-sensitive (retentate retention vs. permeate capture) and is the only metric that may be misaligned with the very low H₂ found in the permeate; harmonizing recovery conventions will resolve this. Overall, the isothermal membrane configuration prioritizes near-total CO₂ capture while preserving H₂ in the retentate, suitable for decarbonized H₂ production with limited polishing. Performance can be tuned by clarifying recovery definitions, choosing the desired product side (retentate vs. permeate), and adjusting stage-cut, pressure ratio, or membrane selectivity to balance H₂ yield against CO₂ capture as needed.

3.3 Model Validation

Model validation is the process of comparing simulation or theoretical results with experimental data or well-established literature values to determine the accuracy, reliability, and predictive power of a model. In chemical engineering, particularly in membrane reactor modeling, validation ensures that the mathematical assumptions, reaction kinetics, transport phenomena, and boundary conditions used in simulations correctly represent real-world behavior.

Table 3: Model Validation for Steady State Isothermal Membrane Reactor			
Parameters	Units	Results	Fernando <i>et al.</i> (2024)
Conversion of CO	%	57.57	68.02
Conversion of H ₂ O	%	28.24	32.15
H ₂ Recovery	%	75.64	77.23
CO ₂ Recovery	%	99.97	97.62
H ₂ in Permeate	mol%	0.33103	0.4183
CO ₂ in Retentate	mol%	0.19527	0.2059

In Table 3, the CO conversion achieved in this study (57.57%) is lower than the 68.02% reported by Fernando *et al.* (2024). Similarly, H₂O conversion is also slightly lower (28.24% vs. 32.15%). However, H₂ and CO₂ recovery (75.64% and 99.97%, respectively) are very close to the reference values (77.23% and 97.62%). This indicates that while the current study (model) slightly underpredicts reactant conversions, it captures product recovery efficiently. The near match in CO₂ recovery shows that the separation and transport modules in the model are reliable, though catalytic reaction parameters may need refinement.

3.4 Variation of CO Mole Fraction Against Reactor Length

The variation of CO mole fractions along the membrane reactor length is depicted in Figure 2. The CO mole-fraction curve declines monotonically with a steep drop near the inlet and an asymptotic tail downstream, indicating fast initial reaction where reactant partial pressures and CO₂-removal driving force are highest, followed by a regime limited by diminishing kinetics, separation driving force, and proximity to equilibrium. The shape confirms effective coupling of reaction and in-situ CO₂ removal relative to a conventional PFR, sustaining conversion deeper into the bed.

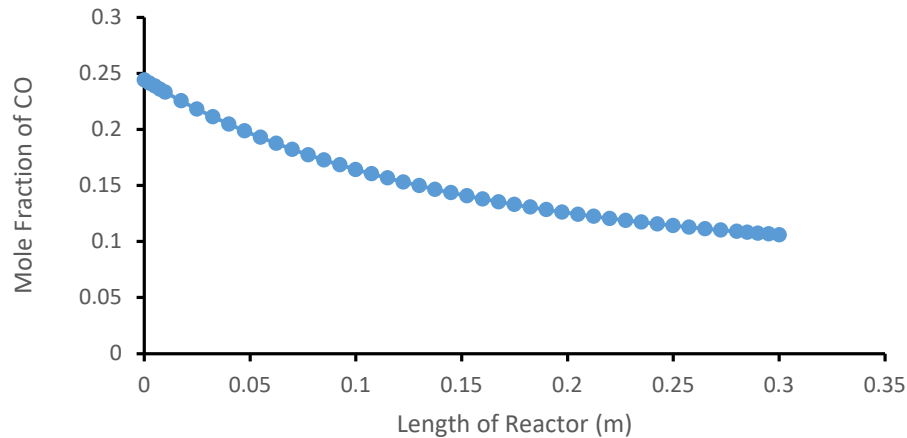


Figure 2: Mole Fraction of CO Versus Length of Reactor

Levers that steepen and depress the curve include stronger CO₂-selective driving force (lower permeate pressure, sweep, staged/graded membrane area), higher steam-to-CO ratio, greater residence time, and improved catalyst effectiveness, while levers that flatten it earlier include excessive temperature or weak downstream separation. Overall, the profile reflects strong front-end conversion with a low but non-zero outlet CO, and further reduction is best achieved by boosting downstream CO₂ removal and/or residence time rather than large upstream changes.

3.5 Variation of Water Vapour Mole Fraction Against Reactor Length

A similar pattern of Figure 2 with CO mole fraction is also experienced with water vapour mole fraction as shown in Figure 3. The H₂O mole-fraction curve declines monotonically with a steep drop near the inlet and an asymptotic tail downstream, indicating fast initial reaction where reactant partial pressures and CO₂-removal driving force are highest, followed by a regime limited by diminishing kinetics, separation driving force, and proximity to equilibrium

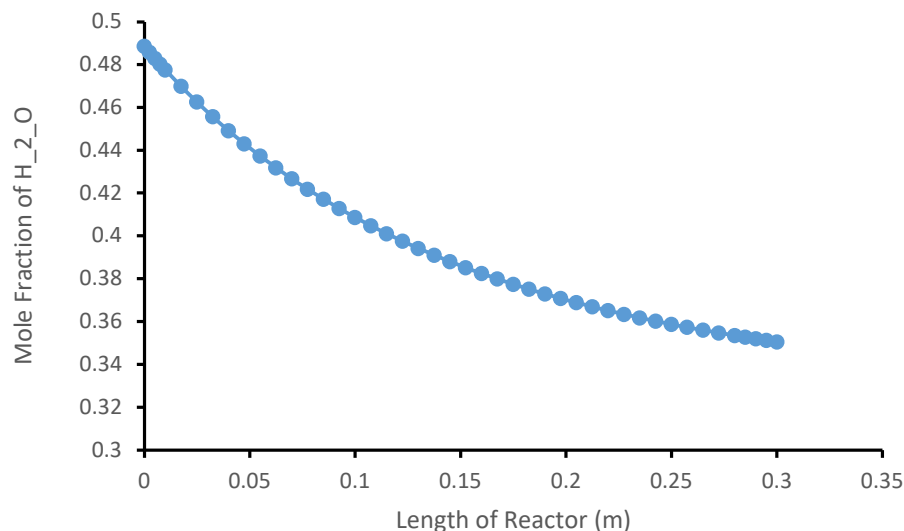


Figure 3: Mole Fraction of H₂O Versus Length of Reactor

The shape confirms effective coupling of reaction and in-situ CO_2 removal relative to a conventional PFR, sustaining conversion deeper into the bed. Levers that steepen and depress the curve include stronger CO_2 -selective driving force (lower permeate pressure, sweep, staged/graded membrane area), higher steam-to- H_2O ratio, greater residence time, and improved catalyst effectiveness; levers that flatten it earlier include excessive temperature or weak downstream separation. Overall, the profile reflects strong front-end conversion with a low but nonzero outlet H_2O , and further reduction is best achieved by boosting downstream CO_2 removal and/or residence time rather than large upstream changes.

3.6 Variation of CO_2 Mole Fraction Against Reactor Length

CO_2 mole fraction increases along the reactor length with a steep rise near the inlet and a gradual leveling downstream. This shape reflects rapid early formation of CO_2 when reactant partial pressures and intrinsic kinetics are highest, and aided by strong initial driving force for transport through the membrane. As CO and steam are consumed, reaction driving force and membrane CO_2 flux both diminish (permeate side becomes richer in CO_2 and the gradient shrinks), so the curve transitions to an asymptotic approach governed by the combined limits of kinetics, separation, and equilibrium. An upward profile of this kind is expected for a product feed; its exact height indicates the balance between formation and in-situ removal. If the goal is minimal CO_2 in the retentate and high capture, the curve can be depressed and flattened by boosting downstream removal (lower permeate pressure or sweep, staged/segmented membranes, higher area per length), increasing residence time, and maintaining a favorable steam/ CO ratio. Conversely, weaker separation, high stage-cut without sweep, or sub-optimal catalyst effectiveness allow more CO_2 to accumulate in the retentate, shifting the curve upward.

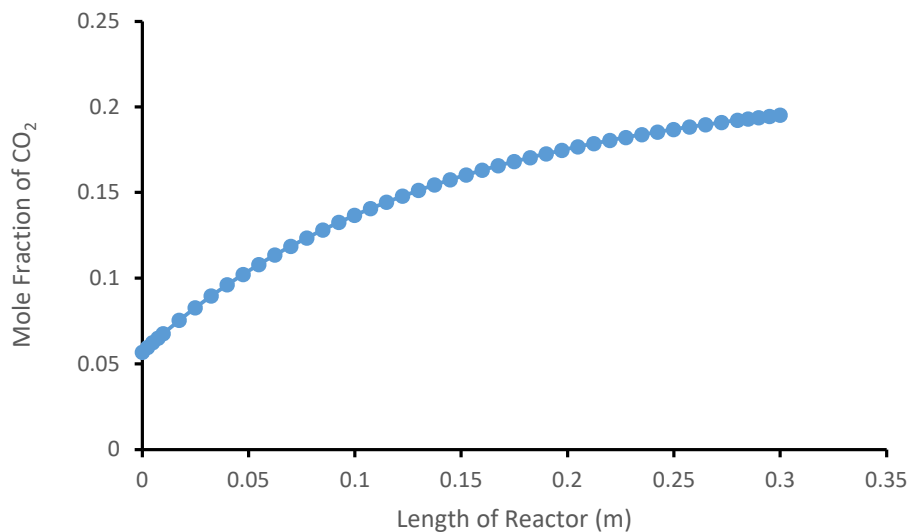


Figure 4: Mole Fraction of CO_2 Versus Length of Reactor

Overall, the trend confirms effective product generation with gradually decreasing incremental gains, typical of isothermal membrane-assisted WGS operation.

3.7 Variation of H_2 Mole Fraction Against Reactor Length

Hydrogen gas mole fraction increases along the reactor length with a steep rise near the inlet and a gradual leveling downstream as shown in Figure 5. This shape reflects rapid early formation of

H₂ when reactant partial pressures and intrinsic kinetics are highest, supported by strong initial driving force for transport through the membrane.

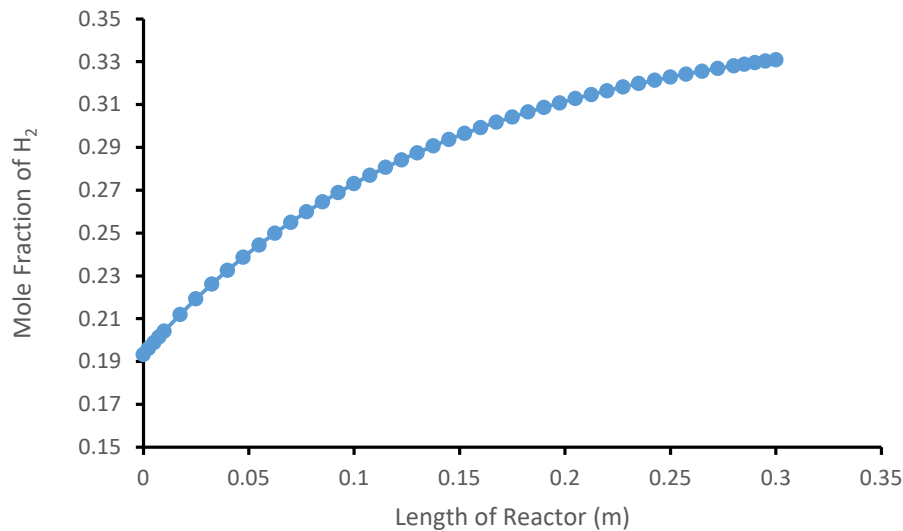


Figure 5: Mole Fraction of H₂ Versus Length of Reactor

As CO and steam are consumed, reaction driving force and membrane H₂ flux both diminish (permeate side becomes richer in H₂ and the gradient shrinks), so the curve transitions to an asymptotic approach governed by the combined limits of kinetics, separation, and equilibrium. An upward profile of this kind is expected for a reaction product; its exact height indicates the balance between formation and in-situ removal. If the goal is minimal CO₂ in the retentate and high capture, the curve can be depressed and flattened by boosting downstream removal (lower permeate pressure or sweep, staged/segmented membranes, higher area per length), increasing residence time, and maintaining a favorable steam/CO ratio. Conversely, weaker separation, high stage-cut without sweep, or sub-optimal catalyst effectiveness allow more CO₂ to accumulate in the retentate, shifting the curve upward. Overall, the trend confirms effective product generation with gradually decreasing incremental gains, typical of isothermal membrane-assisted WGS operation.

3.8 Variation of N₂ Mole Fraction Against Reactor Length

With reference to the nitrogen gas mole fraction, its variation along membrane reactor length is depicted in Figure 6. Thus, N₂ mole fraction rises very slightly along the reactor despite N₂ being non-reactive, thereby leading to gentle, near-linear increase due to concentration effect. As CO and H₂O are consumed and more importantly, CO₂ (and a trace of H₂) are continuously removed through the membrane, so the total retentate molar flow shrinks while the N₂ molar flow remains essentially constant

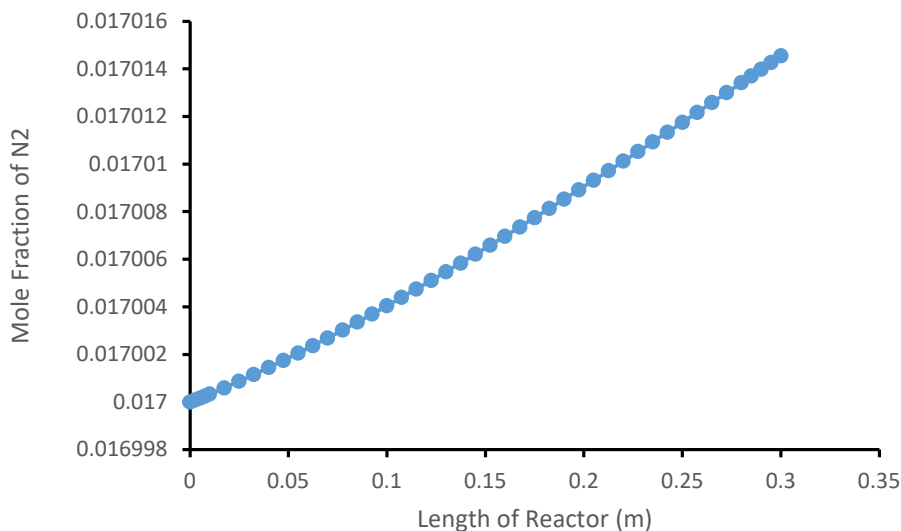


Figure 6: Mole Fraction of N₂ Versus Length of Reactor

With the denominator decreasing, nitrogen mole fraction creeps upward even though its absolute amount changes little. The smooth curvature indicates stable stage-cut and strong CO₂ selectivity with negligible N₂ permeation. The process implications leads to accumulating inert dilutes reactant partial pressures downstream, modestly slowing intrinsic rates, it caps retentate H₂ purity requiring a polishing step if ultra-pure H₂ is desired, and higher CO₂ driving force (lower permeate pressure/sweep or staged membranes) will accentuate this slight rise by further reducing retentate flow. Thus, N₂ molar flow should be constant and any noticeable N₂ loss would signal membrane leakage or non-negligible N₂ permeability. Overall, the profile is the expected signature of a CO₂-selective membrane reactor operating properly with an inert diluent present.

3.9 Temperature Variation Along Membrane Reactor Length

The steady state one-dimensional non-isothermal membrane reactor energy balance results yielded a gradual temperature increase along the reactor length from an inlet temperature value of 855K to an outlet temperature value of 859.96 K over a length of 300cm, corresponding to a net rise of only 4.96 K (~0.58%). This modest temperature change indicates near-isothermal operation

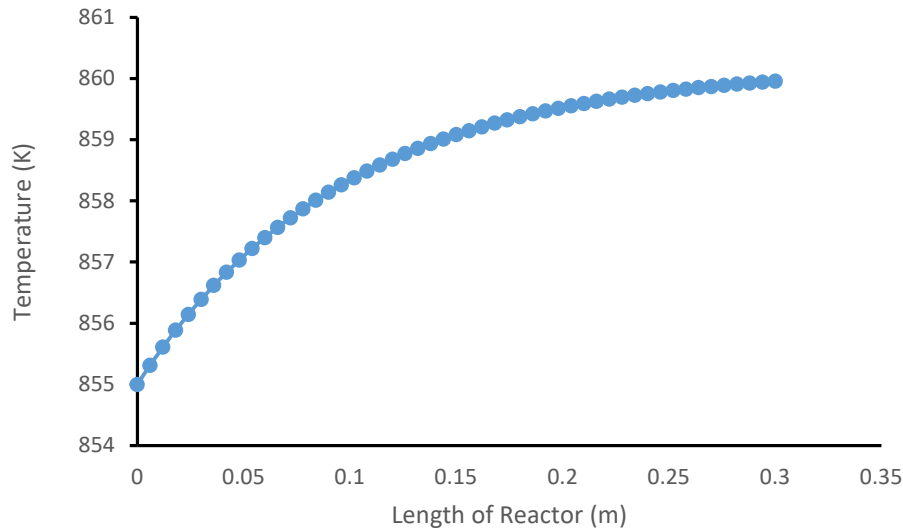


Figure 7: Temperature Versus Length of Reactor

The temperature profile is characterized by a steep initial gradient near the inlet where exothermic reaction heat release is greatest due to high reactant concentrations, followed by a progressively flatter slope as the reaction rate declines with reactant depletion and hydrogen removal. The temperature rise closely follows an exponential approach to an asymptotic value (~ 860.19 K) with a characteristic thermal length of ~ 0.097 m (9.7 cm), meaning that $\sim 95\%$ of the total rise is achieved within the reactor length. This behavior suggests efficient heat management and a well-balanced interaction between reaction kinetics, membrane separation, and heat transfer with minimal thermal deviation from the isothermal case. The results imply that temperature effects on conversion and CO_2 recovery are relatively minor, and further length extension would yield negligible thermal benefit.

4.0 Conclusion

This study successfully developed and simulated a steady-state membrane reactor for CO_2 capture from flue gas using the water-gas shift (WGS) reaction and selective membrane separation. The developed MATLAB model incorporated component material balances, WGS reaction kinetics, membrane permeation, and energy balance to evaluate the reaction, separation, and thermal behaviour of the reactor. The simulated flue gas contained CO (24.4734%), H_2O (49.1474%), CO_2 (5.6169%), H_2 (19.0572%) and N_2 (1.7051%), and the steady-state isothermal results showed 57.57% CO conversion, 28.24% H_2O conversion, 75.64% H_2 recovery, and 99.97% CO_2 recovery. The H_2 concentration in the permeate was 0.33103 mol%, while the CO_2 concentration in the retentate was only 0.19527 mol%, demonstrating highly effective CO_2 removal with limited hydrogen loss. The component profiles along the 300 cm (3 m) reactor showed that CO and H_2O decreased progressively, while CO_2 and H_2 increased along the reactor length. The N_2 mole fraction increased only slightly because N_2 was essentially inert and its concentration increased as other species were removed through the membrane. These trends confirmed the simultaneous occurrence of WGS reaction and membrane separation. Also, the thermal balance analysis showed that temperature increased from 855.0 K at the inlet to 859.96 K at the outlet, representing a rise of only 4.96 K (0.58%). This indicates that the reactor operated under near-isothermal conditions, with the temperature gradually approaching an asymptotic value as the reaction progressed. The

steady state developed model predicted CO conversion, H₂O conversion, H₂ recovery and CO₂ recovery of 57.57%, 28.24%, 75.64% and 99.97% respectively compared with 68.02%, 32.15%, 77.23% and 97.62% reported by Fernando *et al.* (2024). The close agreement in H₂ and CO₂ recovery confirms the capability of the model to reasonably predict the separation performance of the membrane reactor.

References

- [1] Adeloye, O. M., Olisa, E. E. & Igbagara, P. W. (2025). Mathematical Modeling of Membrane System for Hydrocarbon Gas (C₁ – C₃) Recovery in Polyethylene Plant. *Journal of Pakistan Institute of Chemical Engineers*, 53(1), 01-10 <https://doi.org/10.54693/piche.05311>
- [2] Adrover, M. E., López, E., Borio, D. O. & Pedernera, M. N. (2009). Theoretical Study of a Membrane Reactor for the Water Gas Shift Reaction Under Non-isothermal Conditions. *AIChE Journal*, 55(12), 3206–3213. <https://doi.org/10.1002/aic.11929> [American Institute of Chemical Engineers](https://doi.org/10.1002/aic.11929)
- [3] Akpa, J. G., Raphael, K., Adeloye, O. M. & Abowei, M. F. N. (2021). Modeling of Membrane Reactor for Methane Steam Reforming: An Alternative to Conventional Reactor. *Global Scientific Journals*, 9(12), 1466-1479
- [4] Baker, R. W. & Low, B. T. (2014). Gas Separation Membrane Materials: A Perspective. *Macromolecules*, 47(20), 6999–7013. <https://doi.org/10.1021/ma501488s> [ACS Publications](https://doi.org/10.1021/ma501488s)
- [5] Bernardo, P., Drioli, E. & Golemme, G. (2009). Membrane Gas Separation: A review/state of the art. *Industrial & Engineering Chemistry Research*, 48(10), 4638–4663. <https://doi.org/10.1021/ie8019032> [ACS Publications](https://doi.org/10.1021/ie8019032)
- [6] Favre, E. (2007). Carbon dioxide Recovery from Post-Combustion Processes: Can Gas Permeation Membranes Compete with Absorption? *Journal of Membrane Science*, 294(1–2), 50–59. <https://doi.org/10.1016/j.memsci.2007.02.007> [ScienceDirect](https://doi.org/10.1016/j.memsci.2007.02.007)
- [7] Favre, E. (2011). Membrane Processes and Post-combustion Carbondioxide Capture: Challenges and prospects. *Chemical Engineering Journal*, 171(3), 782–793. <https://doi.org/10.1016/j.cej.2011.01.010> [ScienceDirect](https://doi.org/10.1016/j.cej.2011.01.010)
- [8] Fan, Y., Yu, W., Wu, A., Shu, W. & Zhang, Y. (2024). Recent Progress on CO₂ Separation Membranes. *RSC Advances*, 14, 20714–20734. <https://doi.org/10.1039/D4RA00444B> [Royal Society of Chemistry Publishing](https://doi.org/10.1039/D4RA00444B)
- [9] Hla, S. S., Morpeth, L. D. & Dolan, M. D. (2015). Modelling and Experimental Studies of a Water–Gas Shift Catalytic Membrane Reactor. *Chemical Engineering Journal*, 276, 289–302. <https://doi.org/10.1016/j.cej.2015.04.079> [ScienceDirect](https://doi.org/10.1016/j.cej.2015.04.079)
- [10] Kancherla, R., Nazia, S., Kalyani, S. & Sridhar, S. (2021). Modeling and Simulation for Design and Analysis of Membrane-Based Separation Processes. *Computers & Chemical Engineering*, 148, 107258. <https://doi.org/10.1016/j.compchemeng.2021.107258> [ScienceDirect](https://doi.org/10.1016/j.compchemeng.2021.107258)

- [11] Karagöz, S., Da Cruz, F. E., Tsotsis, T. T. & Manousiouthakis, V. I. (2018). Multi-Scale Membrane Reactor (MR) Modeling and Simulation for the Water Gas Shift Reaction. *Chemical Engineering and Processing: Process Intensification*, 133, 245–262. <https://doi.org/10.1016/j.cep.2018.09.012> [ScienceDirect](#)
- [12] Lotrič, A., Sekavčnik, M., Kunze, C. & Spliethoff, H. (2011). Simulation of Water-Gas Shift Membrane Reactor for Integrated Gasification Combined Cycle Plant with CO₂ Capture. *Journal of Mechanical Engineering*, 57(12), 911–926. <https://doi.org/10.5545/sv-jme.2011.100> [Journal of Mechanical Engineering](#)
- [13] Mendes, D., Sousa, J. M., Madeira, L. M. & Basile, A. (2010). The Water-Gas Shift Reaction: From Conventional Catalytic Systems to Pd-Based Membrane Reactors—A Review. *Asia-Pacific Journal of Chemical Engineering*, 5(1), 111–137. <https://doi.org/10.1002/apj.364> [Wiley Online Library](#)
- [14] Merkel, T. C., Lin, H., Wei, X. & Baker, R. W. (2010). Power Plant Post-Combustion Carbon dioxide Capture: An Opportunity for Membranes. *Journal of Membrane Science*, 359(1–2), 126–139. <https://doi.org/10.1016/j.memsci.2009.10.041> [ScienceDirect](#)
- [15] Wei-Hsin, C. & Chia-Yang, C. (2020). Water Gas Shift Reaction or Hydrogen Production and Carbondioxide Capture: A Review. *Applied Energy*, 258, 114078. <https://doi.org/10.1016/j.apenergy.2019.114078> [ScienceDirect](#)
- [16] Wirawan, S. K., Creaser, D., Bendiyasa, I. M. & Sediawan, W. B. (2012). CO₂ Selective Water Gas Shift Membrane Reactor: Modeling and Simulation. *ASEAN Journal of Chemical Engineering*, 12(1), 1–12. [Journal UGM](#)
- [17] Wu, J., Hillman, F., Liang, C.-Z., Jia, Y. & Zhang, S. (2023). Progressing Thin-Film Membrane Designs for Post-Combustion CO₂ Capture: Performance or Practicality? *Journal of Materials Chemistry A*, 11, 17452–17478. <https://doi.org/10.1039/D3TA02842A> [Royal Society of Chemistry Publishing](#)
- [18] Fan, Y., Yu, W., Wu, A., Shu, W. & Zhang, Y. (2024). Recent Progress on CO₂ Separation Membranes. *RSC Advances*, 14, 20714–20734. <https://doi.org/10.1039/D4RA00444B> [Royal Society of Chemistry Publishing](#)
- [19] Liu, B., Tang, C., Li, X., Wang, B. & Zhou, R. (2020). High-Performance SAPO-34 Membranes for CO₂ Separations from Simulated Flue Gas. *Microporous and Mesoporous Materials*, 292, 109712. <https://doi.org/10.1016/j.micromeso.2019.109712> [ScienceDirect](#)
- [20] Chen, W.-H., Tsai, C.-W., Lin, Y.-L., Chein, R.-Y. & Yu, C.-T. (2017). Reaction Phenomena of High-Temperature Water Gas Shift Reaction in a Membrane Reactor. *Fuel*, 199, 358–371. <https://doi.org/10.1016/j.fuel.2017.03.002> [National Cheng Kung University](#)
- [21] Saw, S. Z., Nandong, J. & Ghosh, U. K. (2018). Optimization of Steady-State and Dynamic Performances of Water–Gas Shift Reaction in Membrane Reactor. *Chemical Engineering Research and Design*, 134, 36–51. <https://doi.org/10.1016/j.cherd.2018.03.045> [Colab](#)

- [22] Ovalle-Encinia, O. & Lin, J. Y. S. (2024). Modeling Analysis of Water-Gas-Shift Reaction on Catalyst-Packed Ceramic-Carbonate Dual-Phase Membrane Reactor for Hydrogen Production. *International Journal of Hydrogen Energy*, 64, 39–49. <https://doi.org/10.1016/j.ijhydene.2024.03.245>
- [23] Gan, Z., Sun, Y. & Wang, X. (2024). Highly Efficient and Stable Hydrogen-Permeable Pd-Alloy Membranes and their Use in PDH Membrane Reactors. *Journal of Membrane Science*, 67(9), 121-148.