



Optimizing Hydrogen Production from Methanol Reformers by Temperature Variation and Feed Ratio Using CFD

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ABSTRACT

Steam reformers are typically utilized in hydrogen production industry, demanding pressure vessels within methanol reformer systems operating at temperatures between 250-350°C to ensure cost-effectiveness. This characteristic makes them a superior choice for fuel cell systems. However, challenges arise in enhancing hydrogen gas production efficiency while minimizing carbon monoxide emissions. Computational Fluid Dynamics (CFD) has proven effective in addressing these challenges by simulating fluid behavior. This study delves into product production, reactant consumption using CFD, and investigates changes in physical parameters of methanol reformers to optimize their performance. The research involves 140 numerical simulations that examine the relationship between feeds (steam-to-carbon) and various temperatures, aiming to understand the concurrent effect of physical parameters. The results demonstrate that increasing temperature has a more significant impact on hydrogen production compared to increasing the feed ratio. This effect is particularly notable at lower fuel ratios. For example, at a feed ratio of 1, a temperature increase of 11.4°C leads to a substantial 5.4% rise in hydrogen production. However, at a higher feed ratio (1.98), the increase in hydrogen production is only 1.9% with the same temperature increase.

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NOMENCLATURE

ρ	Density(kg/m ³)	τ	Stress tensor (Pa)
v	Velocity (m/s)	X	Mole fraction
μ	Dynamic viscosity (Pa-s)	Subscripts	
ε	Dissipation rate of turbulent kinetic energy; bed porosity (J/ kg s)	f	Fluid quantity
H	Total enthalpy (J)	r	Reaction quantity
λ	Coefficient of thermal Conductivity (W/ m·K)	j	Reaction indicator
T	Temperature (°C)	i	Species indicator

INTRODUCTION

Fossil fuel resources are rapidly declining worldwide, while energy consumption is continuously increasing. This situation necessitates the search for new and alternative sources of energy. Moreover, fossil fuels currently supply 80% of the primary of world energy,

which poses a significant threat to the environment. Therefore, replacing conventional sources of energy with renewable ones has become an urgent need to prevent the consequences of such high dependency on fossil fuels. Hydrogen, with its high capacity for energy storage, is expected to be a suitable solution to this problem. It is a secondary form of energy that can be produced using three categories of energy supply systems: fossil fuels

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(such as coal, oil, natural gas, etc.), nuclear reactors (such as nuclear fission and breeder reactors), and renewable energy sources (including hydroelectric power, wind power, ocean thermal energy conversion, bio-mass production, photovoltaic power generation, solar thermal systems, etc.).

One of the methods of converting hydrogen into another type of energy such as electricity and heat is the use of fuel cells. A fuel cell is a type of energy converter that directly converts the chemical energy of the fuel into energy, unlike a battery that does not store energy, but converts energy from one state to another, so that the materials inside the cell are not consumed in this conversion [1, 2]. Fuel cells use catalysts in their system that are very sensitive to carbon monoxide because carbon monoxide causes damage to the catalysts and disables them, so the hydrogen that is needed for consumption in the fuel cell must have the highest purity and be free of carbon monoxide. Compared to conventional power generation schemes, fuel cells can reduce carbon dioxide production by 54% due to high efficiency and no solid particle production, and have other advantages such as very long life, negligible noise pollution, reduced fuel consumption and so on. By using this technology, a bright future can be achieved.

The majority of hydrogen is produced by steam reforming of natural gas or other fossil fuels. However, given the Kyoto Protocol and the need to prevent further climate change and reduce greenhouse gas emissions, methods of producing hydrogen that do not emit CO₂ are of particular importance [3].

The choice of method for producing hydrogen depends on its economic feasibility. For example, producing hydrogen by thermal decomposition of methane is not economically viable due to the required difficult operating conditions and purification challenges. In a study conducted by Arzamendi et al. [4], numerical simulation of integrating a methanol reformer with a combustion chamber in microchannel reactors was carried out for hydrogen production. They used computational fluid dynamics for numerical modeling. The results showed that, by reducing the diffusion distance and increasing the surface-to-volume ratio, the flow rates in the reactor would reach 50,000 per hour.

Ribeirinha et al. [5] investigated numerically and experimentally various designs (multi-channel, radial, tubular) of methanol reformers in a high-temperature fuel cell with an electrolyte membrane. Multi-channel reformers exhibited the best performance in terms of methanol conversion, pressure drop reduction, heat transfer, and low operating temperature. They used computational fluid dynamics for numerical simulation. Klenov et al. [6] used computational fluid dynamics to investigate the numerical performance of a compressed methanol processor. They achieved an optimal design for heat transfer between the reformer and combustion chamber as well as control over the temperature of

reformer. The maximum overall efficiency was reported at a methanol injection volume of 24.17 mmol/min for the reformer and 75.8 mmol/min for the combustion chamber, with hydrogen performance equivalent to 7.48 mmol/min and a reformer temperature of 286°C.

Ghasemzadeh et al. [7] used computational fluid dynamics to study reactor performance with dense Pd-Ag membranes in the presence of methanol reformers and self-regulating reformers. They used Cu/ZnO/Al₂O₃ catalysts and studied the effects of parameters such as temperature, pressure, and gas sweep rate. They demonstrated that methanol reactors have better hydrogen performance and recovery compared to self-regulating reformers.

Ziarati et al. [8] developed a comprehensive mathematical model for methanol reformers. The molecular structure factors and convection terms were considered in this model, along with convection terms like heat and mass transfer, using the impact coefficients of two dominant parameters; particle size and wall heat flux. They found that by changing the particle size from 700 to 3200 micrometers, the impact coefficient decreased by approximately 80%, resulting in a decrease in total methanol conversion of about 74%.

Heidarzadeh and Taghizadeh [9] studied the process of steam methane reforming for hydrogen production in a microchannel reactor covered with Cu/ZnO/Al₂O₃ catalysts through laboratory experimentation and computational fluid dynamics simulation. The numerical results were in good agreement with the experimental data. The results showed that increasing the temperature at different feed rates causes a reduction in carbon monoxide and carbon dioxide production, while with a constant temperature, an increase in feed rate reduces the production of carbon monoxide, carbon dioxide, and increases hydrogen production.

Sari et al. [10] numerically studied (using computational fluid dynamics) hydrogen production from a microreactor with thirteen parallel channels. They compared two models: Maxwell-Stefan and mean approximation with experimental data. The results show that the predictions of the Maxwell-Stefan model are more consistent with the experimental data than the average mixture model, especially at lower feed rates.

Perng et al. [11] used computational fluid dynamics to study the numerical effect of diffusers on the performance of methanol reformers. They studied the effect of diffuser length, angle, and wall temperature on hydrogen production, reduction of carbon monoxide production, and methanol conversion.

Ngo et al. [12] introduce a three-dimensional computational fluid dynamics (CFD) model developed for an annulus steam methane reforming (SMR) reactor with the inclusion of a narrow sleeve between the combustor and reactor. The model incorporates various equations and turbulence models to simulate the heat exchange and chemical reactions occurring in the reactor.

The CFD results were validated against experimental data, demonstrating the accuracy of the model. The findings revealed the thermal efficiency, heat flux, and temperature distribution within the reactor. The use of the sleeve in the SMR reactor resulted in improved temperature profiles along the reactor length.

Srivastava et al. [13] addressed the challenges in hydrogen storage for transportation and explores on-board fuel reforming as a solution. It investigates a packed bed-type reactor that utilizes exhaust gas heat energy for sustaining the reforming reaction. The study conducts a numerical analysis, focusing on the impact of operating parameters on reactor performance. The results highlight the significance of temperature as the most influential parameter and reveal the negligible effects of steam/carbon ratio and flow configuration on hydrogen yield and methanol conversion. The study also notes that increased reactant inlet velocity reduces methanol conversion due to decreased residence time for the reforming reaction. This research contributes to the limited literature on on-board hydrogen generation using engine exhaust heat, offering valuable insights for improving engine efficiency and reducing emissions.

Gu et al. [14] explore the heat transfer and storage performance of steam methane reforming in a tubular reactor using a focused solar simulator. Experimental and numerical analyses reveal that methane conversion decreases with increasing inlet flow rate, while thermochemical energy storage efficiency initially increases and then decreases. The maximum efficiency achieved is 11.3% with a central heat flux of 285.6 kW/m². The research highlights the importance of inlet conditions, catalyst bed structure, and heat loss in influencing methane conversion and energy storage efficiency. Increasing inlet temperature, optimizing steam to methane ratio, and utilizing insulation and coating can improve energy storage efficiency.

Based on previous studies, physical parameters can have a significant impact on hydrogen production. However, so far, the simultaneous effect of these parameters and extensive investigations regarding their influence on hydrogen production have not been fully explored. Examining the concurrent effect of these parameters can facilitate optimization and enhance the efficiency of hydrogen production. Furthermore, numerical simulation using computational fluid dynamics can provide a better visualization of heat distribution and fluid behaviors in the process. Therefore, this paper focuses on studying the simultaneous effect of physical parameters on hydrogen production using computational fluid dynamics. This numerical simulation method allows for a more accurate modeling of fluid behavior and enables the investigation of various parameters' impact on hydrogen production. This information can help us improve our understanding of the hydrogen production process and take more appropriate actions to increase efficiency and optimize the process. Additionally, this

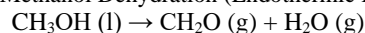
study can pave the road for future research in this area and contribute to the development of hydrogen production-related technologies.

The study explores product production and reactant consumption using Computational Fluid Dynamics (CFD), and investigates alterations in the physical parameters of methanol reformers to enhance their efficiency. This research involves 140 numerical simulations that analyze the correlation between feed ratios (steam-to-carbon) and various temperatures, aiming to comprehend the simultaneous impact of physical parameters, a gap present in previous studies.

Governing equations

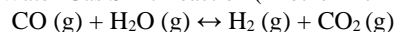
The methanol steam reforming process involves a series of chemical reactions that convert methanol (CH₃OH) and water (H₂O) into hydrogen gas (H₂) and carbon dioxide (CO₂) with the help of a catalyst. This is an essential process for hydrogen production, especially in fuel cell applications. Here are the reactions involved in the methanol steam reforming process:

1. Methanol Dehydration (Endothermic Reaction):



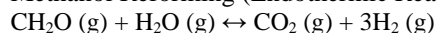
In this step, methanol (liquid) is dehydrated to formaldehyde (gas) and water (gas) in an endothermic reaction, meaning it requires heat input. This reaction prepares the intermediate species for the subsequent reforming reactions.

2. Water-Gas Shift Reaction (Exothermic Reaction):



This is an equilibrium reaction that occurs to shift the balance between carbon monoxide (CO) and hydrogen gas (H₂) by reacting carbon monoxide with water vapor. The reaction is exothermic, releasing heat.

3. Methanol Reforming (Endothermic Reaction):



In this step, formaldehyde (gas) reacts with water vapor to produce carbon dioxide (gas) and hydrogen gas (H₂) in an endothermic reaction. This is the main reforming reaction that yields hydrogen gas.

The transfer of mass and momentum through a porous region is described by the continuity equation and the Navier-Stokes equations for Newtonian fluids. The process under investigation is steady and symmetric, hence all time derivatives and angular gradients must be equal to zero. Due to chemical reactions and extreme temperature changes within the reactor, the fluid is considered compressible which leads to its formulation. Continuity Equation [15].

$$\nabla \cdot \rho \vec{v} = 0 \quad (1)$$

The Navier-Stokes equations can be written using the Brinkman equation as shown in Equation (2). The extended drag force term caused by the catalyst bed can be calculated using constant resistance coefficients obtained from the Ergun equation for solid particles. All time derivatives and angular gradients are equal to zero.

Since the bed porosity is considered a constant, it can be eliminated from the first three terms of the momentum equation and only shown under drag force conditions. Temperature dependencies in the equation arise due to the influence of density ρ , dynamic viscosity μ , and pressure p [15].

$$\nabla \cdot (\rho \cdot \vec{v} \cdot \vec{v}) = -\nabla p + \nabla \cdot (\tau) - (C_{viscous} \cdot \frac{\epsilon}{\mu} \cdot \vec{v}) + C_{inertial} \cdot \frac{\epsilon}{2} \cdot \rho \cdot |\vec{v}| \cdot \vec{v} \quad (2)$$

Energy transfer in the system is described by the energy equation 3. All temporal derivatives are equal to zero because a steady process is assumed. The left-hand side of equation (3) represents the change in total energy (enthalpy and kinetic energy) in the system. The right-hand side terms of the equation describe the mechanisms that create this change in total energy, which from left to right are: change in enthalpy due to chemical reactions, energy transfer via heat conduction, energy transfer via diffusion and viscous dissipation. The strain rate can be described similarly as before [15].

$$\nabla \cdot \left(\vec{v} \cdot \left(H_f + \rho_f \cdot \frac{\vec{v} \cdot |\vec{v}|}{2} \right) \right) = \sum_j \Delta H_{r,j} + \nabla \cdot [\lambda \cdot \nabla T] - \left(\sum_i h_i \cdot J_i \right) + (\vec{\tau} \cdot \vec{v}) \quad (3)$$

RESULTS AND DISCUSSION

Geometry and physical conditions

In order to develop a CFD model, the first step involves creating a suitable geometry and computational grid to enable accurate and stable numerical evaluation of the system equations. The design of the geometry and mesh is carried out using the relevant tools provided by Ansys Fluent. To ensure improved convergence during simulations, the reactor tube is divided into two distinct sections: an inert zone and a catalyst bed. Both sections are filled with porous materials having equal porosity, thereby restricting the occurrence of reactions solely to the second part, which is the catalyst bed. This partitioning allows different properties to be assigned independently to each area. The geometry is simplified to a two-dimensional representation to optimize computational efficiency. To further reduce the computational domain, only half of the cross-sectional area between the wall and the rotational axis is modeled. Consequently, the computational load is decreased while maintaining the essential characteristics of the system.

The hot air flow takes place outside the pipe, ensuring an overall heat transfer coefficient of 110 W/m².K. This

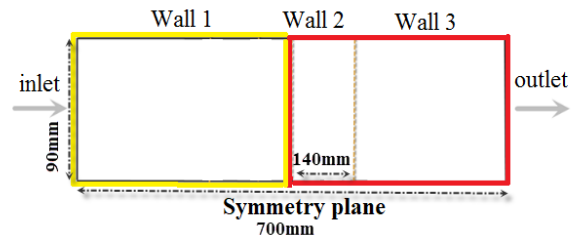


Figure 1. Geometry schematic

heat transfer coefficient governs the rate at which heat is exchanged between the hot air flow and the reactor components. The reactor is filled with CuO/ZnO/Al₂O₃ catalyst, which exhibits a bulk density of 1235.4 Kg/m³ and a bed porosity of 0.4. These parameters directly influence the catalyst's packing and affect the flow behavior and efficiency of the catalytic reactions within the reactor.

Heat transfer through the reactor wall is considered by applying a boundary condition on the inner wall. Conjugate conditions are not considered for the wall in this work. Therefore, heat conduction through the wall is not included in the model under investigation and the reactor walls are not implemented in the geometric design process. Additionally, the names of the geometric components are summarized in Figure 1.

To create a good computational mesh for accurate results, an appropriate meshing strategy has been developed. For both reactors, the catalyst bed is divided into a small separation zone at the beginning of the catalyst bed and a larger section before the reactor outlet. The reason for this division is the high reaction rate and steep gradients at the beginning of the reactor bed, as the reaction activity dominates in the early layers of the catalyst. This will be further validated with a valid reaction rate plot, so the strategy undertaken will be maintained throughout the study.

In terms of meshing, the cell size in the direction of the reactor axis increases until it reaches a maximum predefined value. This cellular growth leads to distorted rectangular cells and the inclusion of triangular cells to keep the aspect ratio sufficiently low. Due to the advanced wall treatment, the maximum size of the first cell layer is limited with a constraint where y^+ should not exceed a unitless number. y^+ is a function of physical properties, radial position, and friction velocity. Since density and dynamic viscosity appear in the equation and these two parameters are temperature-dependent, y^+ is also dependent on temperature. Friction velocity is a function of local shear stress at the wall and fluid density.

Validation

Figure 2 shows the validation of the present numerical step with the work of Chougule and Sonde [16]. This plot

represents the methanol molar fraction. As shown in the figure, there is an acceptable agreement between these two simulations, where the maximum normalized root mean squared error (NRMS) is 1.95%.

RESULTS

The temperature behavior within the catalyst bed, as shown in Figure 3a, reveals interesting insights into the dynamics of the methanol steam reforming process. The initial rapid decrease in temperature is a crucial stage in the reforming reaction, as it signifies the endothermic nature of the reactions involved. During this phase, the heat is absorbed from the surroundings to drive the endothermic reforming reactions and facilitate the conversion of methanol and water into hydrogen and carbon dioxide.

As the reactants progress through the catalyst bed, the temperature starts to increase again before reaching the outlet. However, an intriguing observation is that the temperature also exhibits a decrease contrary to the flow direction, which is not expected in a typical flow process. This unusual behavior can be explained by the complex heat transfer mechanisms occurring within the porous catalyst bed. The interactions between the reactants, the catalyst surface, and the flow patterns create local temperature variations and counter-diffusion phenomena. Analyzing the temperature distribution allows us to deduce the flow direction as the lower temperature region is drawn towards the reactor outlet. This flow pattern has critical implications, especially when dealing with the highest mass flow rate. It suggests that the distribution of reactants and heat transfer within the reformer should be carefully managed to achieve optimal hydrogen production efficiency.

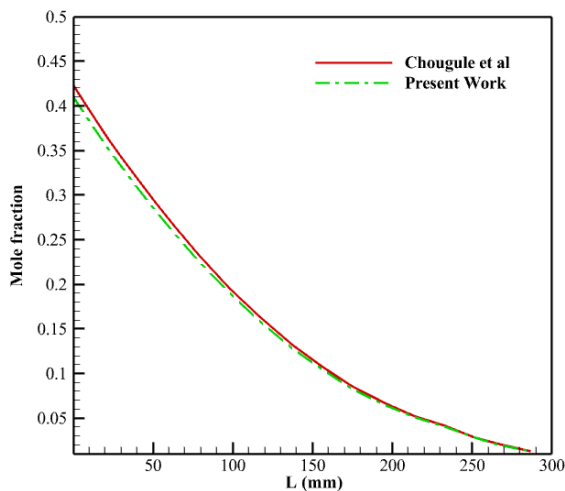


Figure 2. Validation of CH₃OH mole fraction through the research of Chougule and Sonde [16]

Moreover, in regions with low temperatures, we observe remarkable similarities in their spatial extent and shape. This phenomenon is attributed to the thermal boundary conditions set on the reactor wall, where a constant temperature is maintained. Consequently, a higher radial temperature gradient emerges, generating a more pronounced driving force for heat conduction, as described by Fourier's law. The increased heat flux in the reactor wall adjacent to the temperature decrease zone further influences the overall temperature distribution. Figures 3b and 3c, respectively indicate the consumption of methanol in terms of molar flow rate and the production of hydrogen in molar flow rate. As evident from the figures, the reactions initiate within the catalyst bed, and species are consumed or generated throughout this region. The distribution of species is shaped in a wedge-like manner as they move towards the reformer outlet, influenced by the velocity profile within the reformer.

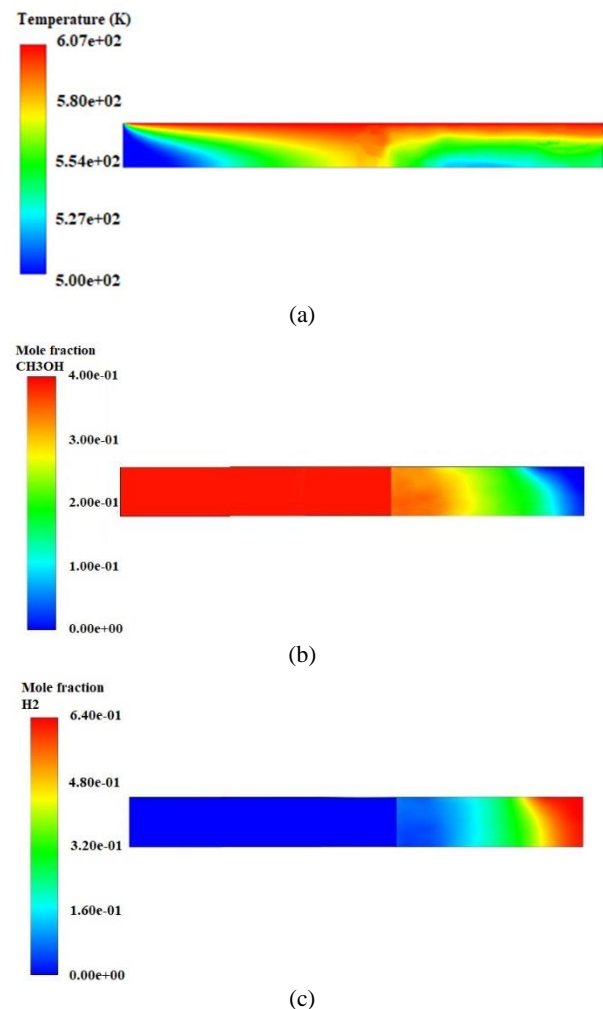


Figure 3. Temperature changes in (a) methanol steam reformer and fractional changes (b) CH₃OH and (c) H₂

Figure 4 compares the molar quantities of H₂, CO₂, H₂O, and CO species. As evident from the figure, the produced amount of carbon monoxide is the lowest in the examined reformer, while the amount of produced hydrogen has the highest value. The percentage difference between the species is provided in Table 1. The equation ϵ has been utilized to obtain η .

$$\eta = \frac{X(H_2) - X(specie)}{X(H_2)} \cdot 100 \quad (4)$$

As indicated in Table 1, the percentage of produced hydrogen to carbon monoxide, which is the most crucial factor, is 95.31%.

Figure 5 presents a comprehensive three-dimensional graph that illustrates the impact of changes in the feed-to-temperature ratio on hydrogen production in methanol reformers. The graph showcases the relationship between the two variables, shedding light on the efficiency of the reforming process under various conditions. Upon analyzing the graph, it becomes evident that the effect of temperature variation on hydrogen production outweighs the influence of changes in the feed ratio. This finding holds particularly true within the studied range of conditions. Intriguingly, this effect is more pronounced when the fuel ratio is lower. For instance, when the feed ratio is set at 1, a mere increase of 11.4°C in temperature leads to a substantial 5.4% surge in hydrogen production. This indicates the sensitivity of hydrogen generation to temperature adjustments in situations where the feed ratio is relatively lower. Conversely, when the feed ratio is higher (1.98), the impact of the same temperature increase on hydrogen production diminishes significantly. In this scenario, the rise in hydrogen production is merely 1.9%, emphasizing that the influence of temperature becomes less influential as the feed ratio increases.

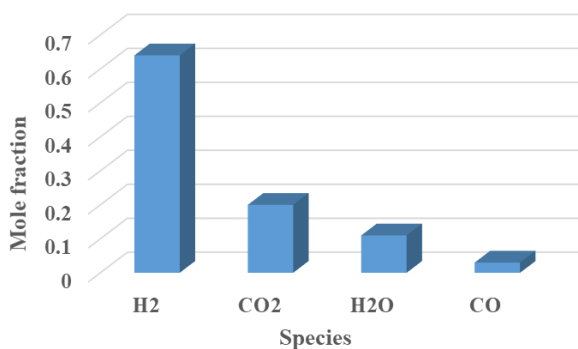


Figure 4. Comparing outlet molar fraction of H₂, CO₂, H₂O and CO

Table 1. Comparing the percentage of hydrogen production relative to the species H₂, CO₂, and CO

specie	CO ₂	H ₂ O	CO
η	68.75	82.81	95.31

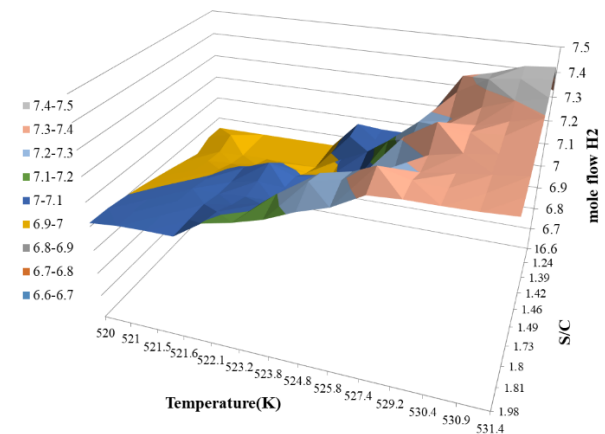


Figure 5. Changes in H₂ molar flow based on feed ratio (S/C) and inlet temperature

CONCLUSION

This study examined alterations in the physical parameters of methanol reformers aimed at enhancing their performance. The geometry was constrained to a two-dimensional and symmetrical model, with due consideration to the preheater space at the onset of the reformer. The study also accounted for the influence of catalyst presence and a porous medium. The results showed that temperature variations in the opposite direction of flow decreased. Moreover, an increase in the amount of methanol in the feed usually led to the expansion of the lower temperature region towards the reactor outlet. The analysis of the graph revealed that temperature variation had a more significant impact on hydrogen production compared to changes in the feed ratio, especially within the studied range of conditions. Notably, this effect was more pronounced when the fuel ratio was lower. For instance, a small 11.4°C increase in temperature at a feed ratio of 1 resulted in a substantial 5.4% increase in hydrogen production, indicating the heightened sensitivity of hydrogen generation to temperature adjustments when the feed ratio was relatively lower. On the other hand, when the feed ratio was higher (1.98), the influence of the same temperature increase on hydrogen production diminished significantly, leading to only a 1.9% rise in hydrogen production. This highlighted that the impact of temperature became less influential as the feed ratio increased.

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**Persian Abstract****چکیده**

ریفرمرهای متانولی به دلیل ویژگی‌های خود توانسته‌اند تا برتری‌های زیادی را در یک سیستم پیل سوختی ایجاد کنند. با این وجود مواردی از قبیل افزایش راندمان تولید گاز هیدروژن، می‌تواند چالش‌های مورد بحث برای این تجهیزات باشد. با توجه به اینکه شبیه‌سازی با استفاده از دینامیک سیالات محاسباتی رفتار سیال را در مسیر حرکتش مدل می‌کند بنابراین می‌تواند در حل چالش‌های مذکور موثر باشد. به همین دلیل در این پژوهش علاوه بر بررسی میزان تولید محصولات واکنش و مصرف واکنش دهنده‌ها با توجه به دینامیک سیالات محاسباتی به بررسی تغییر پارامترهای فیزیکی ریفرمر متانولی در افزایش عملکرد آن نیز می‌شود. این مطالعه شامل ۱۴۰ شبیه‌سازی عددی است که رابطه‌ای بین میزان تغذیه (نسبت بخار به کربن) و دماهای مختلف را برای بررسی تأثیر همزمان پارامترهای فیزیکی مورد مطالعه قرار می‌دهد. نتایج نشان می‌دهد که افزایش دما بر تولید هیدروژن تأثیر بیشتری نسبت به افزایش نسبت تغذیه دارد. این تأثیر در نسبت‌های سوخت پایین‌تر به مراتب مهم‌تر است؛ به عنوان مثال، در نسبت تغذیه ۱، افزایش دما به مقدار ۱۱/۴ درجه سانتی‌گراد به افزایش ۵/۴ درصد در تولید هیدروژن منجر می‌شود. با این حال، در نسبت تغذیه بالاتر (۱/۹۸)، تولید هیدروژن تنها با افزایش یکسان دما به مقدار ۱/۹ درصد افزایش می‌یابد.