

## ASEAN Journal of Process Control

Research Article

# Modeling and Control of Steam Methane Reforming Process Using Model Predictive Control

Tan Li Ting<sup>1</sup>, Nabilla Wahyu Hasanah<sup>1</sup>, Fakhrony Sholahudin Rohman<sup>2</sup>, Dinie Muhammad<sup>1\*</sup> 

<sup>1</sup> Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia (UTM), 81310 Skudai, Johor Bahru, MALAYSIA

<sup>2</sup> Process Systems Engineering Centre (UTM-PROSPECT), Research Institute of Sustainable Environment (RISE), Universiti Teknologi Malaysia (UTM), 81310 Skudai, Johor Bahru, MALAYSIA.

\*Corresponding Author: dinie.muhammad@utm.my

Academic Editor: Jobrun Nandong

Received: 7 December 2023; Accepted: 14 December 2023; Published: 31 December 2023

**Abstract:** This study focuses on modeling and controlling steam methane reforming (SMR) using model predictive control (MPC). The problem in the SMR plant is the limitation of the conventional control in controlling a wide range of operating conditions. The nonlinear dynamic behavior of the SMR process has further complicated the situation, as existing methods lack the adaptability to the changing operating conditions and disturbances. To address these challenges, MPC control scheme is proposed. The development of MPC involves developing a simulation process for Steam Methane Reforming (SMR) using Aspen Plus, creating the process model of SMR using the system identification technique, and designing the MPC control scheme. The development of a simulation plant includes constructing the process flowsheet, determining kinetics parameters, and creating a dynamic model. Model input-output selection and data generation are performed to facilitate the development of the process model. Based on the state space identification technique, the process model is developed with a normalized root mean square error (NRMSE) of 0.8567 for CV<sub>1</sub> and 0.3005 for CV<sub>2</sub>. Then, the core focus lies in designing the MPC control structure and tuning the MPC for enhanced performance. During set point tracking, starting from steady-state hydrogen production and increasing by 20% at 2 minutes, the state-space MPC outperformed the PID controllers, displaying more aggressive capabilities in reaching the desired set point. For the disturbance rejection test, the state-space MPC is able to control the reactor outlet temperature with minimal overshoot, as seen in the CV<sub>2</sub> profile. This behavior is due to the predictive capabilities of MPC, enabling quicker controller actions than PID. By addressing the traditional control limitations, the proposed MPC aims to enhance the operation and control of SMR plants while optimizing hydrogen production through advanced control strategies.

**Keywords:** Steam Methane Reforming (SMR); Model Predictive Control (MPC); dynamic simulation; hydrogen production; process control

---

### 1. Introduction

The availability of continuous electrical energy supply is vital for the progress and development of nations [1]. Currently, the world heavily relies on fossil fuels such as crude oil, coal, and natural gas to meet the growing global energy demand. The majority of electricity production is achieved through the

combustion of conventional fuels, including coal, methane, and petroleum. However, this reliance on fossil fuels for energy generation has led to significant environmental concerns [2].

One of the most pressing environmental issues is the climate crisis, which poses alarming consequences worldwide [3]. The release of greenhouse gases (GHGs), particularly sulfur dioxide (SO<sub>2</sub>), nitrogen oxides (NO<sub>x</sub>), and carbon dioxide (CO<sub>2</sub>) into the atmosphere disrupts the Earth's energy balance, leading to rising temperatures and shifting weather patterns [4]. Addressing the climate crisis requires immediate action to significantly reduce greenhouse gas emissions, aiming for near-zero levels that align with the commitments of the Paris Agreement. This agreement set long-term goals to limit the rise of the global average temperature to 1.5°C above the preindustrial level [1].

To address the challenge, it is necessary to develop alternative energy resources and the corresponding energy generation systems. In this context, hydrogen has emerged as a viable option [5]. Hydrogen is widely acknowledged as a highly promising energy carrier due to its exceptional capacity to efficiently deliver and store significant energy while promoting clean and environmentally friendly properties [6].

There are several ways to produce hydrogen, each with limitations and potential [7]. Presently, the primary method of hydrogen production is through steam methane reforming, accounting for over 40% of global hydrogen output [8]. Approximately 30% of hydrogen is also produced from oil or naphtha reforming, as well as from refinery or chemical industry off-gases. Coal gasification covers around 18% of the capacity, while water electrolysis accounts for 3.9%, and the remaining 0.1% is derived from other sources [7].

With the growing demand for hydrogen production and the exploration of alternative energy sources, steam methane reforming presents a promising approach for efficient electricity generation [8]. To ensure its effectiveness and efficiency and minimize carbon dioxide emissions, achieving optimal control of the SMR process becomes essential. However, modeling, controlling, and optimizing an SMR plant can be challenging due to the complex interactions between process variables and the performance of the reforming reactor. Traditional experimental approaches for such tasks are often time-consuming, expensive, and limited in exploring a wide range of operating conditions [9]. A promising alternative involves investigating the plant behavior through simulation tools such as Aspen Plus, which significantly reduces the experimental costs. Utilizing Aspen Plus offers significant advantages due to its flexibility across various process configurations. This flexibility enables the optimization of diverse operational conditions and the determination of process limitations within these settings [9].

Besides, addressing the challenges posed by the exothermic nature of reactions in steam methane reforming plants is necessary. This prevents issues such as catalyst deactivation and coke formation caused by the excessively high reactor temperatures [10]. To mitigate these concerns, a proposed control scheme should be utilized to regulate the reactor temperature. Traditional control methods, such as standard PID control loops, are commonly employed in reforming plants. While these methods provide simplicity and convenience [11], they often struggle with real-time parameter adjustments and fail to adapt to varying control targets in different operational states, impacting their practical application [12]. The nonlinear dynamic behavior of the SMR process, involving complex interactions between flow, heat, and mass transfer, together with its chemical reactions, further complicates the control efforts. Operators often prioritize safety over economic optimization, leading to difficulties in sustaining desired hydrogen production levels without violating process constraints [13].

To address these challenges and improve the control of the SMR process, the implementation of advanced process control (APC) techniques at the supervisory or regulatory control level has been chosen. Most studies have highlighted that APC applications can reduce variability caused by disturbances. This reduction would reduce energy and utility consumption, improve product quality, minimize losses, and increase throughput [14]. Among the APC techniques, model predictive control is a popular choice. Model predictive control (MPC) is an advanced technique used for controlling dynamic systems subject to constraints [15]. It involves a set of control methods that utilize a process model to predict the future behavior of the controlled system [16]. An extensive review of MPC applications in chemical processes is available in the work by Arumugasamy and Ahmad [17] in 2012.

Different control approaches have been suggested in literature in order to control a methane reformer. In the study conducted by Alatiqi and Meziou [18] in 1991, a proportional-integral-derivative

(PID) controller was implemented to control the methane conversion in the steam methane reforming (SMR) process. By adjusting the steam flow rate, the availability of steam as a reactant can be controlled, influencing the reaction and the conversion of methane. Another study conducted by Sankararao and Lee [19] in 2012 focused on the application of model predictive control. In their research, the controlled variable was the exiting flow rate of hydrogen with the steam-to-methane ratio as the manipulated variable. Meanwhile, in 2016, Kyriakides, Seferlis [20] also conducted a study that focused on using model predictive control to regulate the hydrogen production rate by adjusting methane flow rates entering the SMR reactor.

Then, in 2019, Galusnyak and Dragan [21] conducted a study on the performance of a PID controller to regulate temperature and pressure within the reformer. The PID controller utilized feedback from temperature and pressure sensors to continuously adjust the manipulated variables, which are the heating and cooling rates, to maintain the desired temperature and pressure within the reformer. Overall, the research of Galusnyak and Dragan [21] highlighted the potential of PID control in achieving precise and reliable control of the reformer's temperature and pressure in the SMR process. However, if the operating conditions of the reformer change significantly, PID controllers may not automatically adjust to the new conditions.

From a controller standpoint, both PID and MPC controllers perform well in controlling the steam methane reforming (SMR) process. However, PID controllers may struggle to handle disturbances and can introduce errors in the control response [12]. On the other hand, MPC shows great performance compared to the other controllers. It greatly improves the stability of hydrogen production in the SMR process [13]. However, the specific application of state-space MPC within the context of methane reformers remains unexplored in the existing literature.

This study will focus on the development and implementation of state-space MPC for optimizing a steam reforming plant together with an accurate process model that captures the dynamic behavior and transient response of the SMR process. Aiming to monitor the control of reactor outlet temperature and hydrogen production, model predictive control offers an optimization-based closed-loop control strategy that directly incorporates process input and output constraints into the problem formulation [13]. Recent research highlighted the state-space model as the practical choice for representing process plants due to its ability to encompass a broader range of dynamic behaviors more efficiently than convolution models [22]. Furthermore, the formulation of the state-space model in state-space MPC controller design simplifies relevant system analyses [23]. Generally, state-space MPC is a type of linear MPC which employs the state-space model as its process model. This control technique has been explored across various studies, including nuclear power stations [24], coke furnaces [23], solar power systems [25], refineries, and petrochemical plants. A deeper exploration of the development and challenges of linear-based MPC can be found by referring to the work presented by Darby and Nikolaou [26] in 2012.

The structure of this paper is organized as follows; Initially, an elaboration on the reactor's steady-state and dynamic modeling is provided. Secondly, a brief overview is given regarding the model identification technique and the development of the controller. Thirdly, the outcomes, including reactor validation, sensitivity analysis, linear model identification, and assessments of MPC performance, are presented and discussed. Finally, the paper concludes with research findings and suggestions for future studies.

## 2. Materials and Methods

### 2.1. Reactor Modeling

The reactor considered in this work was adopted from Othman, Imran [27] work in 2019, which resembles a conventional industrial reactor with a length-to-diameter ratio of over 50. The reactor operates at a high temperature of around 730 °C and a pressure of around 1 bar. These severe conditions are needed for the reforming process to take place inside the reactor. The feed to the reactor contains methane gas and steam. Methane, being a key component of natural gas, is preferred for SMR due to its high hydrogen-to-carbon ratio within the hydrocarbon group. This characteristic of methane has resulted in more efficient and selective hydrogen production while minimizing the formation of undesired by-products [28].

Steam methane reforming (SMR) is known to require high temperatures and pressures, which can result in increased operating costs [29]. However, there are ways to address this challenge and

improve the process efficiency. One approach is the use of catalysts, typically nickel-based catalysts, which help reduce energy transfer requirements, minimize reaction time, and increase the yield of hydrogen [30]. Research conducted by Bej, Pradhan [30] in 2013 demonstrated that catalysts containing 10% nickel exhibit excellent performance in terms of methane conversion to hydrogen. At a temperature of 700 °C, they achieved a high conversion rate of 95.7%. These findings highlight the significance of catalyst composition in optimizing the SMR process.

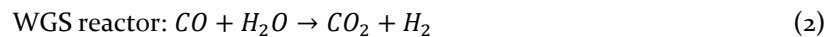
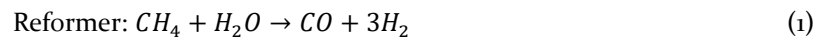
During the reforming process, methane will react with steam, which is moved over a Nickel-based catalyst bed to form a combination of carbon monoxide (CO) and hydrogen [27]. Then, the syngas resulting from reforming undergo a water-gas shift reaction, where carbon monoxide from the initial phase reacts with steam to produce additional hydrogen and carbon dioxide. The resulting mixture can be further processed through  $CO_2$  removal or pressure swing adsorption (PSA) to obtain purified hydrogen with a high level of purity, closely to 100% [29]. The plug flow reactor design features and steady state operating condition work are shown in Table 1 [27]. Based on the table, methane and steam are the feed inputs, while hydrogen, carbon monoxide, and carbon dioxide are the resulting products. All these components are available in the Aspen Plus database for simulation.

**Table 1.** Operating conditions for SMR reactor simulation [27].

	Parameters	Values	Unit
Methane	Flowrate	2550	kg/hr
	Temperature	25	°C
	Pressure	1	bar
Steam	Flowrate	8000	kg/hr
	Temperature	1000	°C
	Pressure	2	bar
Reactor	Temperature	730	°C
	Pressure	1	bar
	Catalyst loading	160	kg
	Length	10	m
	Diameter	0.2	m

## 2.2. Kinetic Model and Parameters

Generally, the main chemical reactions that occur during steam methane reforming (SMR) are represented by Equations 1 and 2, which illustrate the reformer and water-gas shift reactions [28]. These interconnected reactions play a crucial role in hydrogen and carbon dioxide production, and they are fundamental steps in the SMR process.



To gain a better understanding of the kinetics for the SMR reaction, several kinetic models have been developed by researchers such as Chen, Prasad [31], and Singh, Singh [32]. These models follow the Langmuir-Hinshelwood Hougen-Watson (LHHW) kinetic rate equations, which describe the reaction mechanism based on the two main reactions mentioned in Equations 1 and 2. By studying and refining these kinetic models, researchers aim to enhance the understanding of the SMR process and improve its efficiency. The kinetic parameters utilized in this work are displayed in Table 2, referenced from the work of Imran [27]. In order to achieve the desired reactor temperature profile and methane conversion, slight tuning of the reaction kinetic parameters has been performed. These minor adjustments are required due to the difference in modeling techniques used in the Aspen Plus simulation.

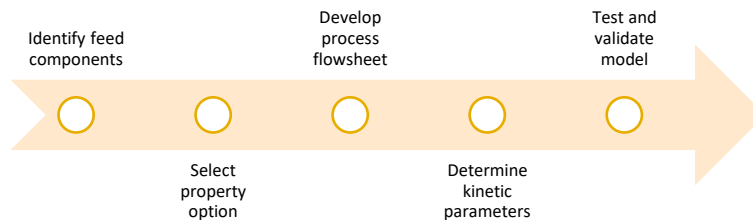
**Table 2.** Kinetic parameter for methane steam reforming [27].

Parameter	Pre-exponential Factor	Ea or ΔH (J/mol)	ln K
$k_1$	$4.2248 \times 10^{15} \left( \frac{\text{mol atm}^{0.5}}{\text{gh}} \right)$	240,100	
$K_1$	$7.846 \times 10^{12} (\text{atm}^2)$	220,200	29.69
$K_{CH_4}$	$6.65 \times 10^{-4} (\text{atm}^{-1})$	-38,280	-7.31
$K_{H_2O}$	$1.77 \times 10^5 (\text{atm}^{-1})$	88,680	12.08
$K_{H_2}$	$6.12 \times 10^{-5} (\text{atm}^{-1})$	-82,900	-9.70
$K_{CO}$	$8.23 \times 10^{-5} (\text{atm}^{-1})$	-70,650	-9.41

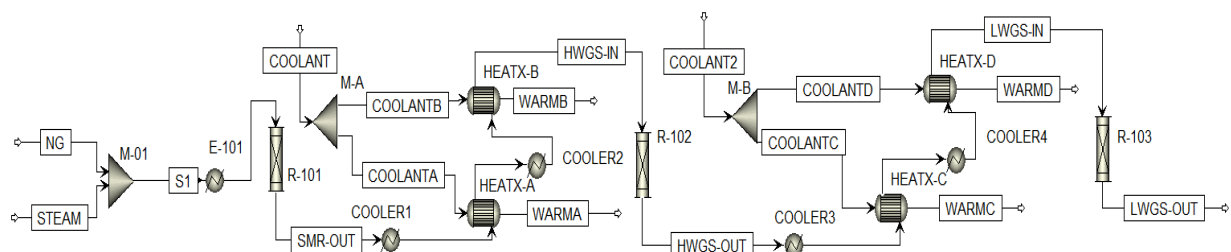
2.3. Steady State Simulation

Figure 1 illustrates the simplified process flow chart used to develop the steady-state model via Aspen Plus. The process involved selecting feed components through Aspen Properties without the need for custom components since all the required components were available in the database. Property method selection in Aspen Plus was used to represent the thermodynamic and phase property of the process. Here, the Redlich-Kwong-Soave equation of state with the Modified-Huron-Vidal mixing rule (RKSMHV2) is used to represent the reforming process [27]. The process continued by building the process flowsheet, as shown in Figure 2. Based on the figure, three plug flow reactors are simulated to represent the reforming process (R-101), high-temperature water gas shift (R-102), and low-temperature water gas shift (R-103) in the system.

Table 3 summarizes the model blocks used in the flowsheet and their corresponding descriptions. The simulation then defined the reaction type and kinetic parameters of the process, as previously discussed. With these settings developed, the model was prepared for simulation and validation.



**Figure 1.** Simplified flow chart of steady state modeling process using Aspen Plus.



**Figure 2.** Process flow diagram of steam methane reforming in Aspen Plus.

**Table 3.** Types of blocks with their description in simulation.

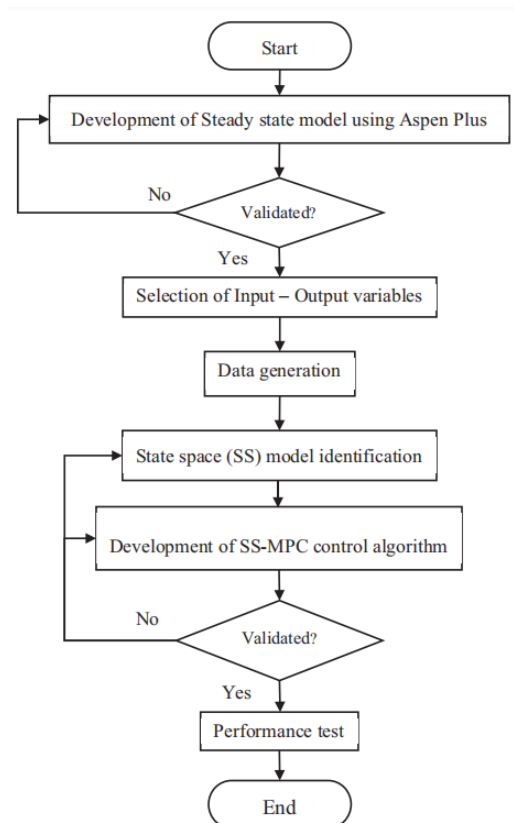
Id Block	Type of Block	Description
M-01	Mixer	Feed methane and steam mixed
E-101	Heater	Pre-heat the mixed gas until the temperature of 730°C
R-101	R-Plug	SMR reaction takes placed
HEATX-A, HEATX-B	Heat-X	Product gas from SMR was cooled to the temperature of 450°C
R-102	R-Plug	High-temperature WGS reactions take placed
HEATX-C, HEATX-D	Heat-X	Product gas from WGS was cooled to the temperature of 210°C
R-103	R-Plug	Low temperature WGS reaction takes placed

*2.4. Dynamic Simulation*

The existing steady-state Aspen Plus model was exported to Aspen Dynamic for dynamic simulation to create a dynamic model suitable for the online control scheme. During the export process, the flow-driven simulation option was chosen. The resulting dynamic model aims to provide real-time plant inputs to the MPC for subsequent control implementation.

*2.5. Control Scheme Development*

Figure 3 shows the flow diagram outlining the development of state-space MPC control. Further elaboration on each step illustrated in the figure will be provided later in this section.



**Figure 3.** Flow diagram for state-space MPC control scheme development.

*2.5.1. Input-output Selection*

Based on the previously mentioned findings, most of the control objectives in methane reformer reactor study focus on hydrogen production and reactor temperature. In practical applications, temperature control involves adjusting either jacket temperature or jacket feed flow rates to maintain stable reactor temperatures and avoid temperature fluctuations. Hydrogen

production is typically managed by manipulating steam and methane flow rates and adjusting the steam-to-methane ratio to enhance production efficiency.

For this study, the manipulated variables chosen are the steam flow rate, methane flow rate, and jacket temperature, labelled MV<sub>1</sub>, MV<sub>2</sub>, and MV<sub>3</sub>, respectively. These variables aim to control hydrogen production and maintain the reactor outlet temperature, labelled as control variables CV<sub>1</sub> and CV<sub>2</sub>. Sensitivity analysis among these variables has been conducted to gain a deeper insight into the system behavior.

### 2.5.2. Data Generation

The identification technique requires the input-output data from the process to determine its parameters according to the desired model type. In this study's identification purpose, a dataset comprising training and validation data was created using the Aspen Dynamic model. By using MATLAB Simulink, the steam flow rate, methane flow rate, and jacket temperature, were induced a variation of  $\pm 20\%$  from their respective steady-state values based on uniform random signals. This dataset, spanning 250 minutes with a sampling time of 0.01 minutes, was generated.

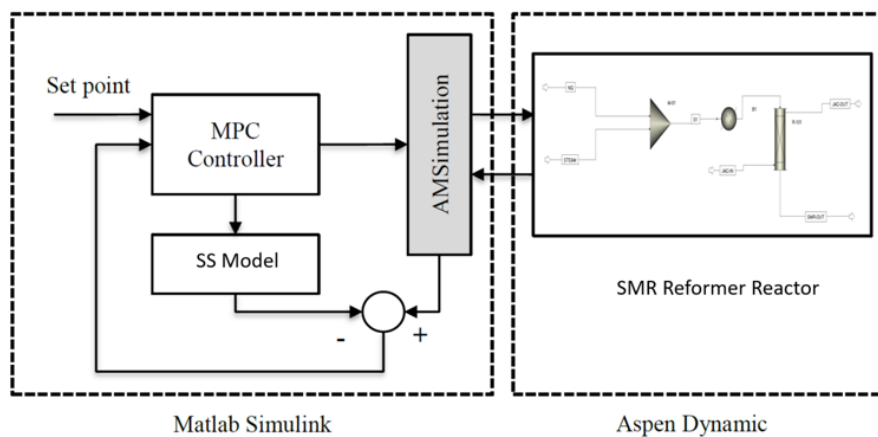
### 2.5.3. State-space Model Identification

Within this study, a conventional Multiple Input Multiple Output (MIMO) model was employed to construct the state-space model. All data were simultaneously generated, in which the model was identified using a state-space identification technique based on the sub-space method [33]. Then, the analysis of model performance was conducted using Normalized Root Mean Square Error (NRMSE). The approved linear model resulting from this process would subsequently be used as the process model for implementation within the MPC framework and as the base model for PID tuning.

### 2.5.4. State-space Model Predictive Control

In this study, a state-space model MPC was developed to control both the reactor outlet temperature and hydrogen production. Typically, MPC operates by solving an optimization problem or objective function at each control interval. The solution derived from this process will provide the optimal manipulated variables to be implemented in the plant until the following control interval [34].

Next, following the development of the model and controller algorithm, the subsequent step involved connecting the control scheme with Aspen Dynamic. Within the MATLAB Simulink environment, the Aspen Dynamic model acted as an actual plant by continuously sending plant information for the MPC to control. This connection between MATLAB Simulink and Aspen Dynamic was established through the AMSimulation block. Figure 4 presents a diagram of the simplified MPC control scheme linked with Aspen Dynamic.



**Figure 4.** MPC control scheme with Aspen Dynamic.

### 2.5.5. Performance Test

In order to evaluate MPC controller performance, the PID controller was developed as a comparison in set point tracking and disturbance rejection tests. During set point tracking, an initial set point value is set, and then a step change is introduced to the set point to a new desired value. In this case, the objective is to step up the hydrogen production to 20%. The controller's response is monitored to observe how quickly and accurately it adjusts the manipulated variables, such as steam flow rate, methane flow rate, and jacket temperature, to bring the process output to the new set point.

While stepping up the hydrogen production, it is necessary to monitor the capability of the controller to maintain the reactor outlet temperature simultaneously during the disturbance rejection. In this case, the disturbance variables were not introduced directly to the model. By conducting these tests, the controller's performance in addressing the challenges of the SMR process can be thoroughly assessed, leading to refinements in the controller design and tuning for optimal process regulation.

## 3. Results and Discussion

### 3.1. Model Validation and Sensitivity Analysis

Model validation is an important step, as the simulation model is valid only if the model is an accurate representation of the actual system. In this study, validation involved evaluating the simulated SMR reaction in Aspen Plus against experimental work conducted by Khzouz and Gkanas [35] in 2018. The SMR reactor modeled in the simulation was based on the operating and design conditions outlined in Table 4. Methane and steam conversion rates and hydrogen yield were compared between the model's outputs and the experimental data shown in Table 5.

The reliability of the model was assured due to the low relative errors observed in the reformer product compositions, specifically under 8.7% for methane conversion. This reliability suggests that the model was sufficiently robust for investigating the performance of the industrial process.

**Table 4.** Operating conditions for validation [35].

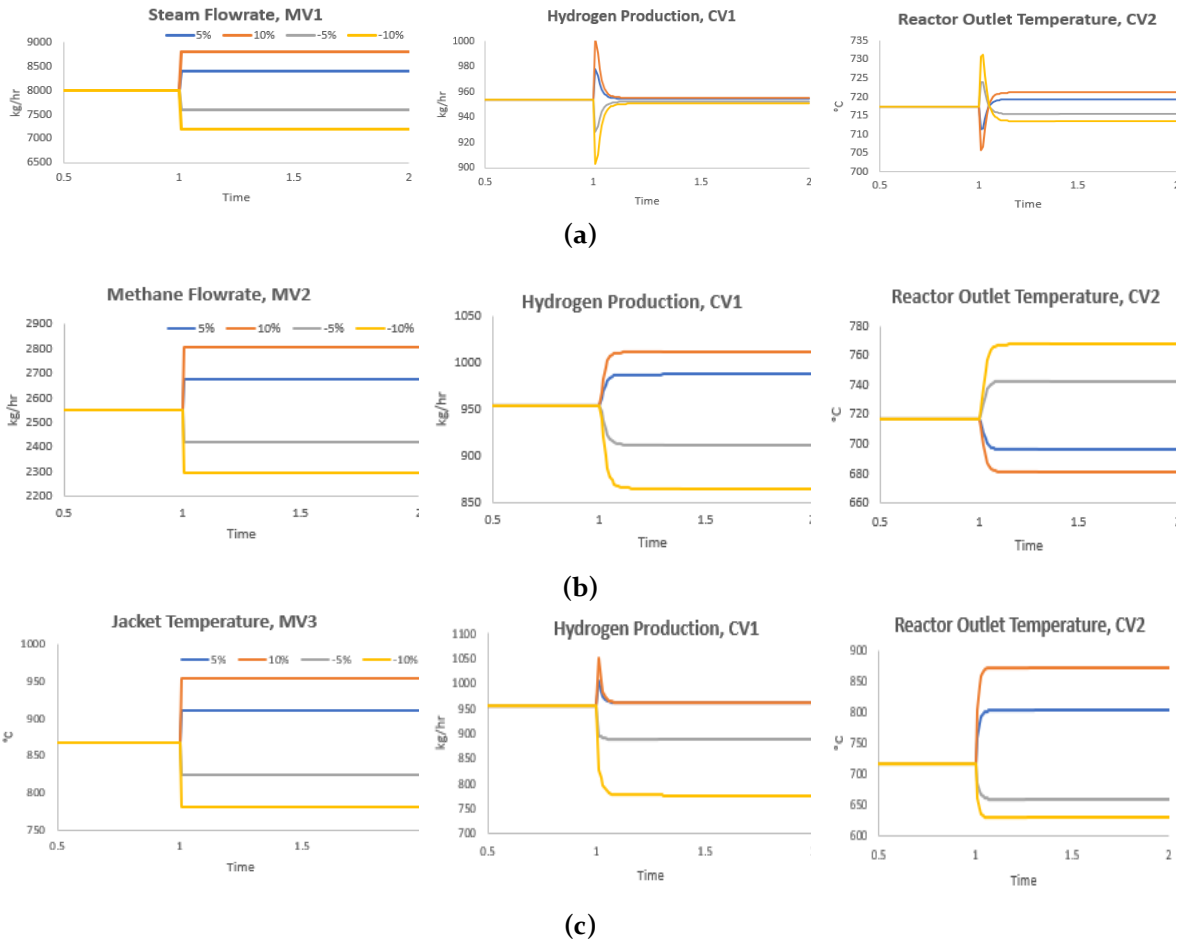
Parameters	Values
Temperature, °C	700
Pressure, atm	1
Steam-to-methane ratio	3
Catalyst used	Ni-based catalyst

**Table 5.** SMR reactants conversion and production validation.

Evaluation	Experimental Data [35]	Simulation Model
Methane conversion (%)	92.00	100.00
Steam conversion (%)	30.00	35.79
Hydrogen yield (mol/mol CH <sub>4</sub> )	2.3	3.0

The sensitivity analysis for the effect of steam flowrate (MV<sub>1</sub>), methane flowrate (MV<sub>2</sub>), and jacket temperature (MV<sub>3</sub>) on hydrogen production (CV<sub>1</sub>) and reactor outlet temperature (CV<sub>2</sub>) is presented in Figure 5.

During the reforming process, an increase in steam and methane flow rate, acting as the reactants of the process, will cause the reaction rate to become higher. This leads to higher hydrogen production, as observed in the figure. Based on the figures, the linear region for hydrogen production and reactor outlet temperature is under  $\pm 5\%$ . Thus, steam and methane flow rate, as well as jacket temperature that is greater than these values, will produce a nonlinear profile as presented in Figure 5 for manipulated variables with a  $\pm 10\%$  change. Besides, observing the hydrogen production profile can be regarded as a second-order process due to its overshoot behavior during substantial step change.



**Figure 5.** Sensitivity analysis results for dynamics model. (a) MV<sub>1</sub>; (b) MV<sub>2</sub>; (c) MV<sub>3</sub>

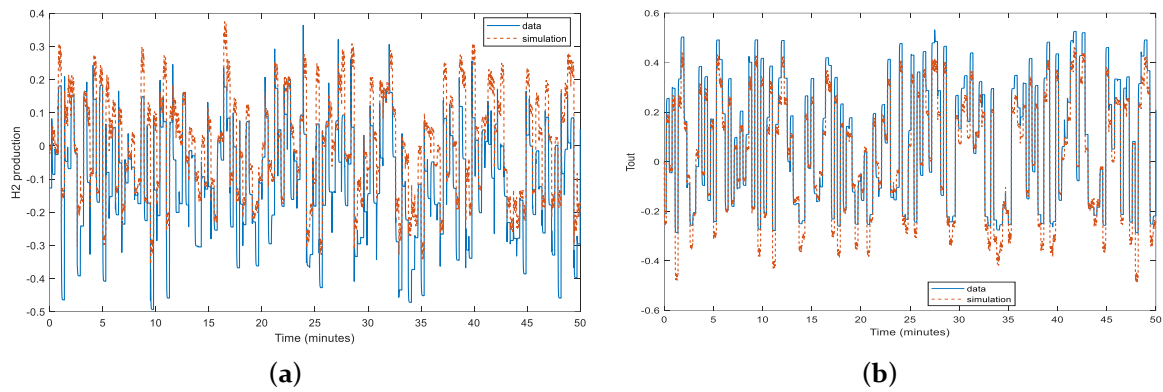
3.2. Linear Model Result

Table 6 outlines the results of the model identification process. Based on the table, CV<sub>1</sub> demonstrated good model identification performance with NRMSE above 0.80. The model identification validation profile for the state space model is illustrated in Figure 6. Examining the identification results for CV<sub>1</sub> and CV<sub>2</sub> reveals limitations in the linear model’s ability to accurately estimate specific regions within the validation data. This inadequacy has resulted from the limitations of linear model identification techniques in capturing higher-order process variables, such as the second-order behavior exhibited by CV<sub>1</sub>, as observed in Figure 5.

Thus, controlling CV<sub>1</sub> and CV<sub>2</sub> profiles will be challenging to MPC, as it heavily relies on the precision of its process model to make error estimation of the current process. To address model inaccuracies, adjusting tuning weights within the MPC framework stands as a potential compensatory measure.

**Table 6.** Identification results for State space model based on validation data.

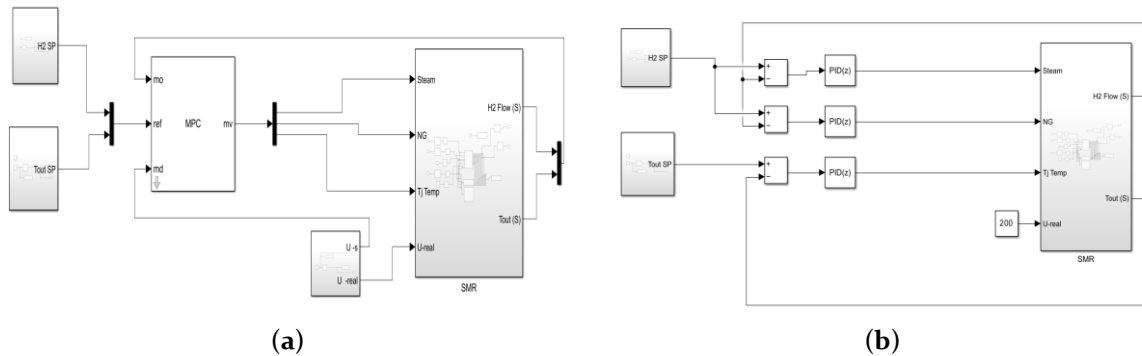
Control Variable	NRMSE
CV <sub>1</sub>	0.8567
CV <sub>2</sub>	0.3005



**Figure 6.** Model identification validation results for the state space model. (a) Hydrogen production; (b) Reactor outlet temperature

3.3. Controller Performance

This section focuses on evaluating the controller performance of both state-space MPC and PID after the development of control scheme presented in Figure 7. The tuning parameters for both controllers are detailed in Table 7. For state-space MPC, the prediction and control horizons were initially determined following recommendations by [36] and [37] were further re-tuned during the online simulation. The tuning weights for state-space MPC were derived by simulating the linear model using MATLAB MPC Toolbox. Initially obtained from the toolbox, these weights were used as the initial tuning for MPC in controlling the SMR reactor online. Meanwhile, the PID tuning parameters were obtained using MATLAB PID Toolbox. The PID was tuned to achieve precise control over outputs and implement more aggressive control moves.



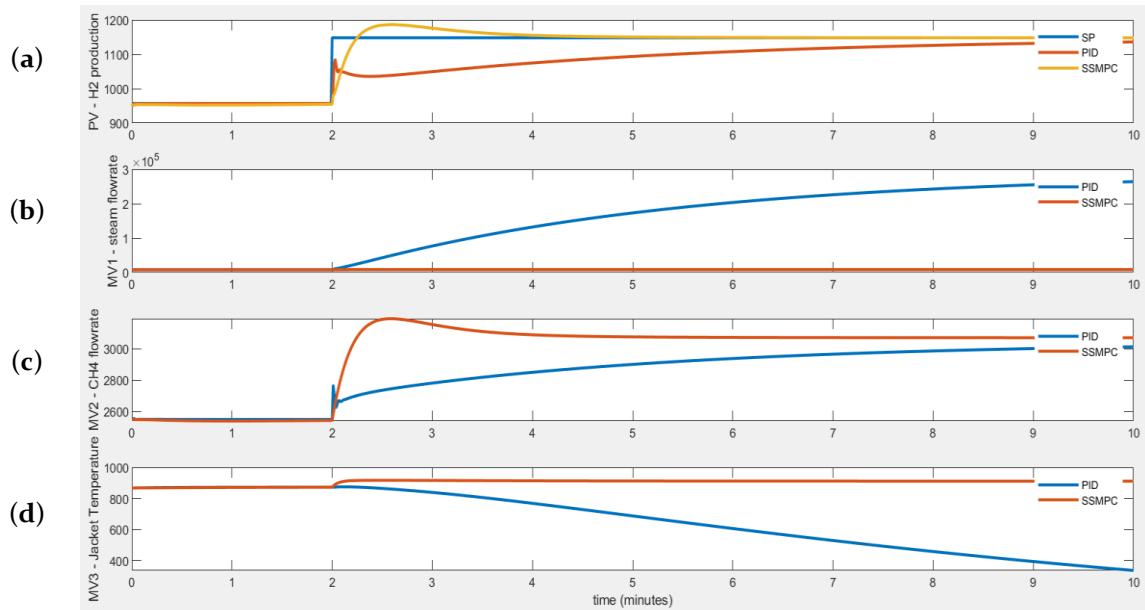
**Figure 7.** Control scheme developed in Simulink. (a) State-space MPC; (b) Multiloop PID

**Table 7.** State-space MPC and PID tuning parameters.

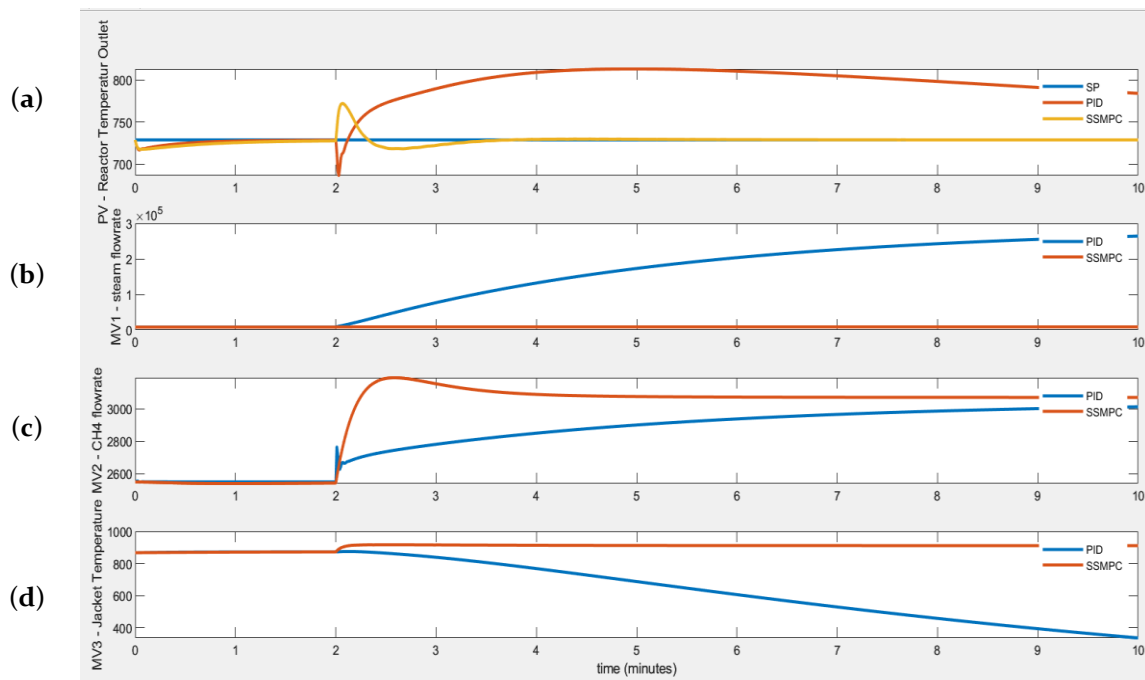
State-space MPC		PID			
		MV1-CV1	MV2-CV2	MV3-CV3	
Prediction horizon	40	Proportional (P)	0.91	1	0.01
Control horizon	10	Integral (I)	181.56	1	0.70
Output tuning weights	[0.135; 0.135]	Derivative (D)	-	-	-
Input tuning weights	[0; 0; 0]				
Input tuning rate weights	[0.739; 0.739; 0.739]				

Figure 8 illustrates the performance of both state-space MPC and PID controllers in setpoint tracking, from hydrogen production at steady state to a 20% increase in hydrogen production at 2 minutes. Assessing the set point tracking in the CV1 profile, the state space MPC controller

demonstrated superior performance compared to PID, performing a more aggressive tracking capability. However, this aggressiveness led to an overshoot in hydrogen production, as observed in the CV<sub>1</sub> profile. Despite the hydrogen production overshoot, the state-space MPC exhibited excellent performance when considering the primary concern of set point tracking, particularly in the CV<sub>1</sub> profile.



**Figure 8.** State space MPC and PID control performance in the setpoint tracking test for each profile. (a) CV<sub>1</sub>; (b) MV<sub>1</sub>; (c) MV<sub>2</sub>; (d) MV<sub>3</sub>



**Figure 9.** State space MPC and PID control performance in disturbance rejection test for each profile. (a) CV<sub>2</sub>; (b) MV<sub>1</sub>; (c) MV<sub>2</sub>; (d) MV<sub>3</sub>

The results of the disturbance rejection test are displayed in Figure 9. Based on the figure, state-space MPC had shown superior performance in maintaining the reactor outlet temperature, as shown in CV<sub>2</sub> profile. State-space MPC rejected the disturbance effect more effectively than PID, as shown in the MV profiles. This improved performance is due to the predictive capabilities enabled by the prediction horizon, enabling the state space MPC to compute controller actions more swiftly than PID.

Referring to Figure 8 and Figure 9, state-space MPC demonstrated outstanding performance in the CV<sub>1</sub> and CV<sub>2</sub> profiles. This capability of MPC to effectively control hydrogen production was also highlighted in a study by Kyriakides, Seferlis [20]. This holds significance as the profitability of

production relies heavily on consistently achieving efficient hydrogen production within the desired capacity. However, the limitation of state-space MPC is due to the inaccuracies in its process model, emphasizing the drawbacks of the linear model identification technique in accurately modeling the process dynamics. Although tuning state-space MPC can compensate for the model's lower accuracy to some extent, addressing the root cause of the problem is essential.

#### 4. Conclusions

In conclusion, this study successfully developed a state-space model predictive controller for optimizing the steam methane reforming process by controlling the reformer reactor's outlet temperature and enhancing hydrogen production. The utilization of Aspen Plus and Aspen Dynamic facilitated the simulation of the reactor model for steady-state and dynamic modeling, respectively. Employing a linear state-space model derived from the reactor's dynamic model data via state-space model identification techniques allowed for the implementation of the state-space MPC control scheme. The model validation results presented the comparable performance of the state space model, leading to its selection as the process model for the MPC. The control objectives within the state-space MPC were effectively addressed using sequential quadratic programming (SQP) techniques. When comparing the overall results, state-space MPC generally outperforms PID in terms of set point tracking and disturbance rejection. Applying the process model for prediction and an optimizer for computing the optimal control output provides state-space MPC an advantage over the PID controllers. Although PID controllers, when fine-tuned, could perform comparably with state-space MPC in regulating the reactor outlet temperature, the study's reliance on linear model identification restricted the state-space MPC's performance. Further improvements could be achieved by adopting more precise nonlinear modeling techniques, offering potential advancements for methane reforming reactor control through nonlinear model-based MPC.

#### References

1. Kabeyi, M.J.B. and O.A. Olanrewaju, *Sustainable Energy Transition for Renewable and Low Carbon Grid Electricity Generation and Supply*. *Frontiers in Energy Research*, 2022. **9**.
2. Hannun, R.M. and A.H. Abdul Razzaq, *Air Pollution Resulted from Coal, Oil and Gas Firing in Thermal Power Plants and Treatment: A Review*. *IOP Conference Series: Earth and Environmental Science*, 2022. **1002**(1): p. 012008.
3. Cao, J., et al., *Current status, future prediction and offset potential of fossil fuel CO<sub>2</sub> emissions in China*. *Journal of Cleaner Production*, 2023. **426**: p. 139207.
4. Bruhwiler, L., et al., *Observations of greenhouse gases as climate indicators*. *Clim Change*, 2021. **165**(1): p. 12.
5. Aziz, M. *Liquid Hydrogen: A Review on Liquefaction, Storage, Transportation, and Safety*. *Energies*, 2021. **14**, DOI: 10.3390/en14185917.
6. Lee, S., et al., *Scenario-Based Techno-Economic Analysis of Steam Methane Reforming Process for Hydrogen Production*. *Applied Sciences*, 2021. **11**(13): p. 6021.
7. Li, S., et al., *Hydrogen Production: State of Technology*. *IOP Conference Series: Earth and Environment*, 2020.
8. Wang, J., et al., *Transient numerical modeling and model predictive control of an industrial-scale steam methane reforming reactor*. *International Journal of Hydrogen Energy*, 2021. **46**(29): p. 15241-15256.
9. Çepelioğullar Mutlu, Ö. and T. Zeng, *Challenges and Opportunities of Modeling Biomass Gasification in Aspen Plus: A Comprehensive Review*. *Chemical Engineering & Technology*, 2020. **43**.
10. Oechsler, B., et al., *Simulation and Control of Steam Reforming of Natural Gas—Reactor Temperature Control Using Residual Gas*. *Industrial & Engineering Chemistry Research*, 2017. **56**.
11. Sartipizadeh, H. and T.L. Vincent, *Robust model predictive control of a catalytic autothermal methane reformer for fuel cell applications*. *Control Engineering Practice*, 2018. **76**: p. 31-40.
12. Li, J., et al., *Improved PID Controller Based on BP Neural Network*. *Journal of Physics: Conference Series*, 2023. **2479**(1): p. 012062.
13. Zanolli, S.M. and L. Orlietti. *Steam reforming plant optimization with Model Predictive Control. in 2013 IEEE 18th Conference on Emerging Technologies & Factory Automation (ETFA)*. 2013.

14. Gous, G.Z., et al., *Advanced Regulatory Control Techniques for Improved Averaging Level Control Performance*. Industrial & Engineering Chemistry Research, 2023. **62**(38): p. 15578-15587.
15. Correa Córdova, M.L., *High Performance Implementation of MPC Schemes for Fast Systems*. 2016, Pontificia Universidad Católica del Perú (Peru): Peru. p. 140.
16. Ławryńczuk, M. *Approximate state-space model predictive control*. in *2015 20th International Conference on Methods and Models in Automation and Robotics (MMAR)*. 2015.
17. Arumugasamy, S.K. and Z. Ahmad, *Model Predictive Control (MPC) and Its Current Issues in Chemical Engineering*. Chemical Engineering Communications, 2012. **199**: p. 472-511.
18. Alatiqi, I.M. and A.M. Meziou, *Dynamic simulation and adaptive control of an industrial steam gas reformer*. Computers & Chemical Engineering, 1991. **15**(3): p. 147-155.
19. Sankararao, B. and J.H. Lee, *Dynamic modeling, simulation and control (using MPC) of an industrial steam reformer*. 2012 12th International Conference on Control, Automation and Systems, 2012: p. 594-600.
20. Kyriakides, A.-S., et al., *Model Predictive Control for Hydrogen Production in a Membrane Methane Steam Reforming Reactor*. Chemical engineering transactions, 2016. **52**: p. 991-996.
21. Galusnyak, S. and S. Dragan, *Mathematical modeling of steam methane reforming process*. Studia Universitatis Babeş-Bolyai Chemia, 2019. **64**: p. 7-18.
22. Simkoff, J.M., et al., *Plant-Model Mismatch Estimation from Closed-Loop Data for State-Space Model Predictive Control*. Industrial & Engineering Chemistry Research, 2018. **57**(10): p. 3732-3741.
23. Zhang, R., S. Wu, and F. Gao, *State Space Model Predictive Control for Advanced Process Operation: A Review of Recent Development, New Results, and Insight*. Industrial & Engineering Chemistry Research, 2017. **56**(18): p. 5360-5394.
24. Wang, G., et al., *State-Space Model Predictive Control Method for Core Power Control in Pressurized Water Reactor Nuclear Power Stations*. Nuclear Engineering and Technology, 2017. **49**(1): p. 134-140.
25. Camacho, E.F., et al. *Incremental State-Space Model Predictive Control of a Fresnel Solar Collector Field*. Energies, 2019. **12**, DOI: 10.3390/en12010003.
26. Darby, M.L. and M. Nikolaou, *MPC: Current practice and challenges*. Control Engineering Practice, 2012. **20**: p. 328-342.
27. Othman, M., U. Imran, and A. Ahmad, *Environment and Economic Assessment of Hydrogen Production from Methane and Ethanol*. 2019.
28. Agyekum, E.B., et al. *A Critical Review of Renewable Hydrogen Production Methods: Factors Affecting Their Scale-Up and Its Role in Future Energy Generation*. Membranes, 2022. **12**, DOI: 10.3390/membranes12020173.
29. Nikolaidis, P. and A. Poullikkas, *A comparative overview of hydrogen production processes*. Renewable and Sustainable Energy Reviews, 2017. **67**: p. 597-611.
30. Bej, B., N.C. Pradhan, and S. Neogi, *Production of hydrogen by steam reforming of methane over alumina supported nano-NiO/SiO<sub>2</sub> catalyst*. Catalysis Today, 2013. **207**: p. 28-35.
31. Chen, Z., et al., *Simulation for steam reforming of natural gas with oxygen input in a novel membrane reformer*. Fuel Processing Technology, 2003. **83**(1): p. 235-252.
32. Singh, A.P., et al., *Steam reforming of methane and methanol in simulated macro & micro-scale membrane reactors: Selective separation of hydrogen for optimum conversion*. Journal of Natural Gas Science and Engineering, 2014. **18**: p. 286-295.
33. Favoreel, W., B. De Moor, and P. Van Overschee, *Subspace state space system identification for industrial processes*. Journal of Process Control, 2000. **10**(2): p. 149-155.
34. Parihar, S., et al. *Model Predictive Control and Its Role in Biomedical Therapeutic Automation: A Brief Review*. Applied System Innovation, 2022. **5**, DOI: 10.3390/asi5060118.
35. Khzouz, M. and E.I. Gkanas *Experimental and Numerical Study of Low Temperature Methane Steam Reforming for Hydrogen Production*. Catalysts, 2018. **8**, DOI: 10.3390/catal8010005.
36. Seborg, D.E., et al., *Process Dynamics and Control, 4th Edition*. 2016: Wiley.
37. Dinie, M., et al., *Temperature control of low density polyethylene (LDPE) tubular reactor using Model Predictive Control (MPC)*. IOP Conference Series: Materials Science and Engineering, 2020.