

Advanced Control of the Steam Reforming Through a Simulation Study

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Abstract

The one-dimensional model was selected to simulate the steam reforming to produce hydrogen in a fixed-bed reactor filled with catalyst particles. The model consists of mass balance of all stream components, heat balance on gas inside the reactor and tube wall reactor. This model was solved by using MATLAB/Simulink. The simulation results have been compared with actual data to validate the model. It was found the good agreement between the main exit molar rate and reformed gas temperature from the reforming reactor and the commercial reformer. Three different control methods were designed which are proportional-integral derivative, cascade and multi-loop to maintain the exit gas temperature. A comparison between these control methods have been made by using step change at different values of feed conditions. These results show that the multi-loop controller has rapidity, very good durability, more suitable, little offset, lower overshoot and less integral absolute error.

Keyword: Fixed bed Reactor, PID Controller, Multi-loop controller, Cascade controller, MATLAB/Simulink.

1.Introduction

A considerable amount of hydrogen is produced by steam reforming of natural gas. Previously most of the hydrogen was used in petroleum refining for treating light naphtha and middle distillates to provide for desulfurization and product stability. Current requirements for hydrogen are in petroleum refining, manufacture of ammonia, methanol, chemicals, welding, etc. The reforming process is carried out in multi-tubular reactors supported by Ni-catalysts at temperatures varying from 500-900C and molar steam to carbon ratios between 2.00 and 9.00. Due to the importance of the operation, the control of the process is subject to continuous improvement, the production of hydrogen using the SRM has been investigated by a lot of authors [1-3]. The fired heater and reformer multi tubular reactors are subject to fluctuations that disturb the production rate quality of hydrogen and the level of the steam drum downstream from the reformer [4]. Steam reforming of methane is a quite complex process. It not only involves the transfer and diffusion of reactants and products, between the bulk phase and catalyst surface, as well as within the catalyst, but also involves several reactions simultaneously in parallel or in series. The earliest SMR modeling efforts focused on steady-state modeling. [5] developed a mathematical model for a top fired steam reformer, including its furnace. A one-dimensional heterogeneous model, with mass transfer limitation in the catalyst pellets, was used to describe the reactor. It was shown that variation of the extinction coefficient of the combustion gas and of the effective emissivity of the reaction tubes might exert significant influence on the reactor wall and process gas temperatures, indicating that these parameters should not be neglected during the analysis of real industrial operations. [6] modeled the conversion process for a single reactor

tube by both chemical reaction models and heat transfer models. The model yields data of temperature, heat transfer and concentrations of hydrogen, carbon monoxide and natural gas along a reactor tube. Simulated temperatures have been validated with measured data from a prototype reformer. [7] developed a one-dimensional mathematical model to simulate methane conversion and hydrogen yield in a fixed-bed reactor filled with catalyst particles. Simulation results show that the steam reforming of methane in a fixed-bed reactor can efficiently store high temperature end thermal energy. [8] developed a dynamic and two-dimensional model for a steam methane reforming process integrated with nuclear heat production is developed. The resulting model fits the reported design conditions of two separate pilot-scale studies. [9] proposed the kinetic-based simulation of methane steam reforming from natural gas and water gas shift reaction for hydrogen production. The results of the simulation show good agreement with results found in the literature. [10] described the combination of chemical-looping combustion (CLC) and steam methane reforming (SMR). The simulation results show a temperature decrease toward the tube center in steady state operation. [11] developed a good computational flow dynamic model. This article discusses some of the issues, challenges, and conceivable arrangements to aid the efficient generation of hydrogen from steam reforming catalytic reactions and membrane reactors of bioproducts and fossil fuels.

[12] investigated the dynamic behavior and control of the low pressure fixed bed reactor . Through the dynamic simulation, the system open loop response has been obtained and the process dynamic is approximated by a simple model. This model is used for the PID controller tuning and the performances of fixed and adaptive PID controllers are compared for load rejection and set point tracking. Finally the proposed optimizer is coupled with a controller for online optimization and hot spot temperature protection. [13] proposed a discrete PI control system and an offset-free linear model predictive controller (MPC) are presented for the co current configuration to address process interactions and sampling delay. MPC offered superior set point tracking relative to discrete-PI control, especially in cases where discrete-PI destabilized the system. [14] designed a control scheme to account for regulation of the reactor outlet temperature, using residual and fuel gas streams as manipulated variables, allowing the analyze of effect of several process variables in reactor performance. The obtained results indicate that the proposed mathematical model can accurately represent the steam reforming process and that the proposed control scheme can allow for efficient operation of the reactor. [15] developed a rigorous computationally efficient closed-loop system with a gain-scheduled model predictive controller (MPC) where a first-principle model of the steam methane reformer is utilized to represent the process dynamics. The gain-scheduled MPC considers critical process parameters of the steam methane reformer such as outlet methane molar concentration and outlet temperature of the reformed gas as the most appropriate and reliable process variables. By simulation of the set-point changes under the influence of the steam methane reformer critical disturbance rejection performances it is shown that reformer tubes could operate in safe temperature range. [16] performed an optimal model predictive control (MPC) strategy was designed to control the hydrogen production rate and the catalyst temperature. Experimental and simulation results indicated that the controller was automated and continuously reliable in the hydrogen production system. In this study initially focuses on selecting mathematical model of an industrial scale steam methane reforming reactor used to produce hydrogen. A simulation program is constructed for steam methane reforming by using the program MATLAB/ Simulink.

It is a powerful software for the simulation of dynamic model analysis and control. It consists of a Simulink part to build the models and study the characteristics of control and dynamic situation. a dynamic model will be developed in Simulink to simulate the transport and used for analysis of control schemes performance under the influence of disturbances in the input variables. In this work, the three type control (PID , Multi-loop , Cascade) is proposed to control the exit reformed gas temperature and evaluate three different feedback control schemes to drive the area-weighted average hydrogen mole fraction measured at the reforming tube outlet to a desired set-point value under the influence of a feed disturbance.

2. Mathematical Models Development

2.1 Static Model Development

The multi tubular reactor to be simulated in this work is placed vertically in a gas fired heater. The heat transfer is by radiation and convection from the fuel gas and flames to the reformer multi tubular reactor and from extended tubes surfaces to the process gas. The reformer tubes were simulated as a one dimensional heterogeneous reactor model. This is applicable for the case where the reformer tube length to diameter ratio is large. Axial dispersion is completely neglected at all flow velocities along the length of the reactor. An equivalent methane feed is calculated at the entry of the reactor, this is based on the assumption that heavier hydrocarbons are very rapidly converted to methane. It is therefore assumed that methane is the primary reactant in the reforming process and heavier hydrocarbons are rapidly hydrocracked to methane at the entrance of the tubular reactor. Consequently, the reaction system inside the reformer tubular reactor is described by the kinetic rate expression for steam-methane reaction, irrespective of the hydrocarbon fed. There are assumptions adopted in this study: 1. axial plug flow for the reforming gases in the tubes is assumed. 2. radial temperature profile is neglected . 3. catalyst particle temperature is uniform and is the same as that of the process gas. 4. heat transfer is by radiation and convection. 5. all the tubes in the reformer are considered to behave similarly. 6. no carbon deposition is assumed to occur in the reformer. Eighth, all hydrocarbons heavier than methane are hydrocracked to methane at the entrance section of the tubes.

2.2. Kinetic Modelling of steam methane reforming

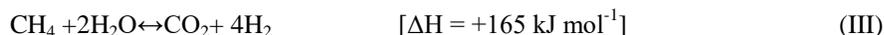
Simulation and most efficient business process projects require information about intrinsic rates of change. The reaction system considered in this study consists of (I)-(III):-Steam Reforming of Methane (SRM);



-Water Gas-Shift (WGS);



-Reverse Methanation (RM).



The rates of reaction were derived from [17] theory of Langmuir-Hinshelwood. They're described by Equations (1) (2) (3) below for SRM, WGS respectively..

$$R_1 = \frac{k_1 \left(P_{\text{CH}_4} P_{\text{H}_2\text{O}} - \frac{P_{\text{H}_2}^3 P_{\text{CO}}}{K_{eq1}} \right)}{p_{\text{H}_2}^{2.5} (\text{Den})^2} \quad (1)$$

$$R_2 = \frac{\frac{k_2}{P_{H_2}} \left(P_{CO} P_{H_2O} - \frac{P_{H_2} P_{CO_2}}{K_{eq_2}} \right)}{(Den)^2} \quad (2)$$

$$R_3 = \frac{\frac{k_3}{P_{H_2}^{3.5}} \left(P_{CH_4} P_{H_2O} - \frac{P_{H_2}^4 P_{CO_2}}{K_{eq_3}} \right)}{(Den)^2} \quad (3)$$

Where Den is :

$$Den = 1 + K_{CO} P_{CO} + K_{H_2} P_{H_2} + K_{CH_4} P_{CH_4} + \frac{K_{H_2O} P_{H_2O}}{P_{H_2}} \quad (4)$$

The reaction rate constants(k_i) are determined by using an Arrhenius approach and steam reforming kinetic parameters for Arrhenius relation are shown in Table [1]:

$$k_i = A_i \exp \left[-\frac{E_i}{RT} \right] \quad (5)$$

Table 1 Steam reforming kinetic parameters for Arrhenius relation[17].

Pre-exponential factor(A_i)	Units	Activation energy(E_i)	Units
$4.225 \cdot 10^{16}$	Kmol Kpa ^{0.5} /kg h	240.1	kJ/mol
$1.995 \cdot 10^4$	Kmol Kpa ⁻¹ /kg h	67.13	kJ/mol
$1.020 \cdot 10^{16}$	Kmol Kpa ^{0.5} /kg h	243.9	kJ/mol

The operating conditions used in the simulation were: feed temperature 500 °C, feed pressure 650 kPa, and speed 15 m/s. The basic characteristics of the steam methane reforming process are shown in Table [2], and the feed composition is shown in Table [3][16].

Table 2- Geometric conditions, catalyst properties, inlet operating conditions parameters [7]

Parameters	value	Parameters	value
Inlet operating conditions		Tube parameters	
temperature of the gas phase inlet, T_g (K)	773	Diameter of tube, D_t (m)	$2.0 \cdot 10^{-2}$
temperature of the solid phase inlet, T_s (K)	733	Length of tube, L_t (m)	$1.8 \cdot 10^{-1}$
temperature of the tube well inlet, T_w (K)	1200	Catalyst properties	
pressure inlet , P_0 (Kpa)	650	Density of catalyst, ρ_{cat} ($\frac{kg}{m^3}$)	2850
Mole fraction(%)		ϵ_{cat}	(-)
CH_4	0.2182	η_1	(-)
H_2O	0.7274	η_2	(-)
H_2	0.0118	η_3	(-)
CO_2	0.0083	K_{CH_4} (Kpa ⁻¹)	$3.247 \cdot 10^{-5}$
CO	0.0343	K_{H_2O} (-)	$2.367 \cdot 10^3$
K_{eq1} (Kpa ⁻²)	$1.871 \cdot 10^6$	K_{H_2} (Kpa ⁻¹)	$5.617 \cdot 10^{-11}$
K_{eq2} (-)	11.069	K_{CO} (Kpa ⁻¹)	$4.765 \cdot 10^{-7}$
K_{eq3} (Kpa ⁻²)	$2.172 \cdot 10^3$		

Table 3- The parameters of the mathematical model used for the simulation[7]

<u>Parameters</u>	<u>value</u>	<u>Parameters</u>	<u>value</u>
volume flow rate , $v_g(m^3/sec)$	0.118	heat capacity of catalyst bed , $Cps \left(\frac{J}{kg.k}\right)$	$\frac{J}{kg.k}$
superficial velocity , $V_{sg}(m/sec)$	15	336	
gravity acceleration, $g (m/sec^2)$	9.81	heat capacity of mixture gas , $Cpg \left(\frac{J}{kg.k}\right)$	$\frac{J}{kg.k}$
spatial time , $\tau (s)$	0.4	0.876	
Gas constant , $R \left(\frac{J}{mol.k}\right)$	8.314	enthalpy of reaction(1) , $\Delta H \left(\frac{J}{kmol}\right)$	$\frac{J}{kmol}$
heat transfer area per volume bed , $a_{gs} \left(\frac{m^2}{m^3}\right)$	150.2	291.83	
heat transfer coefficient between the gas and the solid phase, $h \left(\frac{W}{m^2.k}\right)$	1.735	enthalpy of reaction(2) , $\Delta H \left(\frac{J}{kmol}\right)$	$\frac{J}{kmol}$
heat transfer coefficient between tube wall and gas phase , $hw \left(\frac{W}{m^2.k}\right)$	1000	-37.67	
		enthalpy of reaction(3) , $\Delta H \left(\frac{J}{kmol}\right)$	$\frac{J}{kmol}$
		219.51	
		Gas density, $\rho (kg/m^3)$	
		0.989	

III. Net Rates

$$r_i = \sum_{j=1}^n \sigma_{ij} R_j \eta_i \quad (6)$$

Equation (6) has been used to obtain the net rates of chemical species (r_{CH_4} , r_{H_2O} , r_{H_2} , r_{CO} and r_{CO_2}) as follows:

$$r_{CH_4} = -\eta_1 R_1 - \eta_3 R_3 \quad (7)$$

$$r_{H_2O} = -\eta_1 R_1 - \eta_2 R_2 - 2\eta_3 R_3 \quad (8)$$

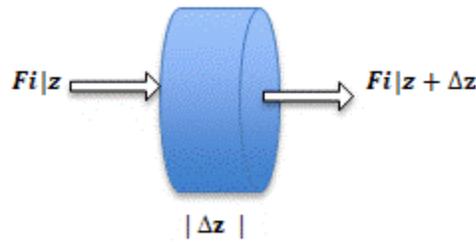
$$r_{H_2} = 3\eta_1 R_1 + \eta_2 R_2 + 4\eta_3 R_3 \quad (9)$$

$$r_{CO} = \eta_1 R_1 - \eta_2 R_2 \quad (10)$$

$$r_{CO_2} = \eta_2 R_2 + \eta_3 R_3 \quad (11)$$

3.Reactor model

The dynamic model includes mass and energy conservation equations for the steam methane reformer and a kinetic model that is part of the larger reactor model. The volume and energy associated with the reformed gas equation are a series of partial differential equations in space and time, while the energy balance equations for the solid phase are a single ordinary differential equation. The total volume of mass and energy consumed or released by the segment is visualized in Fig.



(Figure 1).molar flow rate input and output from the reactor segment with length Δz .

3.1. Mass Balance

The different molar balances for all chemicals on the shell side (CH₄, H₂O, H₂, CO and CO₂) are as follows Silva .

- Mass balance of methane:

$$\frac{V_{sg}}{g} \frac{dF_{CH_4}}{dt} + \frac{4\tau v_g}{\pi d^2} \frac{dF_{CH_4}}{dz} = \pi \rho_s L_z R_p^2 (1 - \varepsilon_b) r_{CH_4} \quad (12)$$

- Mass balance of steam:

$$\frac{V_{sg}}{g} \frac{dF_{H_2O}}{dt} + \frac{4\tau v_g}{\pi d^2} \frac{dF_{H_2O}}{dz} = \pi \rho_s L_z R_p^2 (1 - \varepsilon_b) r_{H_2O} \quad (13)$$

- Mass balance of hydrogen :

$$\frac{V_{sg}}{g} \frac{dF_{H_2}}{dt} + \frac{4\tau v_g}{\pi d^2} \frac{dF_{H_2}}{dz} = \pi \rho_s L_z R_p^2 (1 - \varepsilon_b) r_{H_2} \quad (14)$$

- Mass balance of carbon monoxide:

$$\frac{V_{sg}}{g} \frac{dF_{CO}}{dt} + \frac{4\tau v_g}{\pi d^2} \frac{dF_{CO}}{dz} = \pi \rho_s L_z R_p^2 (1 - \varepsilon_b) r_{CO} \quad (15)$$

- Mass balance of carbon dioxide:

$$\frac{V_{sg}}{g} \frac{dF_{CO_2}}{dt} + \frac{4\tau v_g}{\pi d^2} \frac{dF_{CO_2}}{dz} = \pi \rho_s L_z R_p^2 (1 - \varepsilon_b) r_{CO_2} \quad (16)$$

3.2. Energy Balances

Energy balance of the gas phase;

$$\rho_g C_{p,g} \frac{dT_g}{dt} = -\rho_g C_{p,g} V_{sg} \frac{dT_g}{dz} + h_{gs} a_{gs} (T_s - T_g) + \frac{h_w D_{tube} \pi}{A_{tube} \varepsilon} (T_w - T_g) \quad (17)$$

- Energy balance of the solid phase;

$$(1 - \varepsilon_s) \rho_{cat} C_{p,s} \frac{dT_s}{dt} = \rho_{cat} \sum_{j=1}^3 (-\Delta H_j) \eta_j R_j + h_{gs} a_{gs} (T_s - T_g) \quad (18)$$

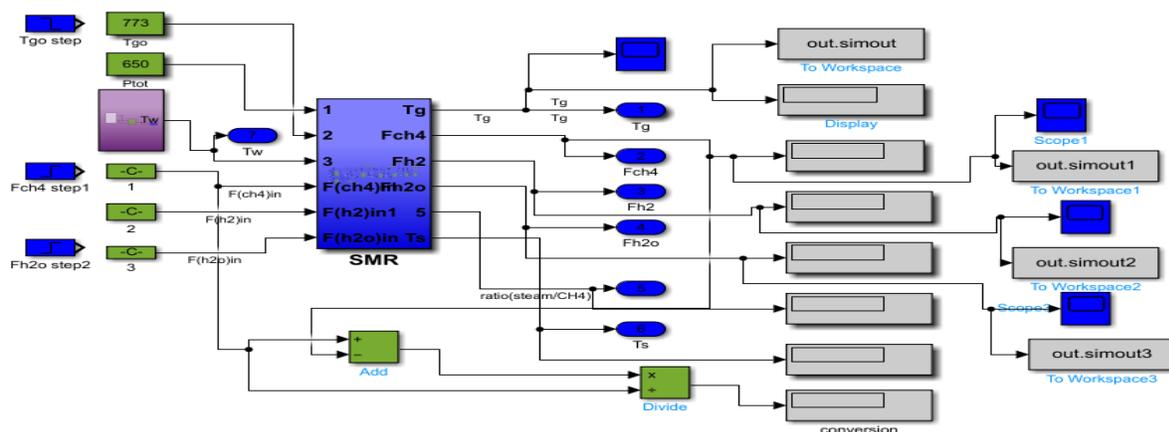
4. Control methods

Embodiments of the invention provide an advanced control system for steam hydrocarbon reformer , especially steam methane reformer reactors. the advanced control system improve the control quality and efficiency of adjusting steam hydrocarbon reformer

operating coefficients. As a result, the steam hydrocarbon reformer operations become more stable, resulting in energy savings and improved reactor yield[18]. All the control systems are built on measurements of the process variables. The outlet temperature is an important parameter that affects the yield. The control variable of the steam methane reformer is the outlet gas temperature, manipulated variable is the fuel gas flow rate. The disturbance variables are the feed temperature, feed molar rate. Three control methods were used which are PID, cascade and multi-loop. The unsteady step change simulation runs were implemented by introducing the fuel gas flow rate and controlling the exit gas temperature.

5. Simulation work

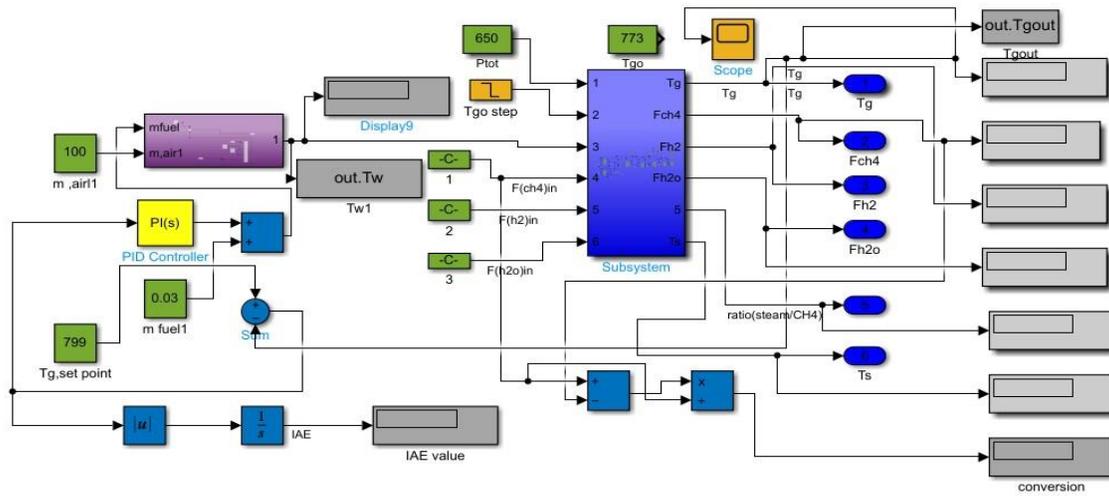
A simulation program was performed using the MATLAB/Simulink program to reform steam methane. Figs 2, 3, 4 and Fig 5 demonstrate the dynamic model's capabilities and the controllers' design, respectively. The mathematical model of the steam methane reformer is composed of a network that represents the mathematical model's equations (mass conservation and energy conservation) from equations 12-18. These equations are used to create a model that is taken from [7].



(Figure 2): Simulation work of the SMR.

5.1. Simulation for PID control

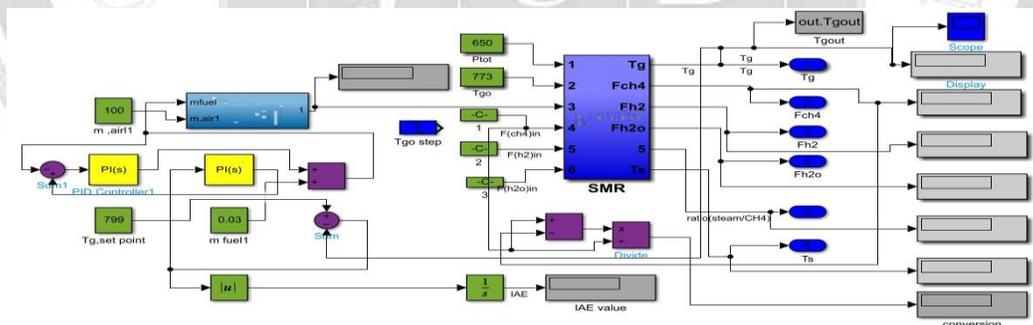
After using Simulink/MATLAB to implement the complex dynamic model, a PID controller is used to control the exhaust gas temperature. After using MATLAB/Simulink to implement the complex dynamic model, a PID controller is used to control the exhaust gas temperature. The purpose of the regulator is to regulate the temperature of the gases leaving the system, the manipulated variable that is used to control the temperature is also employed. In the process and directly affects the output of the process is fuel gas rate and disturbance variables for this process is feed temperature, and feed molar rate, simulation for PID control is shown in Figure(3).



(Figure 3): Simulation work of PID controller for the steam methane reformer.

5.2. Simulation for cascade control

Cascading control loops start out the same as a single control loop. Cascaded controls are used to regulate processes such as temperature and level. The main goal of cascade control is to improve the performance of the process by controlling the initial warning variables to reduce or eliminate the effectiveness of detected disturbances. In this effort, the primary external process variable is the temperature of the exhaust gases, while the secondary internal process variable is the temperature of the burned gases. The basic structure of the simulated flow control system is shown in Figure 4.



(Figure 4): Simulation work of cascade control.

5.3. Simulation of multi-loops control

Systems with only one output that is manipulated by a single input are considered SISO systems. Many procedures do not follow this simple configuration of control. For example, any process that involves manufacturing or refining a product must have a separate control loop. Actually, each unit procedure typically necessitates oversight of at least two variables, for example, the rate of production and the quality of the product. As a result, there is typically at least two control cycles to contend with. Systems with multiple control loops are referred to as

Table 5: Comparison of simulation work (exit reformed gas temperature, conversion, and yield of H₂).

Variable deference %	Actual	Simulated (MATLAB)	Deviation
Conversion(X_{CH_4})	63.8	50.36	21
Yield of H ₂	1.766	1.6	9.3
Exit reformed temperature	850	799	6

Table 6 : Comparison of the simulation exit main composition mol% results with a commercial reformer.

Component deference %	Commercial reformer mol%	Simulated (MATLAB)mol%	Deviation
CH ₄	0.074	0.0939	0.26
H ₂	0.385	0.3035	0.21
Steam(H ₂ O)	0.131	0.495	2.7

6.2. Dynamics of steam methane reforming

This portion discusses the findings of the simulations. The simulation results, including the dynamic behavior and the control strategy of the methane reformer. In open loop systems, the effects of input variables that are disturbances on the output temperature are demonstrated..

6.2.1. Effect of fuel gas

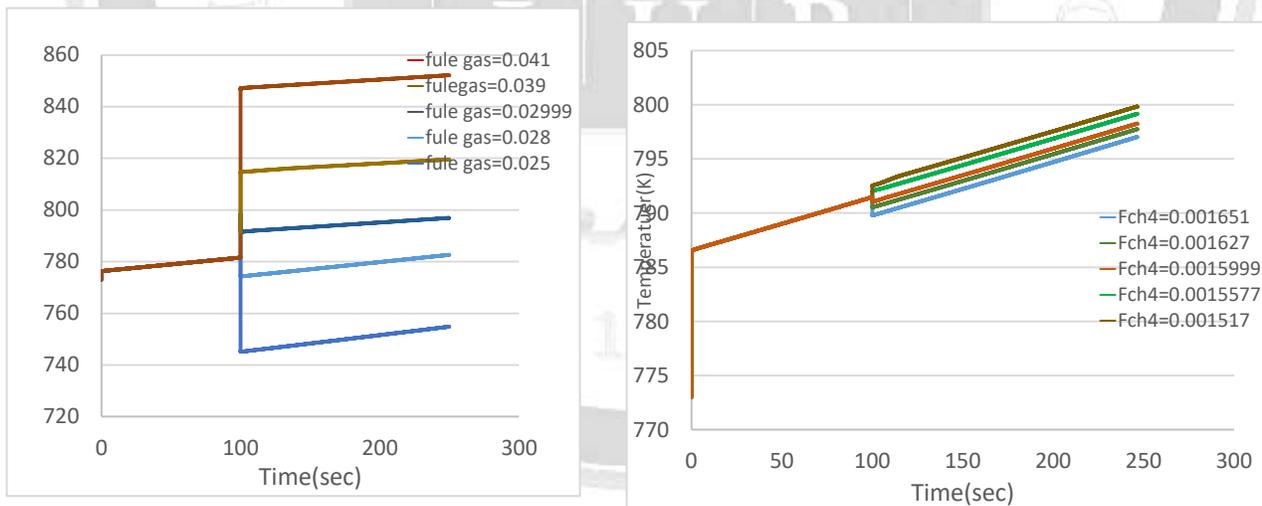
Figure 6 shows the exit gas temperature responses when a fuel gas flow rate is stepped from 0.03 kmol/s to 0.039 kmol/s and 0.041 kmol/s. Initially, the exit gas temperature is 799 K, when the fuel gas flow rate was 0.03 kmol/s, then the exit gas temperature response increased from 799 K to 852.2K and 819.5K, due to a positive step-change in the fuel gas from 0.03 kmol/s to 0.039 kmol/s and 0.041 kmol/sec. It is also known, that increasing the amount of fuel required for combustion, means increasing the temperature of the reactor wall, and as a result, the heat is transferred by radiation from the reactor wall to the tube wall, and then to the gas inside the tube reactor by convection and conduction. Then the gas molecules begin to break down as a result of the increase in the gas temperature inside the reactor. The sensitivity index value due to a positive step change from 0.03 kmol/s to 0.039 kmol/sec and 0.041kmol/s is -0.22 , -0.29 while the exit gas temperature response decreased from 799K to 796.5K ,782.7Kand 754.9 K when a negative step-change in the fuel gas flow rate from 0.03 kmol/s to 0.02999 kmol/s,0.025kmol/sec and 0.028kmol/sec. The decrease in the amount of fuel gas flow rate leads to a decrease in the amount of heat transferred from the reactor wall to the gas inside the tube reactor, and for this reason, the temperature of the gas will decrease. The sensitivity index value due to a negative step-change from 0.03 kmol/s to 0.0299 kmol/s,0.025kmol/sec and 0.028kmol/sec is 0.27,0.23,0.289.

6.2.2. Effect of molar flow rate of methane

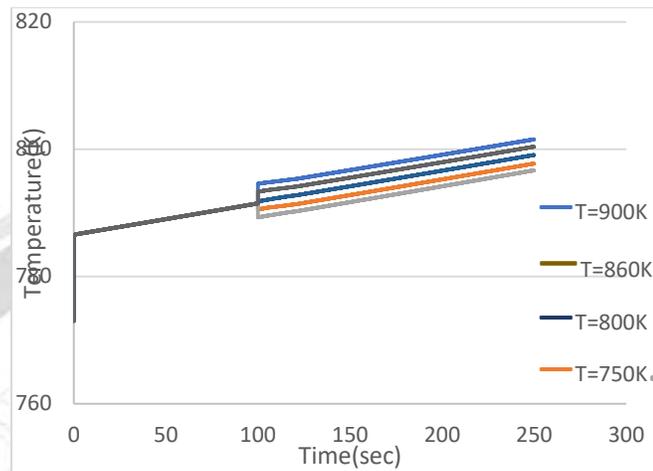
Figure 7 shows the outside gas temperature responses due to a step-change in the feed mole rate of methane . Initially, when the feed rate of methane is 0.001574 Kmol/sec , the out gas temperature from reactor was 799 K, while the feed mole rate of methane stepped to 0.001651 kmol/sec,0.00162kmol/sec and 0.001599 kmol/sec , the exit gas temperature responses decreased to 797K ,797.7 K, and 798.2 K, because of the increase the feed molar flow of methane, means the increase the number of methane moles at constant volume of the reactor, therefor the energy to break down a more methane molecules becomes insufficient. The sensitivity index values for positive steps are (0.022 ,0.035 and 0.0415) respectively. The negative step change in methane mole rate from 0.001574kmol/sec to 0.00155kmol/sec and 0.001517kmol/sec, the exit gas temperature response was increased from 799 K to 799.2K and 799.9 K. The sensitivity index value for a negative step-change is (-0.0425,- 0.044).

6.2.3. Effect of feed temperature

Figure 8 illustrates the response of the gas's exit temperature to the change in feed temperature from 773 K to 900 K, 860 K and 800 K,750 K and 700 K, the initial value of the gas's exit temperature was 799 K, when the feed temperature of the gas was 773 K. However, the feed temperature was changed from 773 K to 900 K, 860 K and 800 K,750 K and 700 K, the gas's exit temperature decreased from 799 K to 796.6 K, and 797.5 with a sensitivity of 0.128. Additionally, when the feed temperature decreased by 10 degrees Celsius from 773 K to 750 K and 700 K, the gas's exit temperature increased by 10 degrees Celsius from 799 K to 801.5 K, 800.35 K and 901.5 with a sensitivity of 0.14..



(Figure 6): Exit gas temperature responses due to a step change In fuel gas rate. (Figure 7): Exit gas temperature responses due to step change in Fch4



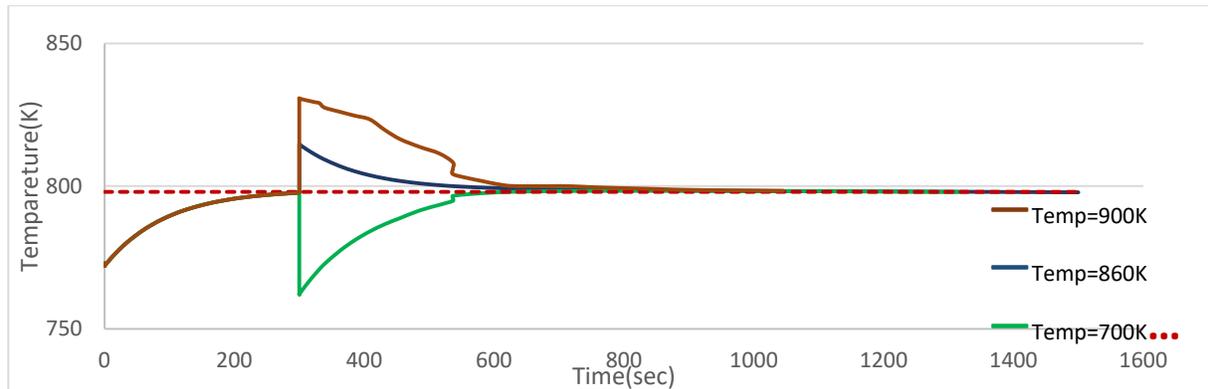
(Figure 8): Exit gas temperature responses due to step change in feed temperature (K).

6.3. Control of steam methane reformer

In this part, a simulation of the closed-loop system is demonstrated. The primary goal is to maintain the temperature of the exit gas in the desired range by utilizing three different control methods, which are PID control, multiple loops control, cascade control, and a controller, the purpose of this is to note the most effective way to maintain the temperature of the exit gas in the SMR system [16].

6.3.1. Proportional Integral Derivative (PID) Controller Tuning

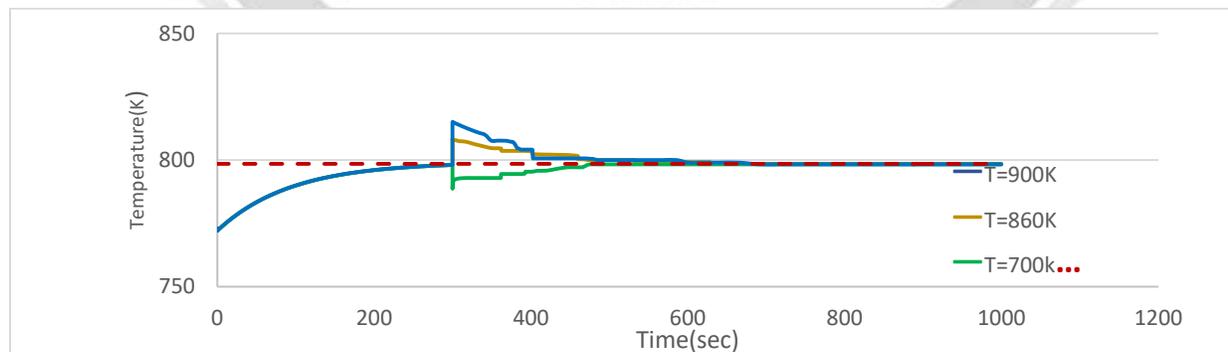
In this method, the first step is to change the set temperature of the gas in the circuit, while setting the parameters I and D to zero, increasing the proportional gain until the output of the circuit starts to oscillate, which is not considered to cause a problem because of the increasing integral component to prevent oscillation.. The term derived from the derivative is increased until the desired position is reached without slowing down the loop. Figure 9 shows the response of the PID system to temperature increases from 773K to 900K, 860K and 700K. If the outlet water temperature is initially 773K, and the PID system outlet temperature control rapidly increases from 773K to 799K (the expected value of the outlet temperature is this), without overshoot or imbalance, the flow temperature increases to 900 K or 860 K, The response of the PID system to this temperature increase increases from 799 K to 830 K or 816 K. Eventually, the response of the PID system to the expected temperature decreased to a temperature corresponding to 799 K, with stabilization times of 775 s and 625 s, respectively. On the contrary, when the feed temperature decreases from 773 K to 700 K, the PID outlet gas temperature decreases from 799 K to 762 K, and then the PID outlet gas temperature increases to the expected temperature of 799 K with a stabilization time of 580.8 seconds.



(Figure 9): PID controller exit gas temperature responses to step-change in feed temperature (K).

6.3.2. Multi-Loops Control of Steam Methane Reformer

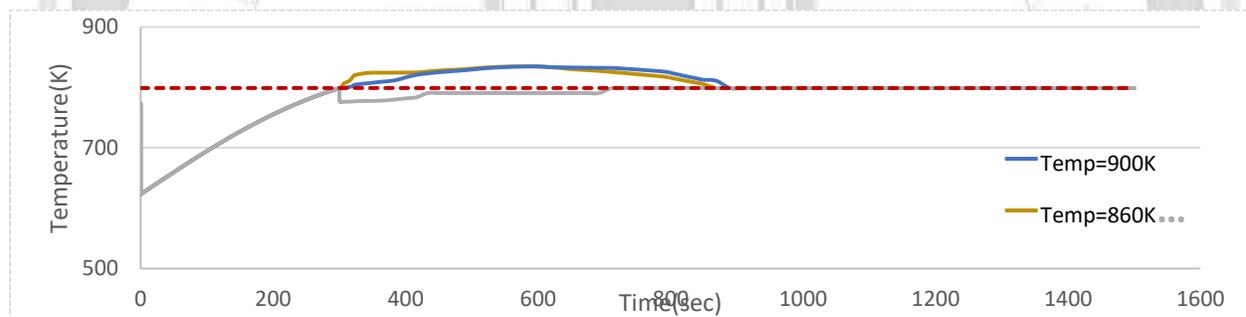
In the Steam Methane Reformer, multiple circuits are employed to regulate two of the variables. In this study, the primary regulating variable is the temperature of the escape gas, and the secondary regulating variable is the rate of the methane's molarity. Through this simulation, numerous experiments were conducted for the purpose of the program that simulates the controller, these experiments involved the response of the gas temperature to a step change in the molar rate of methane, the flow rate of the gas, the feed temperature, and the setpoint in the gas's exit temperature. Figure 10 illustrates the gas temperature at the exit, which is influenced by the temperature change in the feed. When the feed's temperature is increased by 50 degrees Celsius from 773 K to 900 K, the controller's response is increased by 50 degrees Celsius to correspond with the new feed temperature. No overshooting occurs initially, when the feed temperature is 773 K, the gas temperature at the exit is increased rapidly and the controller will reach a consistent state with an error of 9 degrees Celsius at temperature 799 K. After this, the feed temperature is stepped from 773 K to 900 K and 860 K, the gas temperature at the exit is increased to match the new feed temperature. No shift is present between the response and the setpoint temperature at this location...



(Figure 10): Response of multi-loop controller outlet gas temperature to sudden changes in feed temperature (K).6.3.3.

Cascade Control of Steam Methane Reformer

Cascade control has two independent PID controllers and two independent control loops, the first is the temperature at the gas outlet, and the second is the flow rate of the gas. In the cascade system, the first set of parameters derived from the PID controller are the same as the initial values derived from the Ziegler-Nichols method, and in addition, the second set of Parameters are changed automatically by MATLAB and Simulink. The response of the gas outlet temperature to a direct change in feed temperature from 773 K to 860 K, 800 K, and 700 K is shown in Figure 11. When the feed temperature is initially 773 K, the cascade outlet gas temperature response is 798 K. However, as the feed temperature increases from 860 K to 800 K, the cascade outlet gas temperature response increases from 798 K to 834.6 K and 833.2 K, and the outlet gas temperature response decreases to follow the set point until 889 s. A steady state was reached after 869 seconds, and the reaction temperature did not differ from the target temperature. On the other hand, when the supply temperature decreases from 773K to 700K, the cascade outlet gas temperature decreases from 799K to 776K, and then the cascade outlet gas temperature increases to reach the required temperature. However, the response to the cascade temperature was constant at around 11.7 degrees Celsius, with the response not significantly different from the target temperature...

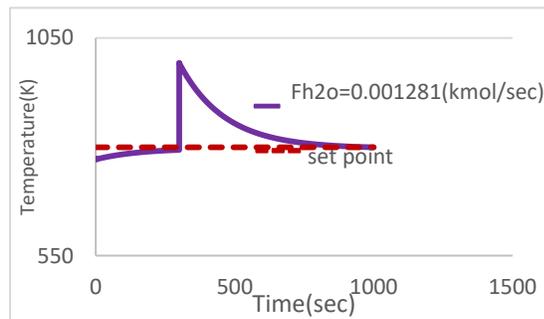


(Figure 11): Cascade controller outlet gas temperature response to sudden changes in feed temperature (K).

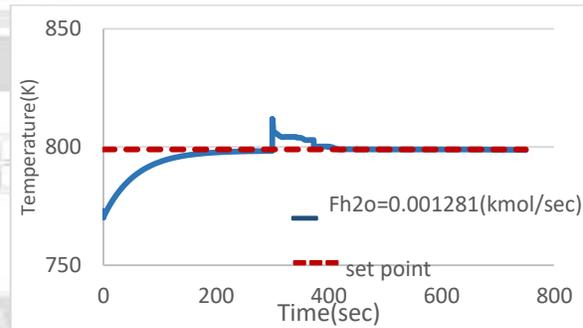
6.3.4. Comparison of control methods

A comparison was made between the multi-loop control system and the traditional control (PID) and cascade control system to find out which is the best method for steam methane reformer operations. Figures 12, 13 and 14 show the PID, the multi-loop and the Cascade temperature responses due to a step-changes in the molar rate of steam. A-step-changes in the molar rate of steam: From Figure 12, PID control the maximum percent step-change in the molar rate of steam from 0.004981 kmol/sec to 0.001281 kmol /sec overshoot is 24% and a settling times of 938.6 sec. From Figure 13, multi-loop control the maximum percent step-change in the molar rate of steam from 0.004981 kmol/sec to 0.001281 kmol /sec overshoot is 1.57% and a settling times of 416.9 sec. From Figure 14, Cascade control the maximum percent step-change in the the molar rate of steam from 0.004981 kmol/sec to 0.001281 kmol /sec overshoot is 10.2% and a settling times of 763.45 sec. The integral absolute errors (IAE) of the PID control when a step change in the the molar rate of steam from 0.004981 kmol/sec to 0.001281 kmol /sec is 3802. The integral absolute errors (IAE) of the multi-loop control when a step change in the the

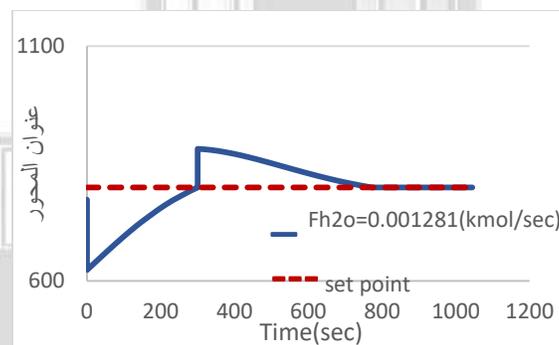
molar rate of steam from 0.004981 kmol/sec to 0.001281 kmol /sec is 852. The integral absolute errors (IAE) of the Cascade control when a step change in the the molar rate of steam from 0.004981 kmol/sec to 0.001281 kmol /sec is 3130.



(Figure 12): PID controller



(Figure 13): Multi-loop controller



(Figure 14): Cascade controller

7. Conclusion

In this study, a dynamic model for a steam-based methane reformer has been chosen and implemented with the help of the MATLAB/SIMULNIK program. A kinetic model was employed to assess the proposed reaction rates from [7]. In the solution of the problem, the method of differential balancing of mass and energy was employed. The simulation results were similar to the data from reformer exit experiments in the same conditions. The Simulation program is employed to portray the behavior of composition, temperature, and pressure as well as the heat flux profile throughout a fixed bed's length. The dynamic behavior demonstrated an effective response to feed rate changes of methane, the feed temperature, and the flow rate of gas. Three methods of control (PID, cascade and multiple loop) were created and employed to maintain the temperature of the outlet of the reformer, based on the overshoot and integral absolute evaluation criterion, it was observed that multiple loop is more effective than others in regards to small displacement and less time spent settling..



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9. References

- [1] D. Karimpourfard, S. Kabiri, and M. R. Rahimpour, "A novel integrated thermally double coupled configuration for methane steam reforming, methane oxidation and dehydrogenation of propane," *Journal of Natural Gas Science and Engineering*, vol. 21, pp. 134-146, 2014/11/01/ 2014, doi: <https://doi.org/10.1016/j.jngse.2014.06.018>.
- [2] A. Zamaniyan, A. Behroozsarand, and H. Ebrahimi, "Modeling and simulation of large scale hydrogen production," *Journal of Natural Gas Science and Engineering*, vol. 2, no. 6, pp. 293-301, 2010/12/01/ 2010, doi: <https://doi.org/10.1016/j.jngse.2010.10.004>.
- [3] A. Zamaniyan, A. A. Khodadadi, Y. Mortazavi, and H. Manafi, "Comparative model analysis of the performance of tube fitted bulk monolithic catalyst with conventional pellet shapes for natural gas reforming," *Journal of Industrial and Engineering Chemistry*, vol. 17, no. 4, pp. 767-776, 2011/07/25/ 2011, doi: <https://doi.org/10.1016/j.jiec.2011.05.028>.
- [4] V. Palma, A. Ricca, and P. Ciambelli, "Structured catalysts for methane auto-thermal reforming in a compact thermal integrated reaction system," *Applied Thermal Engineering*, vol. 61, no. 1, pp. 128-133, 2013/10/15/ 2013, doi: <https://doi.org/10.1016/j.applthermaleng.2013.03.038>.
- [5] A. Zamaniyan, H. Ebrahimi, and J. S. S. Mohammadzadeh, "A unified model for top fired methane steam reformers using three-dimensional zonal analysis," *Chemical Engineering and Processing: Process Intensification*, vol. 47, no. 5, pp. 946-956, 2008.
- [6] E. M. Mokheimer, M. Ibrar Hussain, S. Ahmed, M. A. Habib, and A. A. Al-Qutub, "On the modeling of steam methane reforming," *Journal of Energy Resources Technology*, vol. 137, no. 1, p. 012001, 2015.
- [7] F. A. A. Silva, K. C. Mendes, and J. D. da Silva, "A Simulation Study of the Steam Reforming of Methane in a Fixed-Bed Reactor," *Engineering*, vol. 8, no. 4, pp. 245-256, 2016.
- [8] L. Hoseinzade and T. A. Adams, "Modeling and simulation of an integrated steam reforming and nuclear heat system," *International Journal of Hydrogen Energy*, vol. 42, no. 39, pp. 25048-25062, 2017/09/28/ 2017, doi: <https://doi.org/10.1016/j.ijhydene.2017.08.031>.
- [9] U. I. Amran, A. Ahmad, and M. R. Othman, "Kinetic based simulation of methane steam reforming and water gas shift for hydrogen production using aspen plus," *Chemical Engineering Transactions*, vol. 56, pp. 1681-1686, 2017.
- [10] T. Pröll and A. Lyngfelt, "Steam Methane Reforming with Chemical-Looping Combustion: Scaling of Fluidized-Bed-Heated Reformer Tubes," *Energy & Fuels*, vol. 36, no. 17, pp. 9502-9512, 2022.



- [11] N. Ghasem, "A Review of the CFD Modeling of Hydrogen Production in Catalytic Steam Reforming Reactors," *International Journal of Molecular Sciences*, vol. 23, no. 24, p. 16064, 2022.
- [12] M. Shahrokhi and G. Baghmisheh, "Modeling, simulation and control of a methanol synthesis fixed-bed reactor," *Chemical Engineering Science*, vol. 60, no. 15, pp. 4275-4286, 2005.
- [13] D. Seepersad, J. H. Ghouse, and T. A. Adams II, "Dynamic simulation and control of an integrated gasifier/reformer system. Part II: Discrete and model predictive control," *Chemical Engineering Research and Design*, vol. 100, pp. 497-508, 2015.
- [14] B. F. Oechsler, J. C. Dutra, R. C. Bittencourt, and J. C. Pinto, "Simulation and Control of Steam Reforming of Natural Gas □ Reactor Temperature Control Using Residual Gas," *Industrial & Engineering Chemistry Research*, vol. 56, no. 10, pp. 2690-2710, 2017.
- [15] N. Zecevic and N. Bolf, "Advanced operation of the steam methane reformer by using gain-scheduled model predictive control," *Industrial & Engineering Chemistry Research*, vol. 59, no. 8, pp. 3458-3474, 2020.
- [16] T.-Q. Zhang, S. Jung, and Y.-B. Kim, "Hydrogen Production System through Dimethyl Ether Autothermal Reforming, Based on Model Predictive Control," *Energies*, vol. 15, no. 23, p. 9038, 2022.
- [17] J. Xu and G. F. Froment, "Methane steam reforming, methanation and water-gas shift: I. Intrinsic kinetics," *AIChE journal*, vol. 35, no. 1, pp. 88-96, 1989.
- [18] T. Li and J. J. Wang, "Advanced control system for steam hydrocarbon reforming furnaces," ed: Google Patents, 2013.
- [19] J. De Deken, E. Devos, and G. Froment, "Steam reforming of natural gas: intrinsic kinetics, diffusional influences, and reactor design," ACS Publications, 1982.

"المحاكاة الديناميكية والسيطرة المتقدمة على وحدة التهذيب بالبخار"

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b) drduraid@tu.edu.iq a) hero.a.saef443347@st.tu.edu.iq**الخلاصة**

تم اختيار النموذج أحادي البعد لتمثيل عملية إعادة تشكيل البخار في مفاعل نو قاعدة ثابتة يحتوي على جزئيات محفزة. يتضمن النموذج توازن الكتلة لجميع أجزاء التيار في المفاعل، وتوازن حرارة الغاز داخل المفاعل، وأنابيب المفاعل. تم اشتقاق هذا الحل من خلال استخدام MATLAB و Simulink. وقد تم وضع نتائج المحاكاة جنباً إلى جنب مع الإحصائيات العالمية الفعلية من أجل تقييم صلاحية النموذج... وقد تم اكتشاف أن معدل الخروج الأولي لمفاعل الإصلاح والمفاعل الإصلاحي التجاري كانا متقنين بشكل وثيق. تمت تجربة ثلاث طرق مختلفة وهي تناسبية متكاملة ومنتالية ومتعددة الحلقات، وتهدف هذه الأساليب إلى الحفاظ على درجة حرارة الغاز الخارج. تم إجراء التباين بين طرق التحكم هذه باستخدام زيادة تدريجية في قيمة التغذية عند قيم مختلفة لظروف التغذية. توضح هذه النتائج أن وحدة التحكم متعددة الحلقات سريعة، ولها عمر طويل، وأكثر ملاءمة، ولها إزاحة صغيرة، ولها تجاوز أقل، ولها خطأ مطلق أقل تكاملاً.

الكلمات الدالة: - مفاعل السرير الثابت، جهاز التحكم PID، جهاز التحكم متعدد الحلقات، جهاز التحكم المنتالي، MATLAB/Simulink.