Simulation and Validation of the MIDREX Reformer Process using Aspen Plus and Experimental Data

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محاكاة عملية مصلح الغاز MIDREX باستخدام برنامج Aspen Plus والتحقق من صحة النتائج مقارنة مع البيانات التجريبية

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Abstract

The MIDREX reformer process is a technology used for producing synthesis gas from natural gas. The MIDREX reformer process is consider as combination of carbon dioxide and steam reforming process technology for producing syngas This paper presents a simulation of the MIDREX reformer process using Aspen Plus, a process simulation software, and validation of the simulation results with experimental data. The simulation model was developed based on the process flow diagram of the reformer, and the input parameters were temperature, pressure, and steam-to-carbon ratio. The simulation results were validated by comparing them with the data from actual plant. Simulation results had a maximum error of 2.4% for reformed gas temperature and 8% for compositions compared to actual plant data as per validation results. Simulation studied reformer's operating conditions and can optimize MIDREX process for efficiency.

Keywords: *Aspen Plus, Experimental data, MIDREX reformer, Simulation, Validation.*

الملخص

أدى انتشار ثاني أكسيد الكربون كمنتج ثانوي أثناء تحويل خام الحديد (أكسيد الحديد) إلى حديد نقي إلى بدء عملية كيميائية بديلة لتحويل ثاني أكسيد الكربون إلى خليط من الهيدروجين وأول أكسيد الكربون باستخدام عملية إعادة تأهيل MIDREX. لسوء الحظ، هناك عيب في عملية MIDREX، على الرغم من الحوافز الجذابة المحتملة ذات الفوائد الاقتصادية والبيئية. السبب الرئيسي لذلك هو تفاعل تكوين الكربون على الموقع النشط للمحفز. من أجل تقليل ترسب الكربون، تم تحميل المحفز داخل أنبوب إعادة التشكيل بثلاثة أنواع من نشاط المحفز. تمت محاكاة عملية إصلاح MIDREX بمساعدة ASPEN PLUS V8.8 في هذه الدراسة. تم تنفيذ عملية محاكاة MIDREX المصلح باستخدام ثلاثة أنواع من المفاعلات ذات القاعدة الثابتة على التوالي. تم إجراء المحاكاة الحركية باستخدام كتل نموذج ASPEN PLUS RPLUG مع قانون طاقة معاد ترتيبها. أظهرت النتائج التي تم الحصول عليها أن المحاكاة باستخدام مفاعل السرير الثابت تم التحقق منها باستخدام بيانات المصنع الفعلية. كانت نتائج النموذج قادرة على إعطاء قيمة مرضية لدرجة حرارة الغاز المعاد تشكيلها وتحويل الميثان وثاني أكسيد الكربون لإعادة التشكيل وأول أكسيد الكربون وبخار الماء بحد أقصى للخطأ لا يزيد عن 8٪.

الكلمات الدالة: أسبن بلس، قيم تجريبية، محاكاة، طريقة مادركس، التحقق.

1. Introduction

Carbon dioxide mixed steam reforming is a critical technology for producing syngas, a valuable feedstock for chemicals and fuels (MIDREX Company, 2020). The process converts methane and carbon dioxide to syngas for chemical industry use (Wang et al., 1996). As alternative energy needs grow, this process attracts attention for reducing greenhouse gases and producing products (National Energy Technology Laboratory, 2020). Raju et al. (2009) simulated a combined gasification and reforming process with Aspen Plus, generating flexible H_2/CO ratio syngas from carbon feedstocks. A hydrogasification reactor with steam methane reformer produced syngas with a predetermined ratio adjustable by temperature and CO_2/CH_4 ratio. This unified carbon conversion and produced fixed-ratio syngas by controlling carbon/water and carbon/hydrogen ratios. Ajbar et al. (2011). created an intraparticle mass transfer catalyst tube model for an iron DRI direct reduction reformer. Examining a bottom-fired unit, it assessed temperature profiles and conversions of H_2, CH_4, and CO_2, validating with plant data. They investigated inlet temperature, natural gas flow, and composition effects on outputs. Er-Rbib et al. (2012) showed dry reforming with integrated steam reforming produces synthetic fuel commercially. Their Aspen Plus four-unit process (syngas production, Fischer–Tropsch, hydrocracking, upgrading) analyzed best conditions and equipment while achieving positive carbon balance. Zhang et al. (2014) used Aspen Plus to assess combining DMR with partial methane oxidation for carbon dioxide conversion, finding it used fewer raw materials than SMR to generate equivalent H_2:CO ratio syngas more sustainably. Gopaul & Dutta (2015) compared biogas dry reforms, finding corn cob/stillage biogas optimally produced syngas ratios and yielded thermo-neutral hydrogen oxidation.

This paper simulated the MIDREX reformer using Aspen Plus with three catalyst activities. Results validated with plant data and investigated operating condition effects.

2. Simulation Model of MIDREX Reformer Process

To perform an accurate simulation of the process, it is necessary to have a precise understanding of the details of the process being simulated. Therefore, we will describe the basic processes involved in this method from the beginning. A retrospective cross-sectional study.

2.1. MIDREX Reformer Process

Syngas, a mixture of hydrogen, carbon monoxide and carbon dioxide, enables highly specific chemical and fuel syntheses. It mainly produces ammonia at 120 million Tons yearly and methanol at 30 million Tons in 2000. Syngas also yields 104.4 million Tons of Direct Reduced Iron annually using prevalent MIDREX Technology in shaft furnaces, with roughly 80% of global output through this method as shown in Figure (1) (MIDREX Company, 2020).

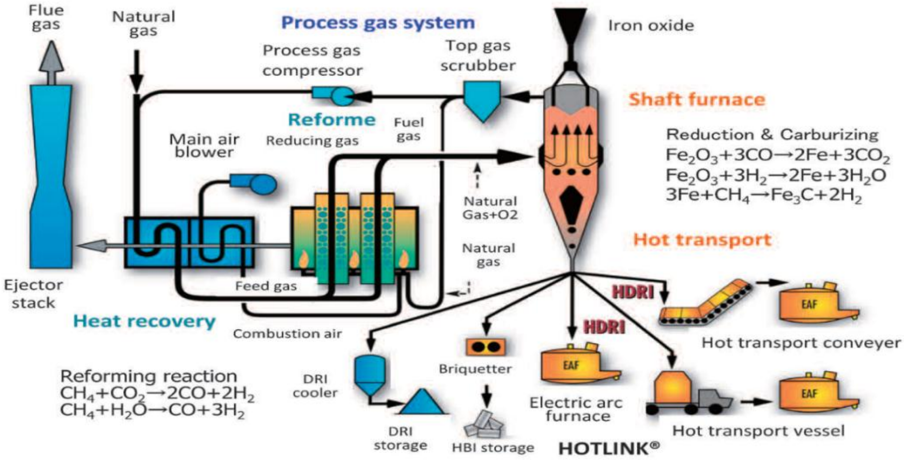

Figure 1. MIDREX process flowsheet (MIDREX Company, 2020)

Feedstock over 600°C avoids carbon deposition from incomplete methane cracking or Boudouard reactions, that lower quality (Nagaoka et al., 2001). The initial inert 1m section applies heat externally to exceed 700°C (MIDREX Company, 2020; and Nagaoka et al., 2001). The 4 m intermediate segment employs lower activity catalyst, slowing the endothermic steam reaction Eqn. (1) and carbon dioxide reaction Eqn. (2) as following;

$CH_4 + CO_2 \leftrightarrow 2CO + 2H_2$ ΔH° 298K= 247 kJ·mol^{-1} ...... (1)

$CO_2 + H_2 \leftrightarrow CO + H_2O$ ΔH° 298K= 41 kJ·mol^{-1} ...... (2)

Higher activity catalyst in the rear 4m portion demands less heat as methane levels fall (MIDREX Company, 2020; and Nagaoka et al., 2001).

As a DRM technique, strict thermal control between reaction onset and maximum sustainable temperature suppresses sintering. Partitioning catalyst properties stages reforming kinetically and thermally (Nagaoka et al., 2001). The second segment experiences sluggish conversions with less active material, while outside heating boosts the front inert section (MIDREX Company, 2020; and Nagaoka et al., 2001).

Strategic placement of the MIDREX reformer and prudent multi-zone design maximizes valuable syngas (H_2, CO, others) production for iron ore pellet reduction alongside natural gas in steelmaking. Judicious catalyst and heating arrangements stage reforming through multiple zones, thereby managing catalyst deactivation (MIDREX Company, 2020; and Nagaoka et al., 2001).

2.2. Simulation Model

The simulation model of the MIDREX reformer process was developed using Aspen Plus. The simulation model was based on the process flow diagram of the MIDREX reformer process as shown in Figure (2). The simulation model included the reformer unit (1st.2nd, and 3rd RPlug reactor), gas mixers, the reformer burners (Stoichiometric reactor), and feed gas heater. A simulation was conducted for a gas reforming unit using three reactors in series arrangement, these were fixed-bed reactors, to achieve the effect of various activities of the catalyst. Also in this mode, a simulation was conducted for the main burners (MB) and auxiliary burners (AB) using a stoichiometric reactor. The input parameters for the simulation model included specifications for the inlet streams, such as temperature, pressure, gas flow rate, and gas composition. The output parameters were the composition and temperature of the Reformed gas (RG) produced as the outlet stream of the reformer unit.

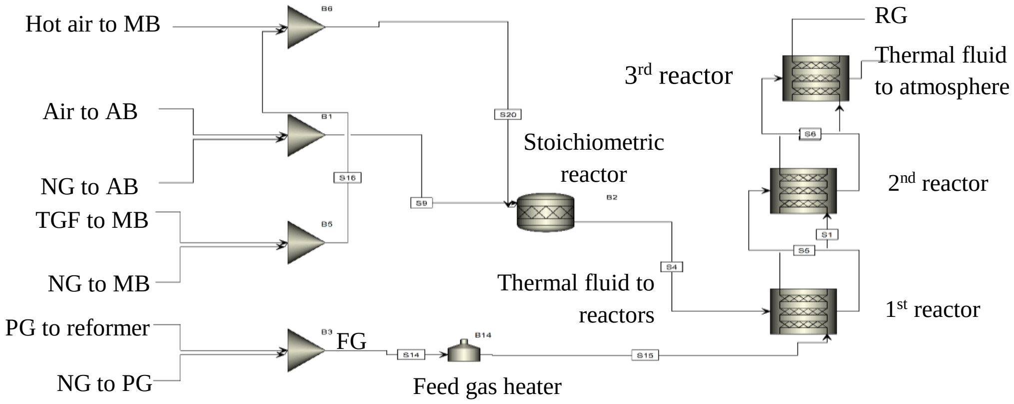

Figure 2. The flow sheet of the simulation process

2.3. Reformer Reactor Model

The simulation uses the RPlug reactor model with co-current thermal fluid type. The heat transfer coefficient per wall area considers thermal conductivity and thickness of reformer tube metal. The first reactor has tubes; 0.2 wide and 1 m long, the second 0.2 m x 3m, and third 0.2m x 4m, with a total of 468 tubes. Each tube contains catalyst: the first region has 42 kg of 0% Ni at 1200 kg/m^3 density, the second 108 kg of 7% Ni at 1100 kg/m^3, and the third 145 kg of 14% Ni at 1100 kg/m^3.

2.3.1 Reaction Kinetics Model

For the purposes of simulation with an RPlug model, reaction kinetics must be specified. The reaction Kinetic of MIDREX process is consider as mixed (steam and dry) reforming of methane reaction kinetic. Because the process gas will be saturated with water vapor after being compressed by compressors and before entering the gas reformer.

Kinetic parameters for the mixed reforming over the similar catalysts were obtained by Park et al. (2015), they found, first-order kinetics for the reaction of combination Equation of Eqns. (1 & 2) as following;

$$2\ CH_4 + H_2O + CO_2 \rightarrow CO + 5\ H_2 \qquad \text{...... (3)}$$

The final expressions used for the combined reaction rate (R_{CH4}) is given bellow;

$$R_{CH4} = 2.98*10^{-9}\ e^{-99,400/RT}\ P_{CH4}P_{CO2}P_{H2O} \qquad \text{...... (4)}$$

Wang et al. (1996) reported that DRM reaction can proceed above 640°C accompanied by SMR reaction, while above 820°C reverse water-gas shift could not occur, then a simple reverse water–gas shift reaction Eqn. (3) is considered bellow 820°C with the following kinetics;

$R_{r} = 1.5*10^{-5}\, e^{-89,000/RT}\, P_{CO2}P_{H2}$ ...... (5)

2.3.2 Reformer Burner Model

The combustion of natural gas and top gas fuel (TGF) with air in the furnace firebox is modeled using a simple RStoic model. The required reaction of fuel with air to provide the heat to the process stream is set as following Eqns. (6-10):

$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$ ...... (6)

$2C_2H_6 + 7O_2 \longrightarrow 4CO_2 + 6H_2O$ ...... (7)

$C_3H_8 + 5\,O_2 \longrightarrow 3CO_2 + 4H_2O$ ...... (8)

$2H_2 + O_2 \longrightarrow 2H_2O$ ...... (9)

$CO + 0.5O_2 \longrightarrow CO_2$ .... (10)

2.3.3 Model Assumptions

The reformer model assumes steady-state uniform conditions, negligible axial/radial dispersion and resistances between fluid and particles. Heat transfer from burners to fluid inside tubes occurs through tube walls by conduction. Heavy natural gas compounds are ignored due to unknown reaction mechanisms.

2.3.4 ASPEN PLUS Molding Steps

Aspen Plus enables modeling chemical processes through the following steps. First, specify process components from databanks, using PENG-ROB for properties (Melhem et al., 1989). Second, define a flowsheet connecting units via streams, with models describing syntheses. Third, label units and connect via streams. Fourth, specify feed streams' composition, flows, temperatures and pressures. Finally, set unit operation models' conditions (Al-Malah, 2022).

2.3.5 Aspen Plus Output

Aspen Plus enables simulating chemical plants when reliable data, conditions, and equipment models are provided. The software calculates important reformer tube parameters to evaluate performance. Pressure drop across the tube is required for flow rate and equipment sizing design. Reformed gas temperature distribution aids material selection and insulation to prevent overheating. Composition profiles of all species allow monitoring reactions and optimization. Reformed gas properties like temperature and quality impact downstream iron production, making simulation crucial for evaluating reforming unit operations.

3. Results and Discussion

The process of synthesis gas (Hydrogen+Carbon Monoxide) production from the Midrex Reformer unit. The Process Gas (PG) reacted with Natural Gas (NG) at reformer backed bed reactor was simulated using flow sheeting software, Aspen Plus V9. Validation was done by comparing the predicted reformed gas (RG) composition and temperature by using Aspen Plus model and data from actual plant.

3.1. The Actual Plant

The plant data were collected from Hot Briquetted Iron (HBI) plant at LISCO company Basis for calculation is 70,080 and 83,000 Nm^3/h of process gas flow rate.

Since the data collected from HBI plant are dry basis analyzer readings, because the devices used in the measurement have a dryer for water vapor from the sample, and the content of water to process gas is calculated in the following way:

The proportion of water vapor in the process gas is calculated by the Antoine equation, from which we get the vapor pressure of water Eqn. (11):

$$\log \mathrm{P}_{\mathrm{H_2O}} = 7.96681 - \left(\frac{1668.2}{\mathrm{T}+228}\right) \qquad \text{...... (11)}$$

where;

$\mathrm{P}_{\mathrm{H_2O}}$= vapor pressure of water, and T is the temperature of the process gas.

The following tables given the wet basis analysis of actual plant data (Table 1 and Table 2).

Table 1. HBI plant operation data on a wet basis analysis for reforming 70,080 Nm^3/h of process.

Stream/ Plant data	NG to PG	PG	TGF	NG to MB	Hot Air to MB	NG to AB	Air to AB
Flowrate Nm^3/h	12166	70080	3890	1700	71960	921.8	9681
Temperature °C	30	80.15	41	30	620	30	25
Pressure barg	1	1.686	0.33	1.228	1.223	1.056	1.173
Volume%							
CO_2	0.008	0.1605	0.1890	0.0079	0	0.0079	0
H_2O	0	0.177	0.055	0	0	0	0
O_2	0	0	0	0	0.21	0	0.21
N_2	0.038	0.0137	0.0157	0.038	0.79	0.038	0.79
H_2	0	0.4208	0.4957	0	0	0	0
CH_4	0.872	0.0133	0.0254	0.872	0	0.872	0
CO	0	0.2148	0.2193		0		0
C_2H_6	0.055	0	0	0.0552	0	0.0552	0
C_3H_8	0.019	0	0	0.0187	0	0.0187	0
C_4H_{10}	0.002	0	0	0.002	0	0.002	0

Table 2. HBI plant operation data on a wet basis analysis for reforming 83,820 Nm^3/h of process gas.

Stream/Plant data	**NG to PG**	**PG**	**TGF**	**NG to MB**	**Hot Air to MB**	**NG to AB**	**Air to AB**
FlowrateNm^3/h	13246	83820	40370	2004	104450	930	9226
Temperature °C	35	78.55	44	35	762	30	35
Pressure barg	1	1.544	0.33	0.58	1.25	1.056	1.173
Volume%							
CO_2	0.0648	0.1605	0.1873	0.0648	0	0.0648	0
H_2O	0	0.177	0.064	0	0	0	0
O_2	0	0	0	0	0.21	0	0.21
N_2	0.0091	0.0137	0.0155	0.0091	0.79	0.0091	0.79
H_2	0	0.4208	0.4911	0	0	0	0
CH_4	0.8454	0.0133	0.0252	0.8454	0	0.8454	0
CO	0	0.2148	0.2172	0	0	0	0
C_2H_6	0.0495	0	0	0.0495	0	0.0495	0
C_3H_8	0.016	0	0	0.016	0	0.016	0
C_4H_{10}	0.005	0	0	0.005	0	0.005	0

3.2. Reformed Gas Temperature Validation

The first experimental data used from HBI plant Table (1) and the current modeling results are shown in Figure (3).

Comparison of the reformed gas temperatures (RGT) measured by the plant thermocouple type B (square symbol), and the predicted gas temperature profiles along with height above tube inlet (HATI) of the reformer by this work for 70,080 Nm^3/h of process gas reacted with 12,166 Nm^3/h natural gas (blue line) are shown in Figure (3).

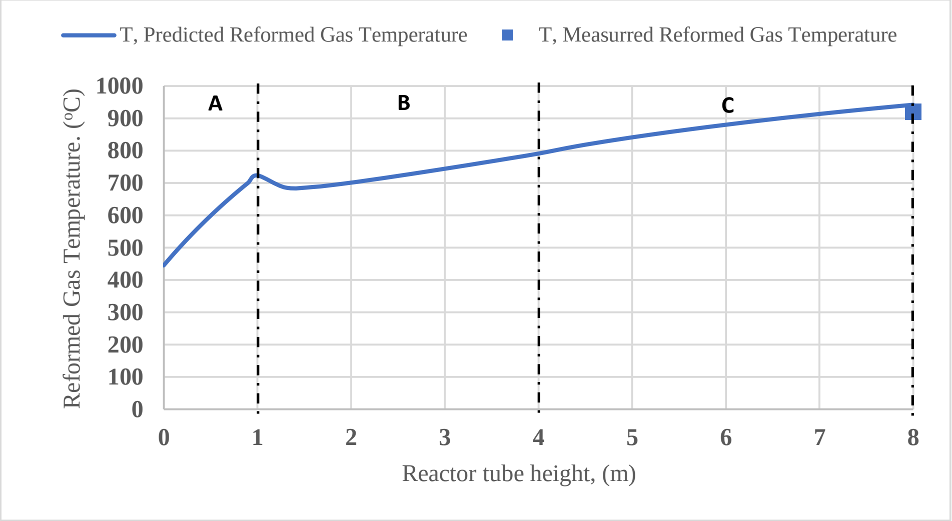

Figure 3 Comparison of the measured given in Table (1) and ASPN Plus model predicted reformed gas temperature profiles.

As can be seen in Figure (3), RGT behavior can be divided into 3 regions. The first region (A) starts at the tube inlet (HATI= 0), where the RGT in this region suddenly increases as a result of methane combustion in the reformer burner, in this reign there isn't reaction occurs because of presence inert catalyst. In the second region (B) where the middle active catalyst presence, the RGT is dropdown at the inlet portion of the region (B) because of the endothermic reaction resulted from Equation (3.1) at same time RGT increases as result of heat supplied by reformer burner. Finally, the third region starts at the (HATI=4) where the height active catalyst the RGT gradually grow up (C) until reaching the maximum methane conversion.

Both the modeled and the experimental temperature profiles in the end of region C showed 935°C, within 8 m above the tube inlet. The prediction of the experimental temperature profile by our developed model was considered successful with a maximum error not more than 2% for the end of region (C).

The second experimental data was given for the same HBI plant as given in Table (2). These data were used to compare the predicted temperature with that of the simulation model.

Comparison of the RGT measured by plant thermocouple (symbols), and the predicted RGT profiles inside the reformer tube by this work for 83,820 Nm^3/h of process gas reacted with 13,246 Nm^3/h natural gas (blue line) are shown in Figure (4).

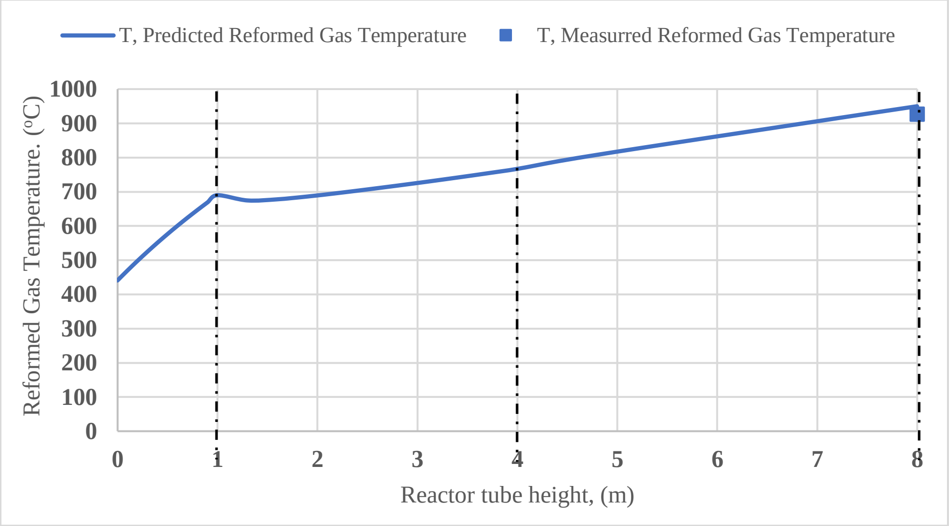

Figure 4. Comparison of the measured given in Table 2 and ASPN Plus model predicted reformed gas temperature profiles.

Figure (4) shown the RGT behavior was divided into 3 regions similar the that given in Figure (3). The model prediction for both experimental data Figure (3) and Figure (4) has at similar behavior in temperature profile. The prediction of the experimental data Table (2) by the current model was considered successful with an error of 2.4%.

3.3 Reformed Gas Compositions Validation

The qualty of syngas production and a good process control in the refoemer unit depends directly reformed gas composation and temperature. In oredr to make good control that reqired to keep CO, H_2 , CO_2, H_2O and CH_4 mole perecent in reformed gas at certine value.

3.3.1 Reactant Composition in Reformed Gas Validation

The methane composition at reformer outlet consider as one of the most important parameter indicate the process is working in normal and safe mode. The MIDREX reformer operation manual recommended that the methane composition should be less than 1 volume %

Figures (5 & 6) depict the percentage of CH_4, CO_2, and H_2O in reformed gas, as calculated by the model, and the corresponding actual data from the plant plotted against process gas flowrates. The solid line along the tube axis indicates the predicted reformed compositions profiles comprising CH_4 mole percent (Blue line), CO_2 mole percent (Orange line) and H_2O mole percent (Green line) with actual data from the plant (symbols), for process gas flowrates of 70,080 and 83,820 Nm^3/h, respectively.

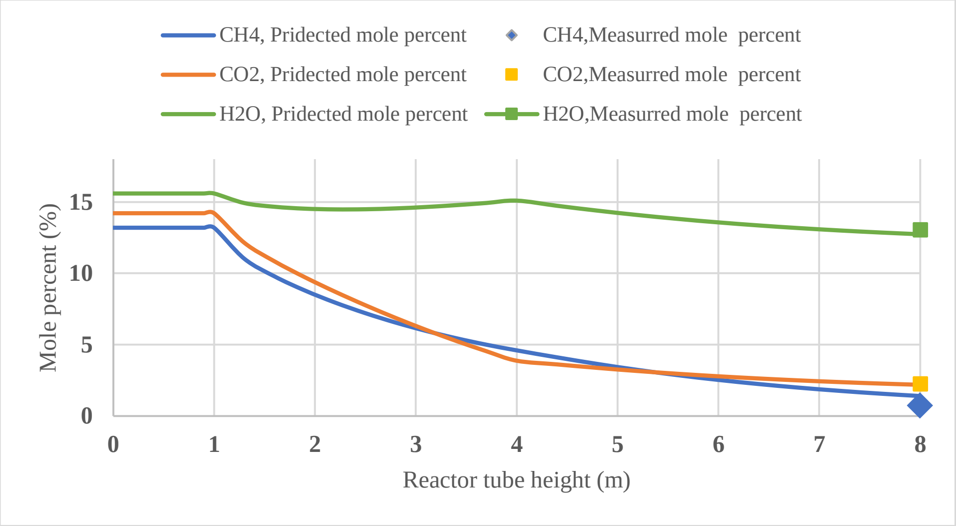

Figure 5. Predicted CH_4, H_2O, and CO_2 mole percent measured reformed gas mole percent for the actual plant data Table (1)

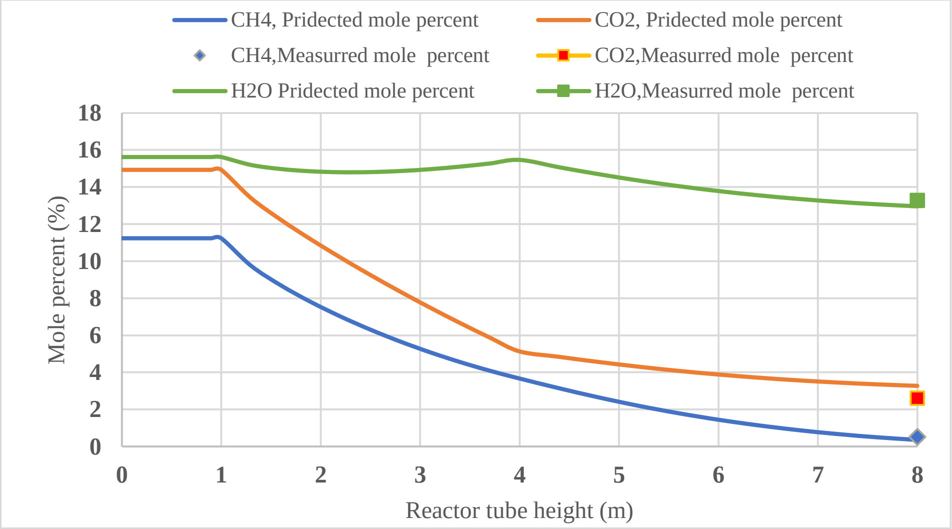

Figure 6. Predicted CH_4, H_2O, and CO_2 mole percent measured reformed gas mole percent for the actual plant data Table (2)

Figure (5) show the methane at reformed gas was less than 1 for both model prediction and the actual plant data. Also Figure (6) shows, that the methane percent was kept to less than 1 even though the natural gas inlet to the tube increased from 12,166 to 13,246 Nm^3/h as shown in Tables (5 & 6). Figures (5 & 6) show that, the model prediction for CO_2 and H_2O at regain B were effected by presence of reverse water–gas shift reaction Eqn. (3). This because of reverse water–gas shift reaction is favored bellow 820°C, where our model shows the RGT at regain B in range of 700 to 800°C. In both cases of the process gas flowrates, the model prediction was in good agreement with the actual plant data

3.3.2. H_2 and CO in Reformed Gas Compositions Validation

The H_2 and CO mole percent in reformed gas are the most important parameter to ensure the reformed gas quality. Figures (7 & 8) show comparisons of the H_2 and CO mole percent in reformed gas that was measured in actual plant and the predicted the H_2 and CO mole percent profiles. The solid line along the tube axis indicates the predicted reformed compositions profiles comprising H_2 mole percent (blue line) and CO mole percent (orange line) with actual data from the plant (symbols), for process gas flowrates of 70,080 and 83,820 Nm^3/h, respectively. Figures (7 & 8) depicted that the model prediction has maximum dive action 8% with the respect actual plant data. This underestimation can be explained as neglecting presence the heavy component in natural gas.

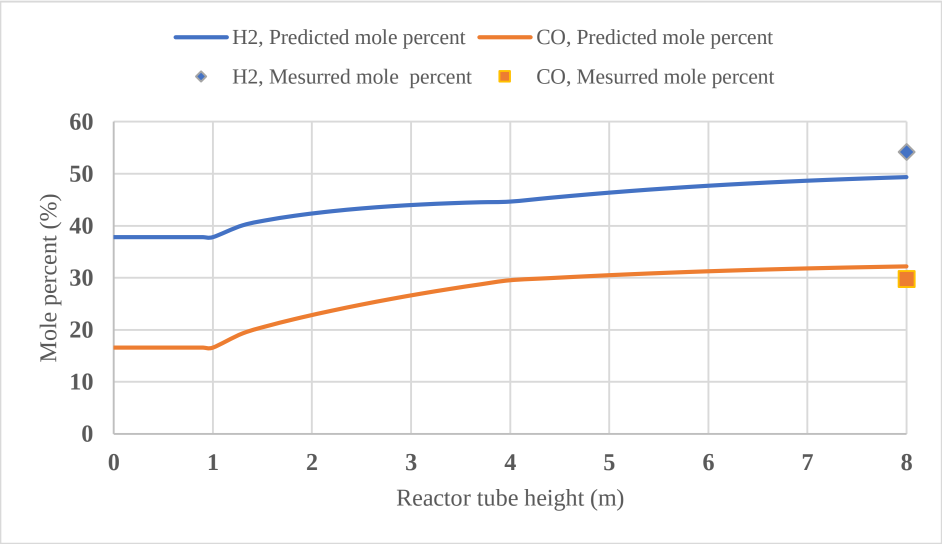

Figure 7. Predicted H_2 and CO mole percent measured reformed gas temperature for expermental data Table (1)

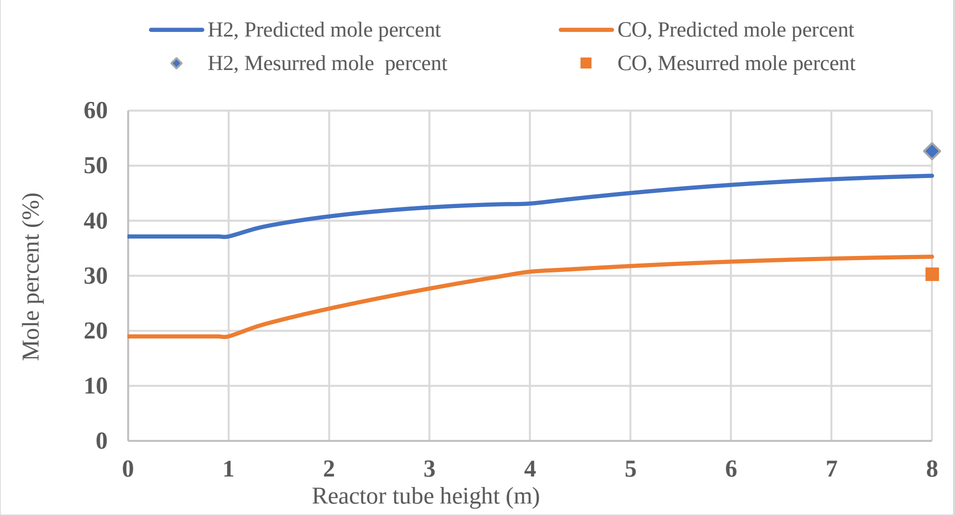

Figure 8. Predicted H_2 and CO mole percent measured reformed gas temperature for expermental data Table (2)

As a conclusion, the simulation results were validated by comparing them with the experimental data from the literature. The validation results showed good agreement between the simulation results and the experimental data. The validation results showed that the simulation model accurately predicted the composition of the synthesis gas and the efficiency of the reformer under different operating conditions.

4. Conclusion

This paper conducted a simulation of the MIDREX reformer process using Aspen Plus, a process simulation software. The simulation results were validated using measured data from the plant analyzer, and showed good agreement with a maximum error of 8% compared to actual plant data. The effect of changing the process gas flow rate from 70,080 to 83,000 m^3/h on the performance of the reformer unit was studied using a simulation model. The results showed that the process gas flow rate can be increased while maintaining the specifications of the reformed gas, such as the reformed temperature and gas composition. The simulation results can be used to optimize the operating conditions of the MIDREX reformer process and improve its efficiency.

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