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Research Article

Fault Detection and Classification in Steam Methane Reforming Process Using Long Short-Term Memory Model

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Abstract: Fault detection and classification using the Deep Learning method, which is the Long Short-Term Memory (LSTM) model, presents an effective approach for enhancing the reliability and efficiency of Steam Methane Reforming (SMR) processes. The timely detection and accurate identification of faults in the SMR process are crucial for minimizing disruptions and optimizing productivity in hydrogen production. LSTM models are particularly suitable for this task, as they can continuously monitor key process variables such as temperature, pressure, and gas composition to detect anomalies. This study develops an LSTM-based fault detection and classification framework for SMR processes, implemented using MATLAB. To generate the necessary process data, a simulation of the SMR process is first conducted using Aspen Plus, followed by the extension of the steady-state model to Aspen Dynamics for dynamic simulation. The faults considered in this study include variations in methane flow rate, steam flow rate, heat duty, and reactor temperature. The monitored conditions are hydrogen production and reactor outlet temperature. Based on these parameters, process data corresponding to both normal and faulty conditions is generated. The first LSTM model is employed for fault detection, with the data labeled according to its operational state (normal or faulty). A second LSTM model is then used for fault classification, wherein the labeled data is categorized based on fault types or normal operations. The classification results demonstrate that the LSTM-based approach offers superior fault detection and classification performance, improving system reliability, safety, and operational efficiency.

Keywords: Fault Detection, Fault Classification, Steam Methane Reforming, LSTM

1. Introduction

Hydrogen energy has the potential to replace fossil fuels as a significant source of energy. Hydrogen functions as an environmentally friendly and adaptable medium for energy, rendering steam methane reforming (SMR) a pivotal procedure in addressing the escalating need for sustainable energy alternatives. Steam methane reforming (SMR) is a chemical process that entails the reaction between methane and steam, conducted under precise conditions, resulting in hydrogen gas and carbon monoxide generation [1].

The process of SMR is a multifaceted and intricate industrial procedure that necessitates meticulous regulation and ideal circumstances to achieve efficient hydrogen production [2]. Deficiencies or anomalies in the functioning of the SMR (Steam Methane Reformer) can result in diminished operational efficiency and potential safety risks. Hence, implementing efficient fault detection and classification systems in SMR processes is of utmost importance to uphold operational reliability, enhance productivity, and guarantee the safety of personnel and equipment[3]

Monitoring key process variables and detecting anomalies or deviations from expected values constitutes fault detection using the LSTM model in SMR. Typically, this requires continuous temperature, pressure, gas flow rates, and composition monitoring via sensors and data acquisition systems [4]. Any anomalies or malfunctions can be swiftly identified by comparing real-time measurements to predetermined thresholds or statistical models. Classifying faults using LSTM models in SMR requires training the model on historical data comprising normal operating conditions and instances of various fault categories. The LSTM model learns the data's patterns and associations, allowing it to distinguish between normal and aberrant conditions. Once the model has been trained, it can classify new or real-time data samples into particular fault categories.

This study focuses on developing a methane steam reforming (SMR) simulation process using Aspen Plus and a fault detection and classification model for the Methane Steam Reforming (SMR) process using the LSTM model. The result of this study is implementing a MATLAB program to label faulty conditions (Fault = 1; Normal = 0), thus establishing the framework for a fault detection system. Then, LSTM is applied to classify the fault condition based on the established labeled data.

2. Materials and Methods

2.1. Process Description of SMR

Methane from natural gas is regarded as a feedstock. This procedure is illustrated in Figure 1. At 1000°C and 2 atm, the methane-only natural gas stream at 25°C and 1 atm is mixed with vapor. Based on the reference, the respective mass discharge rates for steam and methane are 8,000 kg/day and 2550 kg/day [9]. Through the utilization of hot flue gas and a heat exchanger, the gas mixture is heated to 700°C. Following this, the gas mixture is introduced into the SMR reactor at an isothermal temperature of around 700°C and one atmosphere. By employing a Ni-based catalyst, methane and vapor in the reactor are converted to carbon monoxide and hydrogen. In this study, Aspen Plus software was used to develop the SMR process simulation model. During the model development, The ENRTL-RK model was used as the global thermodynamic model in this simulation, while the RKSMHV2 model was used for the MSR and WGS reactors. This thermodynamic model is applied to compositions of non-polar and polar compounds combined with a light gas.

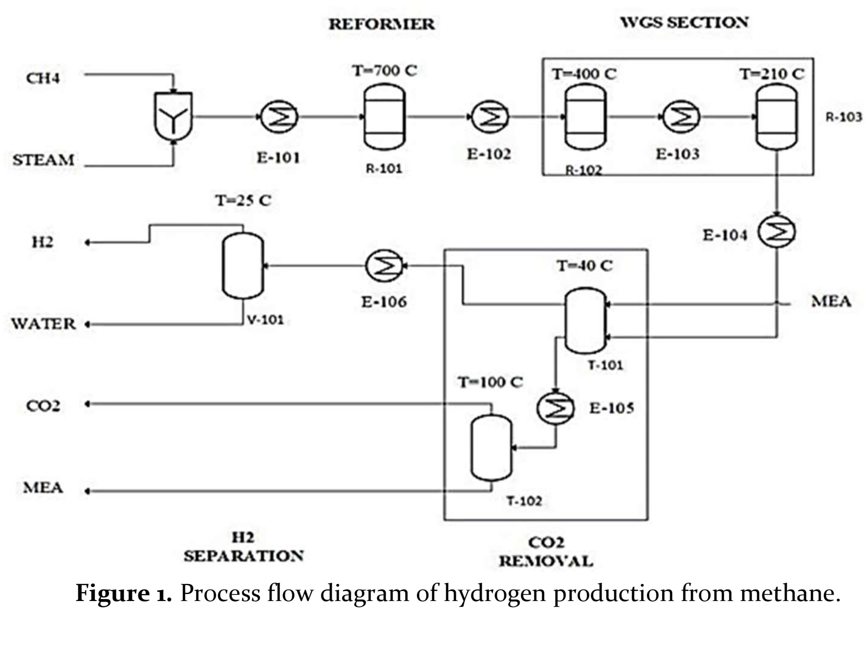


Figure 1. Process flow diagram of hydrogen production from methane.

2.2. Data Generation

Two sets of requirements must be satisfied. The first set demonstrates the program's behavior when everything is functioning ordinarily. The second group consists of four experiments conducted when the mode is unexpected. This conclusion is based on the fact that a single defect alters the normal working condition. The defect scenarios selected for this study were among the most likely to occur in the reactor. Therefore, in this study, we have chosen to study the following faults as tabulated in Table 1.

Table 1. Description of Process Faults in the SMR.

Fault ID	Process Variable	Type	Fault	Normal Condition			Fault
			-20 % (-2)	-10% (-1)	SS	10% (1)	20% (2)
MV1	CH_4 Flowrate	Random	6400	7200	8000	8800	9600
MV2	H_2O Flowrate	Random	2040	2295	2550	2805	3060
MV3	Heat Duty Reactor	Random	160	180	200	220	240
MV4	Temperature Jacket reactor	Random	852	862	867	872	882
CV1	H_2 Production	Random	765	861	957	1052	1148
CV2	Reactor Outlet Temp	Random	583	656	729	802	875

3. Results and Discussion

3.1. Simulation Model

The Aspen Plus simulation of the Steam Methane Reforming (SMR) process is presented in Figure 2. The process begins with mixing natural gas (NG) and steam, which then undergoes pre-treatment in the B1 unit before entering the reformer, where methane reacts with steam at elevated temperatures and pressures to produce hydrogen and carbon monoxide. The product stream is cooled in multiple heat exchangers (COOLER1 to COOLER4) to recover and recycle heat, enhancing energy efficiency. Following cooling, the stream passes through the Water Gas Shift (WGS) reactor, where carbon monoxide reacts with steam to form carbon dioxide. The system employs heat exchange and cooling units (HEATXA, HEATXB, HEATXC, HEATXD) to maintain optimal reaction conditions. The final product streams are separated and directed through various processing units, including separators and additional cooling units, yielding hydrogen-rich output while minimizing waste. The integration of heat recovery and cooling systems throughout the process ensures a sustainable and efficient hydrogen production operation.

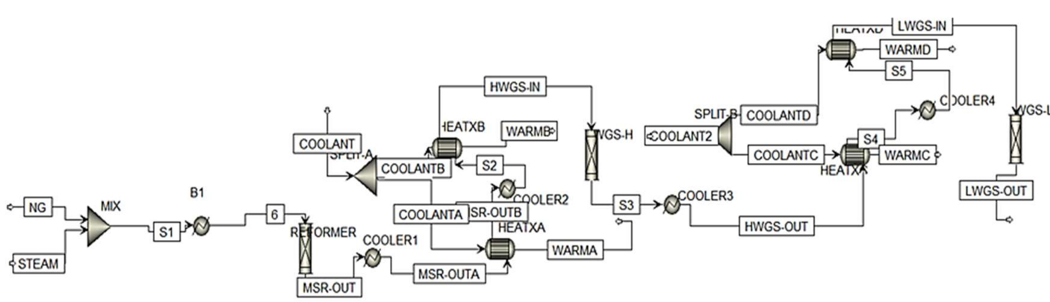
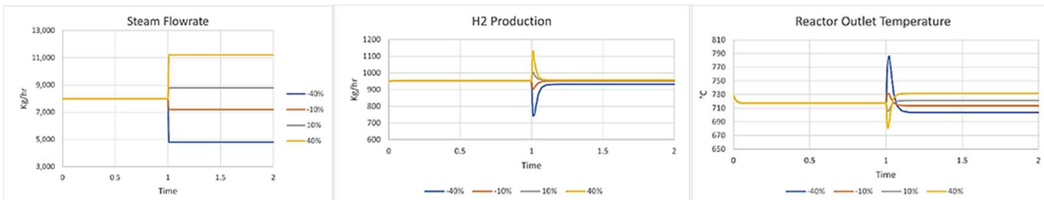


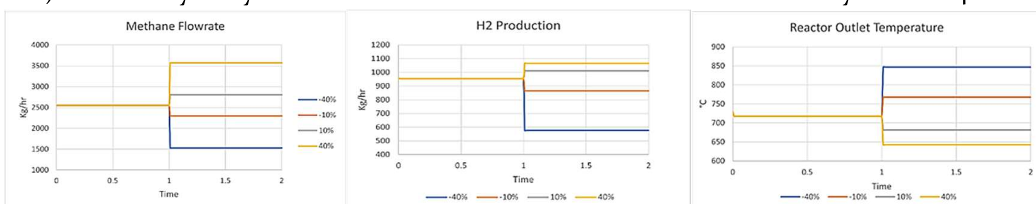
Figure 2. Aspen Plus modeling of Steam Methane Reforming.

3.2. Sensitivity Analysis

A sensitivity analysis is performed to ascertain the extent of sensor bias that might result in a breach of the operational limitations. The analysis is conducted through a heuristic approach, where various sensor biases are simulated under steady state base case conditions. Bias, as described by [10], refers to the divergence from the steady state condition of the base case. The minor sensor bias will prompt the process to transition to a different steady state condition. However, if the bias is substantial, the process will be unable to accommodate this disturbance, ultimately resulting in the system becoming uncontrollable and exceeding the operational limit. The results of the analysis are summarized and depicted in Figure 3.



a) Sensitivity analysis for the steam flowrate is increased and decreased by 10% and 40%



b) Sensitivity analysis for the methane flow rate is increased and decreased by 10% and 40%

Figure 3. Sensitivity Analysis for Steam Methane Reforming.

3.3. Fault Data Generation

Steam flow rate, methane flow rate, reactor heat duty, and jacket reactor temperature data generation take 90 times longer. Data collecting requires careful preparation and execution, including using sensors and monitoring equipment to capture different operational circumstances and accurately portray real-world scenarios. A complete dataset is needed to train a deep learning model with steam and methane flow rates, reactor heat duty, and temperature fluctuations.

Figure 4 shows the four input graphs showing methane flow rate, steam flow rate, heat duty, and jacket reactor temperature, and the two output graphs showing H2 production and outlet reactor temperature. These graphs show pivotal variables' dynamic interactions in operational contexts. These oscillations and patterns in input parameters affect output variables, revealing the system's behavior. Based on this carefully created dataset, an LSTM fault detection system is highly relevant.

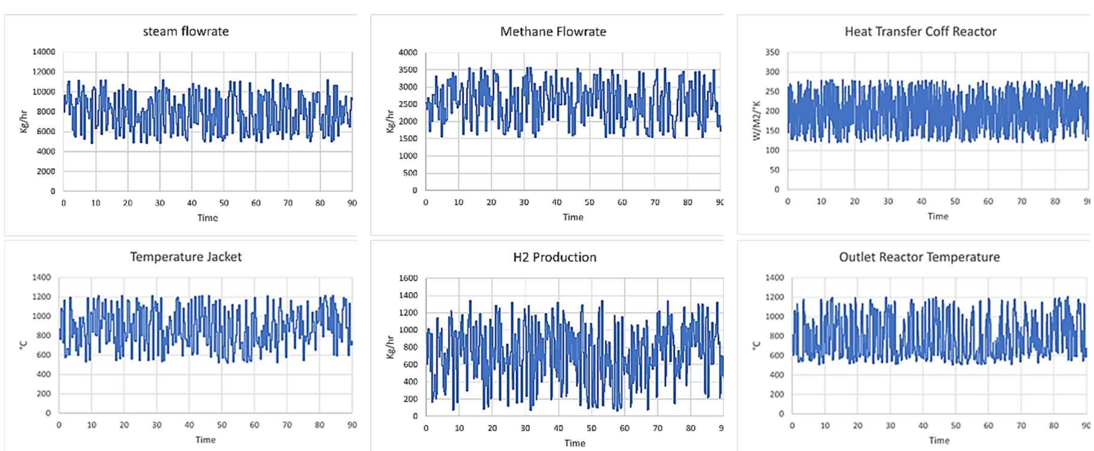
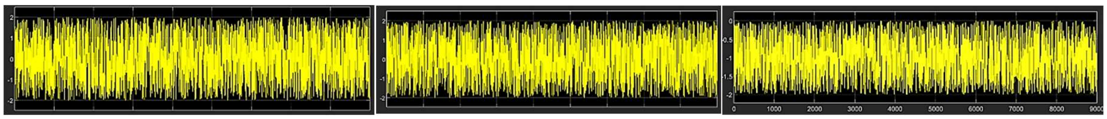


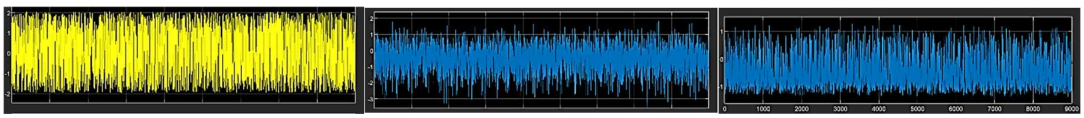
Figure 4. Data Generation from Aspen Dynamic.

3.3. Fault Detection

LSTM model fault identification involves evaluating temporal patterns in generated data to find unusual behavior that suggests chemical process flaws. Figure 5 shows two different plots: the faulty profile (MV1 to Mv4) and the fault effect profile. For the faulty profile, the values between -1 and 1 indicate normal operating conditions, whereas those beyond this range indicate abnormal conditions (or Faults). The effect of this fault can be observed at H_2 Production variation, and Rector Outlet Temperature changes. In this case, the LSTM model learns to identify the normal and fault conditions and assigns it the label FAULT or NORMAL. If any MV1, MV2, MV3, or MV4 has output exceeding the specified range, it would be considered FAULT. The NORMAL condition is only when all the MVs are within the normal operating range. After these detecting and labeling process conditions, another LSTM model is needed to classify the process condition.



a) Faulty data MV1 (CH_4 Flowrate), MV2 (H_2O Flowrate) and MV3 (Heat Duty Reactor)



b) Faulty data MV4 (Temp Jacket Reactor), Fault effect (H_2 Production), and Fault effect (Rector Outlet Temperature)

Figure 5. Fault Detection results.

3.4. Fault Classification

Figure 6 presents the classification model's LSTM training profile and confusion matrix. The training profile shows exceptional outcomes with an overall accuracy of around 95% and a constantly sustained loss below 0.5%. For the classification task, the model is trained using process data as input, and the labeled data as output. The results from the model would be the classified fault condition, whether normal or fault. The confusion matrix in the figure provides a detailed assessment of the classification model's performance by comparing the predicted class labels against the true class labels. The matrix is divided into four distinct quadrants: True Positives (TP), True Negatives (TN), False Positives (FP), and False Negatives (FN). In this case, the True Positives, which represent the correctly predicted true class instances, are recorded as 14,310, while the True Negatives, which correspond to the correctly predicted false class instances, are 690. Notably, there are no instances of False Positives or False Negatives, indicating that the model did not make any incorrect predictions, whether by classifying a false instance as true or a true instance as false.

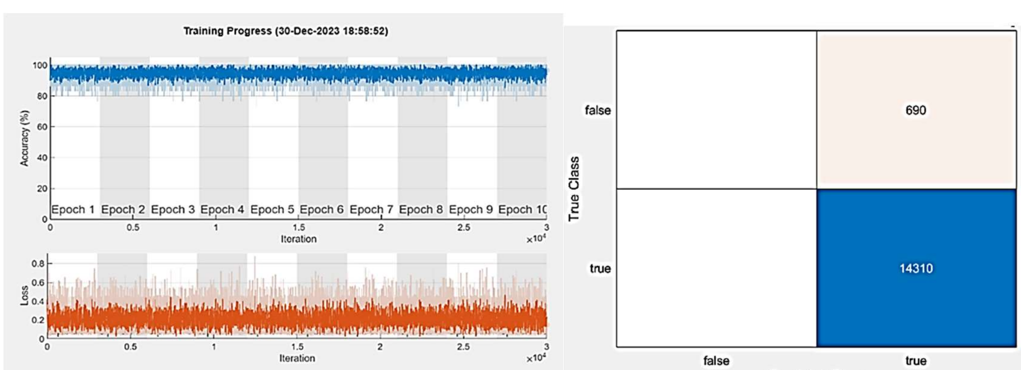


Figure 6. LSTM Training Profile (left) and Confusion matrix of fault classifier (right).

4. Conclusions

This research has succeeded in simulating and detecting faults within the Steam Methane Reforming (SMR) process. By utilizing Aspen Plus and Aspen Dynamic, a comprehensive simulation model was developed, offering valuable insights into the dynamic behavior of the SMR process and laying the groundwork for optimizing operations and further analysis. A MATLAB program was developed to label faulty conditions. The development of a Fault Detection and Classification model for the SMR process, leveraging Long Short-Term Memory (LSTM) neural networks, represents a key achievement in fault detection and classification. The model demonstrates an impressive accuracy rate in correctly identifying and classifying fault conditions in the hydrogen production and reactor temperature output. The next step would be to implement a fault diagnosis technique to identify the root cause of the fault.

Acknowledgments:

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