Thermodynamic analysis of Bi-reforming: An AI-driven optimization study

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1. Introduction

Methane (CH_4) and carbon dioxide (CO_2) are major greenhouse gases (GHGs) making significant contributions to global warming and climate change. One prominent method to transform these gases to value added products is through the production of synthesis gas (syngas), which serves as a precursor for hydrogen (H_2) and various downstream chemicals such as methanol, synthetic diesel, ammonia etc. Processes for converting these GHGs into syngas include steam reforming, dry reforming, bi-reforming, and partial oxidation of methane. Among all these processes, bi-reforming of methane (BRM) combines the advantages of both steam and dry reforming, specifically addition of H_2O can reduce the carbon deposition in the reaction process, and CO_2 is added to adjust the value of the H_2/CO ratio in syngas [1]. BRM process involves many reactants and many intermediate reactions, and the equilibrium changes with slight change in the concentrations. To improve the yield of syngas, it is very important to consider the optimal reaction conditions from the thermodynamics perspective. Employing the Gibbs free energy minimization method to identify suitable operating parameters is tedious, as it would require testing numerous conditions which are computationally expensive, posing significant challenges for the optimization process [2].

In the past decade, the use of artificial intelligence (AI) has become increasingly popular across various fields, with optimization being a crucial aspect. In this study, an efficient and reliable AI-driven process optimization technique was proposed to evaluate the optimal operating conditions (Methane conversion >95% and H_2/CO = 2) with minimum computational load.

2. Methods

AI-driven process optimization: The schematic of the proposed AI-driven process optimization technique is given in Fig. 1. In this study, the optimal process parameters, including temperature, pressure, and feed composition i.e., CO_2/H_2O ratio and with $(CO_2+H_2O)/CH_4 = 1$, are assessed for the BRM process. Initially, experiments are designed using the Taguchi method, incorporating three factors and five levels. The selected ranges for the process parameters are 300-1200°C for temperature, 1-20 atm for pressure, and 0-3 for feed composition (CO_2/H_2O). The Taguchi method efficiently estimates main effects and certain interactions between the process parameters with a minimal number of experiments. The output parameters i.e., methane conversion and syngas ratio at the designed set of experiments are determined through thermodynamic analysis. Further, an AI-based multi-input and multi-output kernel ridge regression (MIMO-KRR) model is trained and optimized to predict output parameters [3]. The trained MIMO-KRR model serves as the fitness function in the particle swarm optimization (PSO) technique to evaluate optimal operating conditions with methane conversion >95% and a syngas ratio of 2.

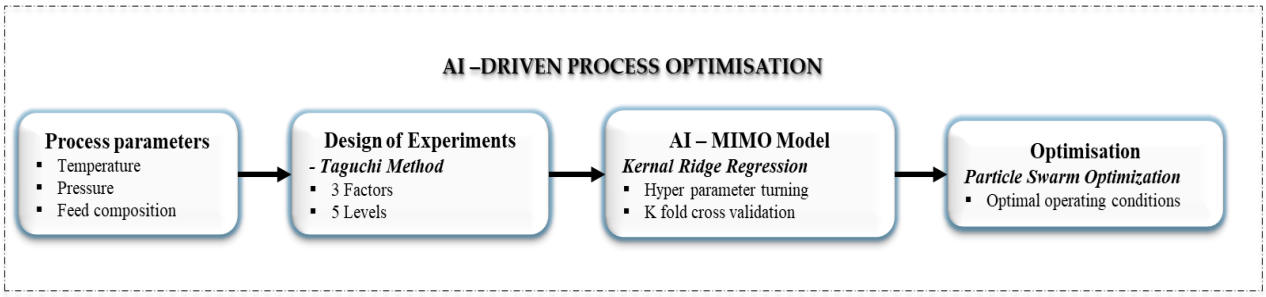

Figure 1. Schematic of AI-driven process optimization.

3. Results and discussion

The Taguchi method resulted in 27 operating conditions, and the output parameters, methane conversion, and syngas ratio, were determined at the designed operating conditions. The complete data are scaled and divided into train and test datasets in a 4:1 ratio. The MIMO-KRR model is trained and optimized using 4-fold cross-validation and the grid search technique. The hyperparameters (ranges/choices) considered for MIMO-KRR optimization are as follows: kernel (linear, poly, rbf, sigmoid); degree (1, 2, 3); and alpha (0.00001, 0.0001, 0.001, 0.01, 0.1, 0.2, 0.5, 0.9). The optimum hyperparameter choices for the MIMO-KRR model were found to be 'rbf,' '1,' and '0.0001' for kernel, degree, and alpha, respectively. The trained model achieved train and test accuracies of >95% in predicting both methane conversion and syngas ratio. Later, the optimized MIMO-KRR model was used as the fitness function in PSO, and the optimum process conditions were evaluated. The complete details about the optimization will be discussed in full in the full-length article.

4. Conclusions

The AI-driven process optimization technique proposed, utilizing thermodynamic data for the BRM process, proved to be efficient and reliable in predicting methane conversion and syngas ratio, as well as in evaluating optimal process conditions. The versatility of this technique allows for its potential extension to other datasets involving catalysts and experimental parameters.

References

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Keywords
Bi-reforming; Thermodynamic analysis; MIMO-KRR; Particle Swarm Optimization