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Physics Informed Neural Networks for a Gasification Reactor

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Abstract. Hydrogen arises as an alternative to decarbonize heavy industries, yet its production remains either expensive or environmentally harmful, prompting the exploration of waste-to-hydrogen gasification as a viable solution. This study addresses the challenges in accurately modeling the gasification reactor, a critical step in waste-to-hydrogen conversion, by confronting issues such as the inherent diversity of biomass and the complex interactions among its constituent properties using Artificial Intelligence. To address these challenges, we propose a methodology that integrates Physics-Informed Neural Networks, merging experimental data with physical principles to develop robust and adaptive models to predict syngas composition. Preliminary results indicate improvements in model accuracy over other models, achieving high predictive accuracies with an R2 value of 0.96 for the syngas composition, as well as greater scalability compared to existing approaches in this field.

Keywords. Artificial Intelligence, Biomass, Gasification, Neural Networks, Syngas

1. Introduction

Gasification is a thermochemical process that, through controlled high-temperature reactions in a limited oxygen environment, transforms organic feedstock into synthesis gas (syngas), which is a mixture of Hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2), and light hydrocarbons. This mixture serves as an intermediate H_2 extraction. Management of operational parameters - which include temperature and feedstock composition, among others - is critical to achieving optimal syngas quality and efficiency.

Recent advances in Artificial Intelligence (AI) have improved waste gasification modeling. Traditional regression and decision tree-based methods provide computational efficiency and interpretability but often sacrifice accuracy [1]. Neural Networks (NNs) offer a solution for learning complex relationships from data, improving predictive performance when trained on sufficiently large datasets. However, this comes at the cost of

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increased computational demands and reduced interpretability. To overcome these limitations and increase performance, even with smaller datasets, Ren et al. [2] proposed integrating experimental data with physical constraints, enhancing NNs performance and scalability.

In this paper, we present a Physics-Informed Neural Network (PINN) approach to achieve accurate predictions of H_2 percentage despite the challenges previously discussed.

2. Methodology

This section outlines the methodology used for structuring PINN approach, focusing on the data mining process and the enhancements applied to the Neural Network method.

2.1. Dataset

A dataset of over 3000 samples was collected from the literature. These samples, coming from over 100 different papers, focused on different aspects of gasification, such as varying temperature ranges, feedstock types, or specific operational conditions. Integrating these diverse datasets lead to a more robust and comprehensive final dataset. To merge the dataset, we converted all the information to the same basis (e.g the elemental composition of the feedstock is all given in ash-free dry basis). Then we erased the rows where the features studied were not taken into account in this work, for example some works have considered the charcoal, or oils produced in the gasification, or the size of the feedstock inserted in the reactor, since in the majority of works this data was missing, we erase this features so the dataset is not biased. We cleaned the dataset, conducting exploratory data analysis to identify and drop columns with high correlations that could cause overfitting. The resulting dataset consisted of 1134 rows with 8 numerical and 5 categorical features. Finally, we applied one-hot encoding to obtain a final dataset with 22 columns. The dataset was split into three subsets: (1) a training set for fitting the neural network, (2) a validation set utilized to monitor performance during training, and (3) a test set from which final metrics and evaluation results were extracted.

The input features to the models consisted of feedstock information and reactor conditions. The feedstock information is divided into ultimate analysis (elemental composition) and proximate analysis (Moisture Content (MC), fixed carbon, and volatile matter). The reactor conditions are divided into operating conditions (amount of oxygen expressed as Equivalence Ratio (ER) and temperature) and categorical variables that describe the reactor (bed material, scale, catalyst presence, reactor type, and gasifying agent). The models predict the percentage of H_2 present in the generated syngas.

2.2. Physics-Informed Neural Network

In this work, we analyze the effect of applying physical constraints in a Neural Network to boost the generalization and ensure compliance with the physical laws that govern the reaction. To do so, we generate two identical Neural Networks, both with the same number of layers, neurons, and activation functions. The only difference between them is that one is trained using traditional data-driven methods only, while the other incorporates

physical constraints directly into the loss function. This comparative analysis provides insights into the benefits of physics-based regularization and serves as a step toward more reliable and physically consistent models in the context of chemical reactions.

Regarding the physical constraints, we adopted the monotonic relationships reported by Silva et al. [3]. H_2 production typically increases with MC due to enhanced steam reforming and water-gas shift (WGS) reactions, which consume CO to form H_2. Additionally, higher oxygen promotes combustion, which consumes carbon, leading to less oxygen.

To incorporate this monotonicity into the Neural Network, a personalized loss function has been created. This loss function consists of two main components: (1) regression loss and (2) monotonicity loss.

- The regression loss is calculated as would be in a standard NN, using the Mean Squared Error (MSE) between the predicted and actual target values.
- The monotonicity loss is defined as the ReLU of the negative of the gradient of the outputs for a selected input parameter. The sign of this gradient is enforced to match the predefined monotonicity. If the sign differs, a penalty is added to the loss function, scaled by a regularization factor λ_m.

The final loss function can be expressed as follows:

$$\mathscr{L}_{\text{total}} = \underbrace{\frac{1}{N}\sum_{i=1}^{N}(\hat{y}_i - y_i)^2}_{\mathscr{L}_{\text{reg}}} + \lambda_{\text{mono}} \cdot \underbrace{\frac{1}{N}\sum_{i=1}^{N}\text{ReLU}\left(m_i \cdot \frac{\partial \hat{y}_i}{\partial x_i}\right)}_{\mathscr{L}_{\text{mono}}} \tag{1}$$

where $\mathscr{L}_{\text{reg}}$ is the mean squared error, and $\mathscr{L}_{\text{mono}}$ enforces monotonicity with respect to selected input features x_j, where $m_j \in \{-1, 1\}$ specifies the desired direction of monotonicity.

Regarding the Neural Network architecture, various layer configurations were tests. None significant improvement ere observed when increasing the number of hidden layers beyond 2. However, due to the notably larger size of our dataset compared to previous studies, we found it necessary to use up to 64 and 32 neurons in the hidden layers to achieve satisfactory prediction performance. For optimization, we employed the Adam optimizer with a learning rate of 10^{-4}.

3. Results

The traditional Neural Network achieved a R^2 score of 0.91 and a MSE of 0.0033, while the PINN achieved a R^2 score of 0.96 and a MSE of 0.0019. Even the PINNS performed better, the most notable difference in both models can be observed in Figure 1. This figure contrasts the H_2 predictions of a traditional Neural Network and a PINN as functions of ER and MC. In the standard model (left), the predicted H_2 output does not consistently follow expected physical trends. Particularly, the relationship between MC and yield appears partially non-monotonic. This suggests the NN may struggle to generalize in low-data regions. Contrarily, the PINN model (right) maintains a more physically consistent pattern, increasing H_2 production smoothly with MC. This can be observed in the regions where the lack of data (MC$<$5 or MC$>$20) leads the NN to generalize poorly, causing

discrepancies where other parameters may incorrectly influence H_2 predictions due to the scarcity of samples, while the PINN remains consistent. The smoother gradients in the PINN output reflect that the physical constraints lead to predictions that are not only more interpretable but likely more robust for real-world applications.

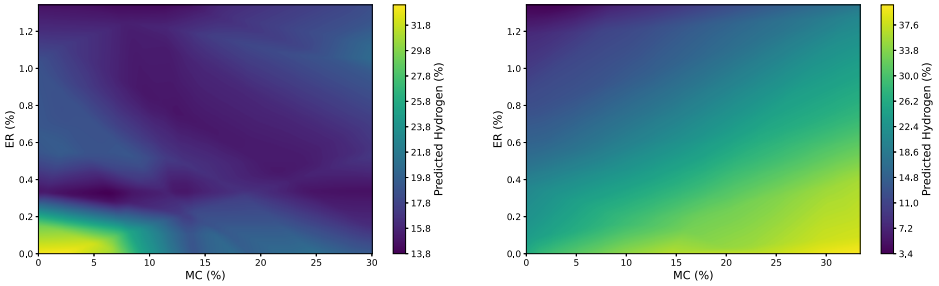

Figure 1. Contour plots showing the predicted H_2 yield as a function of temperature and MC. The left plot shows a standard NN, while the right shows predictions from a PINN. Lighter regions indicate higher H_2 yield.

4. Conclusions

By embedding physical monotonicity constraints into the training procedure, our PINN achieved greater consistency compared to traditional data-driven Neural Networks. Specifically, the PINN demonstrated improved generalization capabilities and adherence to known physical laws, enhancing reliability for real-world application scenarios. These results demonstrate the potential of physically informed machine learning methods as tools to address complex thermochemical modelling, paving the way for more efficient H_2 production from waste.

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