Research on Machine Learning-Assisted Pulse Discharge Plasma Catalysis for Methane-Carbon Dioxide Simulation

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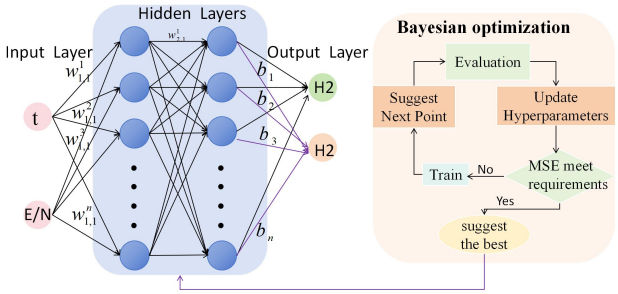
ABSTRACT

Due to the substantial complexity of plasma numerical simulation processes and the significant time required for operation, this paper establishes a dedicated dataset. It investigates deep learning-assisted modeling methods for pulsed discharge plasma catalysis. By employing machine learning, we assess regression algorithms using K-fold cross-validation alongside the coefficient of determination (R^2) metrics. We select the most effective Artificial Neural Network (ANN) to assist in plasma catalysis modeling. Notably, the ANN demonstrates multiple advantages, including improved efficiency and adaptability. To enhance prediction accuracy, we implement Bayesian Optimization (BO) for tuning the ANN parameters. Experimental results indicate that the outcomes derived from the ANN, optimized through Bayesian methods, align well with the numerical results from dynamic models.

INTRODUCTION

As human society continues to develop, the concentration of greenhouse gases steadily rises, making it imperative to reduce these emissions. The 2015 Paris Agreement acts as a global pact that is centered on restraining greenhouse gas emissions in order to avoid severe global warming events [1]. On our planet, CH4 stands as the second largest anthropogenic greenhouse gas, trailing only CO2. Since the onset of industrialization, CH4 has contributed to a global temperature increase of 0.6 degrees Celsius[2].Plasma-catalyzed methane dry reforming represents a process that utilizes plasma catalytic interactions to convert greenhouse gases CH4-CO2 into H2 and CO, thereby reducing atmospheric greenhouse gas levels. However, plasma numerical simulations typically demand substantial computational resources and time, leading to lengthy and costly simulations. Finding a way to overcome this challenge and streamline plasma numerical simulations presents a significant problem in this field.This paper presents a machine learning-assisted approach to plasma methane dry reforming catalyst modeling. First, we apply K-fold cross-validation and utilize the R^2 metric to assess the regression algorithms. Next, we select the best-performing Artificial Neural Network (ANN) as the predictive model's machine learning algorithm. Finally, we implement Bayesian Optimization (BO) to refine the neural network parameters, enhancing model accuracy.

METHODS



DISCUSSION

To validate the performance of the neural network after integrating Bayesian methods, this paper conducted a comparative analysis of the Artificial Neural Network (ANN) and the Bayesian Optimized ANN (BO-ANN). The results are illustrated in Figures 1 and 2. Figure 1 presents the kinetic model of methane-carbon dioxide pulsed discharge plasma and the hydrogen density computed by the ANN, under varying E/N levels. The upper section of Figure 1 displays the hydrogen density results from numerical simulations, while the lower section reflects the hydrogen density values derived from the ANN calculations. Figure 2 similarly illustrates the kinetic model and hydrogen density calculated by the BO-ANN for the methane-carbon dioxide pulsed discharge plasma across changing E/N levels, with the upper half showing the numerical simulation results and the lower half providing the density results calculated using the BO-ANN.

To more distinctly illustrate the effects of incorporating Bayesian optimization, I subsequently created correlation graphs using real data and machine learning simulated data. Figures 3 and 4 display the correlation between the predicted and actual values of hydrogen density generated through ANN and BO-ANN-assisted pulsed discharge plasma catalysis of methane and carbon dioxide. It is evident that the scattering of results from the BO-ANN assisted plasma/plasma-catalyzed modeling is relatively tightly spread across either side of the line Y=X, indicating that the neural network model supported by Bayesian optimization can achieve accurate predictions of target product particle density. The regression parameters are 0.9912 and 0.996, quantitatively demonstrating the accuracy of this predictive methodology. Additionally, the findings indicate a strong consistency between the results derived from deep neural network computations and numerical outcomes obtained from kinetic modeling.

RESULTS

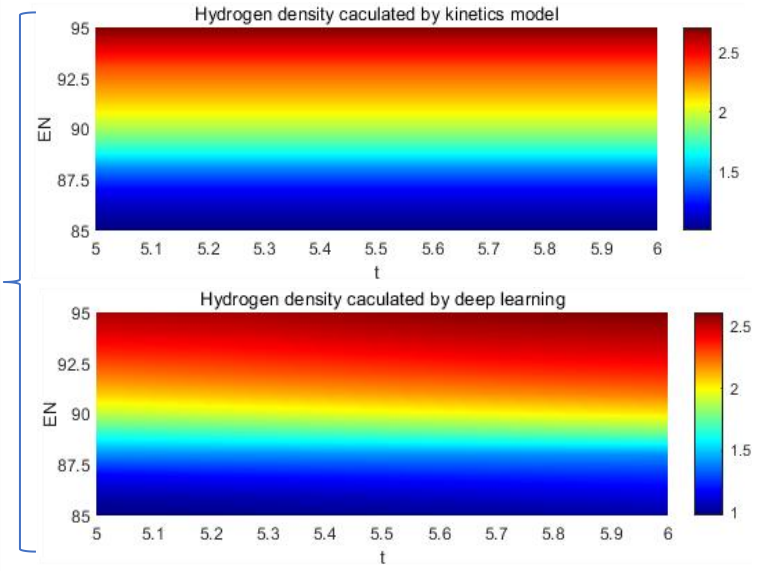


Fig. 1.The computation of H2 density in CH4/CO2 pulse discharge plasma with the use of ANN assisted plasma modeling under diverse E/N and residence times.

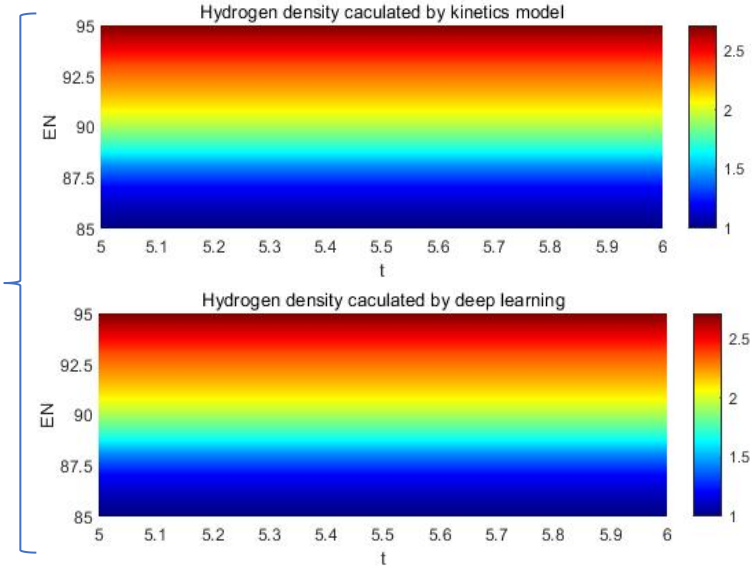


Fig. 2.The computation of H2 density in CH4/CO2 pulse discharge plasma with the use of BO-ANN assisted plasma modeling under diverse E/N and residence times.

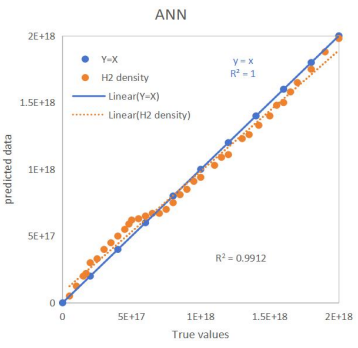


Fig. 3.Correlation graph between the predicted and actual hydrogen density values generated by ANN-assisted pulsed discharge plasma catalysis of methane and carbon dioxide.

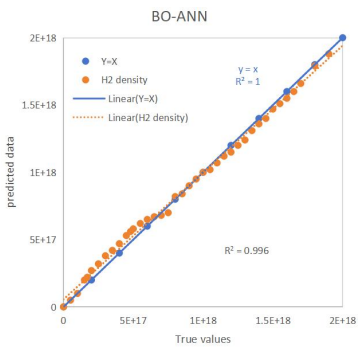


Fig. 4.Correlation graph between the predicted and actual hydrogen density values generated by ANN-assisted pulsed discharge plasma catalysis of methane and carbon dioxide.

REFERENCES

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