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A Deep Learning Model with Greedy Layer-Wise Pretraining Approach for Optimal Syngas Production by Dry Reforming of Methane

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Abstract : Dry reforming of methane (DRM) has sparked significant industrial and scientific interest not only as a viable alternative for addressing the environmental concerns of two main contributors of the greenhouse effect, i.e., carbon dioxide (CO_2) and methane (CH_4), but also produces syngas, i.e., a mixture of hydrogen (H_2) and carbon monoxide (CO) utilized by a wide range of downstream processes as a feedstock for other chemical productions. In this study, we develop an AI-enable syngas production model to tackle the problem of achieving an equivalent H_2/CO ratio [1:1] with respect to the most efficient conversion. Firstly, the unsupervised density-based spatial clustering of applications with noise (DBSAN) algorithm removes outlier data points from the original experimental dataset. Then, random forest (RF) and deep neural network (DNN) models employ the error-free dataset to predict the DRM results. DNN models inherently would not be able to obtain accurate predictions without a huge dataset. To cope with this limitation, we employ reusing pre-trained layers' approaches such as transfer learning and greedy layer-wise pretraining. Compared to the other deep models (i.e., pure deep model and transferred deep model), the greedy layer-wise pre-trained deep model provides the most accurate prediction as well as similar accuracy to the RF model with R^2 values 1.00, 0.999, 0.999, 0.999, 0.999, and 0.999 for the total outlet flow, H_2/CO ratio, H_2 yield, CO yield, CH_4 conversion, and CO_2 conversion outputs, respectively.

Keywords : artificial intelligence, dry reforming of methane, artificial neural network, deep learning, machine learning, transfer learning, greedy layer-wise pretraining
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