Use of Reduced Order Models (ROMs) to Predict SOFC Stack Performance

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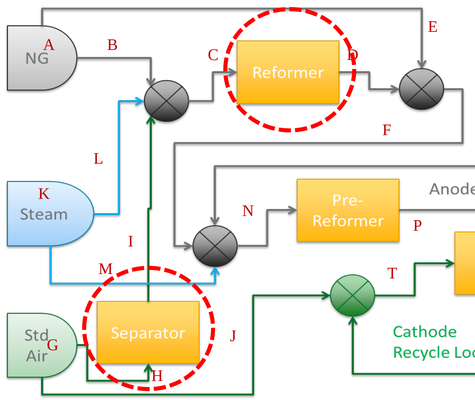
ROM FOR VARIOUS SOFC SYSTEMS

A Kriging regression-based reduced order model (ROM) is created to provide a quick and accurate estimate for the SOFC stack performance. Multiple ROMs have been created for natural gas fuel cell (**NGFC**) and integrated gasification fuel cell (**IGFC**) systems with different gasifier compositions (**conventional, enhanced, and catalytic**), **pressurized systems** (1-5 atm), system configurations with and without **carbon capture and storage** (CCS), and **vent gas recirculation** (VGR). These ROMs serve as key components in Aspen Plus models used to perform system analyses for NETL's Pathway Studies.

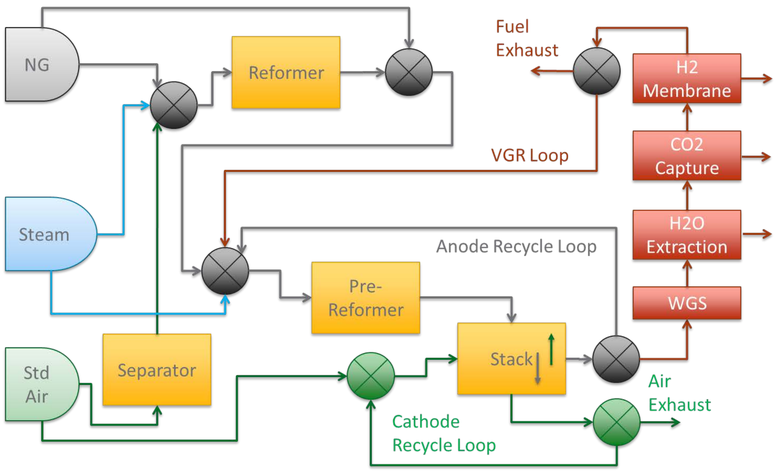
NGFC Flowchart



If no external reformer and syngas used at the inlet "A", NGFC ⟶ IGFC

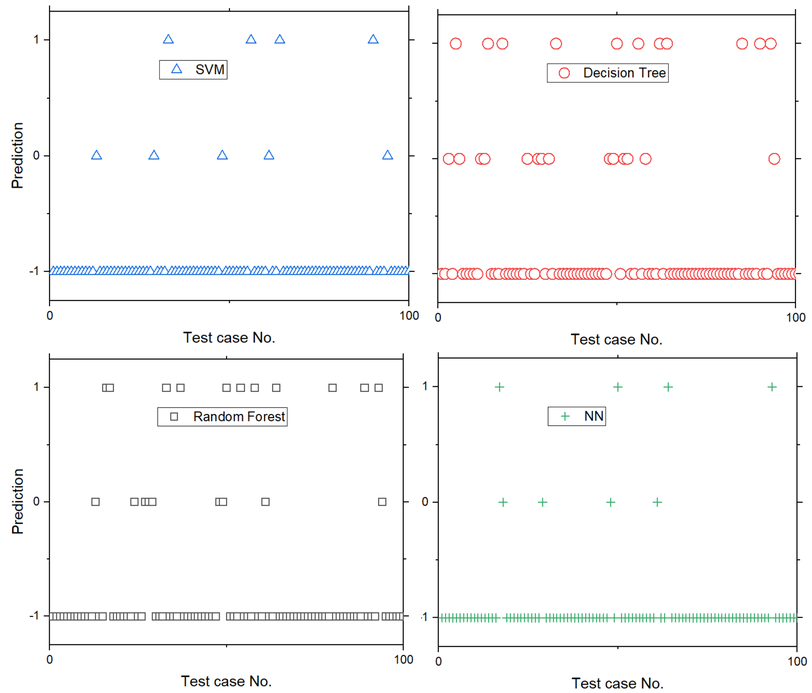
If no air separator, CCS ⟶ w/o CCS

NGFC with VGR Flowchart



MACHINE LEARNING CLASSIFICATION

Machine learning (**ML**) approaches are implemented to identify the physical operating domain of the SOFC stacks, i.e., determine if a given ROM prediction is physical or non-physical. Several traditional ML classification approaches including support vector machine (SVM), random forest, and decision tree together with the advanced neural network (NN) classification method are tested. The results indicate that NN can provide the best prediction accuracy, followed by SVM, random forest, and lastly decision tree.



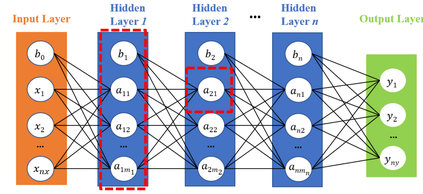
Comparisons of 4 ML Methods for ROM Classification

The ML output indicates whether the given inputs fall in the physical operating domain. More specifically, prediction output **1 indicates PHYSICAL, 0 indicates UNSURE, and -1 indicates NON-PHYSICAL**. The number of training and testing data set are 18,000 and 2,000, respectively. The NN consist of only one hidden layer with 500 neurons.

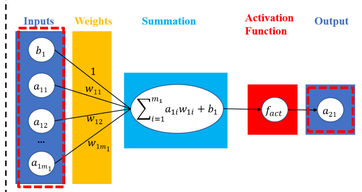
ML Method	Prediction Accuracy
NN	**93.0%**
SVM	**91.4%**
Random Forest	**89.0%**
Decision Tree	**82.6%**

DEEP LEARNING REGRESSION

A deep neural network (**DNN**)-based ROM is also built and serves as an alternative to the Kriging regression-based ROM to predict system level SOFC stack performance. It is demonstrated that DNN ROM can provide **better prediction accuracy and reduce the prediction error by a factor of 2-3** compared with Kriging ROM.

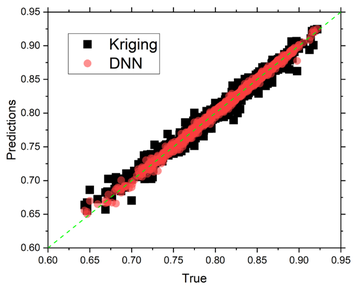


Schematic DNN Framework

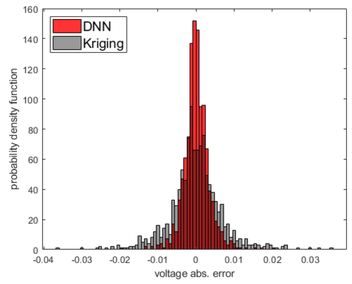


Individual Neuron

The DNN contains a total of 4 layers and the number of neurons in each layer are 32, 200, 200, and 256, respectively. The number of training and testing data set are 10,000 and 1,000, respectively. To perform apple-to-apple comparison, the Kriging regression-based ROM uses the same training and testing data set.



Voltage Prediction Comparison



Voltage Absolute Error PDF Comparison

Parameters from PDF	DNN	Kriging	Improvement Ratio
UB for 95% CI	0.0057	0.0135	**2.36**
LB for 95% CI	-0.0060	-0.0136	**2.27**
Max Error	0.0130	0.0354	**2.72**
Min Error	-0.0140	-0.0362	**2.59**

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