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.

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.

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.

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

DEEP LEARNING REGRESSION
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Schematic DNN Framework
Individual Neuron

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.

Comparisons of 4 ML Methods for ROM Classification

<table>
<thead>
<tr>
<th>Parameters from PDF</th>
<th>DNN</th>
<th>Kriging</th>
<th>Improvement Ratio</th>
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<tbody>
<tr>
<td>UB for 95% CI</td>
<td>0.0057</td>
<td>0.0135</td>
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<tr>
<td>LB for 95% CI</td>
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<td>Min Error</td>
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