Reduced Order Models (ROMs) for SOFC Stack Performance Prediction

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New Features in SOFC ROM GUI

Integrated multiple categories of SOFC systems

Nine different system designs are merged into the ROM construction tool and graphical user interface (GUI)- e.g., NGFC, IGFC with different gasifiers, with/without carbon capture, with/without vented gas recirculation, etc.

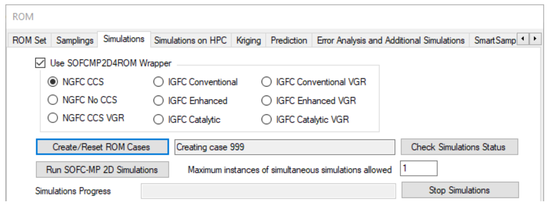

Figure 1: SOFC ROM GUI for selecting different categories of SOFC-based power systems.

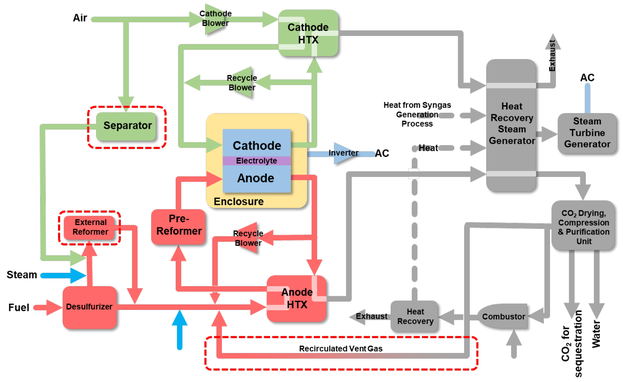

Figure 2: An example of the generic SOFC system flow chart. Different categories of SOFC systems can be modeled by adjusting the fuel inlet composition and enabling/disabling combinations of the oxygen separator, external reformer, and recirculated vent gas modules.

Smart-Sampling

- The Smart-Sampling feature is integrated in SOFC ROM GUI.
- Automatically adds new samples based on the ROM prediction error.
- Achieves higher ROM prediction accuracy with less samples and simulations

Cross-Validation

- The SOFC ROM GUI uses part of the simulation results (e.g., 90% of the samples) as the training set to build the ROM and uses the remaining samples (e.g., 10% of the samples) to verify the accuracy of the constructed ROMs.
- Provides the confidence interval for a user-defined confidence percentage.

Machine Learning Based Prediction

Regression model

Physics-informed machine learning (ML) based regression model is introduced to replace the computationally expensive physics based SOFC simulations (SOFC-MP) for system design and optimization.

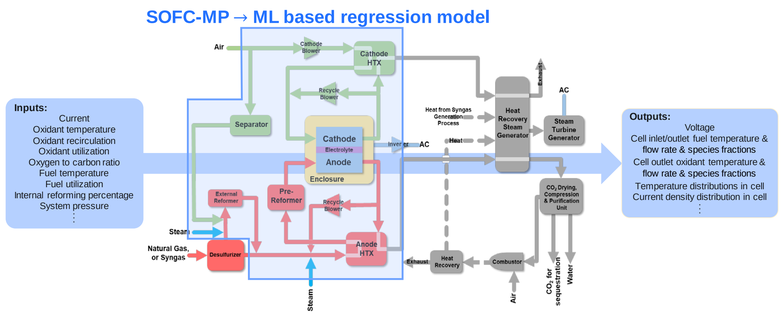

Figure 3: Sketch of regression model that links the input and output parameters.

Deep neural networks (DNN) with mass balance model (MBM) approach can significantly reduce the prediction error (RMSE) compared to Kriging based reduce order model (ROM) and the conventional DNN.

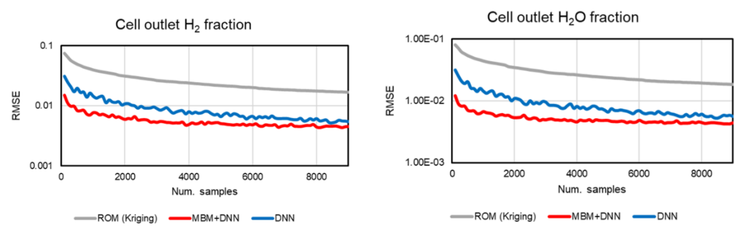

Figure 4: Prediction accuracy comparison for selected outputs: H_2 and H_2O fraction at cell outlet.

Classifier to determine if the system is physically operational

- Not all input parameter combinations can make the fuel cell system physically operational.
- The coupled DNN regression + DNN classifier + MBM can improve the prediction accuracy (purple line).

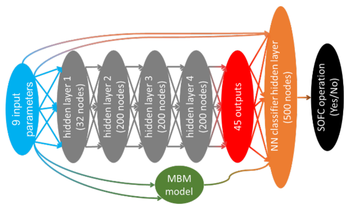

Figure 5: Sketch of the classifier networks.

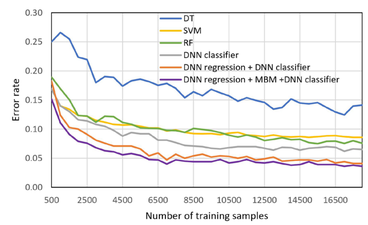

Figure 6: Comparison between different classifiers to characterize viable operation.

Transferring DNN from State-of-the-art (SOA) SOFC to advanced SOFC electrodes

- Advanced SOFC electrode assumes 50% reduction for the activation and ohmic polarization losses compared to the SOA SOFC electrodes
- A well trained DNN for SOA SOFC electrodes can be transferred to advanced SOFC electrode with small amount of training data.

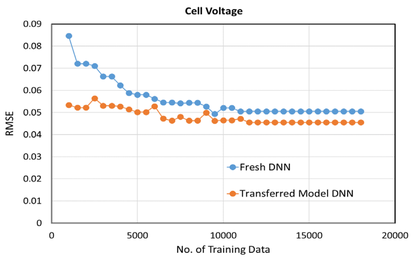

Figure 7: Cell voltage prediction error comparison between fresh and transferred DNN for advanced SOFC electrode using different numbers of training data. The transferred results from the first model provide improved error reduction for the different second model.

Automated ROM Construction on HPC Cluster

- The SOFC-MP ROM GUI provides the capability to transfer the time-consuming simulations to the Linux HPC cluster. However, because of the data transfer between the Windows host computer and remote Linux HPC solver, the whole ROM construction process is not fully automated, e.g., the user needs to implement the construction procedure step by step and check the status of simulation jobs on the Linux HPC.
- To overcome those limitations, a Linux version of an automated ROM construction tool has been developed.
- It provides two strategies for constructing the ROM. One strategy uses a conventional approach and the other uses a smart sampling approach.

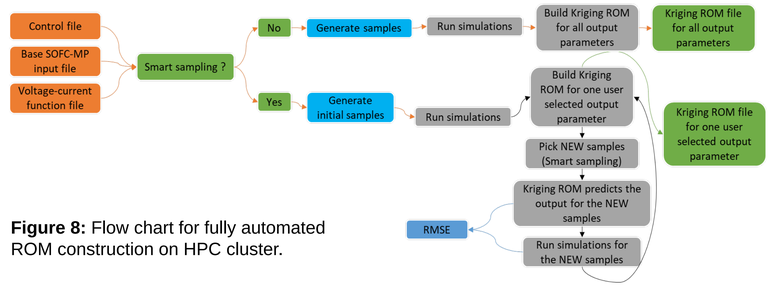

Figure 8: Flow chart for fully automated ROM construction on HPC cluster.

Acknowledgement

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