Improved Capability and Accuracy of a Reduced Order Model (ROM) for SOFC Stacks

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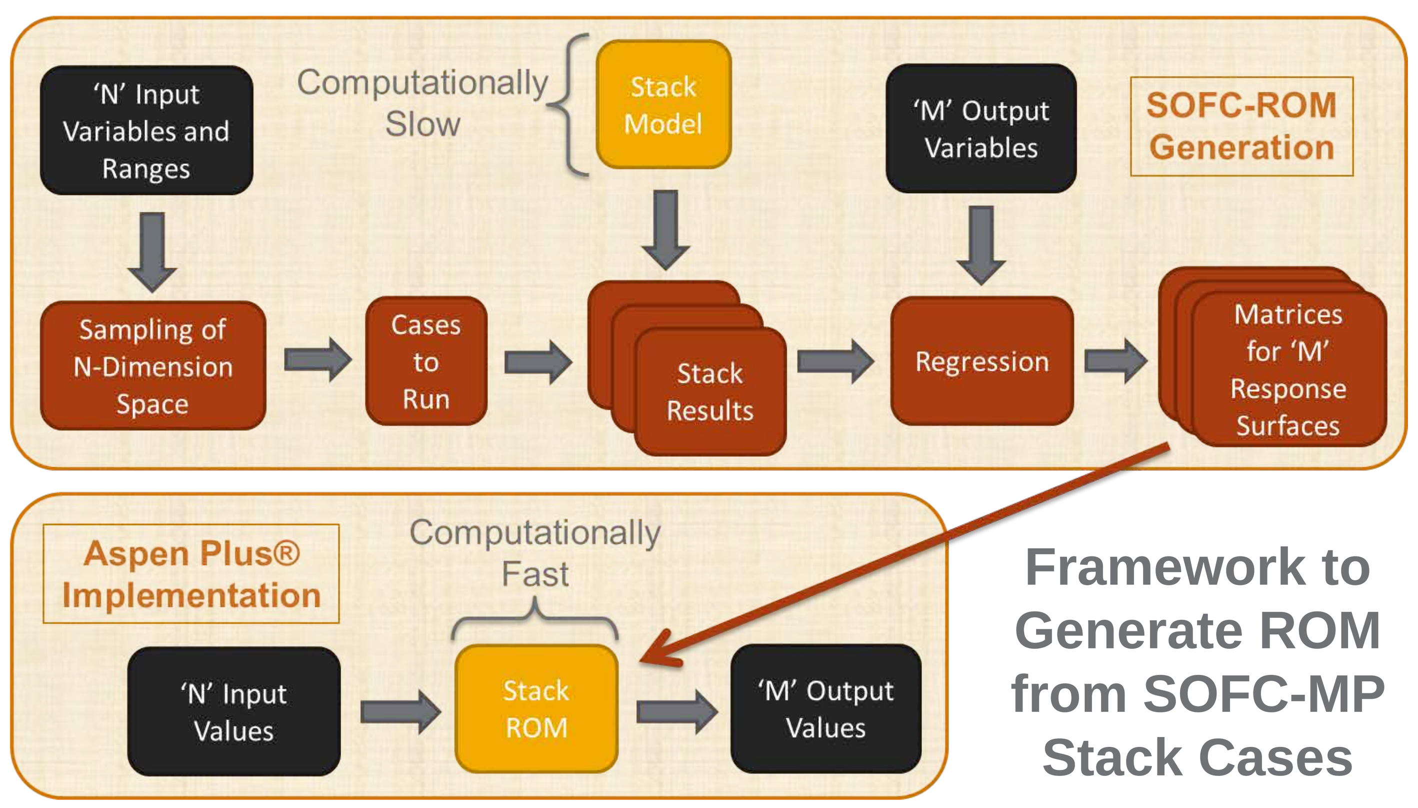
OVERVIEW

PNNL developed an approach to use a reduced order model (ROM) to represent the stack in SOFC power system analyses, and the created ROM was tested in NETL OPPA's natural gas fuel cell (NGFC) system model. This poster presents additional enhancements made to the ROM approach and a method to characterize and reduce the ROM's approximation error.

ROM TECHNICAL APPROACH

Numerical models for design and performance studies of SOFC-based power generation systems require an accurate representation of the fuel cell stack. High fidelity information about the stack can be obtained from detailed models, but these models are too computationally expensive for direct inclusion in the system model. A response surface approach was used to generate a ROM that retains desirable information about the state of the stack.



Framework to Generate ROM from SOFC-MP Stack Cases

ADVANCED ROM DEMONSTRATION

The fuel and oxidant recirculation loops for the SOFC stack were included directly in the ROM rather than in the system model. This allows variable amount of recirculation, includes the effects of exhaust heat recovery from fuel and oxidant stream recuperators, and simplifies the integration in the Aspen Plus system model. This advanced ROM was generated for the counter-flow stack results from PNNL's 2D SOFC-MP software and will be again tested in NETL OPPA's atmospheric NGFC plant model. The wide range of input parameters for the ROM were:

- Average Current Density — 2000-6000 A/m^2
- Internal Reforming — 0-100%
- Oxidant Recirculation — 0-80%
- Oxygen-to-Carbon Ratio Target @ Stack Inlet — 1.5-3.0
- Fuel Utilization (including recirculation loop) — 40-95%
- Oxidant Utilization (including recirculation loop) — 12.5-83.3%
- Oxidant Stack Inlet Temperature — 550-800^{o}C
- Fuel Loop Inlet Temperature — 15-600^{o}C

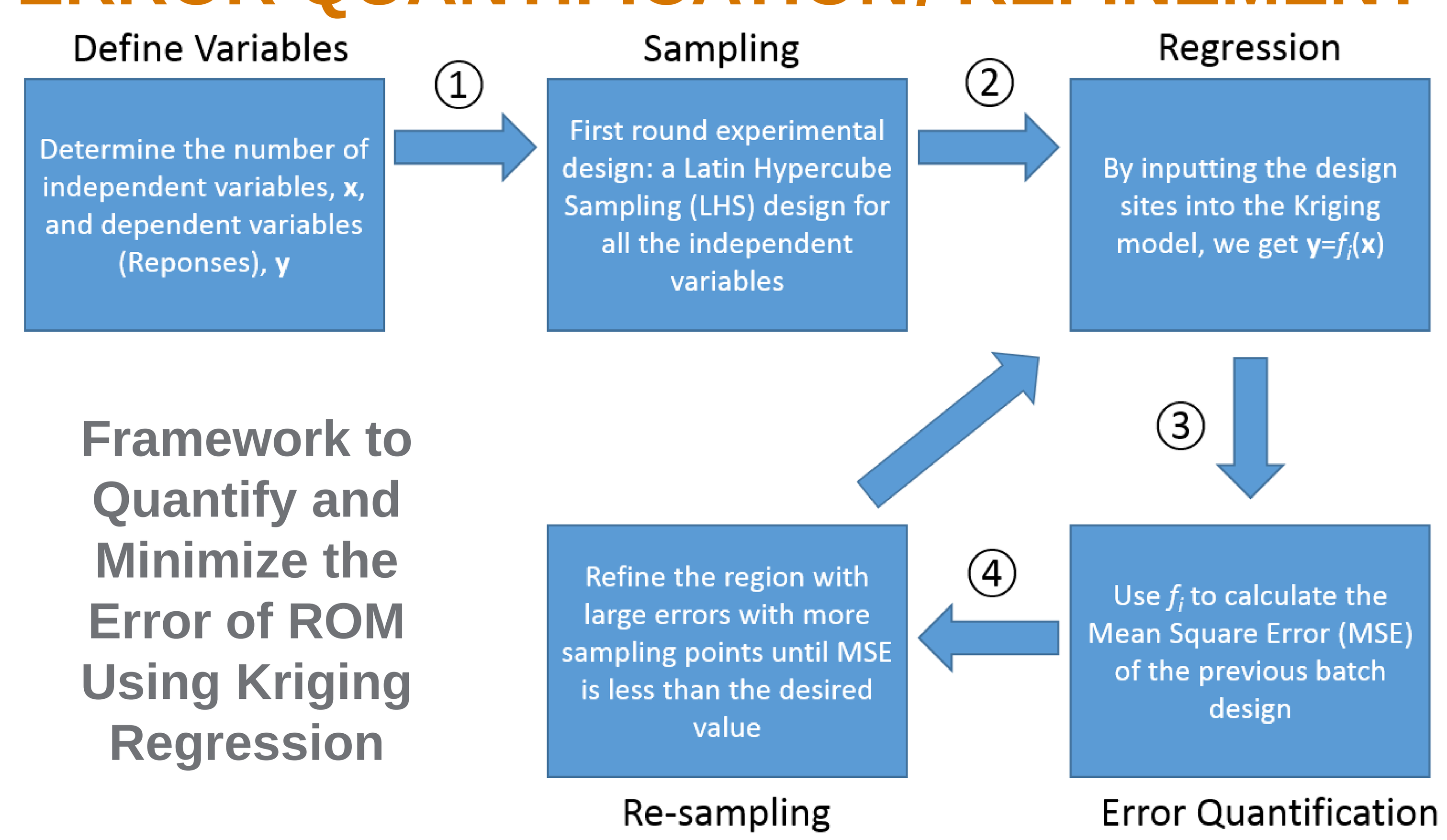
The ROM was built using the Kriging method based on 520 successful cases (296 cases resulted in unviable solutions and were discarded from the ROM set). The estimated mean approximation error for the entire domain based on Kriging was <4% for the stack voltage and <8% for the stack maximum cell temperature.

ROM ERROR FOR TEST CASE RESULTS

Kriging was used as the regression approach to define the response surface. The estimated mean error and mean square error from the solved cases are provided by Kriging. An advanced ROM was generated for the counter-flow stack in an atmospheric NGFC system. The actual error is evaluated by comparison to two test cases, and results for key metrics were acceptable, e.g., <1% error for voltage and temperature.

Test Cases				Actual Results			ROM Results			Approximation Error		
	1	2			1	2	1	2			1	2
J	4000	4000	A/m^2	Current	219.9	219.9	220.2	220.0	A	Current	0.1%	0.1%
FU	90%	80%		Voltage	0.813	0.844	0.820	0.850	V	Voltage	0.9%	0.7%
AU	27.7%	29.0%		CD Max	0.608	0.586	0.447	0.459	A/m^2	CD Max	-26.4%	-21.8%
O/C	2.6	2.1		Tcell Avg	797.8	800.4	795.9	804.2	C	Tcell Avg	-0.2%	0.5%
IR	60%	60%		Tcell Min	722.5	732.3	720.6	735.4	C	Tcell Min	-0.3%	0.4%
Arecirc	50%	50%		Tcell Max	819.2	818.7	817.4	819.7	C	Tcell Max	-0.2%	0.1%
Tfuel	90	90	C	Tair Out	795.9	791.0	794.3	797.6	C	Tair Out	-0.2%	0.8%
Tair	709.4	718.7	C	Tfuel Out	761.5	770.8	760.3	772.0	C	Tfuel Out	-0.2%	0.2%

ERROR QUANTIFICATION/ REFINEMENT



Framework to Quantify and Minimize the Error of ROM Using Kriging Regression

CONCLUSIONS AND FUTURE WORK

- Demonstrated SOFC stack ROM with recirculation features.
- Used cross validation to quantify ROM error distributions.
- DOE useful for pre-identification of sensitive ROM parameters.
- User interface to incorporate DOE approach in ROM analyses, perform error refinement with smart sample augmentation, and export the SOFC ROM is under development.

ACKNOWLEDGEMENT

This work was funded as part of the Solid Oxide Fuel Cell Core Technology Program by the U.S. Department of Energy's National Energy Technology Laboratory.

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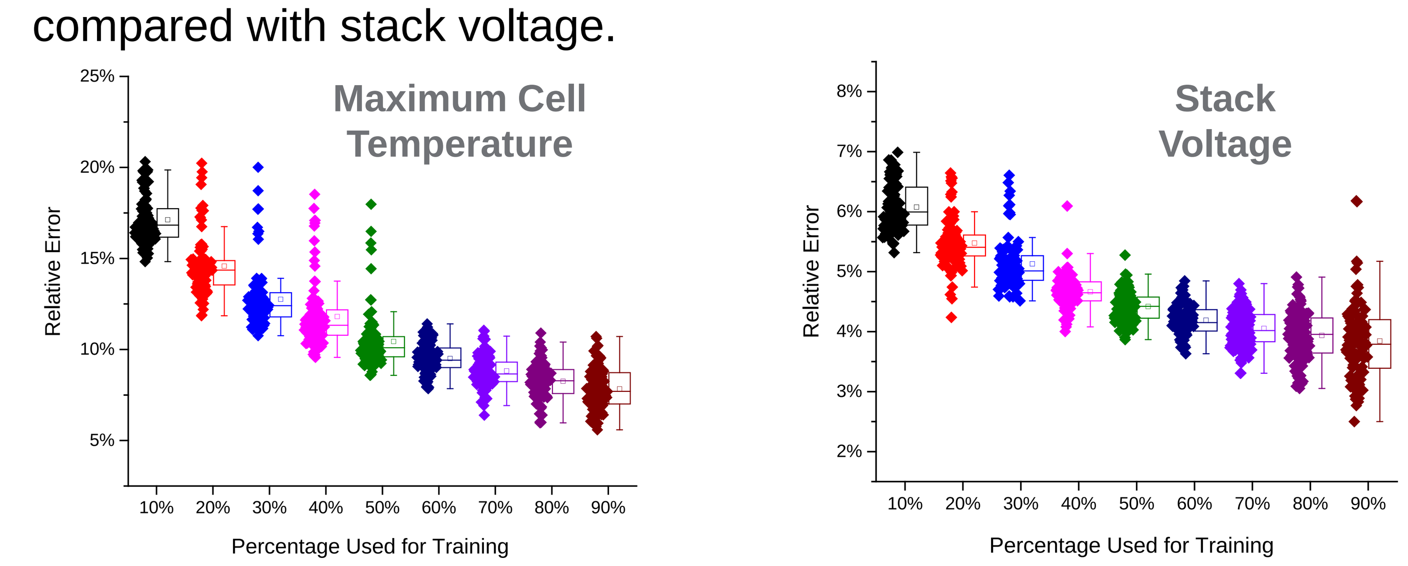
CROSS-VALIDATION AND ERROR DISTRIBUTIONS FOR ROM PREDICTIONS

To obtain the error distribution, results generated from SOFC-MP cases must be partitioned into a training data set and a validation data set. The training data set is used for regression to generate the Kriging approximation, and the error distribution is computed from the remaining validation data set. Multiple partitions are then performed and evaluated.

- Error distribution is plotted using data from 520 SOFC-MP stack cases.
- Error and variance in general decreases with more samples used for training (note the final exported ROM will utilize all available samples).
- Error and variance are slightly greater for maximum cell temperature compared with stack voltage.



DOE METHODS TO ASSESS SENSITIVITY OF ROM INPUT PARAMETERS

Purpose: Evaluate Design of Experiments (DOE) methods to examine the impact of individual effects and interactions of independent variables (factors) on dependent variables (responses).

Approach: Use Yates analysis to divide factors into high and low levels, build the design matrix, and then compute the value of corresponding responses. Use estimate of effect and sum of squares to determine the significance of each factor and interaction.

Example: 2^3 full factorial design with stack data generated by SOFC-MP.

Factors: Average stack current density ***A*** (A/m^2), inlet fuel temperature ***B*** (°C), and inlet oxidant temperature ***C*** (°C).

Response: Maximum cell temperature ***D*** (°C).

Results:

- Main effect comes from Factor A.
- Factor C is next most influential factor.
- Significances of the other factors and interactions are trivial.
- This approach can be used to identify sensitive parameters for fuel cell stack predictions and simplify the ROM.

Design Matrix

A	B	C	D
5000	700	700	871.5
4000	700	700	836.9
5000	600	700	869.7
4000	600	700	836.7
5000	700	600	876.0
4000	700	600	842.8
5000	600	600	878.8
4000	600	600	844.8

Table of Effects

Factors	Estimate of Effect	Sum of Squares	Percent Contribution
A	-33.73	2275.45	95.71
B	0.70	0.99	0.04
C	6.86	94.33	3.96
AB	0.21	0.09	0.00
AC	0.11	0.02	0.00
BC	1.68	5.66	0.23
ABC	-0.60	0.74	0.031