ROM Tool for SOFC-MP Modeling

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Overview

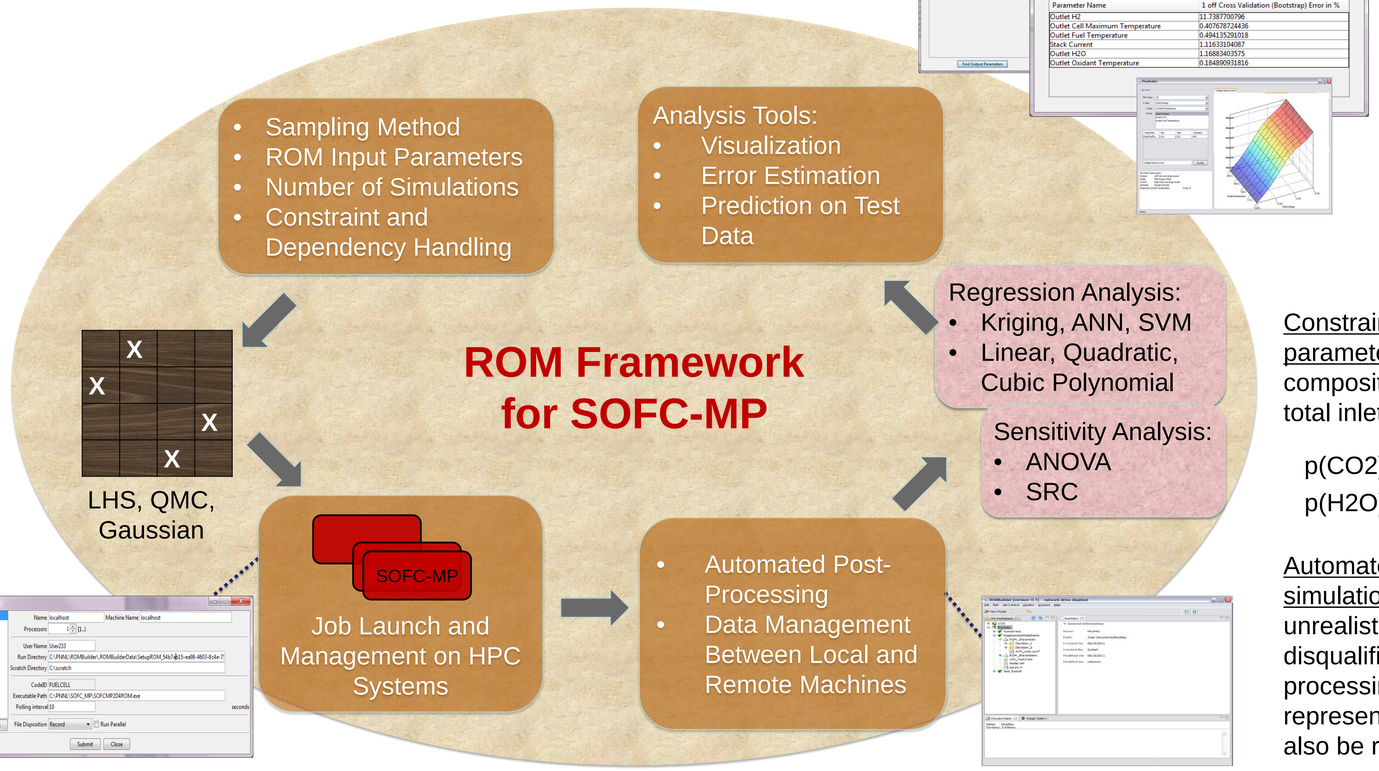
High fidelity SOFC models are computationally expensive to run and hence prohibitive for use in larger scale power system simulations. Reduced Order Models (ROMs) provide approximate representations of such models in O(1) time. REVEAL is a generic, automated framework for building ROMs to use in such scientific and engineering simulations.

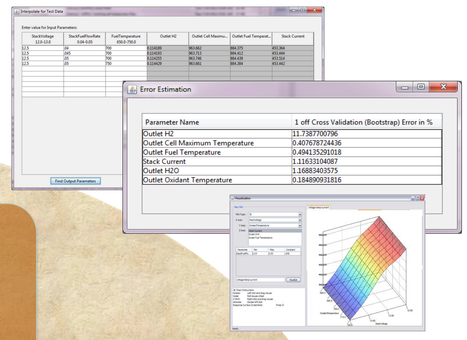
SOFC-MP

SOFC-MP is a simulation tool developed at PNNL to evaluate the tightly coupled multi-physical phenomena in SOFCs. The purpose of the tool is to allow SOFC manufacturers to numerically test changes in planar stack design to meet DOE technical targets. The SOFC-MP 2D module is designed for computational efficiency to enable rapid engineering evaluations for operation of tall symmetric stacks. It can quickly compute distributions for the current density, voltage, temperature, and species composition in tall stacks with co-flow or counter-flow orientations.

ROM Workflow

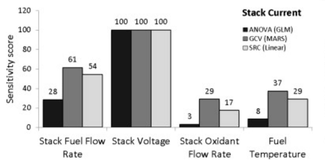
- The SOFC-MP 2D stack model presently serves as the input to the ROM workflow.
- The user can select input parameters to sample, sampling method (LHS, QMC, Gaussian), number of samples, and specify parameter constraints (fuel composition, steam-to-carbon ratio, oxidant composition).
- REVEAL automatically generates samples and prepares simulations to run.
- A generic job launching tool facilitates simulation runs on any HPC machine, collects results, and brings them back to the local machine for analysis.
- User can select between multiple regression and sensitivity analysis methods best suited to their particular model.
- A wide array of analysis tools are available: automated error estimation, 2D/3D visualization, output prediction tool.
- Output of ROM in format compatible with users' system modeling software.



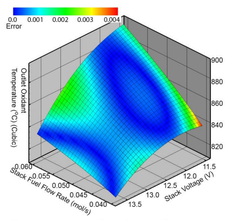


ROM Approach and Analysis

- 16-cell 25x25 cm^2 co-flow stack case
- "A General Approach to Develop Reduced Order Models for Simulation of Solid Oxide Fuel Cell Stacks," *J Power Sources* **232**: 139 (2013).



Parameter Sensitivity Scores for Stack Current



Response Surface for Outlet Oxidant Temperature

Features of the ROM toolkit

- Generic, extensible to other models.
- Portability to both Linux and Windows.
- Built with all open source technology.
- 'Plug and play' semantics between different sampling and regression algorithms.
- Job launching tool with comprehensive set of analysis tools.
- Complete user environment, along with data management and data sharing capabilities.
- Optional: Exports ROM as a module in ACM or Cape Open format to be plugged into process modeling simulations.

Recent Accomplishments

Constraint-based sampling of fuel/oxidant composition parameters: Supports sampling of different fuel and oxidant composition parameters while satisfying the constraints on total inlet partial pressure and steam-to-carbon ratio:

$$p(CO2) + p(CO) + p(CH4) + p(H2O) + p(N2) + p(H2) = 1$$

$$p(H2O) / (p(CO2) + p(CO) + p(CH4)) > user\_threshold$$

Automated identification and handling of unconverged simulations: Selection of wide sampling ranges may lead to unrealistic cases and unconverged solutions. REVEAL disqualifies such cases and discards them from further processing. The resulting ROM is a more accurate representation of the stack model. Additional cases can also be run to augment the solution set if necessary.

Future Work

- Evaluate ROM export capabilities and integration with commercial system modeling tools (e.g. ASPEN) for study of SOFC-based power generation systems.
- Evaluate methods for response surface analysis for cases using constrained variables.
- Release ROM version with examples and documentation.
- Continue 2D/3D framework for SOFC-MP tools:
  - Integrate the pre-processing of generic 3D FEA models with the graphical user interface.
  - Add capability to export generic FEA models for stress analysis.
  - Integrate SOFC-MP 3D modeling approach as input to the ROM tool.

Acknowledgement

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