Enhanced SOFC-MP Software Tool Set

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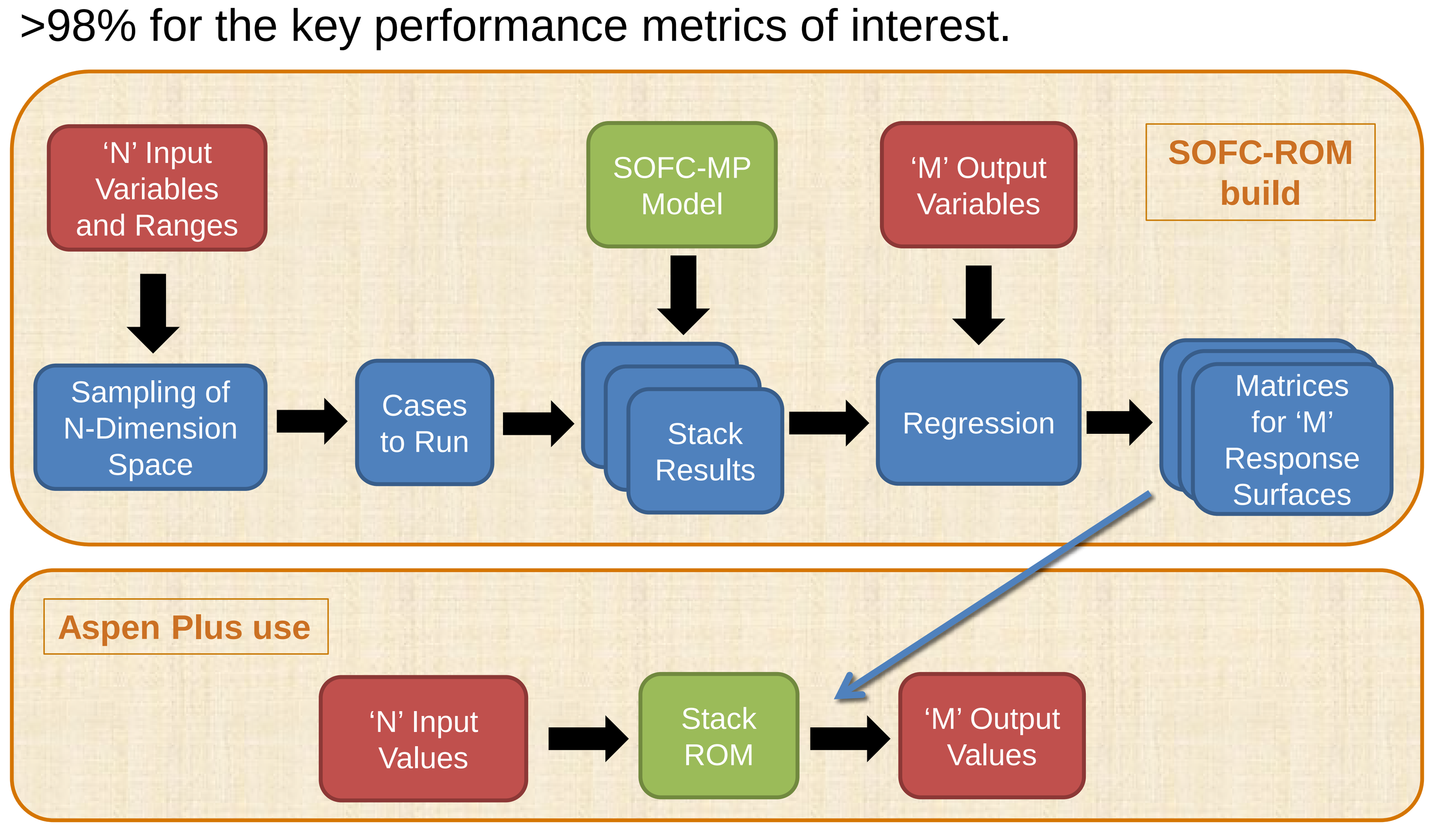
OVERVIEW

This poster presents an overview of PNNL's comprehensive SOFC-MP software tool package and some of the most recent enhancements. The tool set includes:

- SOFC-MP 2D: efficient simulations of co/counter-flow stacks.
- SOFC-MP 3D: detailed simulations of planar stack geometries provide temperature fields for thermal-stress analysis.
- Graphical User Interface (GUI): provides user-friendly integration for 2D/3D modules. It is capable of performing pre-processing, job launching, status monitoring, and post-processing functions.
- Reduced Order Model (ROM) Tool: generates a ROM, based on high fidelity SOFC-MP results and using response surface techniques, to rapidly predict stack performance metrics.
- SOFC-MP/ROM Interface: integrates the stack and ROM tools.

In collaboration with NETL/ESPA last year, the ROM approach was demonstrated by inclusion in the Aspen Plus NGFC power system model to simulate the effect of state-of-art stack performance on cost of electricity projections. Accuracy of the stack ROM was found to be >98% for the key performance metrics of interest.



TECHNICAL APPROACH

Based on the successful demonstration of the ROM approach, improvements to the software tools that could improve the ROM's capability and ease of implementation were identified and pursued:

- Application to other NG compositions.
- Recirculation capability to calculate stack inlet temperature and composition conditions for the fuel and oxidant recycling loops.
- Pressurized electrochemistry operation.
- Use of 3D SOFC-MP models to create a ROM.
- Calculation of the pressure drop in 2D SOFC-MP.
- Variable pre-reformer fraction in the NGFC material flow balance.
- Simplified Aspen Plus integration.
- Application to IGFC.

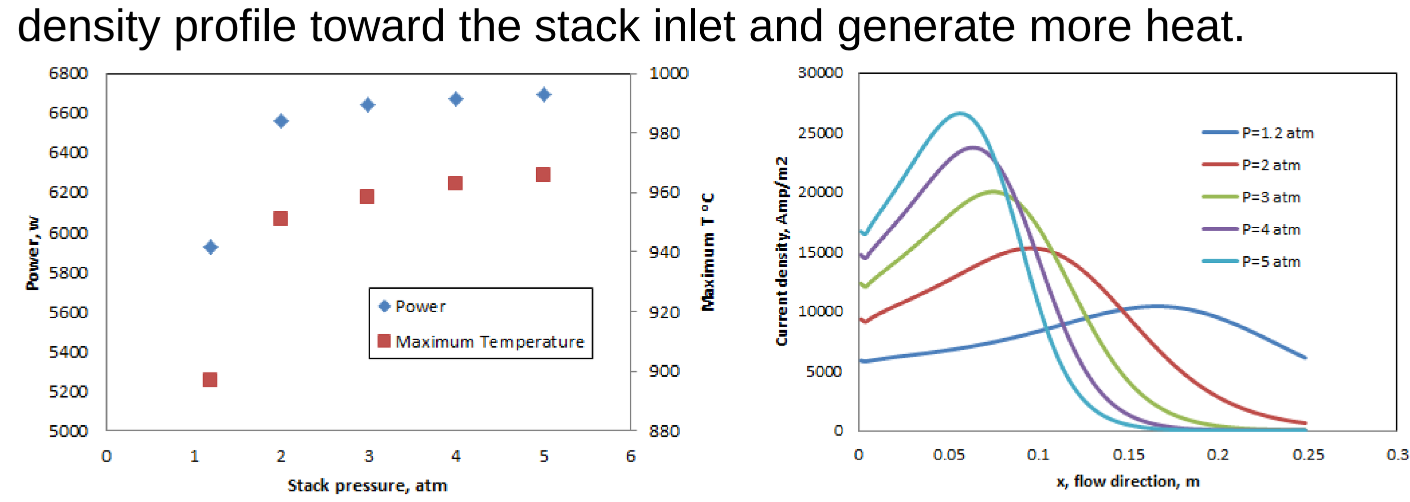
CONCLUSION AND FUTURE WORK

- Improved SOFC-MP/ROM capabilities will support use in NETL OPPA's power generation system models.
- Demonstrate improved ROM capability with added capabilities.

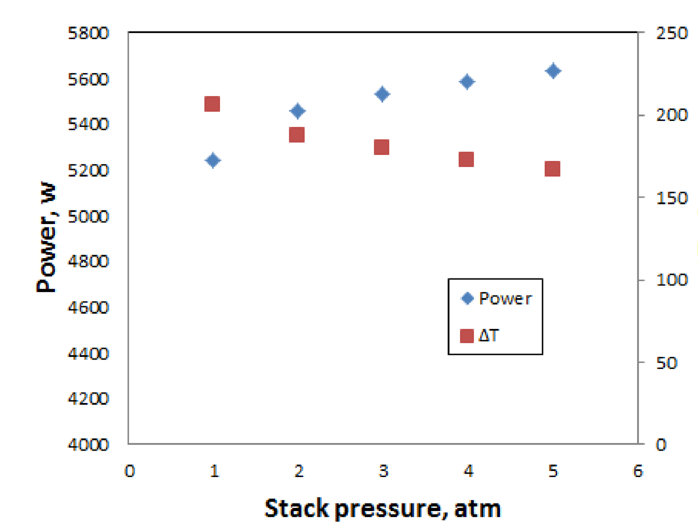
PRESSURIZED STACK PERFORMANCE

The fuel cell system can operate more efficiently at elevated pressure, so the atmospheric electrochemical model of the SOFC-MP 2D module has been enhanced to include beneficial effects of high pressure on the stack performance. Two evaluations were performed to test and demonstrate the high pressure electrochemistry capability.

1. *Fixed cell voltage and air/fuel inlet temperatures*: Higher stack pressure increases cell power as expected. More efficient operation at fixed voltage increases the fuel utilization to shift the high current density profile toward the stack inlet and generate more heat.



2. *Imposing constraints of fixed maximum stack temperature and fixed fuel utilization*: Higher stack pressure improves the overall power generation while also beneficially decreasing the ΔT in the stack to reduce the cell thermal stresses.



PRE-REFORMER FRACTION

For increased flexibility in simulating different operating states of NETL OPPA's NGFC power generation system, the amount of CH_4 pre-reforming must be tuned to control the amount of CH_4 remaining for on-cell reformation. This variable was implemented in the ROM approach. Different stack compositions from the material flow balance are shown to demonstrate the different stack inlet conditions and results from SOFC-MP 2D (at fixed target O/C ratio, current density, and reformer efficiency).

Pre-reform Fraction	H_2 (mol/s)	CO (mol/s)	CH_4 (mol/s)	Fuel Rate (mol/s)	Energy (J)	Tmax (°C)	ΔT (°C)
0.1	1.638e-2	5.607e-3	2.264e-3	3.104e-2	3661.1	802.9	135.3
0.2	1.713e-2	5.858e-3	2.013e-3	3.104e-2	3657.2	803.9	134.9
0.3	1.789e-2	6.110e-3	1.761e-3	3.104e-2	3661.7	805.2	134.6
0.4	1.864e-2	6.361e-3	1.510e-3	3.104e-2	3665.5	806.4	134.4

ACKNOWLEDGEMENT

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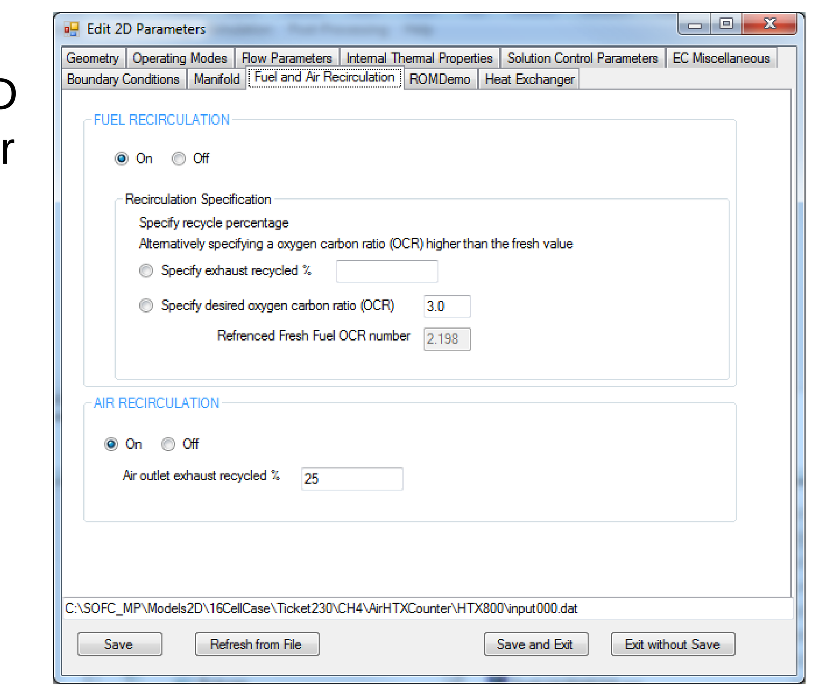
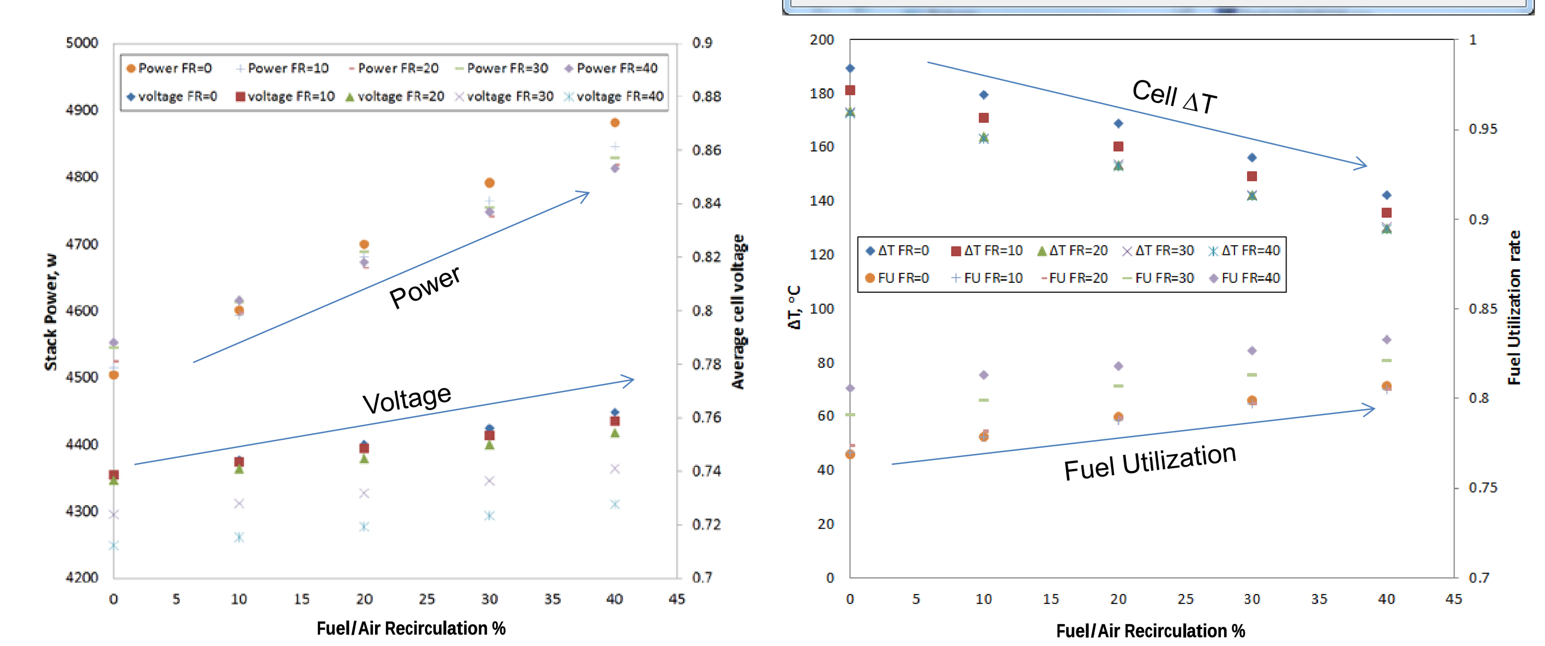
FUEL/OXIDANT RECIRCULATION

Inclusion of the fuel and oxidant recycling loops directly within the ROM was identified as a beneficial enhancement. Recirculation loops consisting of mixing and heat exchanger features were added to SOFC-MP. This was demonstrated to quantitatively analyze stack performance with a 2D model using fixed air heat exchanger effectiveness and constrained to a maximum stack temperature limit.



- 16 cell 25cm x 25cm stack
- Fuel composition: H_2 20%, H_2O 55%, CH_4 20%, CO_2 5% (OCR=2.6)
- Stack temperature < 850°C
- Fuel 0.04112 mol/s
- Oxidant 0.25 mol/s



Benefit of higher fuel/oxidant recirculation under temperature criterion:

- Increases both stack voltage and current resulting in higher power.
- The smoother temperature profile and smaller ΔT is beneficial for stack thermal stresses.

The stack current density distributions below obtained from 3D simulations show that increased recirculation makes the thermal distribution smoother. For fuels with high methane content, higher fuel recirculation showed:

- A higher stack current resulting in a modestly higher power output.
- Slightly smoother stack temperature profile and smaller ΔT.