Reduced Order Model Creation for SOFC Power System Models

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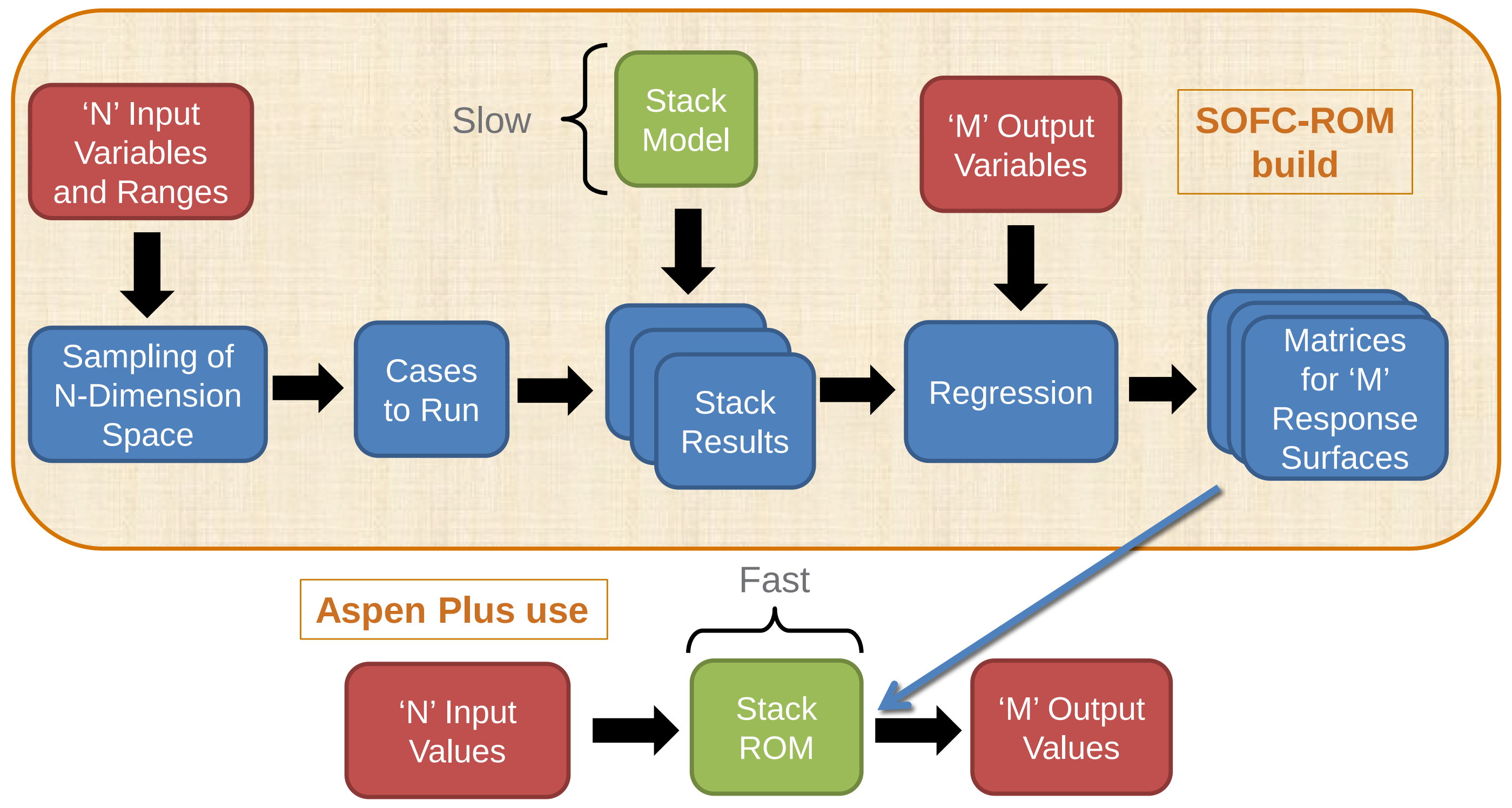
OVERVIEW

This poster presents PNNL's contributions to a collaborative demonstration with NETL for use of a reduced order model (ROM) in SOFC power system analyses, including the technical approach, the ROM generation tool, the SOFC-MP stack model input, the sampled parameter ranges of interest, results, and analysis of the ROM approximation error.

TECHNICAL APPROACH

Numerical models for performance and control studies of SOFC-based power generation systems require an accurate representation of the fuel cell stack. Such high fidelity information about the stack can be obtained from detailed models, but these models are often too computationally expensive to run within the system analysis framework. Response surface analysis techniques were used to generate and demonstrate a ROM for stack performance that retained the important design parameters of interest.



SOFC-ROM build

'N' Input Variables and Ranges

Slow

Stack Model

'M' Output Variables

Sampling of N-Dimension Space

Cases to Run

Stack Results

Regression

Matrices for 'M' Response Surfaces

Aspen Plus use

Fast

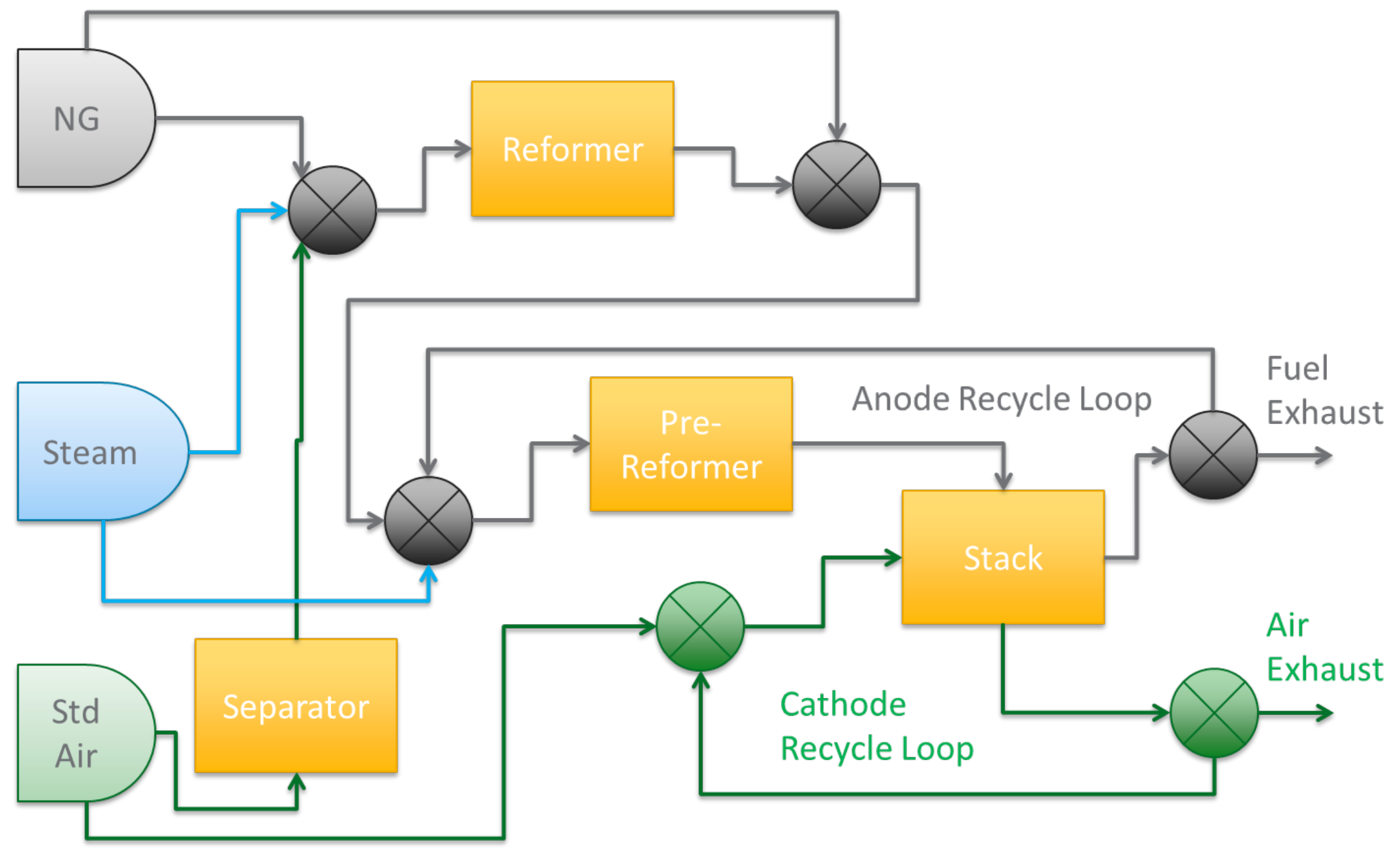
'N' Input Values

Stack ROM

'M' Output Values

SOFC ROM COMPOSITION MODEL

The ROM was generated based on counter-flow stack results from PNNL's 2D SOFC-MP software and implemented/tested in NETL OPPA's NGFC plant model.



A software wrapper calculates species compositions for the stack after pre-reforming to ensure sampling only of viable stack operating states in the design space. This permitted the use of parameters more relevant to the system model perspective (e.g., amount of pre-reforming, recirculation fractions) rather than the original stack model perspective (e.g., inlet species compositions).

ROM DESCRIPTIONS

The ROM was generated based on counter-flow stack results from PNNL's 2D SOFC-MP software for an NGFC system. The ROM was generated from a wide range of input parameters encompassing the expected operating conditions in NETL OPPA's NGFC plant model:

Average Current Density	2000-6000 A/m^2
Internal Reforming	0-100%
Oxidant Recirculation	0-80%
Oxygen-to-Carbon Ratio Target	1.5-3.0
Stack Fuel Utilization	40-95%
Stack Oxidant Utilization	12.5-83.3%
Fuel/Air Inlet Temperature	550-800°C

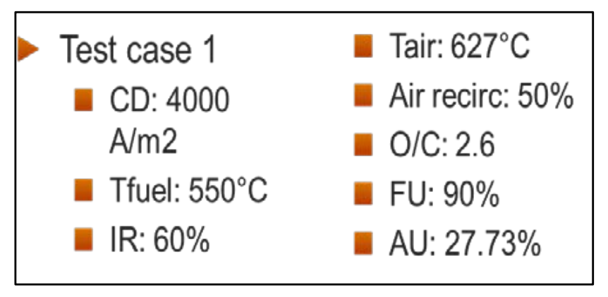
The ROM was built using the Kriging method based on:

- 529 successful cases
- ~200 cases were discarded (out of range temp, non-convergence, etc.)

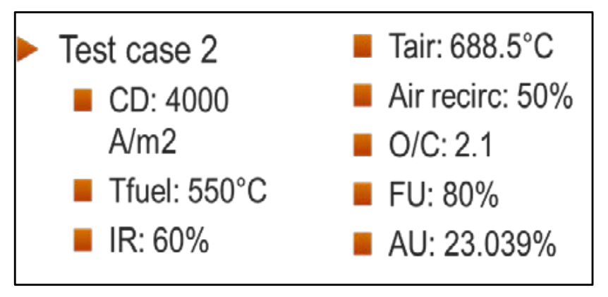
ERROR ANALYSIS AND VERIFICATION

The ROM is an approximation for the detailed stack model, so the error must be quantified to ensure the ROM is sufficiently accurate. ROM predictions were compared to the SOFC-MP case results. Some parameters showed very large errors due to the wide parameter range sampled, but the key metrics were acceptable with only 1-2% error.

#	ROM Output Metric	Mean Error	Std Dev Error	Min Error	Max Error
1	Stack Voltage	1.1%	1.3%	0.01%	13%
2	Stack Current	0.2%	0.1%	0.00%	1%
3	Avg Current Density	0.2%	0.1%	0.00%	1%
4	Max Current Density	12.3%	15.9%	0.03%	222%
5	Min Current Density	16.5%	62.2%	0.01%	1059%
6	Avg Cell Temperature	1.4%	1.5%	0.00%	10%
7	Max Cell Temperature	1.3%	1.4%	0.00%	10%
8	Min Cell Temperature	1.3%	1.4%	0.00%	11%
9	Delta Cell Temperature	13.5%	29.8%	0.00%	400%
10	Outlet Fuel Temperature	1.3%	1.6%	0.00%	12%
11	Delta Fuel Temperature	129.1%	1428.1%	0.01%	31642%
12	Outlet Air Temperature	1.4%	1.6%	0.00%	11%
13	Delta Air Temperature	35.4%	246.1%	0.00%	4022%
14	Fuel Utilization	40.1%	144.0%	0.00%	1264%
15	Air Utilization	3.3%	6.9%	0.00%	64%
16	Outlet Fuel Flowrate	298.9%	336.4%	0.13%	3006%
17	Outlet Fuel H2	2.1%	3.4%	0.01%	39%
18	Outlet Fuel H2O	1.2%	2.0%	0.00%	17%
19	Outlet Fuel CO	3.8%	5.3%	0.00%	51%
20	Outlet Fuel CO2	1.1%	1.6%	0.00%	12%
21	Outlet Fuel CH4	4732.7%	13173.8%	1.12%	102164%
22	Outlet Fuel N2	0.8%	1.2%	0.00%	11%
23	Outlet Air Flowrate	19.1%	32.4%	0.07%	389%
24	Outlet Air O2	0.3%	0.5%	0.00%	5%
25	Outlet Air N2	0.0%	0.0%	0.00%	0%
26	Outlet Air H2O	0.0%	0.0%	0.00%	0%
27	Outlet Air CO2	0.0%	0.0%	0.00%	0%
28	Outlet Air Ar	0.0%	0.0%	0.00%	0%
29	Total Power	1.3%	1.5%	0.00%	14%
30	Air Enthalpy Change	42.7%	150.6%	0.05%	2215%
31	Fuel Enthalpy Change	2.7%	4.4%	0.00%	67%



- Test case 1
  - CD: 4000 A/m2
  - Tfuel: 550°C
  - IR: 60%
  - Tair: 627°C
  - Air recirc: 50%
  - O/C: 2.6
  - FU: 90%
  - AU: 27.73%



- Test case 2
  - CD: 4000 A/m2
  - Tfuel: 550°C
  - IR: 60%
  - Tair: 688.5°C
  - Air recirc: 50%
  - O/C: 2.1
  - FU: 80%
  - AU: 23.039%

For 2 typical NGFC operating states, ROM predictions have small error:

Cell avg T:	0.1% error
Cell min/max T:	0.1-1.2% error
Cell ΔT:	2.2-6.2% error
Tair/Tfuel out:	0.1-0.3% error

CONCLUSIONS AND FUTURE WORK

- The generated ROM is sufficiently accurate for stack electrochemical and thermal performance predictions, and it was successfully implemented and tested in NETL OPPA's NGFC plant model.
- ROM support from SOFC-MP 3D will be added in the future.

ACKNOWLEDGEMENT

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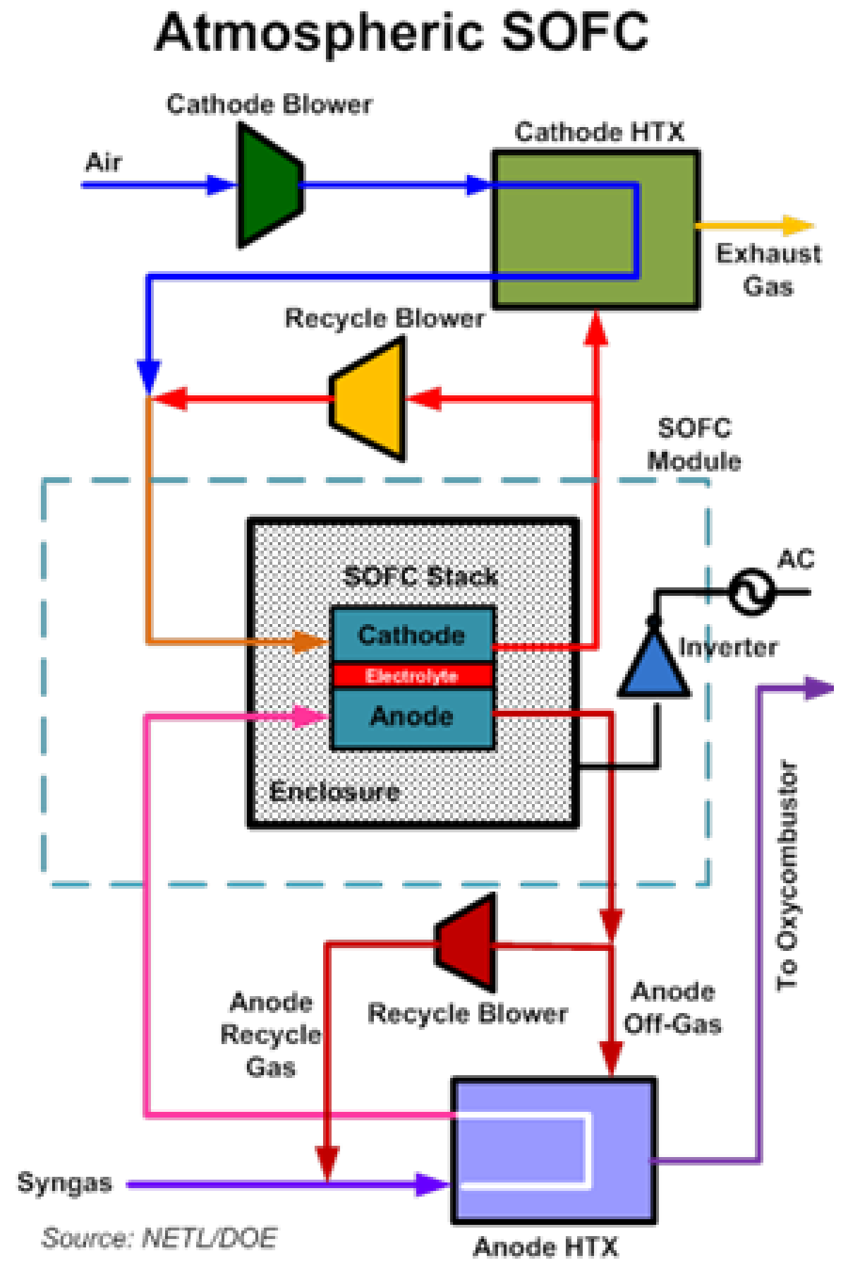
RECENT 2D MODULE ENHANCEMENTS

To improve the ROM accuracy and simplify future integration with Aspen+ system models, the modeling domain of the 2D module was extended to include the mixing and the heat exchangers of the fuel and oxidant recirculation loops. This has enabled faster, more accurate and comprehensive performance evaluations for a given stack geometry and operational constraints.

Limited parametric studies have been performed. For fair comparison, two models are considered comparable if the stacks operate under the same maximum cell temperature constraint (imposed by cell material degradation limitations).



Source: NETL/DOE

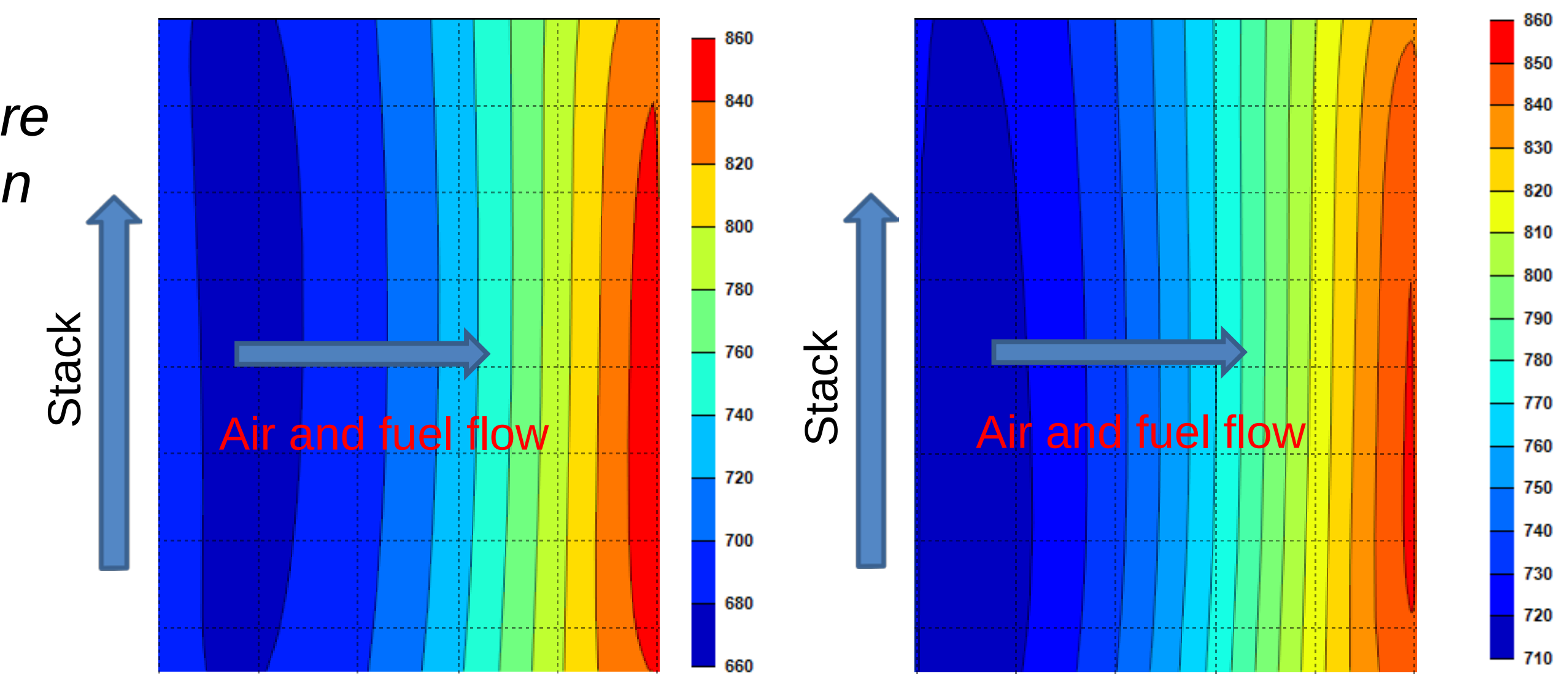
Basic simulation parameters:

- 16 cell 25cm x 25cm stack
- Fuel composition: H_2 20%, H_2O 55%, CH_4 20%, CO_2 5%
- Oxygen/carbon ratio (OCR)
  - OCR=2.6: no fuel recirculation
  - OCR=3: ~11% fuel recirculation
  - OCR=4: ~50% fuel recirculation
- Stack temperature constraint: < 850°C
- Flow rates: fuel 0.04112, air 0.25 (mole/s)

For fuels with high methane content, higher fuel recirculation showed:

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

Stack Temperature Distribution

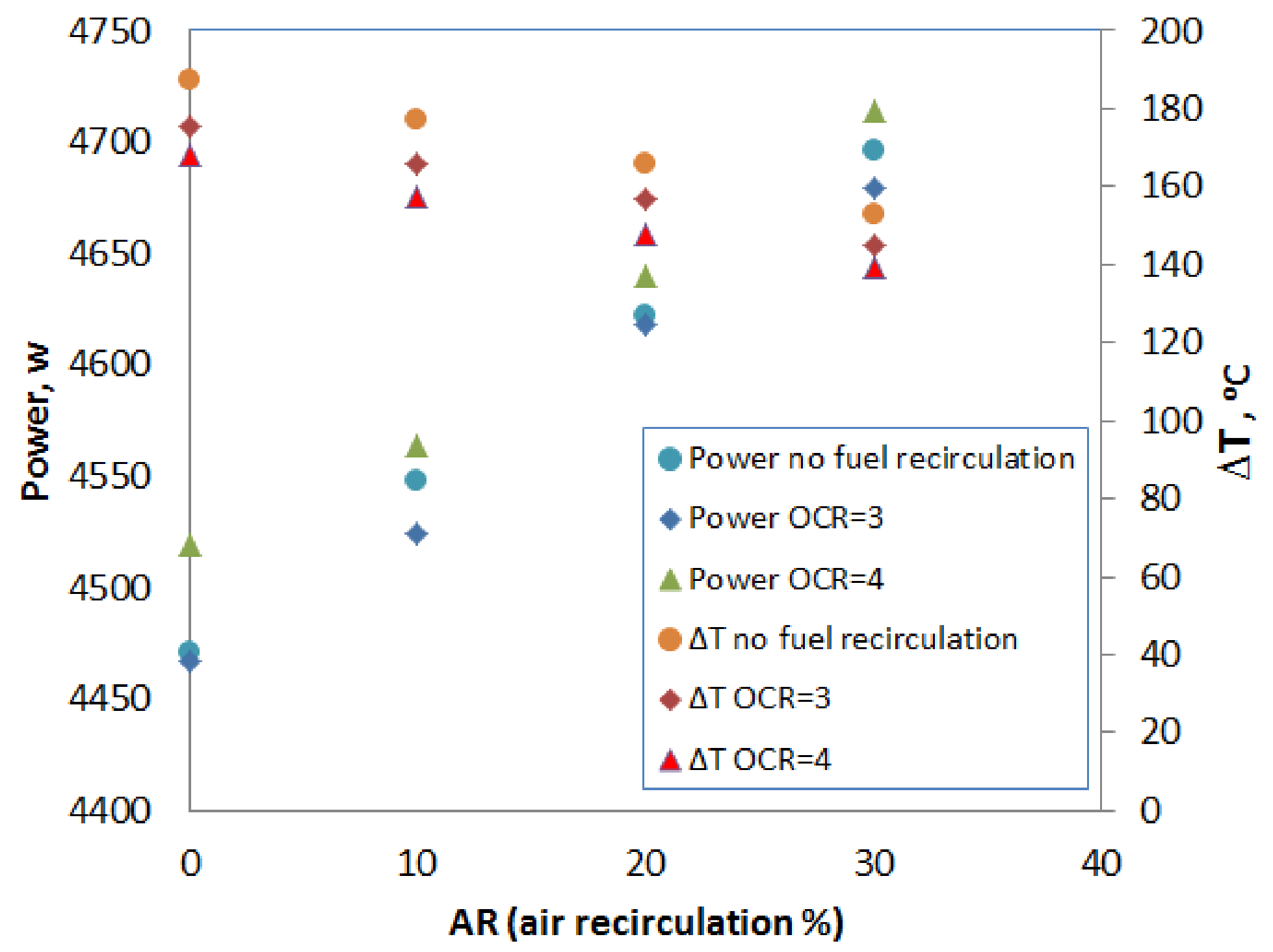


No fuel and air recirculation

Fuel recirculation: 50%
Air recirculation: 30%

The benefit of higher oxidant recirculation is more obvious:

- Increases both stack voltage and current, resulting in a higher power output.
- Smoother cell temperature profile and smaller ΔT beneficial for thermal stresses.



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