Optimal Operating Conditions for Performance and Reliability of Solid Oxide Fuel Cells

Kurtis Recknagle, Naveen Karri, Jie Bao, and Brian Koeppel

Pacific Northwest NATIONAL LABORATORY

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Reliability Overview

Structural reliability of SOFCs define the future prevalence of this technology. Studies at PNNL assessing the structural reliability in conjunction with realistic electrochemistry derived from the in-house SOFC Multiphysics (SOFC-MP) code indicated conflicting requirements for the performance and reliability of SOFCs, thereby necessitating a methodological approach for determining the optimal conditions with minimal tradeoffs. A design-of-experiments (DOE) based response surface methodology (RSM) in conjunction with finite element analysis (FEA) was implemented to arrive at optimal conditions for structural reliability and performance of a generic SOFC design representing present generation planar cells with thin electrodes and interconnects. The influence of flow configuration and fuel composition on the cell thermal gradients and associated reliability for the same target performance was also investigated.

Technical Approach

1. Identify the parameters that influence both performance and structural reliability with screening studies using 2D and/or 3D simulations.
2. Focus on stack performance in a natural gas fuel cell (NGFC) system and abridge NGFC space for 3D reliability simulations using faster 2D models.
3. Within the condensed domain identify the optimal requirements for performance and reliability using DOE based RSM in conjunction with 3D stack FEA simulations.
4. Investigate and determine the preferred flow configuration and fuel compositions for reliability while targeting a specific performance.

Domain for NGFC Systems with 2D Modeling

- The goal of the 2D models is to is to provide an appropriate range of input parameters for the 3-D stack reliability analysis.
- The 2D analysis is centered on operating points from the NGFC pathway evaluations for which the current density is fixed at 400 mA/cm^2 with internal reforming (IR) at 60% (Table 1), which is state-of-the-art, and cases with IR at 100%, representing future operations, with an average stack temperature of 750°C and maximum cell temperature about 800°C.
- The simulation matrix considered three influential parameters along with fuel compositions and flow configurations:
  - Air temperature – T_{air}, Air Utilization – AU, and Fuel Utilization – FU

Table 1. SOFC-MP 2-D Simulations Sample Set #1. Active Area: 400 cm^2, Stack current: 400 mA/cm^2

Set #1: IR 60%, OCR 2.1, FU 84.4%, AU 16.1%, AR 40%, CR 50%.									
Counter-Flow					Co-Flow				
Tair	**Vcell**	**Tmax**	**ΔT**	**Tavg**	**Tair**	**Vcell**	**Tmax**	**ΔT**	**Tavg**
700	0.825	826	98.2	788.3	**700**	0.8066	798.7	105.2	756.9
675	0.8225	802.6	98.7	765.8	**675**	0.8	779.2	106.8	733.6
650	0.8166	779.9	99.9	743.4	**650**	0.7893	760.9	108.9	711.8
625	0.8063	758.7	102.7	721.6	**625**	0.7746	743.6	111.7	691.4
600	0.7916	738.8	107.1	700.3	**600**	0.7554	728.6	116.3	672.9

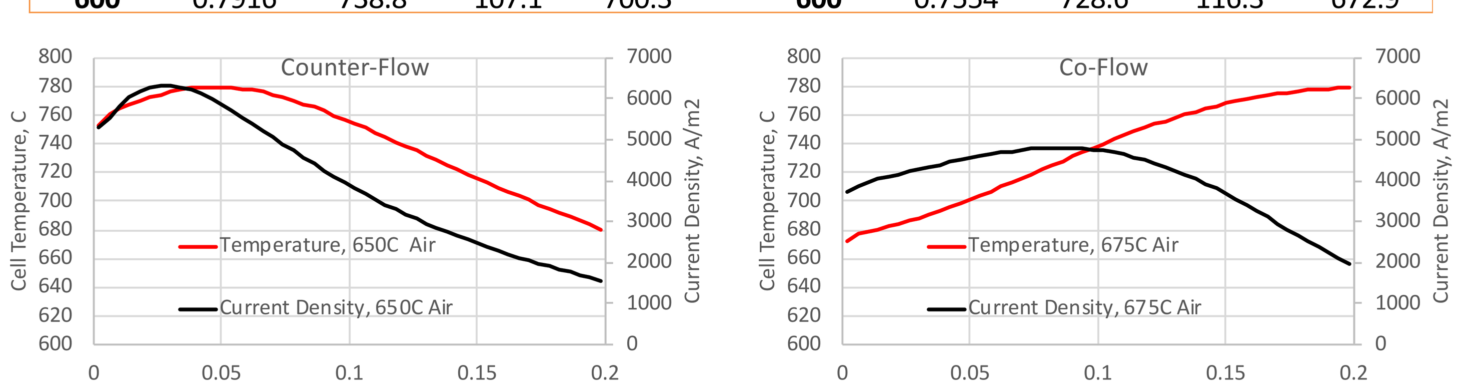

Figure 1: Temperature and current density distributions from: (a) 650°C inflow air temperature for counter-flow configuration, and (b) 675°C inflow air temperature for co-flow configuration, both from simulation set #1.

Table 2. Input Parameter Ranges (Domain) for Use in the Reliability Analyses

	Counter-flow		Co-flow	
	Minimum	Maximum	Minimum	Maximum
Tair, °C	650	700	675	725
UA(stack), %	13.0	16.1	13.0	16.1
UF(stack), %	68.8	84.4	68.8	84.4
Fuel Composition	All 3*	All 3*	All 3*	All 3*

* Compositions Based on IR and Recycling (1): 60% IR, 2.1 OCR (2): 60% IR, 2.6 OCR (3): 100% IR, 2.1 OCR

Results (Table 2) from the 2-D simulation sets showed T_{air} ranges can be focused down to a 50°C range for both flow configurations with stack AU ranging from 13.0% to 16.1% and FU ranging from 68.8% to 84.4% while composition varies based on oxygen to carbon ratio (OCR) ranging from 2.1 to 2.6, and internal reformation (IR) of 60% and 100%.

Stack Reliability, R = 1-Failure Probability (P_f)

Once the domain for 3D simulations is determined, the stack modeling tool SOFC-MP-3D was used to simulate the electrochemistry (performance) and temperature distributions in planar 20 cm x 20 cm single-cell stacks in co-flow and counter-flow configurations. The structural (thermomechanical) analyses was carried out with the commercial FEA software ANSYS® and the P_f of the stack was estimated based on the statistical ceramic reliability theory (Weibull analysis) implemented as a post-processing macro. The stack P_f is based on the individual P_f of all the brittle components: anode, cathode, electrolyte, air seal, fuel seal, PEN seal. The fracture test data for these materials is obtained from literature and past testing at PNNL and ORNL under the SECA program.

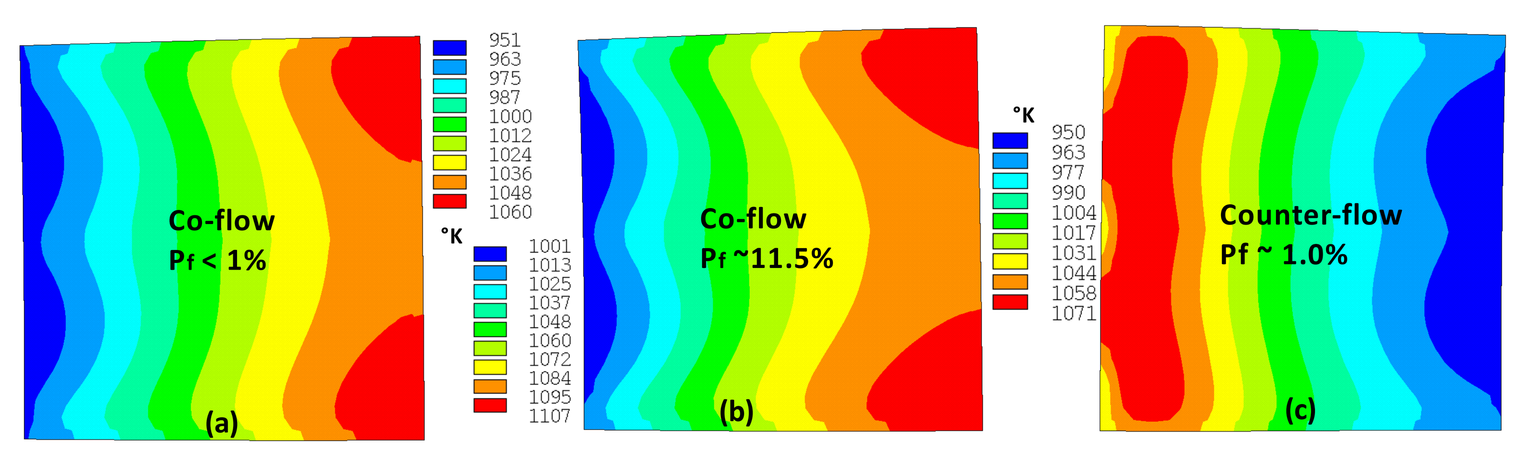

Figure 2: Temperatures and cell P_f in co-flow (a, b) & counter flow (c) configurations for similar power output.

The results from the reliability analysis indicated significant variation in overall stack failure probabilities within the NGFC design space for similar power output. Figures 2(a) and 2(b) show the temperature distribution in a co-flow cell with an average cell temperature of 737°C (ΔT=111°C) and 781°C (ΔT=106°C) resulting in failure probabilities of <1% and 11.5% respectively. The same cell when operated in counter-flow with conditions same as (a) produced an average cell temperature about 732°C (ΔT=121°C) and slightly higher P_f of 1%. All three cases generated ~133W power output. Fuel compositions of higher OCR (2.6) with modified fuel flow rates for similar power reduced the P_f.

Optimal Conditions for Reliability

For DOE based RSM, 2[nd] order quadratic expressions were fit for the desired responses based on the results from methodologically designed experiments. Since our responses are obtained from simulations (not experiments where results may vary with repetition), a central composite design (CCD) with face-centered axial (star) points and no repetitions was used to fit the surfaces for the desired responses: the power output (P), failure probability (P_f), and T_{avg}.

$$P = -201.7 + 0.972T_{air} - 4.21m_{air} + 17.5m_{fuel} - 0.000889T_{air}^2 - 0.0151m_{air}^2 - 13.22m_{fuel}^2 + 0.00781T_{air}\times m_{air} + 0.0732T_{air}\times m_{fuel} - 0.318m_{air}\times m_{fuel}$$

$$\%P_f = 22.6 - 0.098T_{air} + 0.353m_{air} + 7.68m_{fuel} + 0.000119T_{air}^2 + 0.0074m_{air}^2 + 0.97m_{fuel}^2 - 0.001298T_{air}\times m_{air} - 0.02035T_{air}\times m_{fuel} + 0.1223m_{air}\times m_{fuel}$$

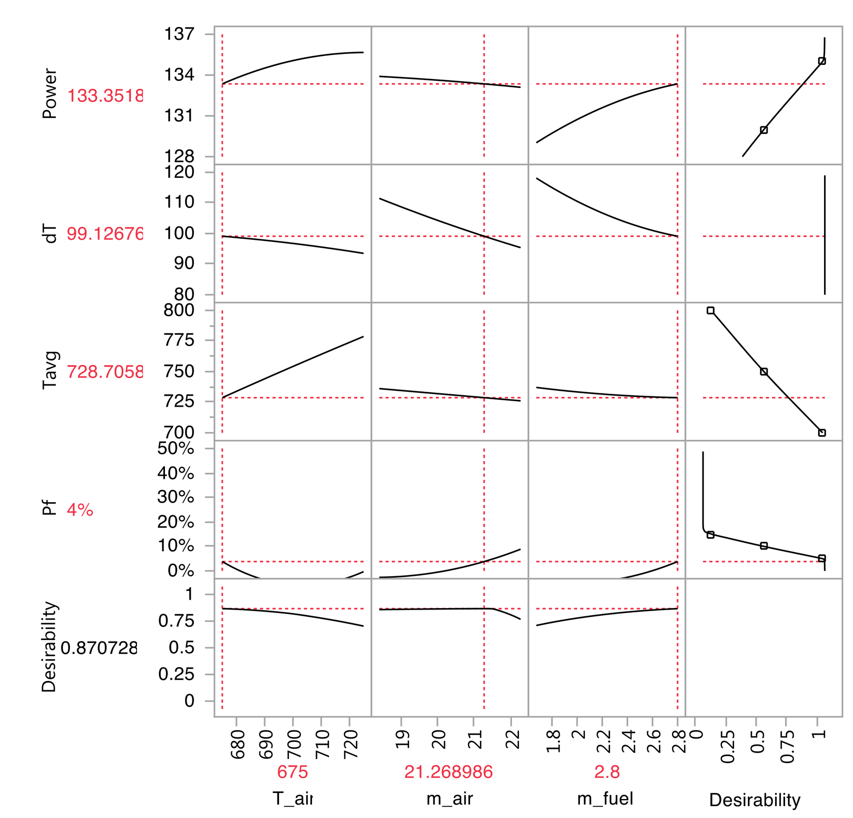

Figure 3: Maximized D=87% for P_f ≤5%, P ≥ 130 W and T_{avg} < 750°C.

For multivariate optimization, the desirability functions approach was used to simultaneously optimize the power output, reliability and T_{avg} with specific constraints. The objective of the desirability function approach is to maximize the overall desirability (D) which is the geometric mean of individual desirabilities (d_i) of all the responses considered.

$$D = (d_1 \times d_2 \times .... \times d_m)^{\frac{1}{m}}$$

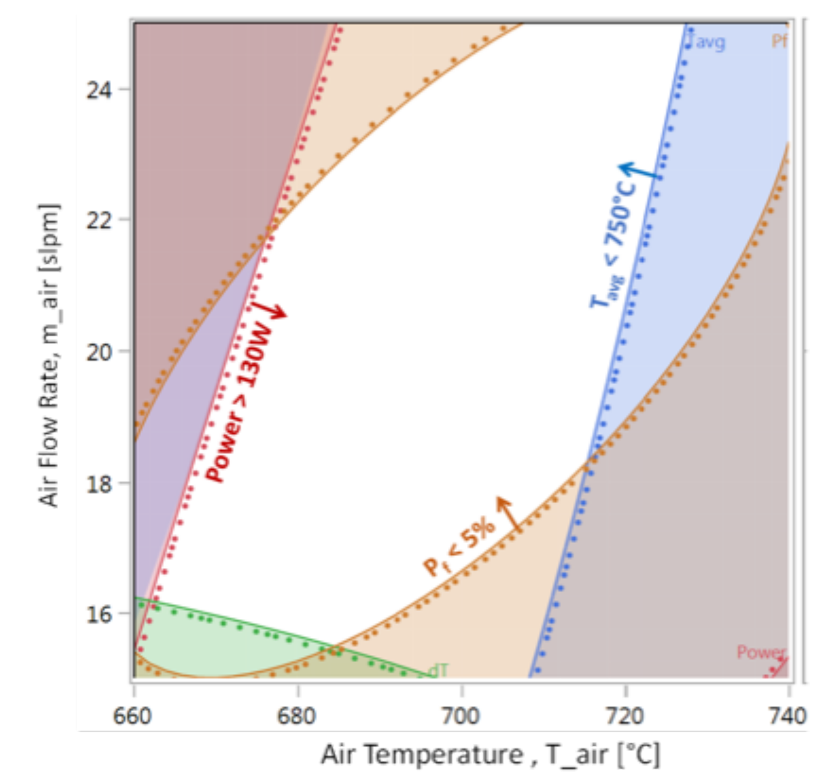

Figure 4: Domain for other solutions with m_fuel =2.8 slpm.

Figure 3 demonstrates a solution (obtained using JMP® software) that maximizes the desirability under the constrains specified for optimal requirements for a co-flow design (D=87%).

Figure 4 illustrates the design space for other solutions which also satisfy the constraints (Power>130W, P_f<5%, T_{avg}<750°C) specified for the optimal operating conditions. The D in these cases will be <87%.

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For additional information, please contact:
Brian J Koeppel
Pacific Northwest National Laboratory
P.O. Box 999, MSIN: K9-89
Richland, WA 99352
brian.koeppel@pnnl.gov

Conclusions and Future Work

- The requirements for SOFC performance and reliability were found to be in conflict.
- SOFC-MP 2D simulations were used to condense the design space for optimization.
- Significant variation in cell reliability was observed within the NGFC design space for similar power output. Higher cell average temperatures and ΔT reduced reliability.
- DOE based RSM techniques with FEA were used to determine optimal requirements.
- Future work will investigate multi-cell stack reliability, including the effect of performance degradation, and integration of predicted responses for reliability into the reduced order model (ROM) for power system evaluations.

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