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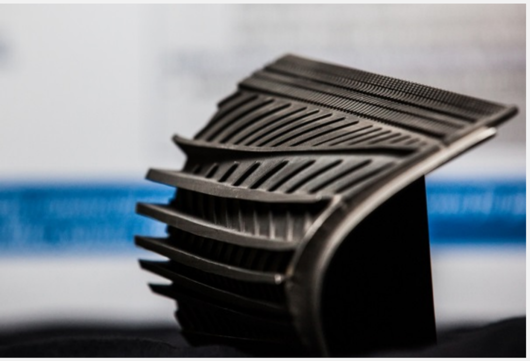
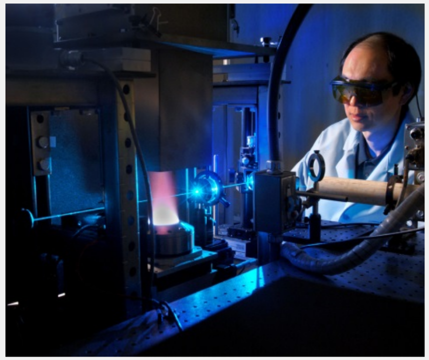
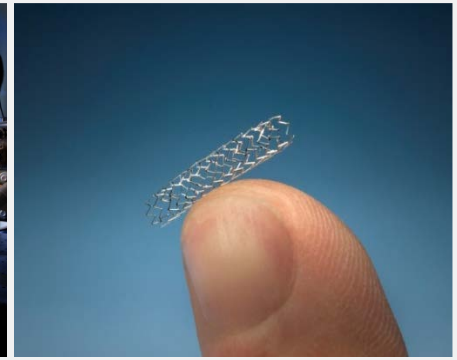
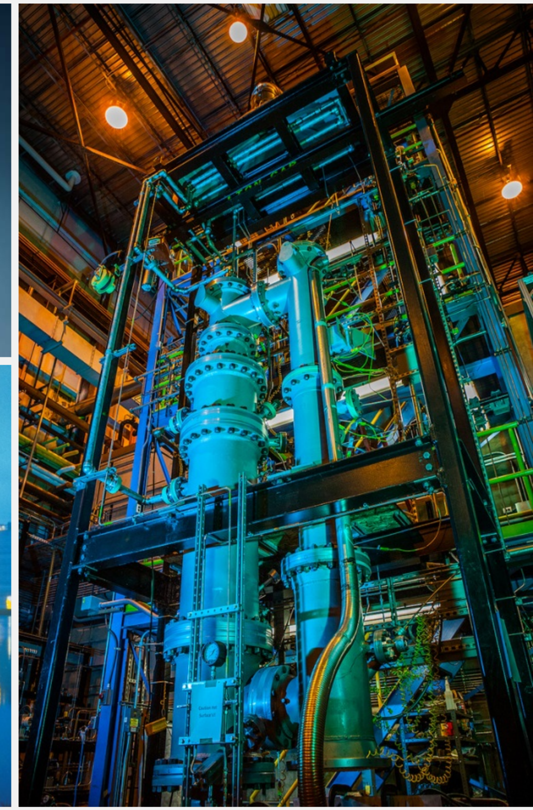

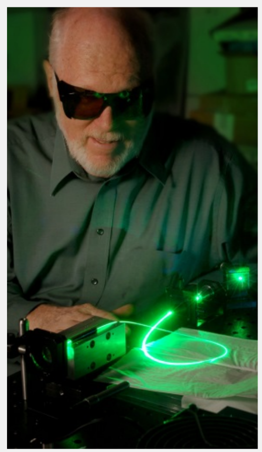


Integrating the PNNL SOFC Multi-Physics Model into the NETL Aspen System Model as a Reduced Order Model

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July 17, 2015

U.S. DEPARTMENT OF ENERGY | National Energy Technology Laboratory

Outline

- **Motivation**
  - Problem Statement
  - Objective
  - Potential Solution
- **Background**
  - PNNL SOFC-MP 2D Model
- **Current Status Overview**
  - ROM Generation
  - ROM Integration
- **Conclusions**
- **Next Steps**

Motivation

PROBLEM STATEMENT: NETL analysis of SOFC systems is limited to what can be described as a "black box" SOFC module within the current Aspen system model

- Consists of two reactors w/ heat and oxygen transfer
- Limited input/output
- Specific overpotential estimates
- Limited optimization from a system perspective

OBJECTIVE: To improve the accuracy and capability of NETL's Aspen-based SOFC system analyses

- Produce a variety of optimization and what-if studies to guide the SOFC program

Motivation

SOLUTION: Integrate the PNNL SOFC-MP model into NETL's system model as a reduced-order model (ROM) to replace the current "black box" approach to:

- Increase the accuracy of SOA SOFC analysis
- Reduce computational time and complexity versus full model
- Allow for additional optimization studies (COE, etc.)
- Allow for the ease of incorporation of other models
  - Such as degradation models, etc.
- Facilitate development of a high fidelity SOFC tool for system analysis
  - An NETL/DOE/PNNL vision
  - SOFC industry team use

Background
PNNL SOFC-MP 2D Model

- **SOFC-MP 2D is a numerical model for the efficient computation of parameters in planar SOFC stacks**
  - Current density
  - Species concentration
  - Temperature distributions
- **Capabilities**
  - Co- or counter-flow geometry
  - Mixed fuel compositions (H_2, H_2O, CO, CO_2, CH_4, N_2)
  - User-defined electrochemistry and CH_4 reforming models
  - Analysis of large area cells, multi-cell stacks
  - Calibrated with state-of-the-art SOFC performance data from industry

SOFC ROM Generation

Current Status Overview
SOFC ROM Generation

- **Initial SOFC ROM generation was completed by PNNL**
  – ROM generation had to be constrained to cover only limited SOFC scenarios with a small range of validity to get viable data points
    - Fixed inlet gas composition (natural gas)
    - Fixed fraction of pre-reforming
    - Counter-flow SOFC configuration w/ no heat loss
    - Single cell at atmospheric conditions
  – ROM validated against full model to be consistent with SOA SOFC technology
  – The accuracy of the ROM was verified by extensive error analysis by PNNL, with key metrics having error of < 3%

Current Status Overview

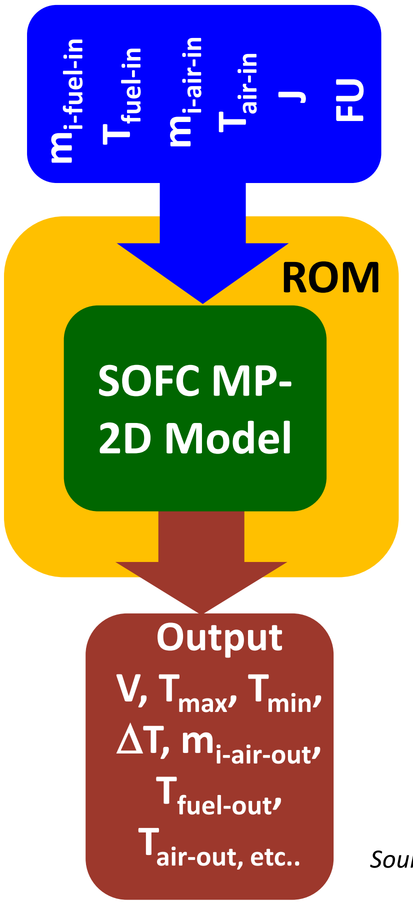
SOFC ROM Generation

- **Methodology used for ROM generation**
  - A spreadsheet material flow model developed for an NGFC system was integrated into the ROM generation process
  - The spreadsheet model ensured that the inputs to the SOFC MP-2D model were physically consistent resulting in an efficient ROM

ROM Input Parameters	Salient ROM Output Parameters
Average current density (J)	Cell voltage (V)
Fuel utilization (FU)	Cell temperature profile (T_{max}, T_{min}, and ΔT)
Inlet NG composition (FIXED)	Stack air outlet conditions
Inlet air composition	Air outlet temperature ($T_{air-out}$)
Fuel inlet temperature ($T_{fuel-in}$)	Species (N_2, O_2, Ar, CO_2, H_2O) mole flows ($m_{i\text{-}air\text{-}out}$)
Air inlet temperature (T_{air-in})	Stack fuel outlet conditions
Anode inlet gas oxygen to carbon ratio (OTC)	Fuel outlet temperature ($T_{fuel-out}$)
Cathode gas recirculation fraction (RF_{cath})	Species (CH_4, H_2, CO, H_2O, CO_2, N_2) mole flows ($m_{i\text{-}fuel\text{-}out}$)
Internal reformation fraction ($X_{int-ref}$)	Current density profile (J_{max}, J_{min}, J_{avg})
Air utilization (AU)	

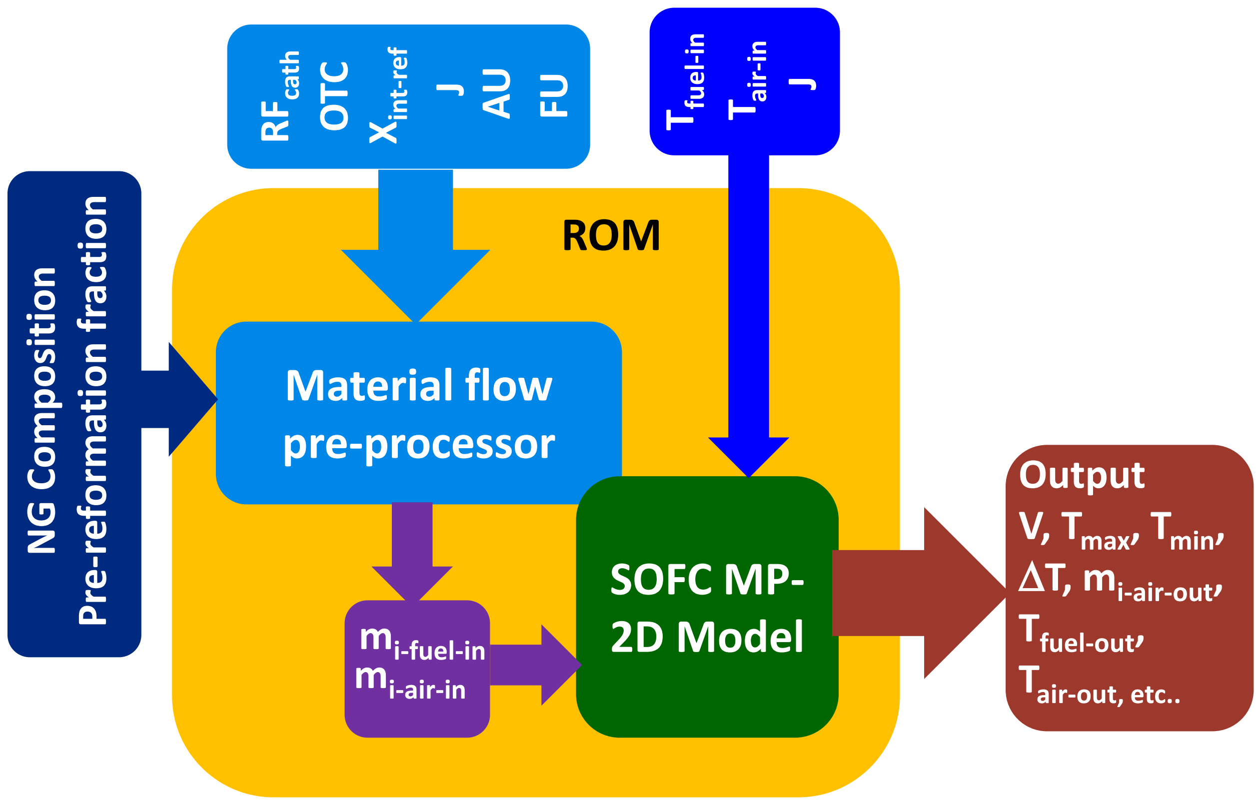
Current Status Overview

SOFC ROM Generation



Source: NETL

Previous ROM generation methodology



Source: NETL

Revised ROM Generation methodology

Current Status Overview
SOFC ROM Generation

- **PNNL generated ROM based on the revised methodology**
  - Supplied ranges for the new input parameters identified
  - SOFC electrochemical model calibrated to SOA SOFC technology was used
  - NG composition is the same as used in the Bituminous Baseline NGCC cases [1]
  - The methane pre-reformation fraction was set to 20 percent (to completely reform higher hydrocarbons, a typical value)

ROM Input Parameters	Ranges
Average current density (J)	2000 – 6000 A/m^2
Fuel utilization (FU)	0.4 – 0.95
Inlet NG composition	Fixed (as in Bituminous Baseline NGCC Cases)
Inlet air composition	Fixed: Standard air (Midwest ISO)
Fuel inlet temperature ($T_{fuel\text{-}in}$)	550 – 800 °C
Air inlet temperature ($T_{air\text{-}in}$)	550 – 800 °C
Anode inlet gas oxygen to carbon ratio (OTC)	1.5 – 3.0
Cathode gas recirculation fraction (RF_{cath})	0.0 – 0.8
Air utilization (AU)	0.125 – 0.833
Internal reformation fraction ($X_{int\text{-}ref}$)	0.0 – 1.0

1. *NETL - National Energy Technology Laboratory. " Cost and Performance Baseline for Fossil Energy Plants Volume 1: Bituminous Coal and Natural Gas to Electricity ," Revision 2a, DOE/NETL -2010/1397, September 2013.*

Integration of SOFC ROM into Aspen System Model

Current Status Overview

SOFC ROM Integration

- **Integration of ROM into system model:**
  - The outputs of the ROM integrated into Aspen were checked against ROM output values generated independently (non-Aspen) using the same input parameter values
    - The airflow, air inlet temperature, fuel outlet temperature, and cell voltage resulting from the routine were specified in the Aspen model
    - The air outlet temperature calculated by the Aspen model was checked against the value of air outlet temperature calculated using the ROM to confirm consistency of energy flows between the models
  - Aspen and ROM species mole flows were confirmed and checked for consistency

Current Status Overview

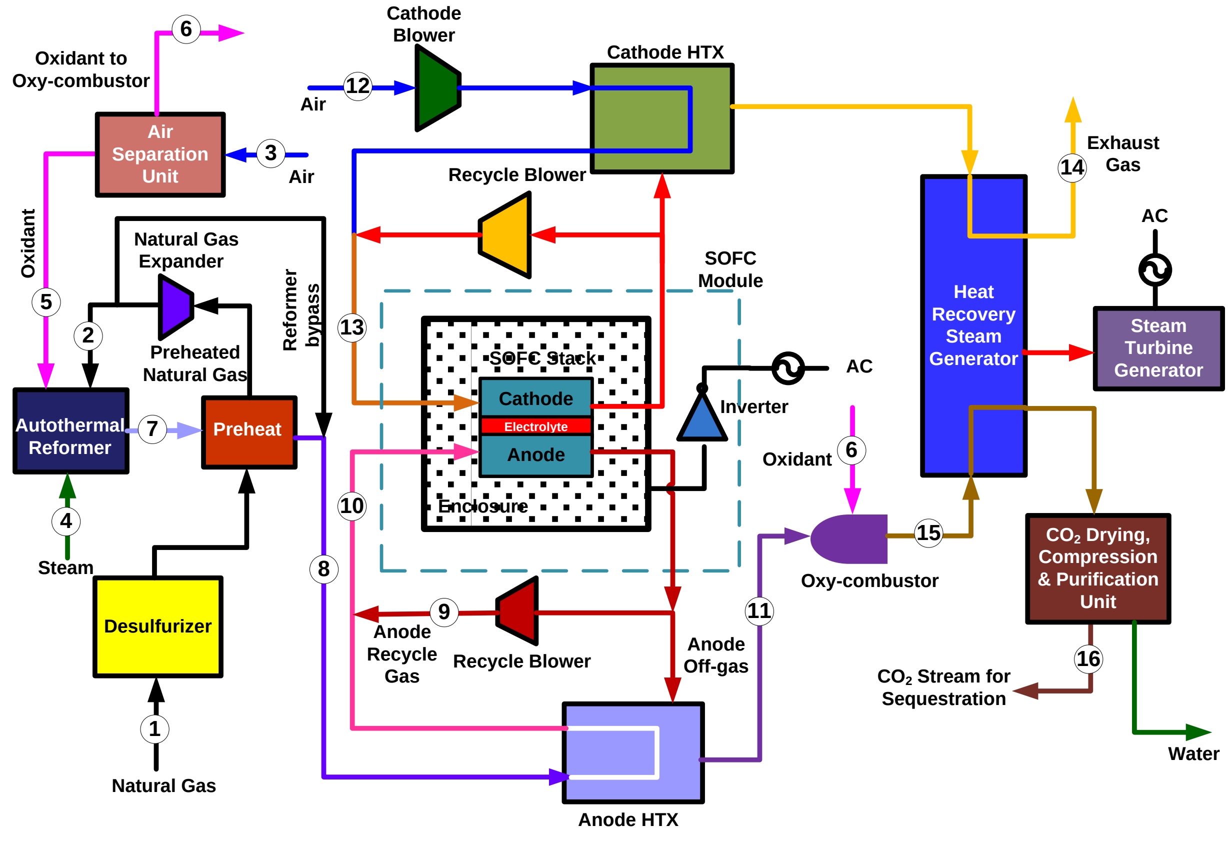
SOFC ROM Integration

- **PNNL generated ROM was integrated into the Aspen model of an NGFC utility-scale system**
  - ROM translation FORTRAN routine is hardwired as a calculation block in the Aspen model
    - PNNL supplied ROM translation routine was modified to seek minimum air flow rate and air inlet temperature combination for a specified cell T_{MAX} and cell ΔT
    - Export/import links to key parameters in the Aspen file established
  - Needs external FORTRAN compiler configured to run with Aspen

Current Status Overview

SOFC ROM Integration

- **NGFC System with CCS**
  - 550 MWe
  - Atmospheric SOFC
  - Auto-thermal O_2 blown reformer
  - Steam bottoming cycle
  - Oxy-combustor
  - Cryogenic ASU provides O_2
  - CO_2 purification unit with auto-refrigeration



Source: NETL

Current Status Overview

SOFC ROM Integration

- **Two sample NGFC cases considered to demonstrate ROM Integration**
  - ROM Case 1 conditions were based on NGFC Case 1-2 [1], which represents SOA technology operating under high fuel utilization conditions
  - ROM Case 2 conditions were chosen to be generally reflective of typical operating conditions for SOA technology

Parameters	Measurement	Case 1-2 NGFC Study (not ROM based)	ROM Based Case 1	ROM Based SOA Case 2
Average current density	mA/cm^2	400		
Fuel utilization		0.9		0.8
Cell maximum temperature	°C	750	750	775
Cell ΔT		100	100	75
Fuel inlet temperature		650	627	688.5
Air inlet temperature		650	550	550
Oxygen to carbon ratio		2.6		2.1
Cathode gas recirculation fraction		0.5		
Air stoichs (Air utilization)		2.9 (0.345)	3.61 (0.277)	4.34 (0.230)
Internal reformation fraction		0.6		

1. NETL - National Energy Technology Laboratory. " Cost and Performance Baseline for Fossil Energy Plants Volume 1: Bituminous Coal and Natural Gas to Electricity ,"Revision 2a, DOE/NETL -2010/1397, September 2013.

Current Status Overview

SOFC ROM Integration

- **The outputs of the ROM runs within Aspen were confirmed to be identical to stand-alone ROM runs with the same input parameters**
- **The air outlet temperature was calculated using Aspen and was found to be nearly the same value as that predicted by the ROM**
  - Confirms consistency of energy flows and heat balance between the ROM and Aspen model

Parameters	Unit	ROM Based Case 1		ROM Based SOA Case 2	
		Aspen	External	Aspen	External
Cell voltage	V	0.788	0.788	0.844	0.844
Cell average temperature	°C	729.0	729.0	700.0	700.0
Cell max temperature	°C	750.0	750.0	775.4	775.4
Cell min temperature	°C	649.5	649.5	700.0	700.0
Cell ΔT	°C	100.5	100.5	75.4	75.4
Fuel outlet temperature	°C	687.0	687.0	727.5	727.5
Air outlet temperature	°C	739.4	739.6	757.3	757.5
Max current density	mA/cm^2	568.8	568.8	499.1	499.1
Min current density	mA/cm^2	205.5	205.5	218.9	218.9

Current Status Overview

SOFC ROM Integration

- **The stack fuel and air inlet flows in the Aspen model were compared to the corresponding flows used in the SOFC-MP model for the same ROM input parameters**
  - The flows were found to be the same within practical limits
  - Serves a check of the consistency of flows between the material flow pre-processor of the ROM and the Aspen model

Parameters	ROM Based Case 1		ROM Based SOA Case 2	
	Aspen	SOFC-MP	Aspen	SOFC-MP
Air inlet species mole-fractions				
O_2	0.1842	0.1842	0.1883	0.1883
N_2	0.7950	0.7951	0.7911	0.7911
Ar	0.0096	0.0097	0.0096	0.0096
Fuel inlet species mole-fractions				
H_2	0.2384	0.2409	0.3263	0.3297
CO	0.0856	0.0831	0.1170	0.1140
CH4	0.0639	0.0639	0.0827	0.0828
H_2O	0.4169	0.4145	0.3175	0.314
CO_2	0.1896	0.1922	0.1508	0.1542

Current Status Overview
SOFC ROM Integration

Parameters	Measurement	Case 1-2 NGFC Study (not ROM based)	ROM Based Case 1	ROM Based SOA Case 2
Internal Reformation Fraction	**%**	**60**		
Average Current Density	**mA/cm^2**	**400**		
Fuel Utilization		**90**		**80**
Cell Maximum Temperature	**°C**	**750**	**750**	**775**
Cell DT		**100**	**100**	**75**
Oxygen to Carbon Ratio		**2.6**		**2.1**
Air Stoichs		**2.9**	**3.61**	**4.34**
Cell Voltage	V	**0.791**	**0.788**	**0.844**
Inlet Nernst Voltage		0.941	0.958	0.966
In Stack Fuel Utilization	%	80	80	69
Plant Output				
SOFC Power	kWe	525,700	516,708	515,495
Natural Gas Expander Power		18,400	18,200	19,000
Steam Turbine Power		79,000	78,300	89,000
Total Gross Power		**623,100**	**613,208**	**623,495**
Auxiliary Load				
ASU Auxiliaries	kWe	321	318	464
ASU Main Air Compressor		15,090	14,680	21,460
CO_2 Compressor		18,570	22,451	23,535
CO_2 Refrigeration		14,499	0	0
Boiler Feedwater Pumps		1,371	1,359	1,545
Condensate Pump		102	101	115
Circulating Water Pump		2,090	2,180	2,400
Cooling Tower Fans		1,080	1,120	1,240
Steam Turbine Auxiliaries		33	33	37
Cathode Air Blower		7,610	8,222	9,224
Cathode Recycle Blower		7,690	8,273	9,541
Anode Recycle Blower		2,110	1,955	1,368
Miscellaneous Balance of Plant		398	394	413
Transformer Losses		2,070	2,011	2,072
Total Auxiliary Load		**73,035**	**63,097**	**73,414**
Net Plant Power		**550,065**	**550,111**	**550,081**
Net Plant Efficiency (HHV)	%	**55.9***	**56.5**	**53.9**
Net Plant Heat Rate (HHV)	**kJ/kWhr (Btu/kWhr)**	**6,441 (6,105)**	**6,372 (6,039)**	**6,681 (6,332)**
Condenser Duty	**GJ/hr (MMBtu/hr)**	**464 (440)**	**454 (430)**	**517 (490)**
Natural Gas Feed Flowrate	kg/hr (lb/hr)	67,551 (148,925)	66,828 (147,330)	70,069 (154,475)
Thermal Input	kWth	984,164	973,623	1,020,841
Raw Water Consumption	m^3/min (gpm)	4.1 (1,071)	4.29 (1,132.4)	4.84 (1,278.1)

** The NGFC case 1-2 uses externally refrigerated CPU unlike the ROM based cases, which use autorefrigerated CPU; the HHV efficiency of the case 1-2 can be projected to be ~57.4% (1.5 percentage points higher than listed) if an autorefrigerated CPU was employed.*

Conclusions

Conclusions
ROM Generation

- **Developed a methodology for ROM generation**
  - Results in an efficient ROM generation process
  - The resultant ROM input parameters closely mimic the design and operational parameters of a typical SOFC system
  - Enables the ultimate vision of the development of a tool that is useful for SOFC system calculations since the methodology can be extended to ROM representation of high fidelity SOFC-MP 3D models
- **Successfully generated a ROM based on the revised methodology**
  - Utilized the SOFC electrochemical model that was calibrated to be consistent with SOA SOFC technology
  - Range of input parameters covered the gamut of values encountered in a typical NGFC system
  - The accuracy of the ROM was verified by extensive error analysis and was found to be acceptable (<3%) for the key parameters

Conclusions
ROM Integration

- **The ROM was successfully into the Aspen model of NGFC system**
  - The outputs of the ROM integrated into Aspen were checked against ROM outputs values generated independently (external to Aspen) using the same input parameter values
  - A routine that iterated the ROM calculations to find the lowest air flow and the corresponding air inlet temperature for specified values of cell maximum temperature and cell ΔT was developed
  - Aspen and ROM species mole flows were confirmed and checked for consistency
  - Two sample NGFC cases were analyzed using the ROM based and compared to a previous NGFC case

Conclusions

Next Steps – ROM Development

- **The next phase of the ROM development will focus on:**
  - Modifications to the SOFC-MP 2D model to include:
    - Cathode and anode recirculation
    - Cathode and anode heat exchangers representations
    - Pre-reformer routine
    - Pressure drop calculations
  - Extension to other fuel compositions
    - Other natural gas compositions
    - Syngas compositions (for IGFC system analyses)
  - Extension to pressurized SOFC operation
  - Inclusion of cross-flow SOFC configuration

Conclusions

Next Steps - ROM Integration

- **The next step of ROM integration into the Aspen system model is to develop a custom user SOFC model based on the ROM that can be easily called within the Aspen model**
  - Enables ROM customization without affecting the Aspen model
  - Enables user-friendliness and portability of the ROM model
- **Application of the ROM integrated Aspen model to different systems-level optimization**
  - COE, based on voltage/current operating point
  - Re-visitation of SOFC pathway based on new capability and accurate SOA analysis
  - Guide SOFC program with meaningful and achievable goals, such as a reduction in ASR rather than overpotential

Acknowledgments

- Arun Iyengar, Booz Allen Hamilton
- Brian Koeppel and Kevin Lai, PNNL
- Dale Keairns, BAH
- Briggs White, NETL
- Travis Shultz, NETL
- Heather Quedenfeld, NETL
- Shailesh Vora, NETL

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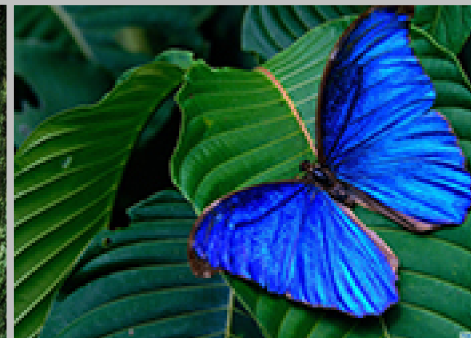
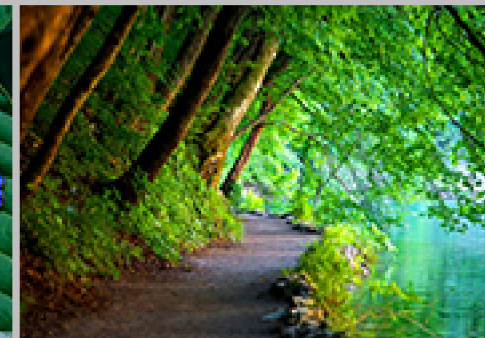

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