SOFC Modeling for IGFC System Analysis

10th Annual SECA Workshop

Pittsburgh, PA

July 16, 2009

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Coal-Based Power Systems

US DOE Targets

- 250-500 MW net power output
- HHV efficiency: 45-50% (2010), 60% (2015)
- 90+% carbon capture, ready for sequestration
- 99% SO_2 removal, 90% Hg removal
- NOx emissions < 0.01 lb/MMBtu
- COE increase <10% w/sequestration
- Reduced water requirement desired

Coal Industry Concerns

- Capital cost, reliability
- Efficiency traditionally less important – low fuel cost
- Cost of Electricity (¢/kWh)

Toward a Competitive Coal Power System

Key approaches for 60% HHV efficiency, competitive COE:

- High-efficiency gasifier, methane-containing syngas
- SOFC-based power block
- Large air temperature rise across SOFC subsystem

SOFC requirements and trends:

- Increasing operating voltage
- Increasing power density
- Increasing internal reforming
- Increasing ΔT (air and cell)

SOFC Cooling

Air blower/compressor major equipment parasite in IGFC power block

- Air flow is primary source of cooling for SOFC
- Reducing air enables more SOFCs to be driven for the same compressor power

Increasing air temperature rise reduces air flow requirements

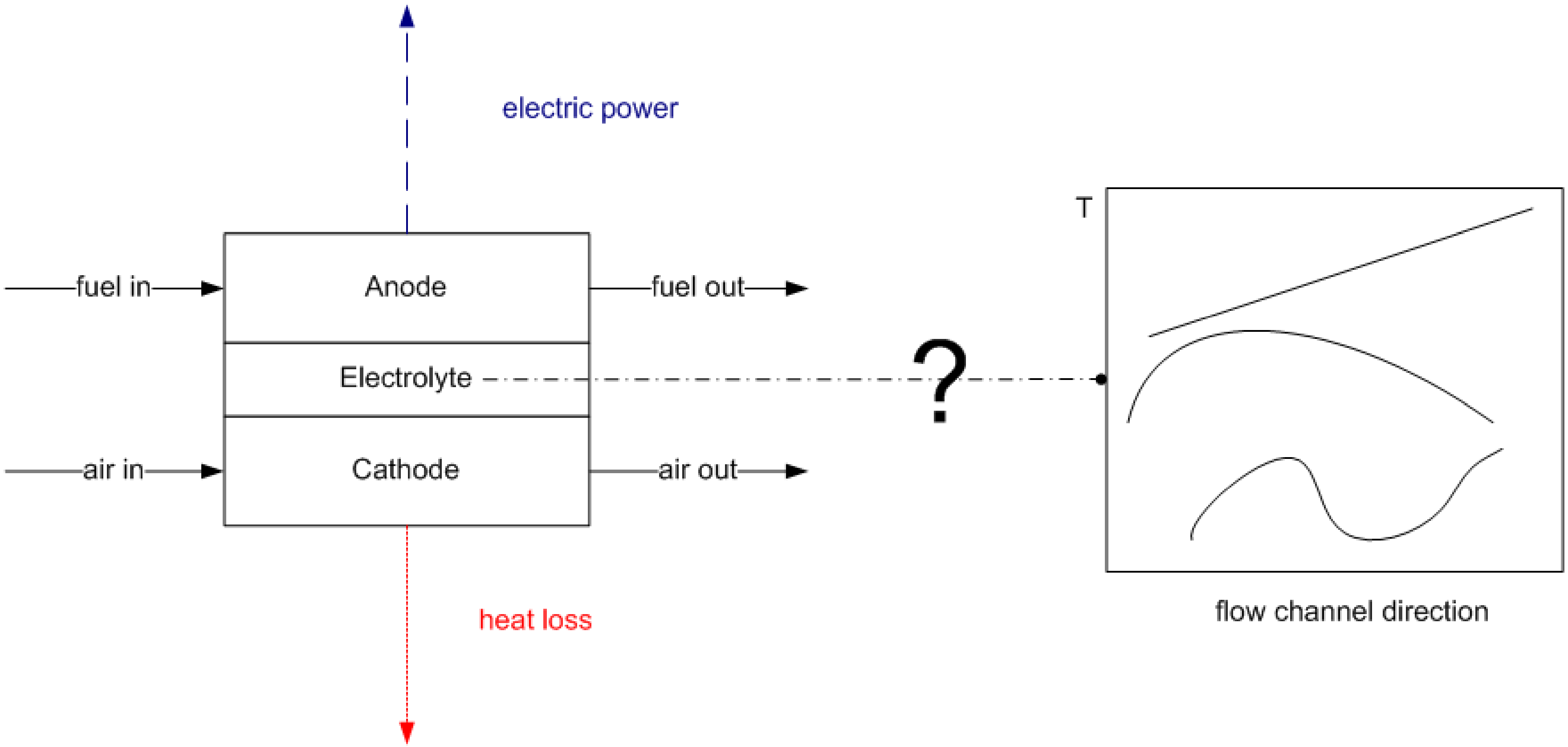
- Modern planar SOFCs operate in 600°C – 850°C range
  - High temperatures, limited by interconnect degradation
  - Low temperatures, limited by SOFC performance
- Desirable to achieve 150-200°C temperature rise (in SOFC subsystem)

High-methane fuel enables endothermic internal reforming

- Methane-free fuel, <20% Ua achievable for 150-200°C ΔT
- Methane content >20% enables 40-50% Ua for the same ΔT
- With high-methane fuel, details inside fuel cell become important

Thermodynamic vs. Dimensional SOFC Model

- Thermodynamic model
  - Global mass & energy balance
- Dimensional model
  - Dimensional distribution of temperature, species concentrations, current density, local Nernst potential, etc.



SOFC Dimensional Model Development

Concomitant reformation, water gas shift, electrochemistry, heat transfer, and mass transport processes must be understood and resolved for robust SOFC design in IGFC

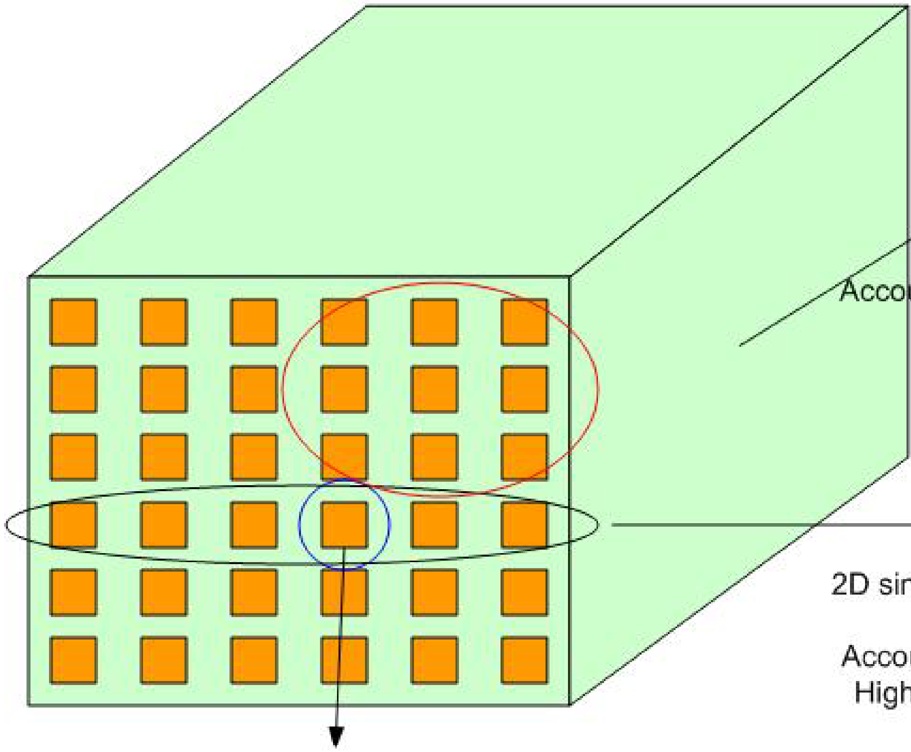
Desired:

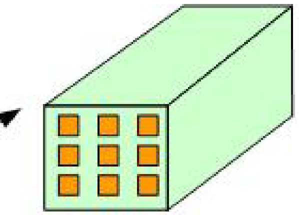
- Dimensional model for SOFC
- Stand-alone
- Compatible with system models

Approach:

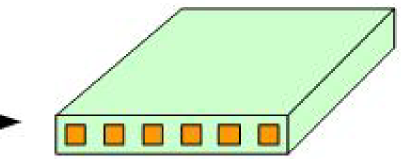
- Use finite volume method, develop quasi-2D model
- Develop and evaluate in Matlab
- Create stand-alone model in C++, capable of linking with system models (Aspen+)
- Version also developed in Fortran (also linkable)

Dimensional SOFC Model Approach

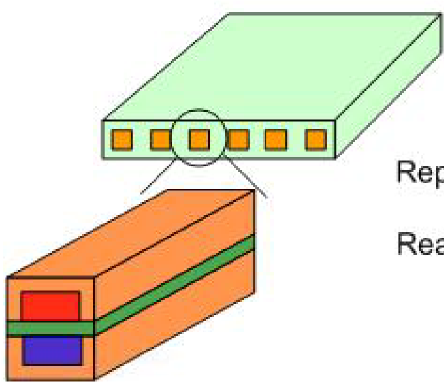




3D multi cell model, co-flow, counter-flow, (cross-flow)
Representative of the stack corner
Accounting for radiation heat loss at front, back, left (right) and upper (lower) edges
Challenging in numerical method



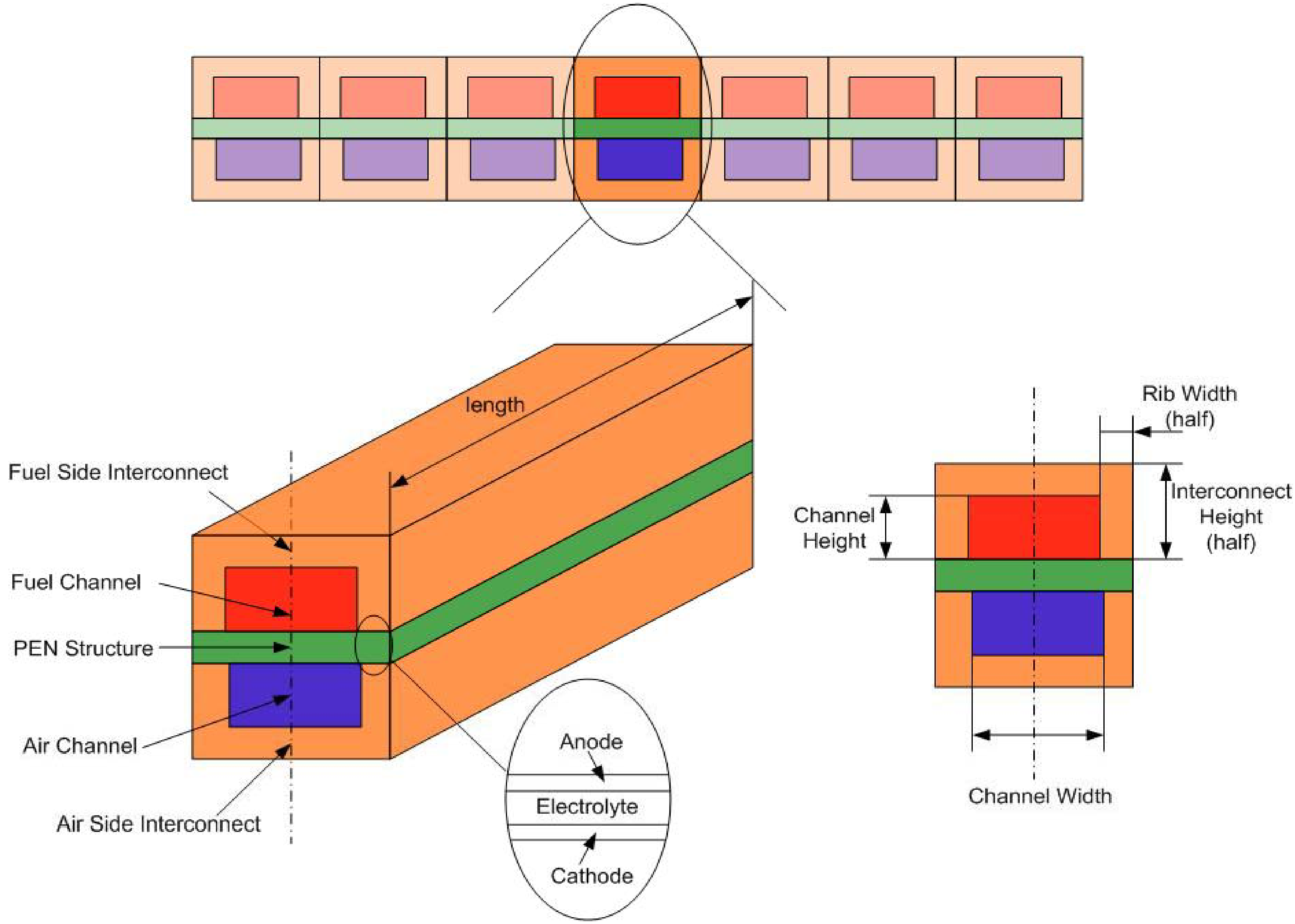
2D single cell model (multi channel), co-flow, counter-flow, cross-flow
Representative of the centered cell layer in stack
Accounting for radiation heat loss at front, back, left and right edges
Higher calculation expense, may be linked to system analysis tool



1D single cell model (single channel), co-flow or counter-flow
Representative of the "most" centered channel in the centered cell in stack
Accounting for radiation heat loss at front and back edges
Reasonable calculation expense, good to be linked to system analysis tool

Planar SOFC Model Geometry

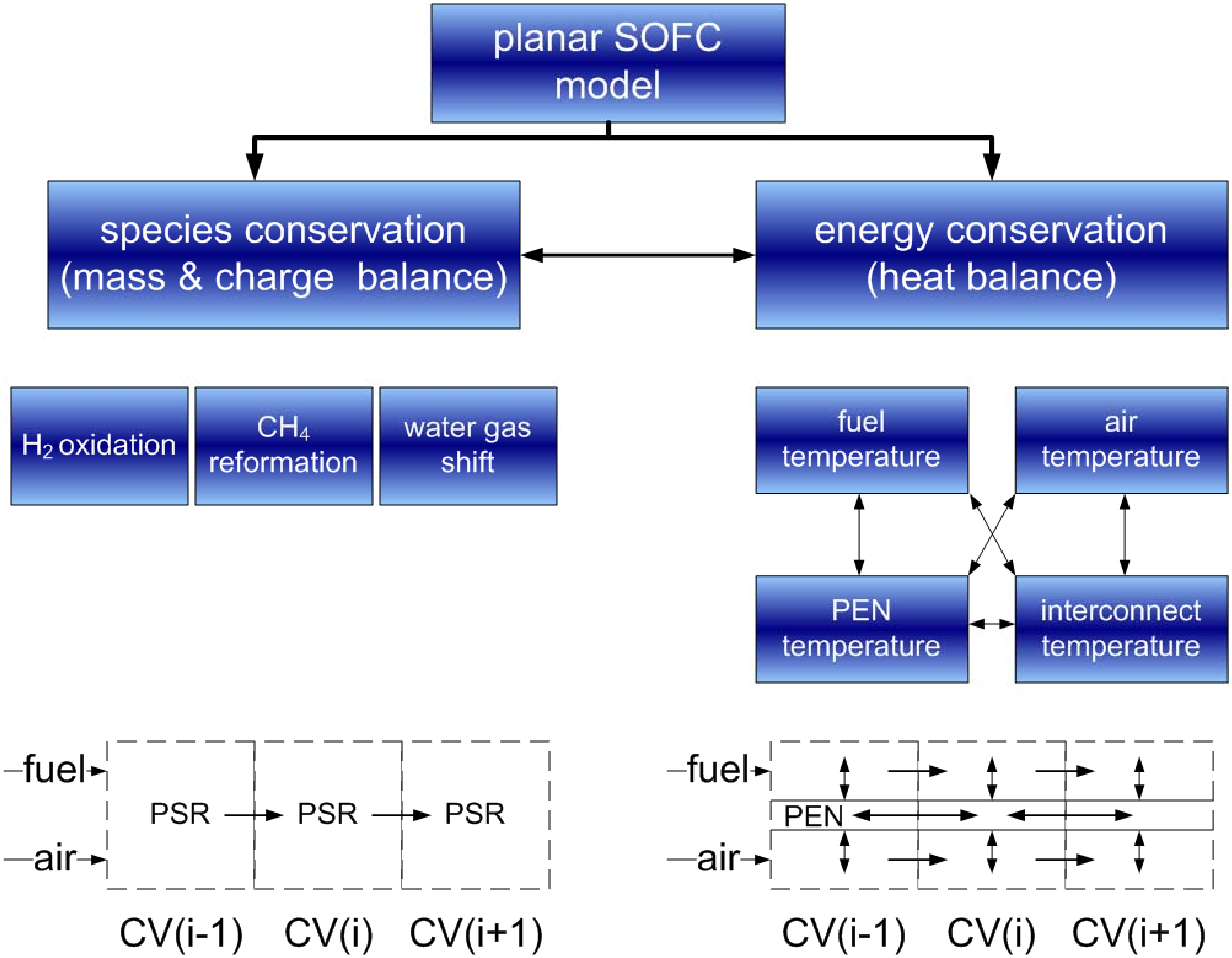
Quasi-2D co/counter flow planar SOFC model



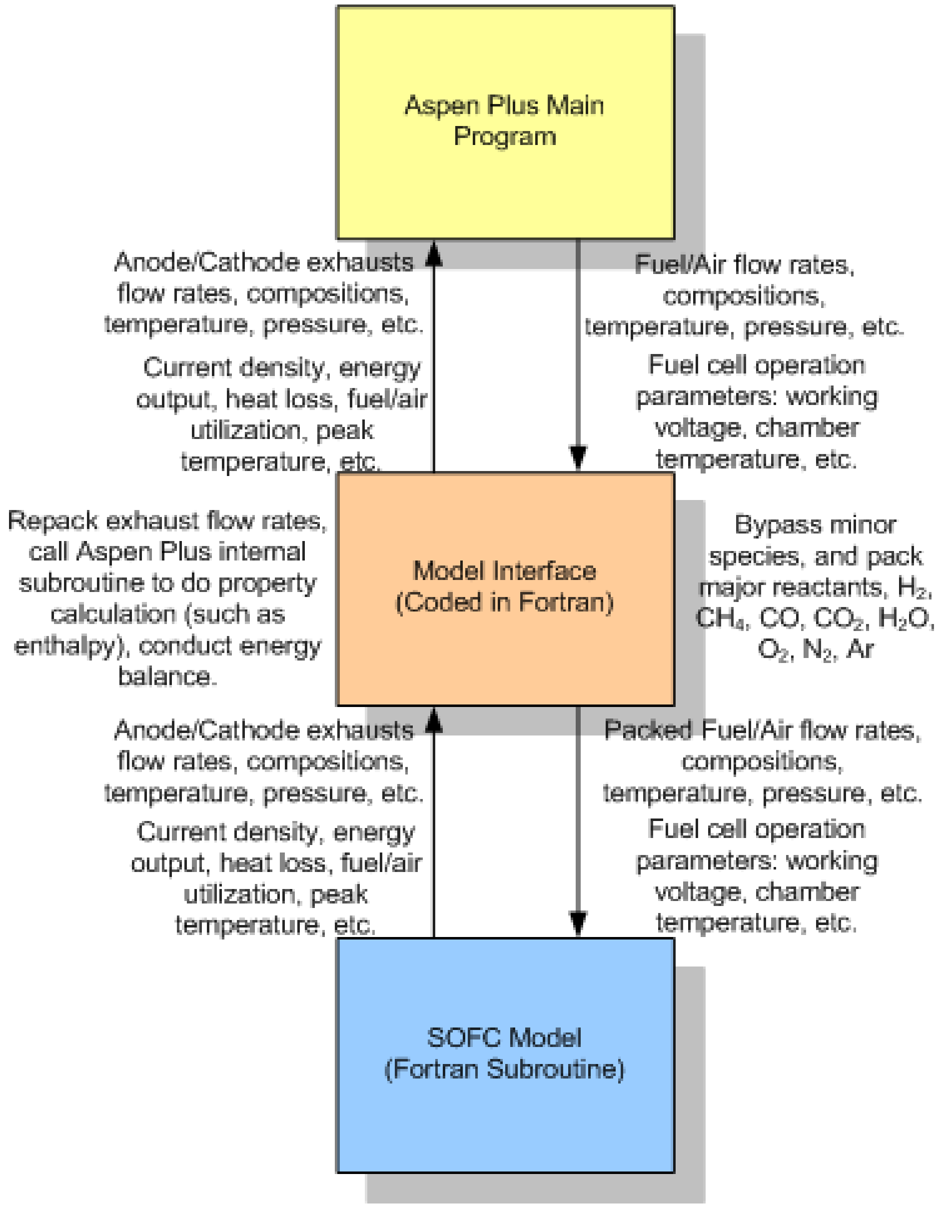
Key Simplifications & Assumptions

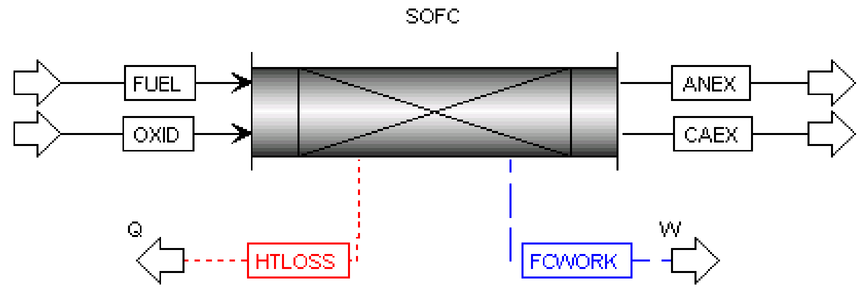
- Steady state modeling
- Four separate temperatures: PEN structure, air flow, fuel flow, interconnect
- Each control volume has uniform species concentration in fuel or air channel
- H_2 electrochemical oxidation only, CO oxidized through water-gas shift
- Water-gas shift always at equilibrium
- Methane reformation controlled by kinetics
  - Multiple approaches implemented – Achenbach, PNNL
- External heat loss by radiation only
- Large Peclet number: negligible axial heat conduction in gases

Numerical Scheme



Cooperation with System Analysis Tool





Number of parameters

Integer: 6 Real: 20 Character: 20

Values for parameters

	Integer	Real	Character
1	12506	0.8	STACK NUMBER & WORKING VOLTAGE (V)
2	100	1045	CELL NUMBER & ENV TEMPERATURE (K)
3	100	0	CHANNEL NUMBER & DP AT ANODE SIDE (PA)
4	40	0	CONTROL VOLUME NUMBER & DP AT CATHODE SIDE (PA)
5	8	0.1	SPECIES NUMBER & GEOP1: LENGTH (M)
6	1	0.003	RADIATION HEAT LOSS CONTROL & GEOP2: WIDTH (M)
7		0.00242	GEOP3: RIBWIDTH (M)
8		0.001	GEOP4: FUEL CHANNEL HEIGHT (M)
9		0.002	GEOP5: AIR CHANNEL HEIGHT (M)
10		0.00325	GEOP6: OVERALL HEIGHT (M)
11		0.0006	GEOP7: ANODE THICKNESS (M)
12		3E-05	GEOP8: CATHODE THICKNESS (M)
13		5E-06	GEOP9: ELECTROLYTE THICKNESS (M)
14		6677.60428	AVERAGE CURRENT DENSITY (A/M2)
15		0.85000983	FUEL UTILIZATION FACTOR
16		0.18545413	AIR UTILIZATION FACTOR
17		1061.8604	AVERAGE SOLID TEMPERATURE (K)

Model Verification: IEA Benchmarks

Benchmark 1, Humidified H_2

Parameter	Benchmark 1 Data	Campanari Parameter	Costamagna Parameter
Voltage (V) High Low	0.722 0.702	0.715	0.704
Current Density (A/m2)	High/Low		
Max	3957/3725	3961	3780
Min	1366/1020	977	1190
Solid Structure Temperature (K)	High/Low		
Max	1371/1321	1333	1337
Min	1203/1182	1190	1189
Outlet Gas Temperature (K)	High/Low		
air	1340/1321	1332	1335
fuel	1341/1321	1333	1337

Benchmark 2, Pre-reformed Natural Gas

Parameter	Benchmark 2 Data	Campanari Parameter	Costamagna Parameter
Voltage (V) High Low	0.649 0.633	0.626	0.607
Current Density (A/m2)	High/Low		
Max	3665/3040	3686	3718
Min	2508/1748	1663	1586
Solid Structure Temperature (K)	High/Low		
Max	1307/1294	1298	1304
Min	1135/1120	1120	1120
Outlet Gas Temperature (K)	High/Low		
air	1299/1289	1296	1301
fuel	1299/1294	1298	1304

Toward Modern Performance Parameters

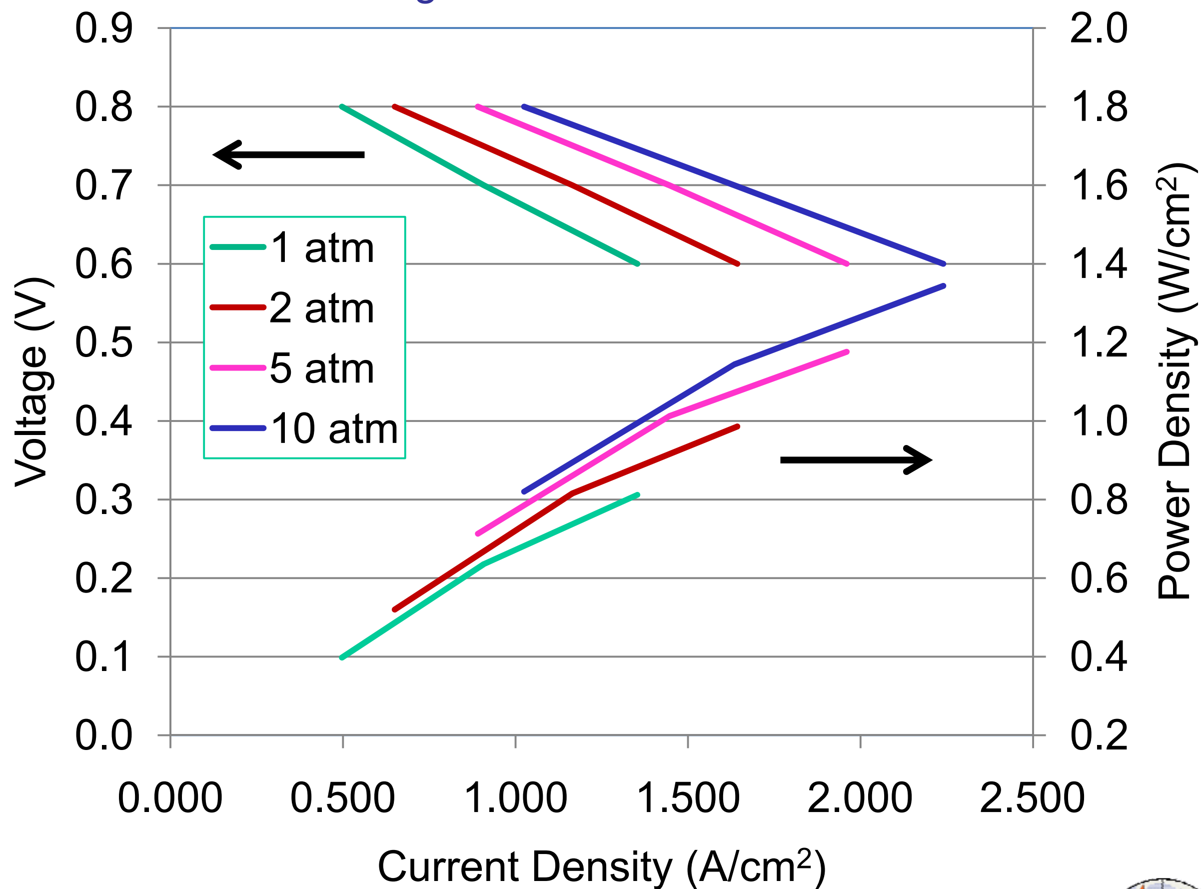
- Sensitivity Analyses:
  - Fuel: 90% H_2 + 10%H_2O (molar fraction)
  - Air: 21% O_2 + 79% N_2 (molar fraction)

	Baseline	Test 1	Test 2	Test 3	Test 4
$E_{a,\ anode}$ (kJ/mol)	100	75	50	50	50
$E_{a,\ cathode}$ (kJ/mol)	120	120	120	100	80
Fuel inlet flow rate (10^{-6}mol/s)	2.3799	3.4336	3.5425	22.013	56.558
Fuel utilization	0.850	0.850	0.850	0.850	0.850
Air utilization	0.143	0.143	0.143	0.143	0.143
Average current density (A/cm^2)	0.0648	0.0935	0.0964	0.5995	1.5405
Average power density (W/cm^2)	0.0518	0.0748	0.0772	0.4796	1.2324
Anode activation loss (mV)	45.92	4.32	0.26	1.73	4.54
Cathode activation loss (mV)	91.53	133.12	137.13	101.99	26.49
Ohmic loss (mV)	3.35	4.87	5.04	33.27	85.02
Anode diffusion loss (mV)	0.78	1.12	1.16	7.26	20.54
Cathode diffusion loss (mV)	0.024	0.033	0.034	0.22	0.64
Fuel outlet temperature (K)	1126.9	1127.9	1127.9	1132.7	1138.4
Air outlet temperature (K)	1126.8	1127.7	1127.8	1128.9	1128.5

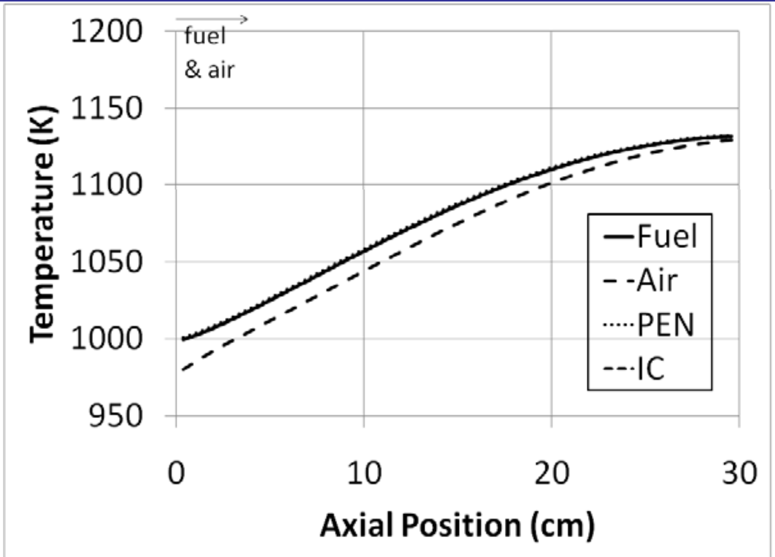
SOFC Performance

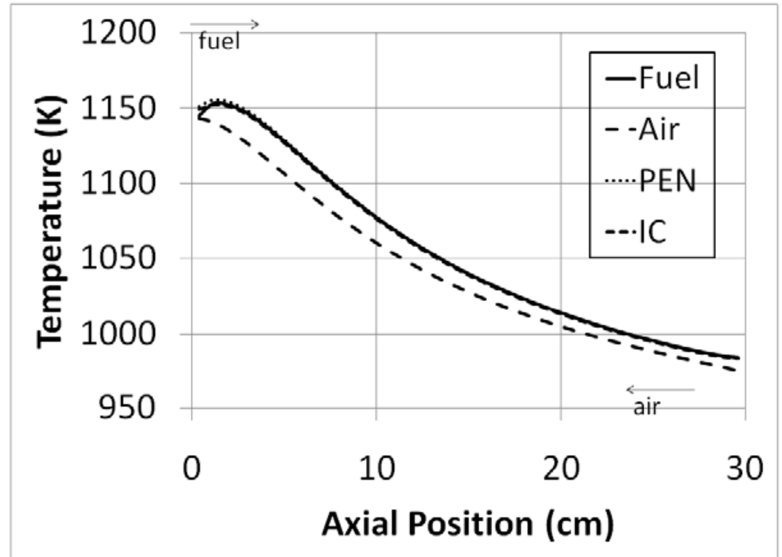
- Targeting state-of-the-art performance
  - IGFC systems for the next decade
- 0.400 W/cm^2 at 1 atm, 0.8 V
- Significant performance increases with pressure: $P^{1/4}$ improvement in cathode polarization
- Working toward parameter validation

Fuel: 80% H_2, 10% H_2O, 10% N_2
80% Fuel Utilization
Avg. Cell T: 770°C



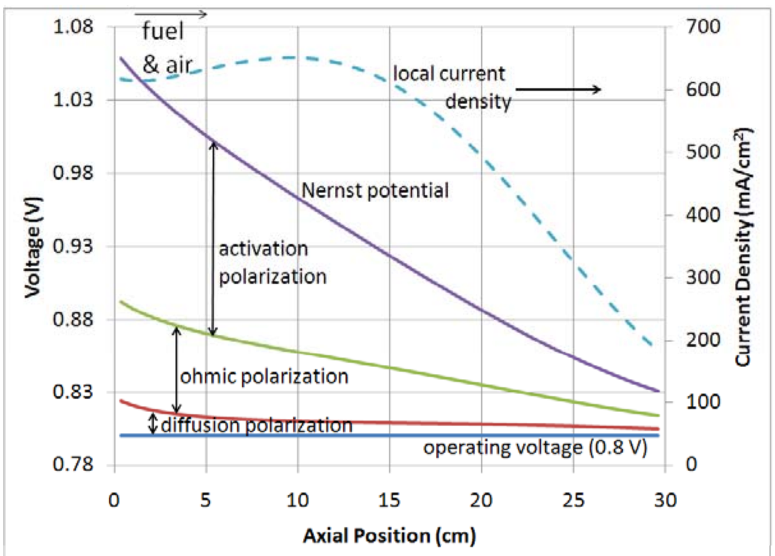
Sample Model Results on Humidified H_2

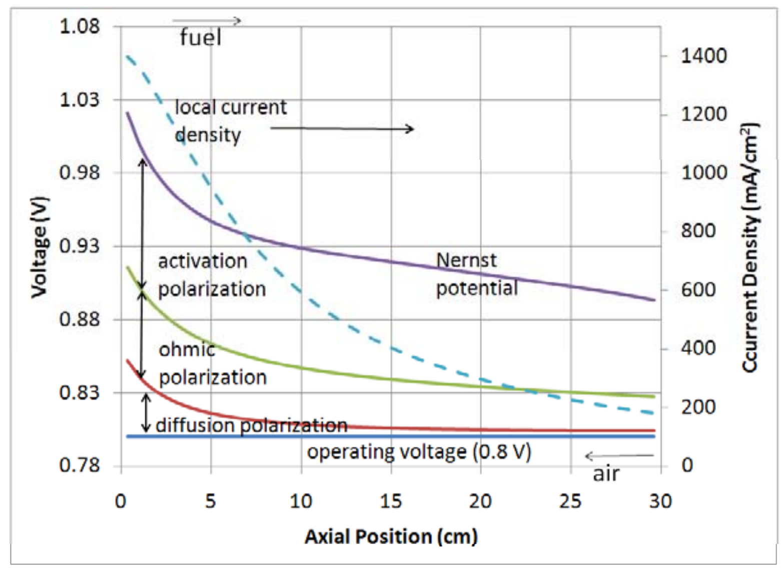




co-flow

counter-flow

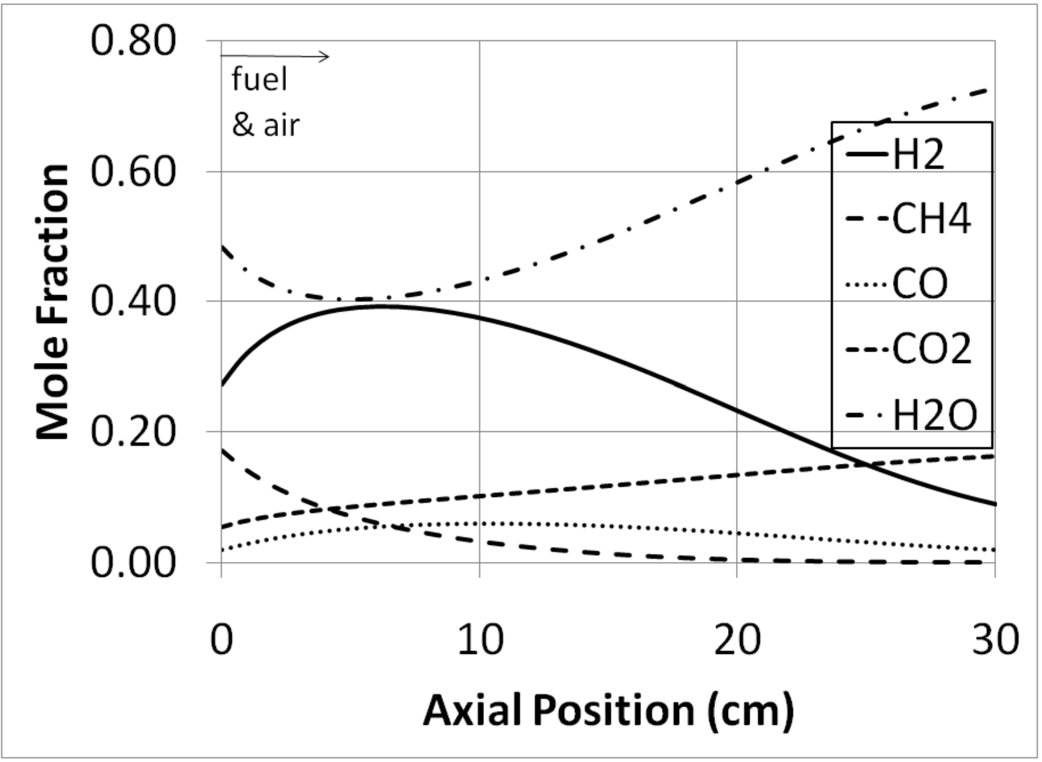




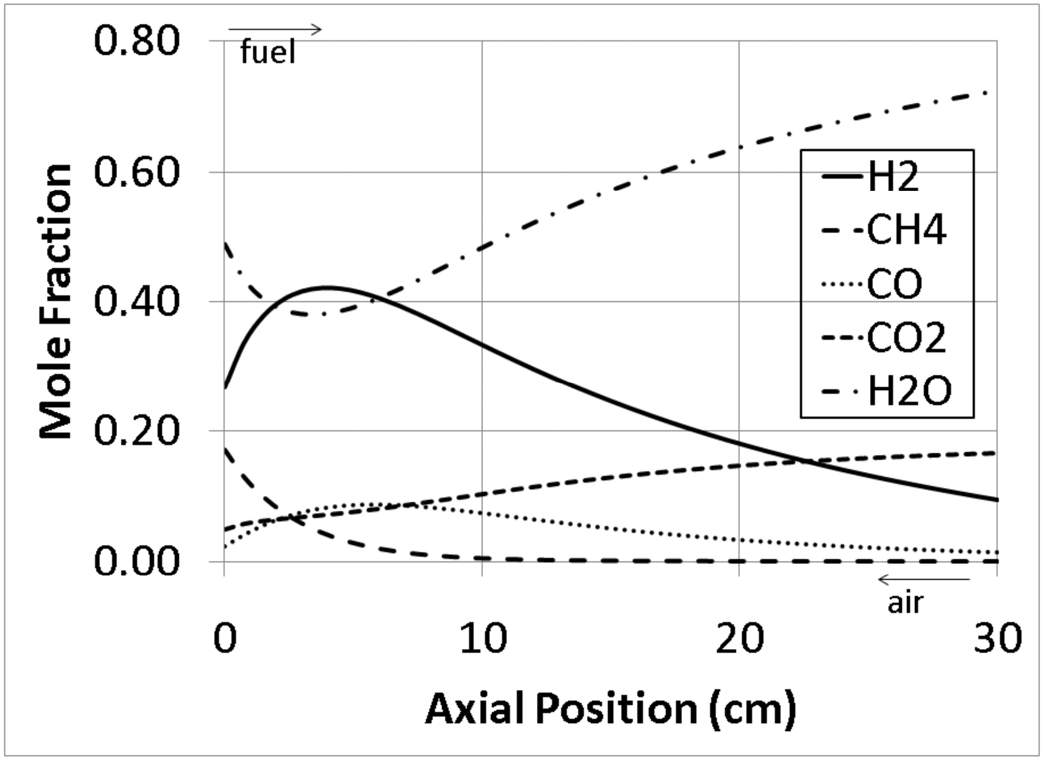
fuel: 90 mol.% H_2, 10 mol.% H_2O
adiabatic, atmospheric operation 85% fuel utilization, 14.3% air utilization

Sample Model Results: Syngas

co-flow
species distribution



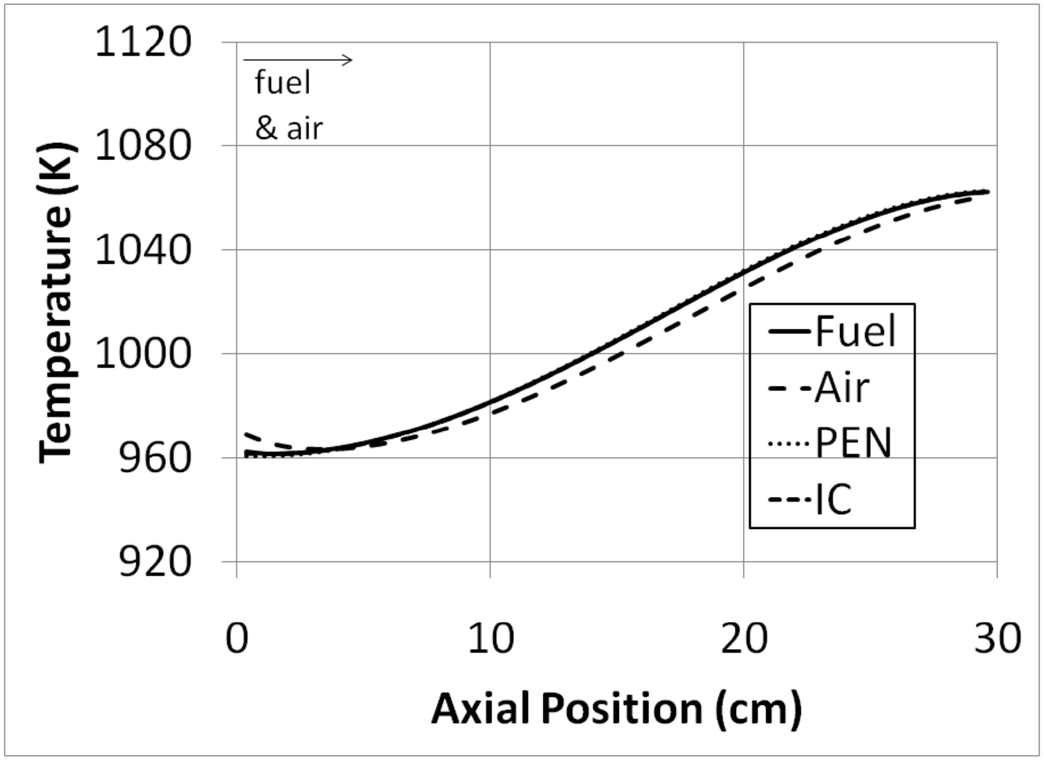
counter-flow
species distribution



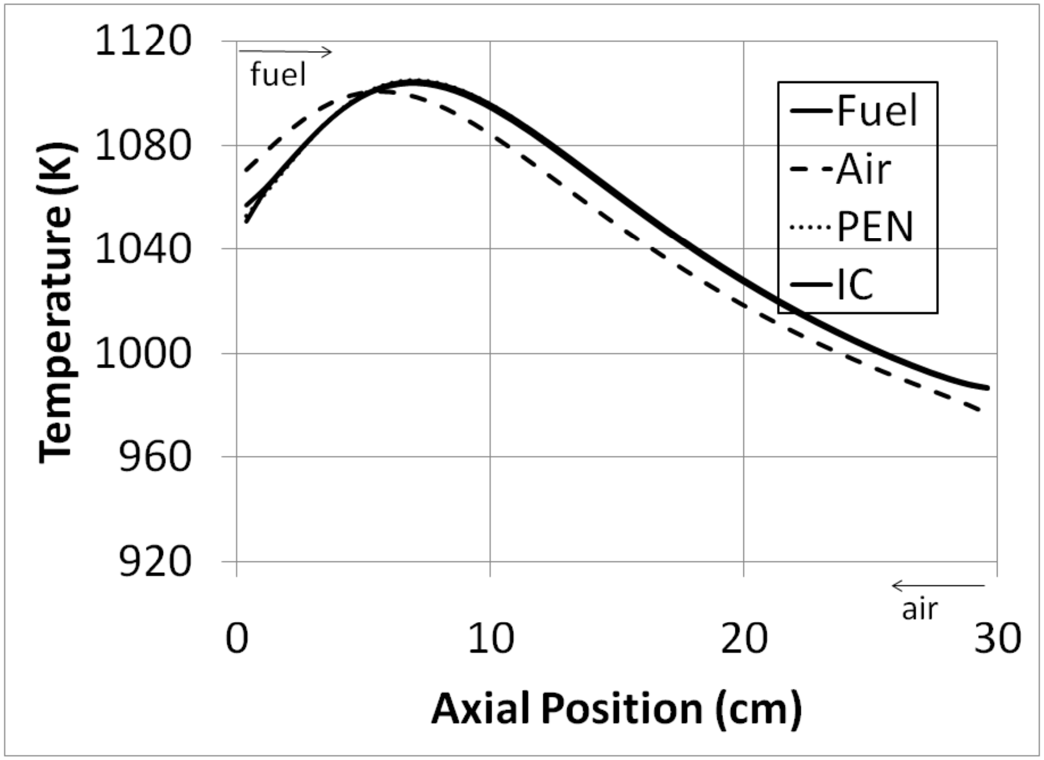
- o fuel mole composition:
  26.26% H_2, 17.1% CH_4, 2.94% CO, 4.36% CO_2, 49.34% H_2O
- o adiabatic, atmospheric operation
- o 85% fuel utilization, 14.3% air utilization

Sample Model Results: Syngas

co-flow temperature



counter-flow temperature



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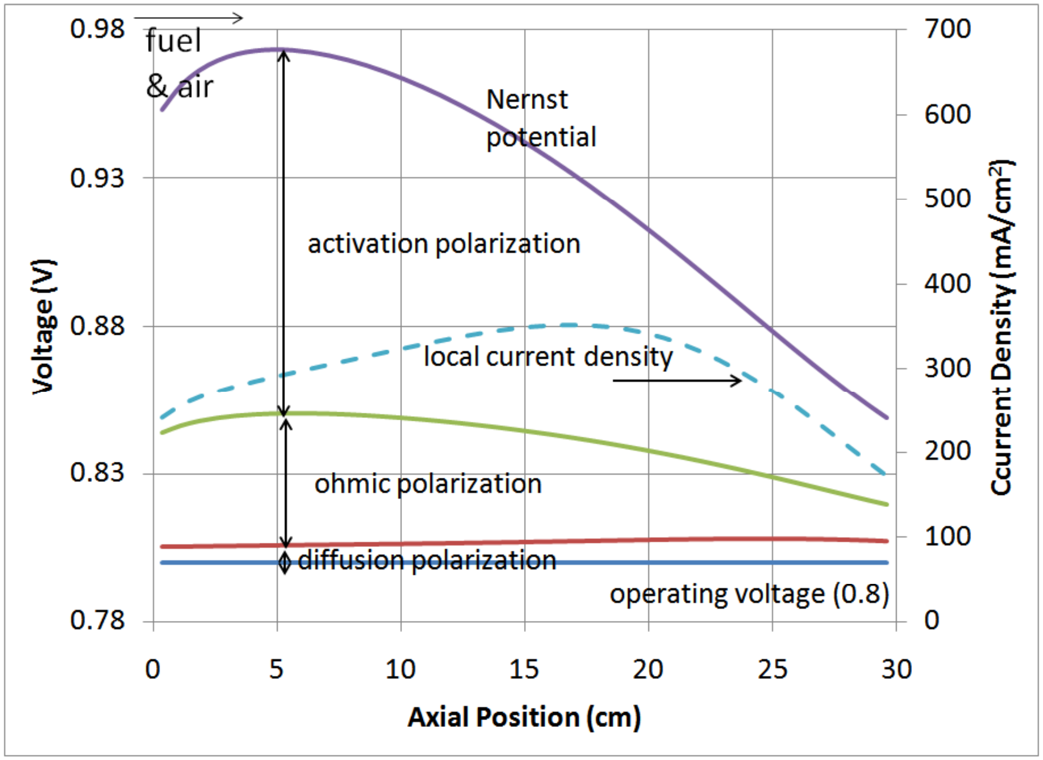
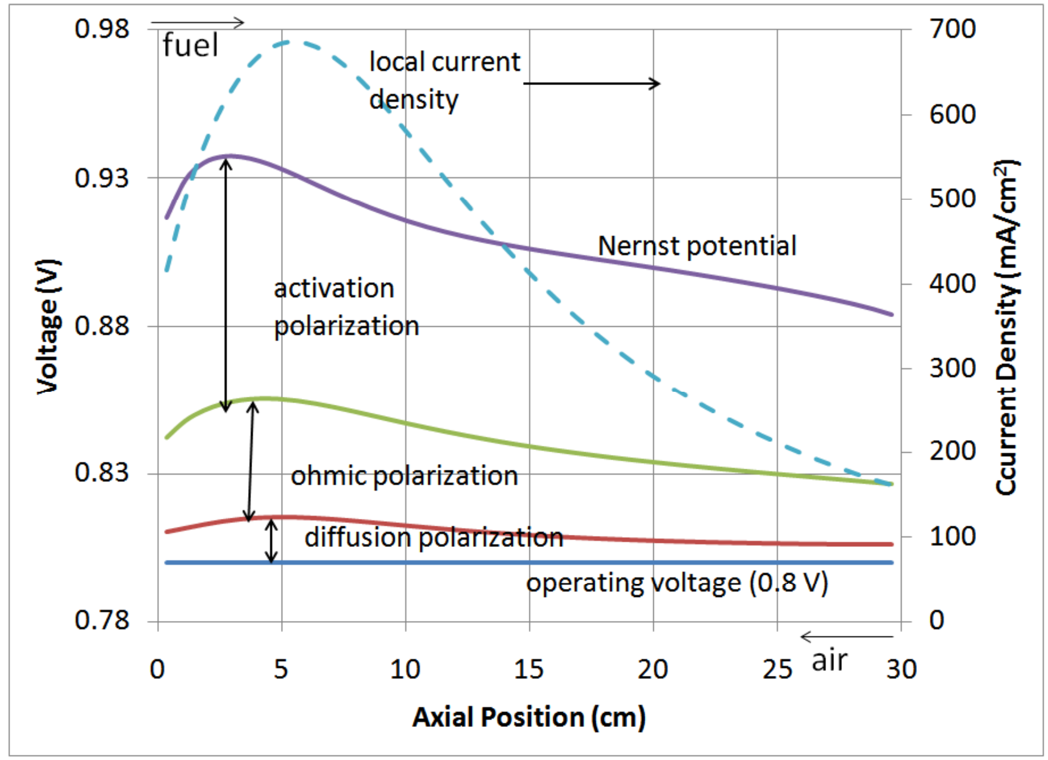
Sample Model Results: Syngas

co-flow electrochemical performance



counter-flow electrochemical performance



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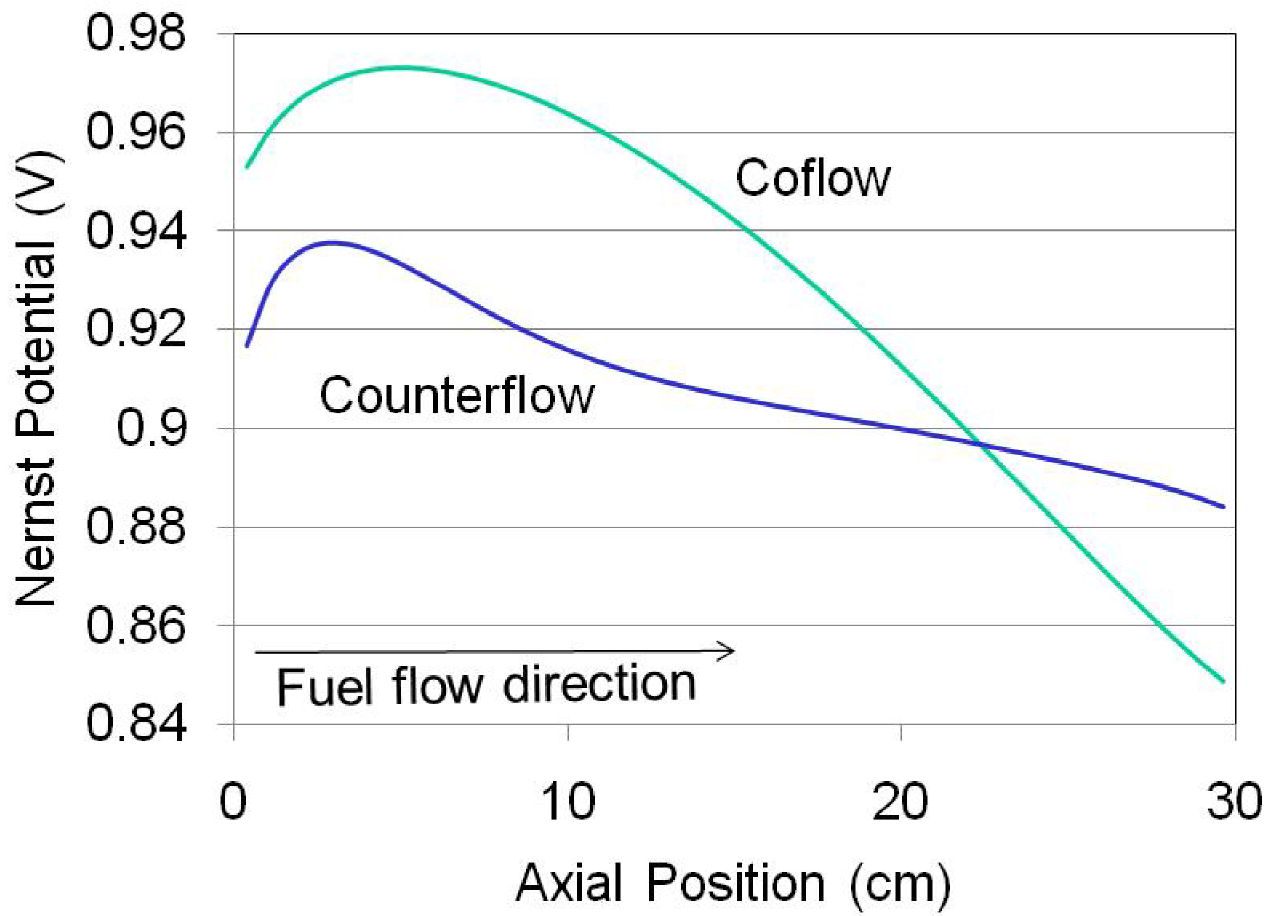
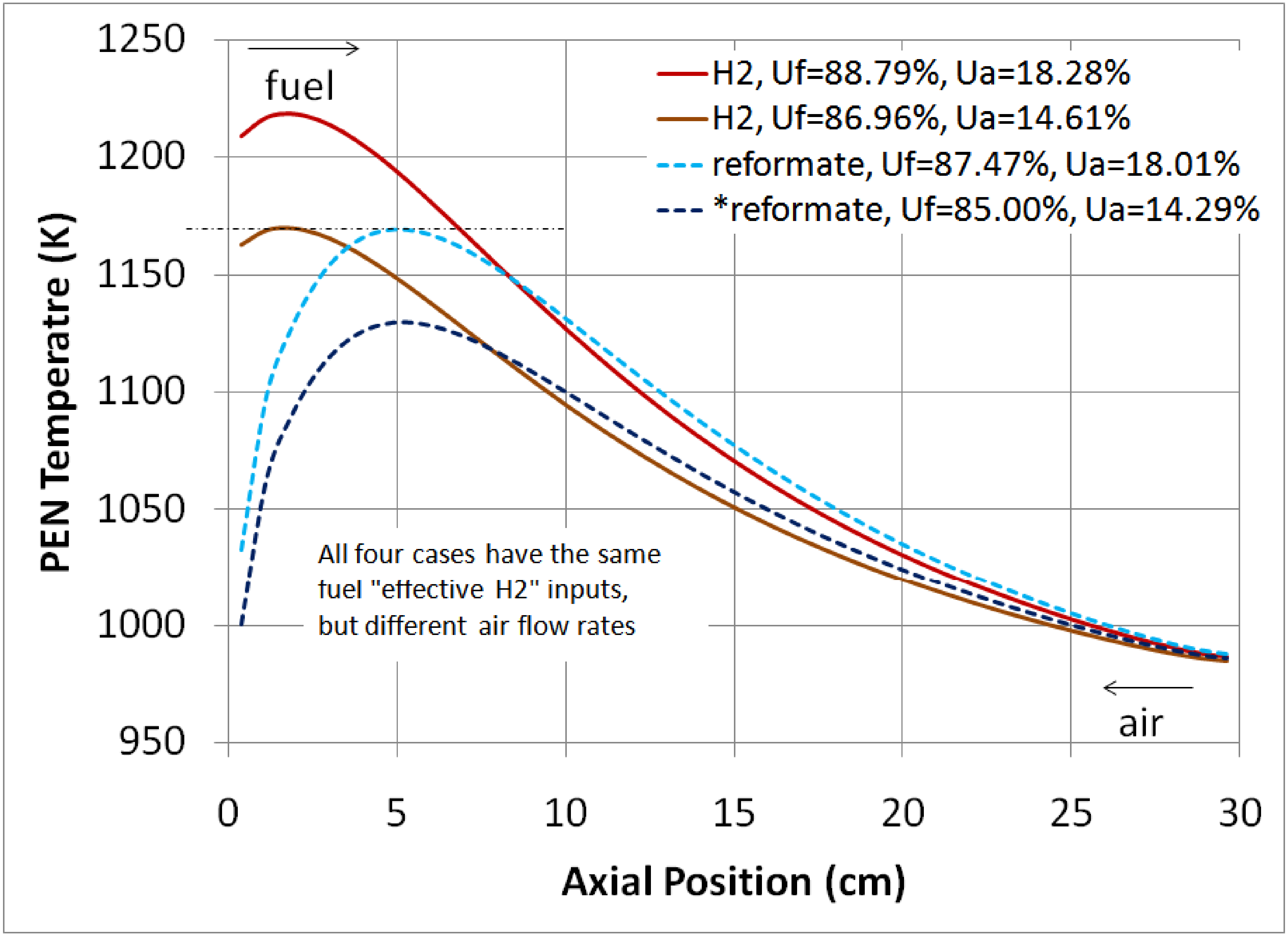
- o adiabatic, atmospheric operation
- o 85% fuel utilization, 14.3% air utilization

Nernst Potential

- Nernst varies significantly with flow configuration
- In many cases, counterflow enables improved operating voltage



Effects of Internal Reforming



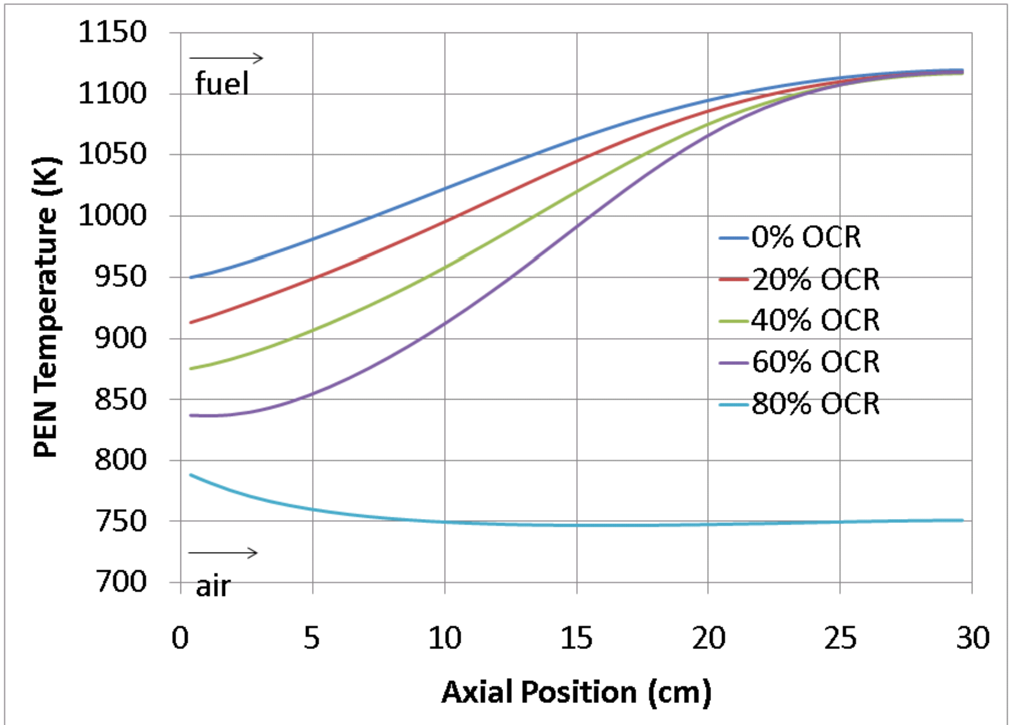
Implications for IGFC Systems

- Best system performance, cost:
  - High methane content syngas
  - High air temperature rise through SOFC
  - High fuel cell power density

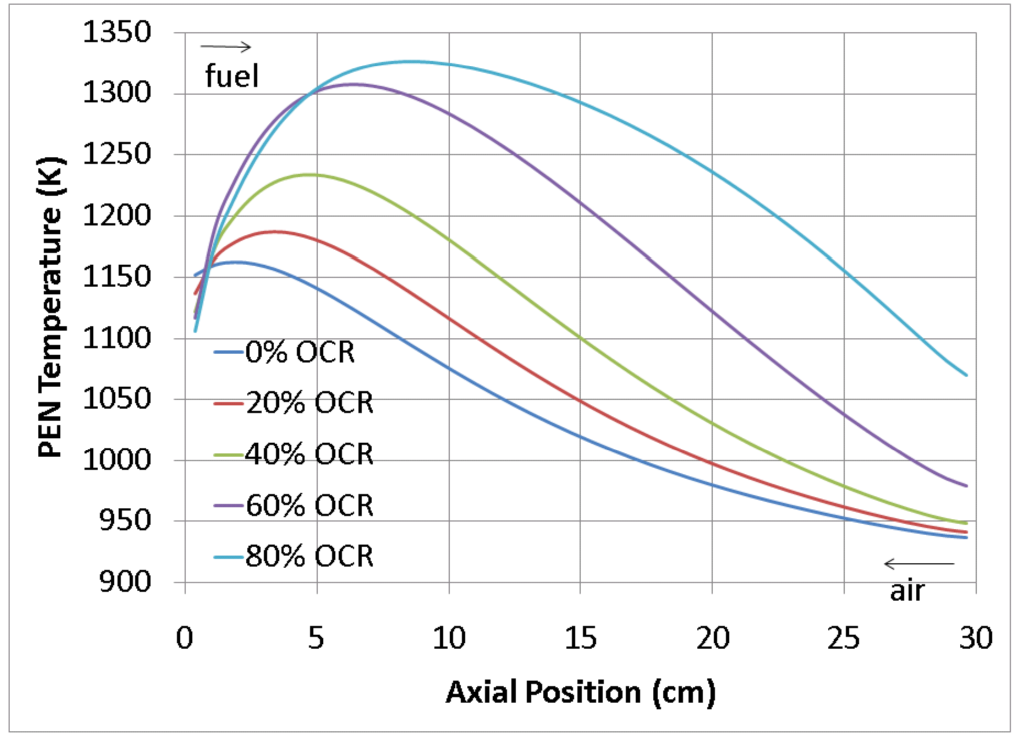
- For these conditions, internal details of SOFC important
  - Performance dependent on flow configuration
  - Peak temperatures may not be at inlet and outlet
  - Need to integrate dimensional models with system analysis

Increasing Methane and Temperature Profiles

Methane composition & flow configuration



co-flow case
PNNL CH_4 reformation kinetics
U_f = 85% (except for 80% OCR), V = 0.8 V
U_a varied to achieve about 200K ΔT at air side
higher OCR, higher CH4 (0→20.2% vol.)



counter-flow case
PNNL CH_4 reformation kinetics
U_f = 85%, V = 0.8 V
U_a the same as corresponding co-flow cases
higher OCR, higher CH4 (0→20.2% vol.)

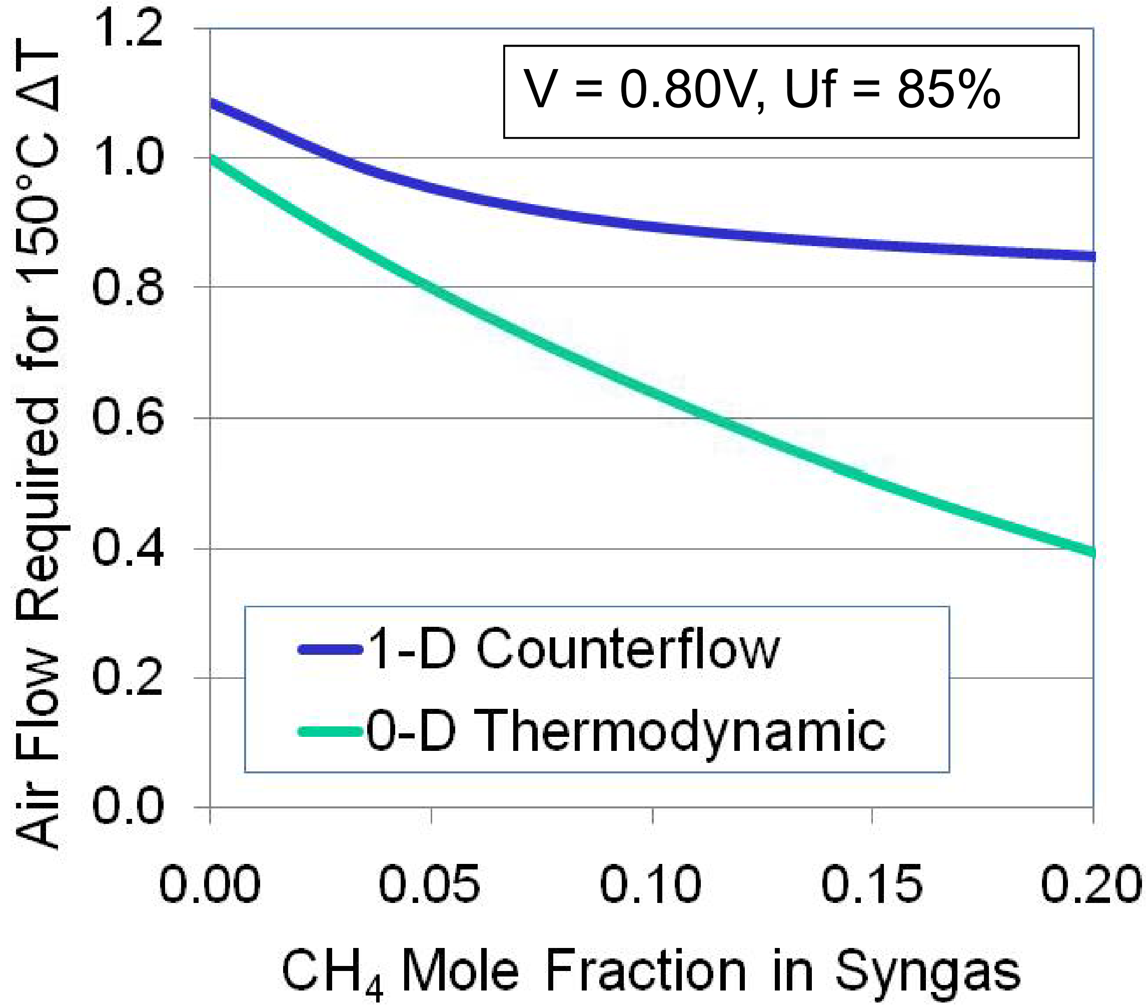
0-D vs. 1-D Comparison

Temperature rise set to 150°C

- 0-D: Air temperature rise
- 1-D: Solid temperature ΔT

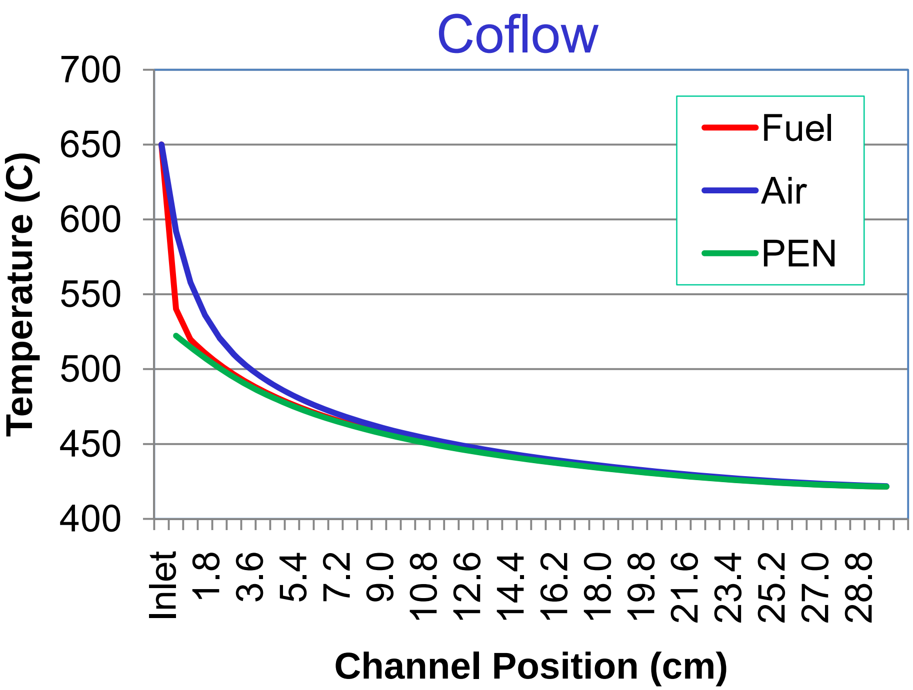
Internal reforming does reduce air-flow requirement

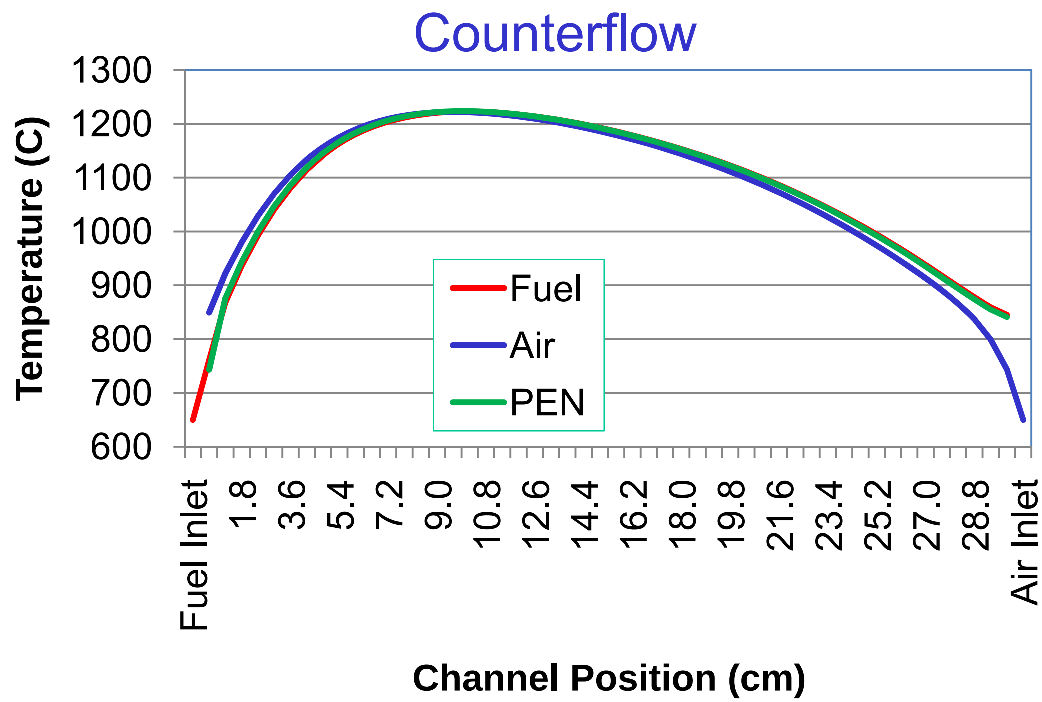
- Air temperature rise is not a good proxy for solid ΔT
- 0-D model overestimates cooling benefit



Sample Results: IGFC System

1 atm, 0.80 V, 85% Uf, 200°C air T rise (~50% Ua), ~30% CH_4 in syngas





- System analysis (w/0-D thermodynamic model) results in Ua = 50%

- Coflow configuration: fast reformation leads to excessive cooling at inlet
- Counterflow configuration: significant internal temperature spike

Strategies for Mitigating High ΔT Challenge

- Increase air flow through SOFC
  - Increased parasitic loss and lesser reformation cooling benefit
- Recycle air and/or fuel
- Increase interconnect thickness
  - Improved in-plane thermal conduction
  - Increased material cost
- Increase operating voltage
  - Improved efficiency, lower heat generation
  - Reduced power density, increased SOFC cost
- Retard reformation kinetics
- Cascade stacks: series air, parallel fuel
- Move reforming off anode: reforming channels

Summary & Conclusions

IGFC system design requires dimensional SOFC analysis

- Capture synergies and limitations inherent to SOFC
- Thermodynamic SOFC modeling not sufficient
- Design strategies exist to mitigate SOFC internal thermal limitations

SOFC steady-state performance and thermal behavior highly dependent on stack configuration

Detailed quasi-2D planar SOFC model developed for IGFC system analysis

- Designed for use in conjunction with IGFC design and analysis
- Integrates with system modeling software
- Calculates thermal, species, potential profiles

Acknowledgements

- This work was supported by the U.S. Department of Energy (DOE) under Contract DE-AC26-04NT41817.313.01.05.036.

- The authors gratefully acknowledge the technical guidance and insights provided by Wayne Surdoval and Travis Shultz of the U.S. DOE.

- The authors thank Dale Keairns, Mo Khaleel and Kurt Recknagle for very useful discussions.