Theory Based Process Modeling for Evaluation of Fuel Cells in Advanced Energy Systems

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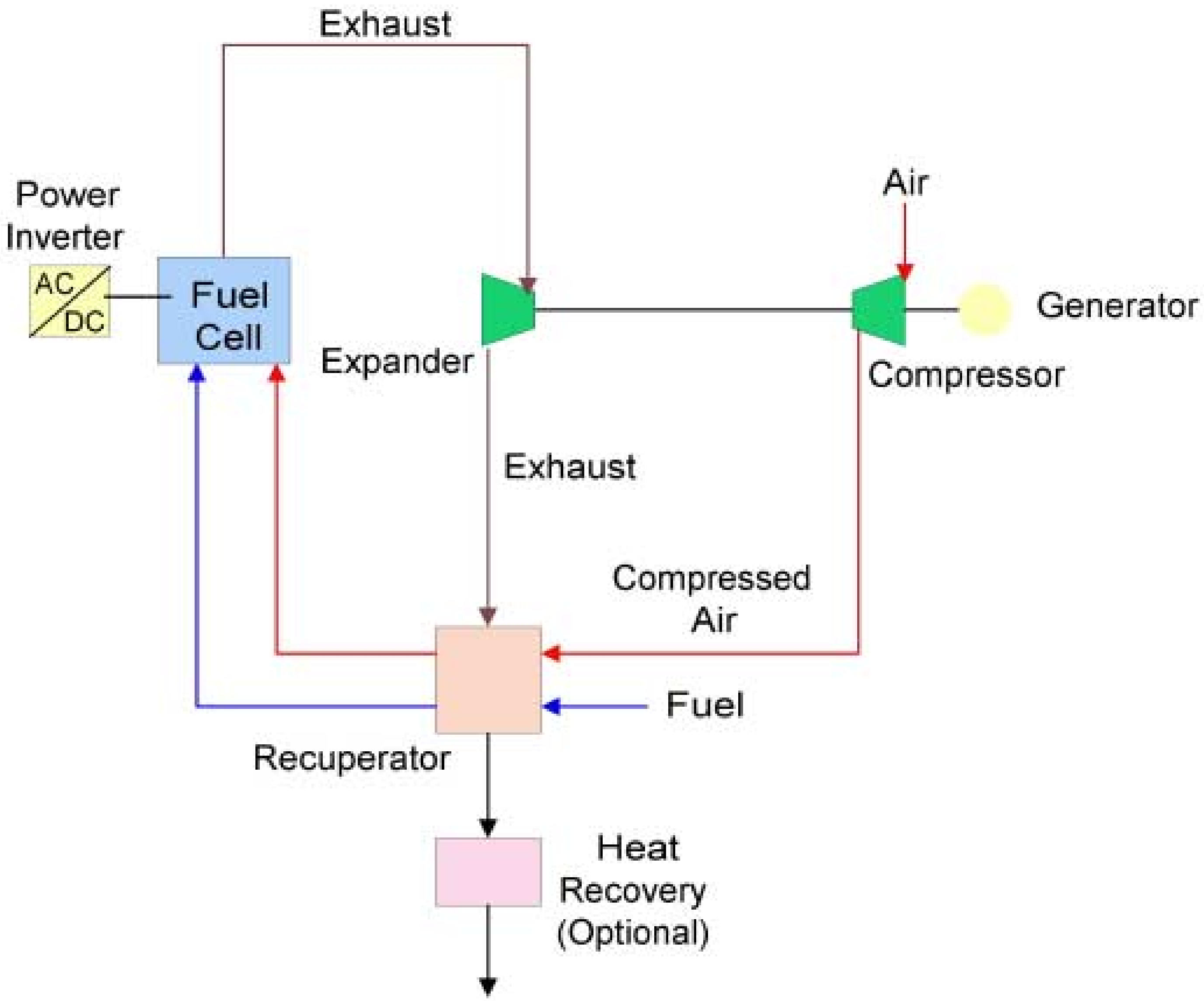
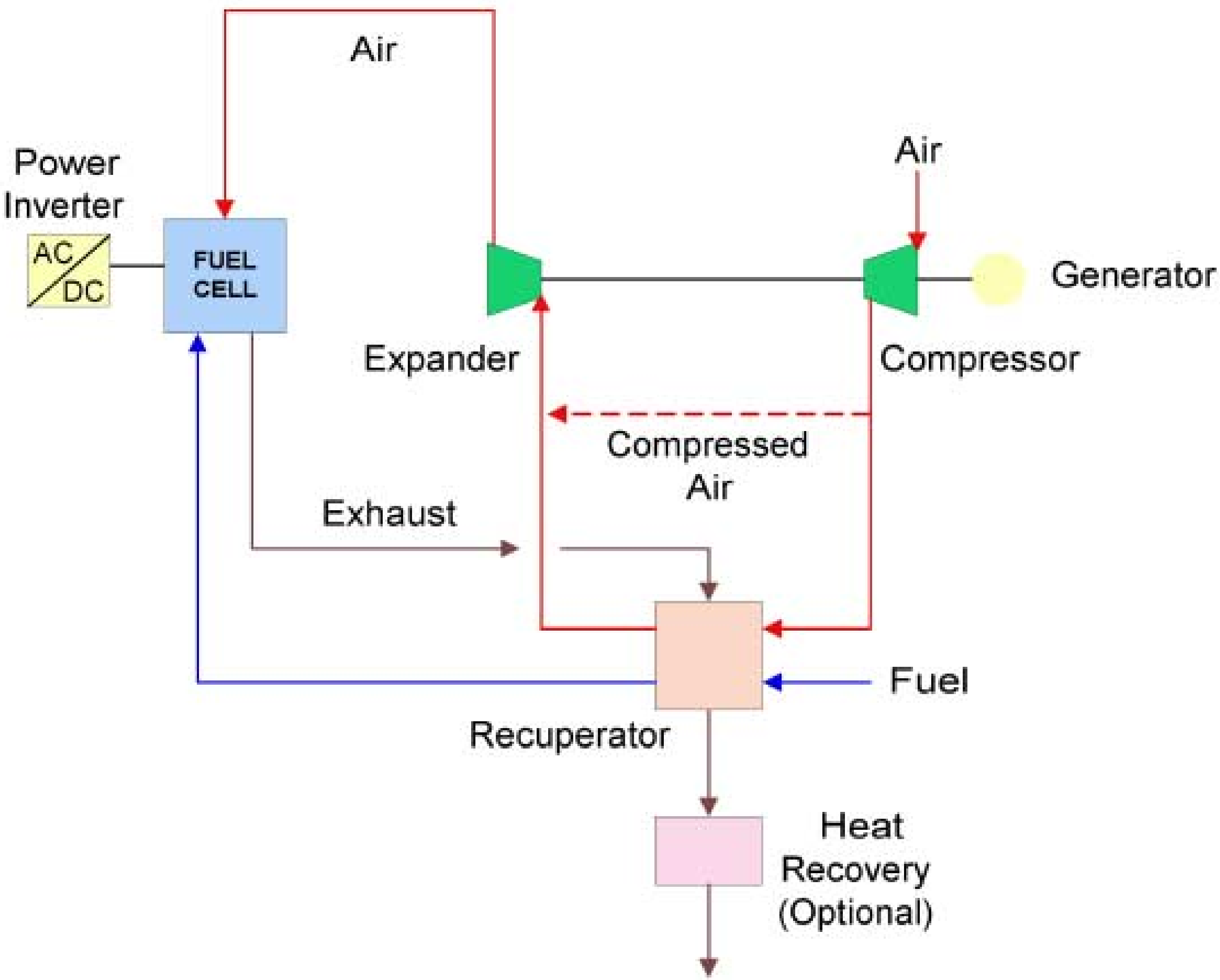
Fuel Cell/Heat Engine Cycles in Hybrid Systems

	Fuel Cell Cycle (fuel side)		**Heat Engine Firing**	
	Topping	**Bottoming**	**Direct**	**Indirect**
Hybrids/V21 Programs				
SW	SOFC *t-coflow-iir*	-	GT	-
MTI	SOFC *p-crossflow*	-	-	GT
HW	SOFC *p-coflow*	-	-	GT
MCP	MCFC *p-coflow*	-	GT	-
FCE	MCFC *p-crossflow-dir*	-	-	GT
Other Concepts				
SOFC-PEMFC	SOFC *p-coflow-iir*	PEMFC *p-coflow*	-	-
POXHE-SOFC	-	SOFC *p-crossflow*	GT/ICE	-

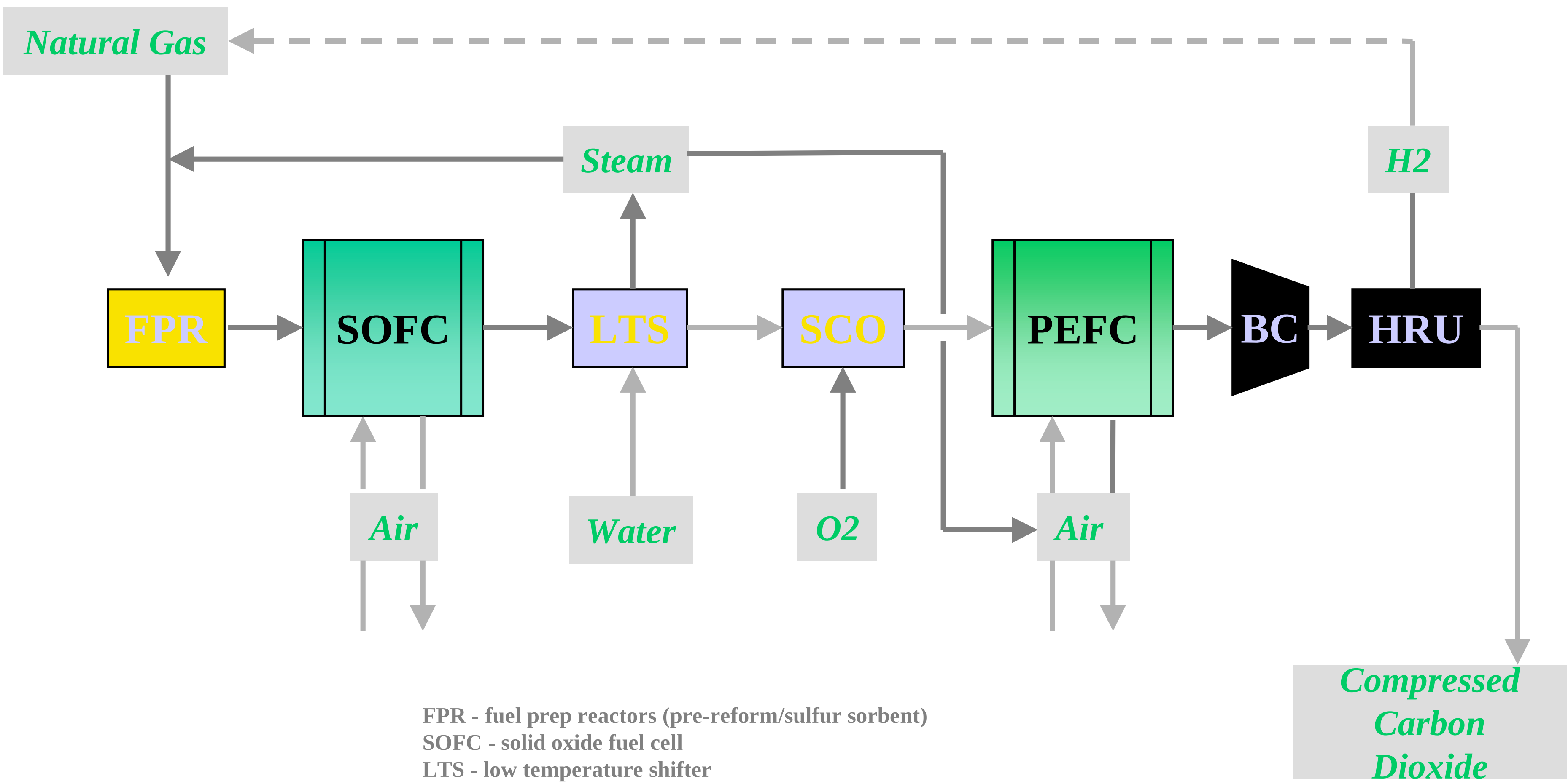
Turbine Bottoming Cycle



Turbine Topping Cycle

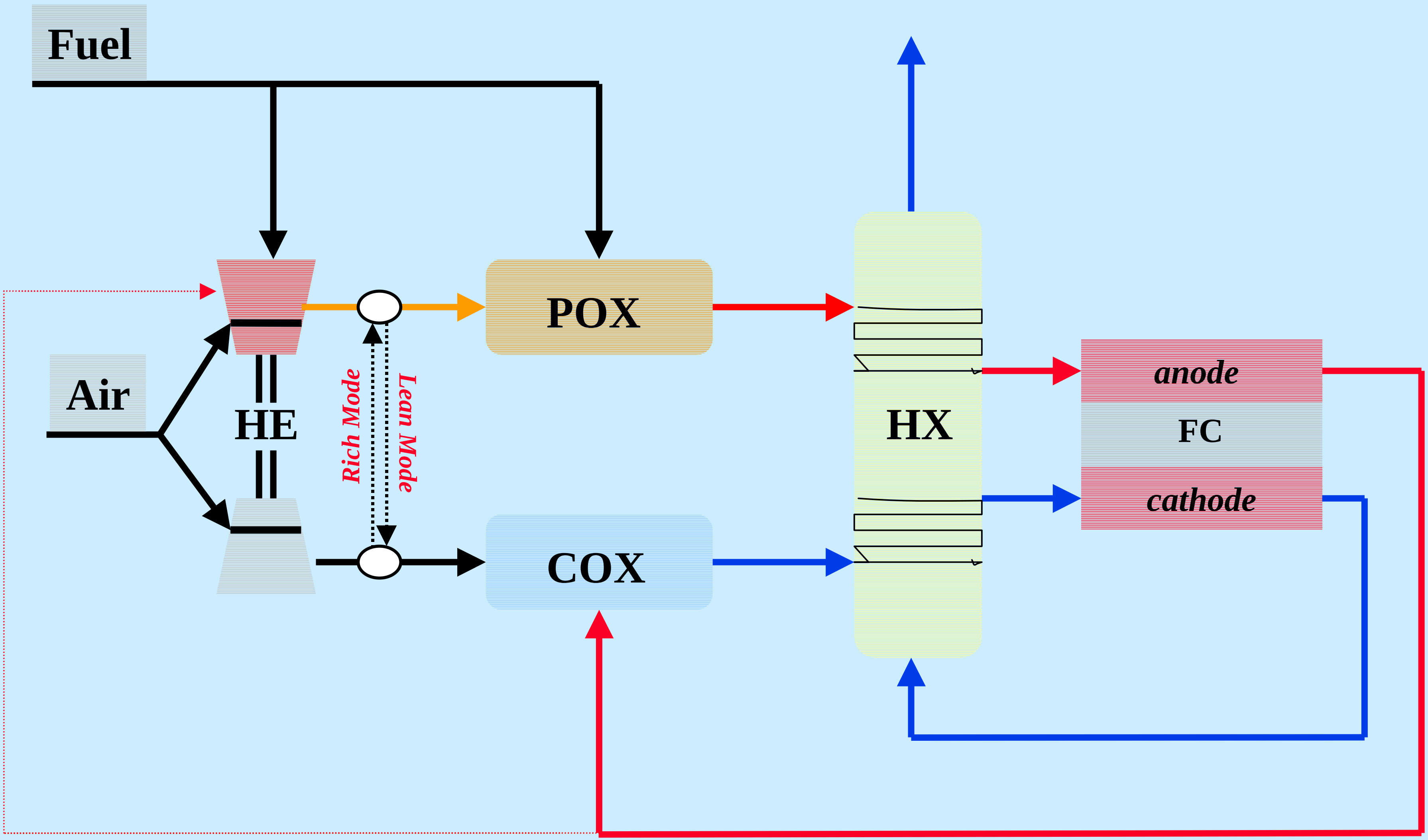


SOFC-PEMFC Hybrid
Sequestering Version

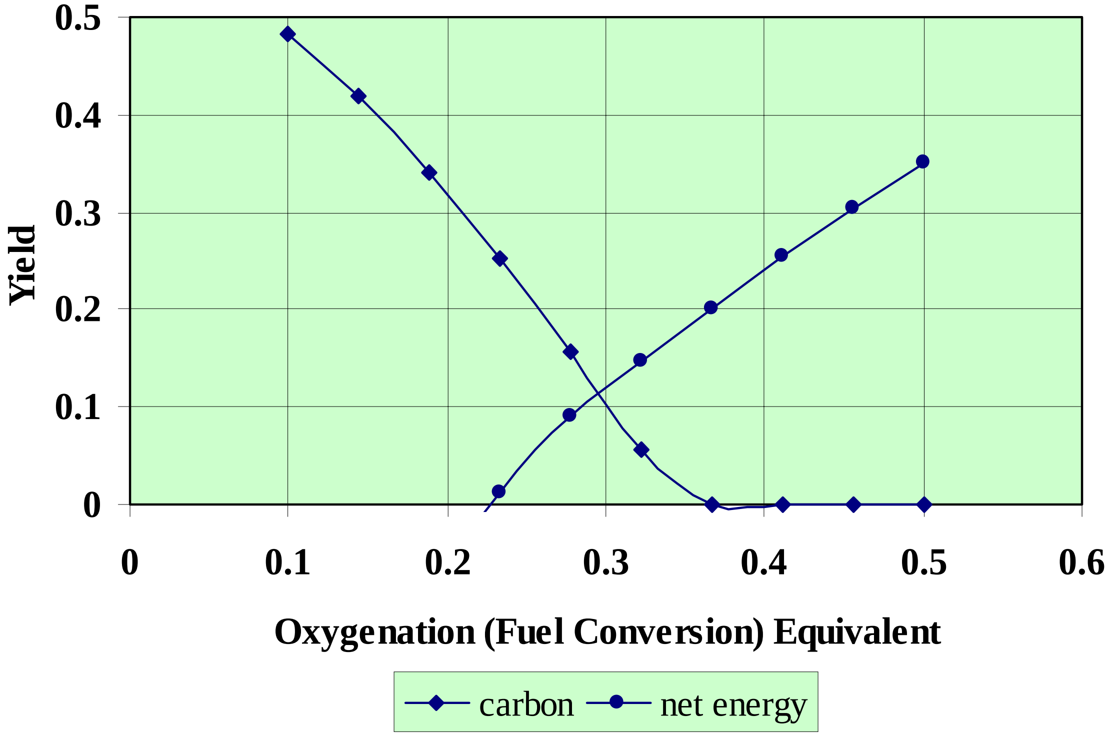


FPR - fuel prep reactors (pre-reform/sulfur sorbent)
SOFC - solid oxide fuel cell
LTS - low temperature shifter
SCO - selective catalytic oxidizer
PEFC - polymeric electrolyte fuel cell
BC - booster compressor
HRU - hydrogen recovery unit

Direct Fired Reforming Heat Engine-Bottoming Fuel Cell Hybrid



Motivation for Engine Based POX Reforming



Direct POX Reforming of CH4 with Dry Air to Equilibrium at 1400 F and 10 ATM.

Basic Aspects of Fuel Cell Process Modeling

- Heat and Material Balances – System Integration

- Current Density Distribution – Fuel Cell Sizing

Current Density Distribution for Coflow with Constant Resistivity

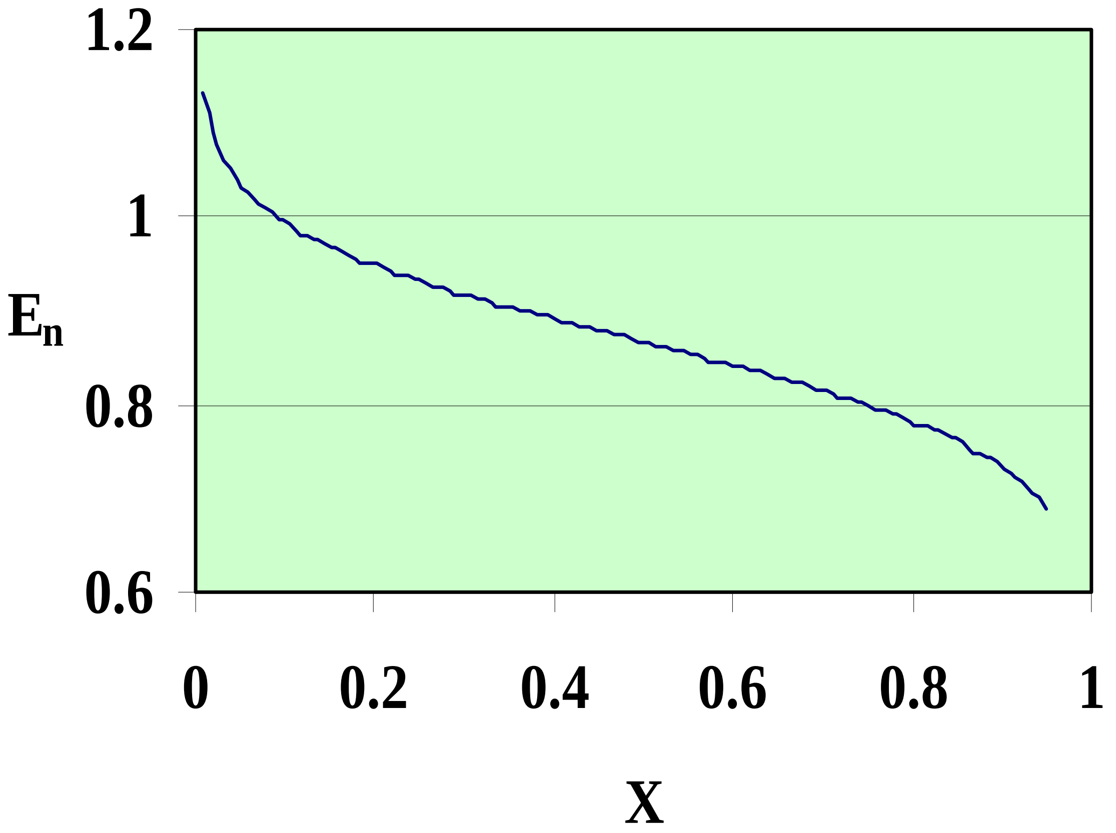
$$\mathbf{i_m/i_r = \{(\int^{X_r} ((E_r - E_c) / (E - E_c))\, dX) / X_r\}^{-1}}$$

where:

$i_m \equiv$ average current density

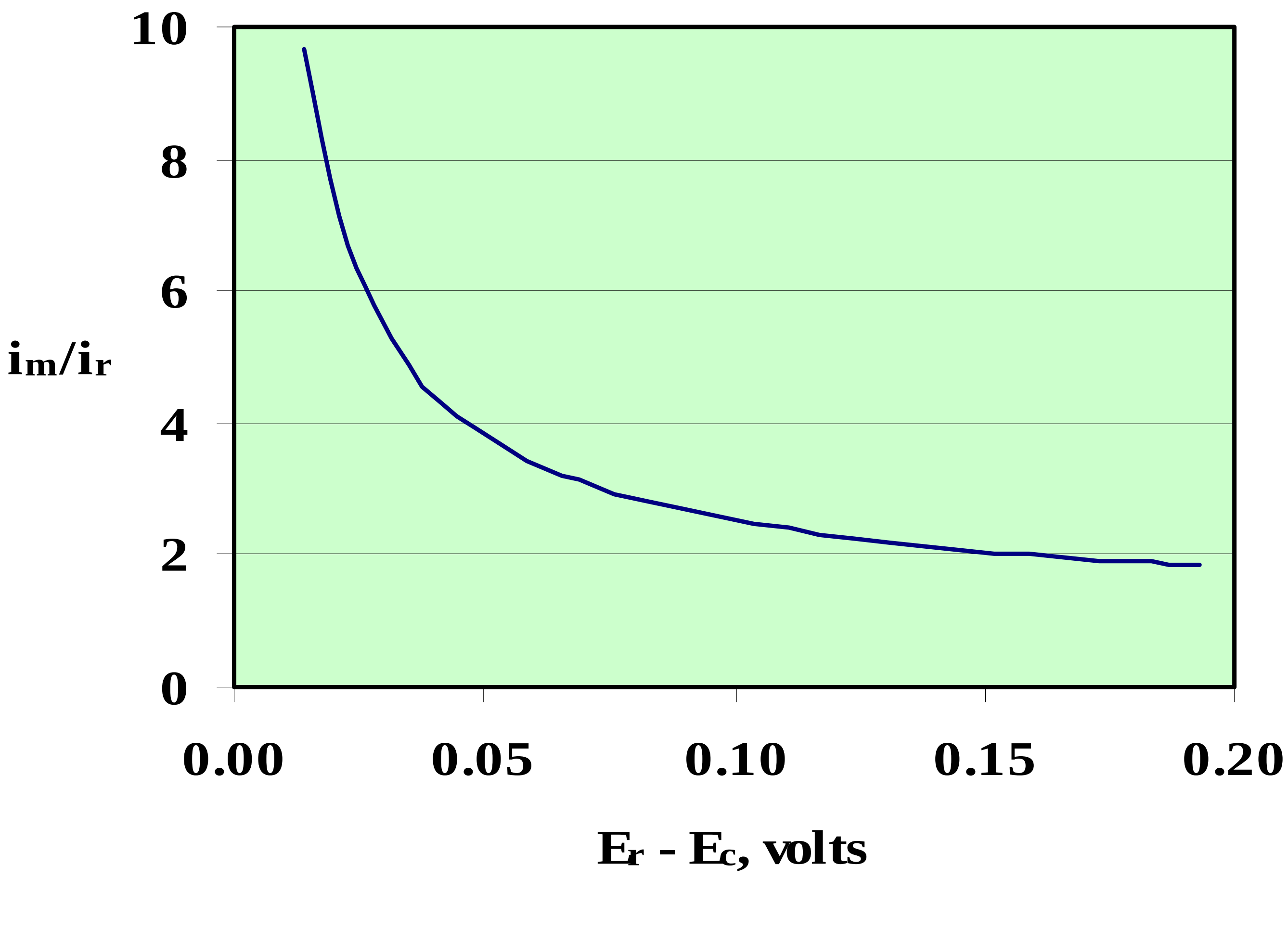
$i_r \equiv$ reference current density = $(E_r - E_c) / \Omega$

Typical Nernst Potential Curve for SOFC



1000C, 1 ATM, 1.5 Air:Fuel Equivalence Ratio, 50% Dry H2

Typical Current Density Distribution Index



Fuel Cell Process Model

Rating Stage Sequence

- *splitters, mixers, heaters, restricted equilibrium reactors*
- *executed repeatedly during flowsheet convergence*
- *uses cell voltage or voltage efficiency as an input*

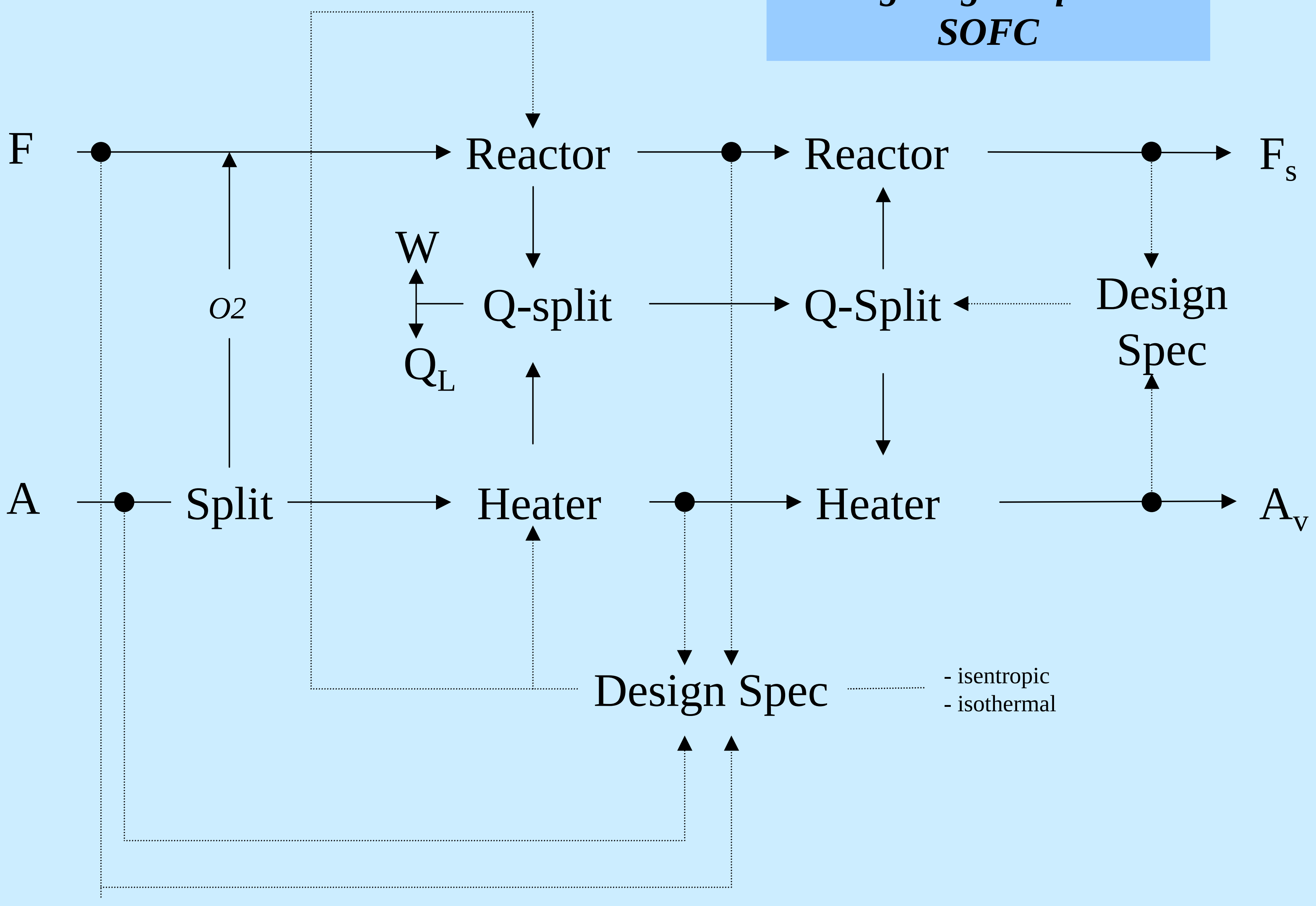
Design Stage Sequence

- *same models and physical properties packages*
- *executed once - after flowsheet convergence*
- *uses a Fortran Tear Variable for discretized calculations*

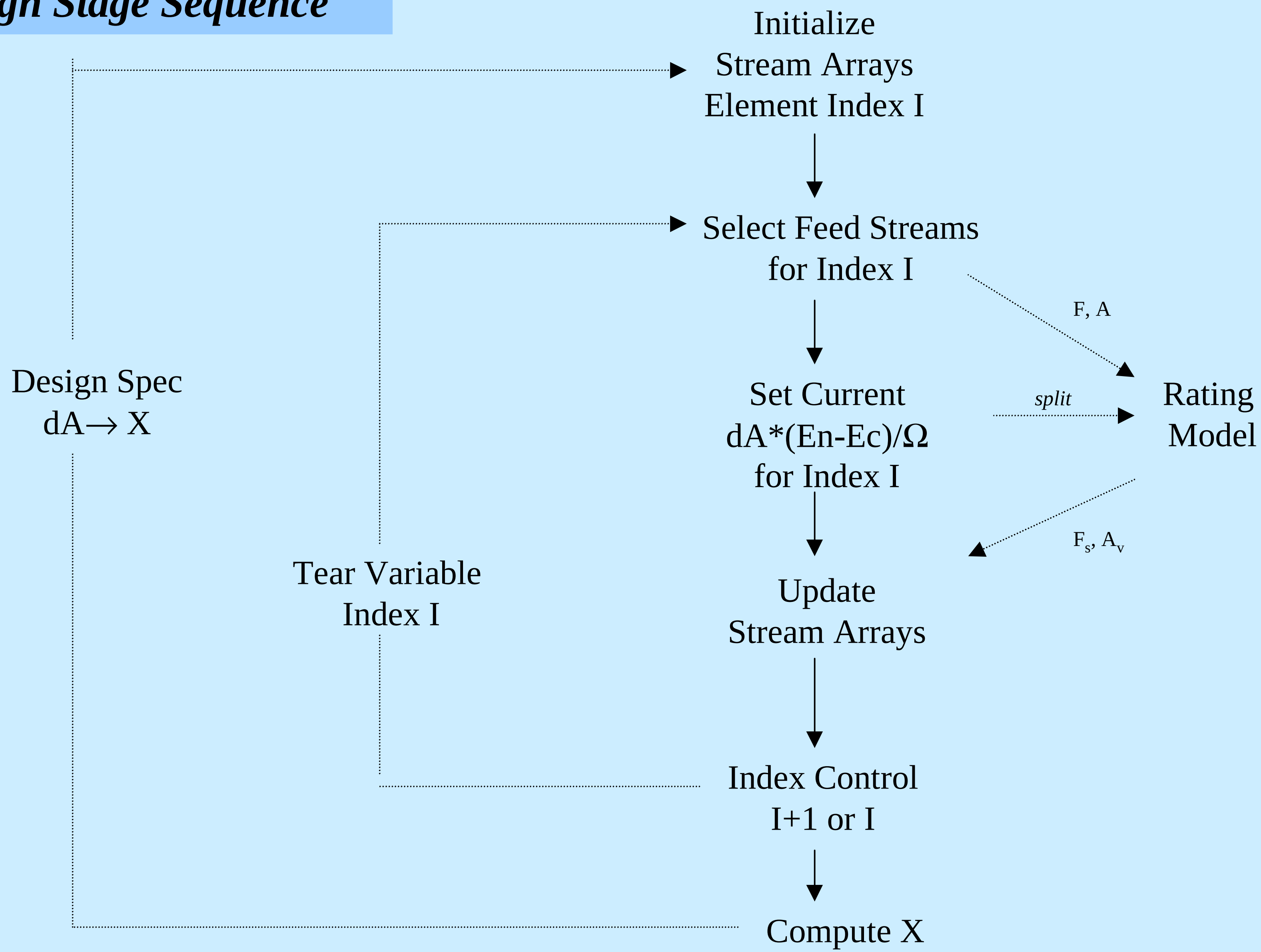
Important Features

- Reactant Manifolding
  - *coflow, crossflow, counterflow*
- Reaction Thermodynamics and Kinetics
  - *reforming, shifting, carbon formation*
- Temperature Effects
  - *ohmic resistances, electrode activation*
- Gas Diffusion Resistances
  - *anode, cathode*

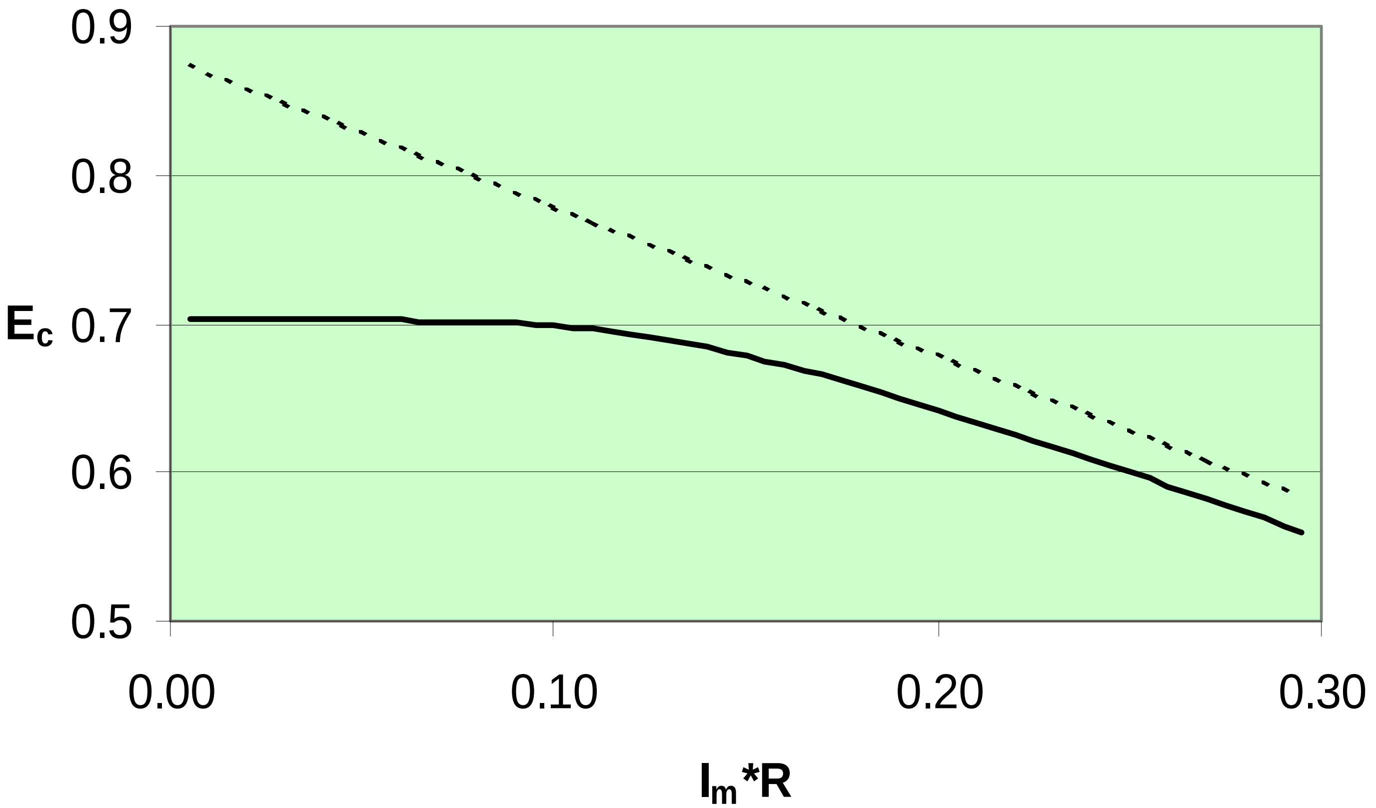
Rating Stage Sequence - SOFC



Design Stage Sequence

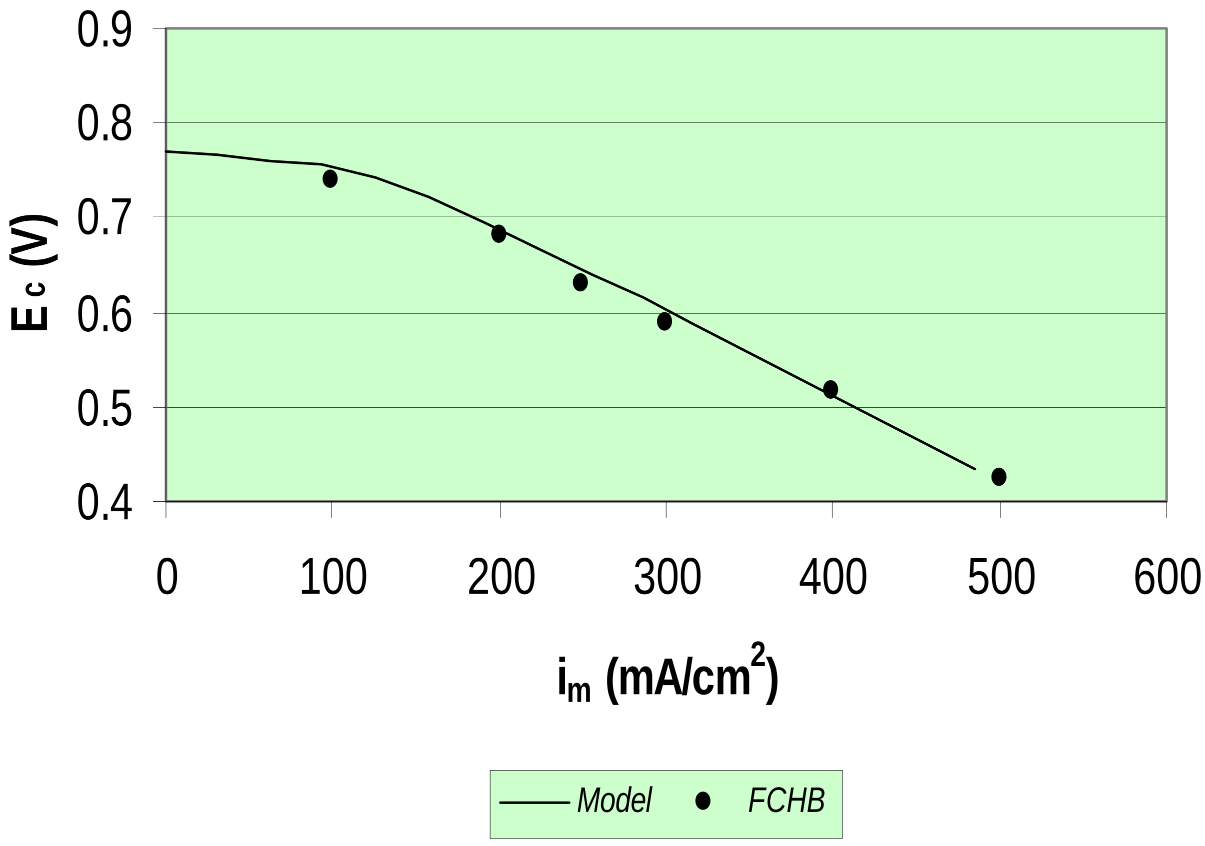


Predicted V-I Curve with High Nernst Potential Losses



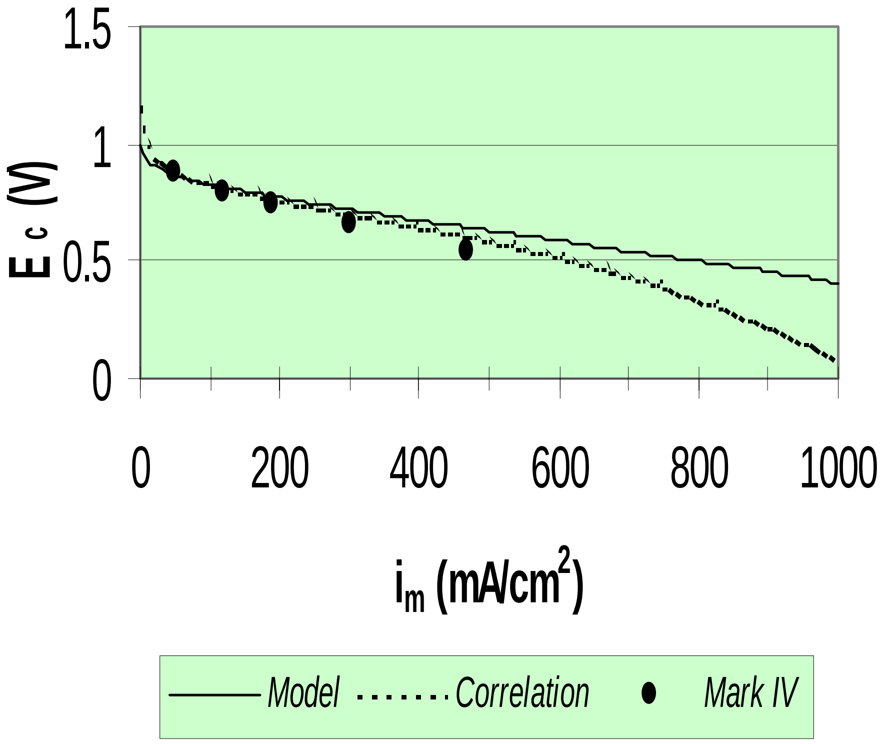
Co-flow SOFC @ 1000C/1ATM/Dry H2/2.5 AFR/95% Fuel Conversion.

Model vs SOFC Benchmark



SOFC Performance per FCHB, Fig. 5-11 at 1000C, 85% Fuel Utilization and 25% Air Utilization. Fuel (67% H2/22% CO/11% H2O).

Model vs PEMFC Benchmark



PEMFC Performance per Mark IV (Amphlett et al., 1995) for H2/ and Air at 70 C and 3 Atm.

SOFC Model Parameters

	PST (Kinoshita, 1988)	AES (Singhal, 1998)
cathode thickness, cm	0.07	0.22
anode thickness, cm	0.01	0.01
electrolyte thickness, cm	0.04	0.004
interconnect thickness, cm	0.04	0.0085
tube diameter, cm	1.27	2.2
interconnect chord length, cm	0.60	0.6 (estimated)

	Derived from Kinoshita, 1988	Reference @ 1000C (FCHB)
cathode, ohm-cm	Exp(-5.48+1210/(T+273.))	0.013
interconnect, ohm-cm	Exp(-4.51+4770/(T+273.))	0.5
anode, ohm-cm	Exp(-6.03-1100/(T+273.))	0.001
electrolyte, ohm-cm	Exp(-6.01+10510/(T+273.))	10

Computed Network Equivalent Cell Resistance @ 1000C

ohm-cm^2	0.92	0.6

PEMFC Model Parameters

Resistivities

apparent cell resistivity, ohm-cm^2	0.35	derived from Fig. 6-3, FCHB for 7 mil Nafion 117
ionic resistivity, ohm-cm^2	0.19	7 mil Nafion at .09 S/cm (Jacoby, 1999)
	---------	
apparent electronic resistivity, ohm-cm^2	0.16	

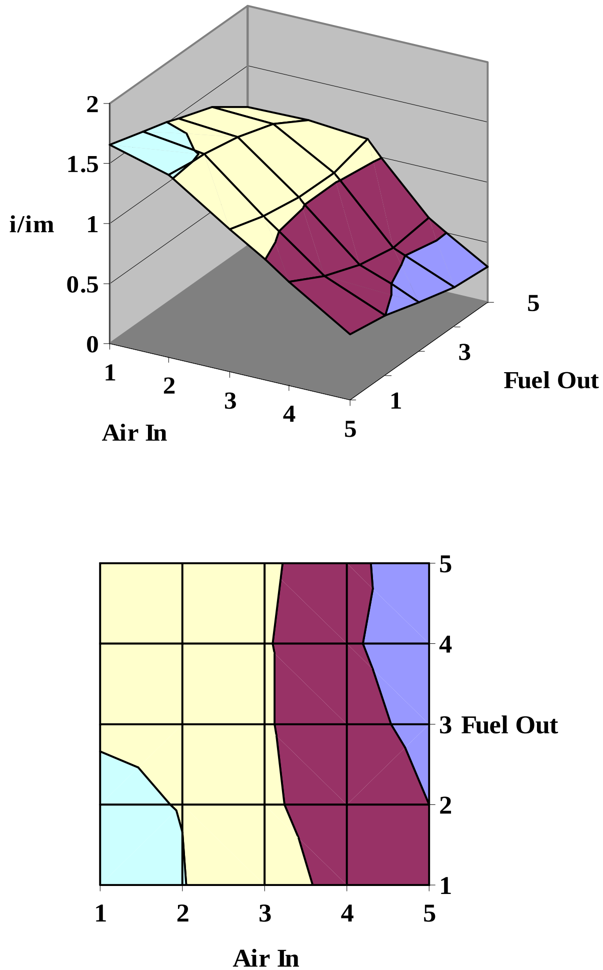
Activation

Tafel slope, volts/decade	0.07	Amphlett et al.,1995
apparent exchange current density, mA/cm^2	0.04	(.0037 @ .15 mg/cm^2 Pt/C, Fischer and Wendt, 1996)

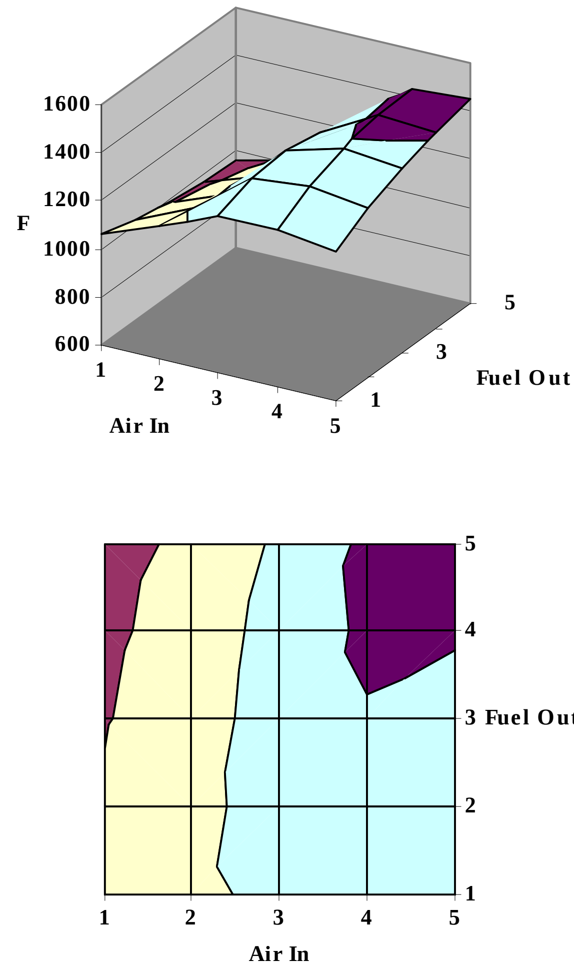
Diffusion

limiting current density, mA/cm^2	1100	estimated/arbitrary cutoff point

Hypothetical Crossflow MCFC with DIR to Equilibrium

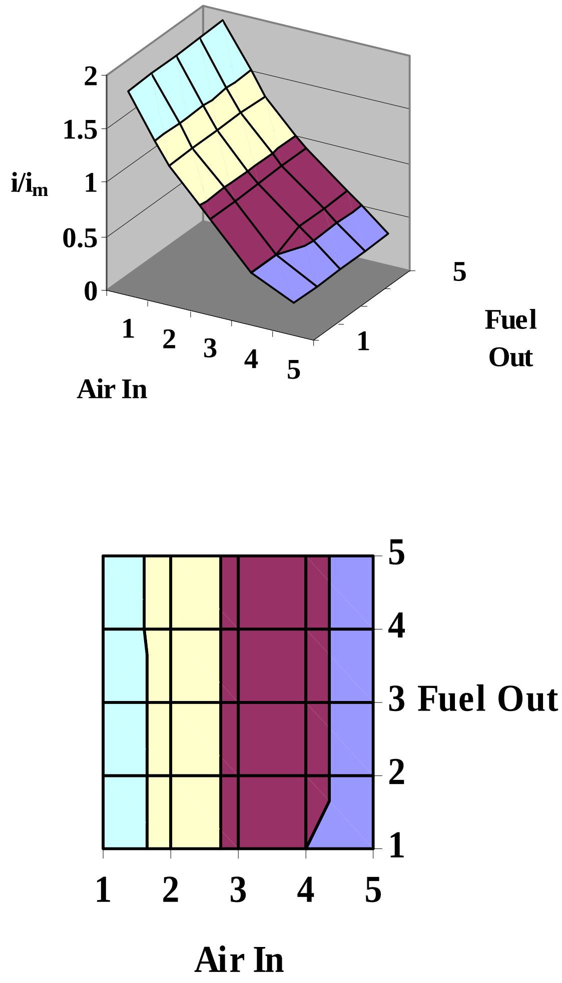


current density

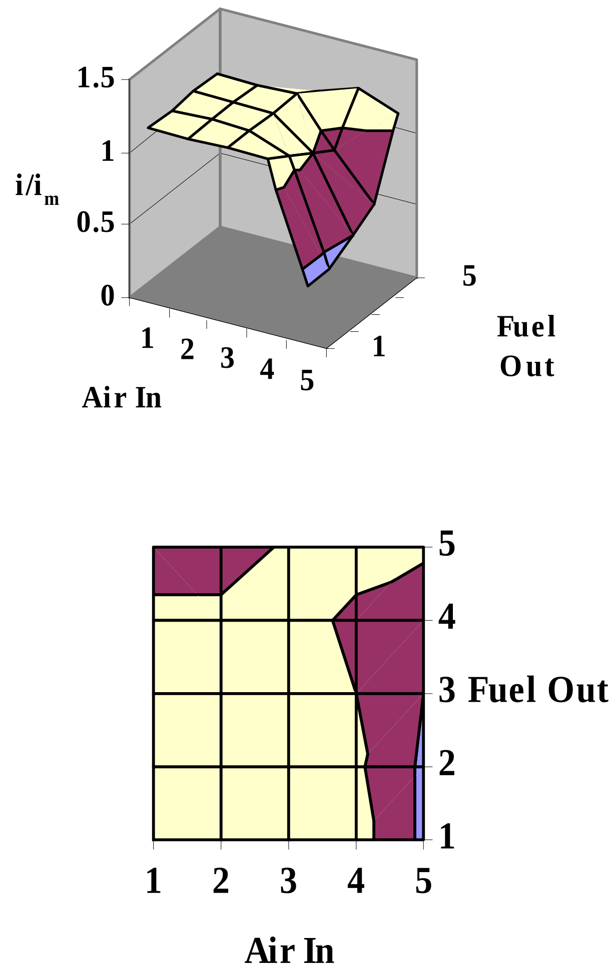


temperature

Hypothetical Crossflow SOFC without DIR

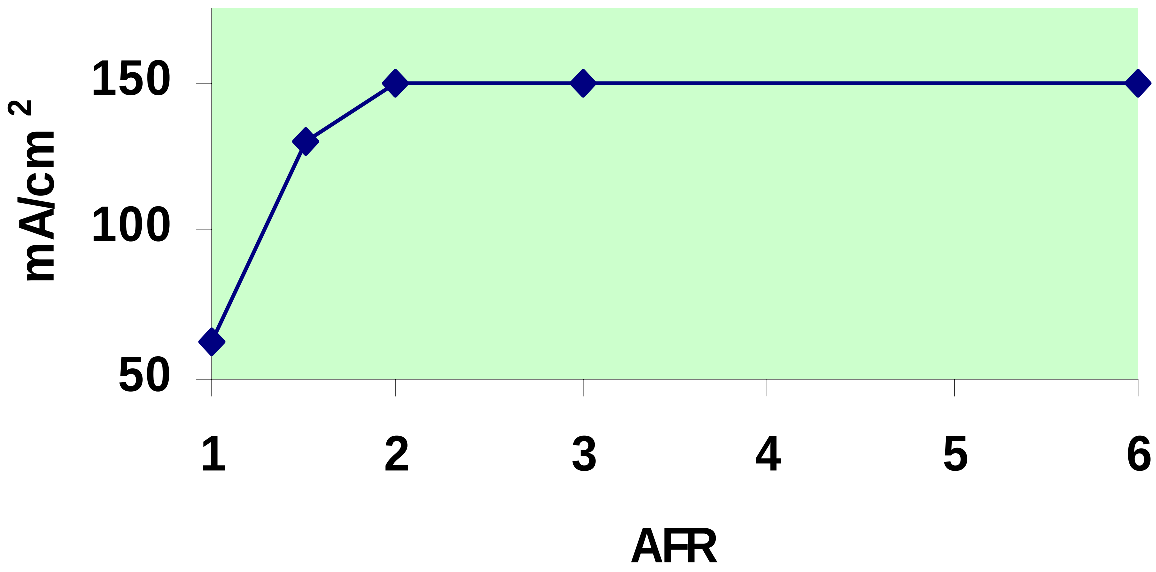


high AFR



low AFR

Assuming AFR is Independently Variable



Acknowledgements

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