"Dynamic Modeling of Fuel Cell Hybrid Systems"

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HYBRID SYSTEMS COMPONENT MODELS

DYNAMIC MODELS FOR A REFORMER, SOFC, AND GAS TURBINE

GENERAL MODEL ASSUMPTIONS

- 1D process flow
- Well-stirred at nodal level
- Slow pressure transients

FUEL CELL ASSUMPTIONS

- H_2 electrochemically oxidized only
- CO consumed via water-gas shift
- Shift always at equilibrium (constraint)
- Equipotential: $V_{cell} = V_{node\ 1} = V_{node\ n}$

HYBRID SYSTEMS COMPONENT MODELS

DYNAMIC MODEL BASIC EQUATIONS

Equation of State

$$C = \frac{P}{R_u T}$$

Mass Conservation Equations

$$V\frac{dC_j}{dt} = \dot{N}_{in,j} - \dot{N}_j + r_j$$

$$VC\frac{d\mathbf{?}}{dt} = \dot{N}_{in}\left(\mathbf{?}_{in} - \mathbf{?}\right) - \mathbf{?}\sum r_j + \mathbf{R}$$

- **Calculates changes in mole fraction based on inlet molar flows and reaction rates**

HYBRID SYSTEMS COMPONENT MODELS

DYNAMIC MODEL BASIC EQUATIONS

Energy Conservation

- **Gaseous**

Molar Flow Through Electrolyte (Fuel Cell Only)

$$\frac{d}{dt}\left(CC_{v,molar}T\right)=\left(\dot{N}h\right)_{in}-\dot{N}h+\overbrace{\left(\dot{N}h\right)_{solid\rightarrow gas}}$$

$$+\left(\text{heat transfer}\right)+\left(\text{heat of reaction}\right)$$

- **Solid**

Molar Flow Through Electrolyte (Fuel Cell Only)

$$\frac{d}{dt}\left(rC_{mass}T\right)=\overbrace{\left(\dot{N}h\right)_{gas1\rightarrow solid}-\left(\dot{N}h\right)_{solid\rightarrow gas2}}$$

$$+\left(\text{heat transfer}\right)+\left(\text{heat of reaction}\right)$$

HYBRID SYSTEMS COMPONENT MODELS

STEAM REFORMATION – IN REFORMER AND FUEL CELLS

Methane reformation reaction

$$CH_4 + H_2O \xrightarrow{\text{reform}} 3H_2 + CO$$

- **Reaction rates on nickel based catalysts:**

Lee et al. (1990) and Ross et al. (1972)

$$r_{CH_4} = -kP_{CH_4}^{m} P_{H_2O}^{n}$$

From Stoichiometry…

$$r_{CO} = -r_{CH_4}$$

$$r_{H_2} = -3r_{CH_4}$$

$$r_{H_2O} = r_{CH_4}$$

HYBRID SYSTEMS COMPONENT MODELS

REFORMATE: WATER GAS SHIFT

Shift reaction

$$\mathrm{CO} + \mathrm{H_2O} \xleftrightarrow{\text{shift}} \mathrm{CO_2} + \mathrm{H_2}$$

- **Reaction proceeds fast enough at elevated temperatures to assume equilibrium**
- **Algebraic constraint at exit of each node**

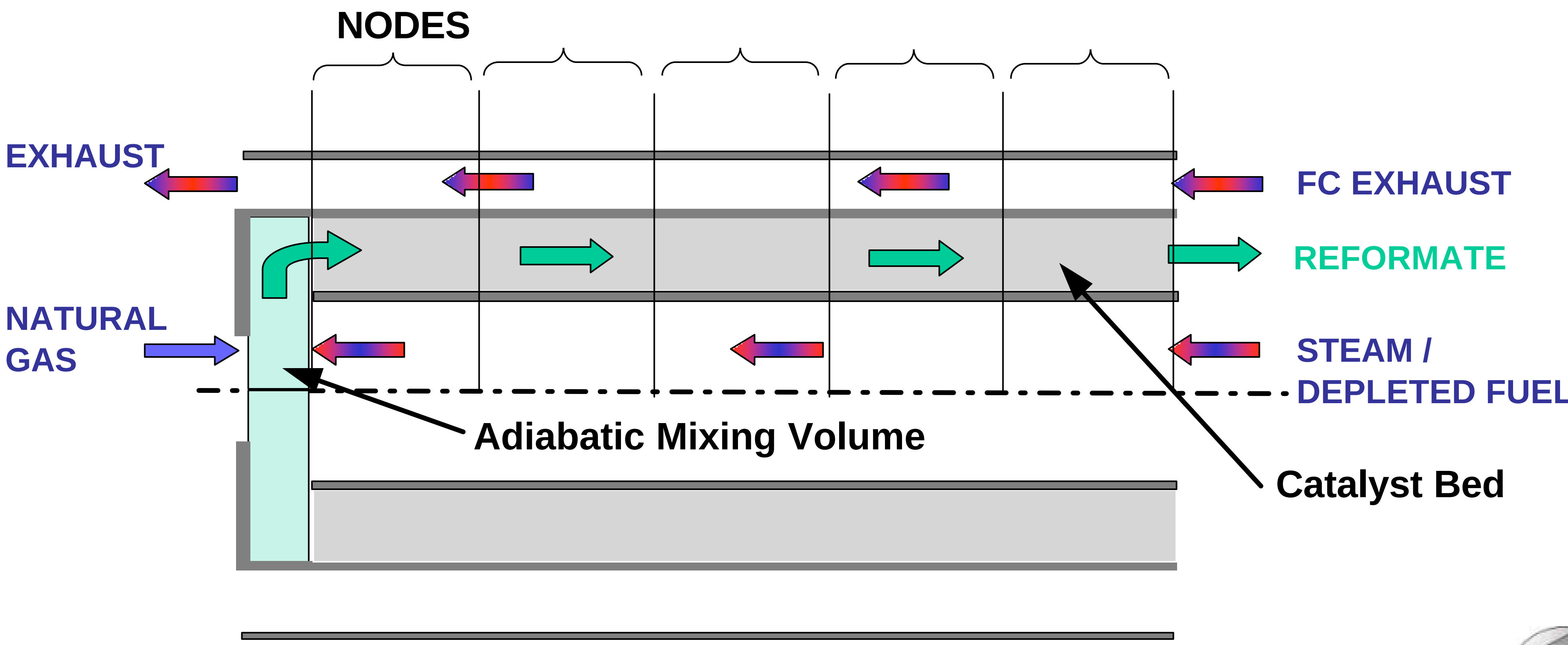
Provides the non-electrochemical reaction source for CO_2!

$$K(T) = \frac{c_{CO_2} c_{H_2}}{c_{CO} c_{H_2O}}$$

REFORMER MODEL

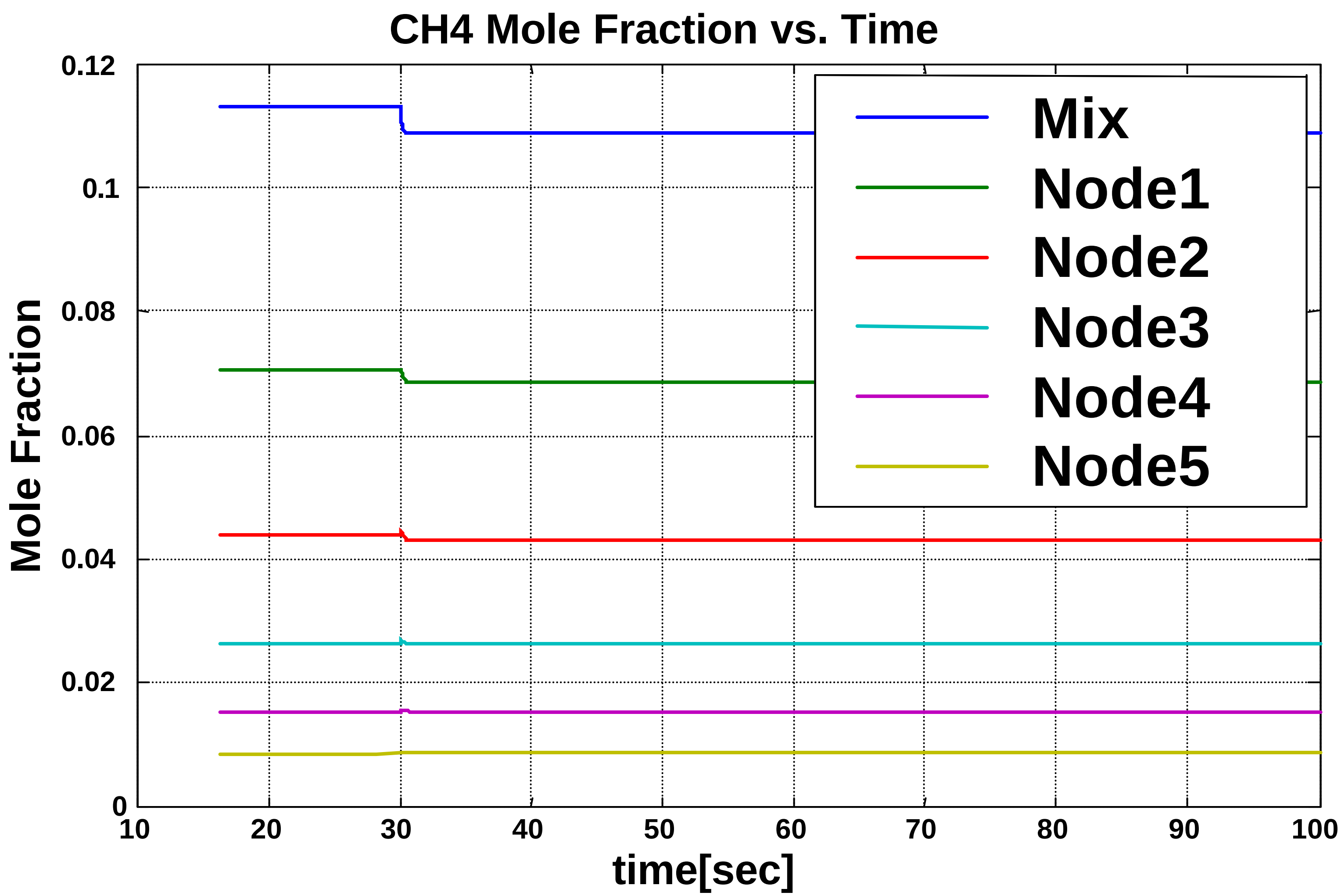
REFORMER

- 5 node model
- Concentric cans
- Heat from exhaust gas heat exchange



REFORMER MODEL

REFORMER SAMPLE OUTPUT: 5% INCREASE IN RECIRCULATION OF DEPLETED FUEL



FUEL CELL MODEL(S)

FUEL CELL OPERATION

Actual operating voltage

$$V = E - h_A - h_C - h_R$$

- **Polarization losses are due to kinetics, mass transport and electrical resistances**

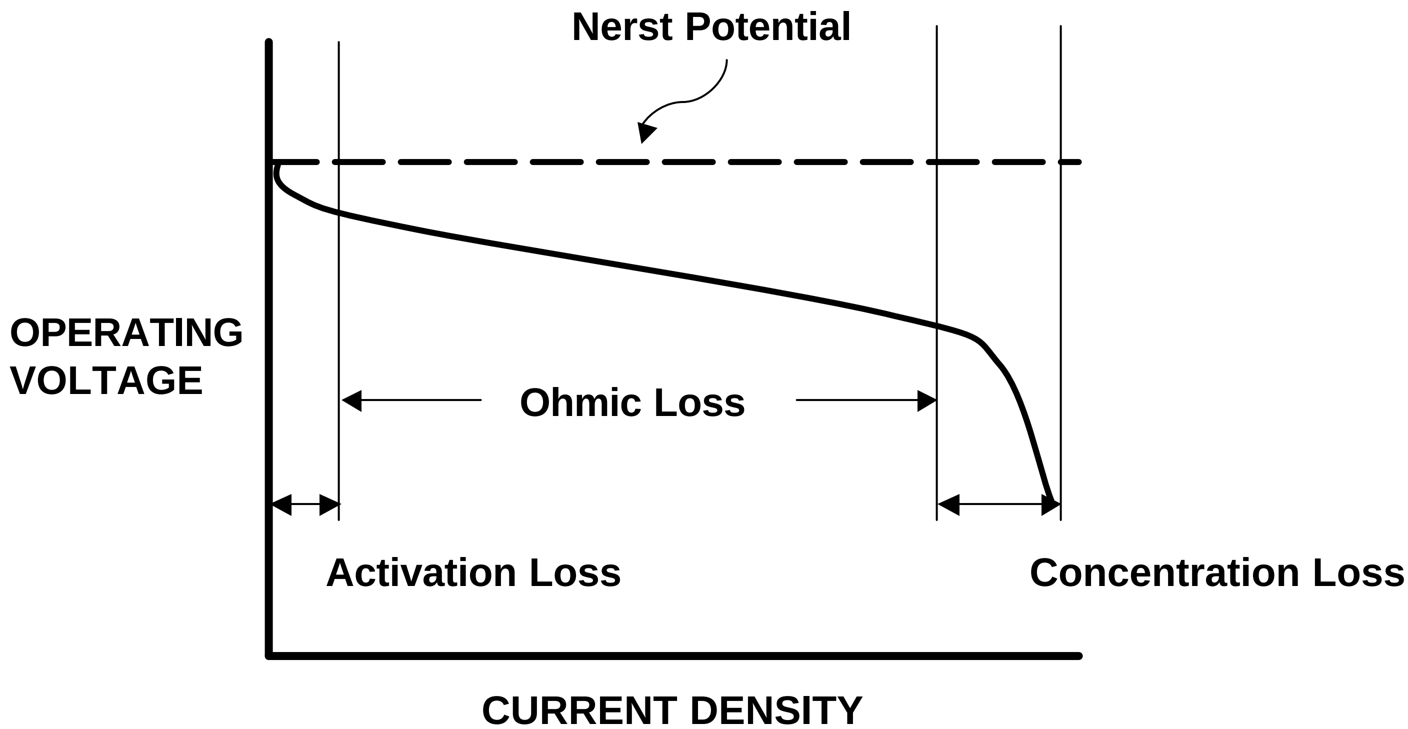
$$h_A = \frac{R_u T}{anF} \ln\left(\frac{i_{node}}{i_0}\right)$$

$$h_C = -\frac{R_u T}{nF} \ln\left(1 - \frac{i}{i_L}\right)$$

$$h_R = iR$$

FUEL CELL MODEL(S)

FUEL CELL OPERATION



Actual operating voltage characteristic

FUEL CELL MODEL(S)

SOLID OXIDE FUEL CELL ELECTROCHEMISTRY

Cell Reactions

$$H_2 + O^{2-} \xrightarrow{anode} H_2O + 2e^-$$

$$\tfrac{1}{2} O_2 + 2e^- \xrightarrow{cathode} O^{2-}$$

Nerst Potential

$$E = E_0 + \frac{R_u T}{2F} \ln\left(\frac{c_{H_2} c_{O_2}^{1/2}}{c_{H_2O}} P_{CATHODE}^{1/2} \right)$$

- **Ideal operating voltage with respect to partial pressures of cell reactants**

FUEL CELL MODEL(S)

HEAT TRANSFER

Conduction

- Axially from node to node through solids

Convection

- From surface to gas
- Based on Nusselt number

Radiation

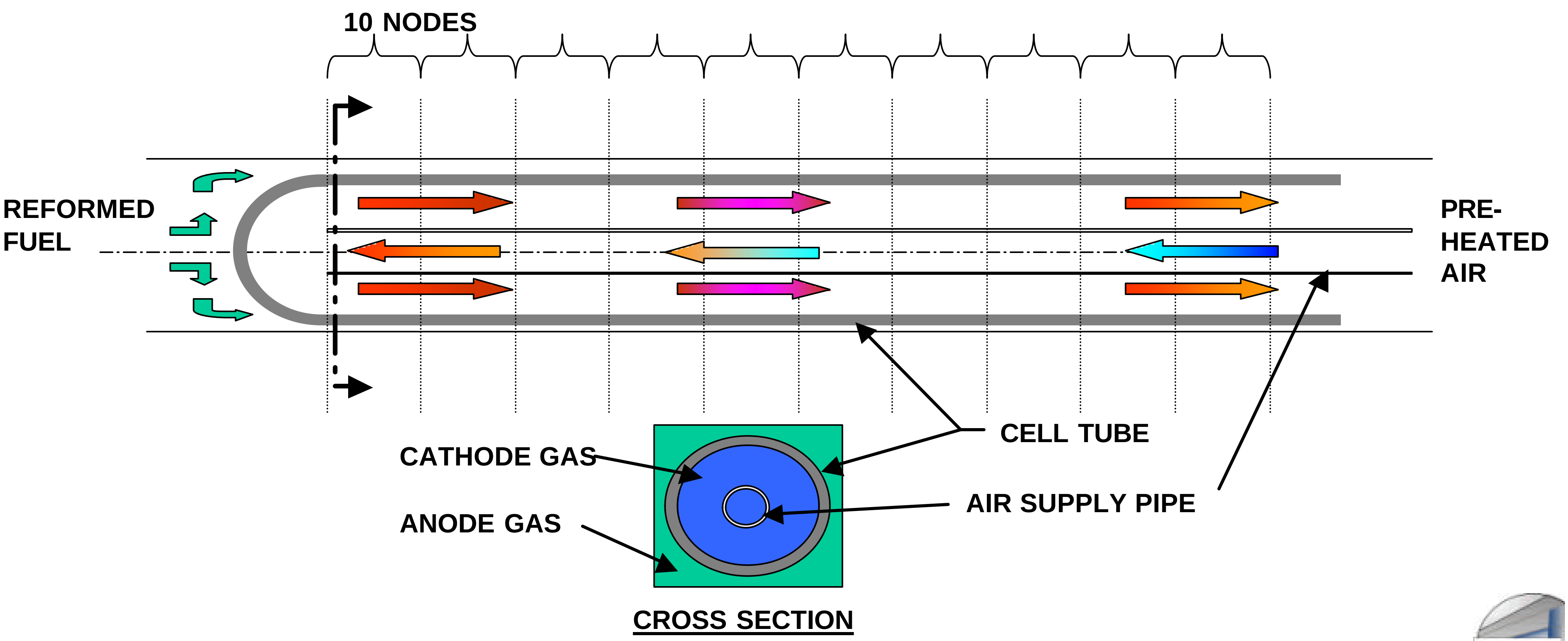
- From surface to surface
- Geometry is an issue
  - Concentric cylinders: TSOFC
  - Parallel planes: PSOFC

FUEL CELL MODEL(S)

TUBULAR (TSOFC) FUEL CELL DISCRETIZATION

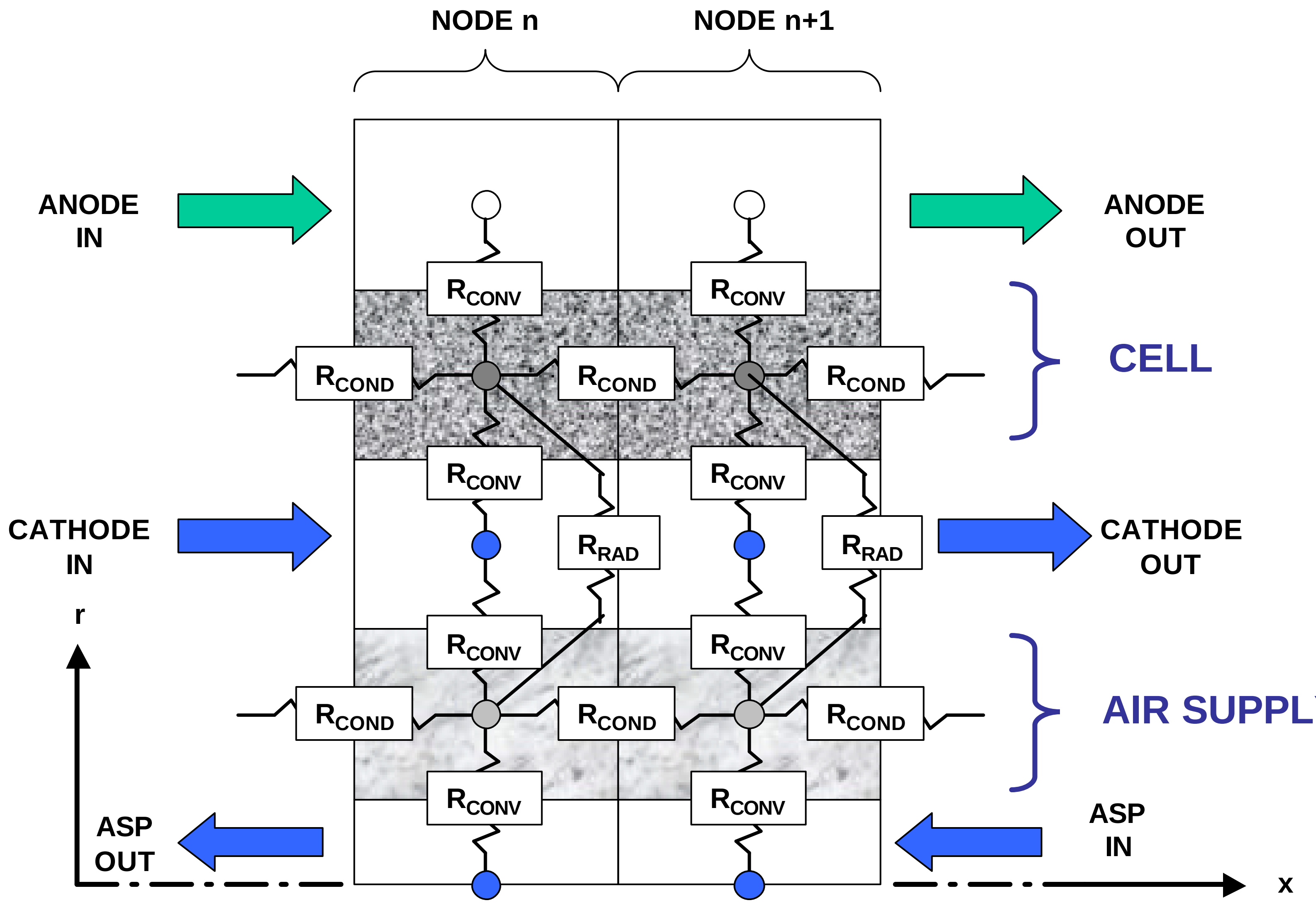
10 Discrete Computational Nodes

- Anode Gas
- Cathode Gas
- Cell Solid
- Air Supply Pipe Solid
- Air Supply Gas



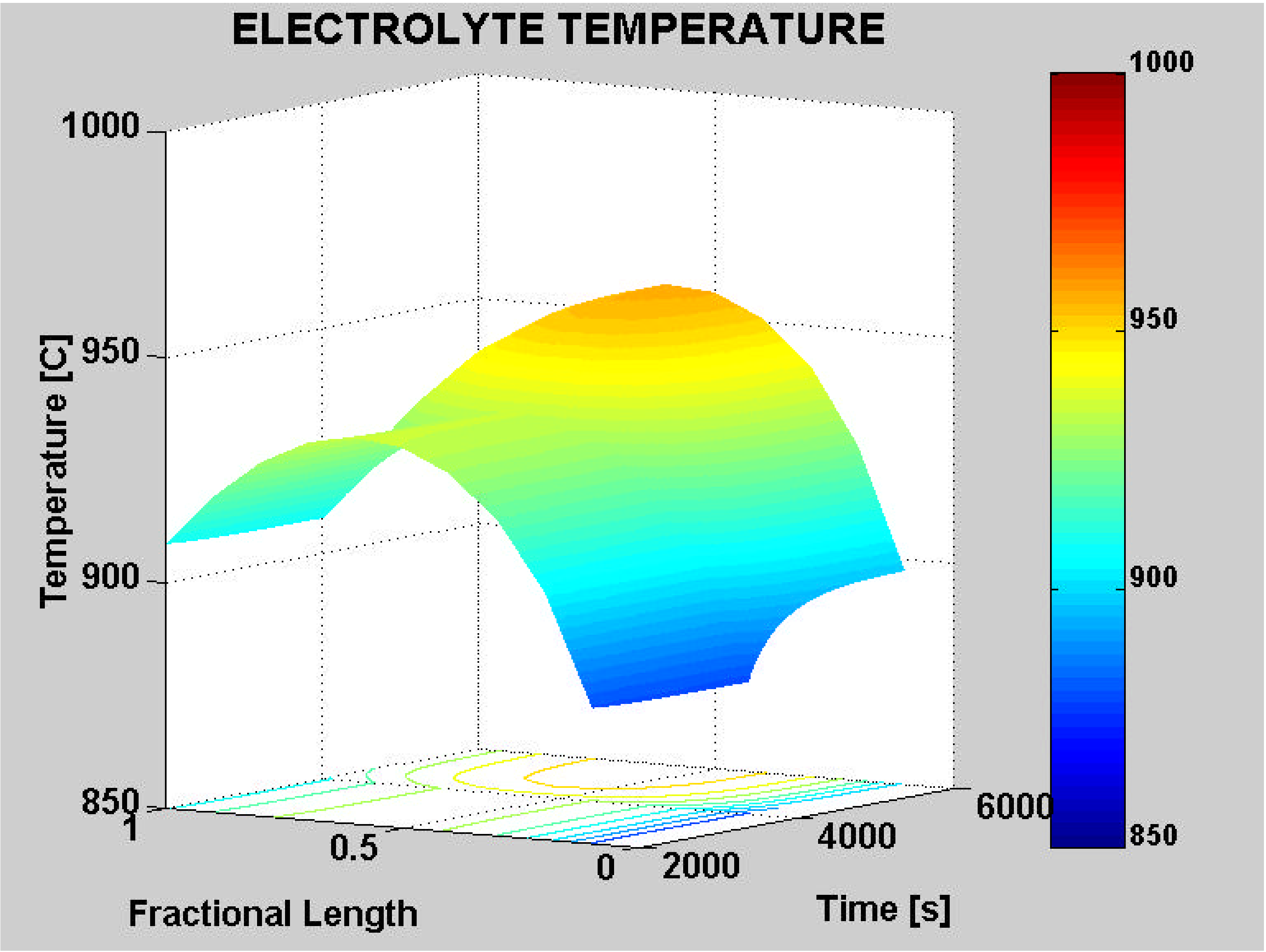
FUEL CELL MODEL(S)

TSOFC NODAL FUEL CELL HEAT TRANSFER RESISTANCES



FUEL CELL MODEL(S)

SAMPLE TSOFC OUTPUTS: 10% LOAD INCREASE



FUEL CELL MODEL(S)

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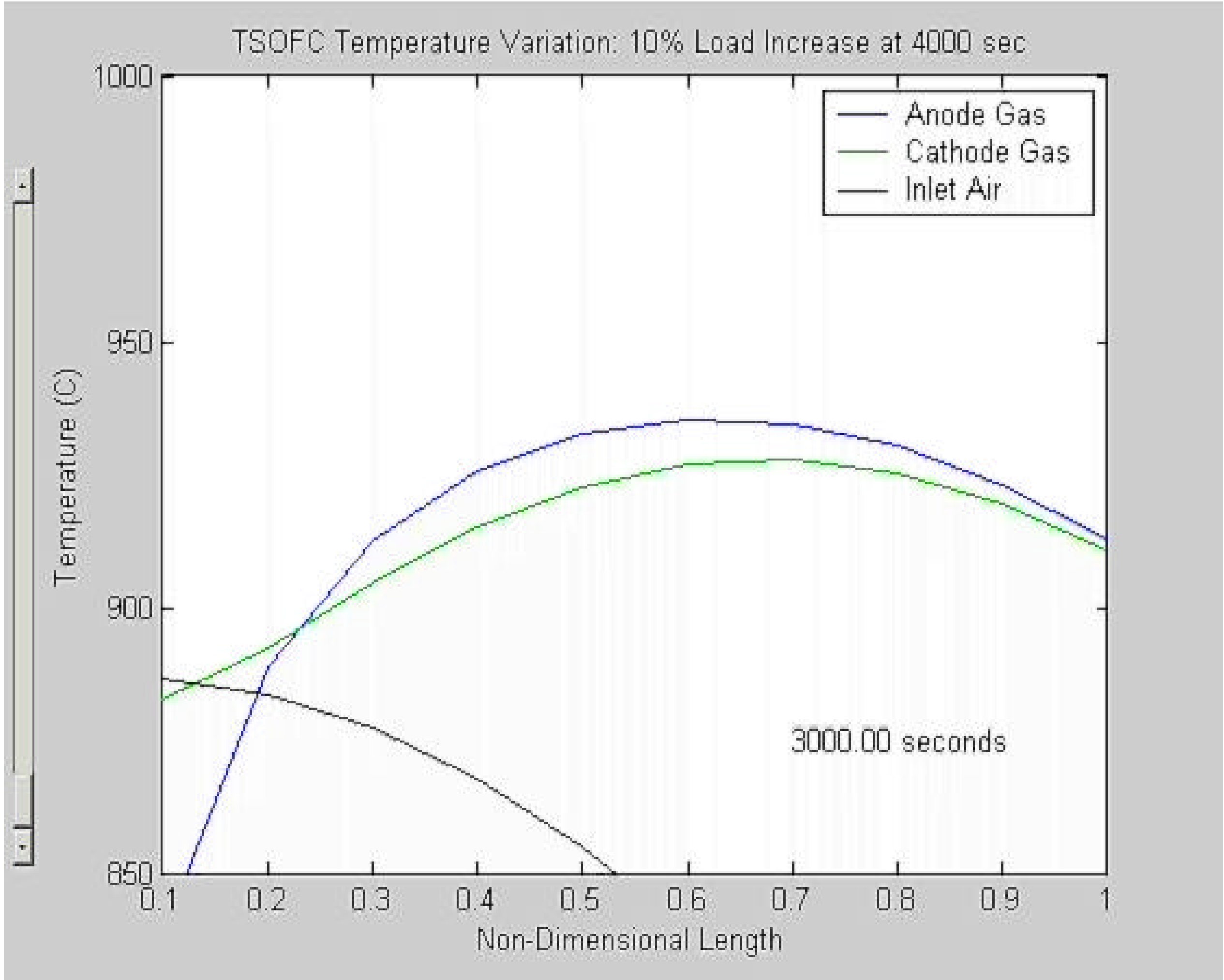
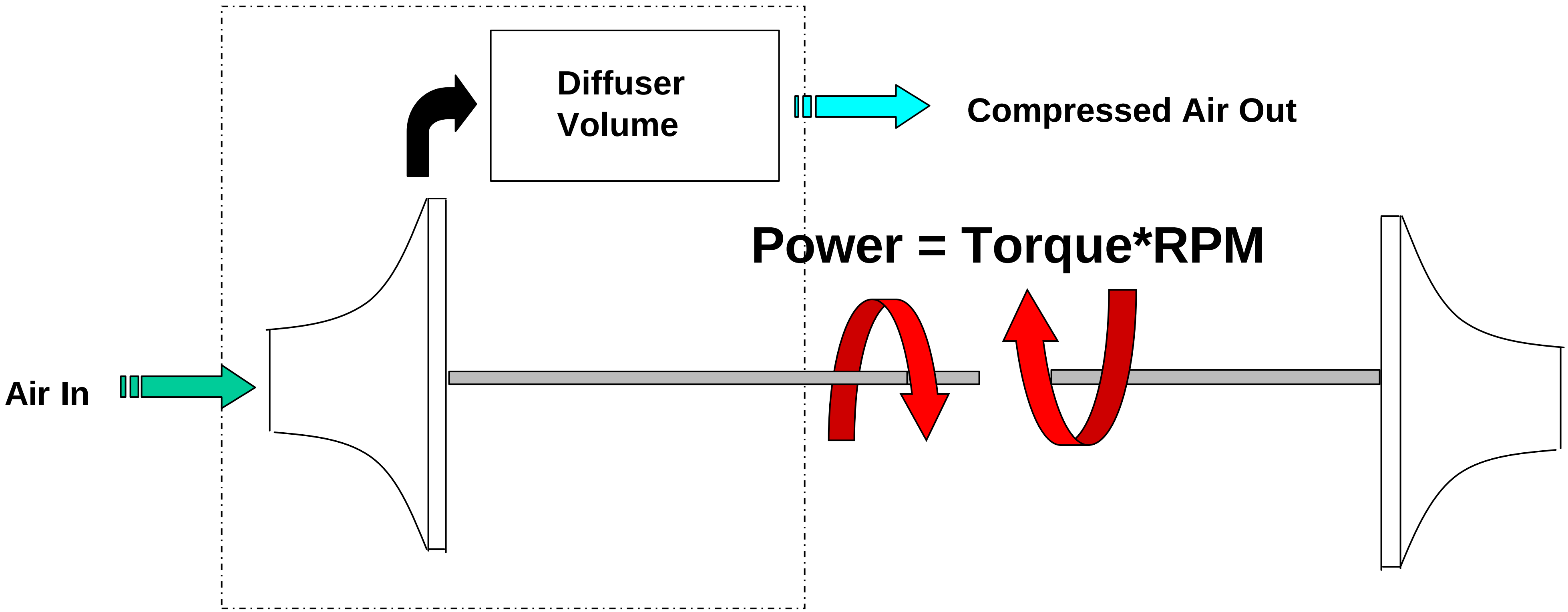


GAS TURBINE MODEL

COMPRESSOR

- **Lumped Parameter**
  - **Incompressible Compressor**
  - **Compressible representative diffuser volume**

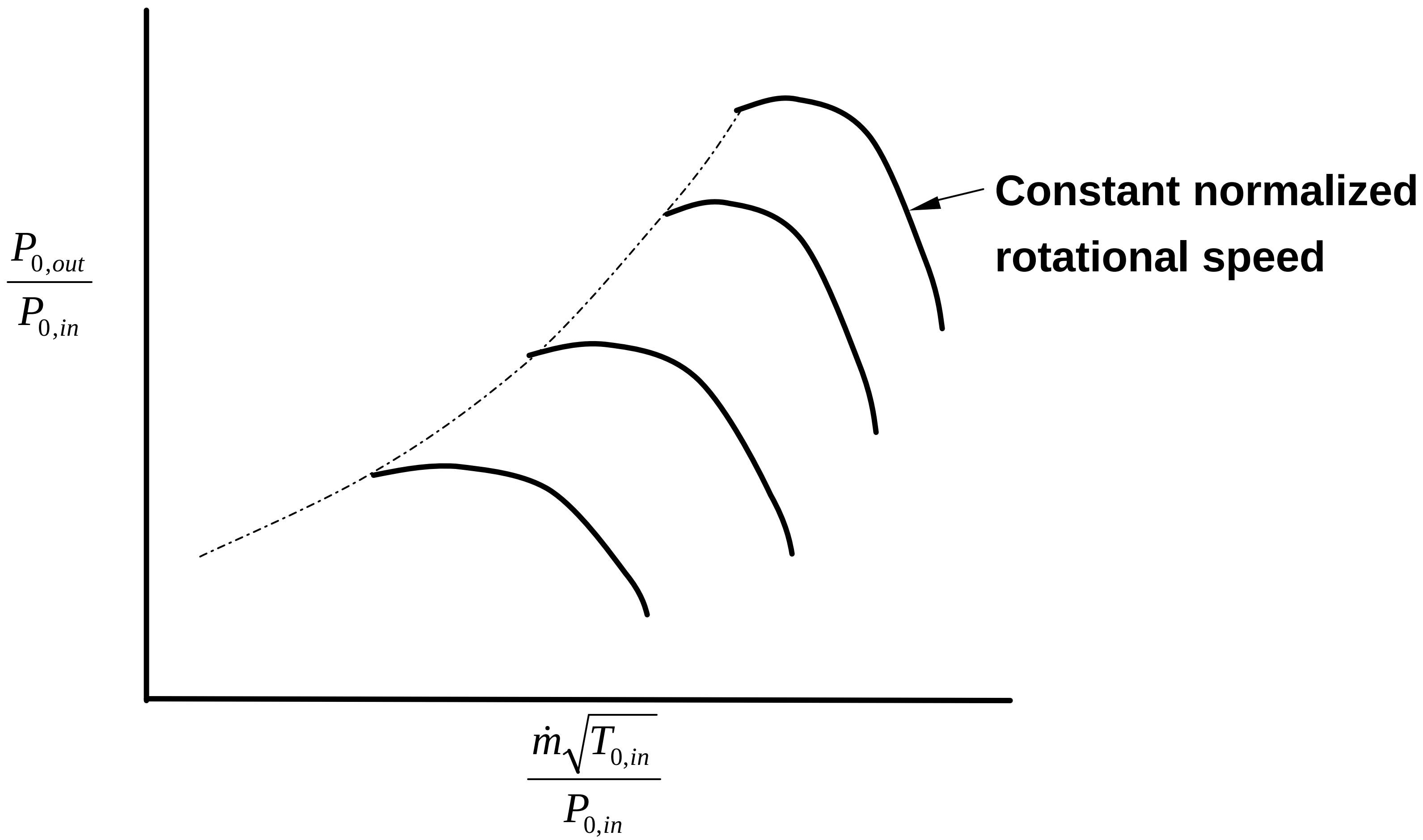


Compressor Control Volume

GAS TURBINE MODEL

COMPRESSOR MAPS

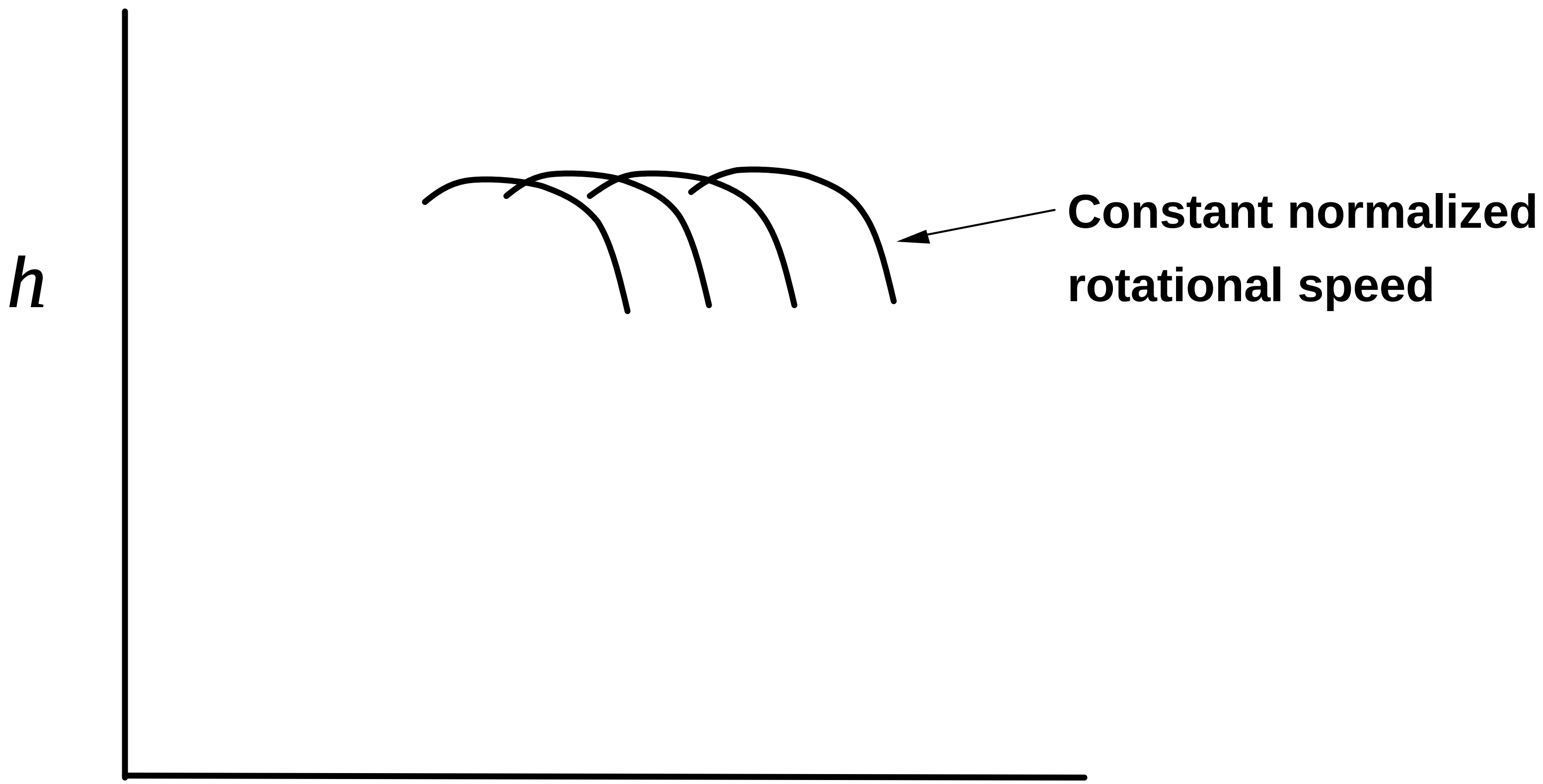
- **Total pressure ratio vs. normalized mass flow**



GAS TURBINE MODEL

COMPRESSOR MAPS

- Isentropic efficiency vs. normalized mass flow



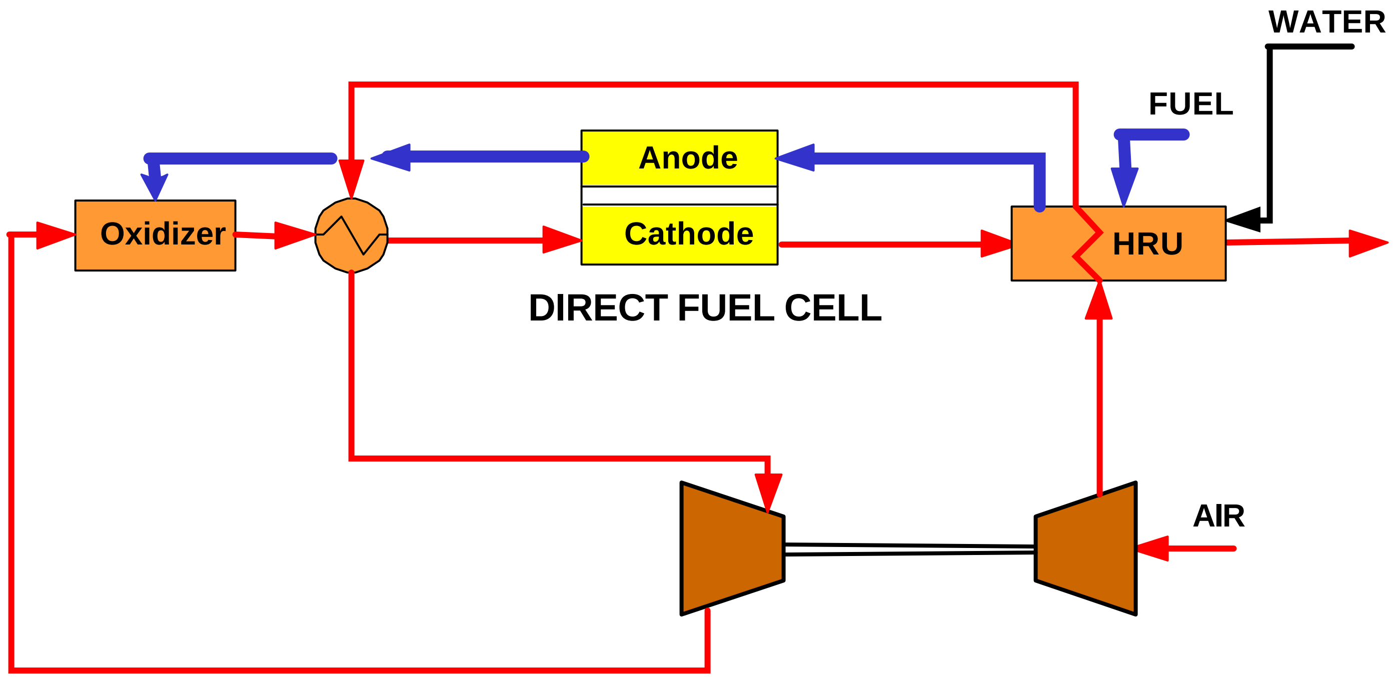
$$\frac{\dot{m}\sqrt{T_{0,in}}}{P_{0,in}}$$

HYBRID SIMULATION

Dynamic Modeling Tools – Example Results - MCFC

FCE Direct FuelCell™ / Gas Turbine Hybrid System

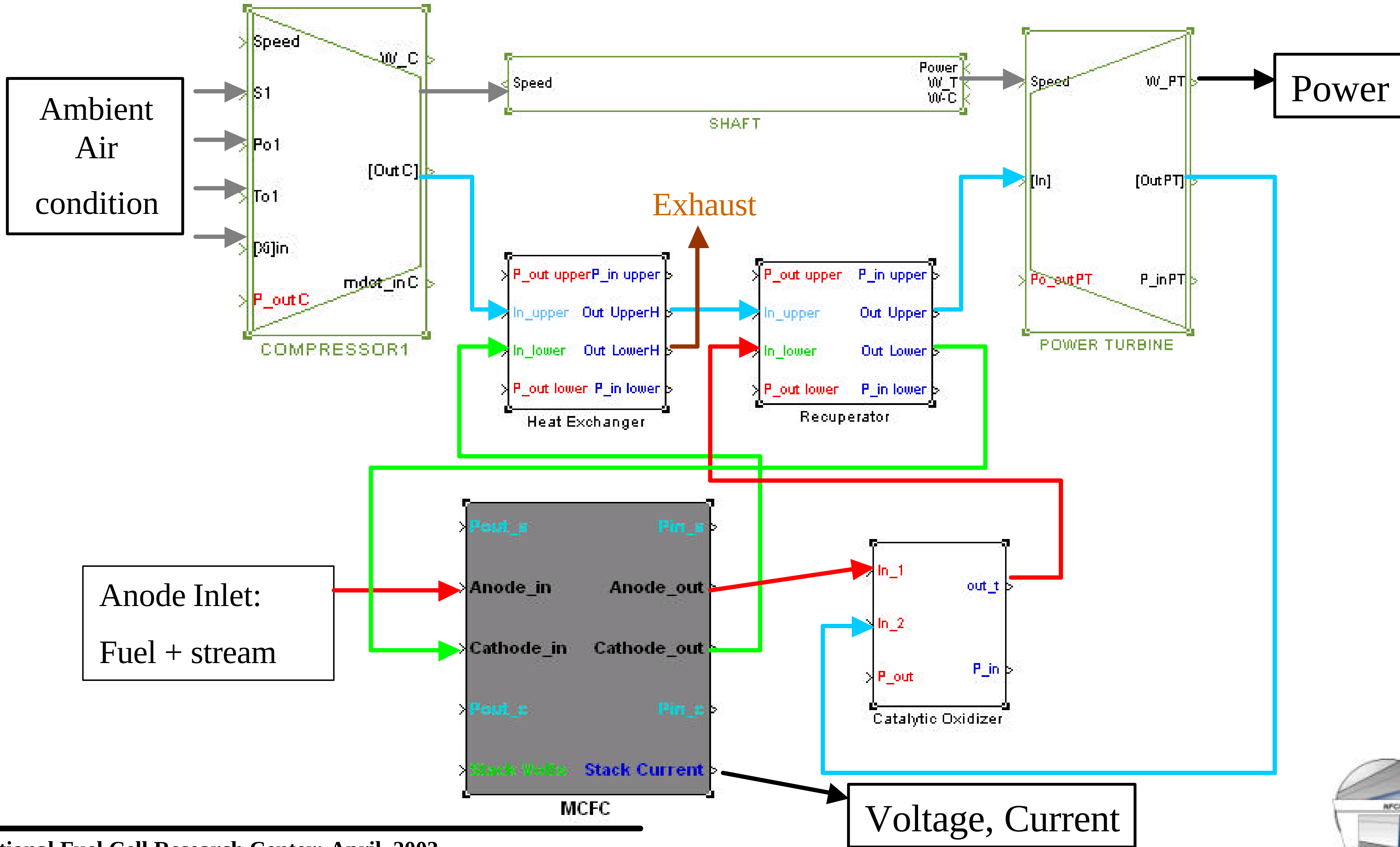
Compressed Air is Heated with Fuel Cell Waste Heat, Expanded, and then Used as the Fuel Cell Oxidant



- ***Efficiencies of ~ 75% are possible***
- ***Potential to Significantly Lower $/kW Cost***

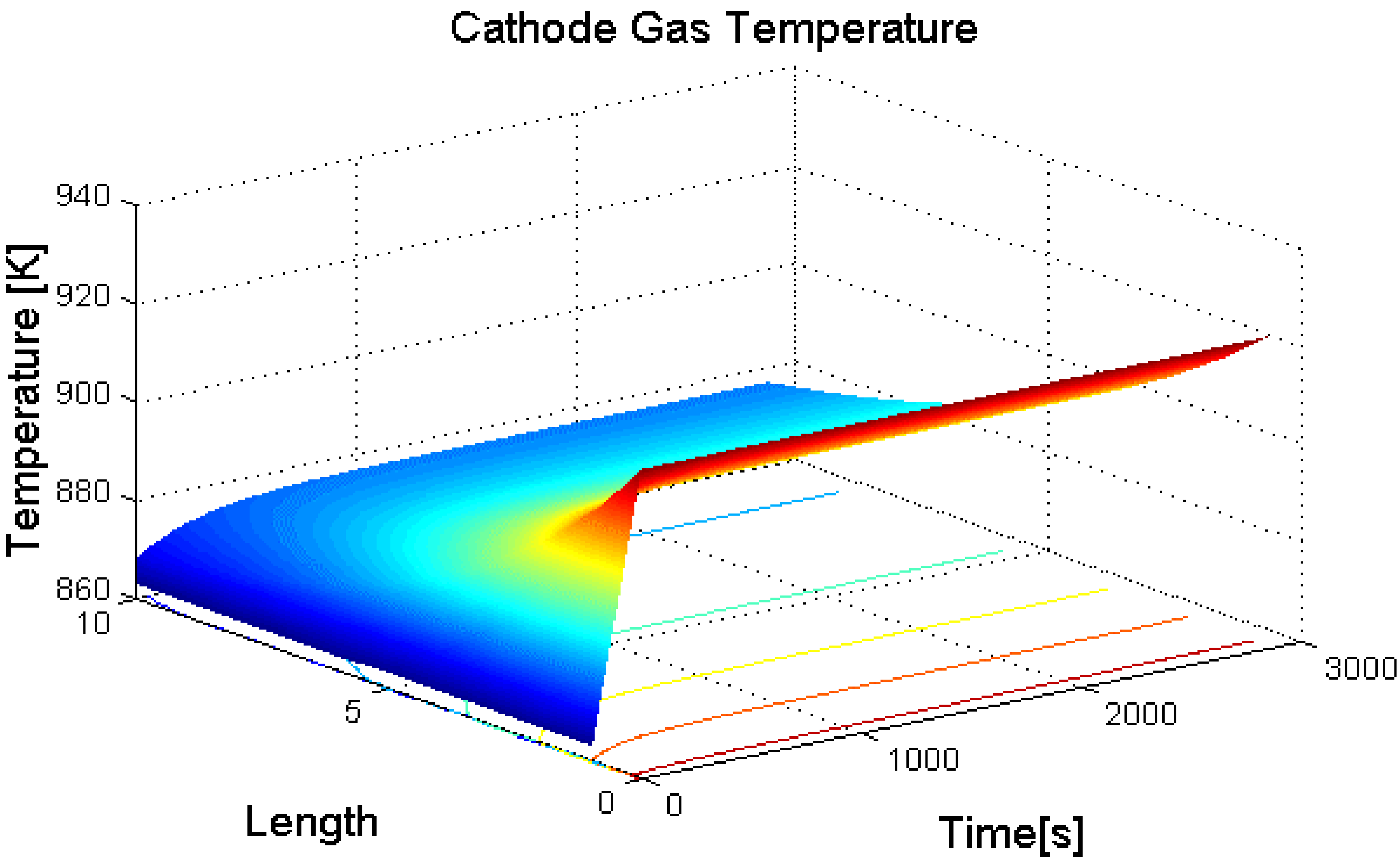
HYBRID SIMULATION

MCFC Hybrid Implementation



HYBRID SIMULATION

Sample MCFC Hybrid Results



DATA AND VALIDATION

SINGLE CELL MCFC MODULE