Expedited Real Time Processing for the NETL Hyper Cyber-Physical System (FE0030600)

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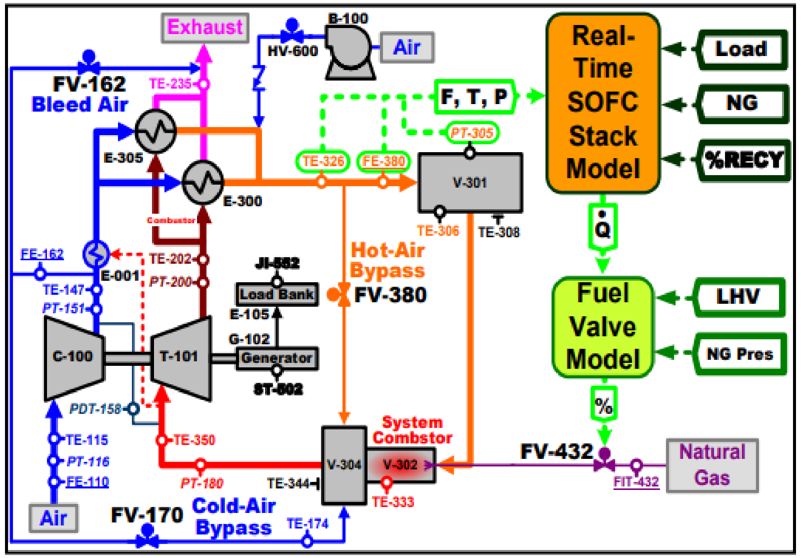
Cyberphysical Systems and Fuel Cells Research

- The National Energy Technology Laboratory houses the Hyper cyberphysical solid oxide fuel cell/gas turbine system
- Research on the system allows for the development of efficient power systems and control strategies for such systems
- The solid oxide fuel cell stack in the system is a computational model that allows for rigorous testing of the system and definition of design spaces without damaging real, expensive fuel cells



Project Objectives

- Provide the National Energy Technology Laboratory’s Hybrid Performance (Hyper) Facility the needed numerical methods algorithm(s), software development and implementation support to enact real time cyber-physical systems (CPSs) that simulate process dynamics on the order of five milliseconds or smaller

- The proposed paths forward comprise three distinct approaches to hasten transient simulations (each of these three classes were proposed independently as options for improvement, yet in some cases one class of approach may complement another):
  1. Implementing alternatives to the presently employed explicit-implicit blended finite difference (spatio-temporal) approach
  2. Introducing an “informed” processing approach wherein *a priori* computations expedite real time attempts
  3. Optimizing key parameters within the facility’s present real time processing scheme

Two Thermal Modeling Subtopics in this Project

1. Real-time adaptive meshing for computational solid oxide fuel cell models in cyberphysical systems for enhanced accuracy at reduced computational burden

   (GRA: Alana Homa)

2. Computationally designing and testing thermally robust solid oxide fuel cells and observing their thermal transient implications

   (GRA: Gared Colton)

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Real-time adaptive meshing for computational solid oxide fuel cell models in cyberphysical systems for enhanced accuracy at reduced computational burden

Fuel Cell Model Characteristics

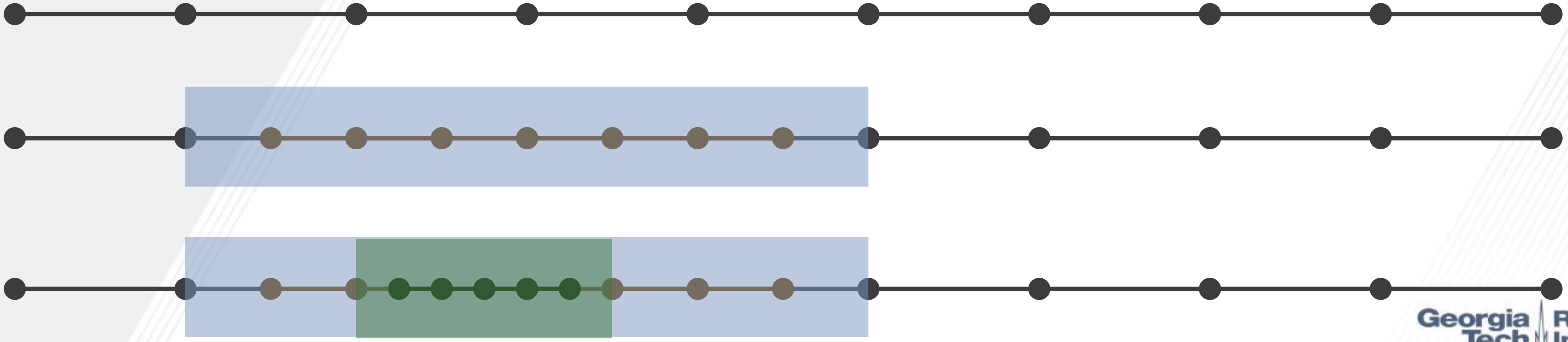
- Desire to reduce sampling time for cyber-physical components requires matching reductions in computation time for SOFC model
  - <5-10 ms target
- Smaller computational windows means reducing resolution, potentially leading to:
  - Greater error in bulk outputs

Adaptive Meshing

- Actively changing the problem discretization in response to a developing solution, allows for more strategic allocation of limited computational resources
- Many well-developed mathematical methods for 1D cases
    - For real-time application, need to identify algorithms that can operate reliably within strict time limits
    - Trade-off between mesh quality and computational speed

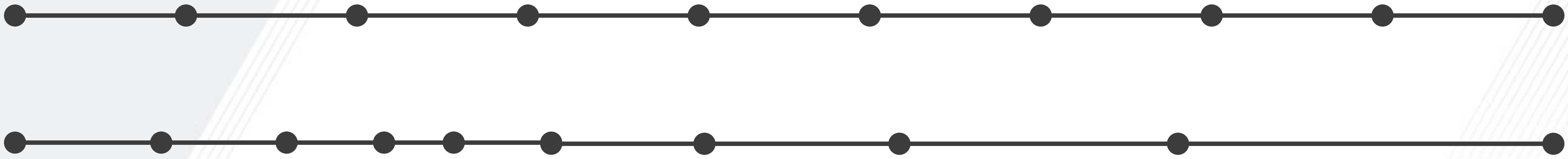
h-Methods

- Structured local refinement, done in layers
- Change total number of nodes
  - Need for nested data structures – not compatible with our code
  - Greater change in computation time – not ideal for Hyper



r-Methods

- “Relocation” methods
- Keep same number of nodes, concentrating more densely in needed areas
    - More consistent calculation times, more varying slice sizes – preferable for a real-time application



Evaluation Criteria

- "Heat Imbalance Percentage" - $\left|\frac{Q_{gen}-Q_{dissipation}}{Q_{gen}}\right|$
  - Decreases towards 0 with higher uniform resolution (at steady state conditions)
- Comparison with uniform, higher-resolution results
  - Total heat generation
  - Internal profiles, transient + steady state
    - Solid/gas temperatures
    - Current density
    - Fuel composition
    - Potential losses

Rediscretization Algorithm

- Based on de Boor’s algorithm error equidistribution

$$\int_{x_j^n}^{x_{j+1}^n} M\big(f(x,t^n)\big)dx = \frac{1}{m}\int_{x_1^n}^{x_{m+1}^n} M\big(f(x,t^n)\big)dx$$

- M(f(x,t)) – monitor function, used as a representation of the error
    - Algorithm works by allocating a greater density of nodes where the value of M is higher and vice versa
    - In practice, because f will not be a continuous function but a collection of distinct values at each node, interpolation and numerical integration is required

Monitor Function

- Selection of appropriate monitor function M is key
- One approximation, in absence of rigorous error calculation, is scaled arc length, based on local gradient:

$$M(f(x,t)) = \sqrt{1 + \alpha^2 \left(\frac{\partial f}{\partial x}\right)^2}$$

- α scales how closely solution is based on gradient, to ensure sufficient remaining nodes in areas of flat gradients
- SOFC model is not a single variable f – it is a combination of many tracked variable such as solid temperature, gas temperature, current, voltage, fuel stream composition, etc.

Selection of Monitor Function

$$M_s = \sqrt{1 + \alpha^2 \left(\frac{\partial T_s}{\partial x}\right)^2}$$

$$M_G = \sqrt{1 + \alpha^2 \left(\frac{\partial T_G}{\partial x}\right)^2}$$

$$M = kM_S + (1 - k)M_G$$

Goal: Improve accuracy via appropriate monitor function

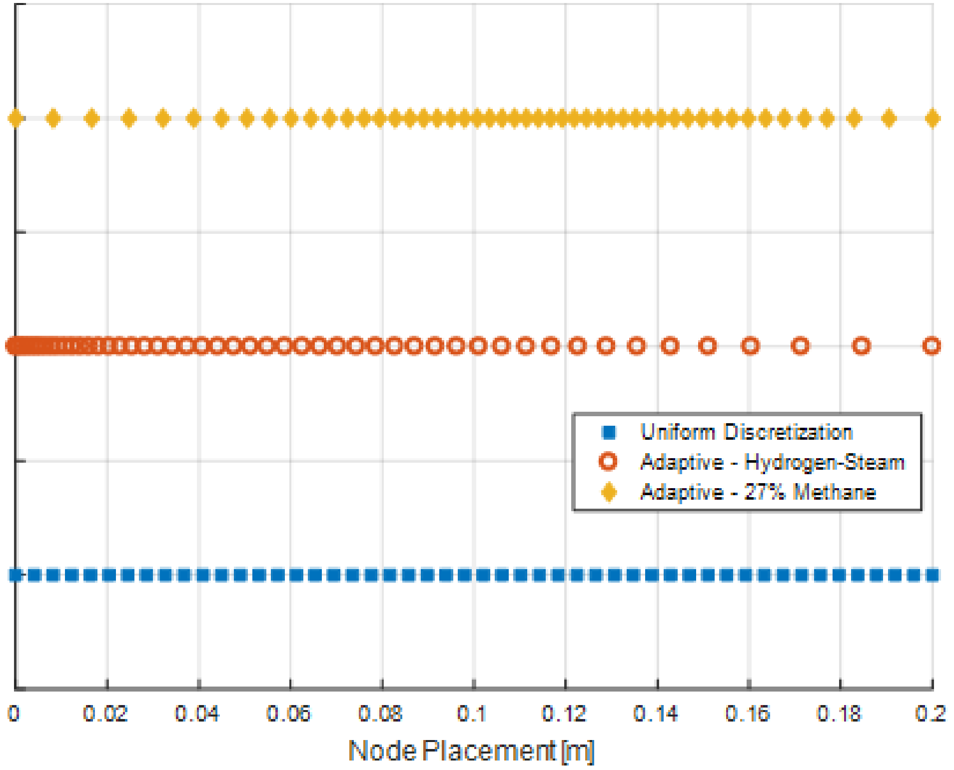


Fig. 1 - Demonstration of Rediscretization upon Fuel Stream Composition Change

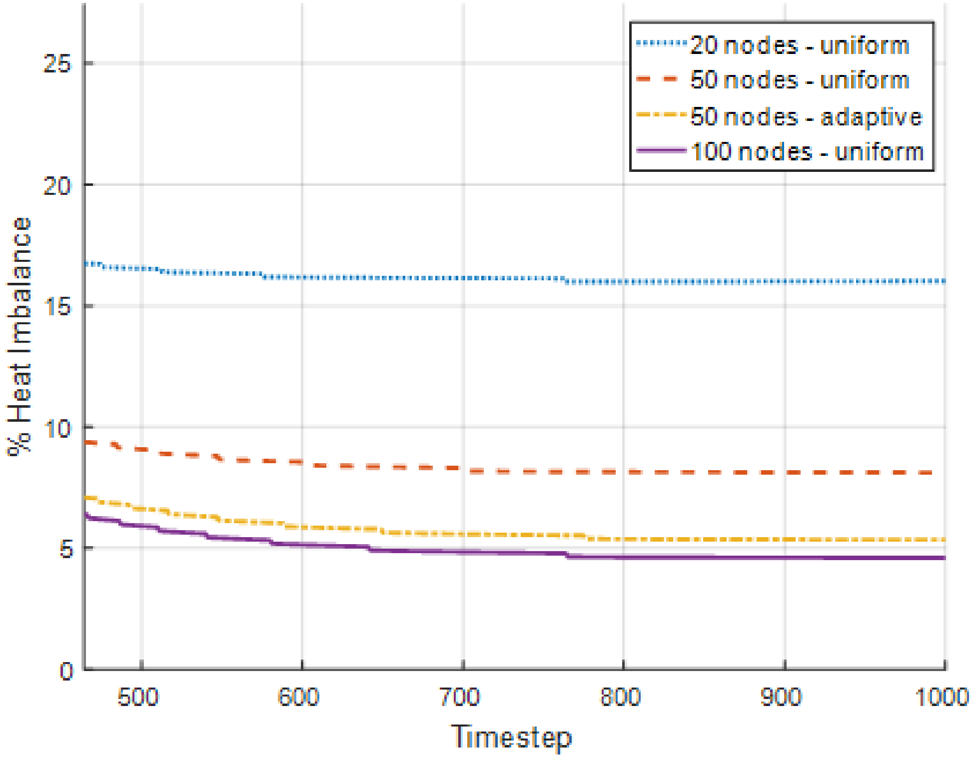


Fig. 2- Demonstration of Steady-State Heat Imbalance Reduction with Adaptive Meshing

Timing in MATLAB

- Timing of adaptive algorithm linked to number of interpolation points used, but overall represents a negligible amount of the total fuel cell algorithm time (~1-5% increase over non-adaptive algorithm depending on number of interpolation points used)
    - Bulk of computation still in rootfinders in electrochemical algorithm

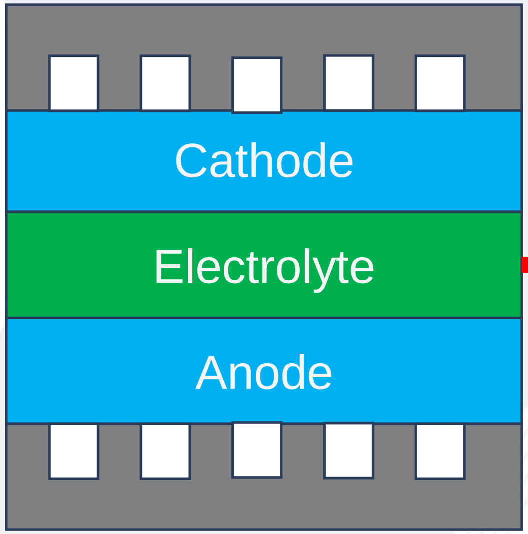
- We were not able to implement within Hyper given the coronavirus pandemic

Computationally designing and testing thermally robust solid oxide fuel cells and observing their thermal transient implications

Scope of Research

Conceptual Fuel Cell and Interconnect Designs

Oxidant Side Interconnect



Fuel Side Interconnect

Inputs:
Fluid Inlet Temperature, Electrical Load, Fuel Type, etc.

Computational Models of Fuel Cell and Interconnects:

Thermal
Fluid
Electrical
Electrochemical

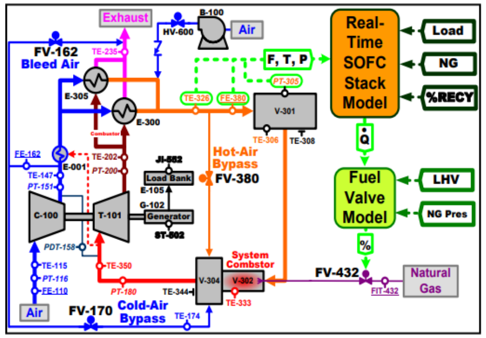
Outputs:
<u>Axial Temperatures and Temperature Gradients</u>, Cell Voltage, etc.

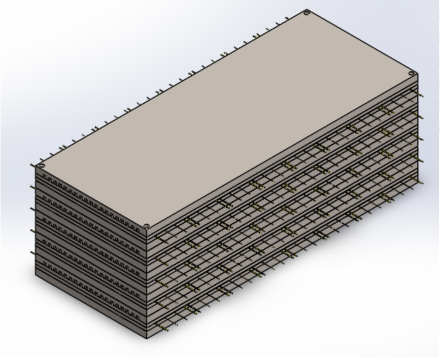
Determine Designs and Inputs that Produce Desirable Outputs

Implement Computational Model of Designs and Inputs in a Cyber physical System

- or -

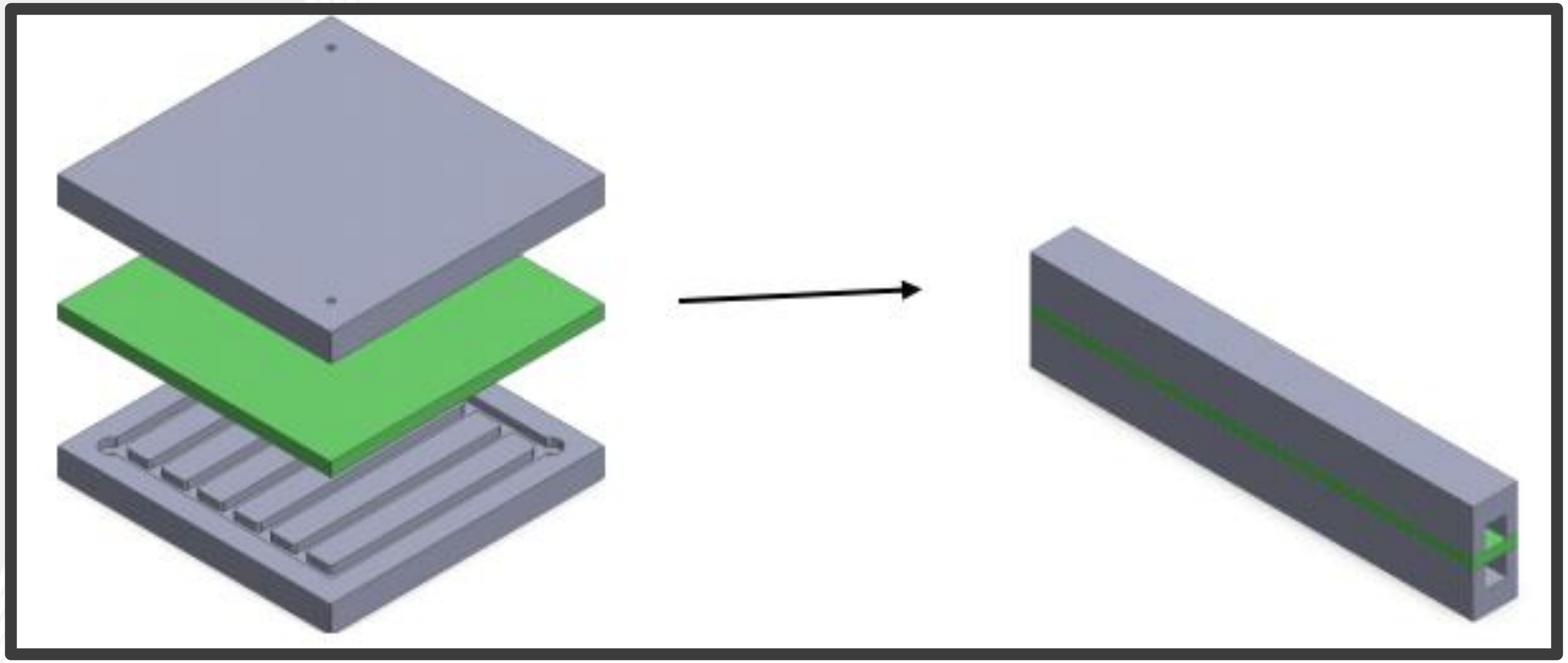
Fabricate Designs based Upon Computational Results and Collect Experimental Data



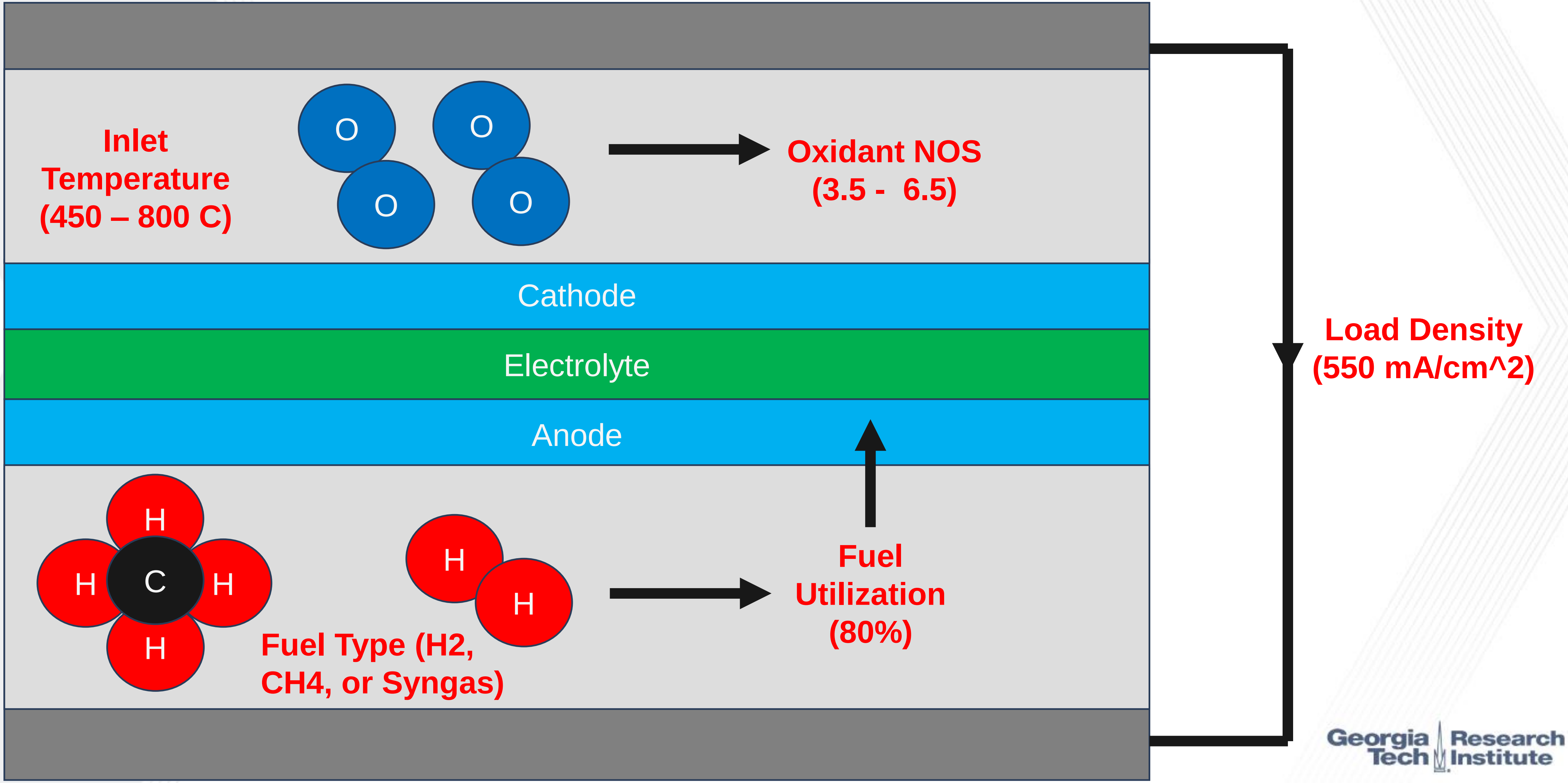


Interconnect Designs

- Standard interconnects for co-flow (shown below)
- Thermally redesigned, geometrically altered interconnects for co-flow (underway)



Inputs: Fuel Cell Operating Parameters Investigated



Inlet Temperature (450 – 800 C)

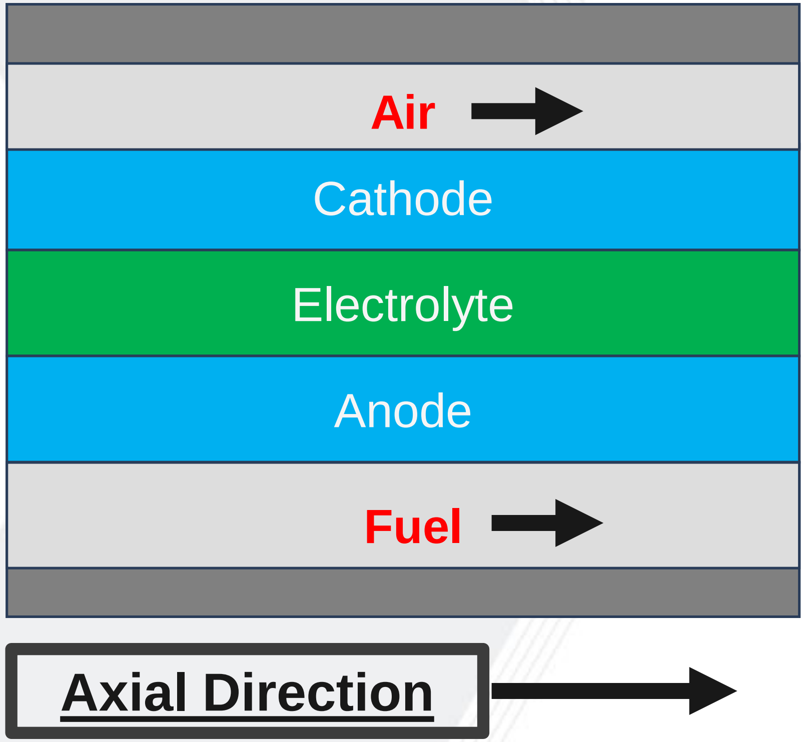
Oxidant NOS (3.5 - 6.5)

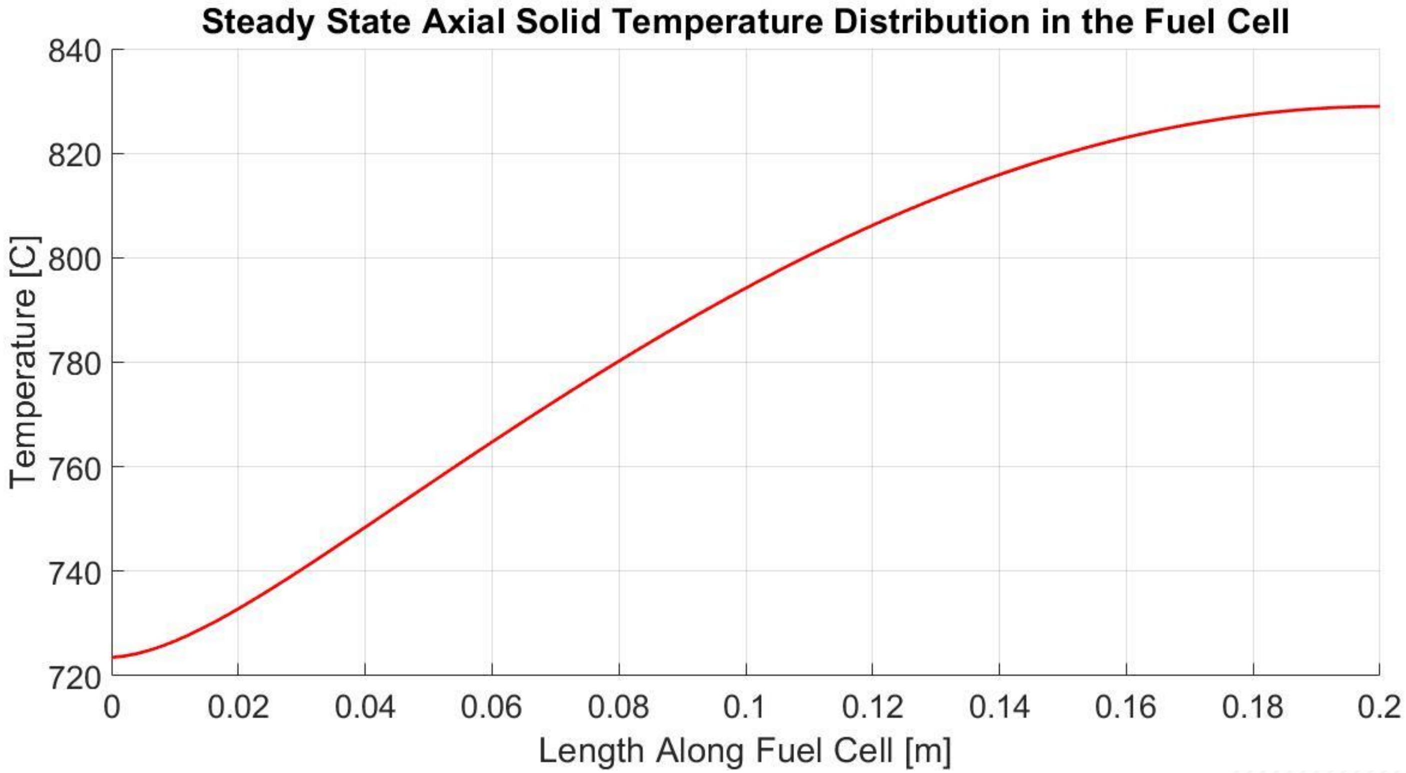
Load Density (550 mA/cm^2)

Fuel Type (H2, CH4, or Syngas)

Fuel Utilization (80%)

Output Examples





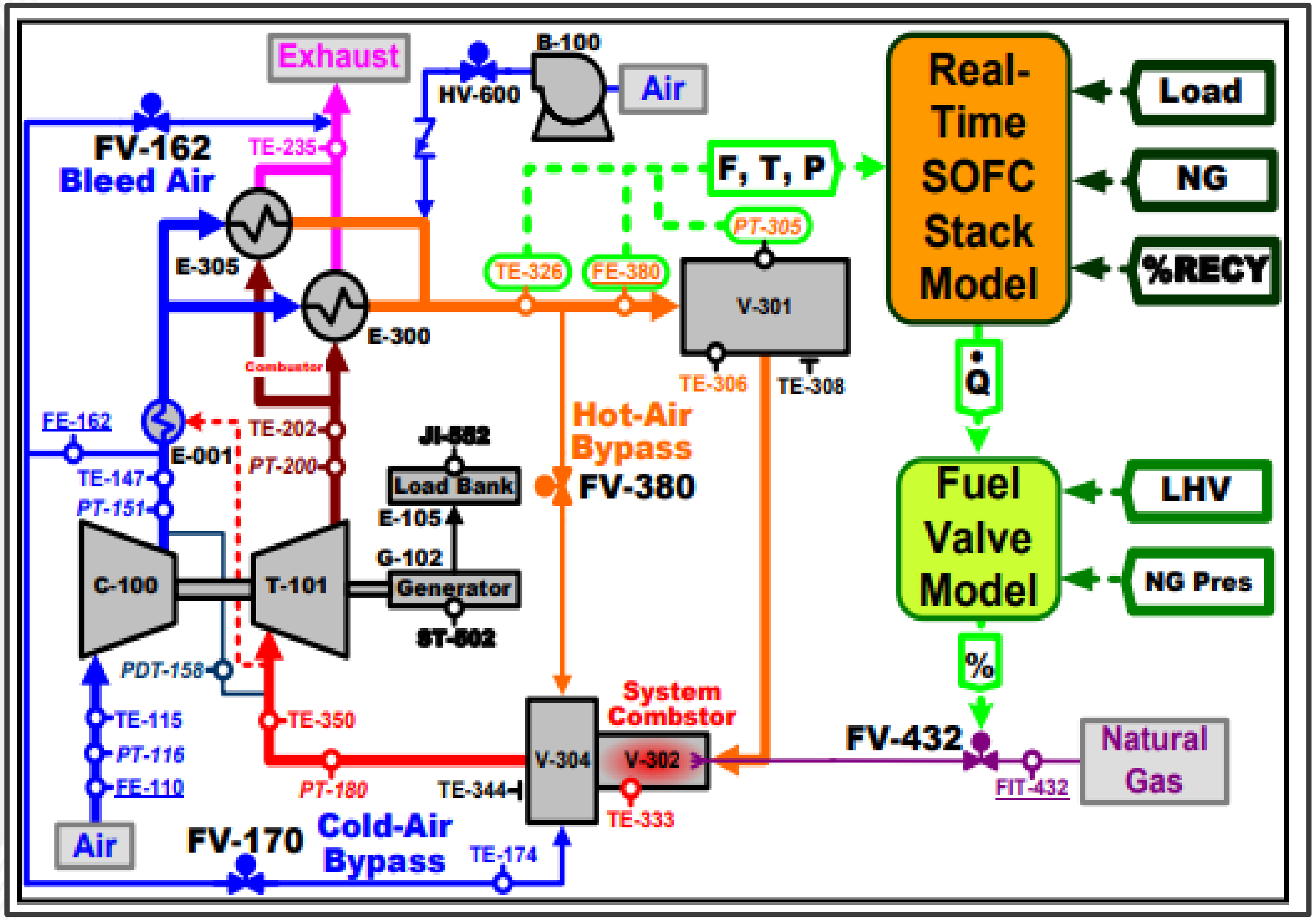
Fuel: Hydrogen Gas
Fuel Utilization = 80%
NOS = 6.5
Inlet Temperature = 650 C
Load Density = 550 mA/cm^2

Desirable Outputs: Interpretation of Results

- The sets of parameters that often led to non-convergence were:
    - Lower flow inlet temperatures
    - 27% methane as the fuel
    - Therefore, this planar solid oxide fuel cell model should not be implemented within Hyper for low temperature tests when the fuel is methane

- Converging conditions that resulted in the most desirable thermal management of the fuel cell were:
    - Higher flow inlet temperatures
    - Hydrogen gas as the fuel
    - Therefore, these parameters not only constitute feasible models that can be implemented within Hyper, but also desirable models that are viable for improving solid oxide fuel cell system efficiencies through their promotion of desirable thermal management of the fuel cell

Conclusions and Future Work



Implement Designs and Parameters in a Cyberphysical System for Systems-Level Analyses

Acknowledgement and Disclaimer

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