Overview of the Rolls-Royce Fuel Cell Multi-Physics Code Project

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28 July 2011

 This material is based upon work supported by the U.S. Department of Energy under Award Number DE-FE0000773.

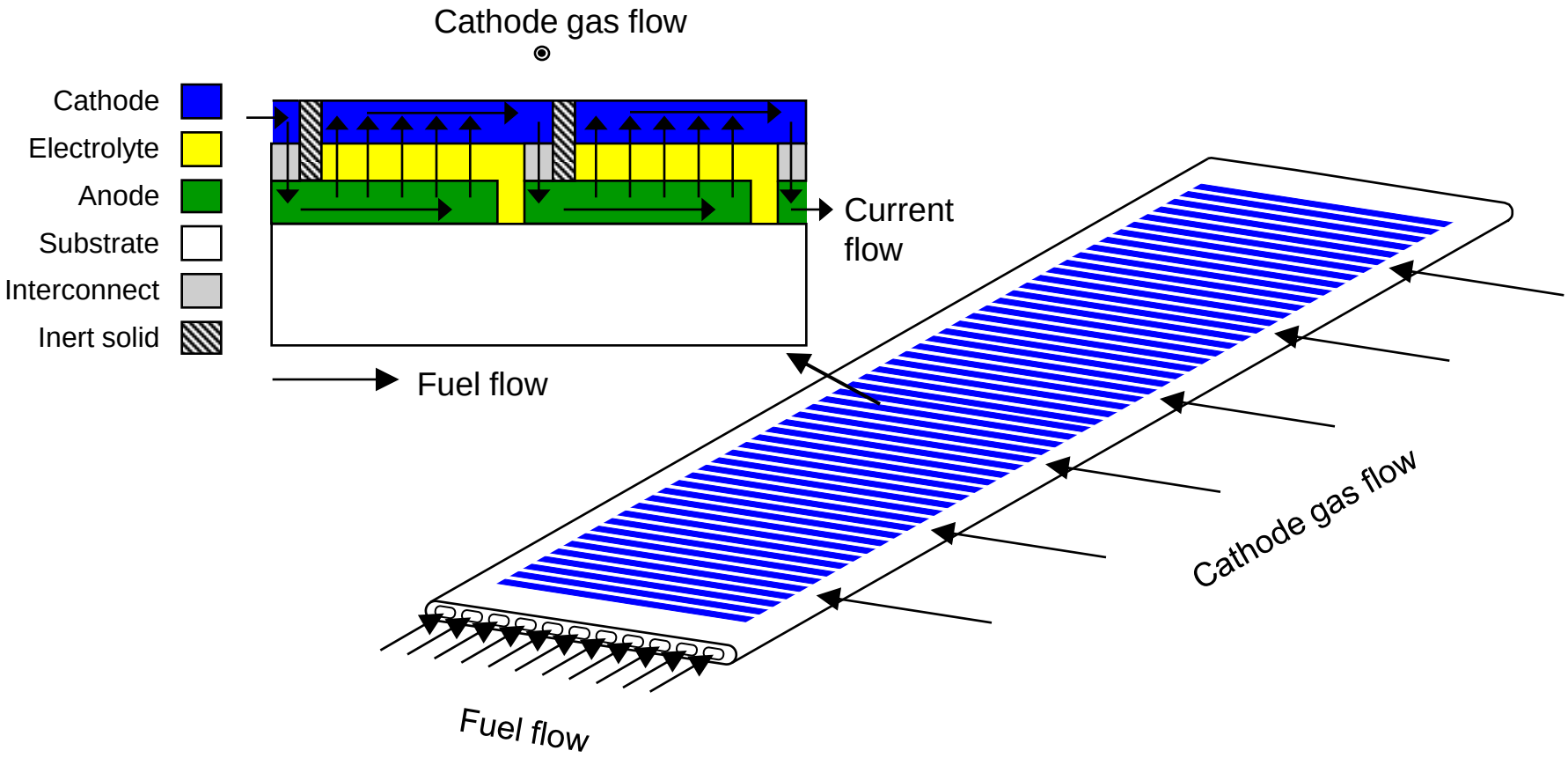
Acknowledgements

- This material is based upon work supported by the Department of Energy National Energy Technology Laboratory under Award Numbers DE-FE0000773 and DE-FE0000303.
- DOE project manager Patcharin Burke
- UK and US based RRFCS team

Overview

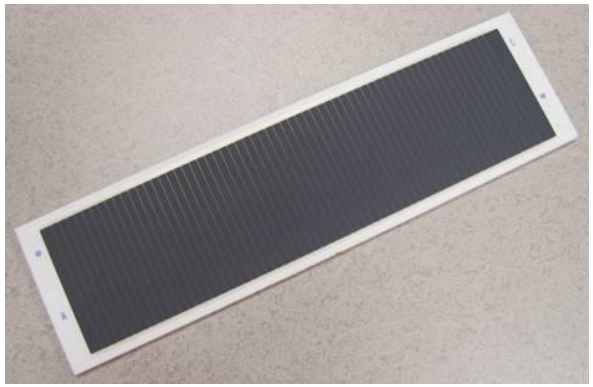
- IP-SOFC Technology
- Project Objectives
- Work Program
- Multi-Physics Code Demo
- Validation
- Conclusions

IP-SOFC Technology

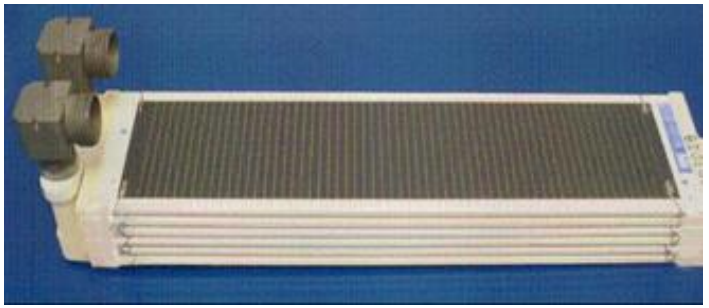


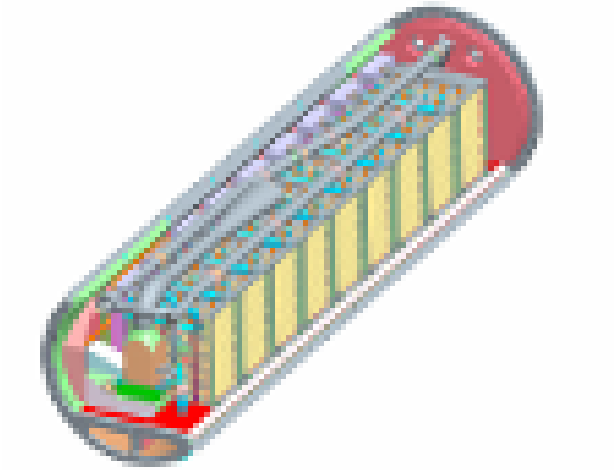
Current Stack Configuration

Substrate assembly, 60W



Bundle assembly, ~350W





1MW System will be 250kW tiers

Design Tool Applications

- Multiple scales
  - Single Cell ⟶ Bundle ⟶ Strip ⟶ Block ⟶ System
- Analysis of current design
  - Nominal operation (steady state and transient)
  - Effect of geometric and material tolerances
  - Extreme operating modes and conditions
  - Degradation data and rates
  - Lifetime and reliability
- Support SECA activities
- Diagnostic analysis
  - Explain test anomalies
- Improve future designs
  - Cost reduction
  - Performance enhancements
  - Feasibility studies
- Non SOFC applications
  - Peripheral components
  - Fuel processing

Overview

- IP-SOFC Technology
- **Project Objectives**
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- Multi-Physics Code Demo
- Sample Results
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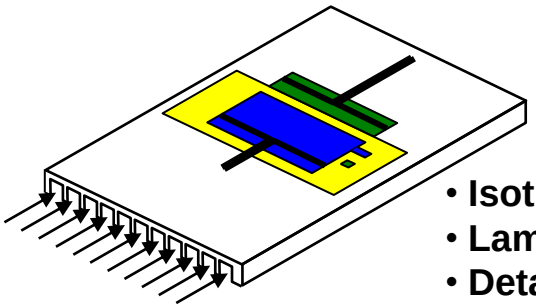
MPC Objectives

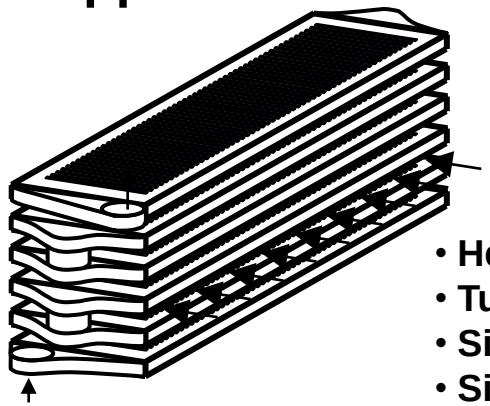
- Scope
  - Model scale: cell → bundle
  - Steady-state & transient
- Models
  - Fluid flow & heat transfer
  - Porous flow
  - Chemical & electrochemical reaction
  - Current flow
  - Degradation
- Support product development & design activities
  - Interface with Strip & Block models
  - Interface with mechanical models (lifetime, reliability)
  - CFD & heat transfer analysis
- Professional Use
  - Non expert user

Project Strategy

- STAR-CCM+ (CD-adapco) chosen for MPC
- Program divided into 4 Code Releases
  - Prioritize implementation of simplest models
    - Initial code release provides basic SOFC platform
  - Verification and validation throughout
    - Parallel computing resources
- Model choice application dependent
  - Interchangeable models available
  - Step by step approach to new applications



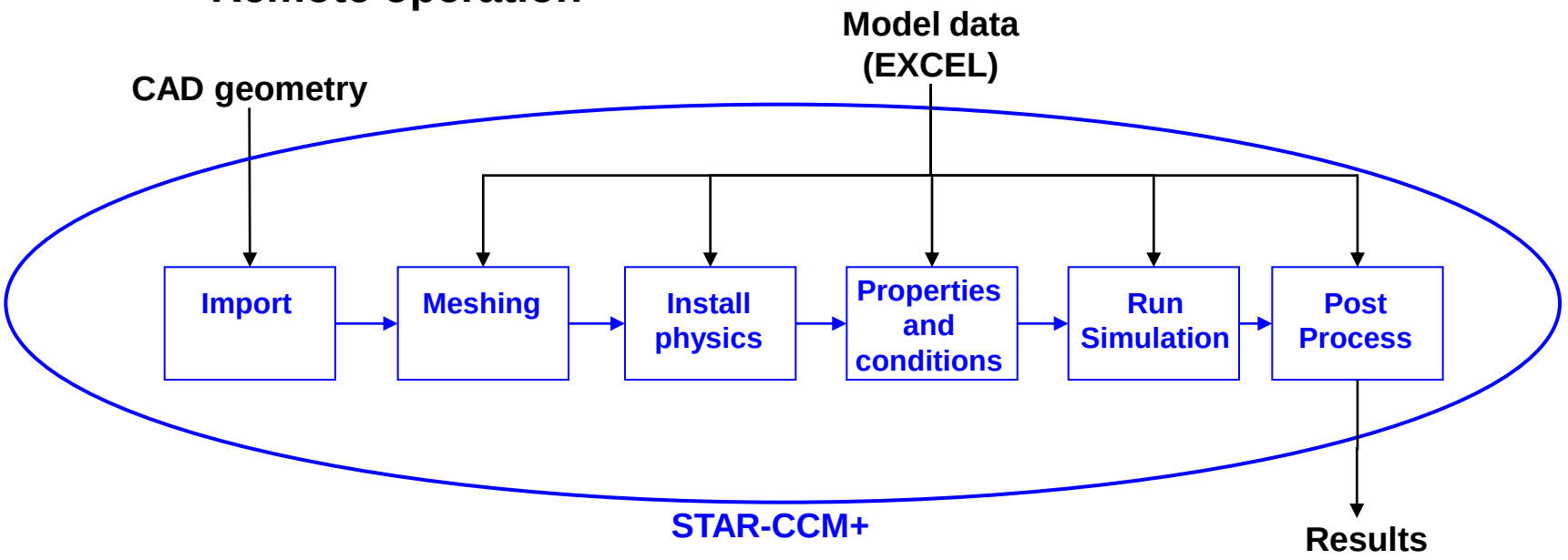
- Isothermal
- Laminar
- Detailed current flow
- Advanced chemistry



- Heat transfer + Radiation
- Turbulence
- Simplified current flow
- Simplified chemistry

Project Strategy

- **Provide SOFC expertise to professional user**
  - **Extensive use of JAVA macro programming**
  - **Automate processes**
    - **Reduce error and time**
    - **Ensure best practice**
    - **Remote operation**



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Code Enhancement Program

Physical model	Interchangeable fidelity level	
	Low (1)	High (2)
Fluid flow	1D Plug flows (Steady state laminar)	CFD calculations
Porous flow	Darcy model	CPIM model
Heat transfer	Isothermal	Convection, conduction + radiation
Chemistry	Global one step reactions	Multi-step reactions – chemistry solver
Electrochemistry	Uniform current density	Integrated with current flow simulation
Current flow	Analytical Ohmic loss model.	3D numerical model
Degradation	Empirical models for time dependent changes	Kinetic models

Code Release

- R1
- R2
- R3
- R4

Model Verification/Validation Program

Applications/ Models	1D Single Cell	2D Single/ Penta Cell	3D Penta Cell	3D Substrate	3D Bundle
Porous Flow	2	2	2	2	2
Fluid Flow	2	2	2	2	1 2
Heat Transfer	1	1	1	2	2
Chemistry	1 2	1 2	1 2	1	1
Electrochemistry	1	2	2	1 2	1 2
Current Flow	-	2	2	1 2	1 2
Degradation	-	1 2	1 2	1	-

Code Release

- R1
- R2
- R3
- R4

Low Fidelity – 1
High Fidelity – 2

Progress To Date

- Code Release 3 complete
  - Fully coupled physics
    - 1D, 2D and 3D
    - Interchangeable model fidelity
  - Validated models up to substrate
  - Simulation spreadsheet and macros
- Capabilities beyond previous tools
- Effective methodology
  - Common platform development

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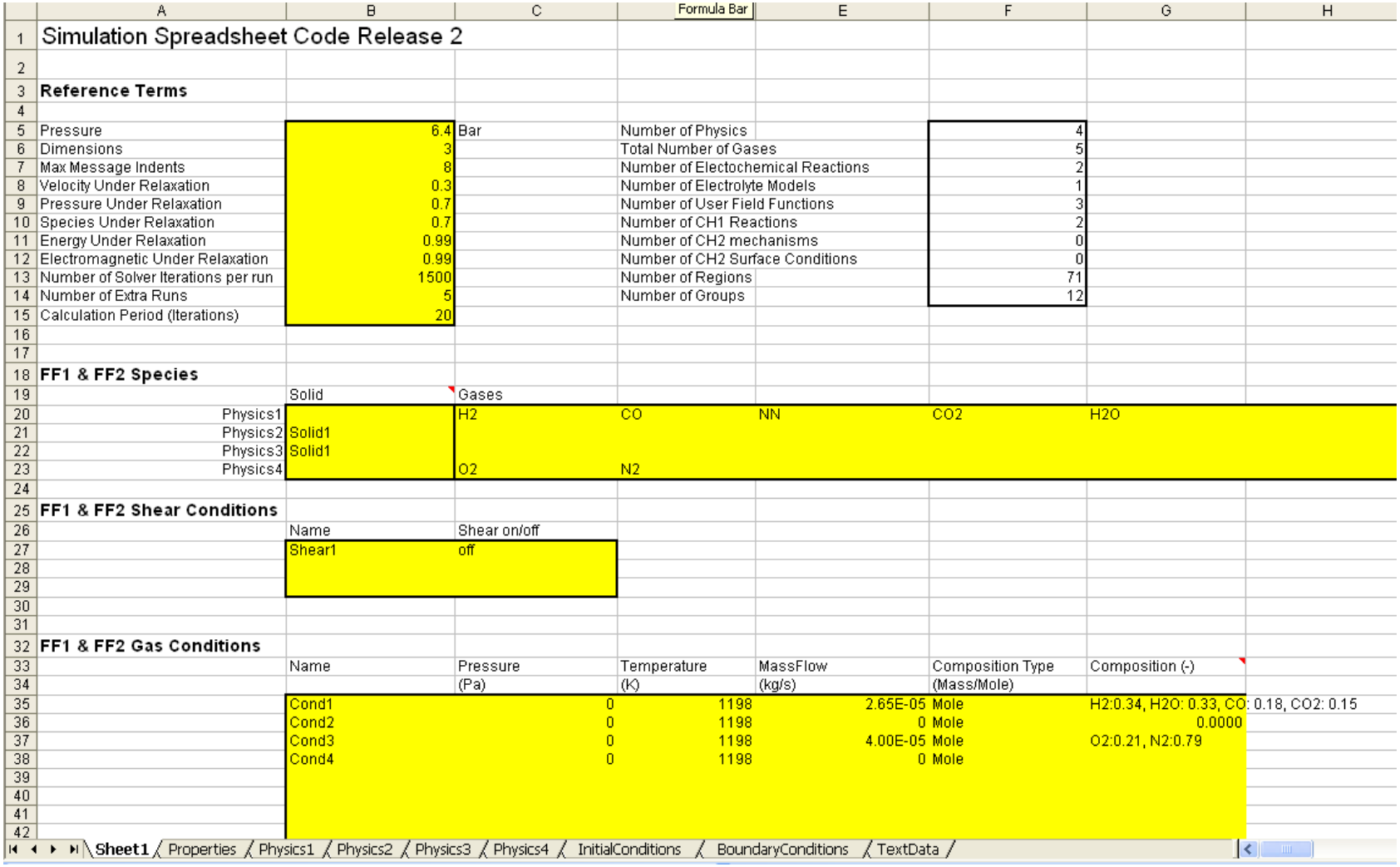
EXCEL Simulation Spreadsheet

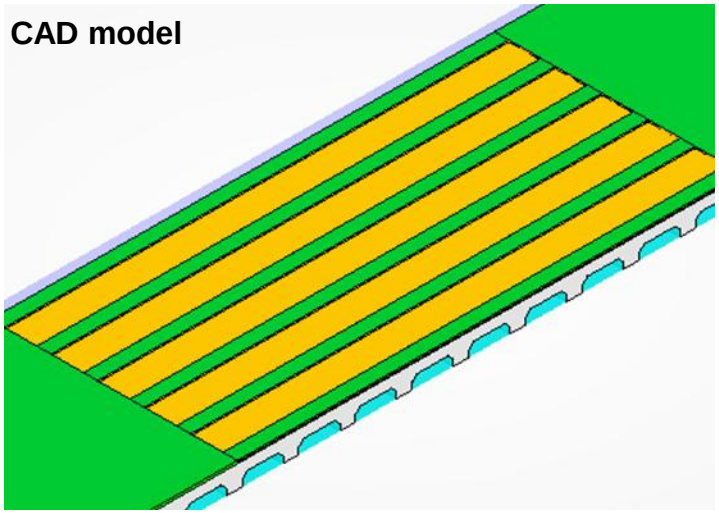


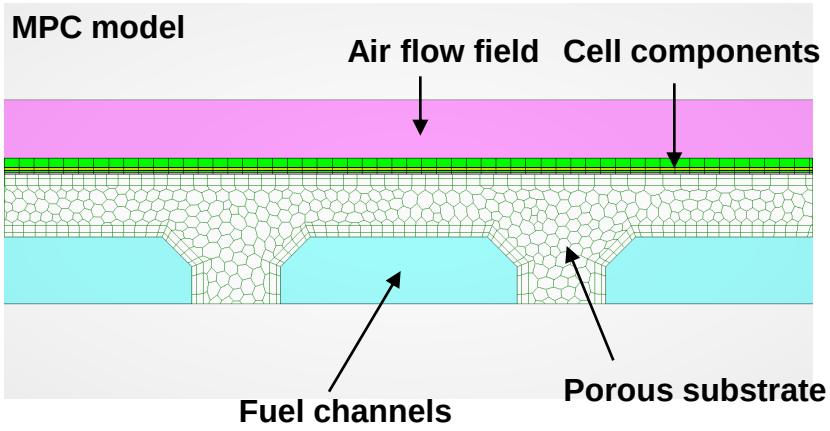
	A	B	C	Formula Bar	E	F	G	H
1	Simulation Spreadsheet Code Release 2							
2								
3	**Reference Terms**							
4								
5	Pressure	6.4	Bar	Number of Physics		4		
6	Dimensions	3		Total Number of Gases		5		
7	Max Message Indents	8		Number of Electochemical Reactions		2		
8	Velocity Under Relaxation	0.3		Number of Electrolyte Models		1		
9	Pressure Under Relaxation	0.7		Number of User Field Functions		3		
10	Species Under Relaxation	0.7		Number of CH1 Reactions		2		
11	Energy Under Relaxation	0.99		Number of CH2 mechanisms		0		
12	Electromagnetic Under Relaxation	0.99		Number of CH2 Surface Conditions		0		
13	Number of Solver Iterations per run	1500		Number of Regions		71		
14	Number of Extra Runs	5		Number of Groups		12		
15	Calculation Period (Iterations)	20						
16								
17								
18	**FF1 & FF2 Species**							
19		Solid	Gases					
20	Physics1		H2	CO	NN	CO2	H2O	
21	Physics2	Solid1						
22	Physics3	Solid1						
23	Physics4		O2	N2				
24								
25	**FF1 & FF2 Shear Conditions**							
26		Name	Shear on/off					
27		Shear1	off					
28								
29								
30								
31								
32	**FF1 & FF2 Gas Conditions**							
33		Name	Pressure	Temperature	MassFlow	Composition Type	Composition (-)	
34			(Pa)	(K)	(kg/s)	(Mass/Mole)		
35		Cond1	0	1198	2.65E-05	Mole	H2:0.34, H2O: 0.33, CO: 0.18, CO2: 0.15	
36		Cond2	0	1198	0	Mole	0.0000	
37		Cond3	0	1198	4.00E-05	Mole	O2:0.21, N2:0.79	
38		Cond4	0	1198	0	Mole		
39								
40								
41								
42								

Sheet1 | Properties | Physics1 | Physics2 | Physics3 | Physics4 | InitialConditions | BoundaryConditions | TextData

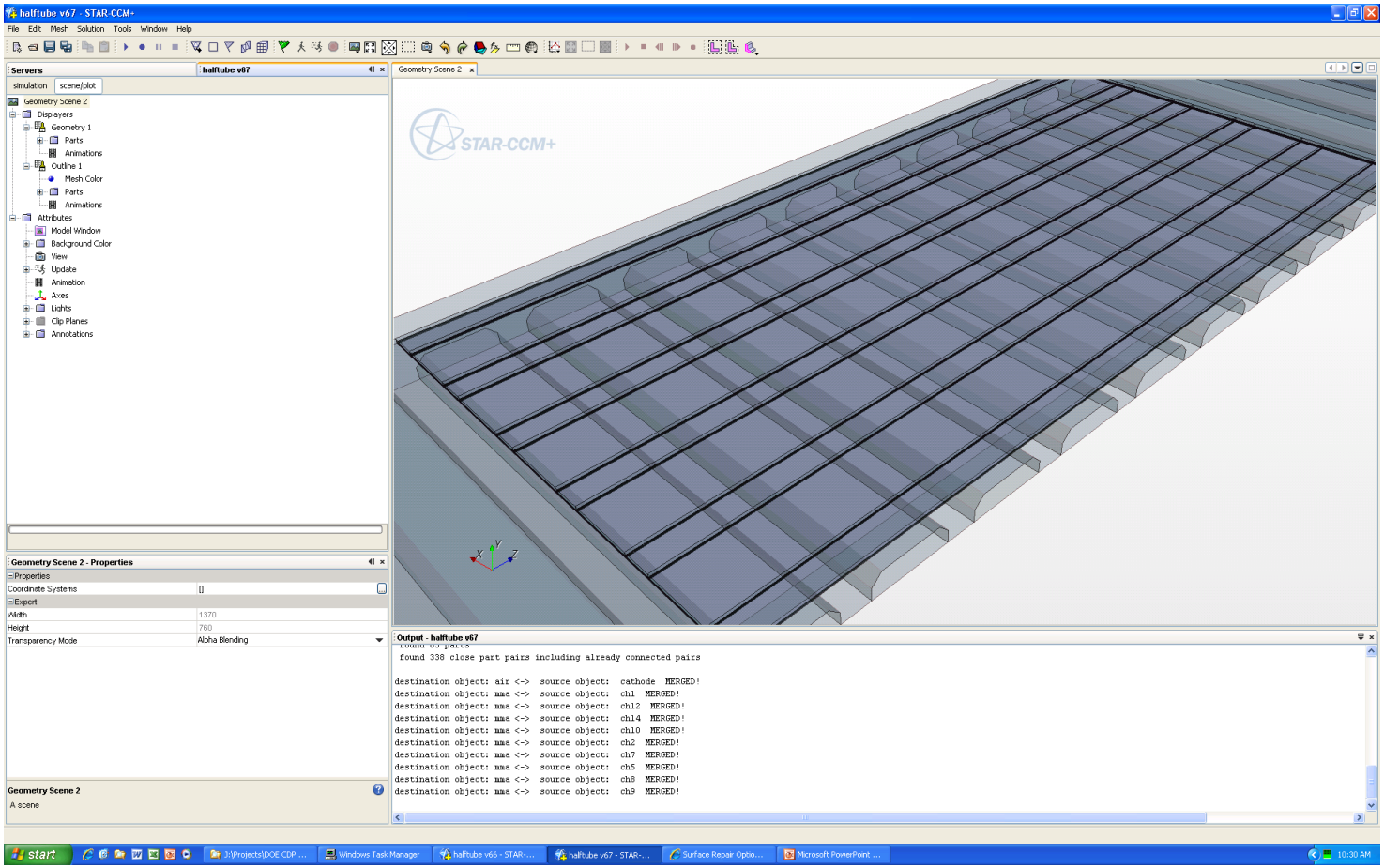
Model

Penta cell model
Consider only the active length of the tube
Neglect the unused region

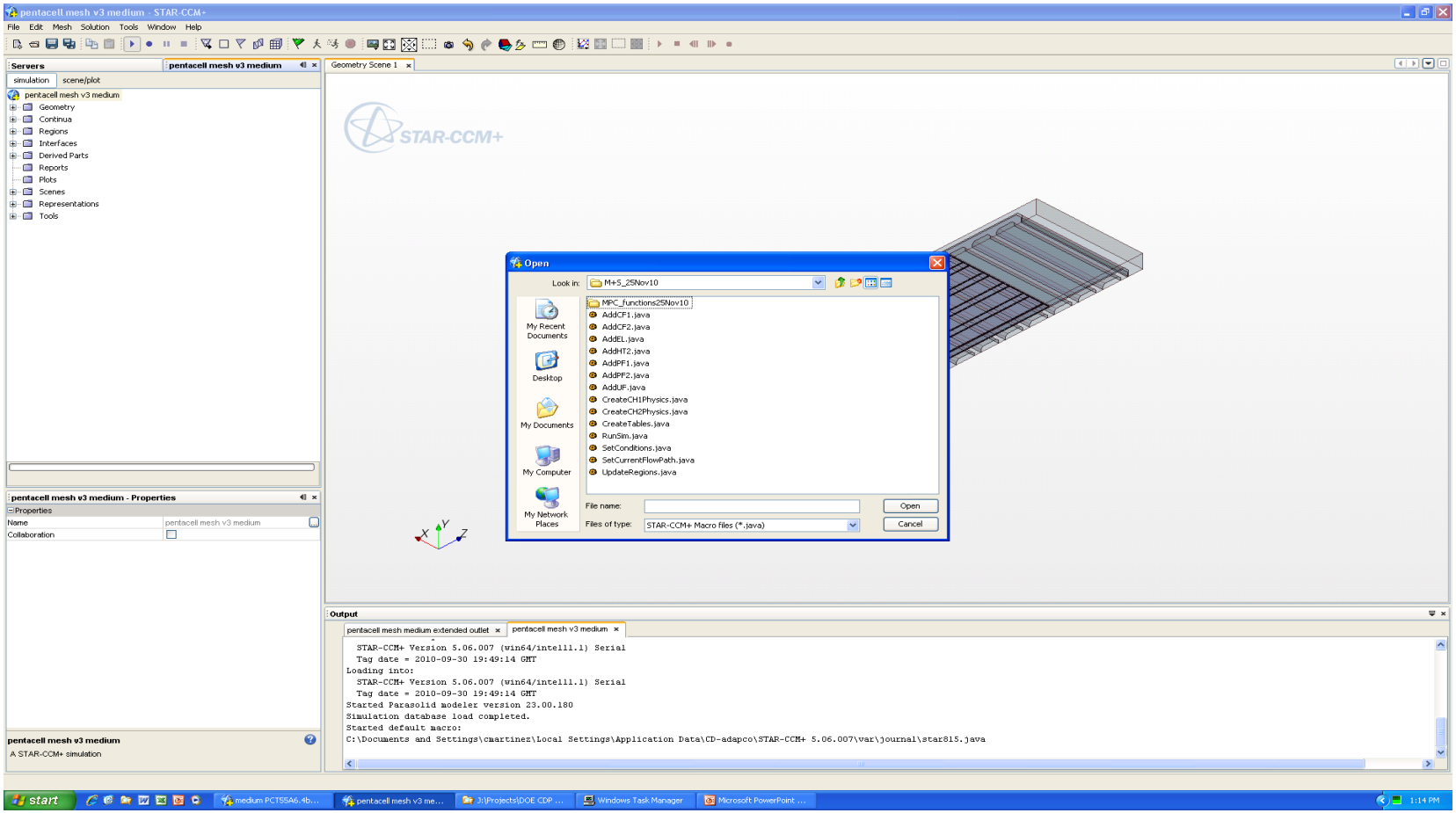




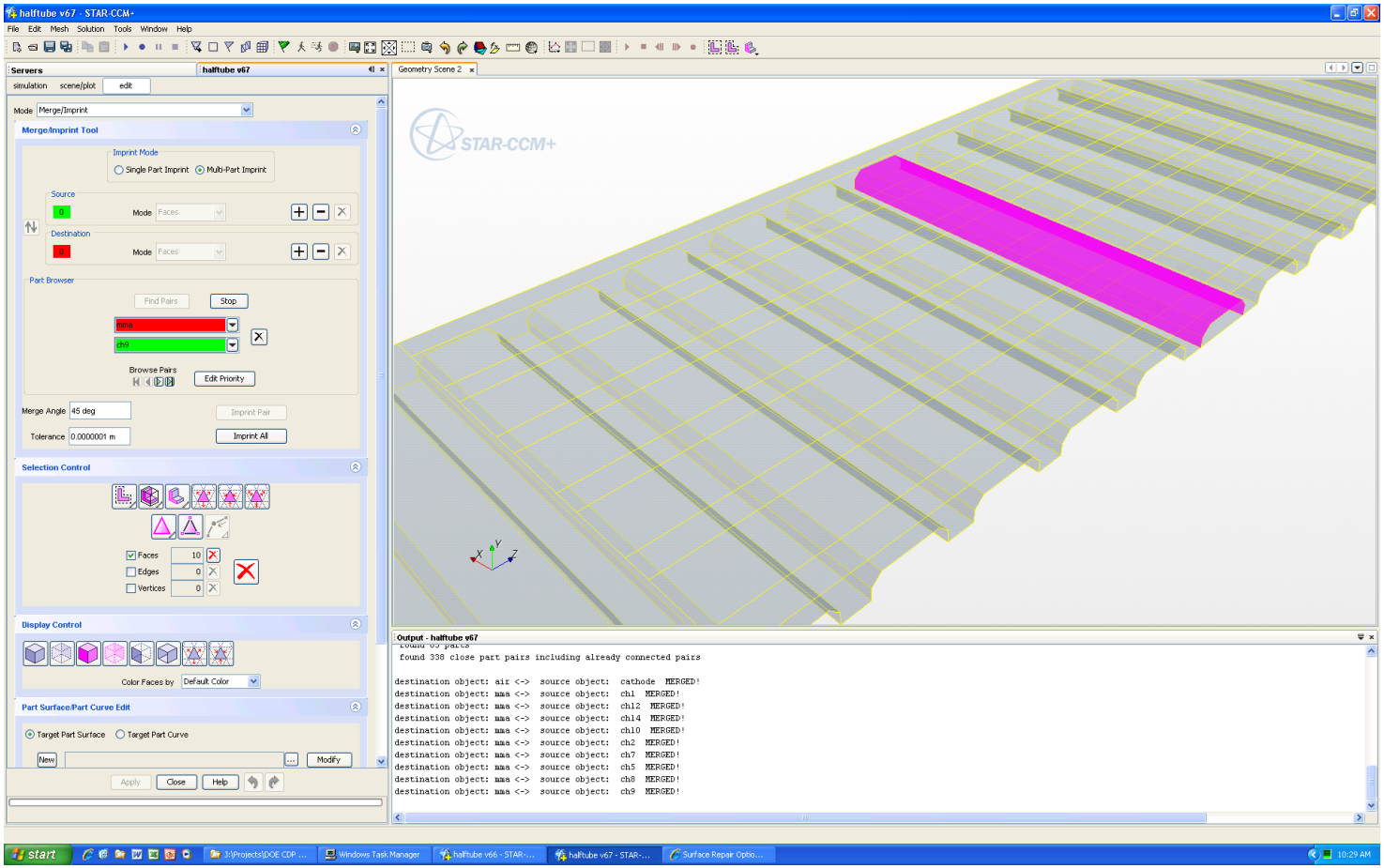
STAR-CCM+



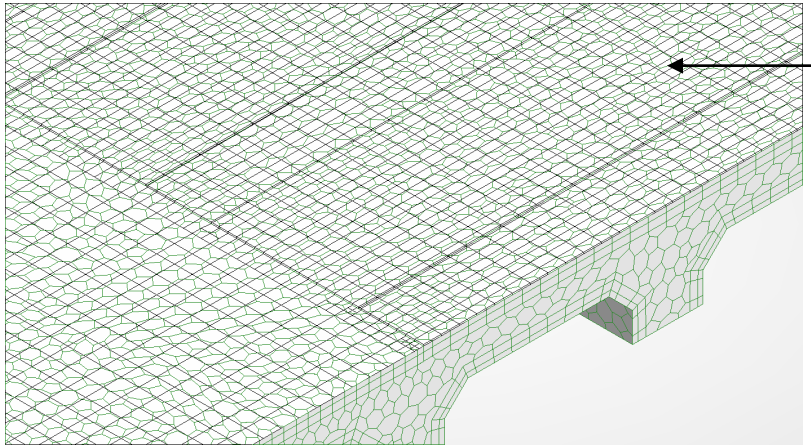
STAR-CCM+ Macros



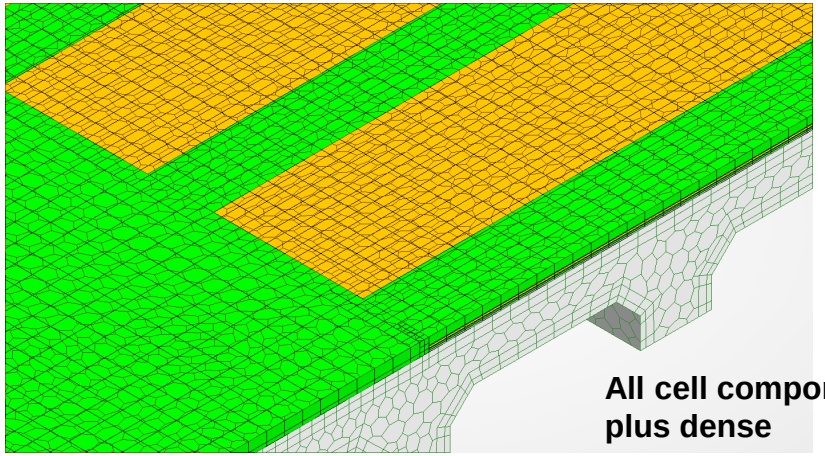
Automatic Interface Creation



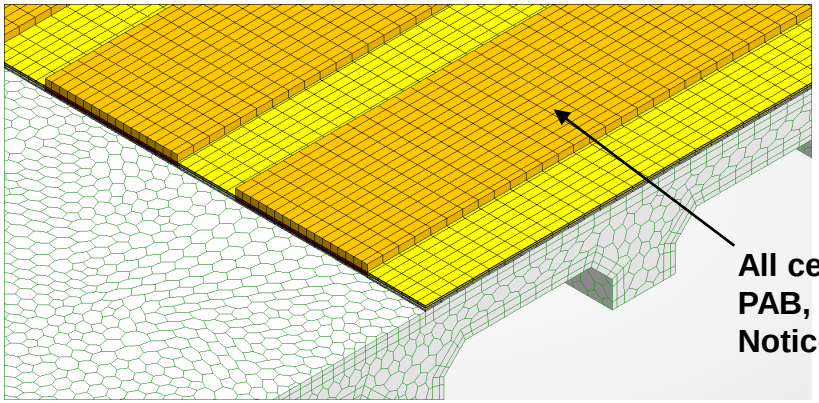
Meshing Capability



Model's grid on the porous substrate with marked lines from the cell regions sitting on its surface

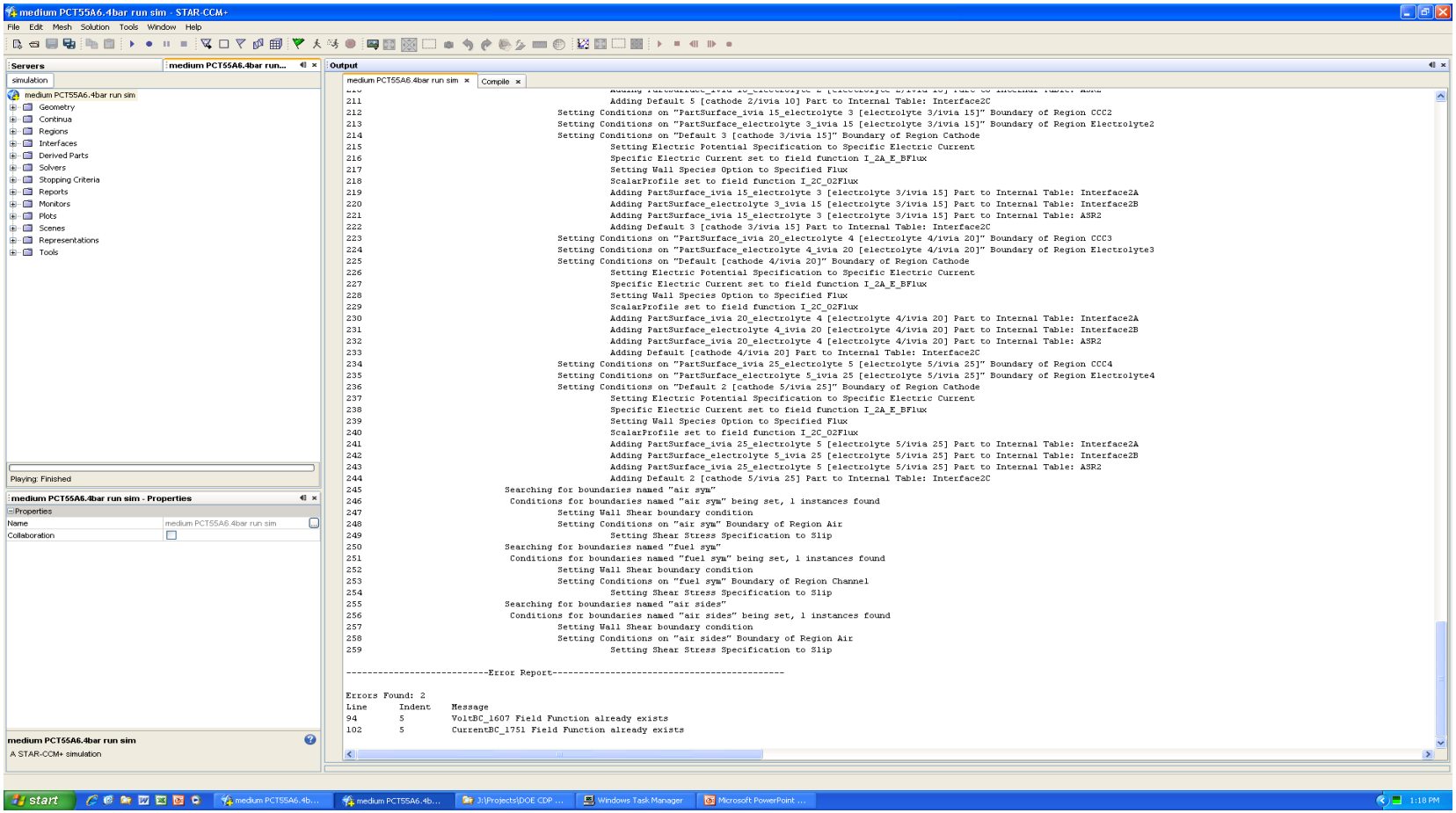


All cell components plus dense



All cell elements included:
PAB, anode, acc, electrolyte, cathode, ccc and interconnects.
Notice the change in mesh type

STAR-CCM+ Output

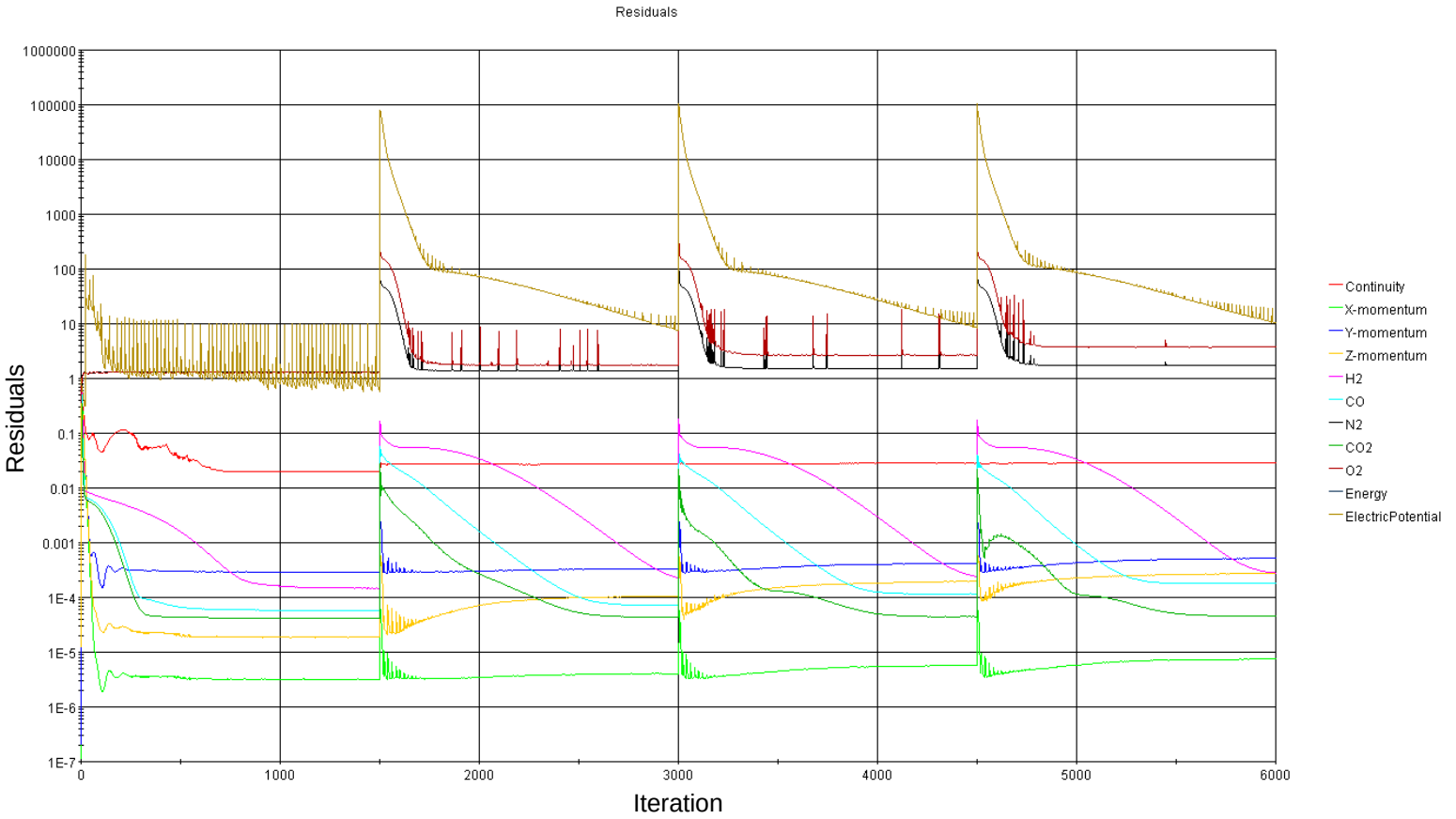


Chosen Models

- High fidelity fluid flow
  - CFD
- Low fidelity heat transfer
  - Isothermal
- High fidelity porous flow
  - CPIM
- Low fidelity chemistry
  - Water gas shift
- High fidelity electrochemistry and current flow
  - Integrated electrochemistry & numerical current flow

Iterations and Residuals

This model ran four points, each taking 1500 iterations, with a 20 iteration calculation period. In each run the current withdrawn from the cell increased by 2000 A m^-2

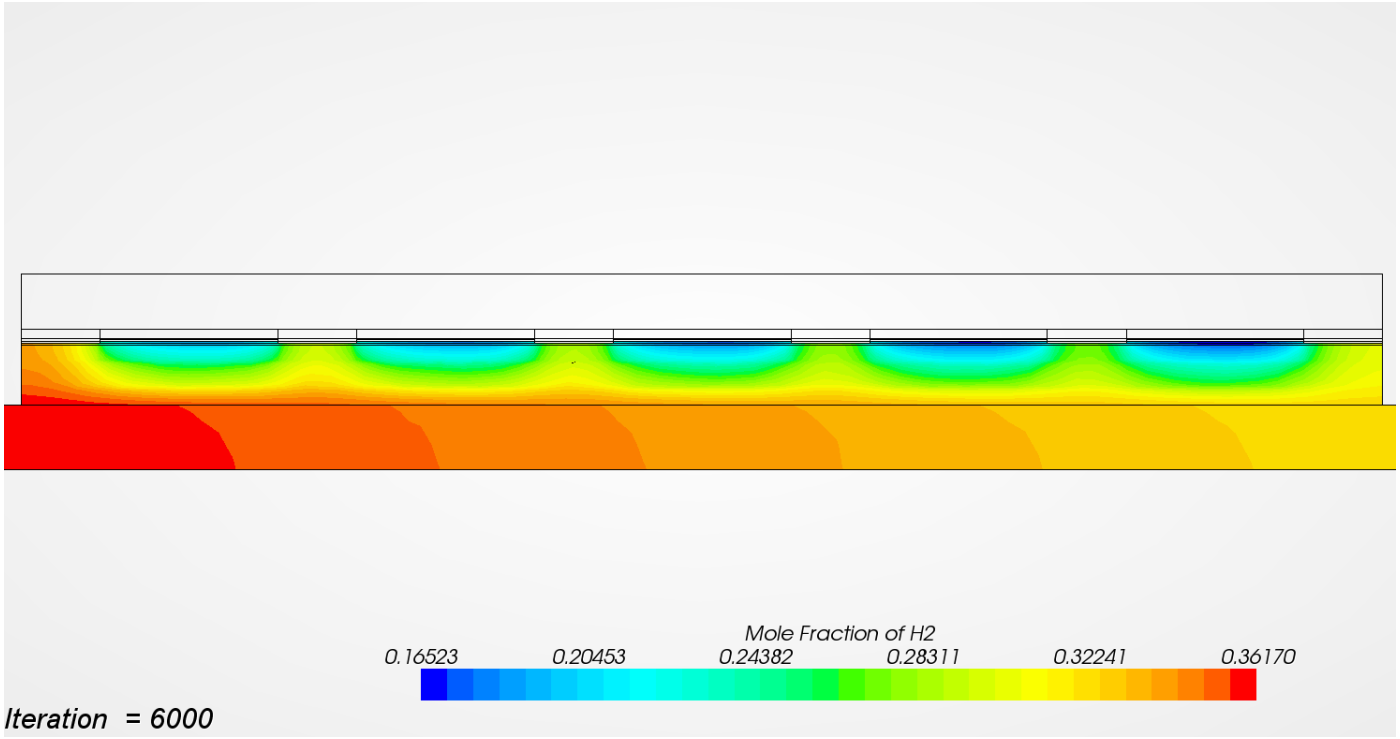


Hydrogen Mole Fraction

Contour plots demonstrate how hydrogen is being consumed by the electrochemical reaction.

Section planes across and along the tube show hydrogen diffusing across the porous substrate and how it is being consumed at the cell layers.

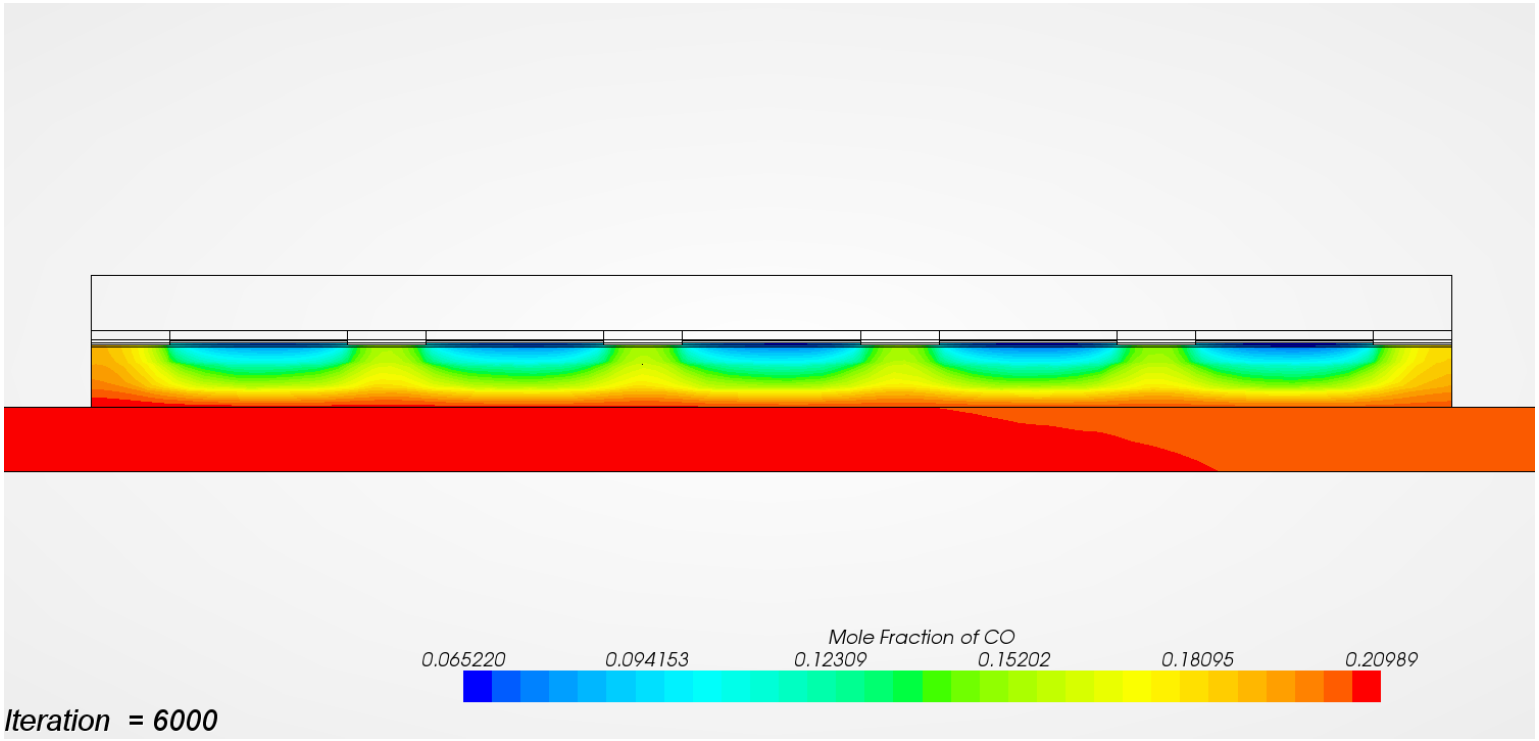
Variations in hydrogen mole fraction confined to porous regions where flow resistance is high.



Carbon Monoxide Mole Fraction

Contour plots demonstrate how carbon monoxide is being consumed by the WGS chemical reaction.

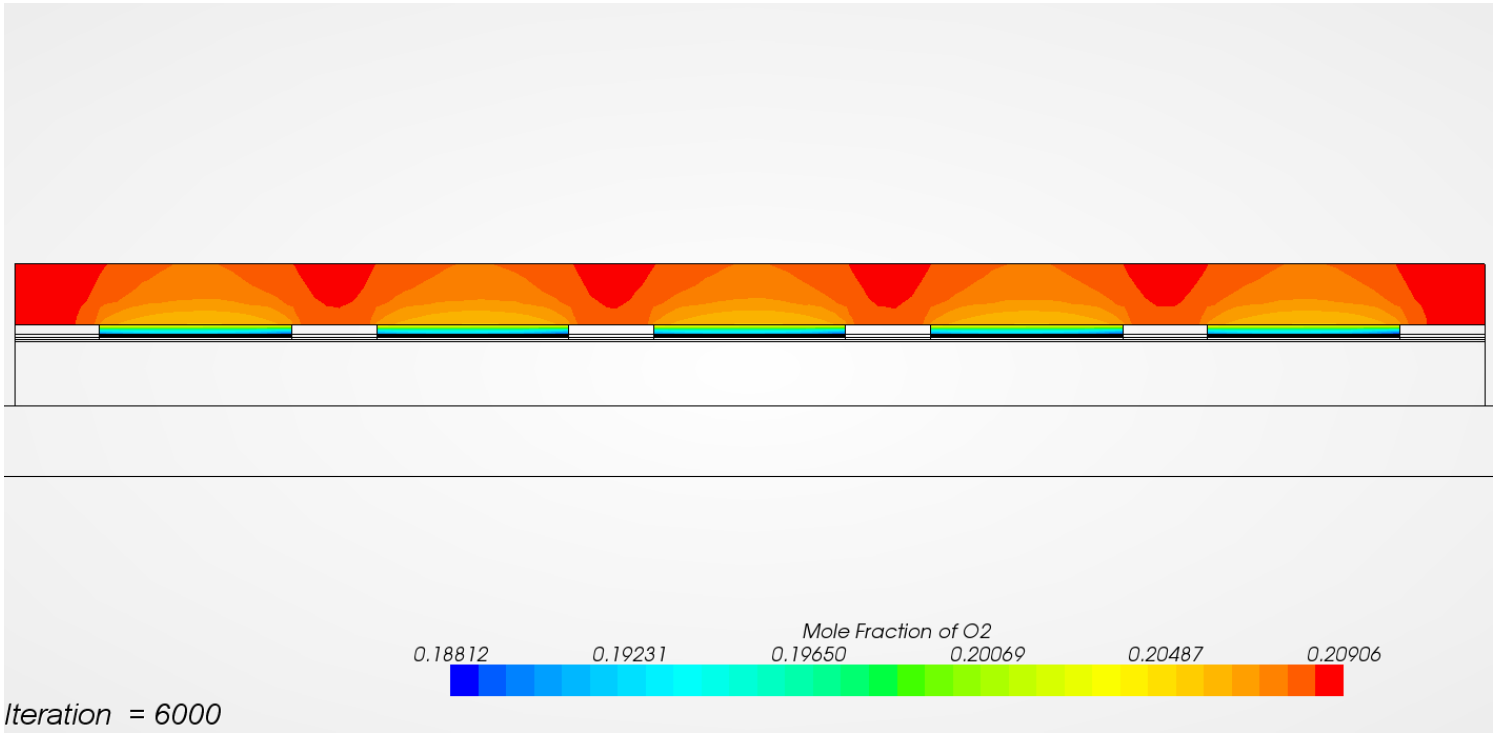
Section planes across and along the tube show carbon monoxide diffusing across the porous substrate towards the cell layers.



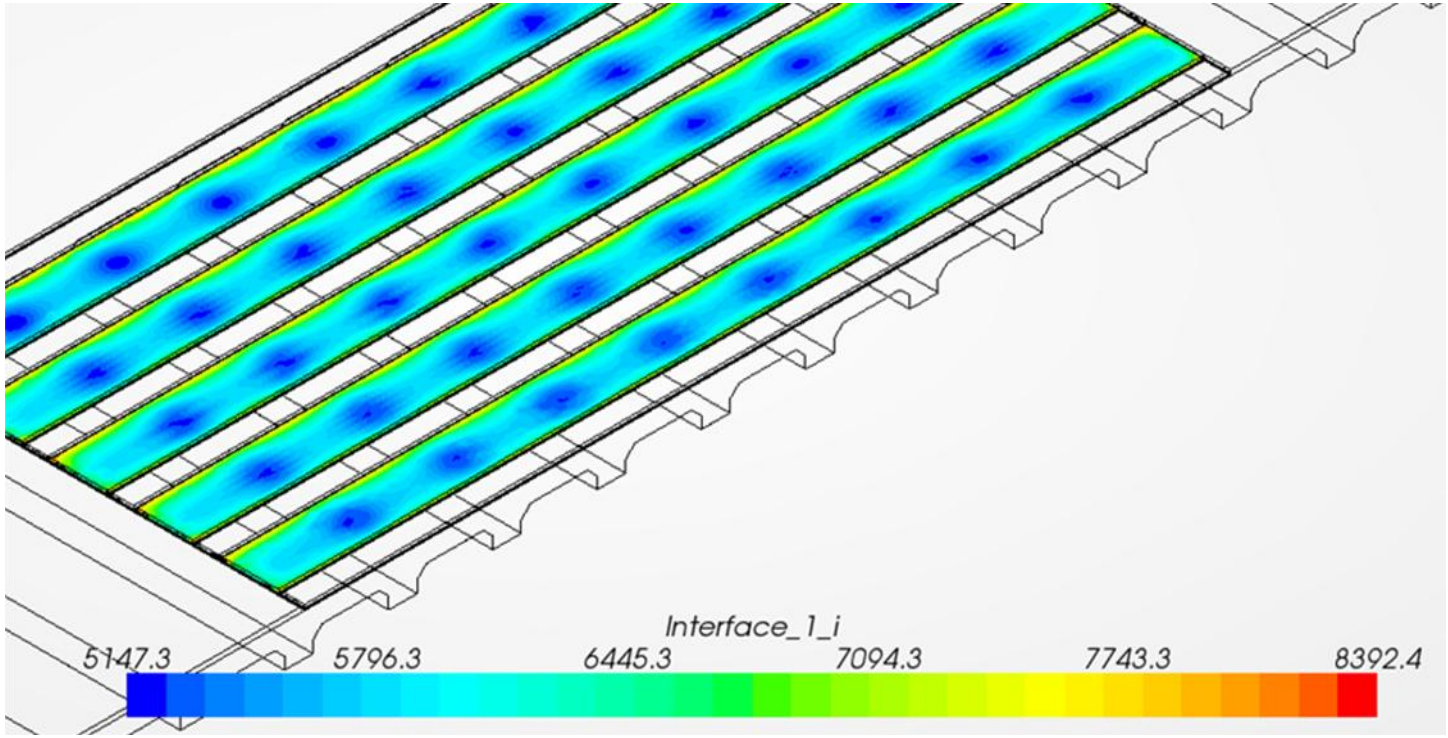
Oxygen Mole Fraction

Contour plots demonstrate how oxygen is consumed by the electrochemical reaction.

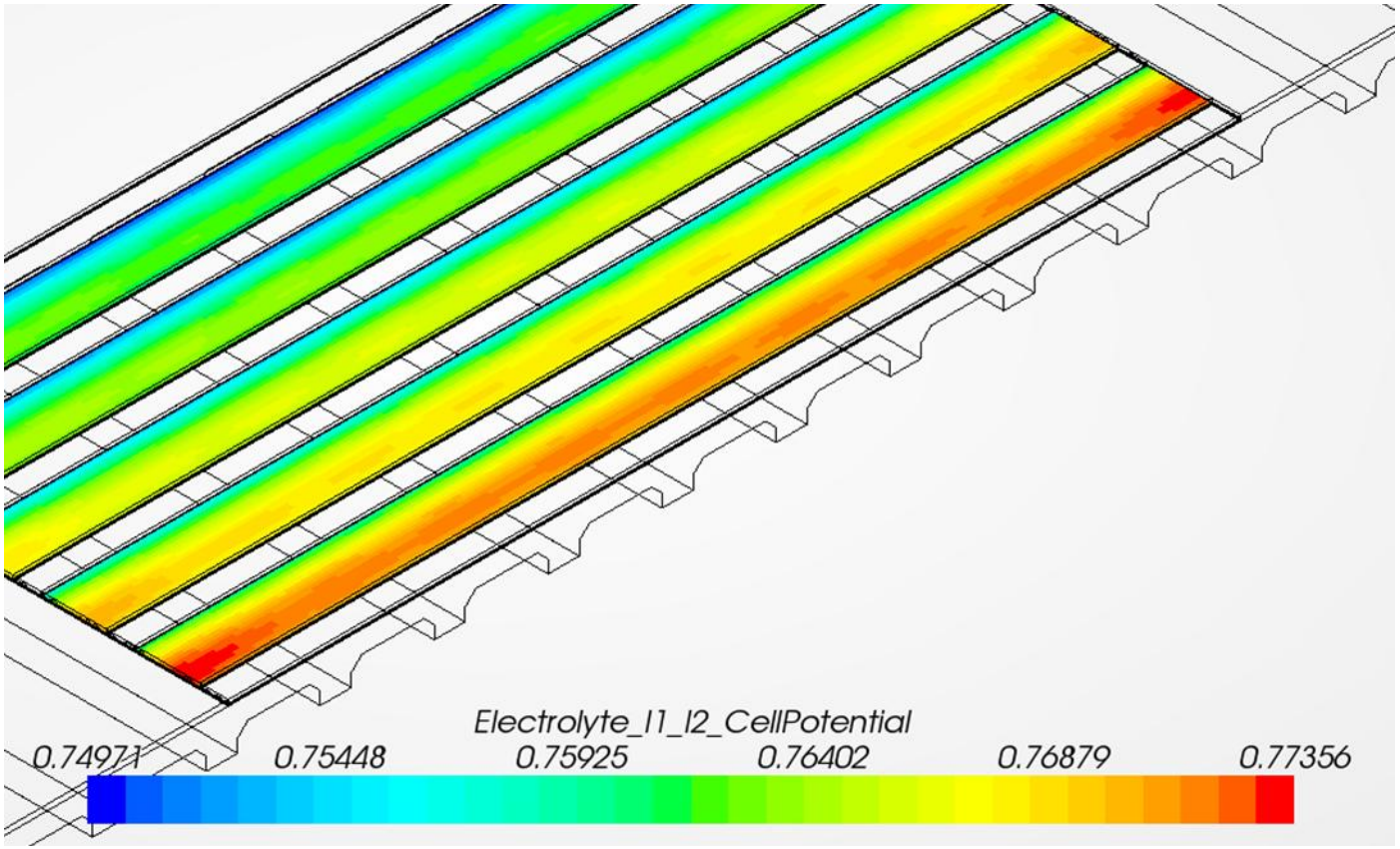
Section planes across and along the tube shows gradient of oxygen decreasing along the air flow field and how its mole fraction is reduced near the cell regions.



Current Density Distribution



Cell Potential



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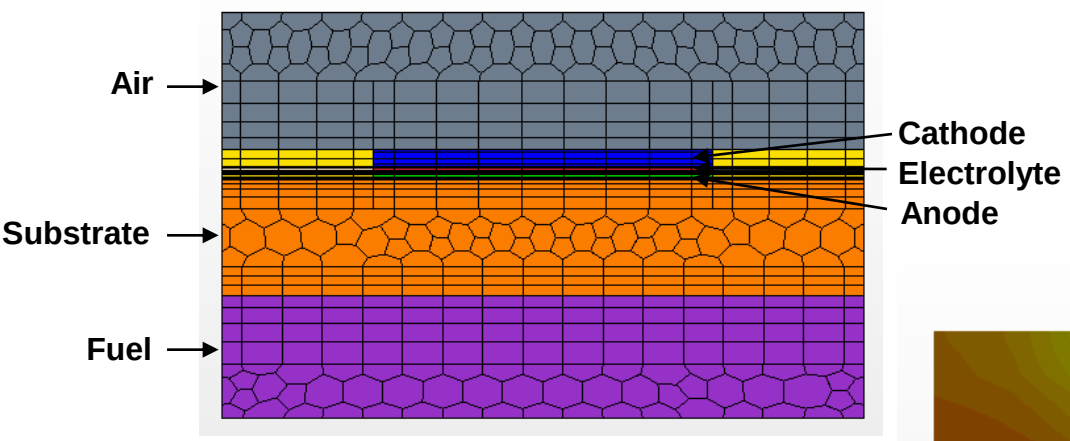
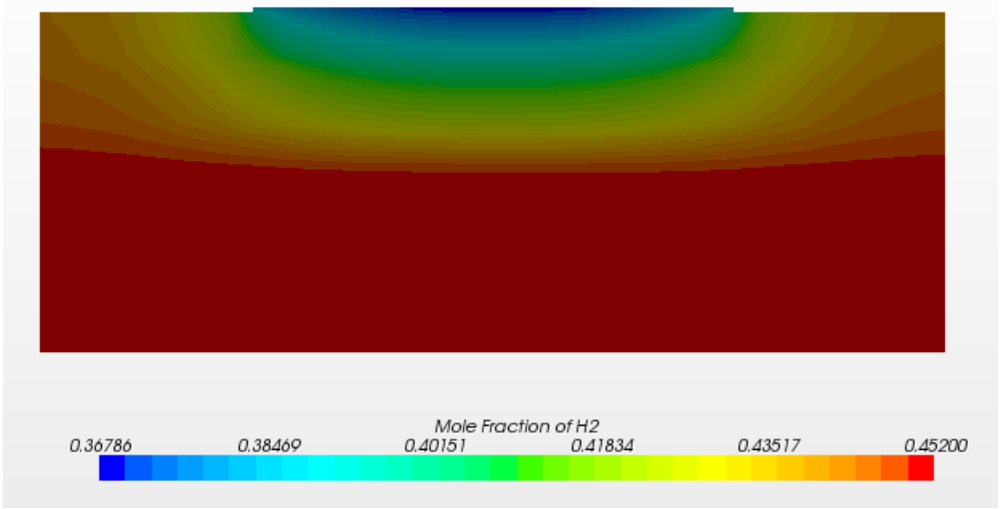
- **Validation**
- Conclusions

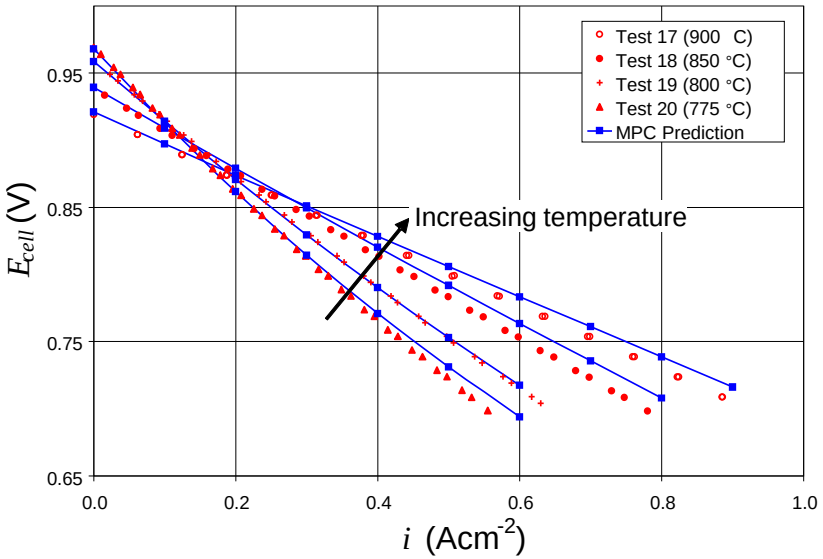
2D Single Cell Model Validation

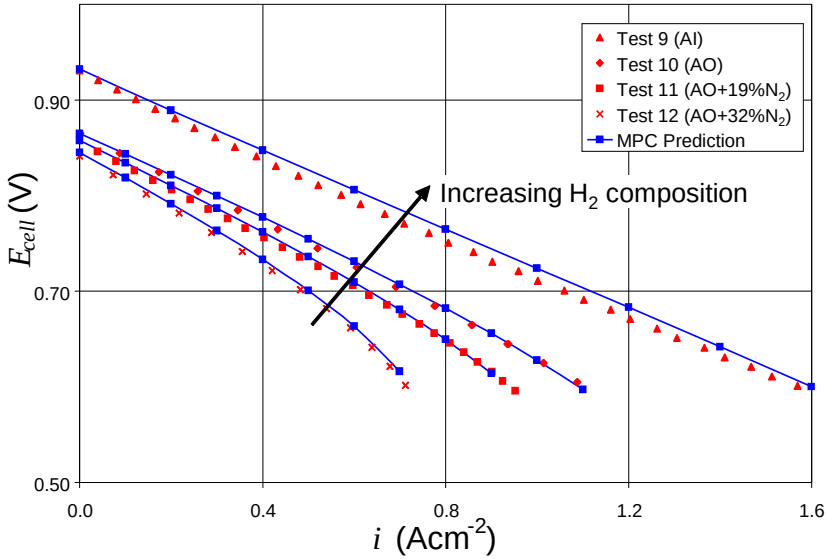
- 31 IV curve test matrix





Results



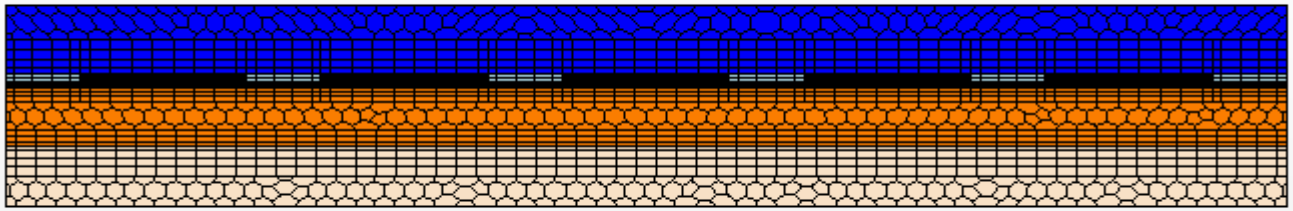


Mean Errors

E_{cell}(OCV): 0.3%, E_{cell}(Imax): 1.7%, ASR 4.4%

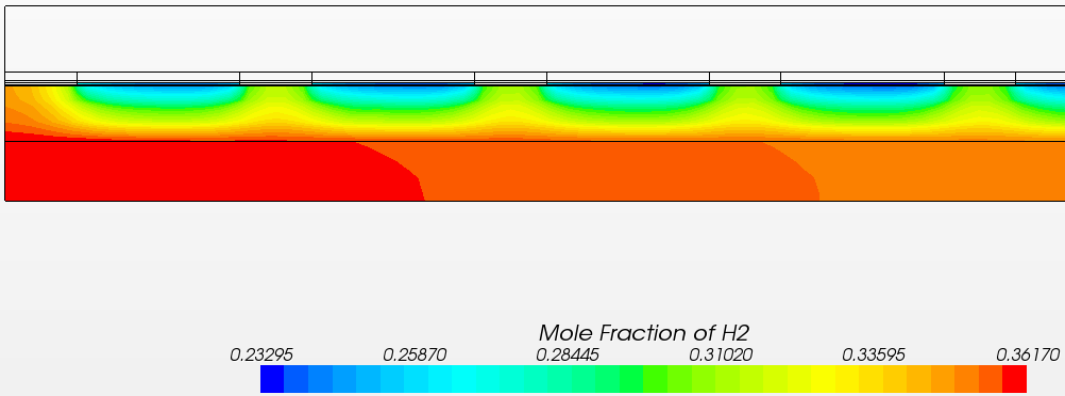
2D Penta Cell Model Validation

- **34 IV curve test matrix**



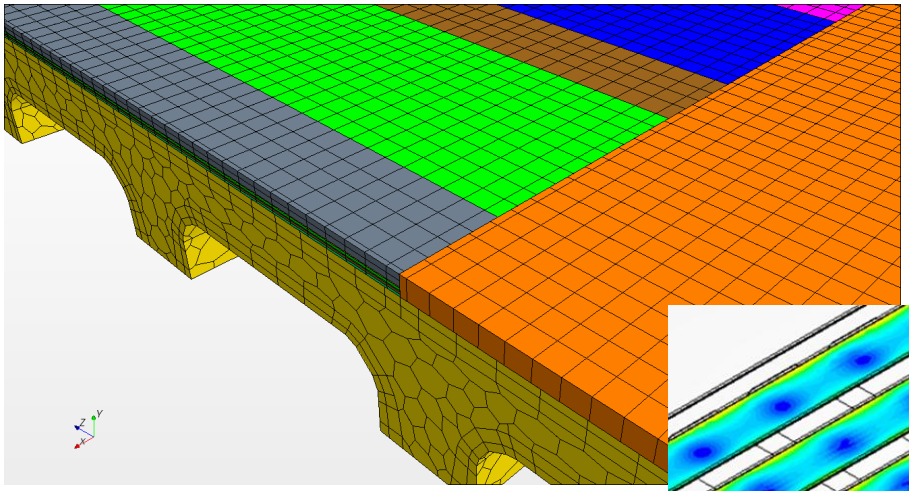
Mean Errors

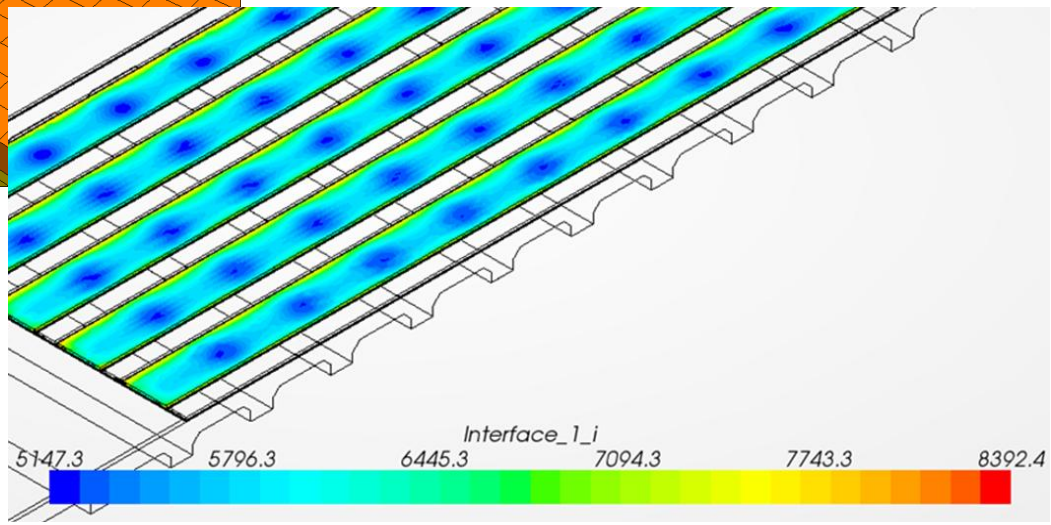
- E_{cell}(OCV): 0.7%
- E_{cell}(Imax): 1.8%
- ASR 6.0%



3D Penta Cell Model Validation

- **5 IV curve test matrix**



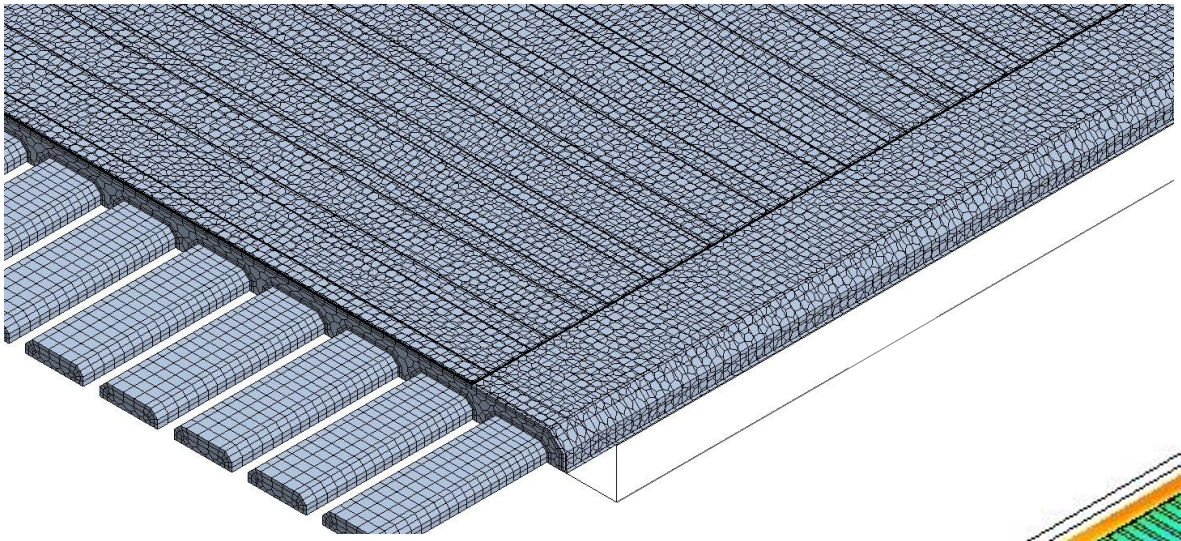


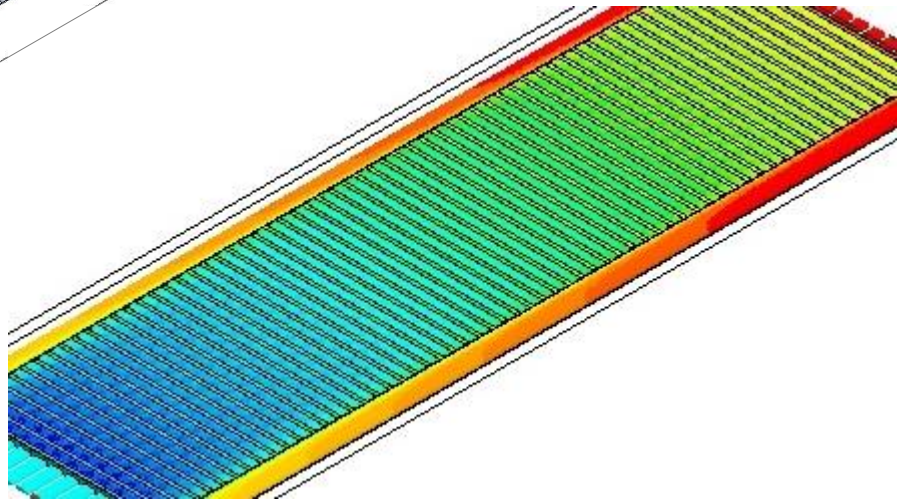
Mean Errors

- **Unchanged from 2D analysis**

3D Substrate Model Validation

- **Test matrix being built**





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Conclusions

RRFCS requires a design tool for detailed calculations

- **MPC being developed in commercial software**
  - **STAR-CCM+ (CD-adapco)**
  - **Customized for SOFC**
  - **Coupled SOFC physics**
  - **Automated operation**
- **Development on schedule**
  - **Code Release 3 complete**
  - **Models validated up to substrate level**
  - **Bundle validation underway**
- **Predictive capabilities being used by RRFCS**