



# Rolls-Royce

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

Ben Haberman, Carlos Martinez Baca, Greg Rush  
28 July 2011

**©2011 Rolls-Royce Fuel Cell Systems (US) Inc. This material is based upon work supported by the U.S. Department of Energy under Award Number DE-FE0000773.**

The information in this document is the property of Rolls-Royce Fuel Cell Systems (US) Inc. and may not be copied or communicated to a third party, or used for any purpose other than that for which it is supplied without the express written consent of Rolls-Royce Fuel Cell Systems (US) Inc.

This information is given in good faith based upon the latest information available to Rolls-Royce Fuel Cell Systems (US) Inc. No warranty or representation is given concerning such information, which must not be taken as establishing any contractual or other commitment binding upon Rolls-Royce Fuel Cell Systems (US) Inc. or any of its subsidiary or associated companies. This document does not contain any Export Controlled Data.

# Acknowledgements

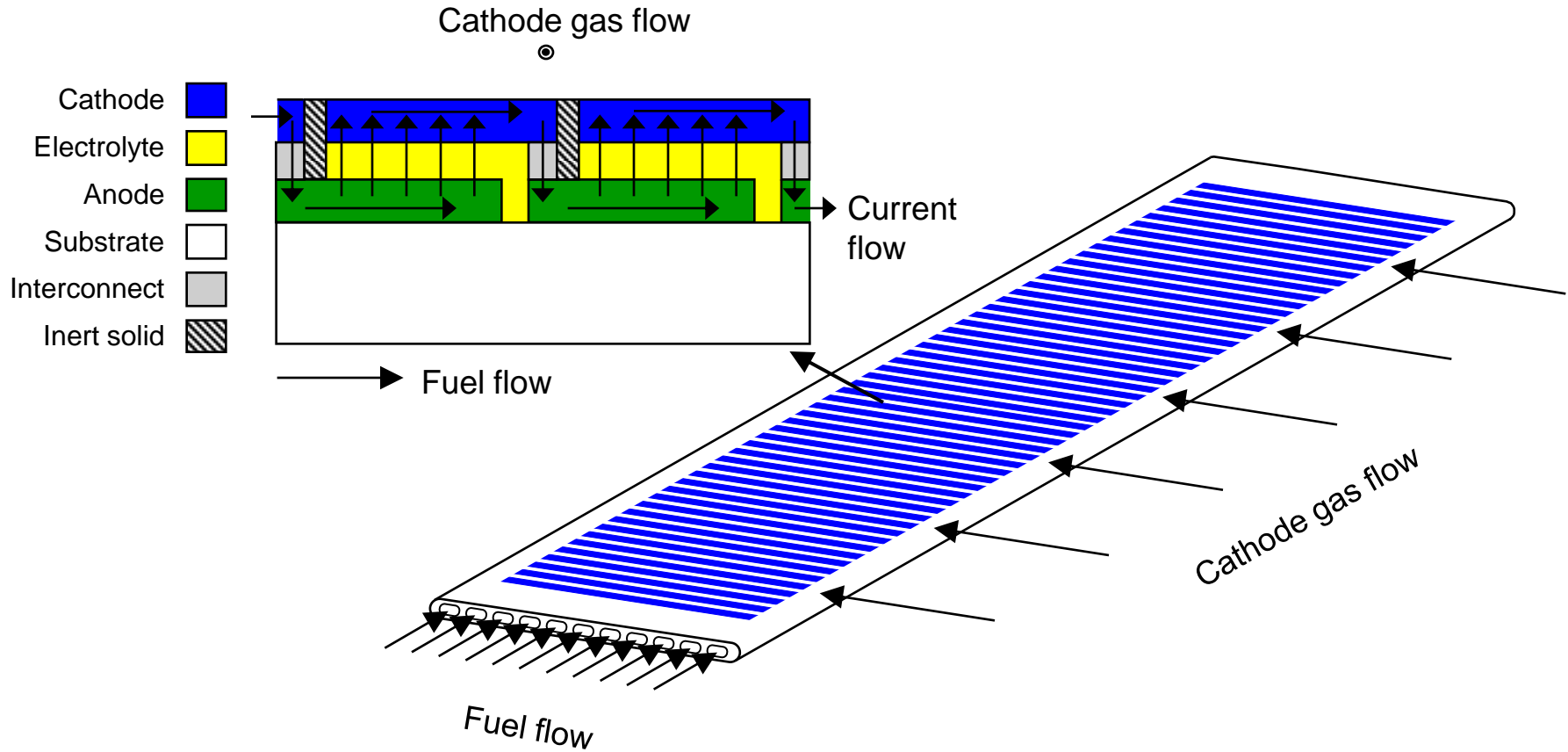
- **This material is based upon work supported by the Department of Energy National Energy Technology Laboratory under Award Numbers DE-FE0000773 and DE-FE0000303.**
- **DOE project manager Patcharin Burke**
- **UK and US based RRFCS team**

This material was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

# Overview

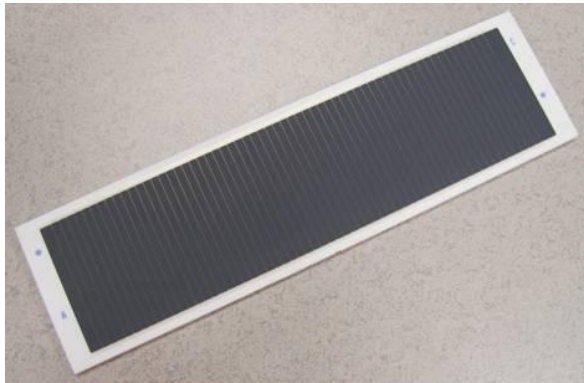
- **IP-SOFC Technology**
- **Project Objectives**
- **Work Program**
- **Multi-Physics Code Demo**
- **Validation**
- **Conclusions**

# IP-SOFC Technology

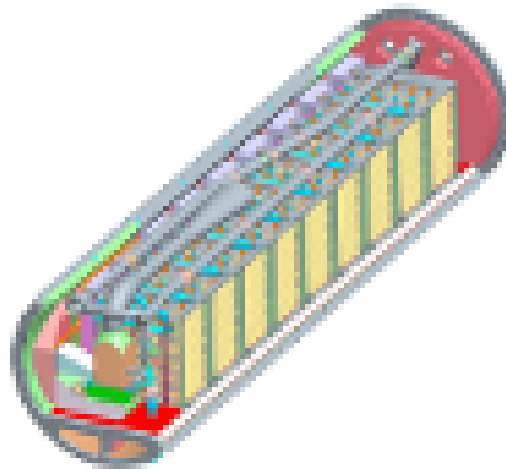
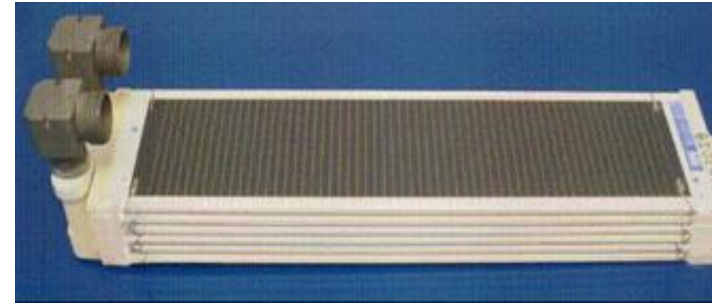


# Current Stack Configuration

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**
- Work Program
- Multi-Physics Code Demo
- Sample Results
- Conclusions

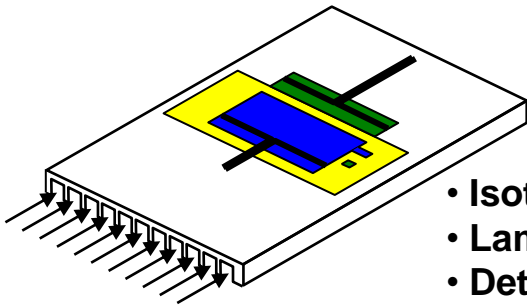
# MPC Objectives

- **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

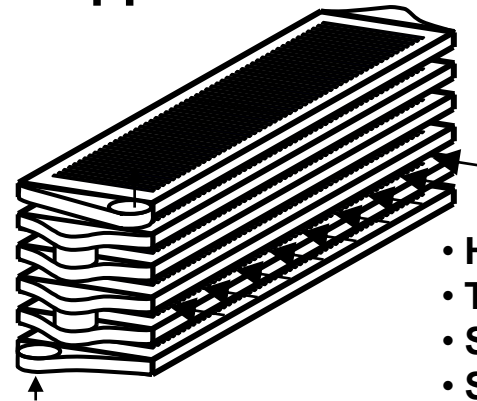


# Project Strategy

- 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



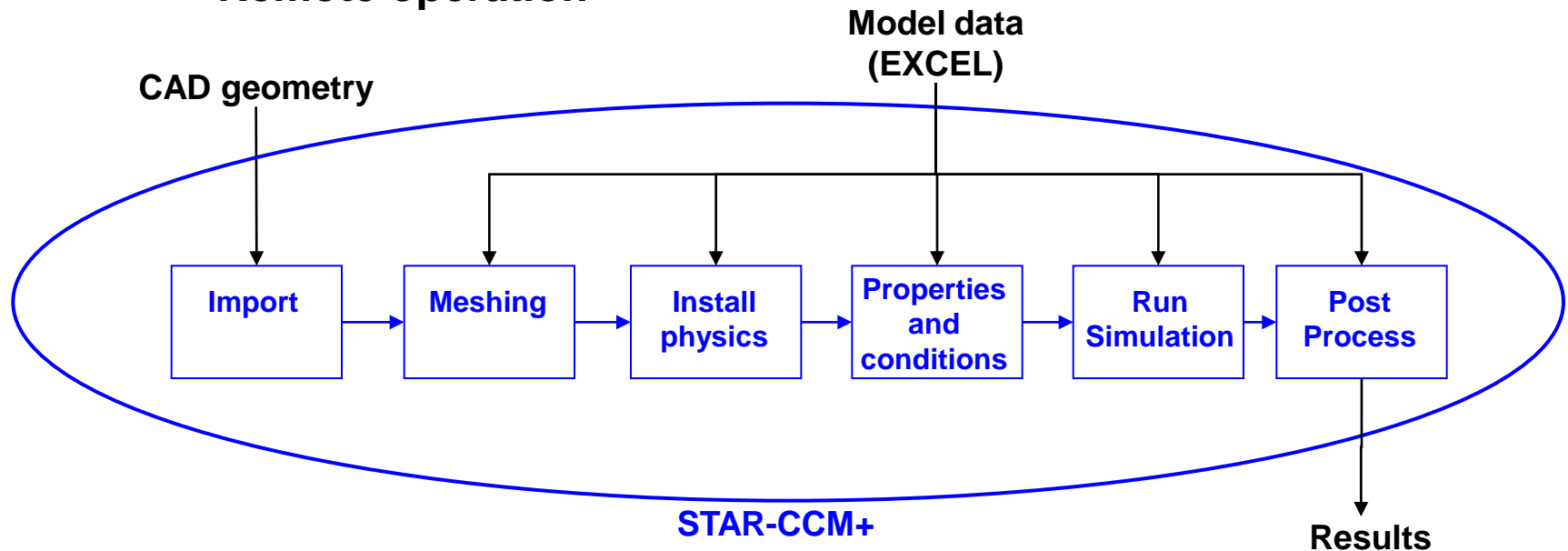
- Isothermal
- Laminar
- Detailed current flow
- Advanced chemistry



- 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







# Overview

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

# 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

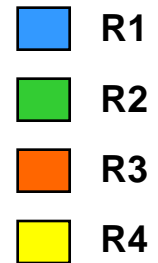
## Code Release

-  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



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**

# Overview

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

# EXCEL Simulation Spreadsheet

	A	B	C	Formula Bar	E	F	G	H
1	Simulation Spreadsheet Code Release 2							
2								
3	<b>Reference Terms</b>							
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 Electrochemical 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	<b>FF1 &amp; FF2 Species</b>							
19		Solid	Gases					
20	Physics1		H2	CO	NN	CO2	H2O	
21	Physics2	Solid1						
22	Physics3	Solid1						
23	Physics4		O2	N2				
24								
25	<b>FF1 &amp; FF2 Shear Conditions</b>							
26		Name	Shear on/off					
27		Shear1	off					
28								
29								
30								
31								
32	<b>FF1 &amp; FF2 Gas Conditions</b>							
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								

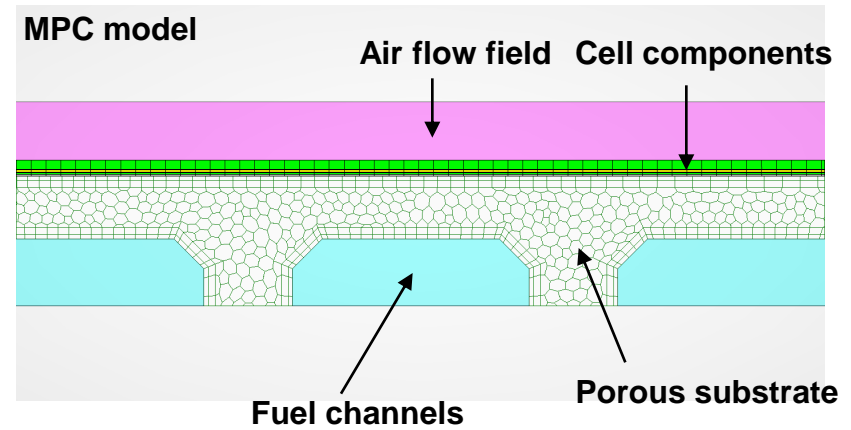
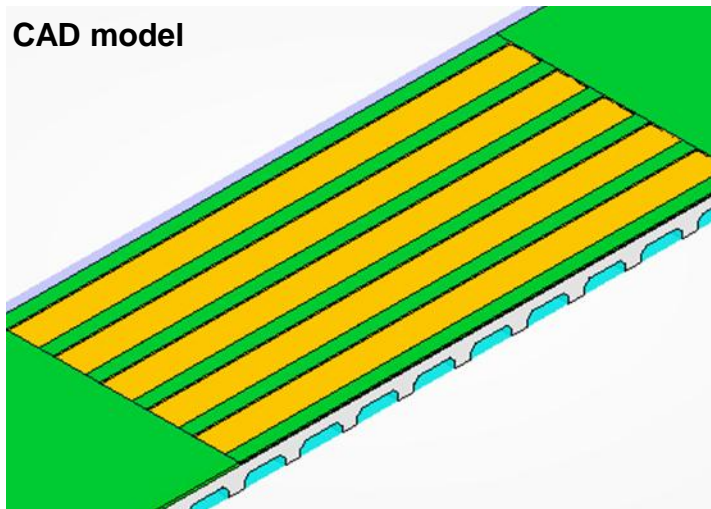
Sheet1 | Properties | Physics1 | Physics2 | Physics3 | Physics4 | InitialConditions | BoundaryConditions | TextData



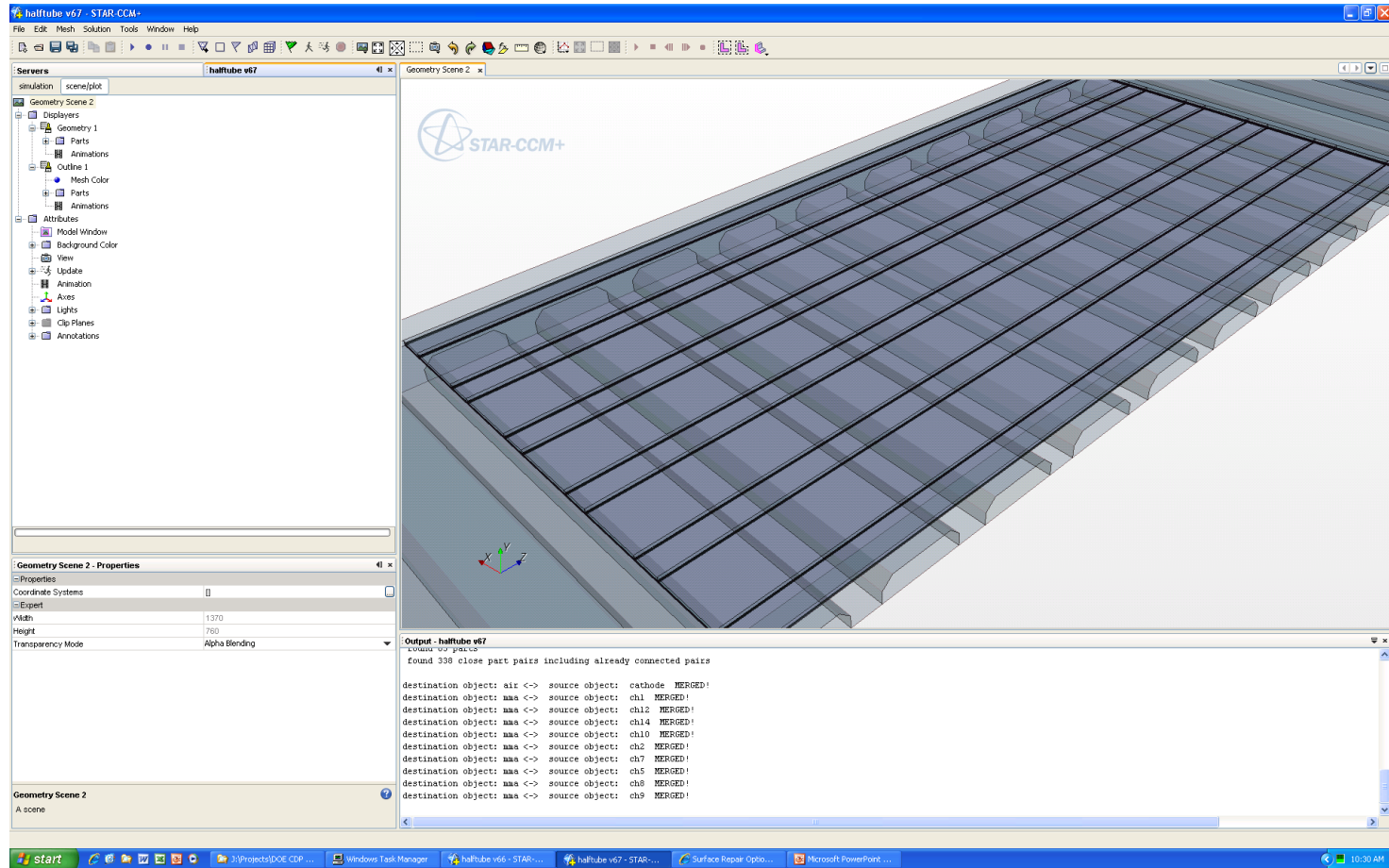
# Model

## Penta cell model

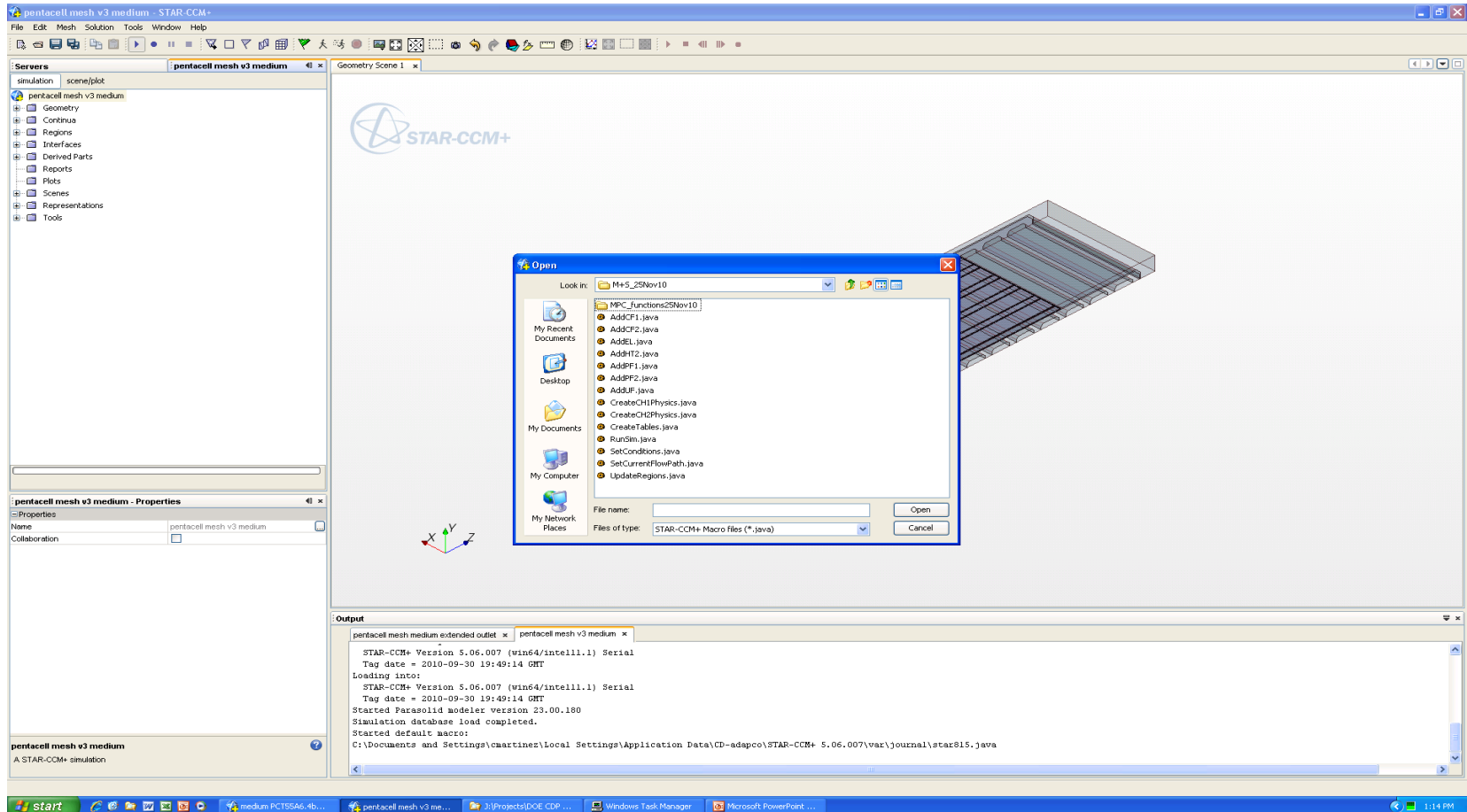
Consider only the active length of the tube  
Neglect the unused region



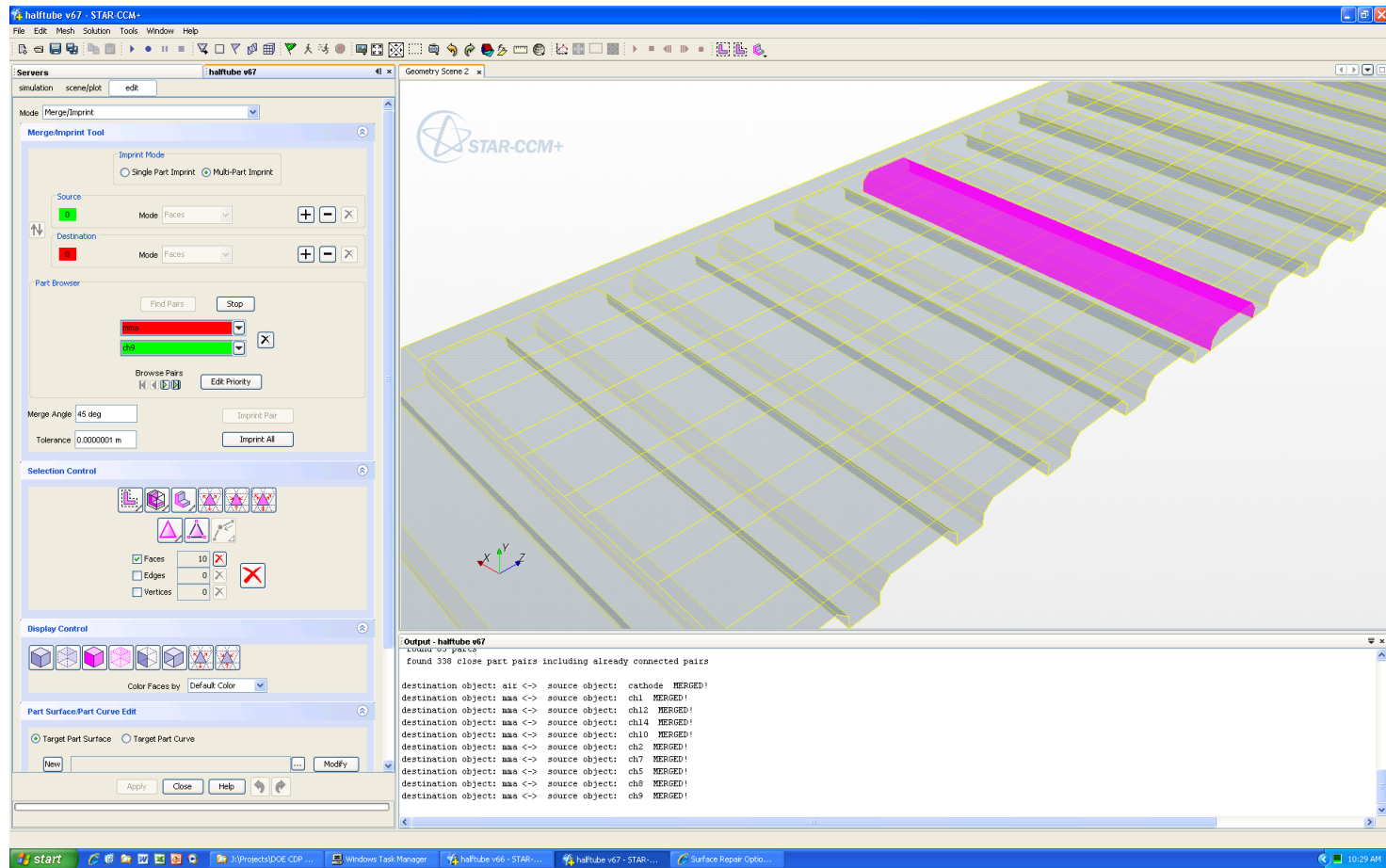
# STAR-CCM+



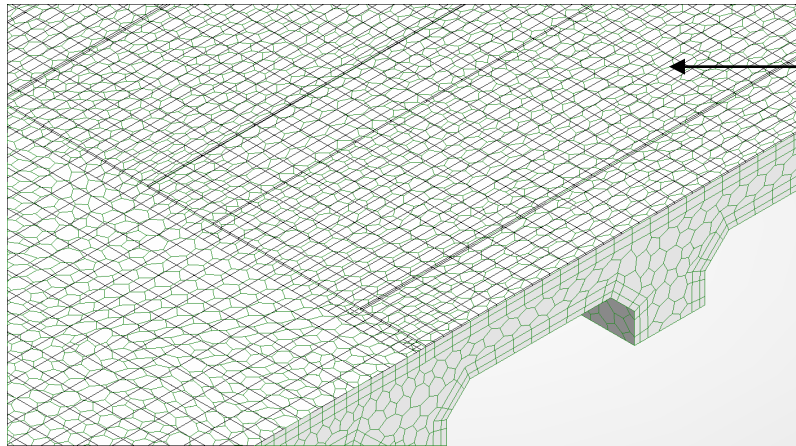
# STAR-CCM+ Macros



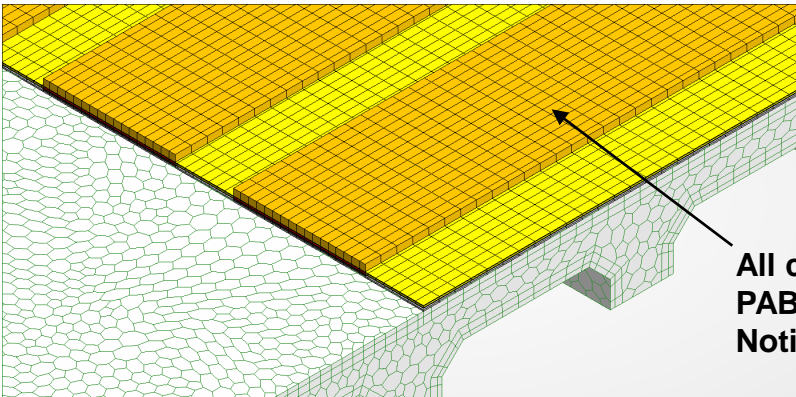
# Automatic Interface Creation



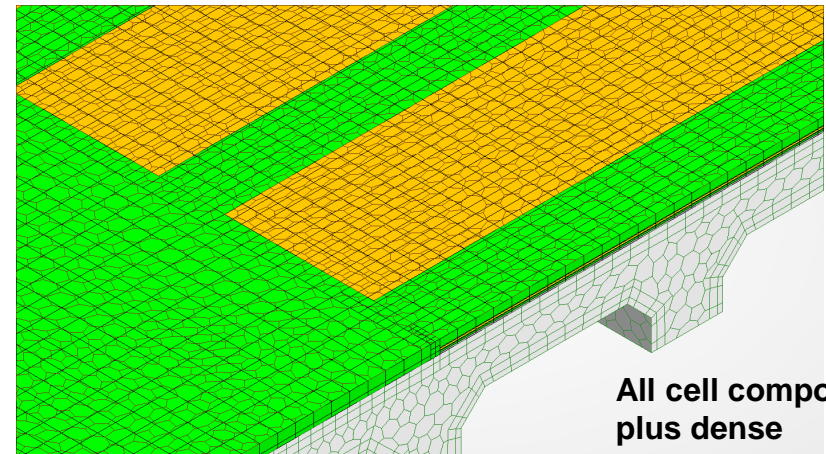
# Meshing Capability



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



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



All cell components plus dense

# STAR-CCM+ Output

The screenshot displays the STAR-CCM+ software interface. The main window shows the simulation output for a case named "medium PCT55A6.4bar run sim". The output log contains the following text:

```

211
212 Adding PartSurface_ivia 15_electrolyte 3 [electrolyte 3/ivia 15] Part to Internal Table: Interface2C
213 Setting Conditions on "PartSurface_ivia 15_electrolyte 3 [electrolyte 3/ivia 15]" Boundary of Region CCC2
214 Setting Conditions on "Default 3 [cathode 3/ivia 15]" Boundary of Region Cathode
215 Setting Electric Potential Specification to Specific Electric Current
216 Specific Electric Current set to field function I_2A_E_BFlux
217 Setting Wall Species Option to Specified Flux
218 ScalarProfile set to field function I_2C_O2Flux
219 Adding PartSurface_ivia 15_electrolyte 3 [electrolyte 3/ivia 15] Part to Internal Table: Interface2A
220 Adding PartSurface_electrolyte 3_ivia 15 [electrolyte 3/ivia 15] Part to Internal Table: Interface2B
221 Adding PartSurface_ivia 15_electrolyte 3 [electrolyte 3/ivia 15] Part to Internal Table: ASR2
222 Adding Default 3 [cathode 3/ivia 15] Part to Internal Table: Interface2C
223 Setting Conditions on "PartSurface_ivia 20_electrolyte 4 [electrolyte 4/ivia 20]" Boundary of Region CCC3
224 Setting Conditions on "PartSurface_electrolyte 4_ivia 20 [electrolyte 4/ivia 20]" Boundary of Region Electrolyte3
225 Setting Conditions on "Default [cathode 4/ivia 20]" Boundary of Region Cathode
226 Setting Electric Potential Specification to Specific Electric Current
227 Specific Electric Current set to field function I_2A_E_BFlux
228 Setting Wall Species Option to Specified Flux
229 ScalarProfile set to field function I_2C_O2Flux
230 Adding PartSurface_ivia 20_electrolyte 4 [electrolyte 4/ivia 20] Part to Internal Table: Interface2A
231 Adding PartSurface_electrolyte 4_ivia 20 [electrolyte 4/ivia 20] Part to Internal Table: Interface2B
232 Adding PartSurface_ivia 20_electrolyte 4 [electrolyte 4/ivia 20] Part to Internal Table: ASR2
233 Adding Default [cathode 4/ivia 20] Part to Internal Table: Interface2C
234 Setting Conditions on "PartSurface_ivia 25_electrolyte 5 [electrolyte 5/ivia 25]" Boundary of Region CCC4
235 Setting Conditions on "PartSurface_electrolyte 5_ivia 25 [electrolyte 5/ivia 25]" Boundary of Region Electrolyte4
236 Setting Conditions on "Default 2 [cathode 5/ivia 25]" Boundary of Region Cathode
237 Setting Electric Potential Specification to Specific Electric Current
238 Specific Electric Current set to field function I_2A_E_BFlux
239 Setting Wall Species Option to Specified Flux
240 ScalarProfile set to field function I_2C_O2Flux
241 Adding PartSurface_ivia 25_electrolyte 5 [electrolyte 5/ivia 25] Part to Internal Table: Interface2A
242 Adding PartSurface_electrolyte 5_ivia 25 [electrolyte 5/ivia 25] Part to Internal Table: Interface2B
243 Adding PartSurface_ivia 25_electrolyte 5 [electrolyte 5/ivia 25] Part to Internal Table: ASR2
244 Adding Default 2 [cathode 5/ivia 25] Part to Internal Table: Interface2C
245
246 Searching for boundaries named "air sym"
247 Conditions for boundaries named "air sym" being set, 1 instances found
248 Setting Wall Shear boundary condition
249 Setting Conditions on "air sym" Boundary of Region Air
250 Setting Shear Stress Specification to Slip
251
252 Searching for boundaries named "fuel sym"
253 Conditions for boundaries named "fuel sym" being set, 1 instances found
254 Setting Wall Shear boundary condition
255 Setting Conditions on "fuel sym" Boundary of Region Channel
256 Setting Shear Stress Specification to Slip
257
258 Searching for boundaries named "air sides"
259 Conditions for boundaries named "air sides" being set, 1 instances found
260 Setting Wall Shear boundary condition
261 Setting Conditions on "air sides" Boundary of Region Air
262 Setting Shear Stress Specification to Slip

```

Below the output log, an error report is displayed:

```

-----Error Report-----
Errors Found: 2
Line      Intent      Message
94         5           VoltBC_1607 Field Function already exists
102        5           CurrentBC_1751 Field Function already exists

```

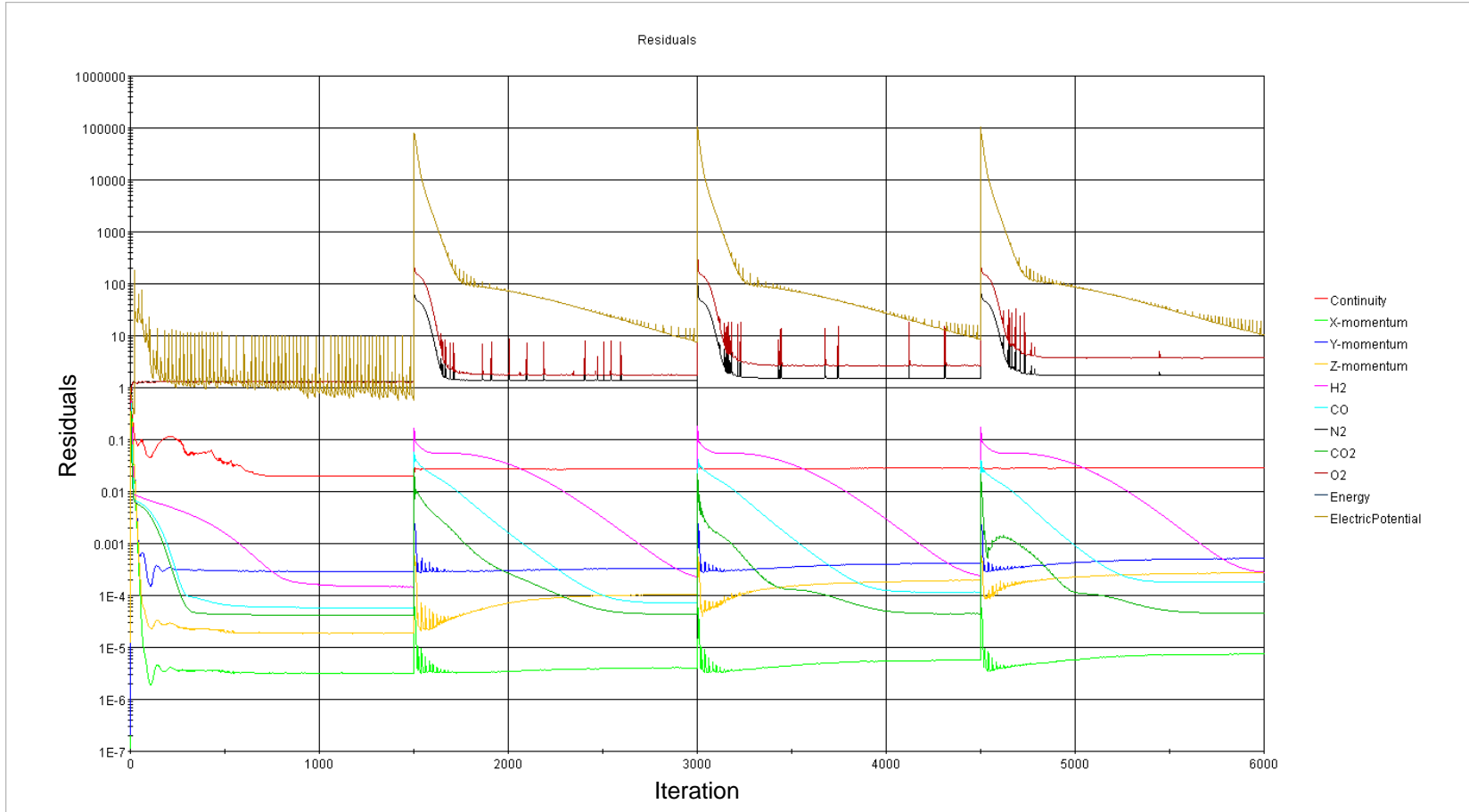
The interface also shows a "Servers" panel on the left with a tree view of the simulation hierarchy, including Geometry, Continuum, Regions, Interfaces, Derived Parts, Solvers, Stopping Criteria, Reports, Monitors, Plots, Scenes, Representations, and Tools. A "Properties" panel is visible at the bottom left, showing the simulation name and collaboration status. The Windows taskbar at the bottom indicates the system time as 1:18 PM.

# 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<sup>-2</sup>



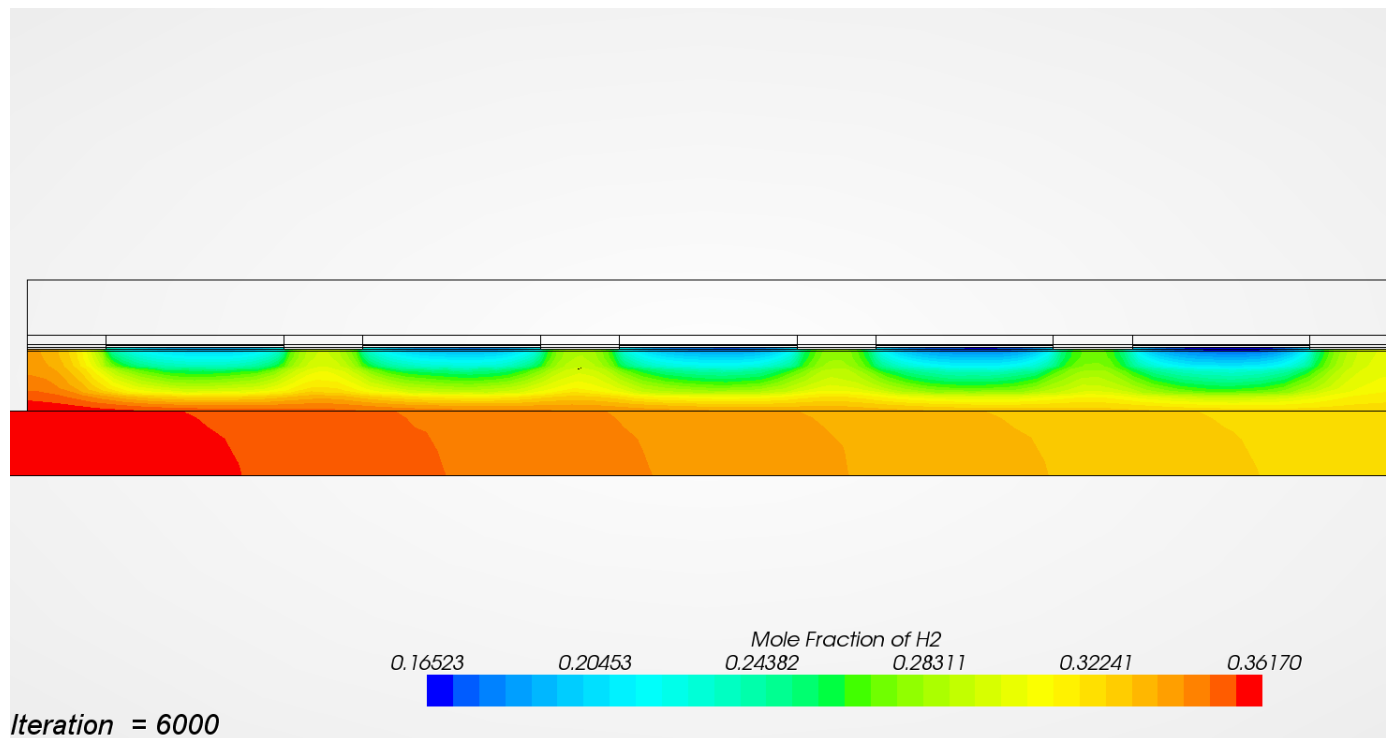


# Hydrogen Mole Fraction

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.

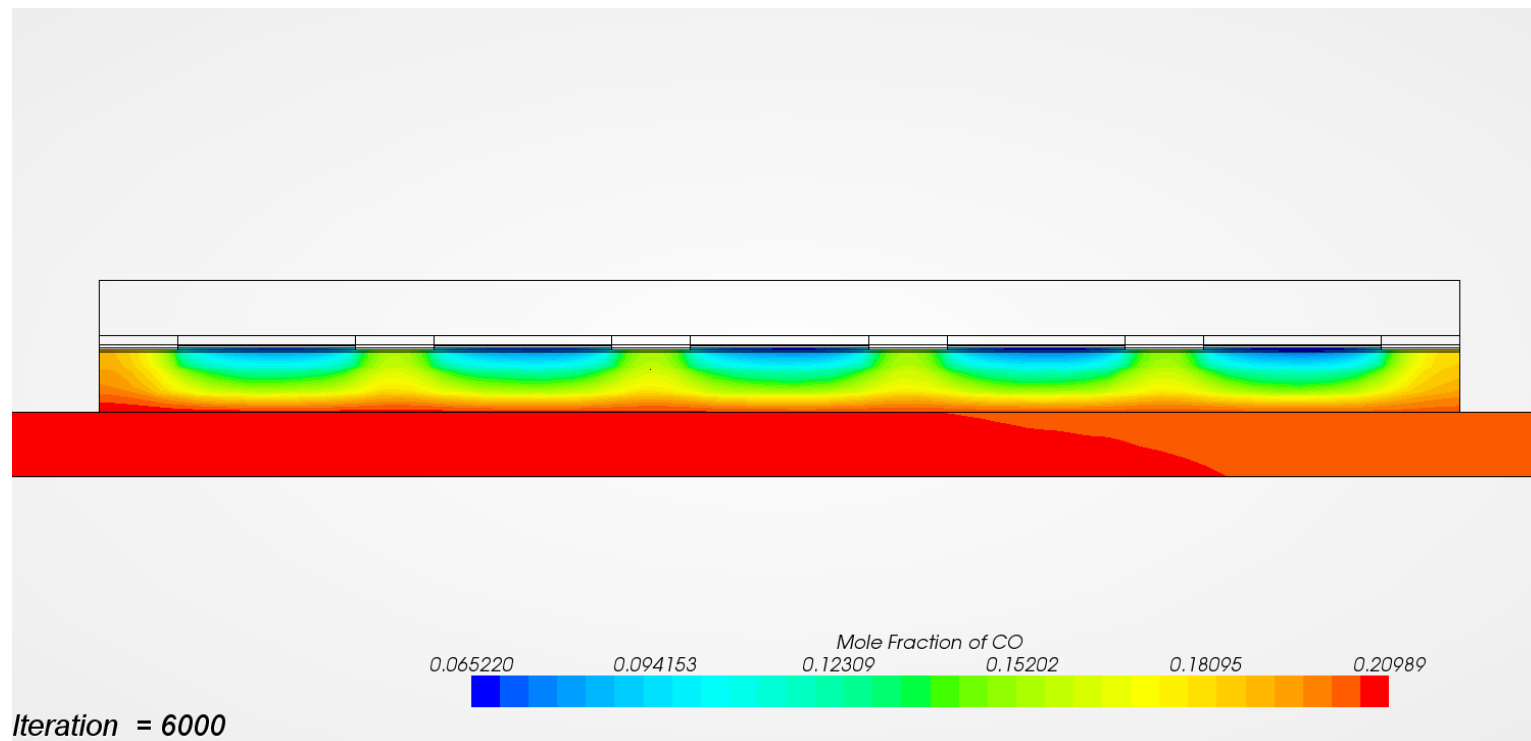
Variations in hydrogen mole fraction confined to porous regions where flow resistance is high.



# Carbon Monoxide Mole Fraction

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

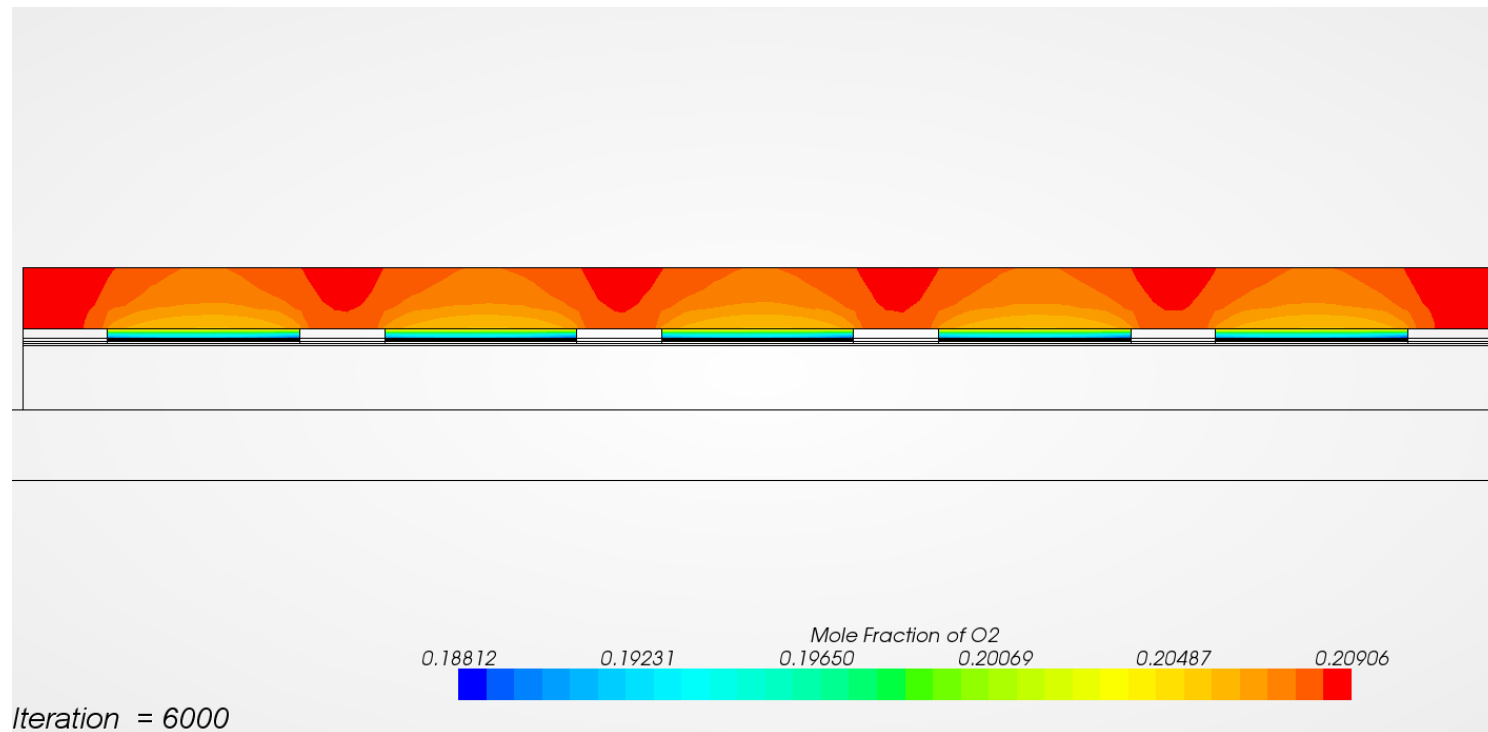
Section planes across and along the tube show carbon monoxide diffusing across the porous substrate towards the cell layers.



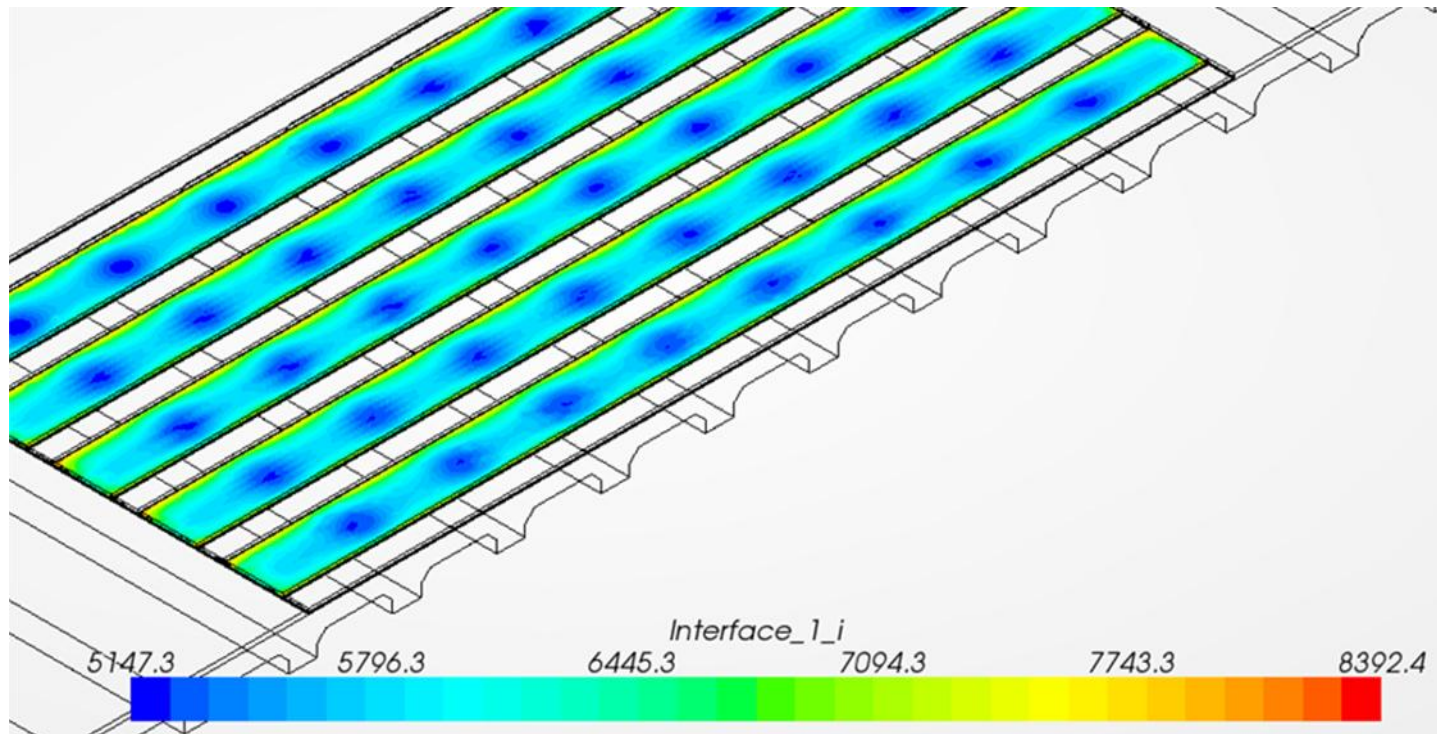
# Oxygen Mole Fraction

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

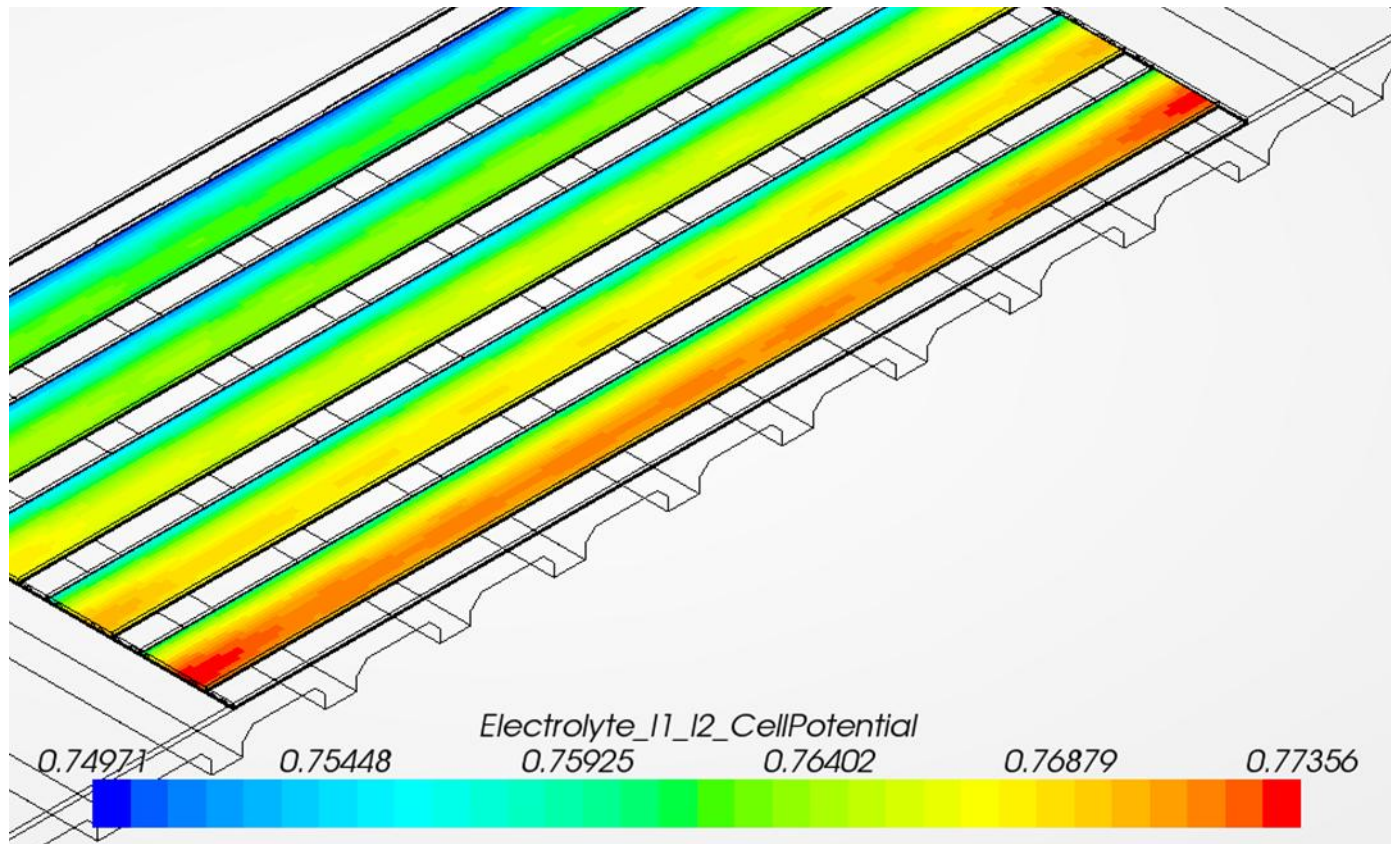
Section planes across and along the tube shows gradient of oxygen decreasing along the air flow field and how its mole fraction is reduced near the cell regions.



# Current Density Distribution



# Cell Potential

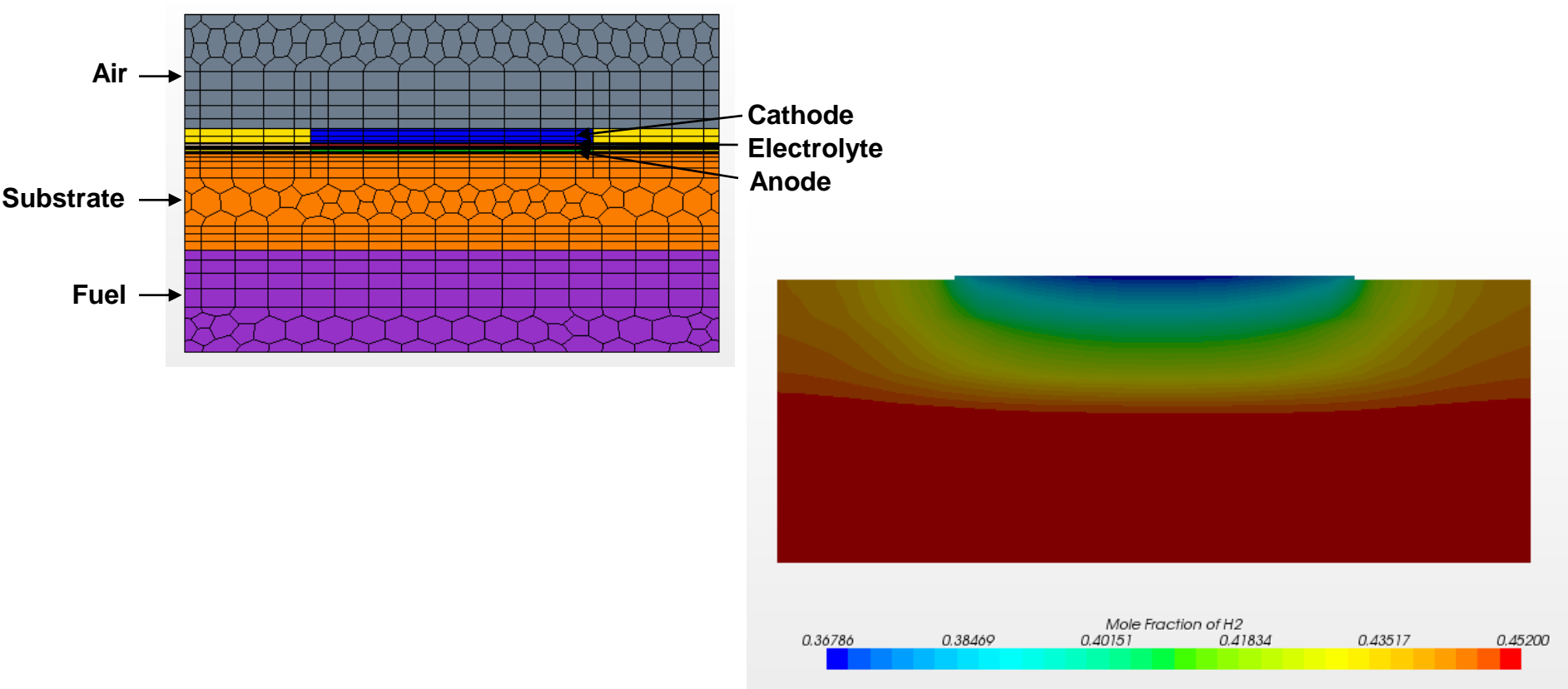


# Overview

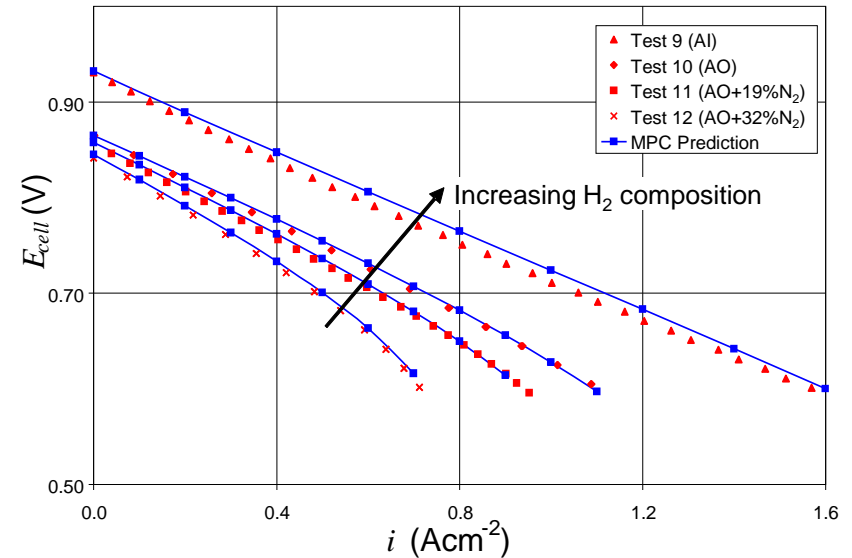
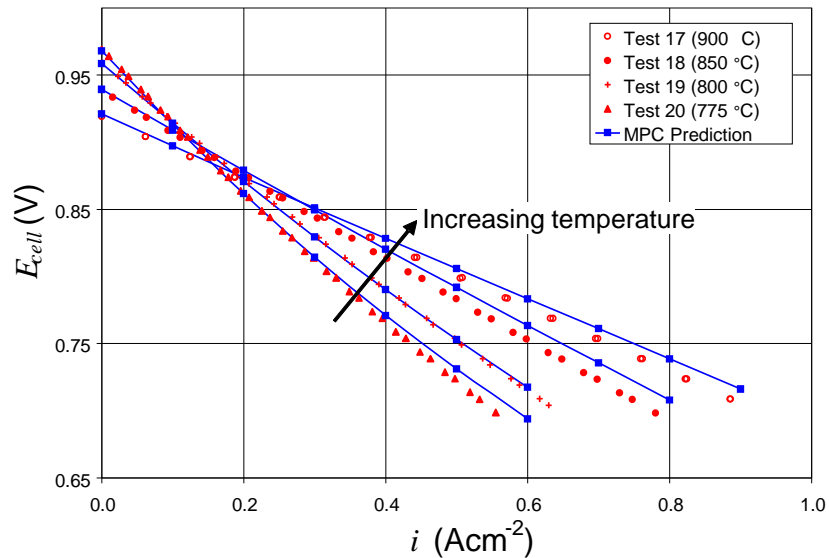
- IP-SOFC Technology
- Project Objectives
- Work Program
- Multi-Physics Code Demo
- **Validation**
- Conclusions

# 2D Single Cell Model Validation

- 31 IV curve test matrix



# Results



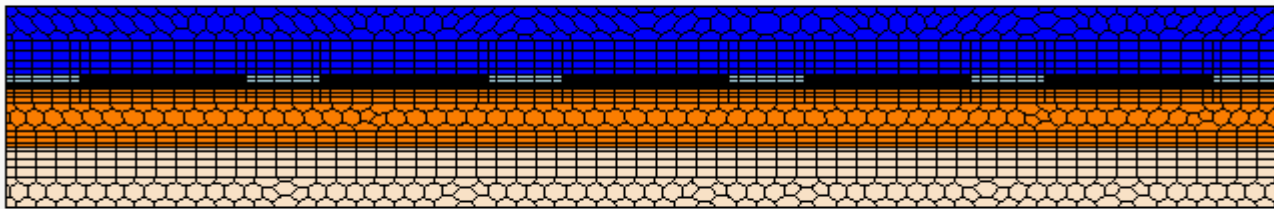
## Mean Errors

$E_{cell}(\text{OCV})$ : 0.3%,  $E_{cell}(\text{I}_{max})$ : 1.7%, ASR 4.4%



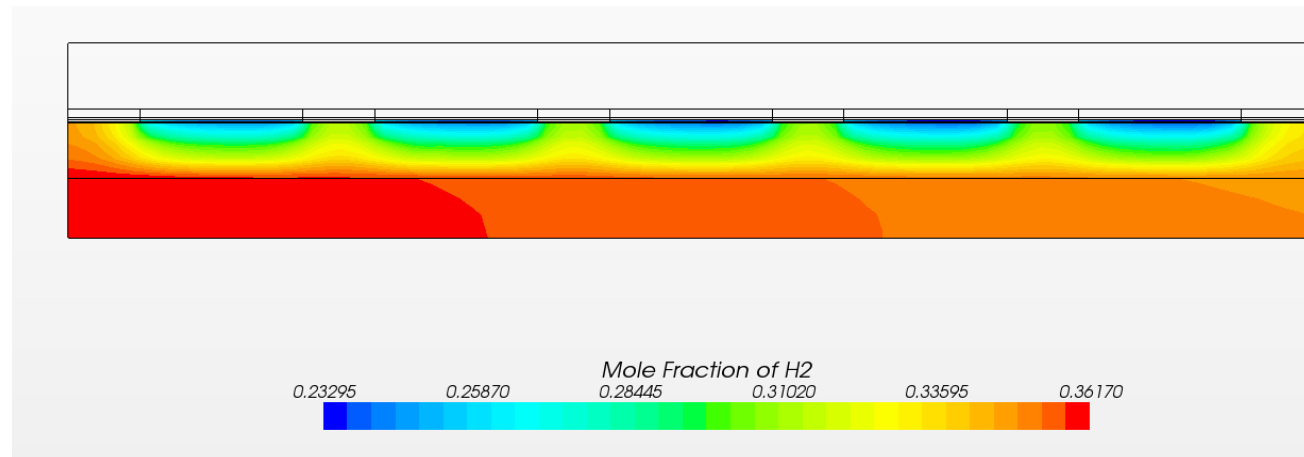
# 2D Penta Cell Model Validation

- 34 IV curve test matrix



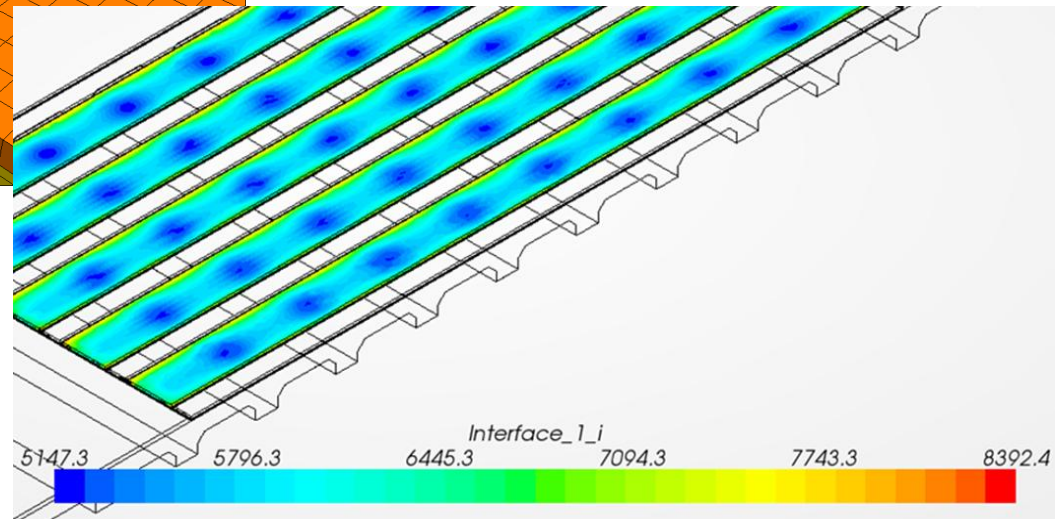
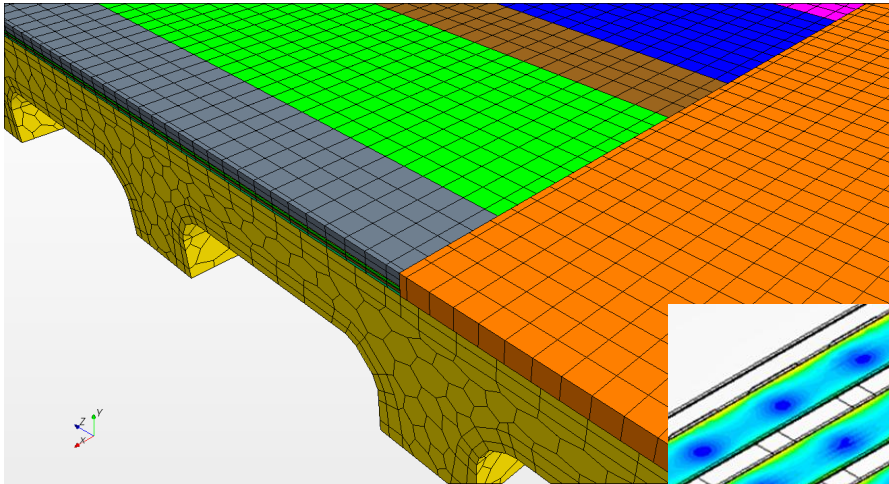
## Mean Errors

- $E_{\text{cell}}(\text{OCV})$ : 0.7%
- $E_{\text{cell}}(\text{I}_{\text{max}})$ : 1.8%
- ASR 6.0%



# 3D Penta Cell Model Validation

- 5 IV curve test matrix

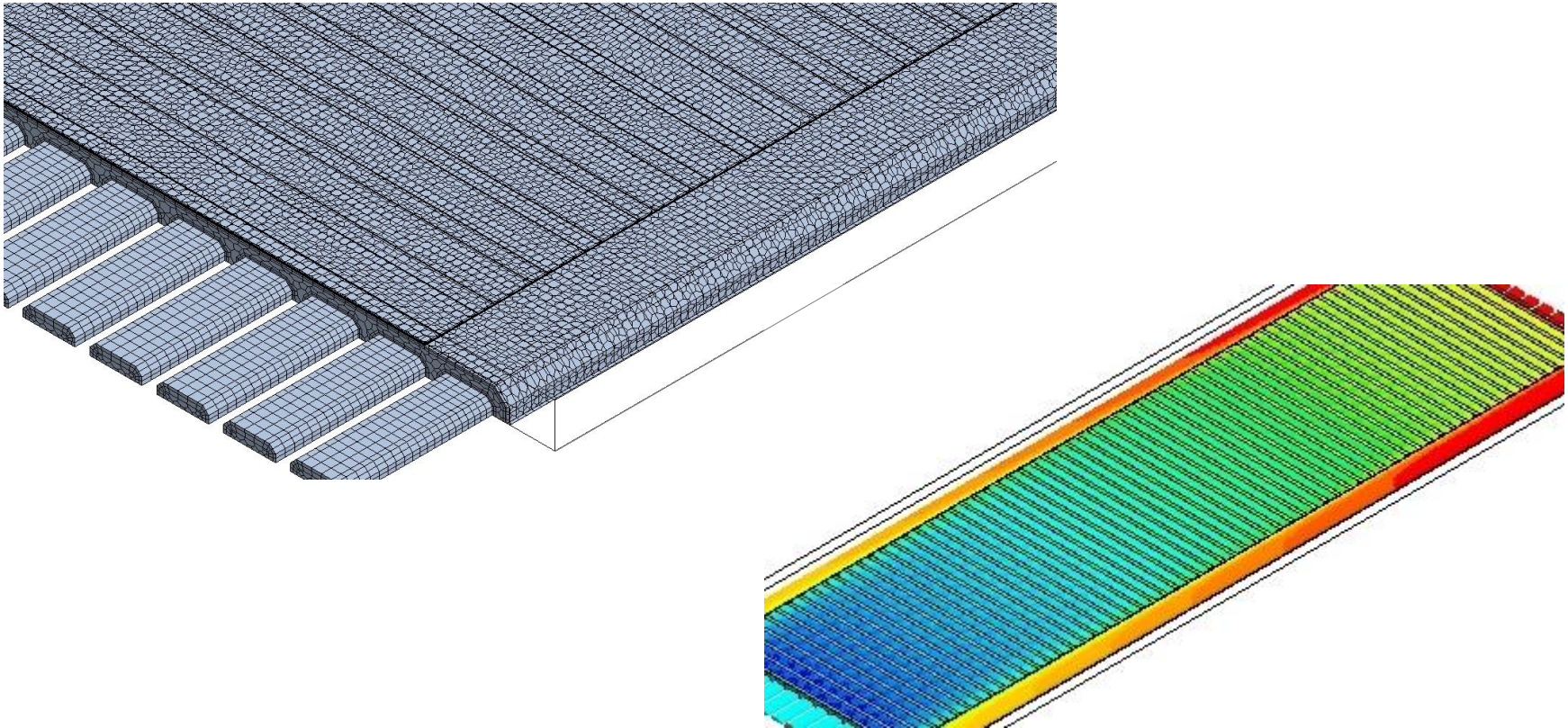


## Mean Errors

- Unchanged from 2D analysis

# 3D Substrate Model Validation

- Test matrix being built



# Overview

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

# 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**