

# CD adapco Group OVERVIEW



CD adapco  
Group

# The CD adapco Group in Short

The CD adapco Group is a global partnership of companies specializing in CFD software as well as industrial computer aided engineering (CAE) services. Our mission is to be a full service provider of software tools and engineering services to assist our clients in integrating virtual technology into their overall engineering process.

Our main centers, adapco in New York and Computational Dynamics Ltd in London are involved in the development of the industrial CFD code, STAR-CD, as well as several innovative new CFD codes and associated CAE tools. Over 400 experienced professional staff and CFD specialists are employed, We have subsidiary offices providing local CFD support, training and CFD/CAE consultancy and engineering services throughout the world.



# WORLD-WIDE CD adapco Group ORGANIZATION

- Established in 1980 - 1987
  - Global staff of 400 researchers and engineers, 50% with PhD
    - Development 30%
    - Technical support and engineering services 40%
    - Sales and Marketing 20%
  - Computational Dynamics Ltd
    - Head quarters in London
    - 3 offices in Europe
    - 1 office in USA
  - adapco
    - 5 offices in USA
  - CD-adapco Japan
    - 2 offices in Japan
    - 1 office in China
  - CD-adapco France
  - CD-adapco Korea
  - Agents and distributors throughout the rest of the world
- Global user base of over 3000
  - Annual turnover of over \$40,000,000
  - Average annual growth of around 20%
  - Largest supplier of CFD technology to the automotive industry
  - Largest supplier of CFD technology in Germany and Japan
  - Second largest supplier of CFD technology in the world
  - Group's long-term aim is to remain the best CFD technology supplier on the market
    - Recognizing the changing needs of the industrial users
    - Developing the best tools to address the industrial users needs



# About adapco

## Organization

CFD Consulting Group providing flow and thermal analyses using CFD tools and methods

FEA Consulting Group providing thermal, structural, and dynamic analyses using FEA methods

Advanced Methods Development Group providing leading edge analysis method development and solutions for multi-physics and other challenging applications

Software Development Group providing general purpose and application specific pre- and post-processing tools

Software Sales Group providing software licenses, training, and user support for engineering software

*adapco's Quality System is certified as conforming to the ISO 9001 standard. Our certification extends to all five of adapco's service groups.*



# adapco CFD Applications Group

**adapco's CFD Applications Group provides World Class analysis support to New Product Development and Product Upgrade Design Teams**

**Support includes**

- **Flow path performance evaluation and optimization**
- **Heat transfer analysis to predict temperatures or provide Boundary Conditions for FEA analyses**
- **Specialty applications such as reacting, fluid-solid interaction, and two-phase flows**

## **CFD Group Make-up**

- **Degrees in Mechanical or Aerospace Engineering with concentrations in CFD or Numerical Heat Transfer**
- **60% Master's Degrees, 30% PhD, 10% Bachelor's Degrees**
- **Members of the group have an average of nine years experience in CFD with an average of five years at adapco**



# INDUSTRIAL LINKS AND PARTNERSHIPS

- **ENGINSOFT**
  - FRONTIER (optimization)
- **FLOWMASTER International**
  - FLOWMASTER (1D/3D coupling)
- **Gamma Technology**
  - GT-Power (1D/3D coupling)
- **INTES**
  - PERMAS (fluids structures interaction)
- **LMS International**
  - SYSNOISE (aeroacoustics)
- **Collins and Aikman**
  - COMET ACOUSTICS
- **Reaction Design**
  - CHEMKIN (complex chemistry)
- **Siemens Axiva**
  - MiXpert (mixing vessels simulation)

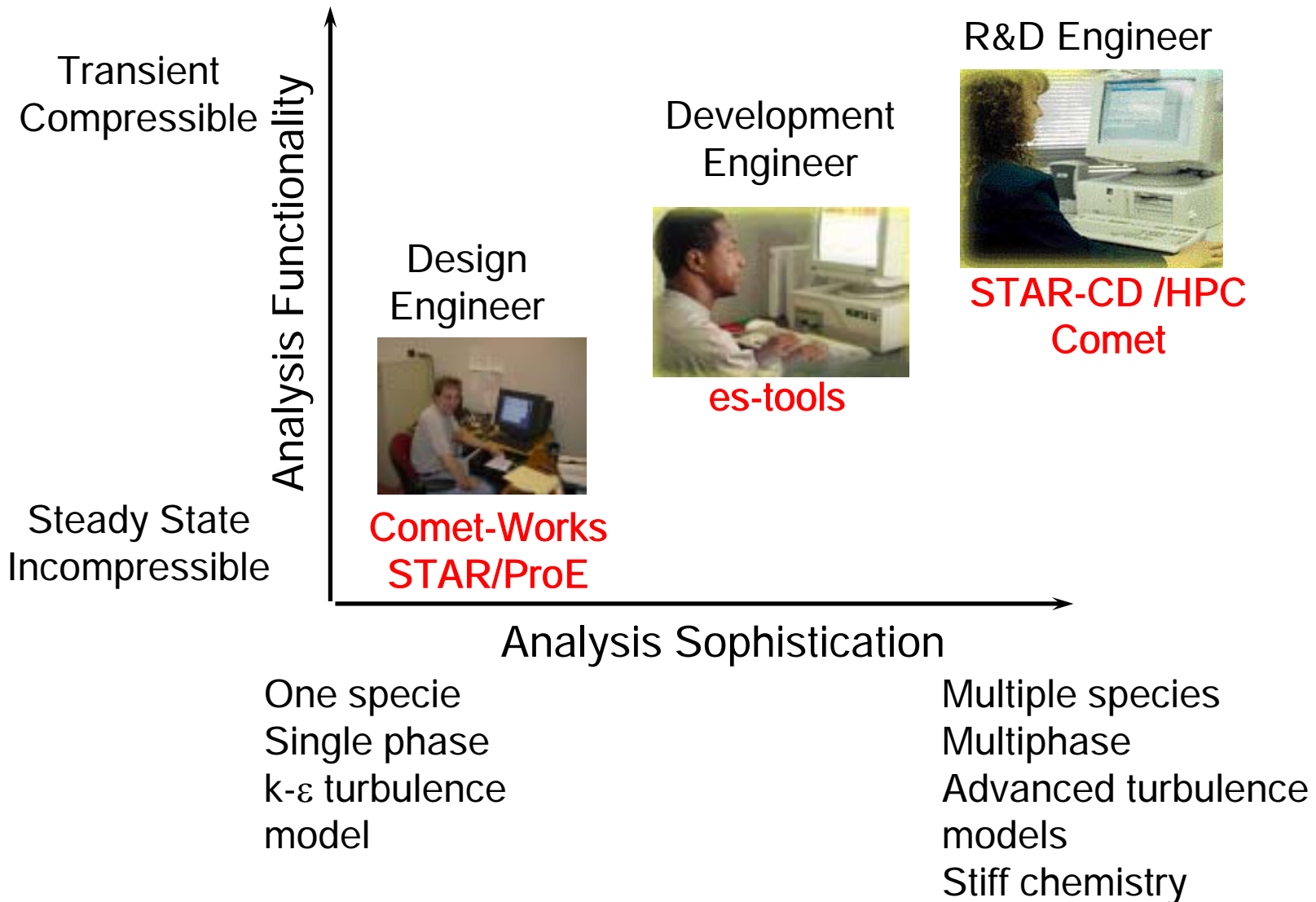


# ACADEMIC LINKS AND PARTNERSHIPS

- **Imperial College**
  - General CFD technology
- **U Hamburg-Harburg**
  - Marine hydrodynamics
- **U Karlsruhe**
  - Aeroacoustics
- **Penn State University**
  - Aeroacoustics
- **U Leeds**
  - Combustion technology
- **UMIST**
  - Turbulence modeling technology
- **RWTH-Aachen**
  - Combustion technology
- **TU Berlin**
  - Turbulence modeling, aeroacoustics
- **U South Carolina**
  - PEM Fuel cell technology
- **U Stanford**
  - Turbulence modeling technology
- **U Wisconsin**
  - Combustion technology
- **U Nevada Las Vegas**
  - Surface chemistry technology



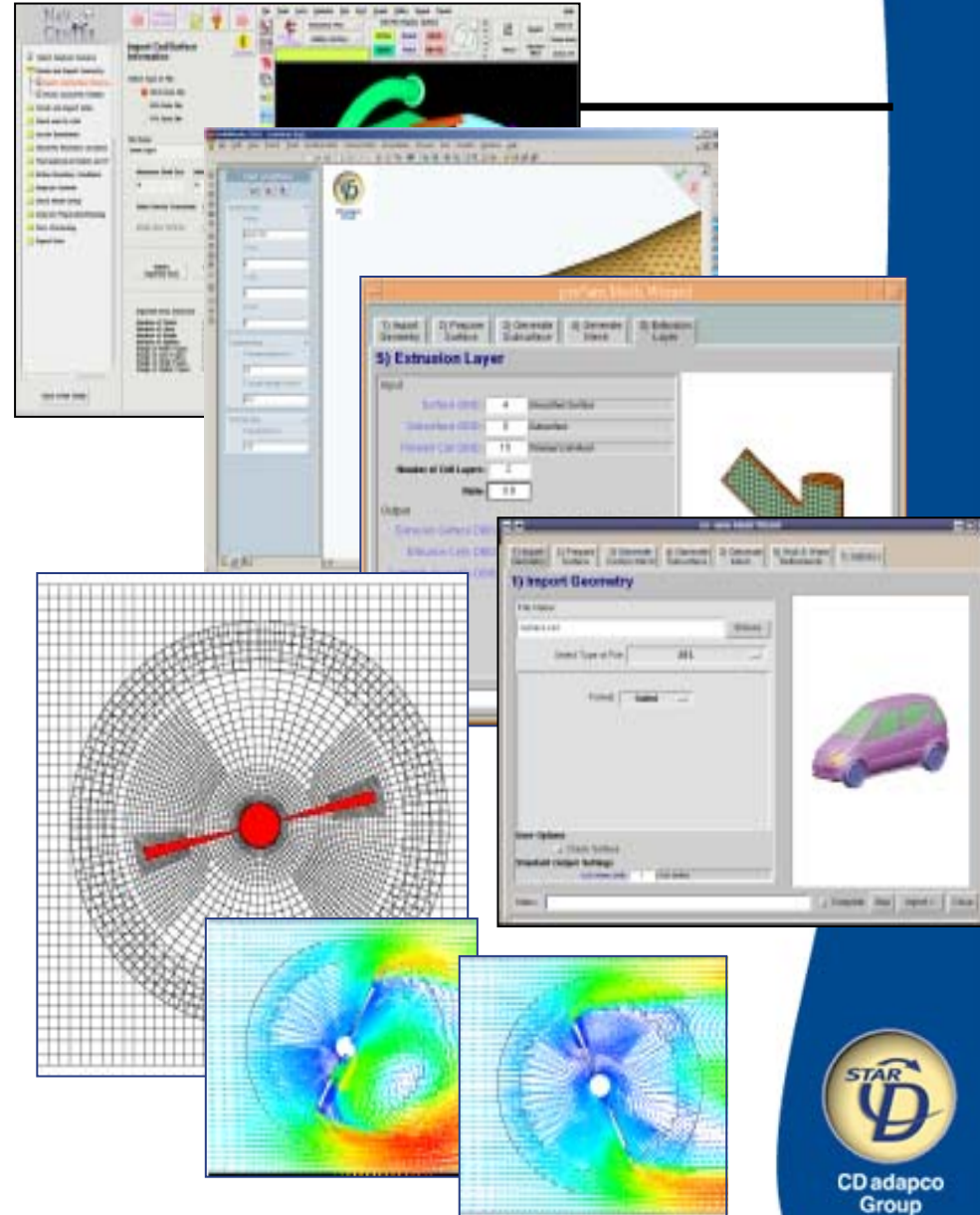
# PRODUCT POSITIONING





# ADDRESSING THE NEEDS OF INDUSTRY

- Easy to use and learn and graphical use interface
  - Both general and application specific
- Flexible CAD interface and CAD/CAE integration
  - Including surface cleaning and repair
  - Code coupling
- Automatic meshing
  - Both general and application specific
- Complete mesh handling flexibility
  - Any cell shape or grid structure
  - Any mesh movement
- State of the art numerics and solvers
  - Stability and accuracy
  - Speed and efficiency
- Extensive physics modeling capability
  - Both general and knowledge based tuning
- Utilization of latest computer technology
  - Hardware optimization
  - Parallel processing
- Advanced analysis and post-processing tools
  - Innovative data processing and visualization
- Technical support and know-how
  - Knowledgeable, experienced and industry aware engineering team



# Software Product Summary

- General solvers and CFD analysis codes
  - STAR-CD
  - COMET
  - Two new solvers under development
- General pre/post-processor GUI
  - PROSTAR
- CAD
  - pro-surf
  - pro-cad
- Automatic Mesh Generation
  - pro-am
- Integration
  - STAR/ProE
  - STAR-Works
  - COMET-Works



## Knowledge based expert systems

- es-aero
- es-uhood
- es-aftertreatment
- es-pass
- es-ice
- es-brake
- es-turbo
- es-fsi
- **es-pemfc**





# *Samples of PEM Fuel Cell GUI*



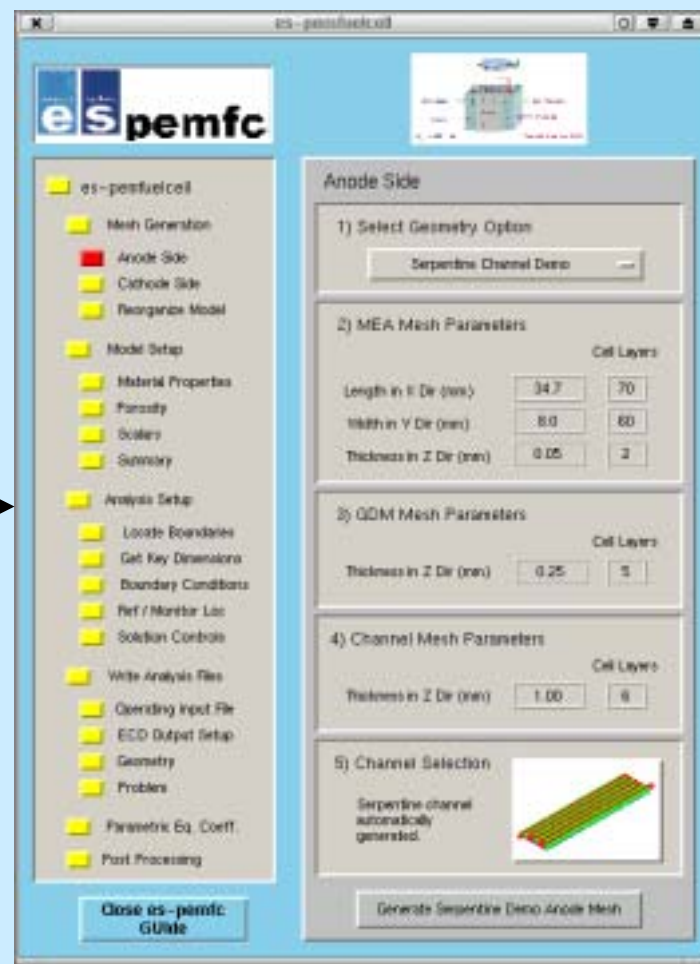
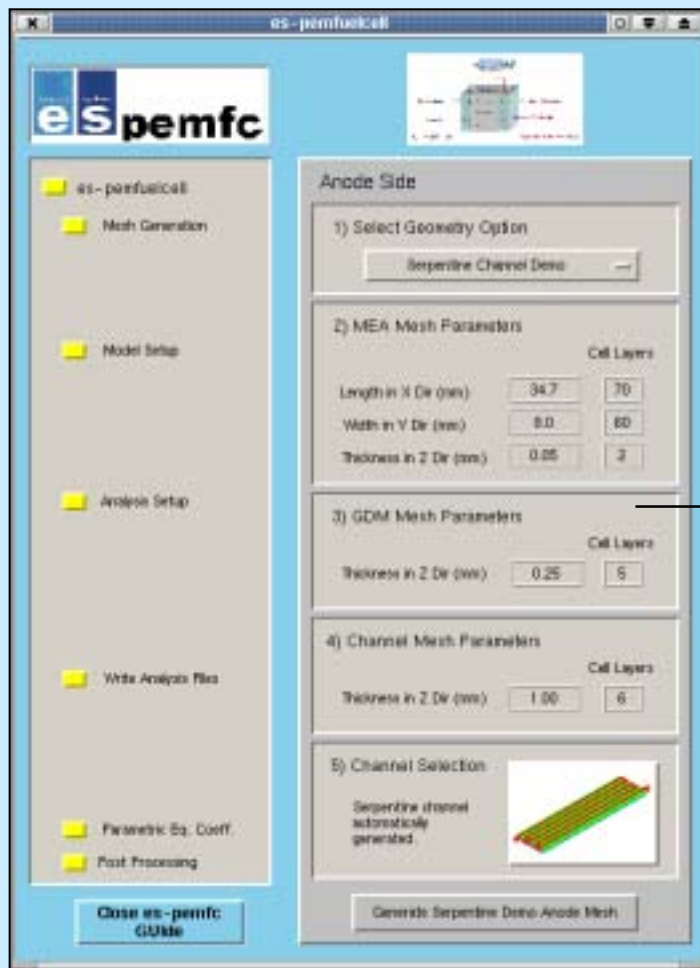


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**Process-oriented GUI steps user through all needed set-up and post processing for PEM analysis**

# *es-pemfc Panel*

es-pemfc Documentation



# Anode Options

Anode Side

1) Select Geometry Option

Serpentine Channel Demo

2) M

Serpentine Channel Demo  
Straight Channel Demo  
Customized Rectangular Geometry  
Customized Square Geometry  
User Grid Supplied

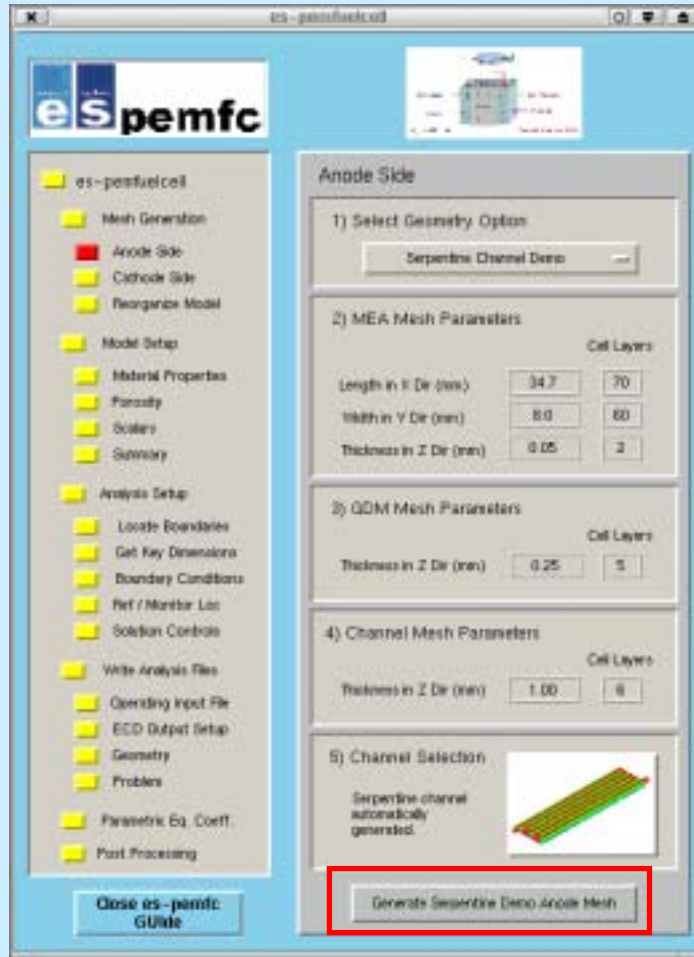
Len

Width in Y Dir (mm)

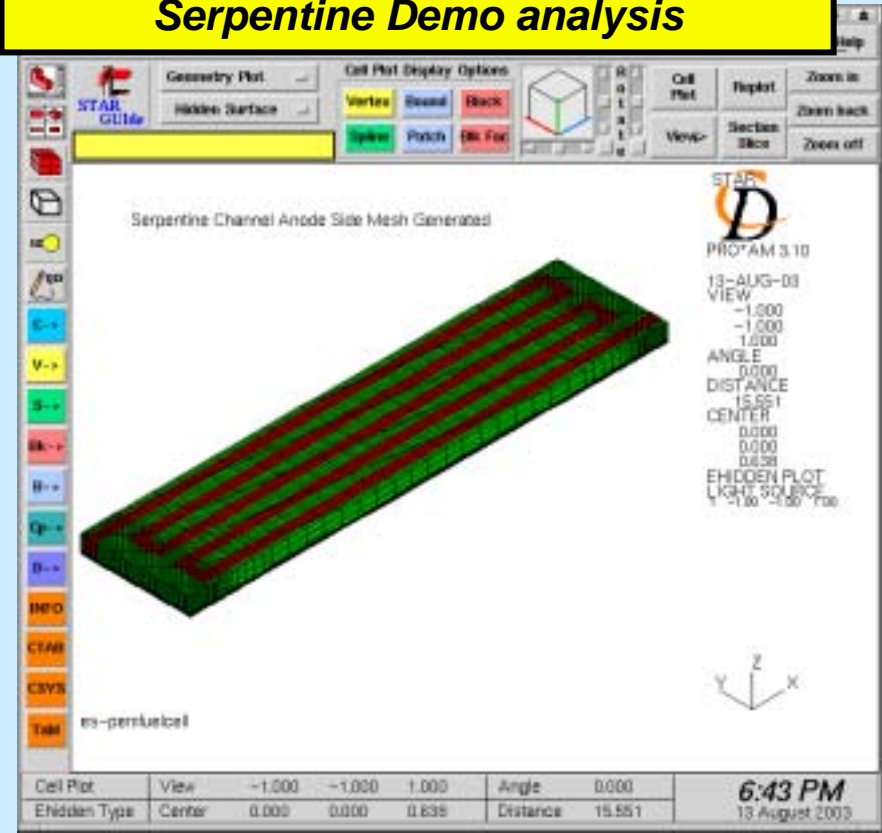
Thickness in Z Dir (mm)

**Included in GUI are two complete demonstration analyses with realistic input, user defined rectangular or square geometry with auto mesh generation, plus flexibility to import complex grids generated by user by other means**

# Serpentine Demo



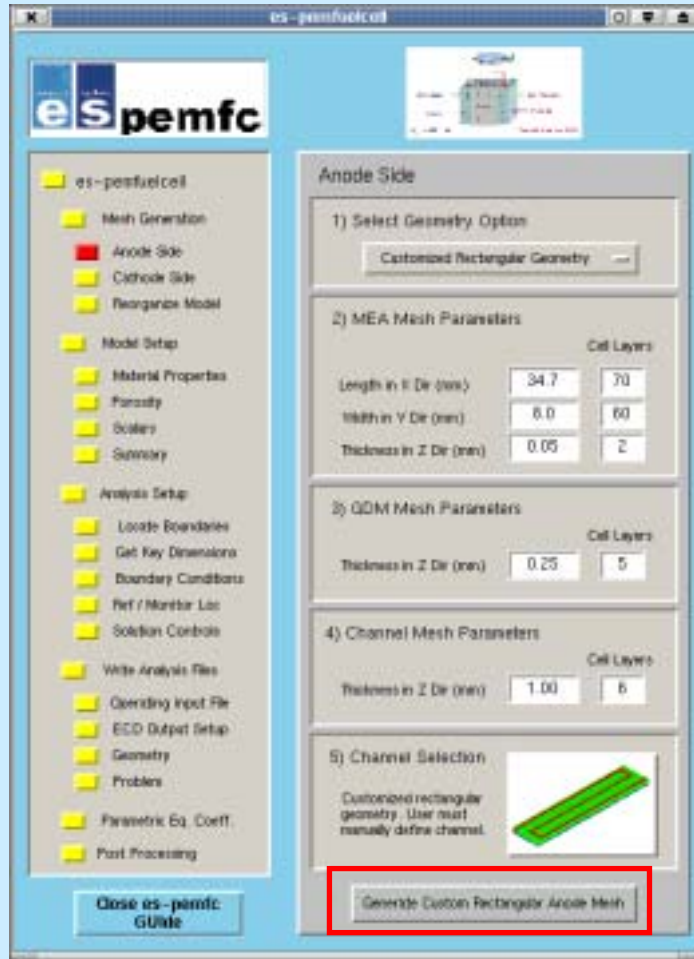
**Mesh generation example for Serpentine Demo analysis**



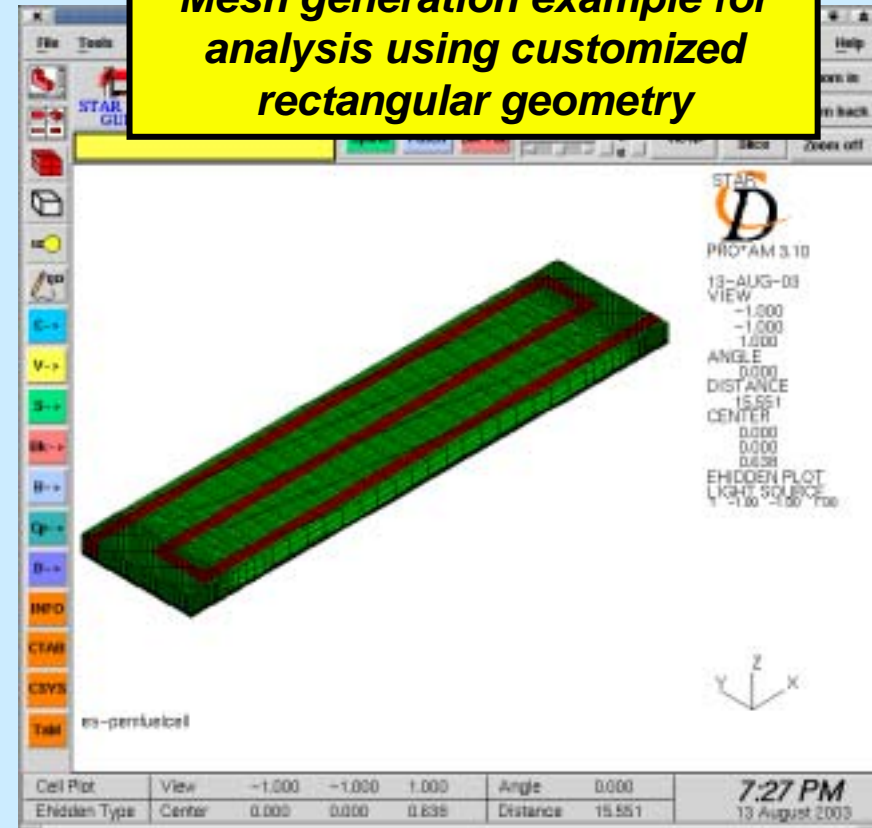
Construct Anode Side Mesh



# Custom Rectangular Geometry



Mesh generation example for analysis using customized rectangular geometry



Construct Anode Side Mesh



# User Grid Supplied

**Facility to import user supplied grid, restructure mesh, and convert to cell types required by PEM Subroutines**

es-pemfc Documentation

**Re-Organize Fuel Cell Model**

The cell types in your custom grid must follow the convention shown in the figure. Use the table shown below to change your cell types.

Description	Current Cell Type Nos.	New Type
MEA		→ 6
Anode GDM - 1st Layer		→ 5
Anode GDM - 2nd Layer		→ 11
Anode GDM		→ 4
Anode Gas Channel		→ 1
Cathode GDM - 1st Layer		→ 8
Cathode GDM - 2nd Layer		→ 10
Cathode GDM		→ 7
Cathode Gas Channel		→ 9
Bipolar Plates - Both		→ 2

Buttons: Close es-pemfc GUI, Reorganize Model

**Re-Organize Fuel Cell Model**

The cell types in your custom grid must follow the convention shown in the figure. Use the table shown below to change your cell types.

Description	Current Cell Type Nos.	New Type
MEA	101 102 103	→ 6
Anode GDM - 1st Layer	44	→ 5
Anode GDM - 2nd Layer	67 60	→ 11
Anode GDM	18	→ 4
Anode Gas Channel	200 201	→ 1
Cathode GDM - 1st Layer	33	→ 8
Cathode GDM - 2nd Layer	44	→ 10
Cathode GDM	56	→ 7
Cathode Gas Channel	68 69	→ 9
Bipolar Plates - Both	55 56 57	→ 2

Buttons: Close es-pemfc GUI, Reorganize Model

Steps 3: Restructure Model





# Material Properties

**Material Property specification with realistic defaults**

es-pemfc Documentation

The screenshot shows the 'es-pemfc' software interface. On the left is a navigation tree with categories like Mesh Generation, Anode Side, Cathode Side, Reorganize Model, Model Setup, Material Properties (highlighted in red), Porosity, Scales, Summary, Analysis Setup, Locate Boundaries, Get Key Dimensions, Boundary Conditions, Ref / Material List, Solution Controls, Write Analysis Files, Operating Input File, ECO Output Setup, Geometry, Problems, Parametric Eq. Coeff, and Post Processing. The main area is titled 'Material Properties' and contains four sections:

- Material 1: Anode Side Fluid**
  - Density (ρ): Ideal gas H<sub>2</sub>, Water Vapor
  - Viscosity (μ): multiconp H<sub>2</sub>, Water Vapor
  - Conductivity (k): multiconp H<sub>2</sub>, Water Vapor
  - Spec Heat (Cp): multiconp H<sub>2</sub>, Water Vapor
- Material 2: Cathode Side Fluid**
  - Density (ρ): Ideal gas N<sub>2</sub>, O<sub>2</sub>, Water Vapor
  - Viscosity (μ): multiconp N<sub>2</sub>, O<sub>2</sub>, Water Vapor
  - Conductivity (k): multiconp N<sub>2</sub>, O<sub>2</sub>, Water Vapor
  - Spec Heat (Cp): multiconp N<sub>2</sub>, O<sub>2</sub>, Water Vapor
- Material 3: MEA Solid**
  - Density (ρ): constant 200 kg/m<sup>3</sup>
  - Conductivity (k): constant 0.15 W/m-K
  - Spec Heat (Cp): constant 500 W/m-K
- Material 4: Bipolar Solid Phases**
  - Density (ρ): constant 200 kg/m<sup>3</sup>
  - Conductivity (k): constant 0.15 W/m-K
  - Spec Heat (Cp): constant 500 W/m-K

At the bottom, there are buttons for 'Apply' (highlighted with a red box), 'Reset to Defaults', and 'Close es-pemfc GUI'.

The screenshot shows the STAR CDD GUI. The main window displays a 3D model of a PEMFC stack with alternating green and red layers. The title bar reads 'STAR CDD GUI'. The menu bar includes File, Tools, Lists, Modules, Plot, Post, Graph, Utility, Panels, AutoMesh, Favorites, and Help. The toolbar contains various icons for geometry, hidden surfaces, and cell plot display options. The main area is titled 'Material Types and Properties Set' and shows the 3D model. On the right, there is a STAR logo and the text 'PROGRAM 3.10', '13-AUG-03', 'VIEW', and 'HIDDEN PLOT'. At the bottom, there is a table with the following data:

Cell Plot	View	-1.000	-1.000	1.000	Angle	0.000
Hidden Type	Center	0.000	0.000	0.000	Distance	15.250

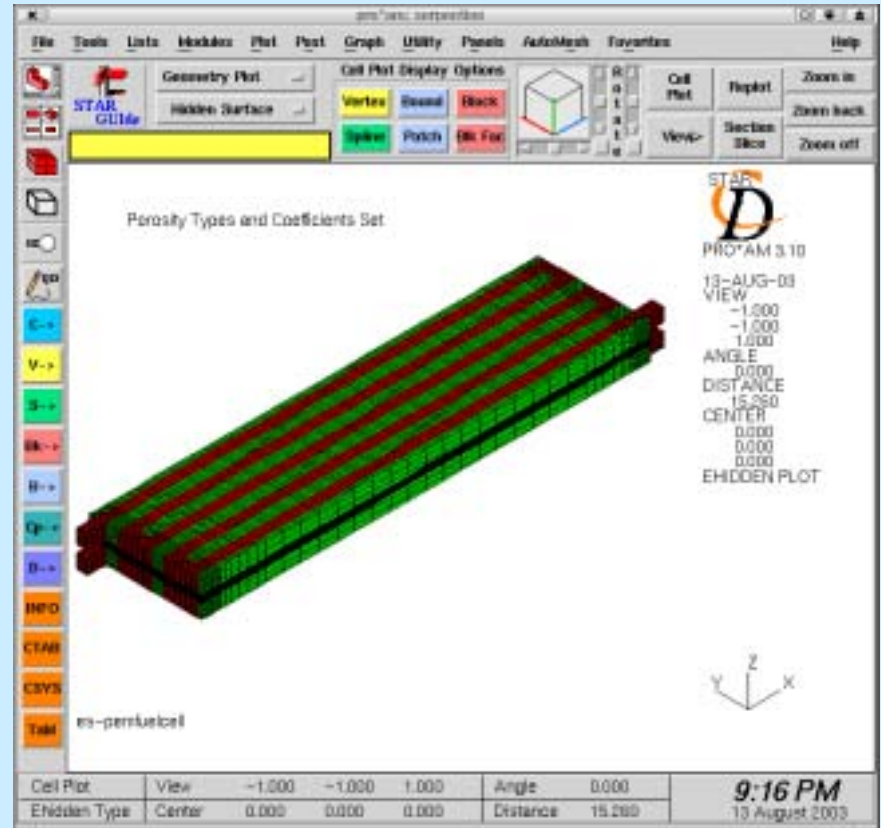
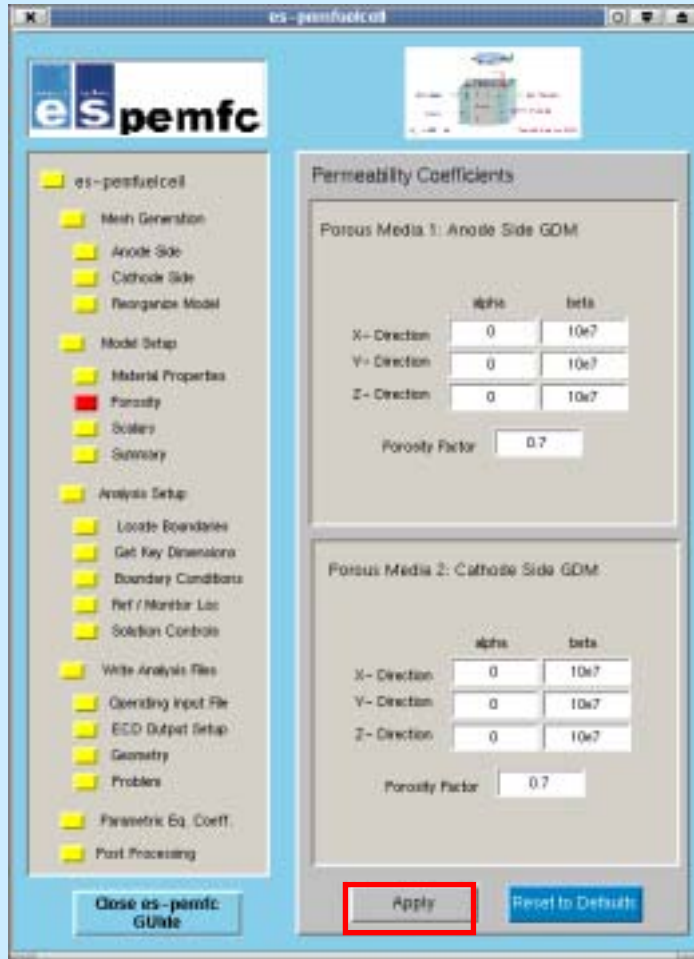
The bottom right corner shows the time '9:15 PM' and the date '13 August 2003'.



# Porosity

**Porosity specification with realistic defaults**

es-pemfc Documentation





# Scalars

**Automatic set-up of  
scalars needed by PEM  
Subroutines for  
electrochemistry**

es-pemfc Documentation

Active Scalars			
Description	No.	Name	
Nitrogen Gas	1	N2	
Hydrogen Gas	2	H2	
Oxygen Gas	3	O2	
Water Vapor - Anode	4	WVA	
Water Vapor - Cathode	5	WVC	
Liquid Water - Anode	6	LWA	
Liquid Water - Cathode	7	LWC	

Passive Scalars			
Description	No.	Name	
Current Density	8	CD	
Net Water Fluxes Proton	9	ALPHA	
Kinetic Over Potential	10	KOP	
Anode Over Potential	11	ADP	
Cathode Over Potential	12	CDP	
Membrane Conductivity	13	MC	
Water Diffusivity	14	WDC	
Water Content inside MEA	15	LAMECA	
Anode Activity	16	AA	
Cathode Activity	17	CA	
MEA Liquid Film Thickness	18	LFT	

STAR CDM PROGRAM 3.10  
13-AUG-03  
VIEW  
-1.000  
-1.000  
1.000  
ANGLE  
0.000  
DISTANCE  
15.260  
CENTER  
0.000  
0.000  
0.000  
HIDDEN PLOT

es-pemfuelcell

Cell Plot View -1.000 -1.000 1.000 Angle 0.000  
Hidden Type Center 0.000 0.000 0.000 Distance 15.260

9:17 PM  
13 August 2003



# Model Summary

**Summary panel to quickly check cell types and material properties**

es-pemfc Documentation

**Model Summary**

**Material 1: Anode Side Fluid**

Description	Cell Type	Porous Media	Porous Index
Anode GDM - L1	5	Yes	1
Anode GDM - L2	11	Yes	1
Anode GDM	4	Yes	1
Anode Gas Channel	1	No	0

**Material 2: Cathode Side Fluid**

Description	Cell Type	Porous Media	Porous Index
Cathode GDM - L1	8	Yes	2
Cathode GDM - L2	10	Yes	2
Cathode GDM	7	Yes	2
Cathode Gas Channel	9	No	0

**Material 3: MEA Solid**

Description	Cell Type
MEA	6

**Material 4: Bipolar Solid Plates**

Description	Cell Type
Bipolar Plates - Both Sides	2

Print



Anode Side



Cathode Side



MEA



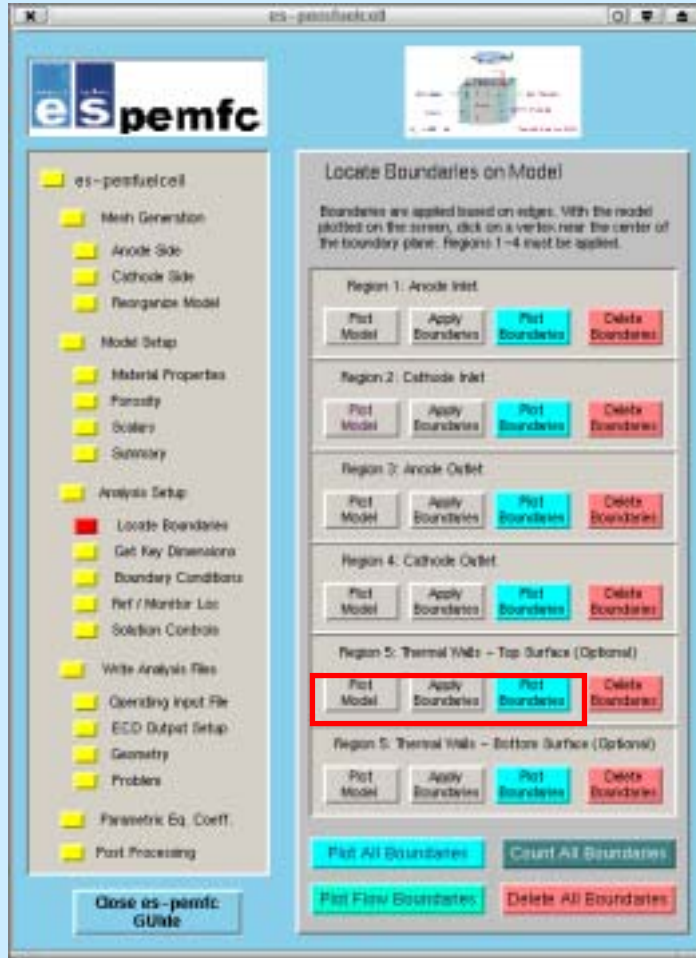
Bipolar Plates



# Locate Boundaries

**Graphical boundary condition locator**

es-pemfc Documentation



Plot Model

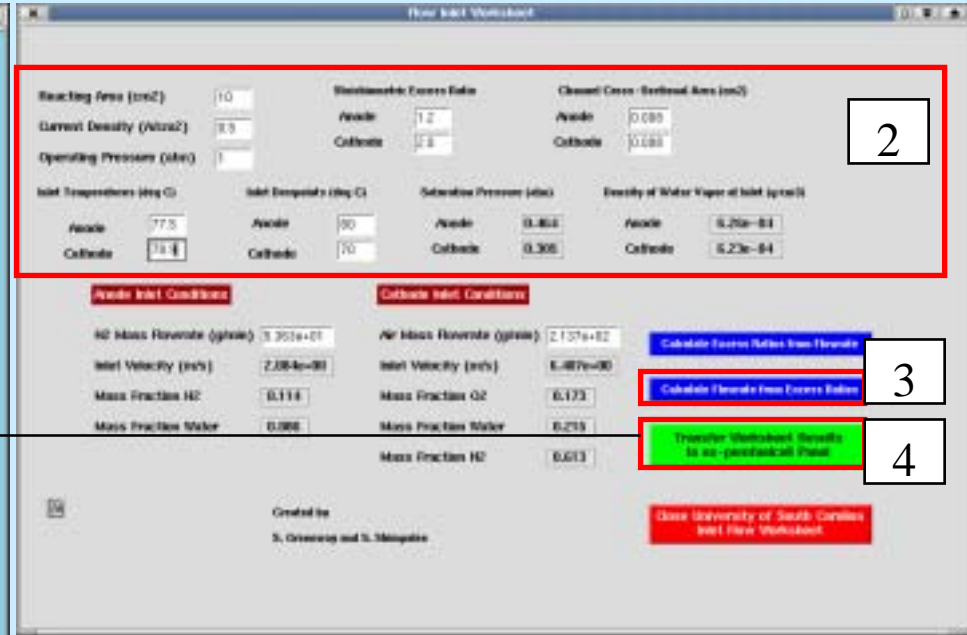
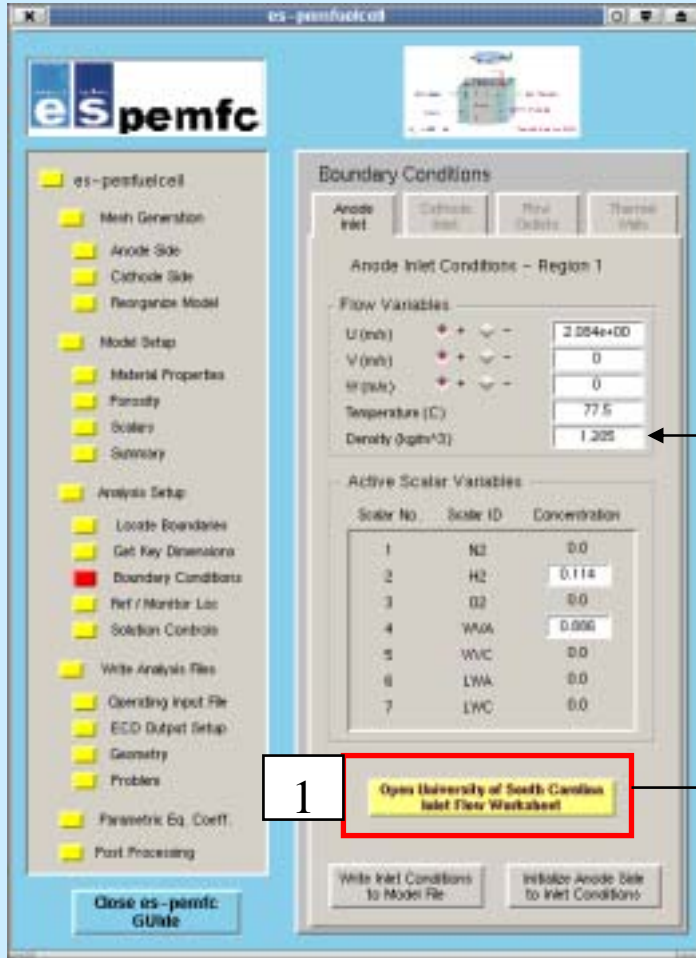


Apply Boundaries



Plot Boundaries

# Boundary Conditions



**Boundary condition specification using University of South Carolina Worksheet. User puts in independent values and dependent values computed automatically**

Flow Inlet Worksheet



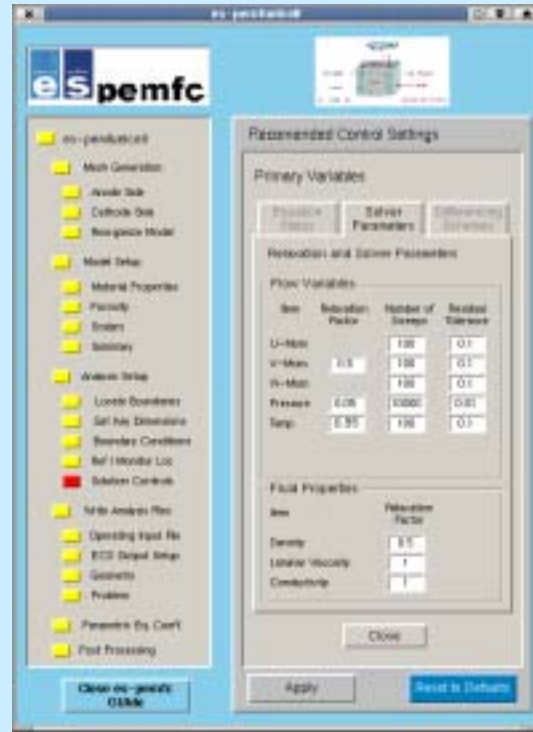
# Control Settings

**es-pemfc Control Panels apply default the solver and differencing scheme choices recommended for PEM fuel cell analysis (may be different than STAR-CD defaults)**

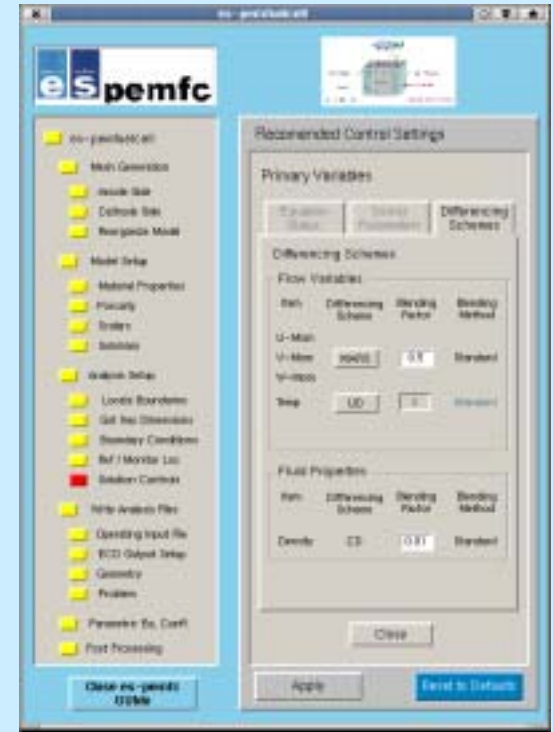
es-pemfc Documentation



Equation Status

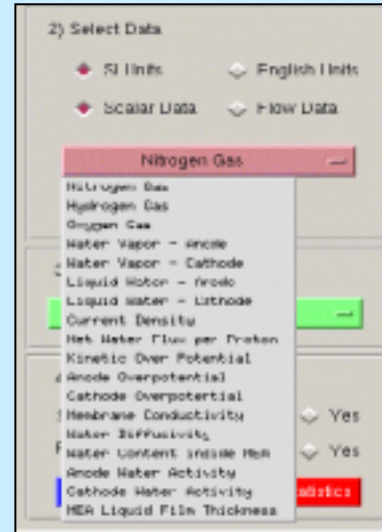


Solver Parameters

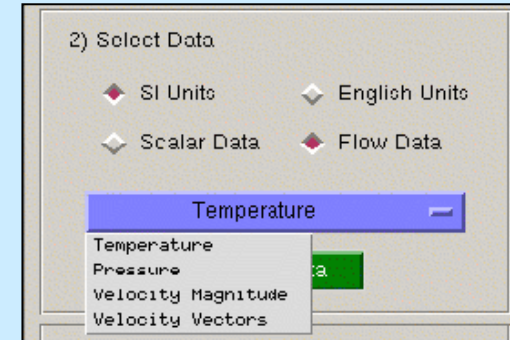


Differencing Schemes

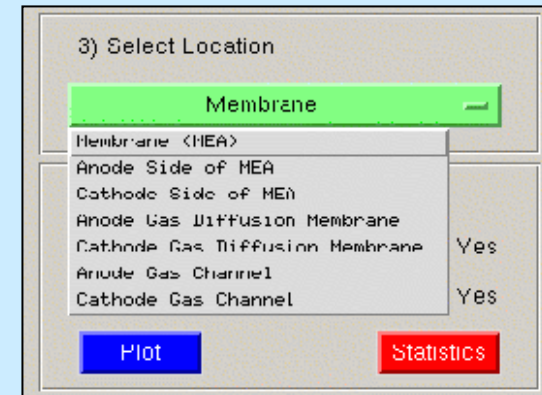
# Post Processing



Scalar Data



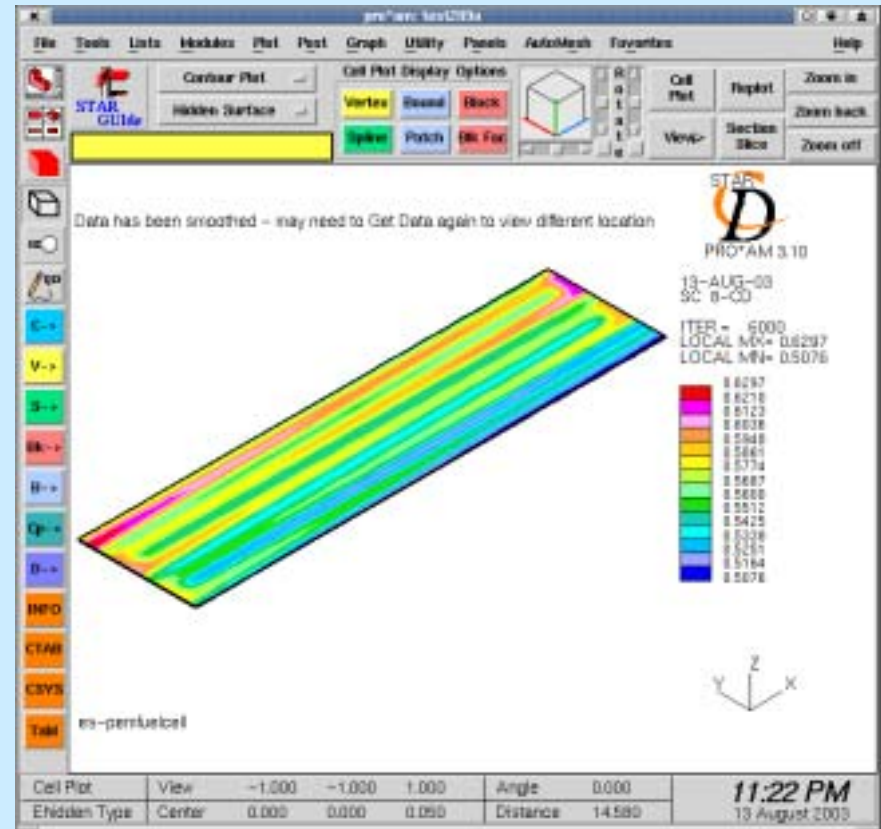
Flow Data







# Post Processing – Ex. 1a

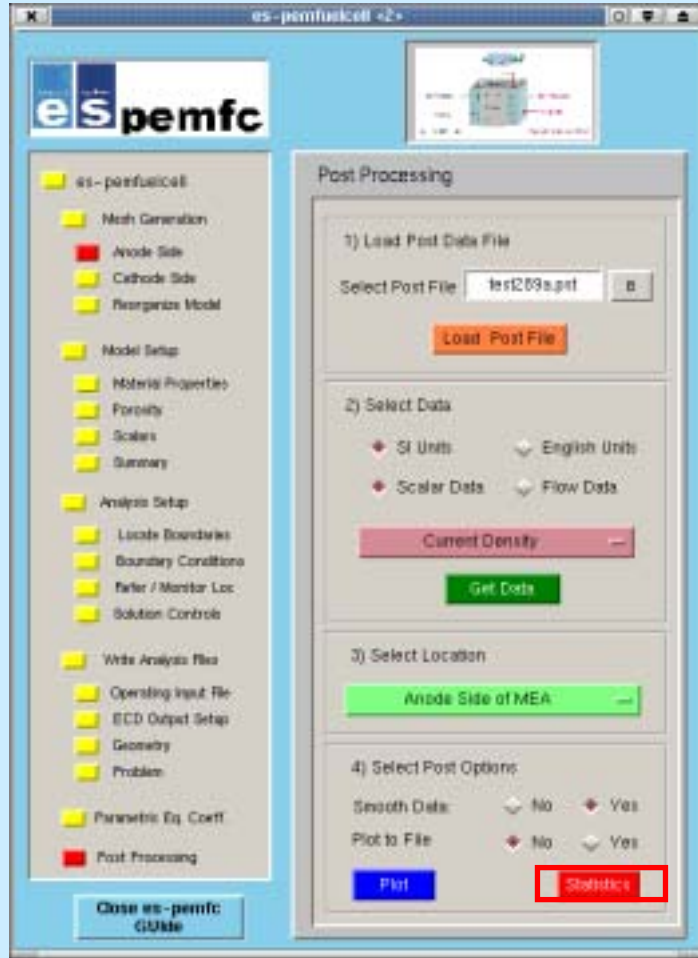


Plot: CD – Anode Side of MEA



# Post Processing – Ex. 1b

es-pemfc Documentation



4	FLUI	9000	0
5	FLUI	3000	3000
6	SOLI	12000	0
7	FLUI	9000	0
8	FLUI	3000	0
9	FLUI	10584	0
10	FLUI	3000	0
11	FLUI	3000	0

UTIL\*->  
sum,cset

SUMMARIES FOR STORED CELL DATA USING SET

REG 4  
COOB

SUM 1704.7  
MIN LOC 8941  
MIN VAL 0.50764  
MAX LOC 6054  
MAX VAL 0.62991  
AVG VAL 0.56824

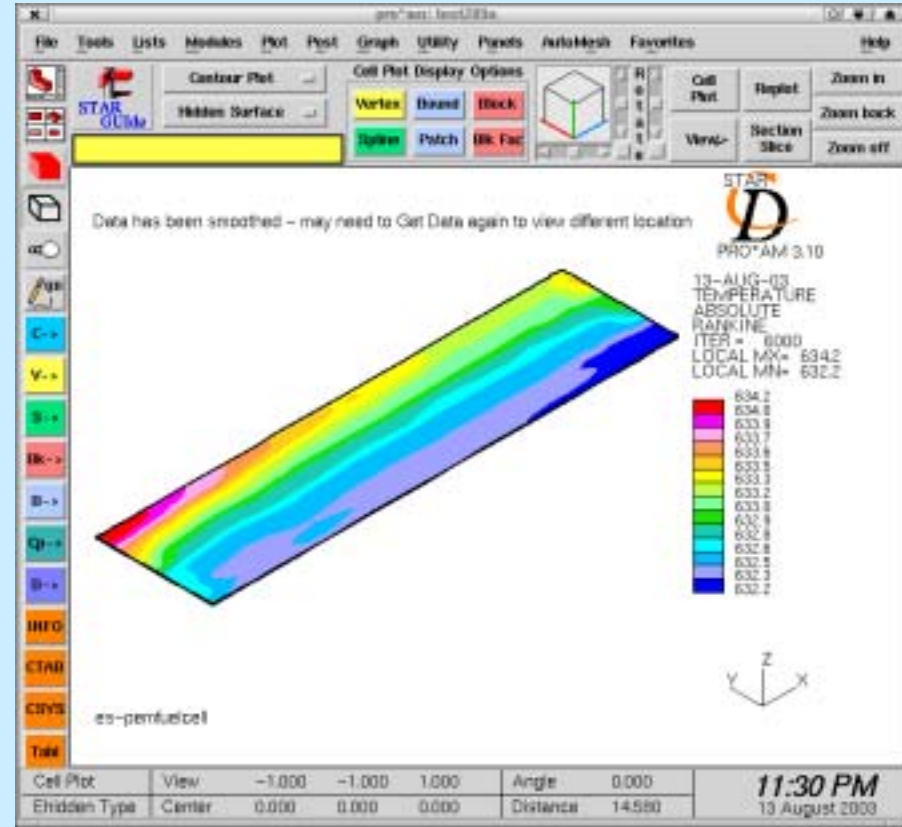
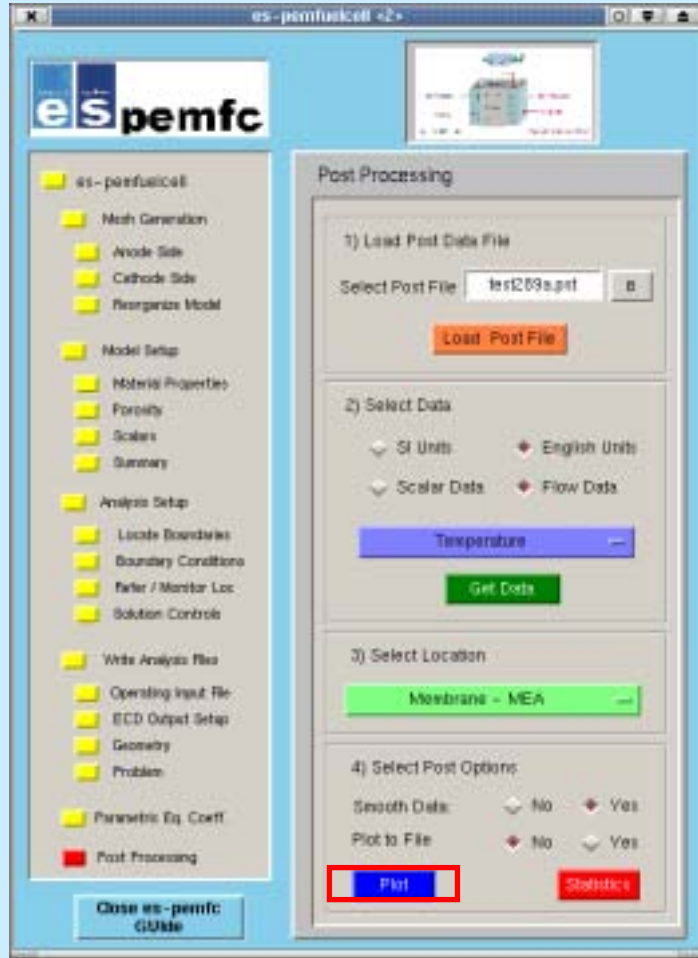
Statistics: CD – Anode Side of MEA

# Post Processing – Ex. 2



Plot: Pressure – Anode Gas Channel

# Post Processing – Ex. 3



Plot: Temperature – MEA

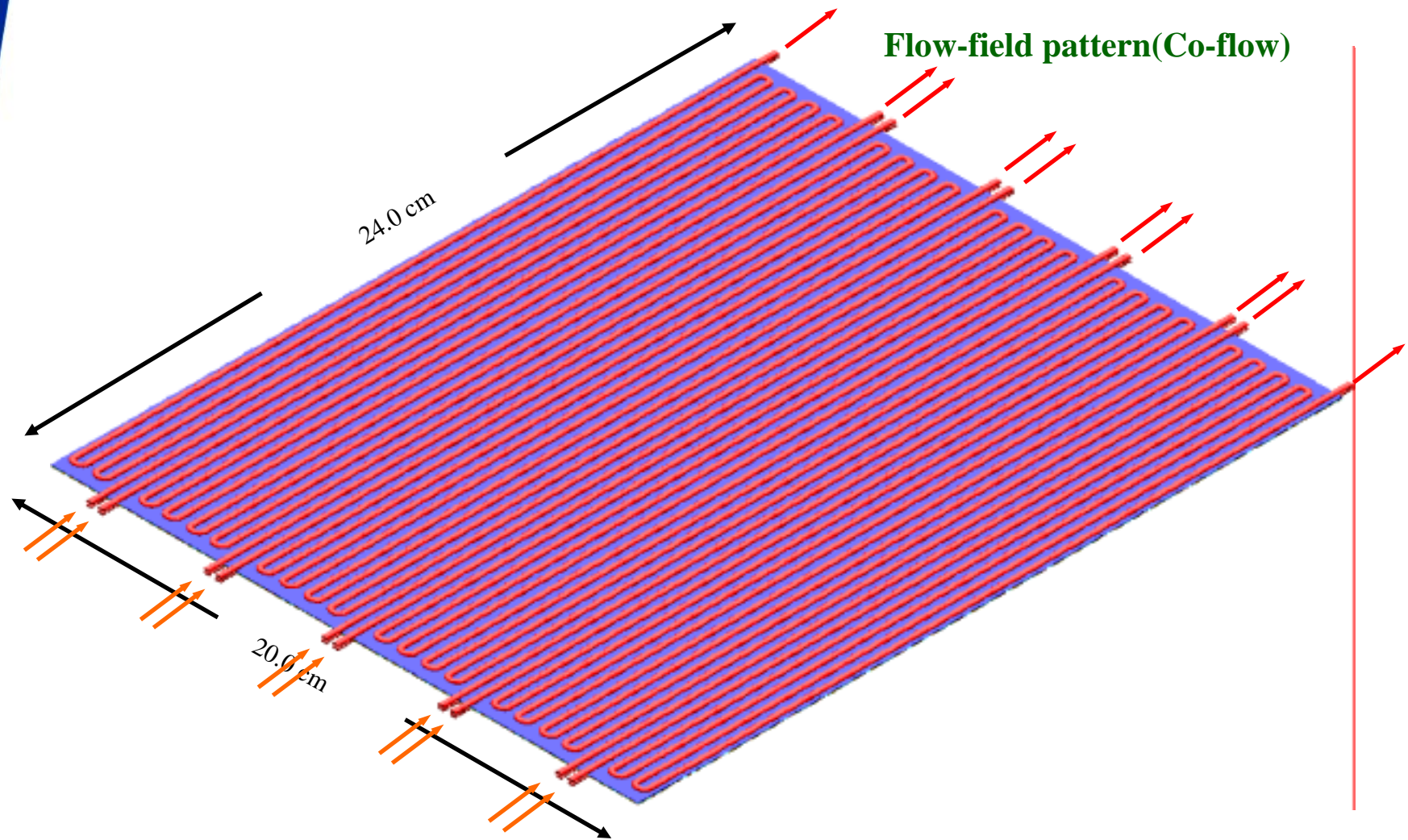
# Predicting Water and Current Distribution of a Commercial-size PEMFC

# Objectives

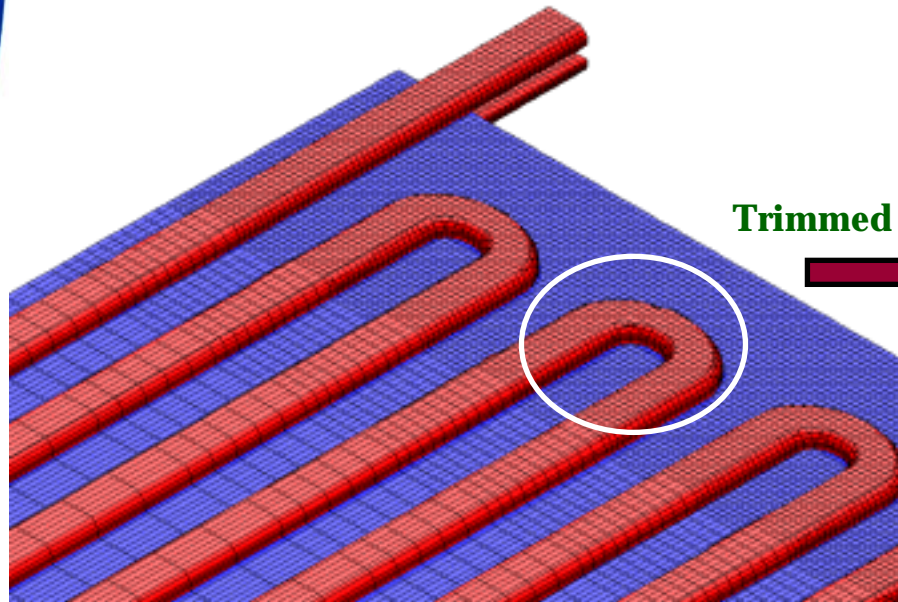
- Model the performance of an 480-cm<sup>2</sup> patented automotive flow-field under humidified and dry cathode conditions
- Examine water and current distributions for the two cases and determine causes of the performance differences
- Report the metrics for problem solutions



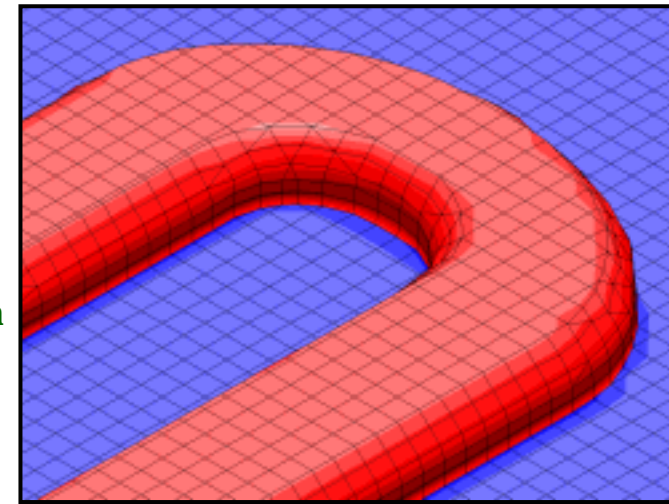
# 480-cm<sup>2</sup> PEMFC components used for computational analysis (J. A. Rock, U.S. Patent # 6,099,98)



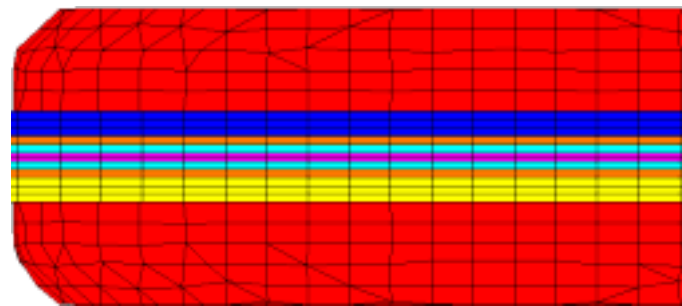
# Meshing and geometry details



Trimmed cell mesh



Cross-section view



Anode flow channel

Anode GDL

MEA

Cathode GDL

Cathode flow channel

## Geometry detail

- Total cell = 4,951,440. Number of channel = 10. Number of pass = 5. Channel length = ~120 cm.
- MEA thickness (membrane+catalyst layers) = 0.050 mm. GDL thickness = 0.250 mm (permeability =  $1\text{E-}12 \text{ m}^2$  with 0.7 porosity).
- Flow channel area =  $\sim 1.1 \text{ mm}^2$ , Reaction Area =  $480 \text{ cm}^2$ .



# Computational Procedure

- Computations were carried out in parallel on a Linux Cluster
- A commercial version of STAR-CD with integrated PEMFC electrochemistry subroutines was used for the calculations
- MPICH was used for message passing between the nodes
- The effect of the number of processors used on calculation time was measured



# Condition of Interested

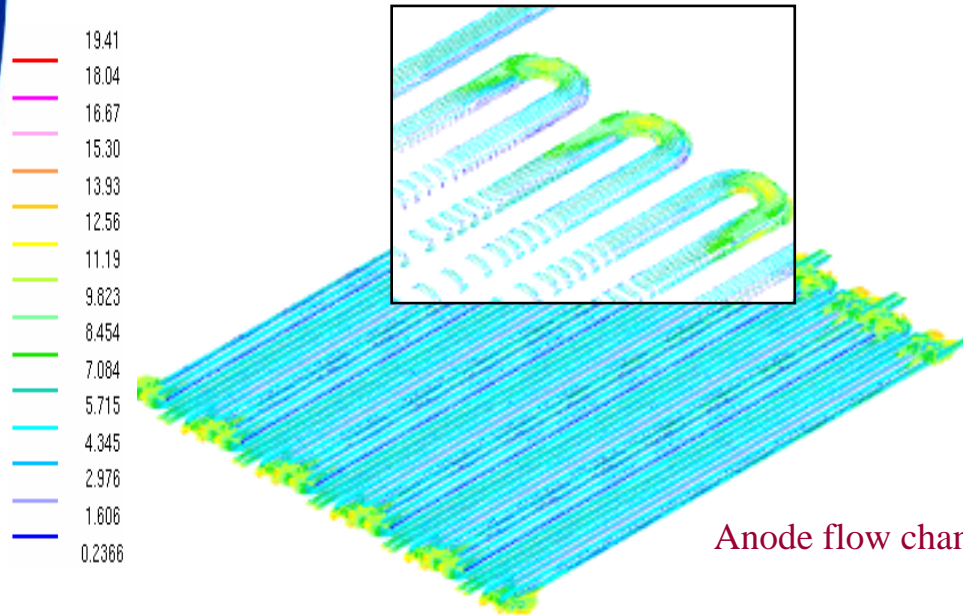
- Normal condition:

- 1.2/2.0 stoich, 40% H<sub>2</sub>/Air
- 70°C/70°C anode/cathode dew point temperature (i.e 100% relative humidity both anode and cathode)
- 70°C cell temperature
- 101 kPa back pressure

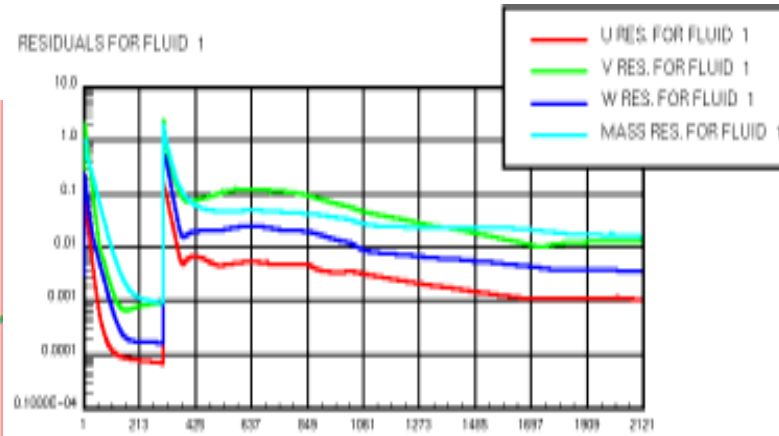
- Cathode By-pass (Cathode bypasses humidifier):

- 1.2/2.0 stoich, 40% H<sub>2</sub>/Air
- 70°C/by-pass anode/cathode dew point temperature (i.e 100% relative humidity anode, 0% relative humidity cathode)
- 70°C cell temperature
- 101 kPa back pressure

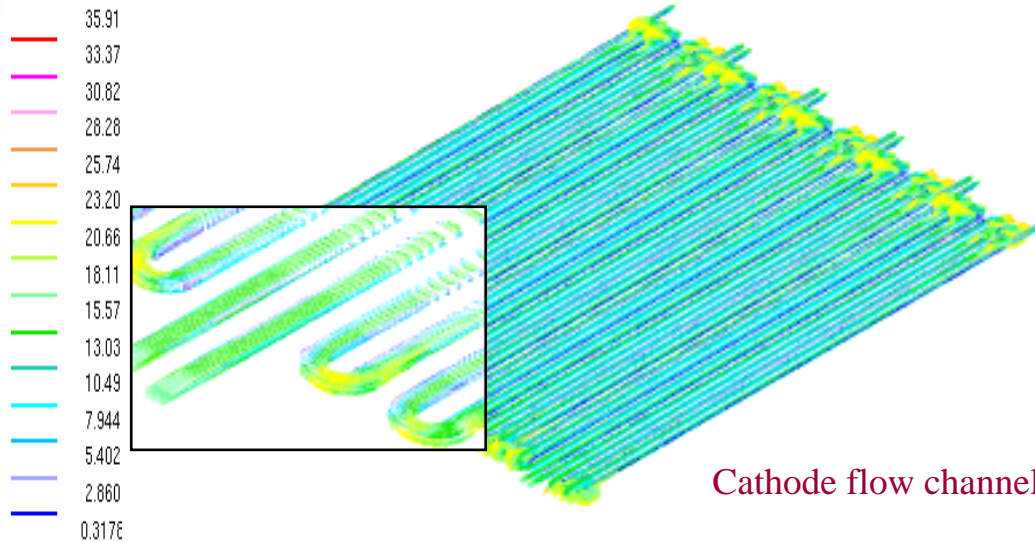
# Velocity vectors, velocity magnitudes, and residuals plots for anode and cathode



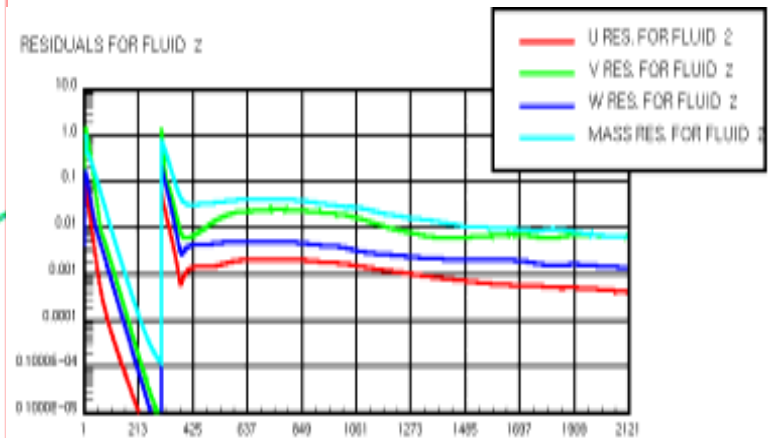
Anode flow channel



Anode residuals

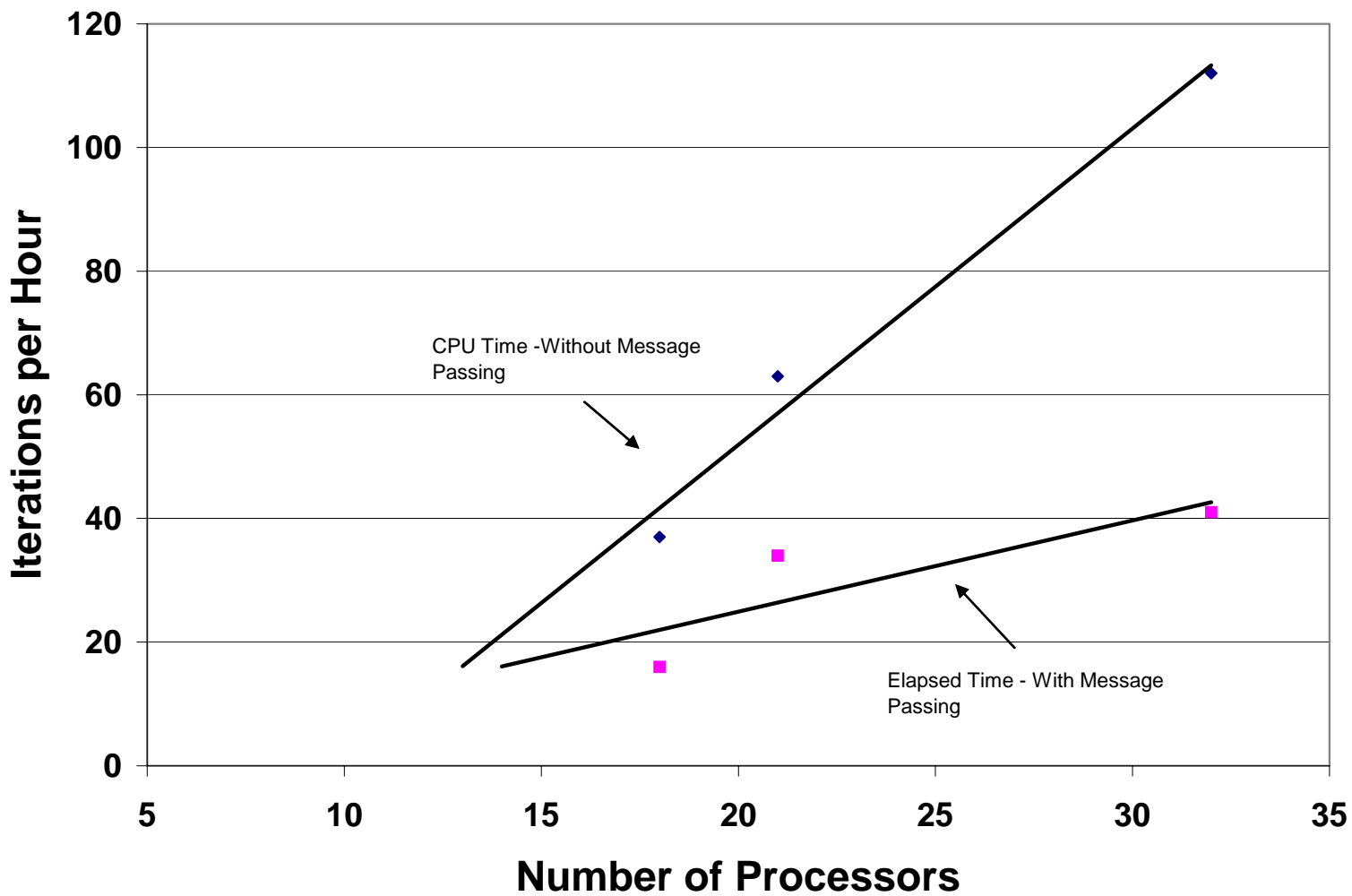


Cathode flow channel



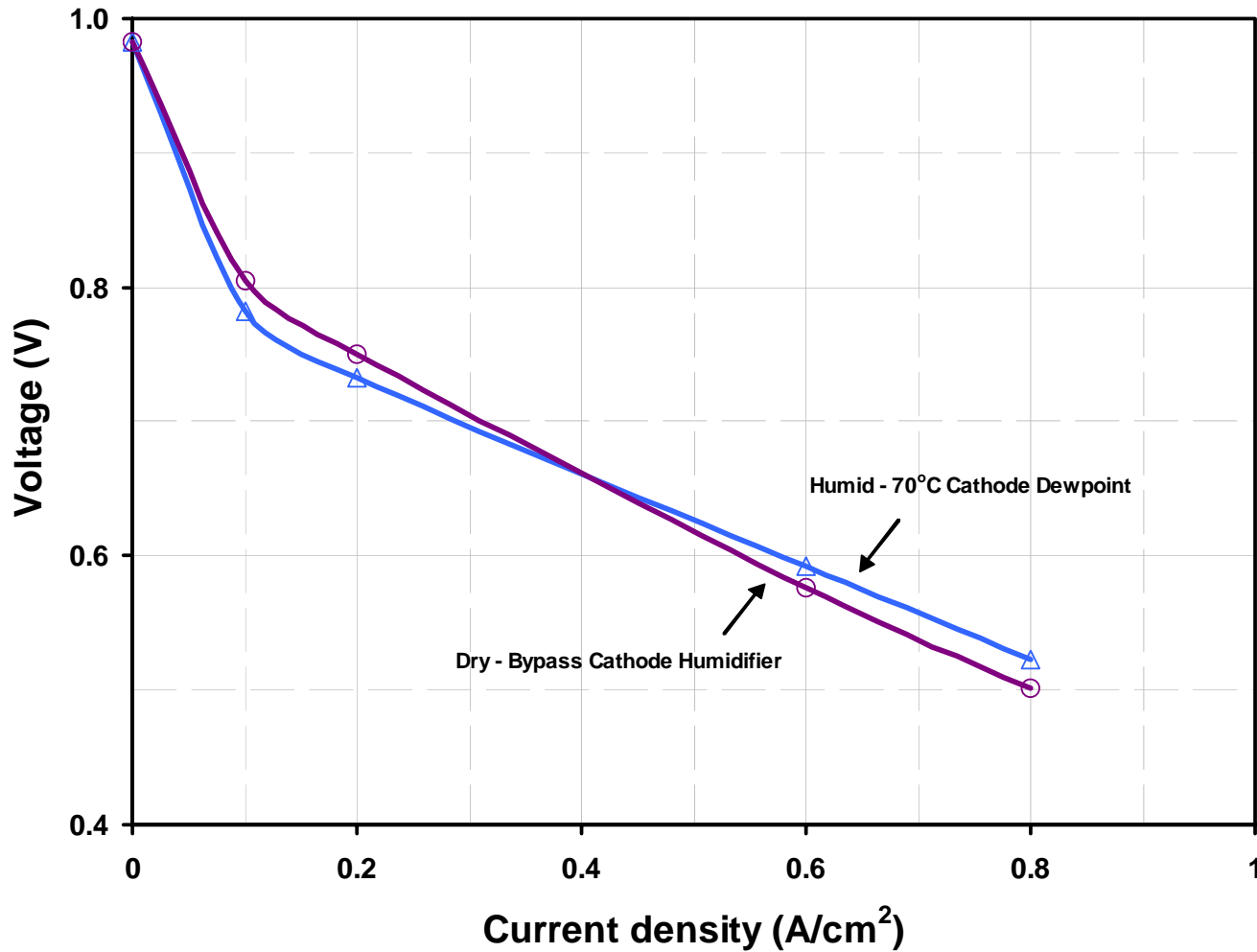
Cathode residuals

# Parallel performance

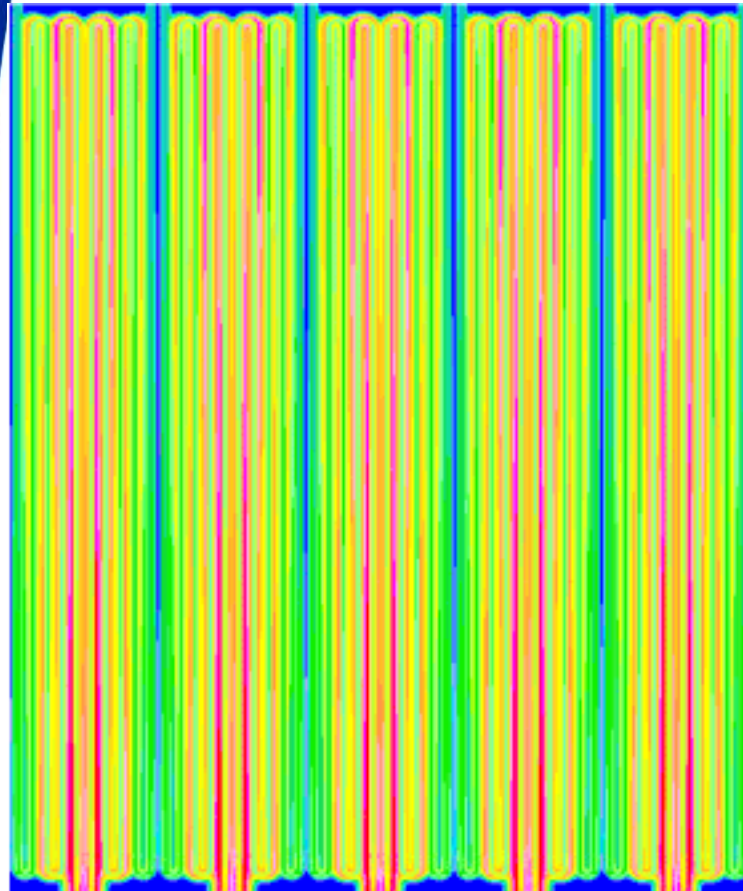


# Polarization curves for PEM fuel cell.

( $T_{cell} = 70\text{ }^{\circ}\text{C}$ , Pressure(A/C) = 1/1 bar, Stoic.= 1.2/2.0)

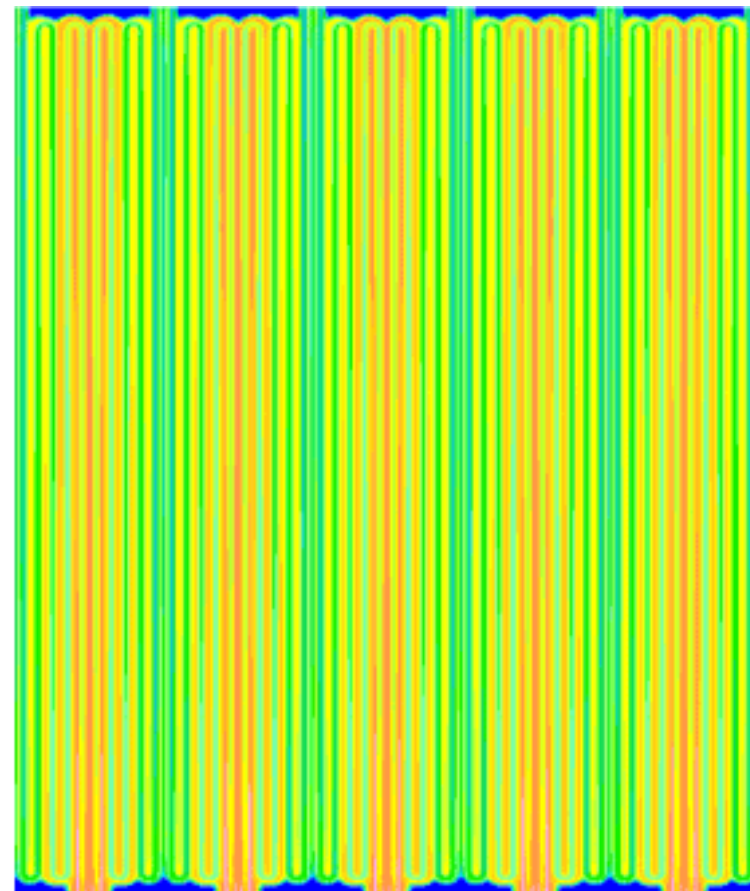


# Local current density ( $A/cm^2$ ) distribution on MEA surface at $I_{avg}$ of $0.6 \text{ mA}/cm^2$ between Normal case and Cathode by-pass case



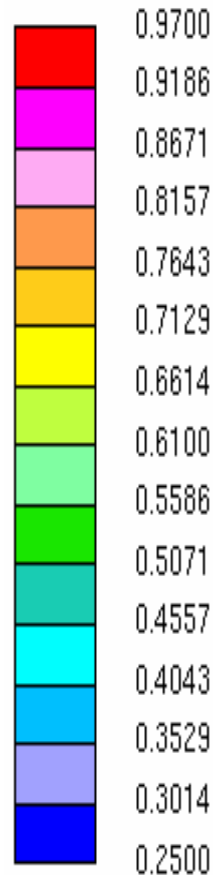
Normal case

$I_{avg} = 0.6 \text{ A}/cm^2$ ,  $V_{cell} = 0.59V$

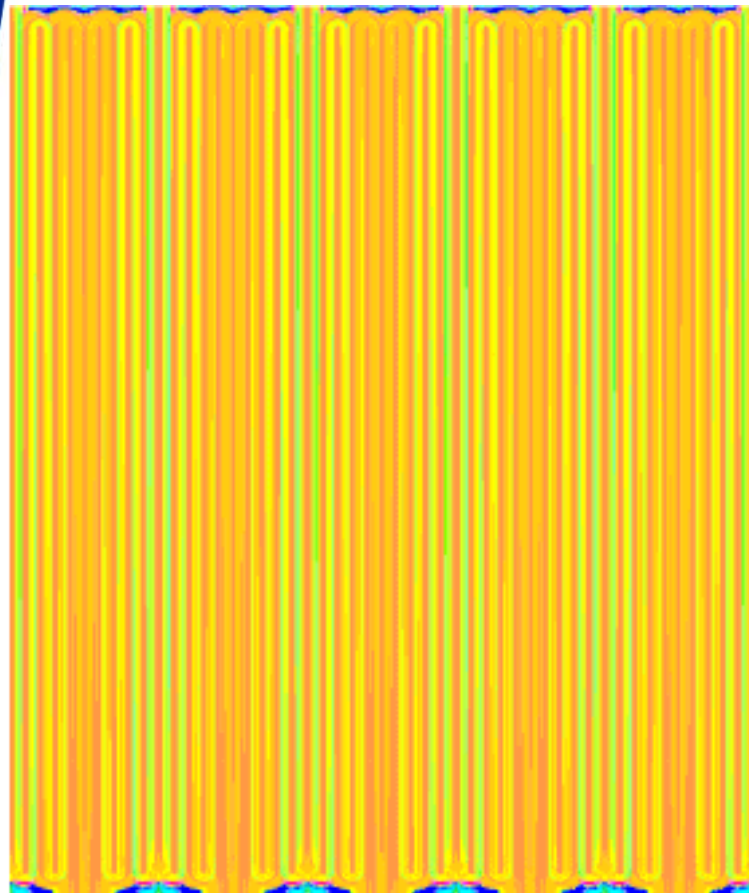


Cathode by-pass case

$I_{avg} = 0.6 \text{ A}/cm^2$ ,  $V_{cell} = 0.57V$

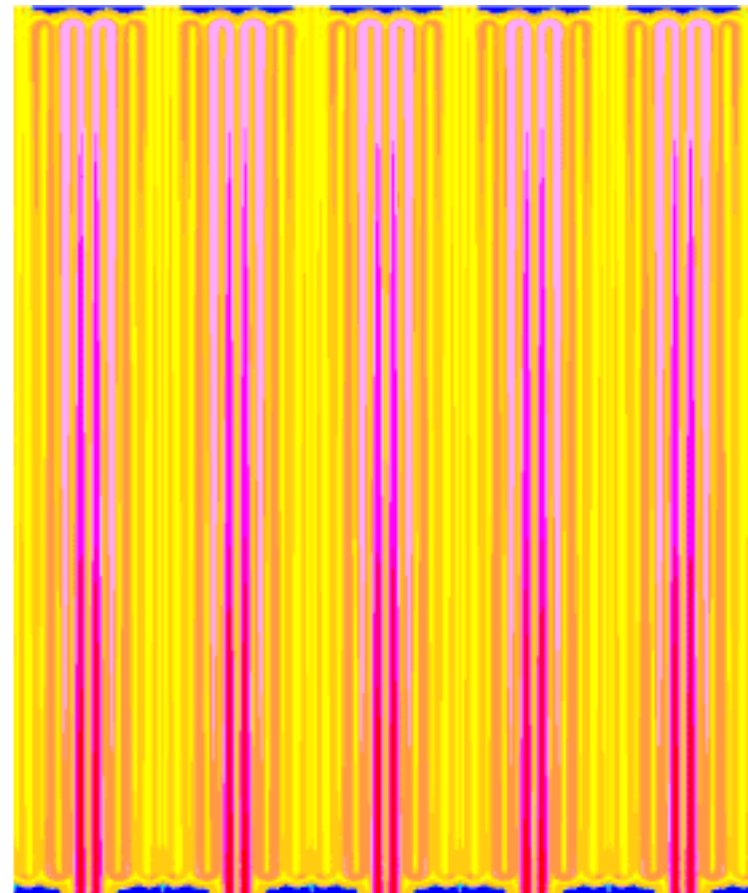


# Net water flux per proton ( $\alpha$ ) distribution on MEA surface at $I_{avg}$ of $0.6 \text{ mA/cm}^2$ between Normal case and Cathode by-pass case



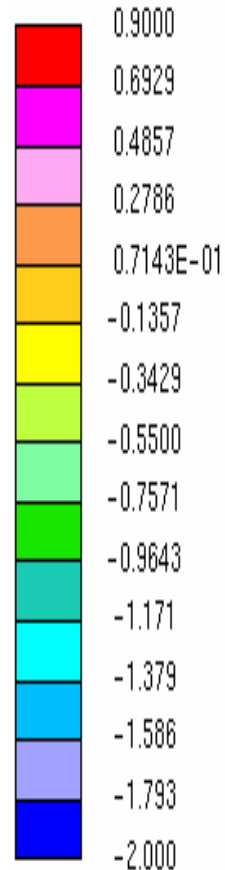
Normal case

$\alpha_{avg} = -0.13$ ,  $V_{cell} = 0.59V$

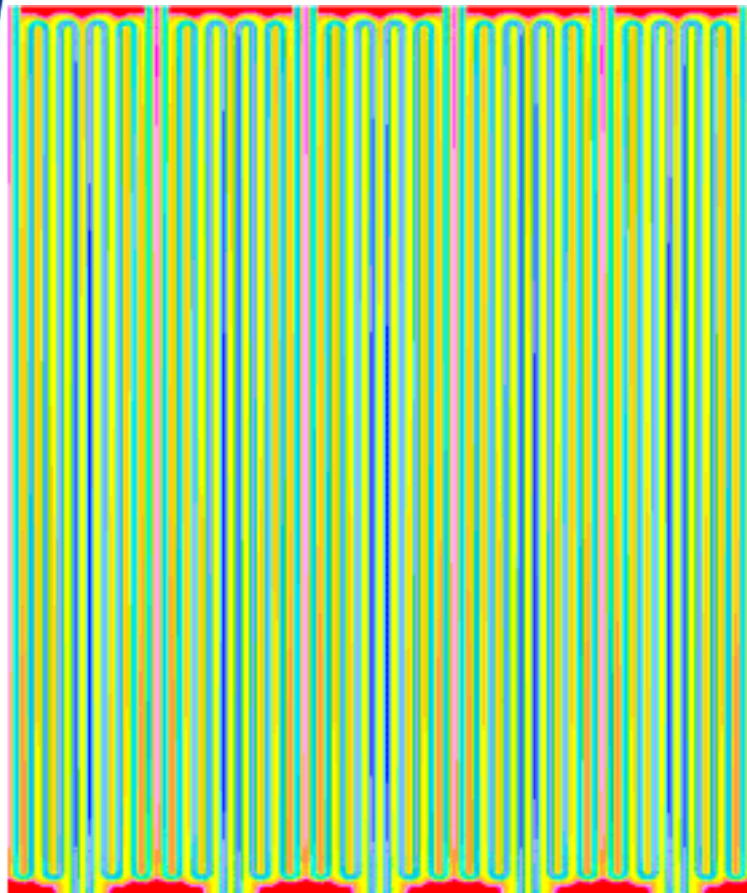


Cathode by-pass case

$\alpha_{avg} = -0.0028$ ,  $V_{cell} = 0.57V$

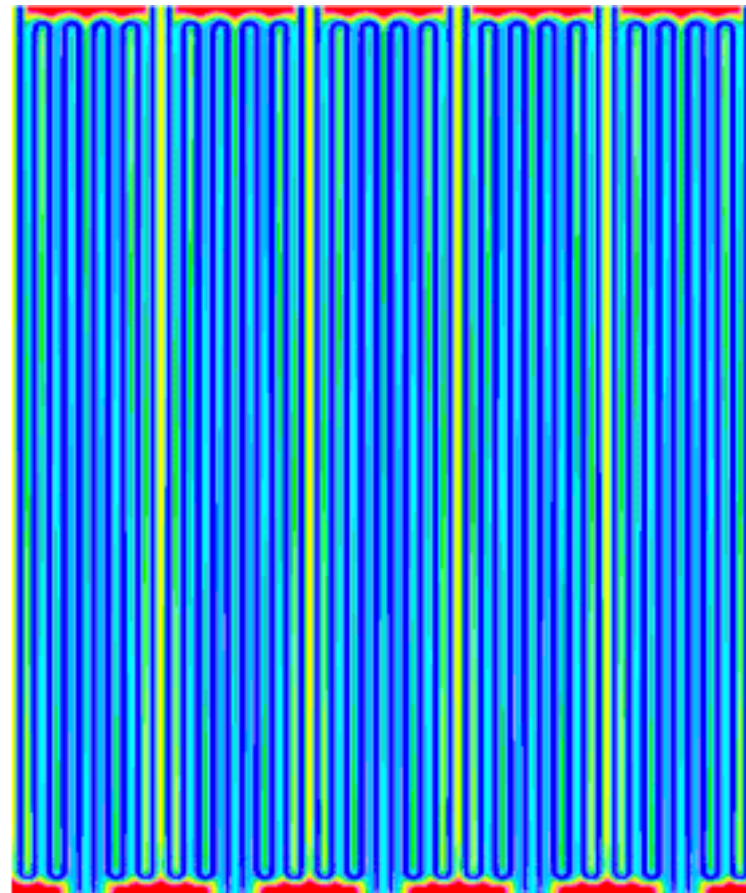


# Water content ( $\lambda$ ) distribution on MEA surface at $I_{avg}$ of $0.6 \text{ mA/cm}^2$ between Normal case and Cathode by-pass case



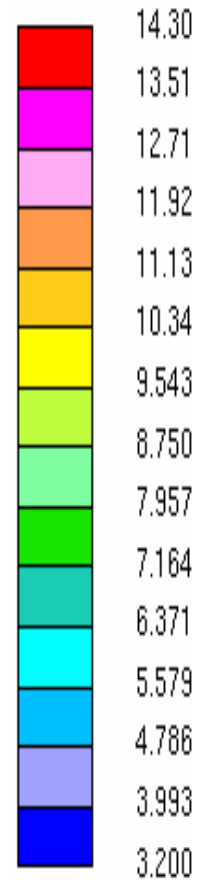
Normal case

$\lambda_{avg} = 8.6, V_{cell} = 0.59V$



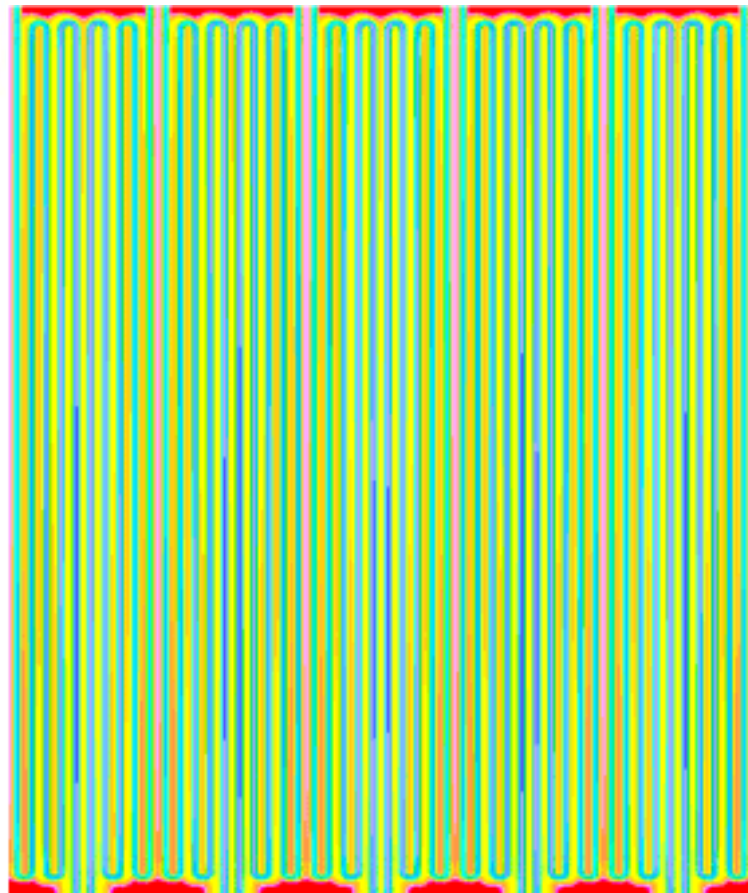
Cathode by-pass case

$\lambda_{avg} = 5.9, V_{cell} = 0.57V$



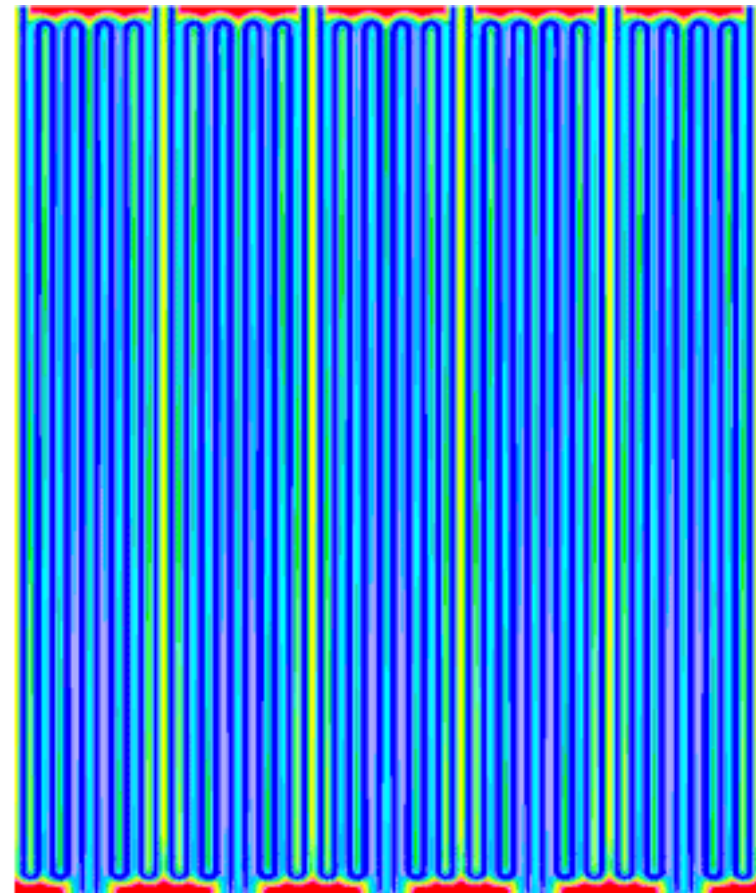


# Membrane conductivity (S/m) distribution on MEA surface at $I_{avg}$ of $0.6 \text{ mA/cm}^2$ between Normal case and Cathode by-pass case



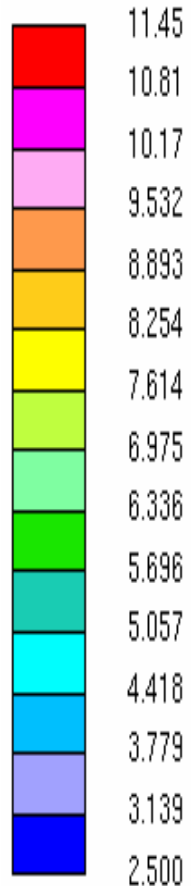
Normal case

$\sigma_{avg} = 6.89$ ,  $V_{cell} = 0.59V$

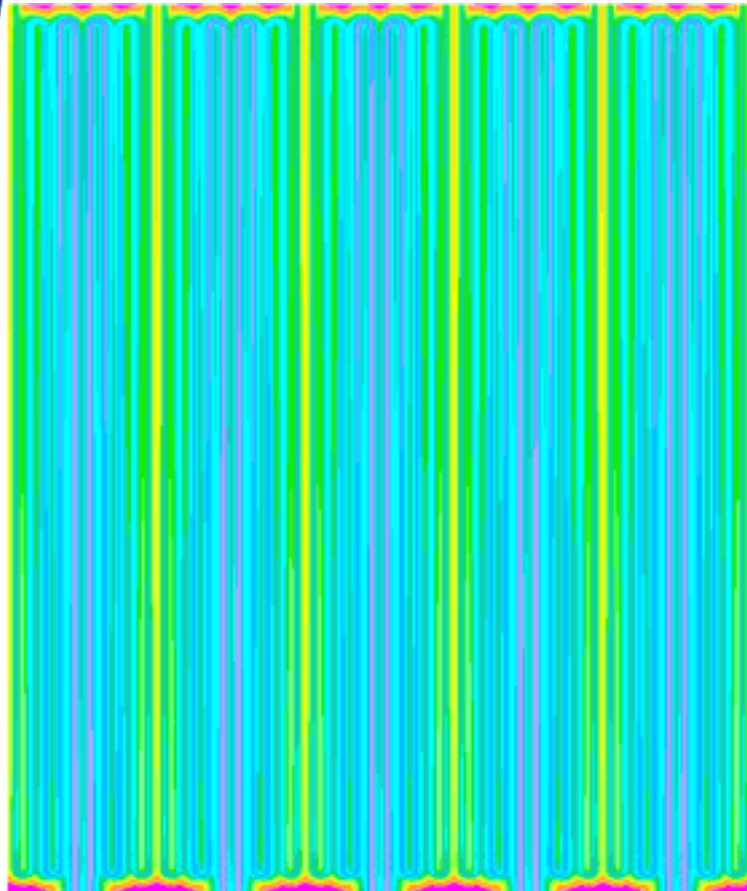


Cathode by-pass case

$\sigma_{avg} = 4.60$ ,  $V_{cell} = 0.57V$

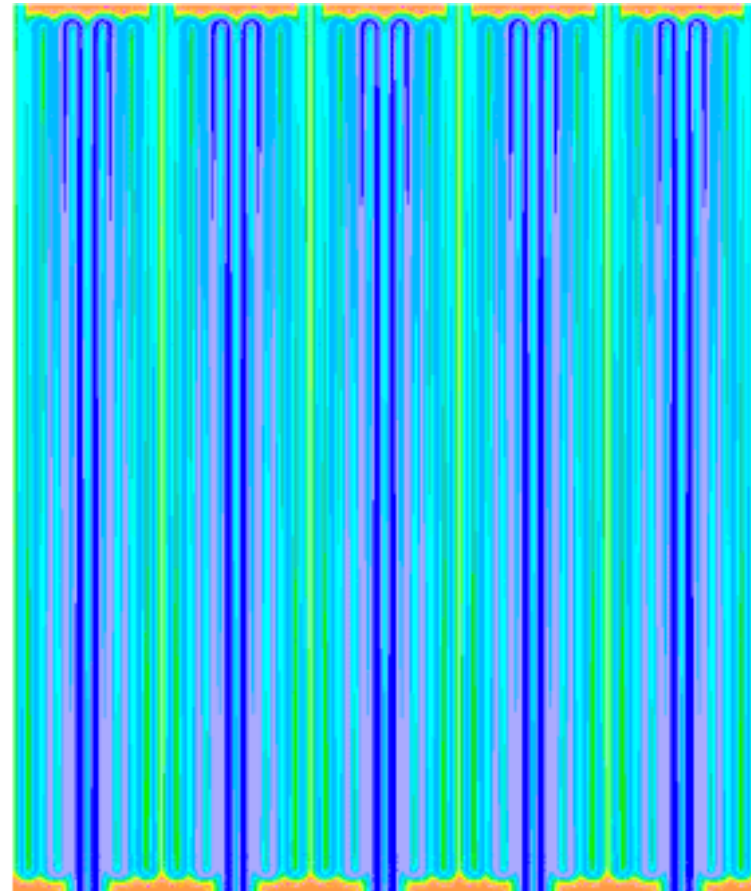


# Cathode over-potential (V) distribution on MEA surface at $I_{avg}$ of $0.6 \text{ mA/cm}^2$ between Normal case and Cathode by-pass case



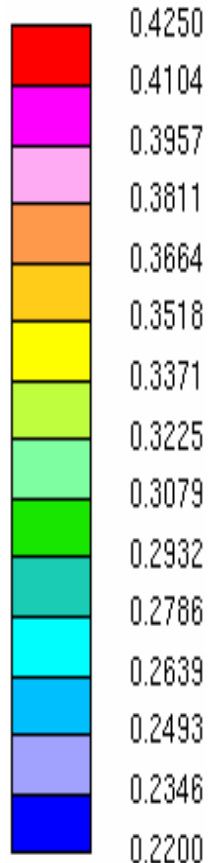
Normal case

$\eta_{O_2,avg} = 0.28$ ,  $V_{cell} = 0.59V$

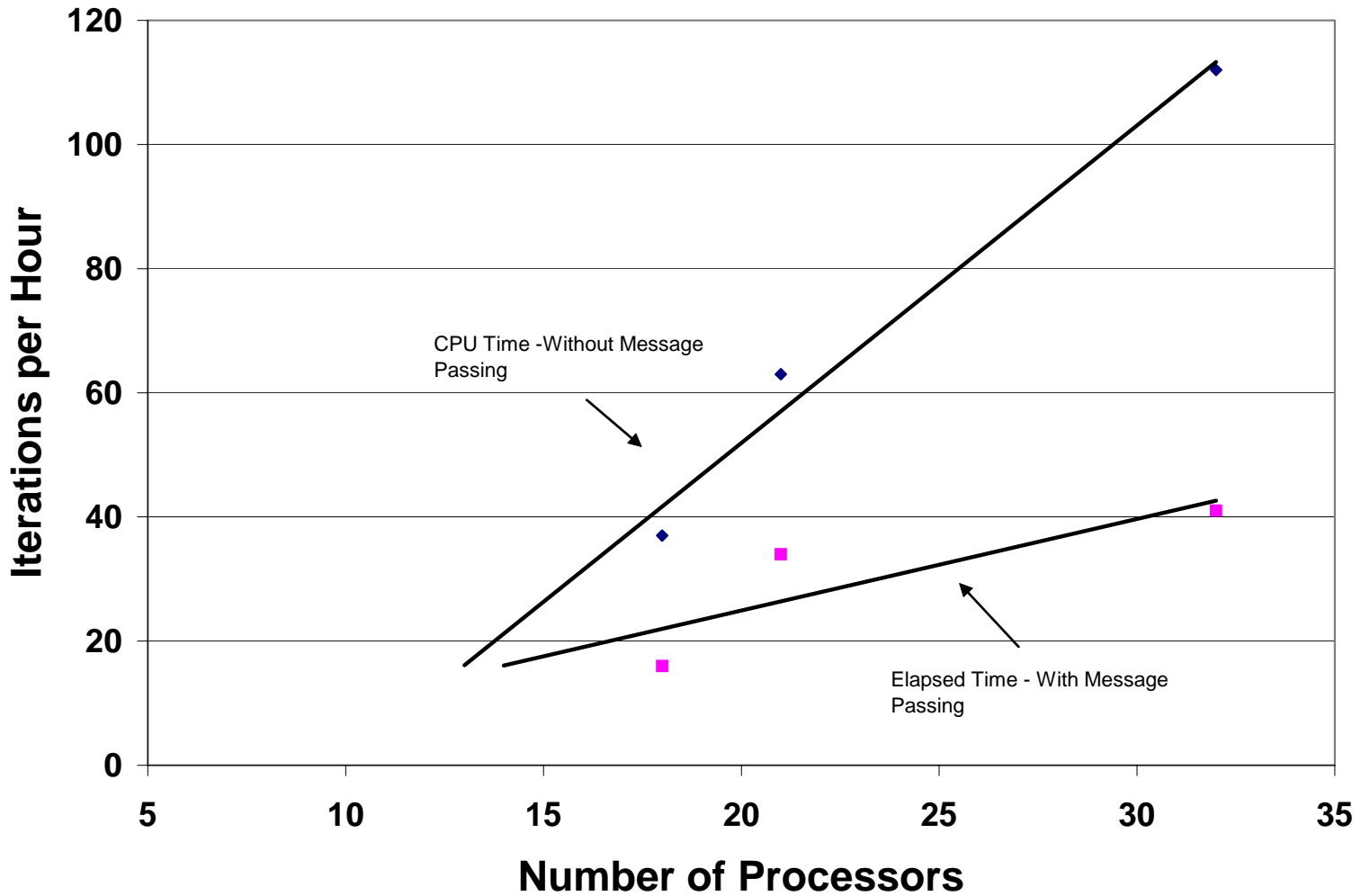


Cathode by-pass case

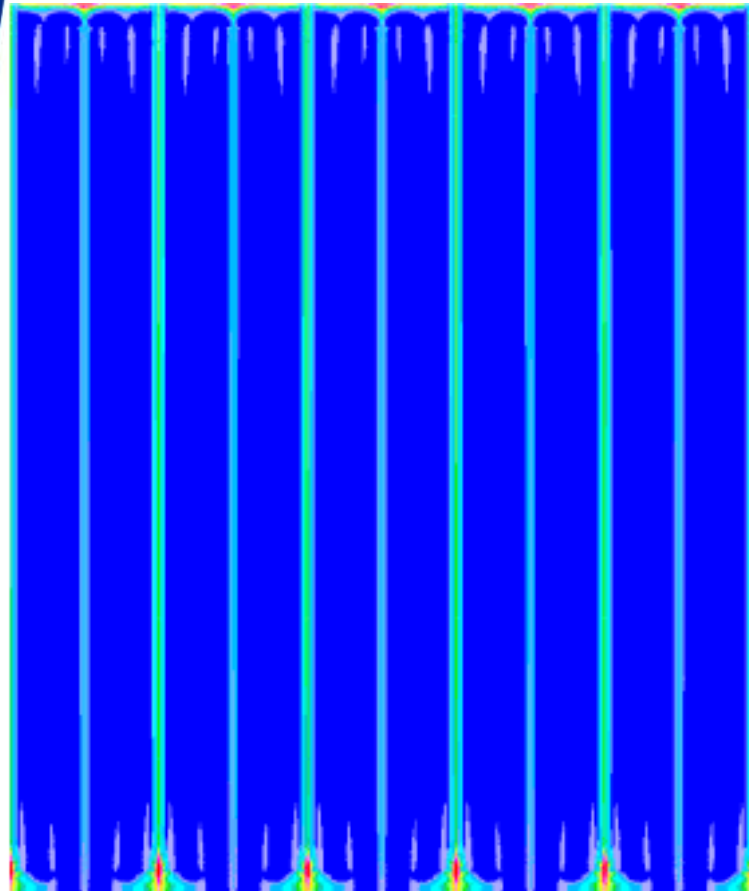
$\eta_{O_2,avg} = 0.24$ ,  $V_{cell} = 0.57V$



# Parallel performance

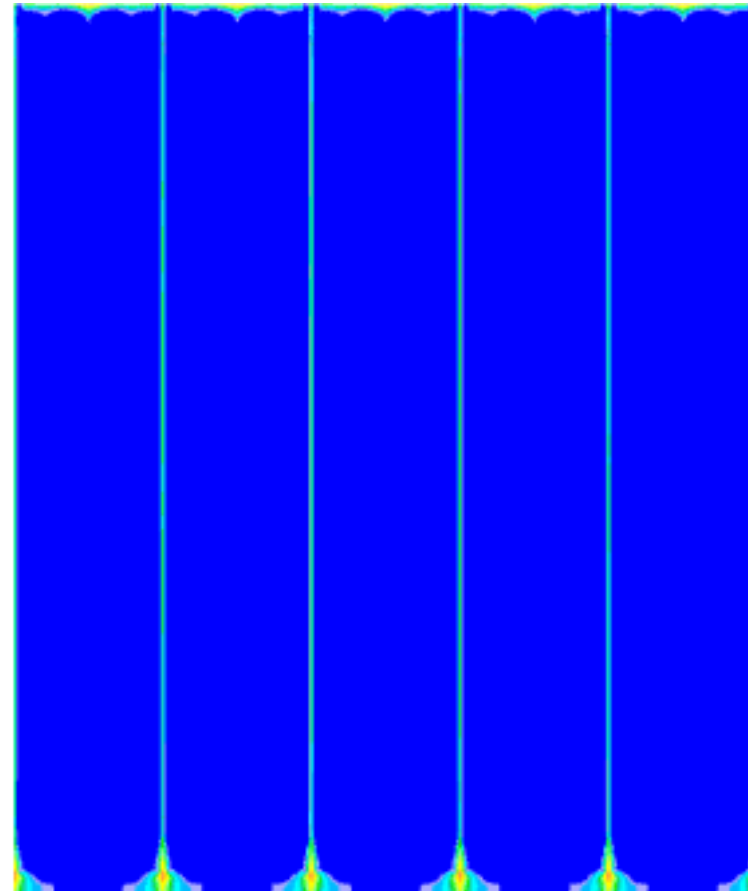


# Liquid water fraction distribution on cathode MEA surface at $I_{avg}$ of $0.6 \text{ mA/cm}^2$ between Normal case and Cathode by-pass case



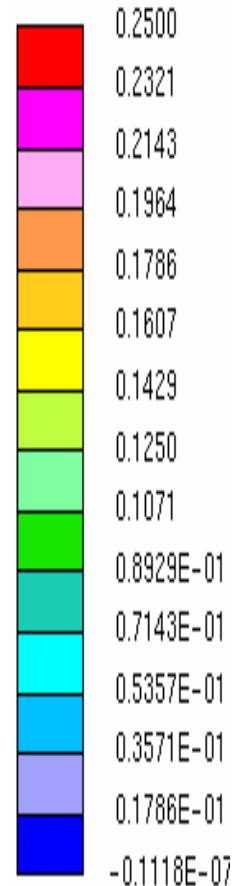
Normal case

$CW_{avg} = 0.02$ ,  $V_{cell} = 0.59V$

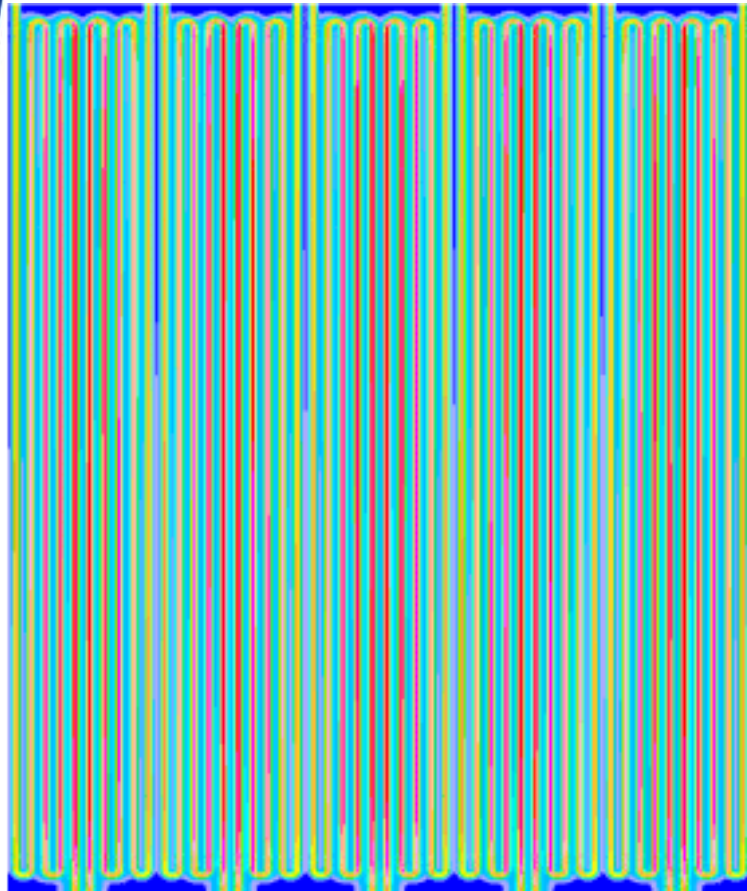


Cathode by-pass case

$CW_{avg} = 0.008$ ,  $V_{cell} = 0.57V$

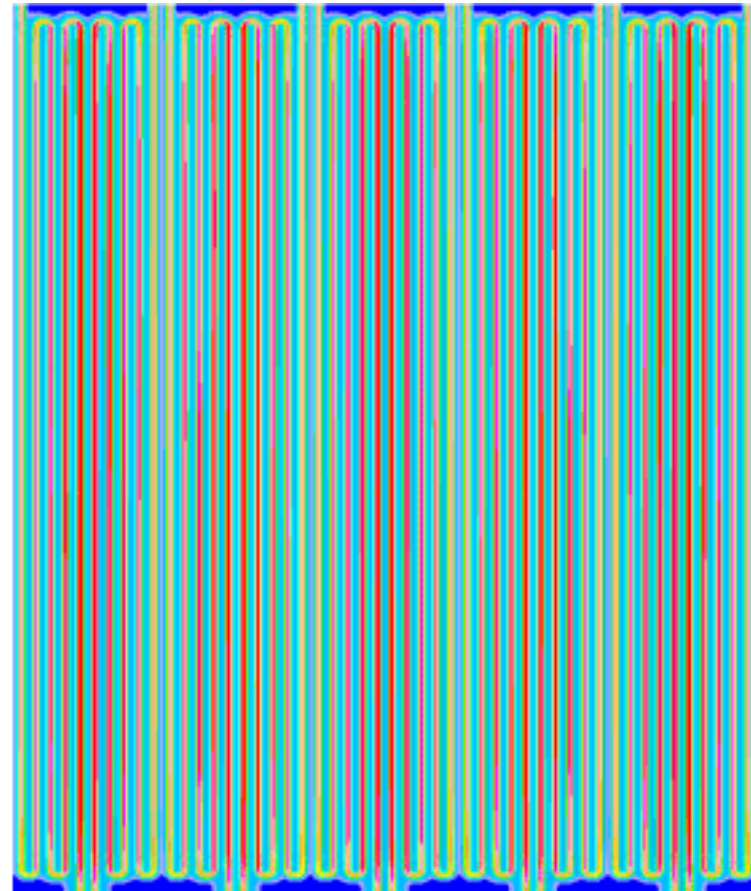


# Temperature (K) distribution on anode MEA surface at $I_{avg}$ of $0.6 \text{ mA/cm}^2$ between Normal case and Cathode by-pass case



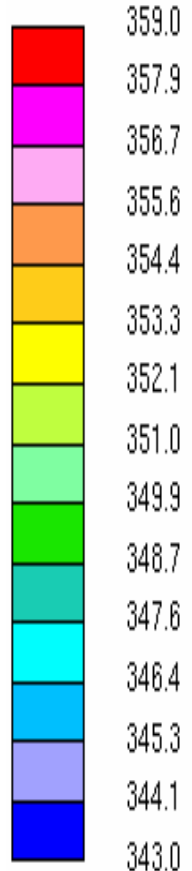
Normal case

$T_{avg} = 349$ ,  $V_{cell} = 0.59V$

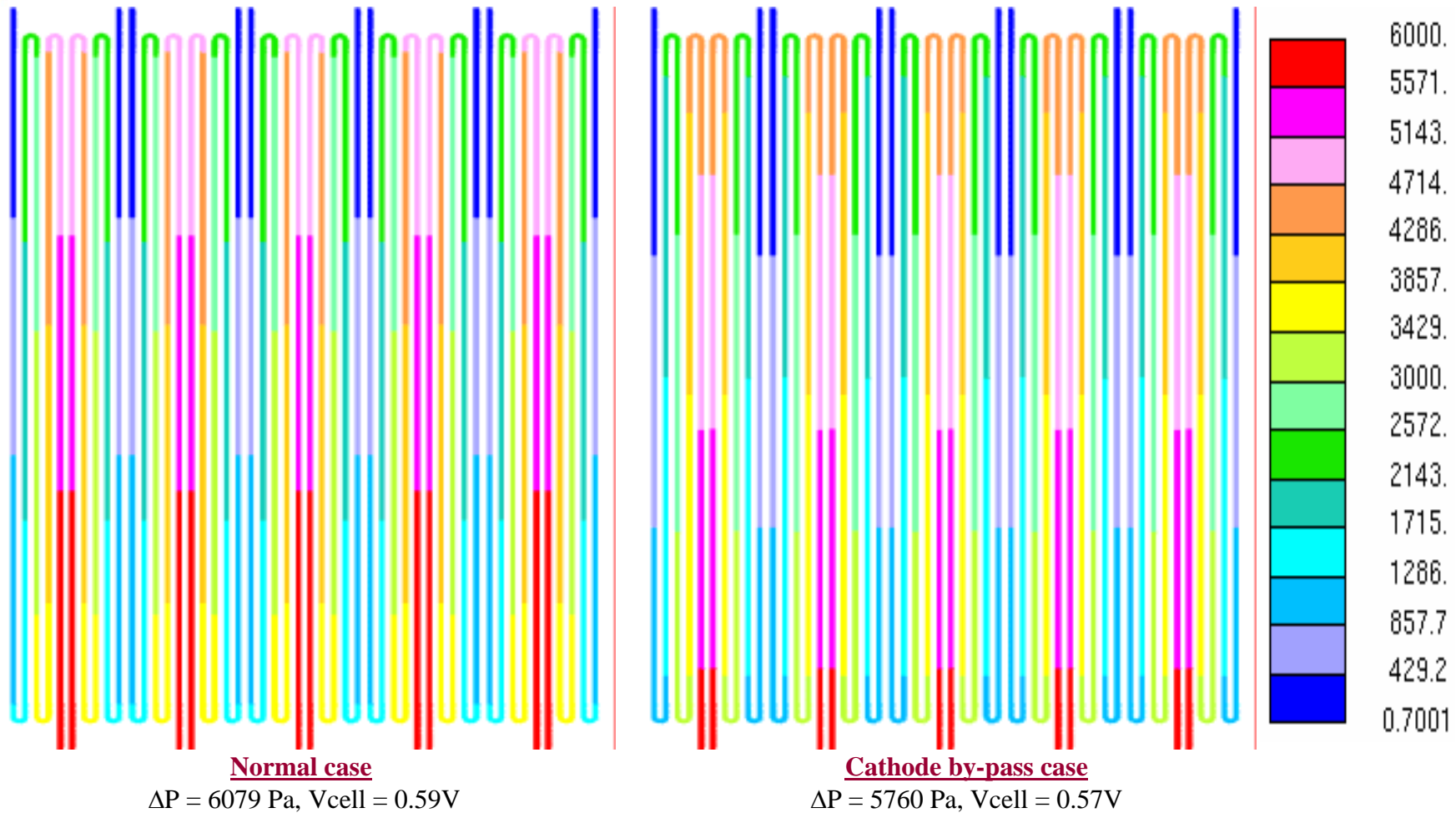


Cathode by-pass case

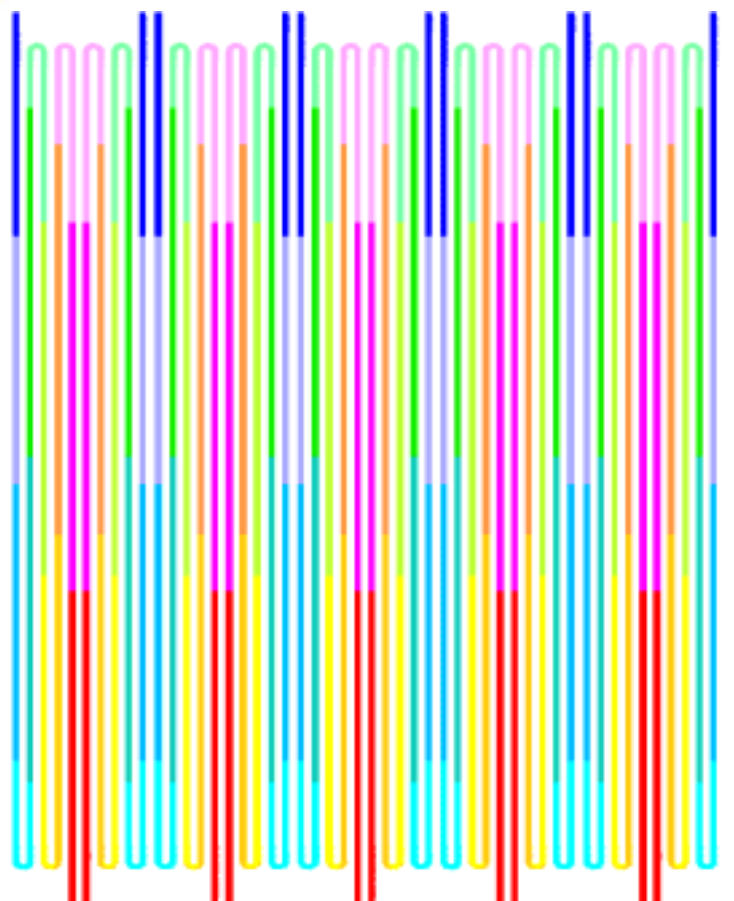
$T_{avg} = 349$ ,  $V_{cell} = 0.57V$



# Relative Pressure (Pa) distribution on anode flow channel at $I_{avg}$ of $0.6 \text{ mA/cm}^2$ between Normal case and Cathode by-pass case

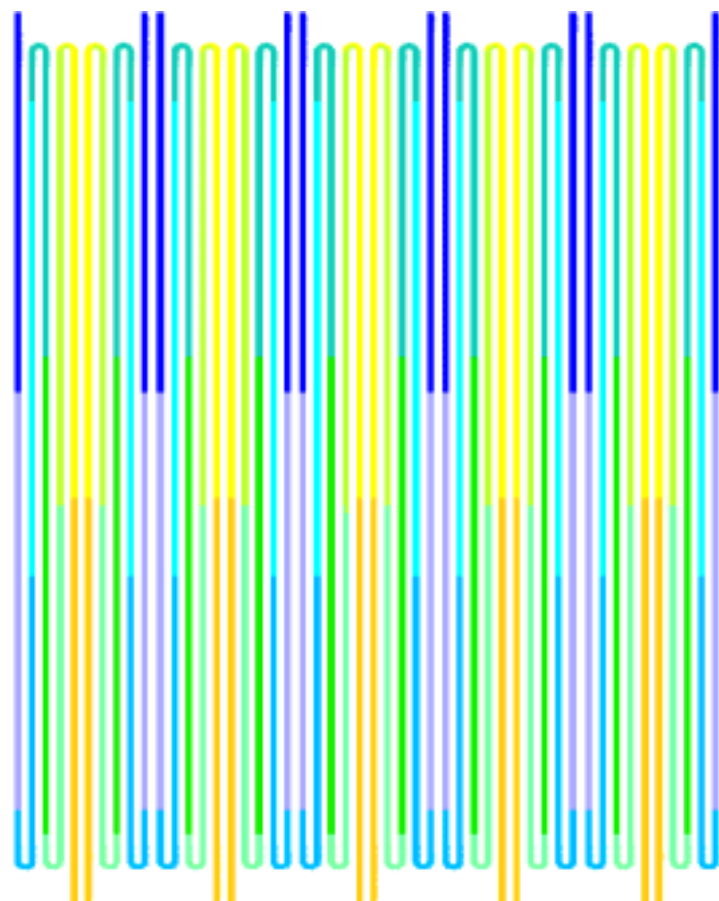


# Relative Pressure (Pa) distribution on cathode flow channel at $I_{avg}$ of $0.6 \text{ mA/cm}^2$ between Normal case and Cathode by-pass case



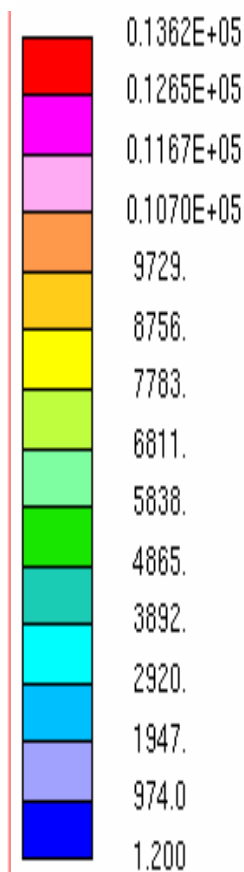
Normal case

$\Delta P = 13618 \text{ Pa}$ ,  $V_{cell} = 0.59V$



Cathode by-pass case

$\Delta P = 9632 \text{ Pa}$ ,  $V_{cell} = 0.57V$



## Summary

- Using similar membrane parameters, results were obtained for a well hydrated and dry membrane conditions.
- Polarization data for the two cells were similar, but distributions of electrochemical variables were different
  - Membrane Water Content and thus Membrane Conductivity were lower in the dry case
  - Cathode Overpotential was lower for the dry case due to the very low concentration of liquid water





## Conclusions

- The performance of the dry cell is lower, but not significantly lower
- The decrease in Cathode Overpotential in the dry case nearly compensated for the lower Membrane Conductivity
- The lower pressure drop in the cathode bypass case makes the flow-field better suited for automotive applications

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