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# Computational Modelling of Solid Oxide Fuel Cells

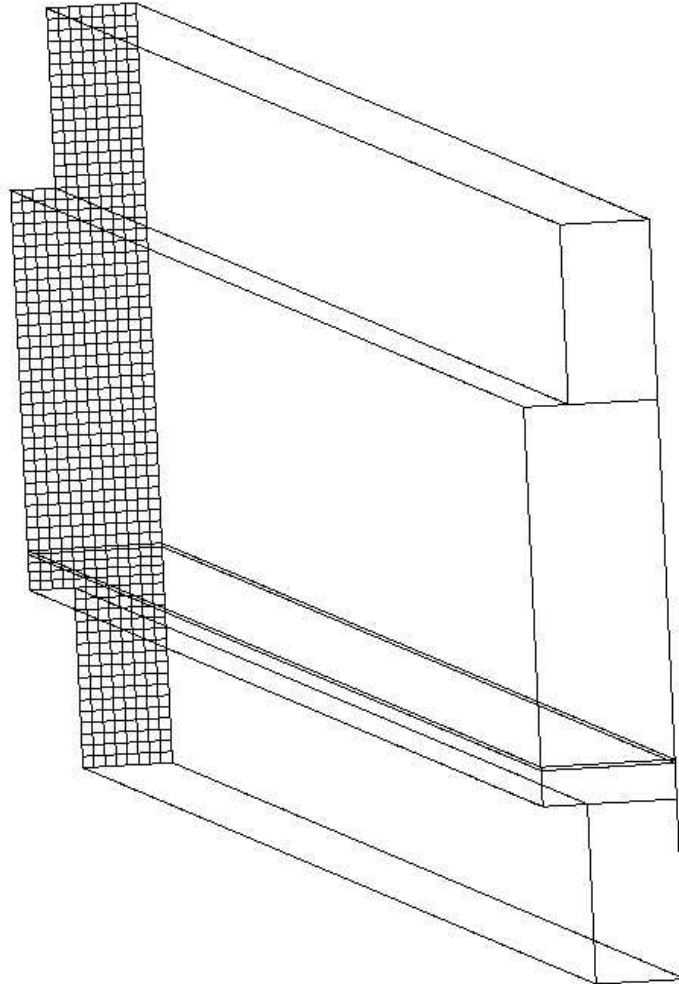
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# Project Objectives

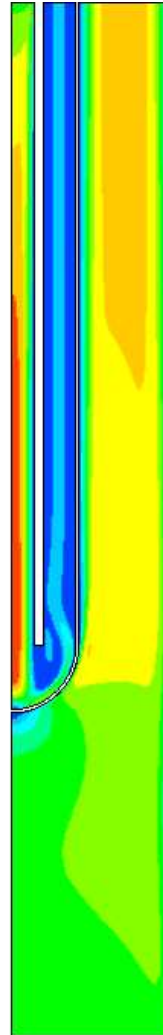
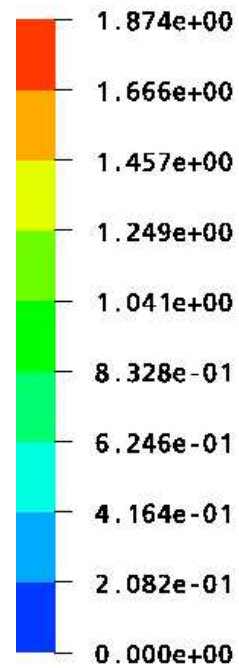
- To model tubular SOFC stacks including:
  - Electrochemistry
  - Internal reforming
  - Heat transfer including participating medium radiation
  - Combustion of exhaust streams
- To apply CFD to optimize component design

# Planar Geometry



# Tubular Geometry

Velocity  
(Contour 1)



# SOFC Modelling: Process and Flows

- Electrochemical reaction leads to
  - Charge generation  $\rightarrow$  *current flow*  $\rightarrow V$
  - Chemical conversion  $\rightarrow$  *mass flow*  $\rightarrow c$
  - Heat generation  $\rightarrow$  *heat flow*  $\rightarrow T$
- Transport in porous media
- In addition–radiation and eforming
- Highly non-linear, coupled

# Modelling Accomplishments

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- Laminar flow and heat transfer in flow channels

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- Turbulent flow and heat transfer in tubes
- Laminar flow in porous media (Darcy model)
- Heat and species transport in porous media
- Diffusion dominated mass transport
- Multicomponent diffusion and conservation of species

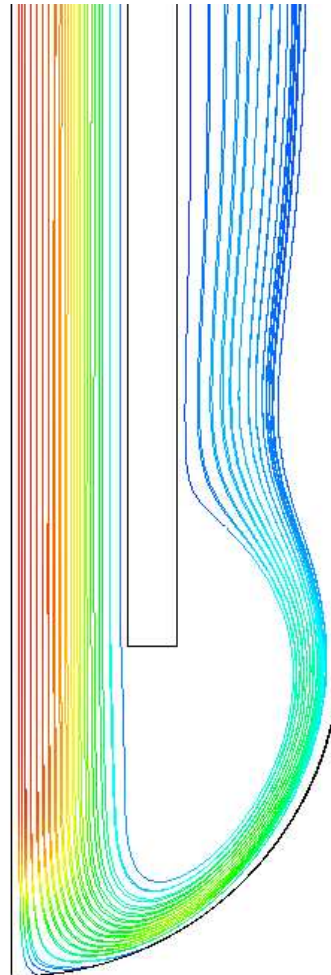
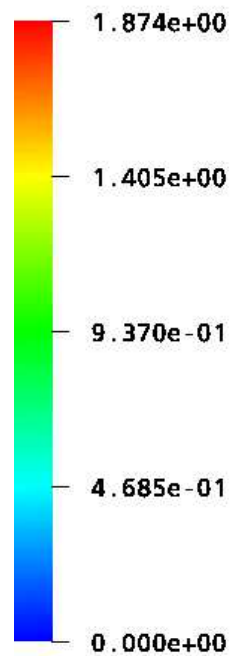
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- Laminar flow in porous media (Darcy model)
- Heat and species transport in porous media
- Diffusion dominated mass transport
- Multicomponent diffusion and conservation of species
- Electrochemical reaction via sources and sinks in catalyst

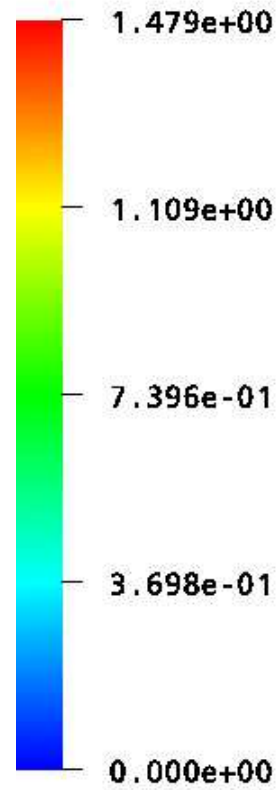
# Flow and heat transfer in channels

Velocity  
(Streamline 1)

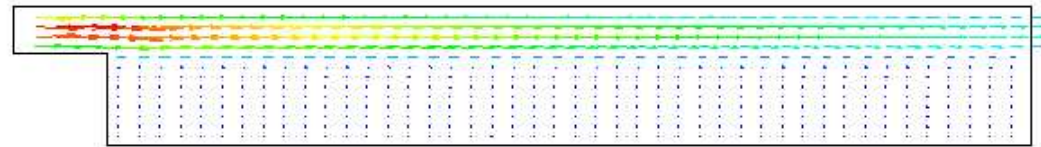
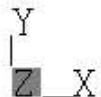


# Laminar flow in porous media

Velocity  
(Vector 1)

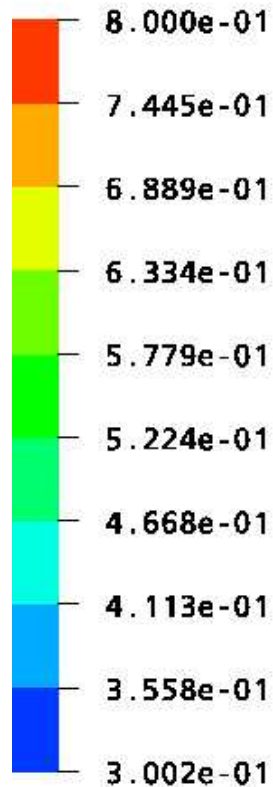


[m s<sup>-1</sup>]



# Heat and species transport in porous media

H2 . Mass Fraction  
(Mass Fraction)



Y  
|  
■ X

# Current Work–Model Development

- Develop/refine individual sub models
- Constantly testing/improving models
- Representative geometry
- Tubular and planar
- Radiation with participating medium
- Conference paper, Rochester

# Radiation

- Ignored in most SOFC models
- Nothing on participating media
- Planar and tubular
- Preliminary results show
  - Difference of 50° when using radiation model
  - Little effect from gas in planar
- Tubular geometry is very different

# On Going Work

- Activation overpotentials - Butler-Volmer
- Ohmic losses - electronic / ionic potential field
- Reforming
- Refine and combine sub-models
- Stefan-Maxwell multi-component diffusion
- Validate porous media model (Knudsen Diffusion)
- Our needs - validation data and transport properties