MATHEMATICAL MODELING AND EXPERIMENTAL STUDIES OF HYDROGEN COMBUSTION IN MICROTUBULAR SOLID OXIDE FUEL CELLS

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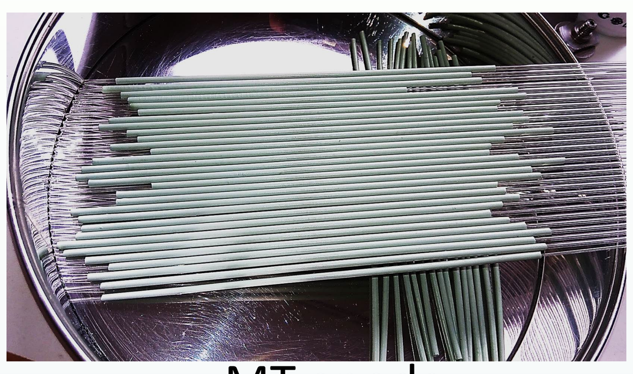
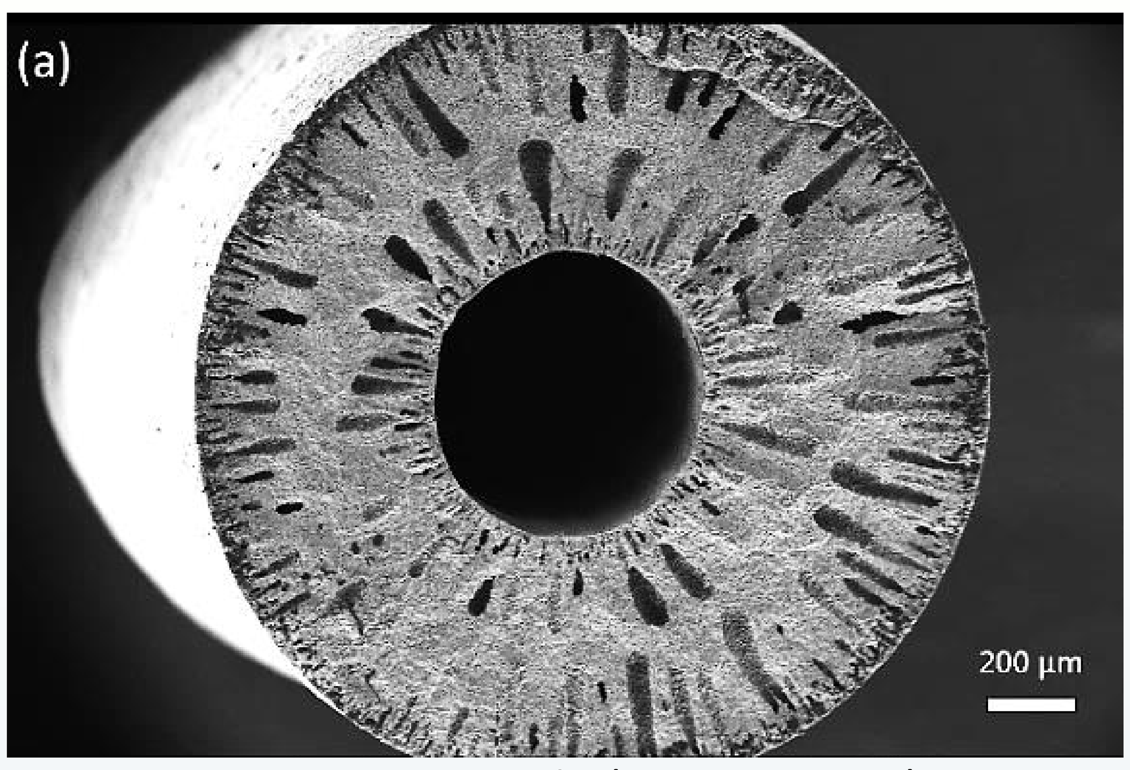
MICROTUBULAR SOLID OXIDE FUEL CELLS:

- MT SOFCs – tubular elements whose outer diameter < 5 mm
- Gastight thin layer (electrolyte) sandwiched between porous layers (anode and cathode)
  - High oxygen flows
  - Mechanical strength
  - Thermal stress resistance
- Cathode and anode reactions:
  - $O_2 + 4\bar{e} \rightarrow 2O^{2-}$
  - $2H_2 + 2O^{2-} \rightarrow 2H_2O + 4\bar{e}$
- The limiting factor in MT SOFC wide application in electrical devices is reactor design and performance
- The mathematical modeling is meant to help this problem solution



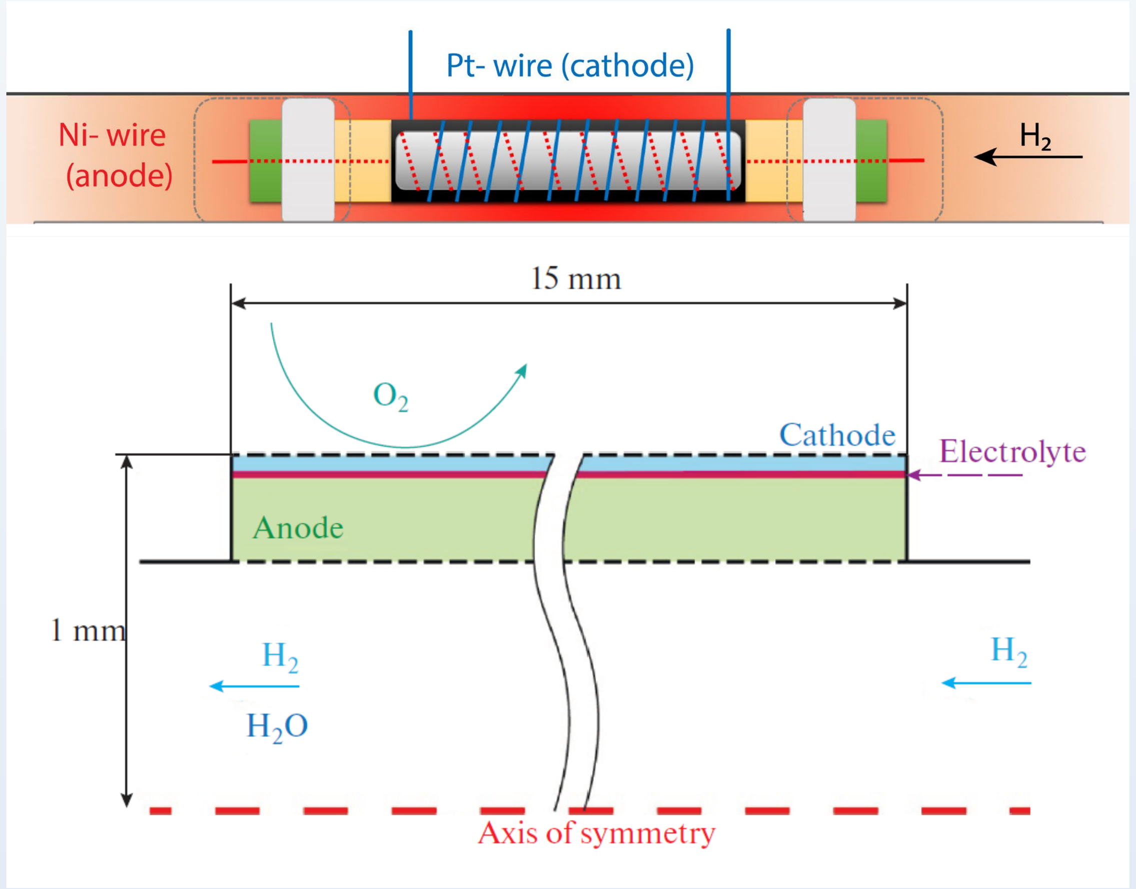
MT anode



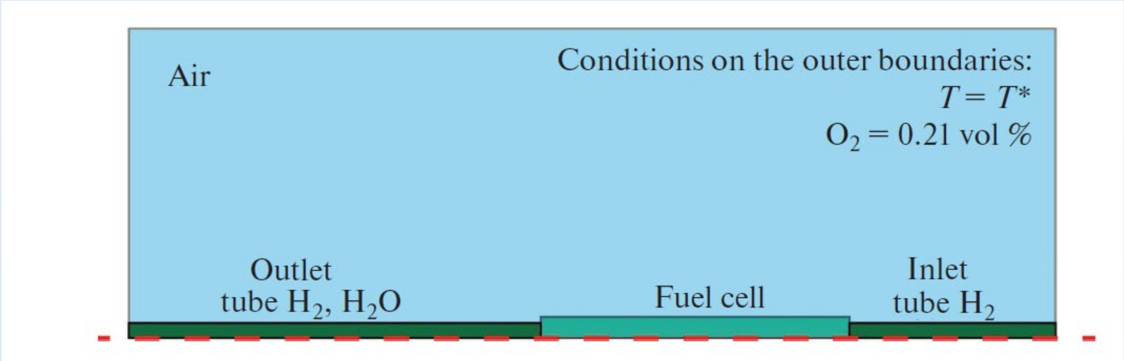
MT anode (cross-section)

Mathematical model (COMSOL Multiphysics, 2D-axisymmetric geometry):

- Species transport (free and porous media):
  - $\nabla \cdot j_i + \rho(u \cdot \nabla)\omega_i = 0$
  - $j_i = -\left(\rho\omega_i \sum_k D_{ik}\left[\nabla x_k + \frac{1}{p}\left((x_k - \omega_k)\nabla p\right)\right]\right)$
  - $x_k = \frac{\omega_k}{M_k}M_n, \quad M_n = \left(\sum_i \frac{\omega_i}{M_i}\right)^{-1}$
  - Boundary reaction
    - $-n \cdot j_i = \sum_k M_i R_{i,k}$
- Species transport (electrolyte):
  - $-\nabla \cdot (D_{O2}^s \nabla c^-) = 0$
  - Boundary reaction
    - $-n \cdot j_i = \sum_k R_{i,k}$
- Momentum balance (free and porous media)
  - $\rho(u \cdot \nabla)u = \nabla \cdot \left[-pI + \mu(\nabla u + (\nabla u)^T) - \frac{2\mu}{3}(\nabla \cdot u)I\right]$
  - $\nabla \cdot (\rho u) = 0$
- Heat balance
  - $\rho C_P u \cdot \nabla T - \nabla \cdot \left(\left(1-\varepsilon_p\right)\lambda_s + \varepsilon_p \lambda\right)\nabla T = 0$
  - Boundary reaction heating
    - $-n \cdot q = Q$



MT SOFC general scheme



Computational domain view

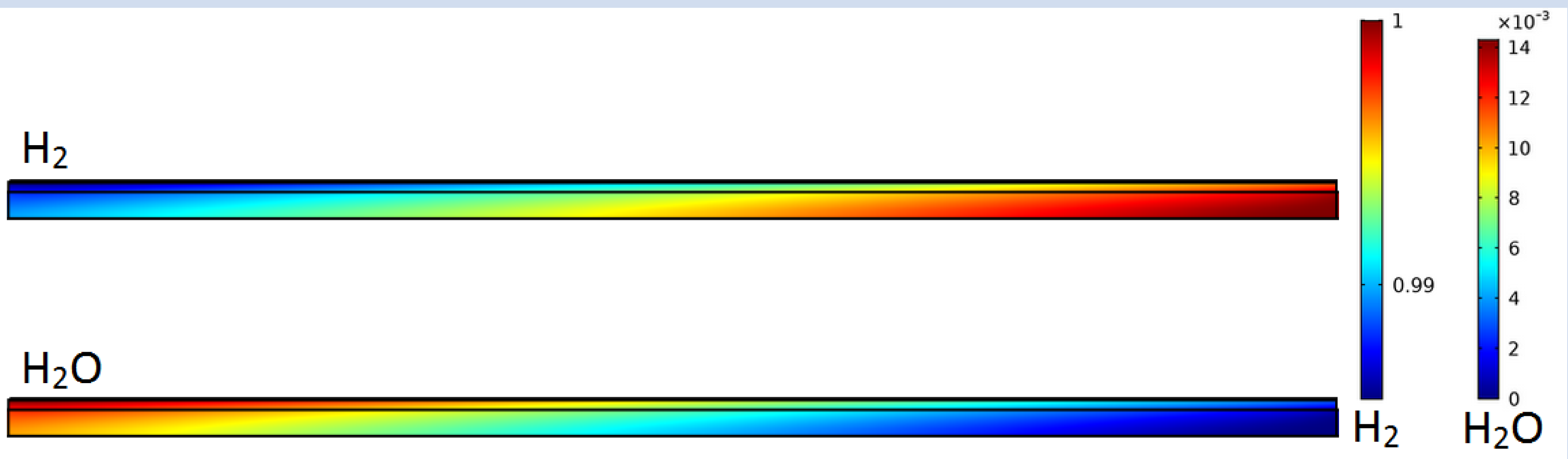
Model parameters:

- Gas inlet conditions:
  - H2 inlet concentrations – 1 mole fraction
  - Gas flow rate 300 ml/min
  - 600<T*<850
- Reaction rates:
  - $R_1 = k_1\left(c_O - \frac{c^-}{k_{eq}}\right)$
  - $R_2 = k_2 x_H c^-$
- Solid-phase diffusivity
  - $D_{O2}^s = 1.5 \times 10^{-8}\exp(-8120/T)$ m²/s

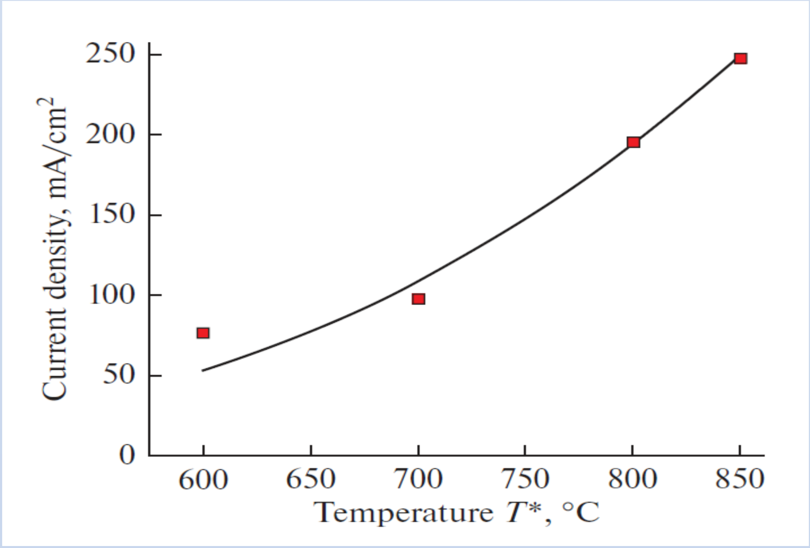
i	1	2	eq
E_i, J/mol	40 000	70 000	2 365
k_i^0	1, mol/m²/s	10, m/s	20 800

Estimated kinetic parameters

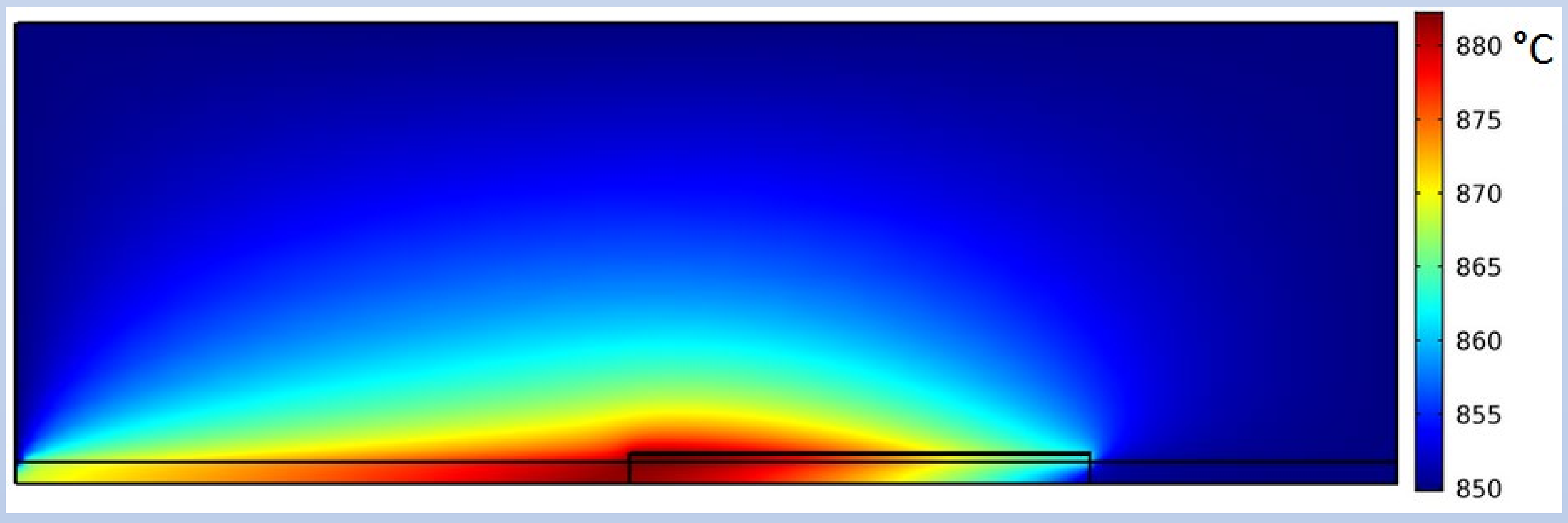
RESULTS (T*=850 °C):



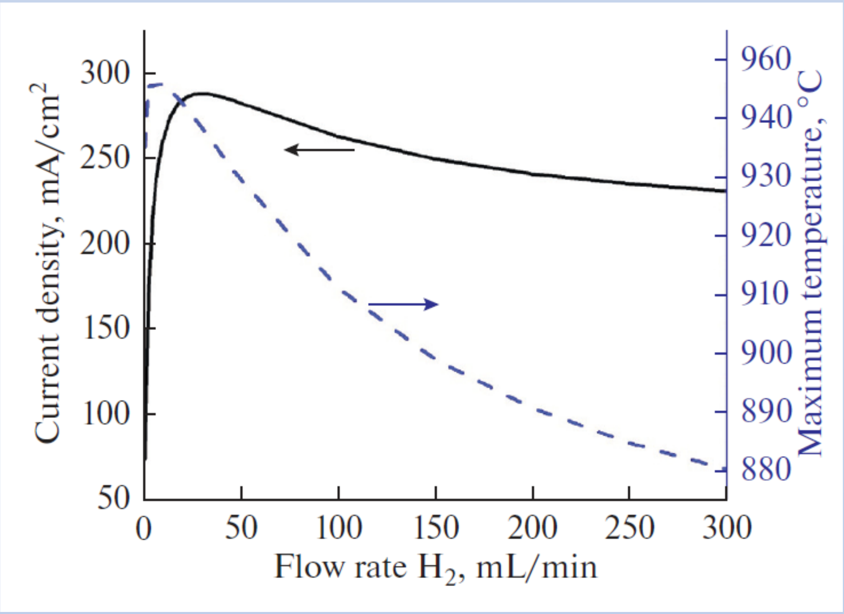
Hydrogen and water concentrations inside the tube, mole fraction

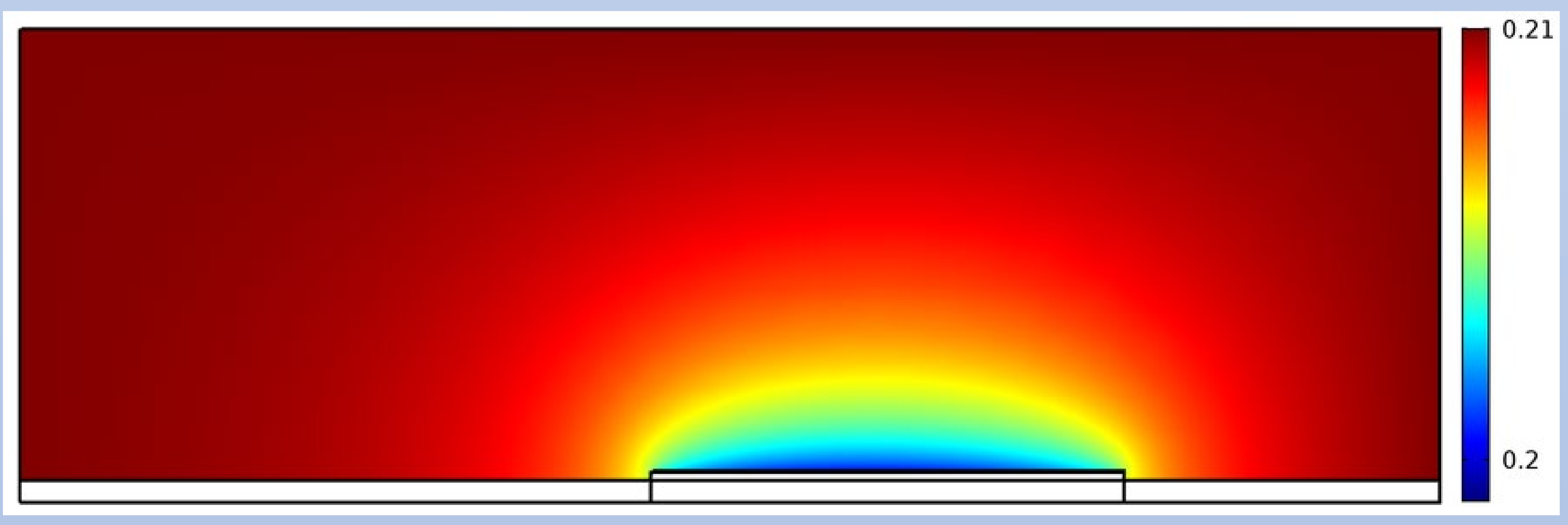


model vs. experiments(red dots)

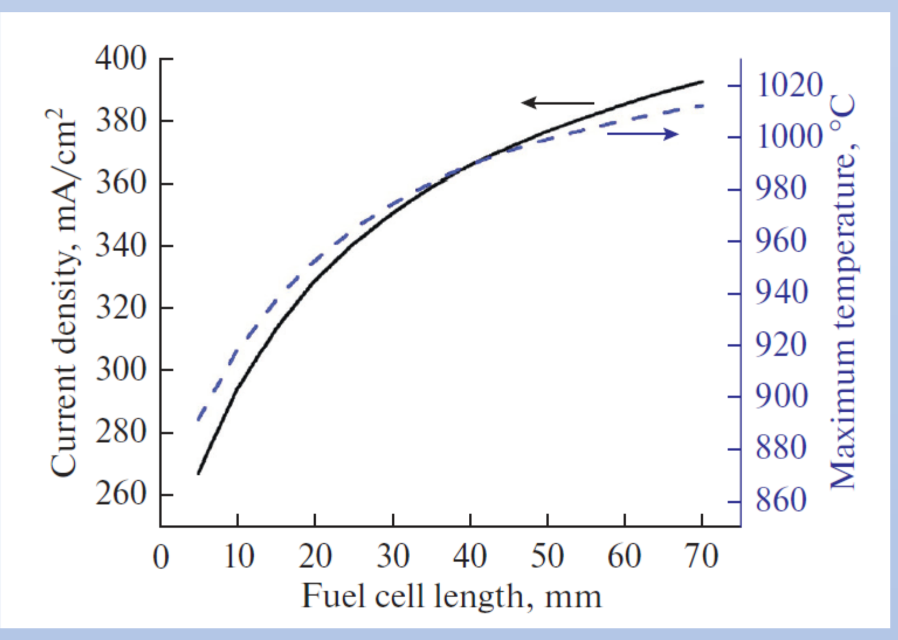


Temperature distribution in the whole domain





Outer oxygen concentration, mole fraction



- Conclusion
  - High hydrogen flow rate leads to current density decreasing
  - Too long tubes may lead to overheating