INSTITUTE OF CHEMICAL TECHNOLOGY PRAGUE

Development of mathematical modelling tool for analysis and optimization of the High Temperature Solid Oxide Steam Electrolysis process

STARRING

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Hydrogen production

Utilization

- Chemical industry
- Hydrogen economy

Production methods

- Steam reforming
- Water electrolysis
  - Minor
  - Sustainable
  - Pure
  - Electric energy storage/consumption

Alkaline water electrolysis

Water electrolysis

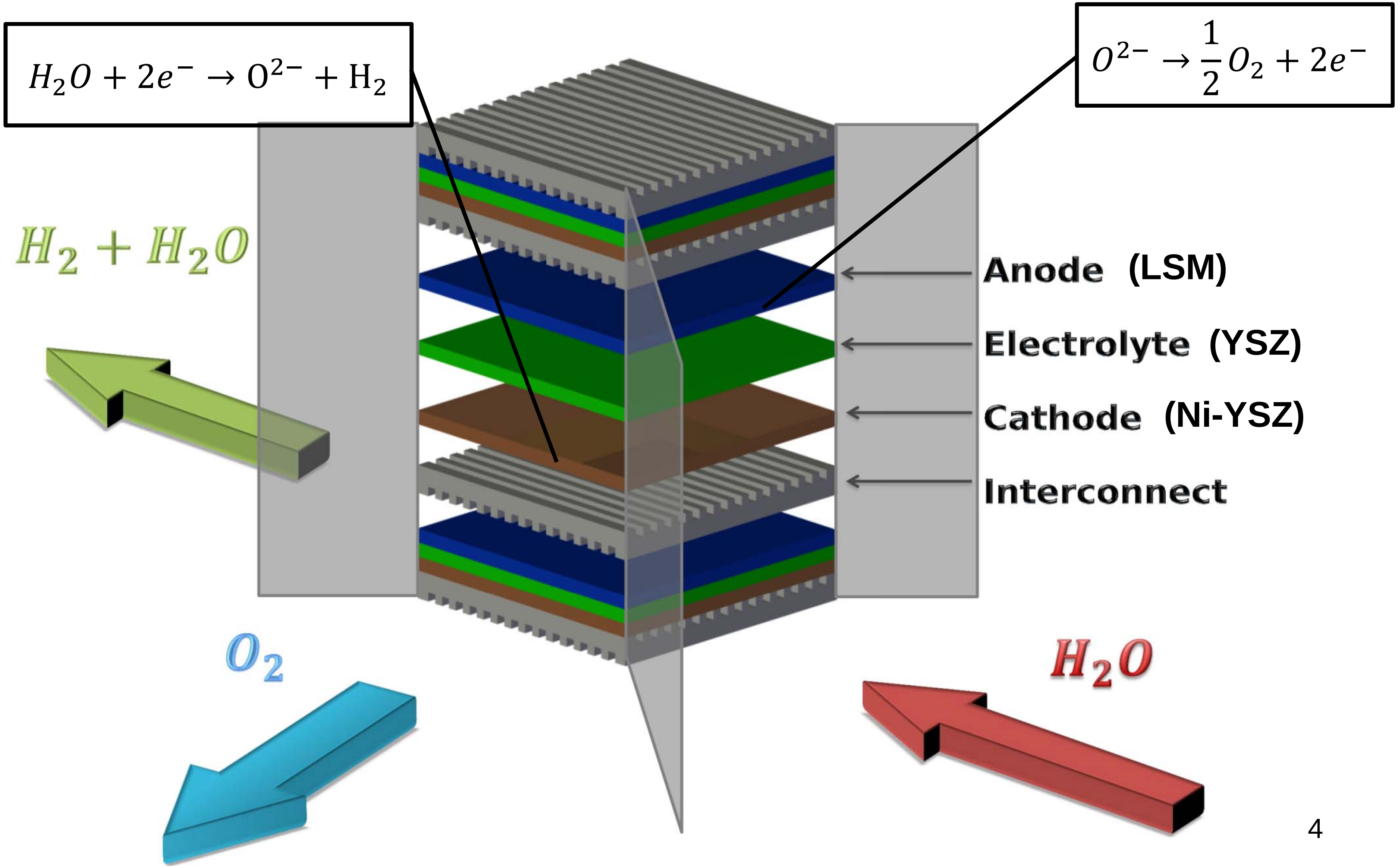
Conventional

- Alkaline Water Electrolysis
- High electric energy requirement

Alternative

- High Temperature Steam Electrolysis
- Lower electric energy input
- Economical only with appropriate heat source (cheap, stable, high temperature)

HTSE - planar arrangement



Objectives

Long-term goals

- Mathematical modeling the HTSE process
  - Understanding
  - Prediction
  - Optimization
  - Scale-up

Presentation objectives

- History and current stage of development in ICTP
- Peculiarities of HTSE system

Mathematical background

Charge transfer

$$\nabla \cdot j_{io} = \nabla \cdot (-\sigma_{io} \nabla \Phi_{io}) = j_R \cdot a_{TPB}$$

$$\nabla \cdot j_{el} = \nabla \cdot (-\sigma_{el} \nabla \Phi_{el}) = -j_R \cdot a_{TPB}$$

$$j_R = j_0 \left(\frac{c_{red}}{c_{red}^*} e^{\beta_{ox} \eta \frac{zF}{RT}} - \frac{c_{ox}}{c_{ox}^*} e^{-\beta_{red} \eta \frac{zF}{RT}} \right)$$

Heat transport

$$\nabla \cdot \left(\vec{\hat{\dot{h}}} + \vec{\hat{\dot{q}}} \right) = \nabla \cdot \left(C_p \vec{\hat{\dot{n}}} T - \lambda \nabla T \right) = q_R$$

Mathematical background

Material transport - porous structures

$$\nabla \cdot \vec{\hat{\dot{n}}}_{H_2O} = \nabla \cdot \left(-D_{H_2O} \nabla p_{H_2O}\right) = n_{R,H_2O} \cdot a_{TPB}$$

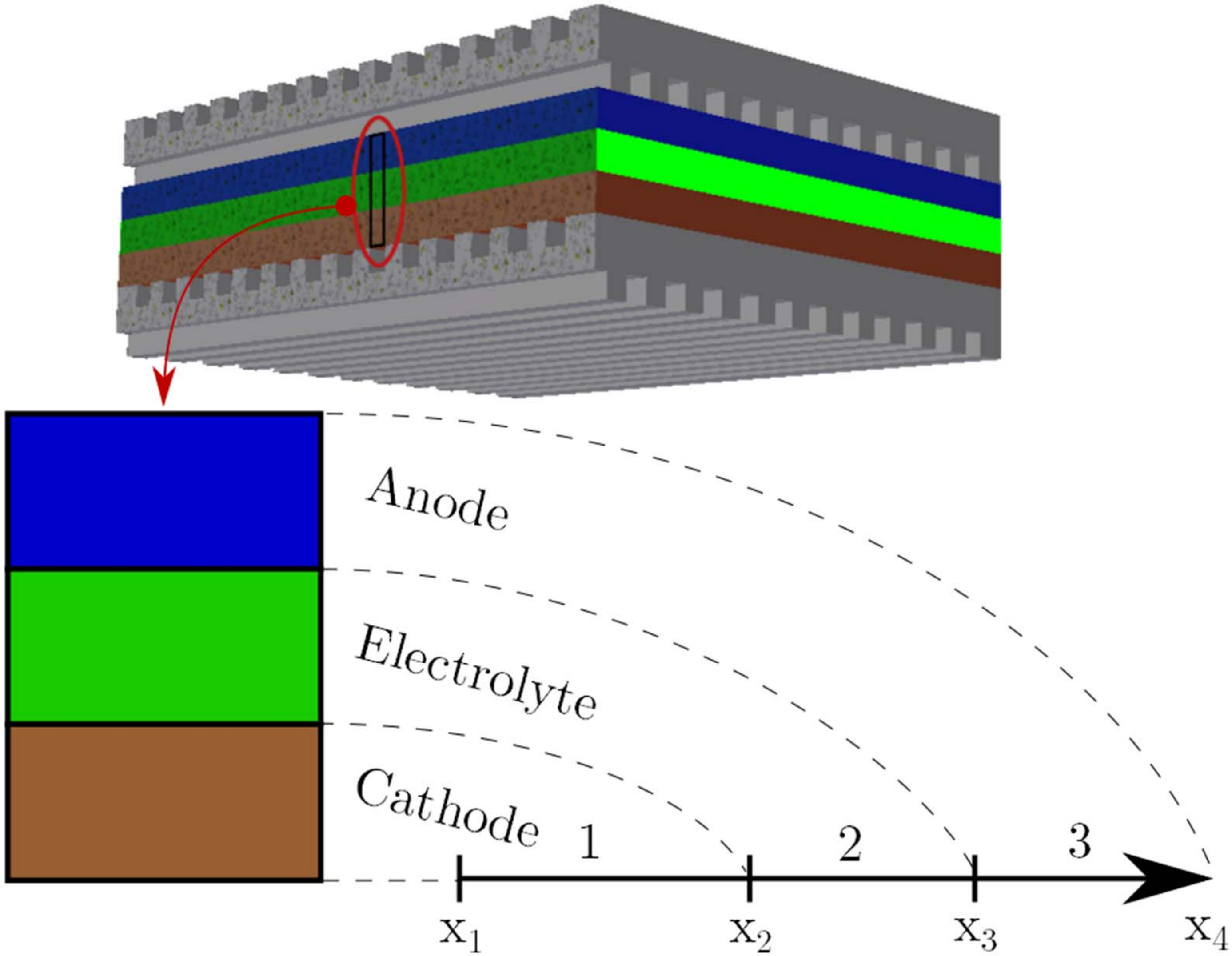
$$\nabla \cdot \vec{\hat{\dot{n}}}_{O_2} = \nabla \cdot \left(-D_{O_2} \nabla p_{O_2}\right) = n_{R,O_2} \cdot a_{TPB}$$

$$p_{H_2} = p - p_{H_2O}, \qquad D^{eff} = \frac{\varepsilon}{\xi}\left(\frac{1}{D_{Knudsen}} + \frac{1}{D_{Transport}}\right)^{-1}$$

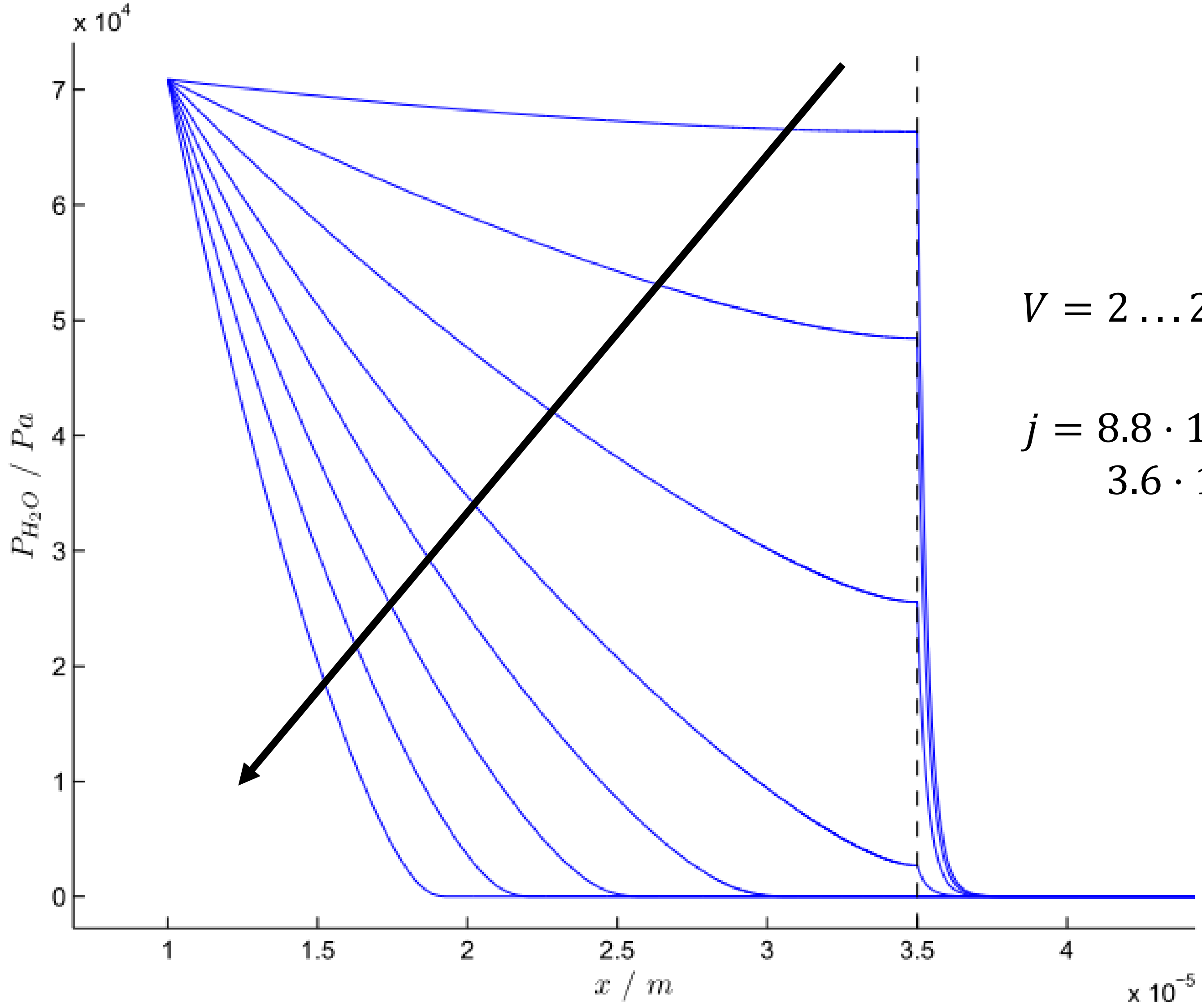
Material transport – flow channels

- Navier-Stokes equation (laminar flow)
- Continuity equation (compressible)

1D modelling



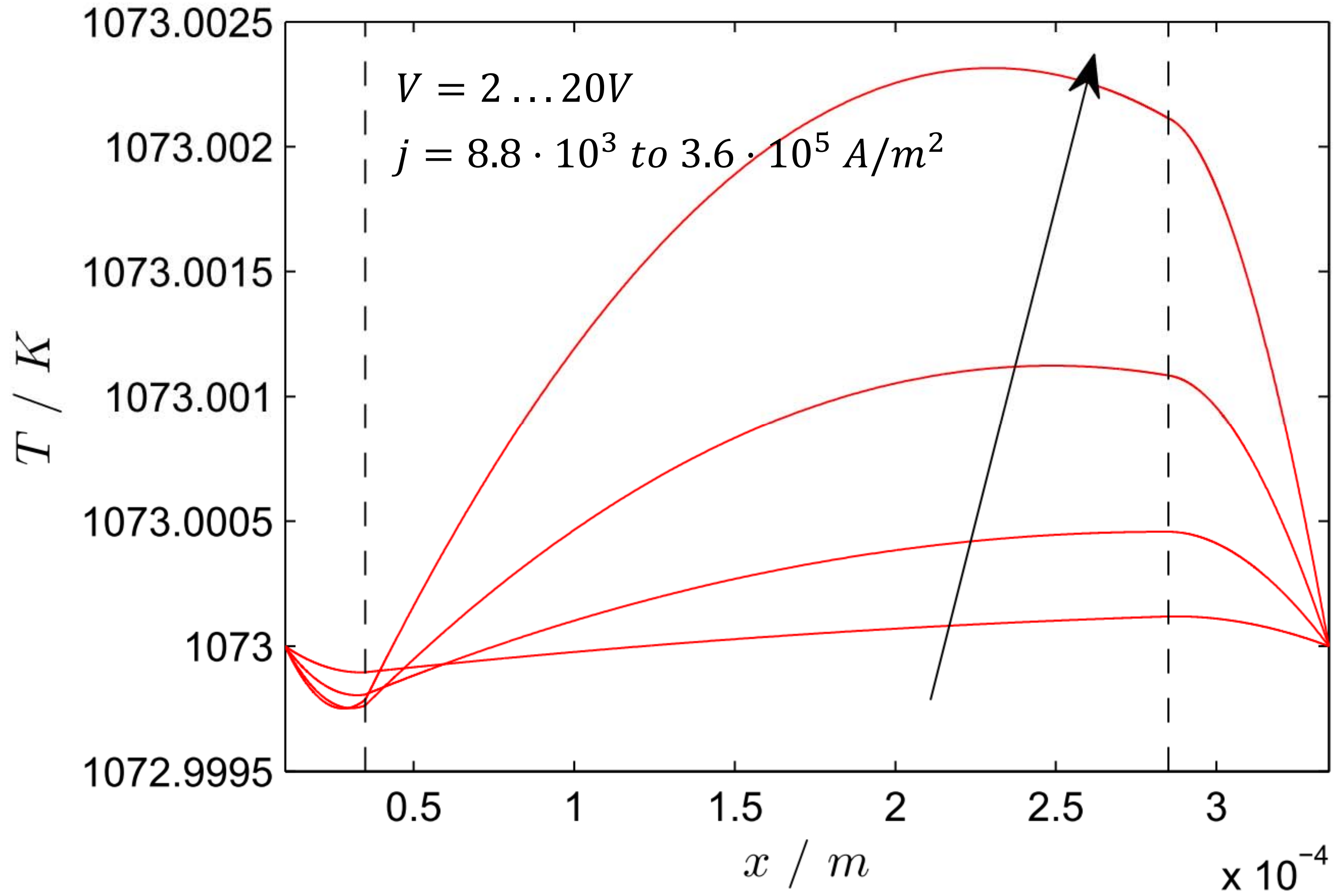
1D modelling



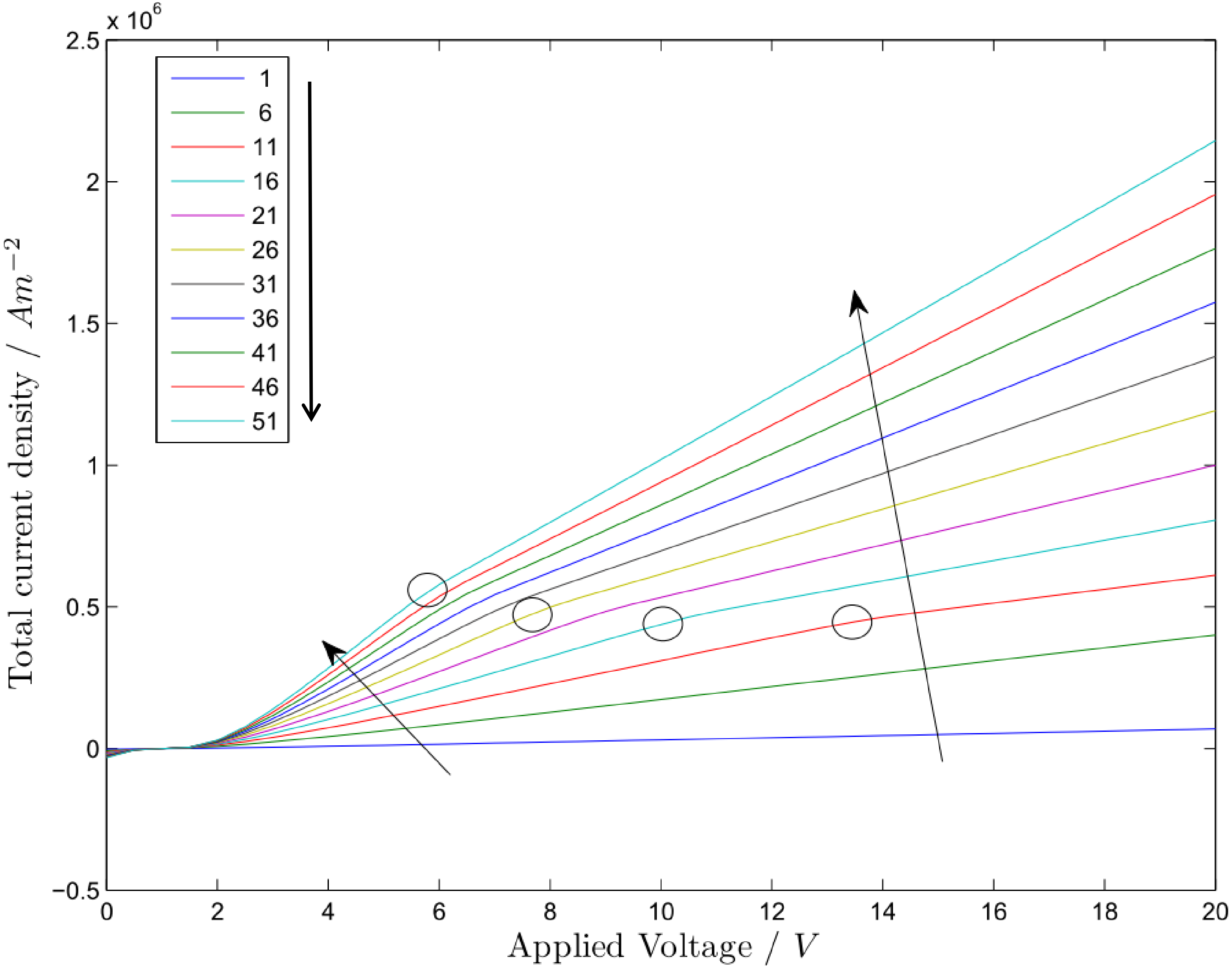
$V = 2 \ldots 20V$

$j = 8.8 \cdot 10^3 \ldots$
$3.6 \cdot 10^5\ A/m^2$

1D modelling – temperature



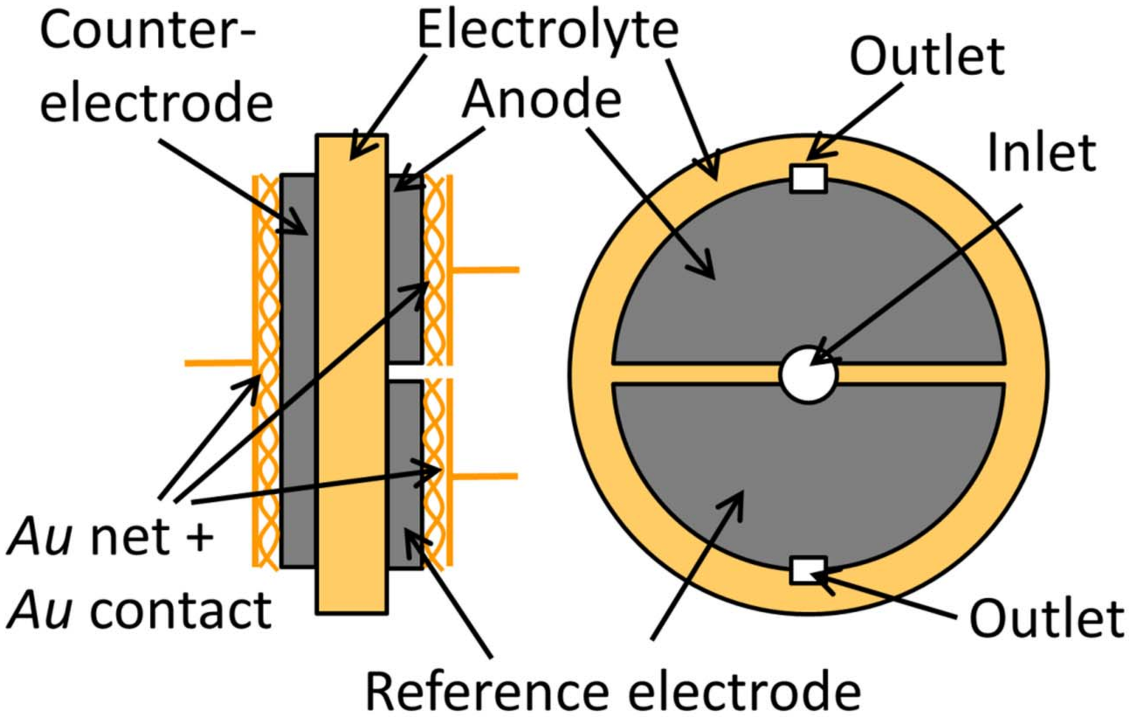
1D modelling – YSZ conductivity



Evaluation of kinetic data of anode reaction

- 1st step: potentiodynamic measurements of LSM anode in symmetric cell

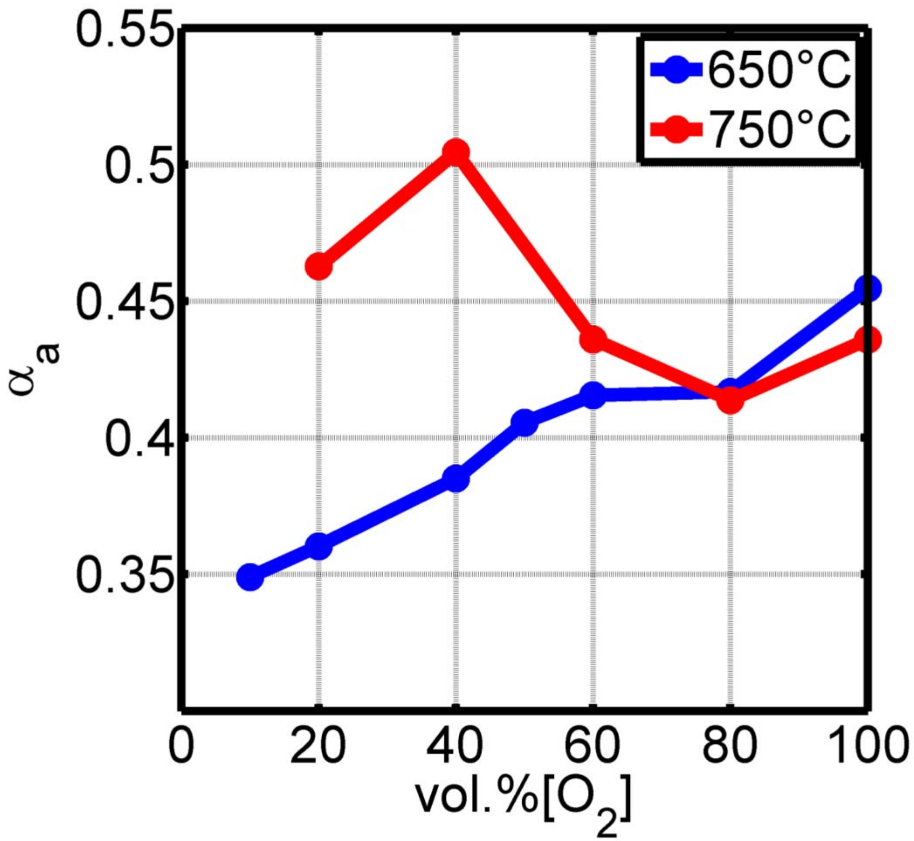
$$O^{2-} - 2e^{-} \rightarrow \frac{1}{2}O_2$$



Anode/Reference electrode: O_2+N_2, 20-100 vol.%[O_2], **Counter electrode:** air
Temperature 650 °C, 750 °C, **Pressure:** atmospheric

Evaluation of kinetic data of anode reaction

- 2nd step: Tafel analysis of anodic region of overvoltage



Tafel's equation

$$\eta = -\frac{RT}{\alpha_a F}\ln\left(I_{o,a}\right) + \frac{RT}{\alpha_a F}\ln(I)$$

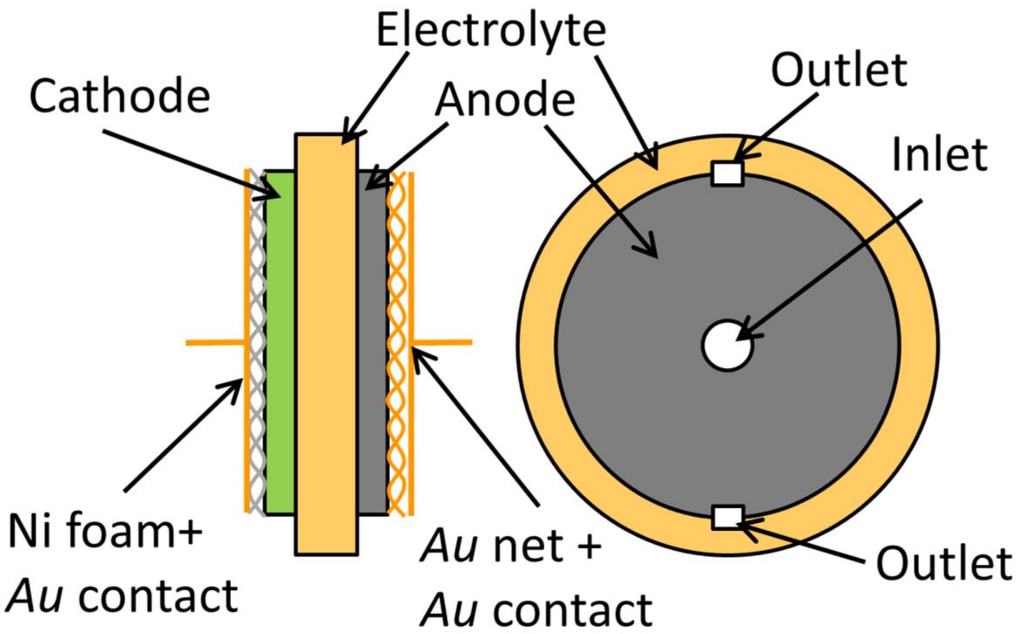
60 vol.%[O_2]

750 °C

Evaluation of kinetic data of cathode reaction

- 1st step: measurements of current density – voltage curves on an experimental HTSE cell

$$H_2O + 2e^- \rightarrow H_2 + O^{2-}$$



Temperature 800 °C; Pressure atmospheric;
Anode: air, Cathode: H2O+H2; 15, 25 and 50 vol.%[H2O]

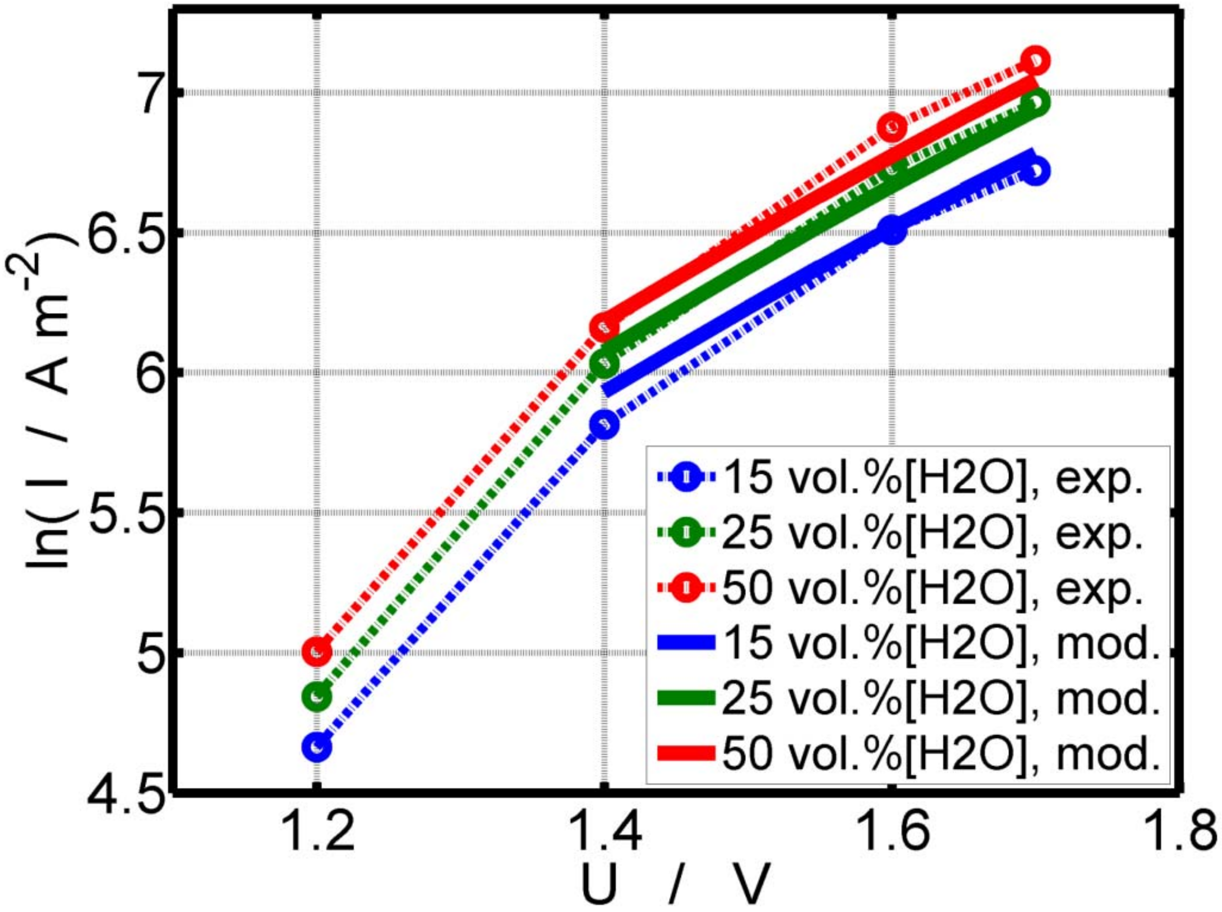
Evaluation of kinetic data of cathode reaction

- 2nd step: development of a Pseudo-2D model of HTSE cell having two fitting kinetic parameters αc and I0,c
- Cylindrical symmetry - coordinate is *r* (radius) oriented from center to the cell perimeter
- Electric current flow normal to cell plane
- Stationary, isobaric, isotermic (800 °C)

$$U = U_{OCV} - \left(\frac{RT}{\alpha_a F}\ln\left(I_{o,a}\right) + \frac{RT}{\boldsymbol{\alpha_c} F}\ln\left(\boldsymbol{I_{o,c}}\right)\right) +$$

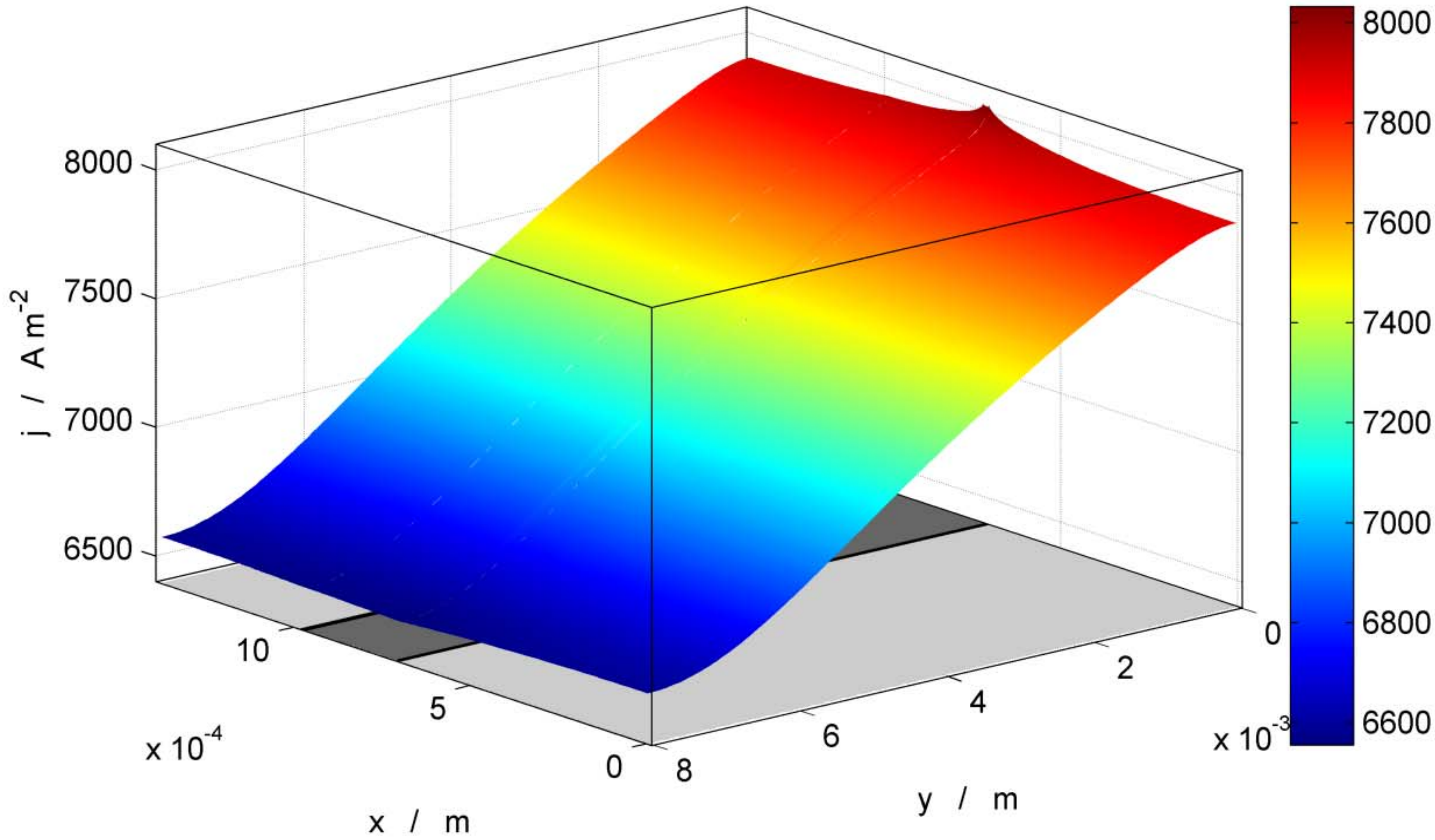
$$+ \left(\frac{RT}{\alpha_a F} + \frac{RT}{\boldsymbol{\alpha_c} F}\right)\ln(I) + \frac{RT}{\boldsymbol{\alpha_c} F}\ln\left(\frac{p_{H_2O}}{p^0}\right) + R_{s,cell} I$$

Evaluation of kinetic data of cathode reaction



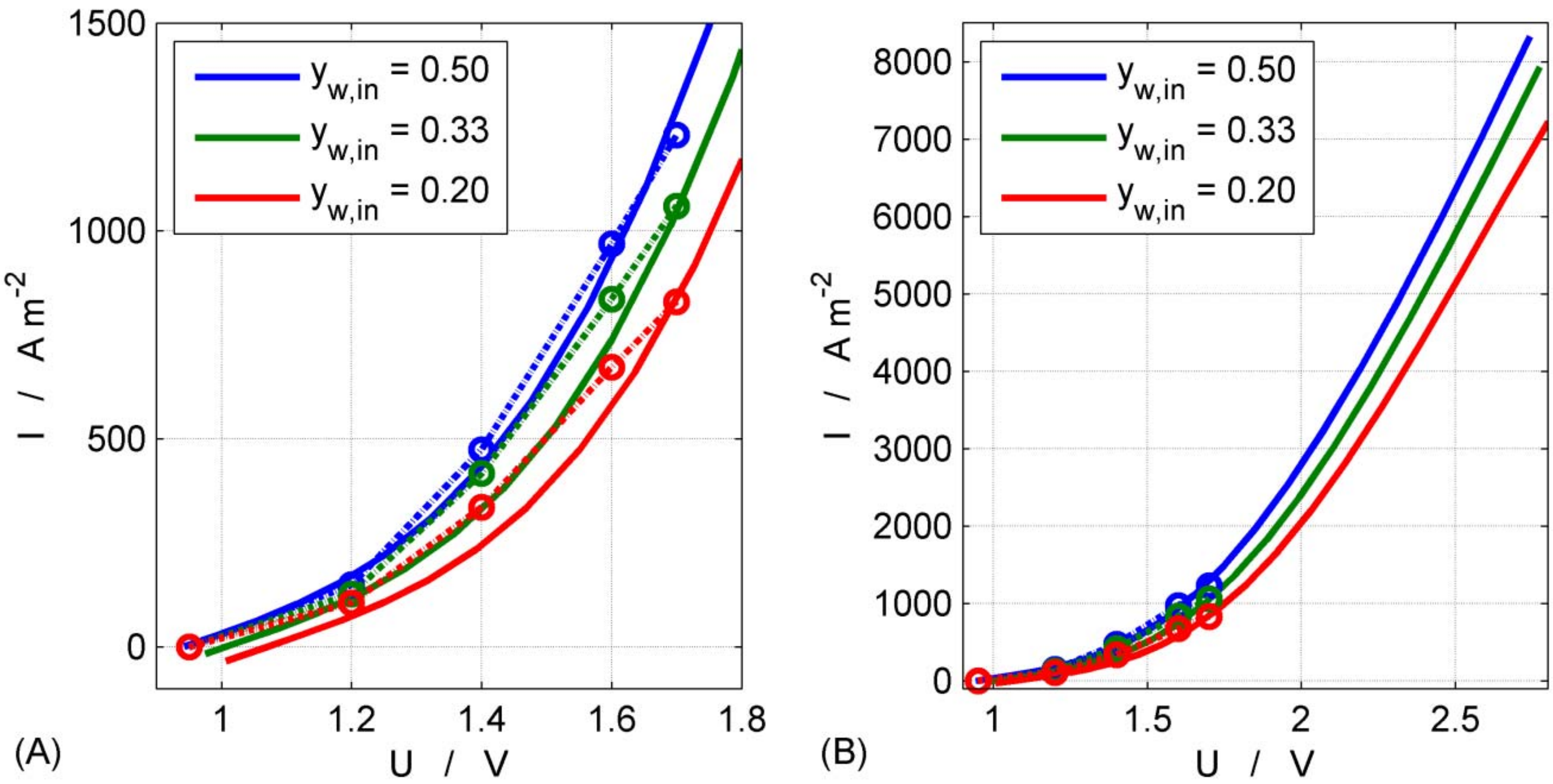
α_a = 0.45 (750°C), 0.40 (650°C); $I_{o,a}$ = 15.03 A m^{-2} (750°C), 8.14 A m^{-2} (650°C);
α_c = 1.19 (800°C); $I_{o,c}$ = 4.79 A m^{-2} (800°C)

2D modelling



T= 800 °C, $y_{w,in}$ = 0.2; U = 2.8 V; I = 7249 A m-2

2D modelling



T= 800 °C