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Multiphysics Modeling and Simulation of a Solid Oxide Electrolysis Cell

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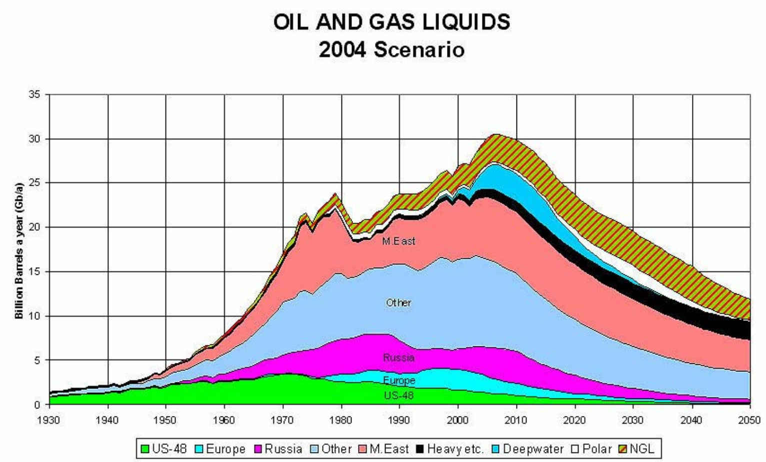
Summary

- High Temperature Electrolysis (HTE)
- Model
- Electrochemical Kinetic Description Influences
- Effective Diffusion Coefficient Sensibility
- Feeding Configuration Effects
- Conclusions

High Temperature Electrolysis

- Decrease of oil production in the future → need in changing the energy economy

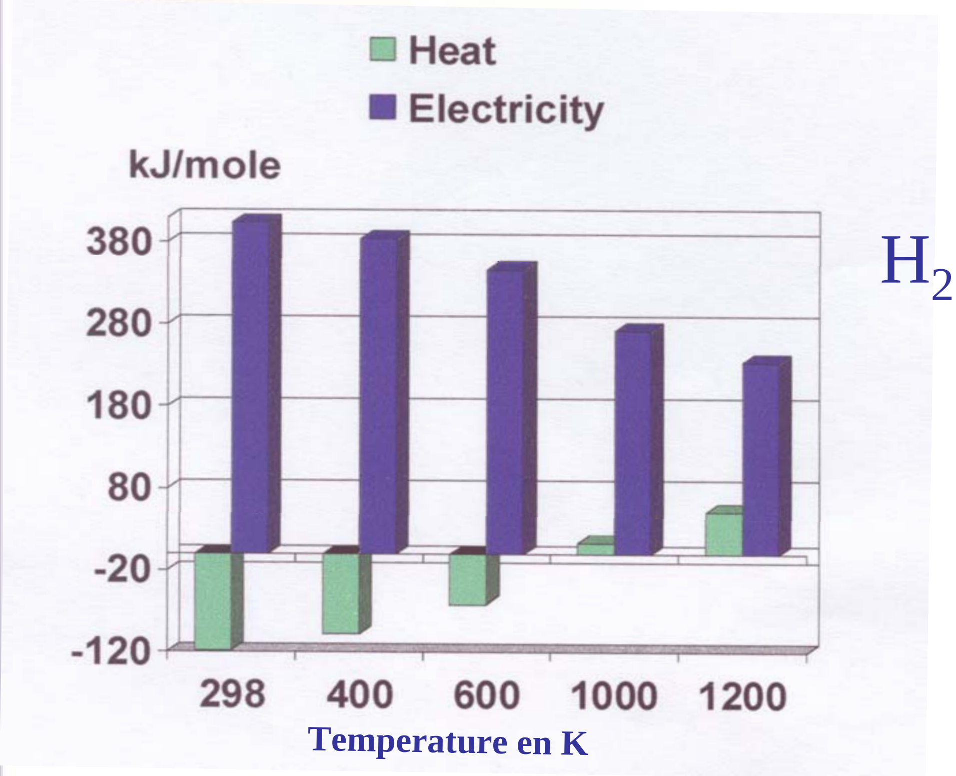


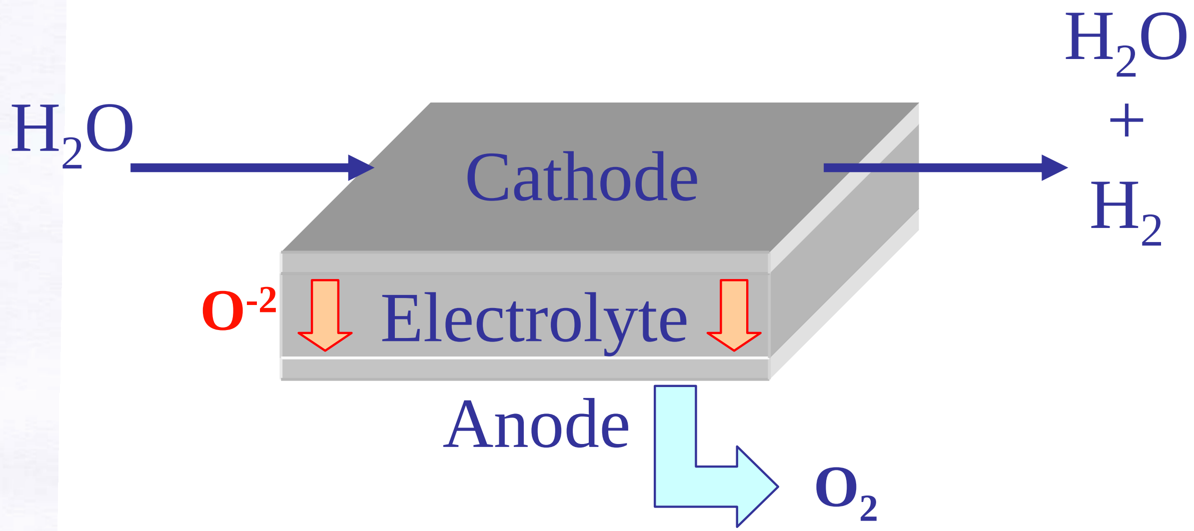
- Pollution and Global warming issues → hydrogen consumption is environmentally friendly

➢ Problem : major hydrogen production by hydrocarbons reforming

- Water electrolysis with clean energy sources is a promising solution

High Temperature Electrolysis



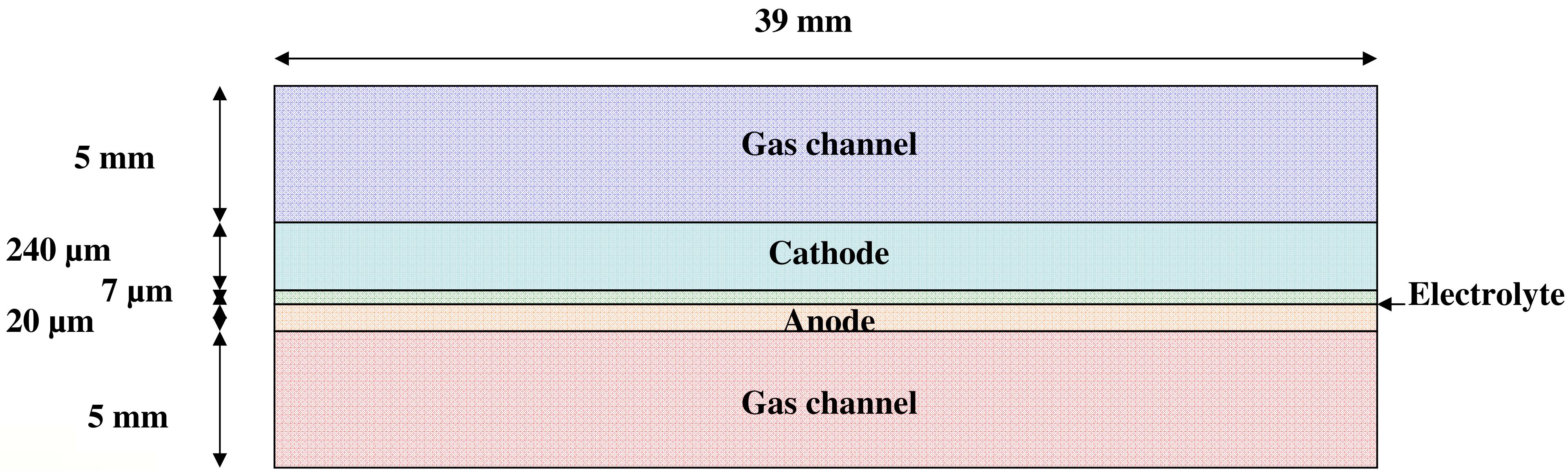


- No noble metals are required at high temperature
- Ceramic materials usually used for HTE:

Hydrogen electrode: Cermet (Ni / YSZ)
Electrolyte: Yttria Stabilized Zirconia (YSZ)
Oxygen electrode: LaSrMnO3 (LSM)

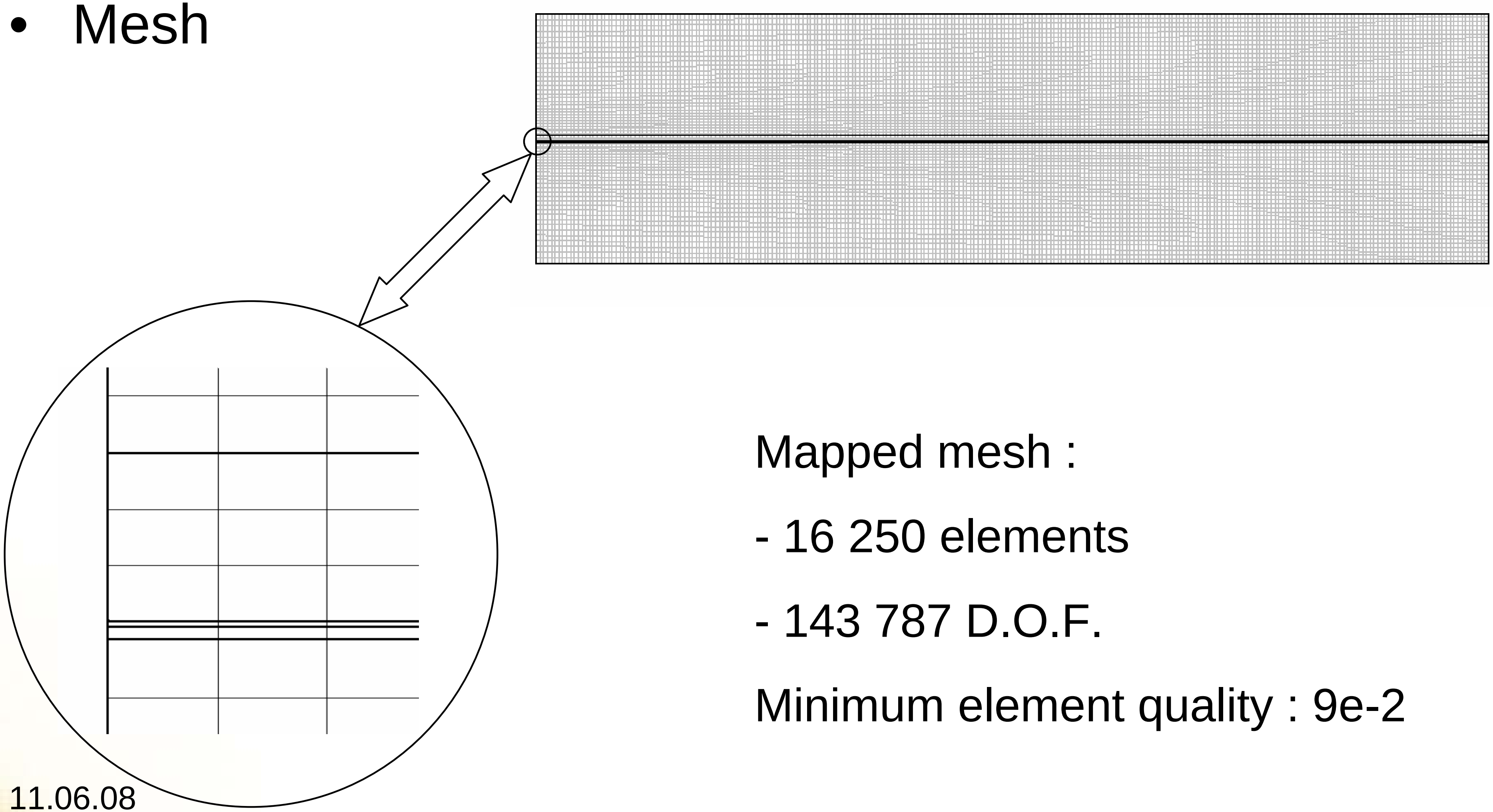
Model

- Geometry



Model

- Mesh



Mapped mesh :

- 16 250 elements

- 143 787 D.O.F.

Minimum element quality : 9e-2

Model

- Charge balances

  - Ionic current: *Conductive Media DC* in electrodes and electrolyte

  - Electric current: *Conductive Media DC* in electrodes

  - Current sources are given by Butler-Volmer equation

$$\mathbf{j}_{\mathbf{a,c}} = \mathbf{j}_{0\mathbf{a,c}}\left(\frac{\mathbf{C}_{\mathbf{red}}}{\mathbf{C}_{\mathbf{red},0}}\exp\left(\frac{\alpha\mathbf{n}\ \mathbf{F}\eta}{\mathbf{RT}}\right)-\frac{\mathbf{C}_{\mathbf{ox}}}{\mathbf{C}_{\mathbf{ox},0}}\exp\left(\frac{-(1-\alpha)\mathbf{nF}\eta}{\mathbf{RT}}\right)\right)$$

$$\eta = V_{elec} - V_{ionic}$$

Model

- Mass balances

Convection and Diffusion for Water concentration:

- Electrode:

$$\nabla.\left(-D_{eq}^{eff}\nabla c_{H_2O}\right)=R_c \qquad R_c=-\frac{j_c}{2F}$$

$$^{*}\quad D_{eq}^{eff}=\frac{1}{D_{H_2O,k}}+\frac{1}{D_{H_2O,N_2}^{eff}}+(1-y_{N_2})\left(\frac{1}{D_{H_2O,H_2}^{eff}}-\frac{1}{D_{H_2O,N_2}^{eff}}\right)-\frac{\alpha y_{H_2O}}{D_{H_2O,H_2}^{eff}}$$

- Gas channel:

$$\nabla.\left(-D_{eq}\nabla c_{H_2O}\right)=-u.\nabla c_{H_2O}$$

$$D_{eq}=\frac{1}{D_{H_2O,N_2}}+(1-y_{N_2})\left(\frac{1}{D_{H_2O,H_2}}-\frac{1}{D_{H_2O,N_2}}\right)-\frac{\alpha y_{H_2O}}{D_{H_2O,H_2}}$$

* Suwanwarangkul *et al.*, Journal of Power Sources **122** (2003) 9-18

Model

<u>*Convection and Diffusion* for Oxygen concentration:</u>

- Electrode:

$$\nabla.\left(-D^{eff}\nabla c_{O_2}\right)=R_a-u_e.\nabla c_{O_2}$$

$$u_e=-\frac{k}{\eta}\nabla p \qquad D^{eff}=\left(\frac{1}{D^{eff}_{O_2,N_2}}+\frac{1}{D_{O_2,k}}\right)^{-1} \qquad R_a=\frac{j_a}{4F}$$

- Gas channel:

$$\nabla.\left(-D_{O_2,N_2}\nabla c_{O_2}\right)=-u.\nabla c_{O_2}$$

Model

- Heat balance

Convection and Conduction

$$\nabla.\left(-k\nabla T+\rho C_p T u\right)=Q_{a,c,e}$$

$$Q_{a,c}=\boxed{\sum Q_{a,c}^{irreversibility}}+\boxed{\sum Q_{a,c}^{joule}}$$

In the cathode:

$$Q_c=\boxed{\left(\frac{-T\Delta S}{2F}-\eta\right)j_c}+\boxed{Q_{elec}^{joule}+Q_{ionic}^{joule}}$$

In the anode:

$$Q_a=\boxed{\eta j_a}+\boxed{Q_{elec}^{joule}+Q_{ionic}^{joule}}$$

In the electrolyte:

$$Q_e=Q_{ionic}^{joule}$$

Model

Conductive media DC (ionic)

Conductive media DC (electric)

Convection and Diffusion (water)

Convection and Diffusion (oxygen)

Darcy's Law

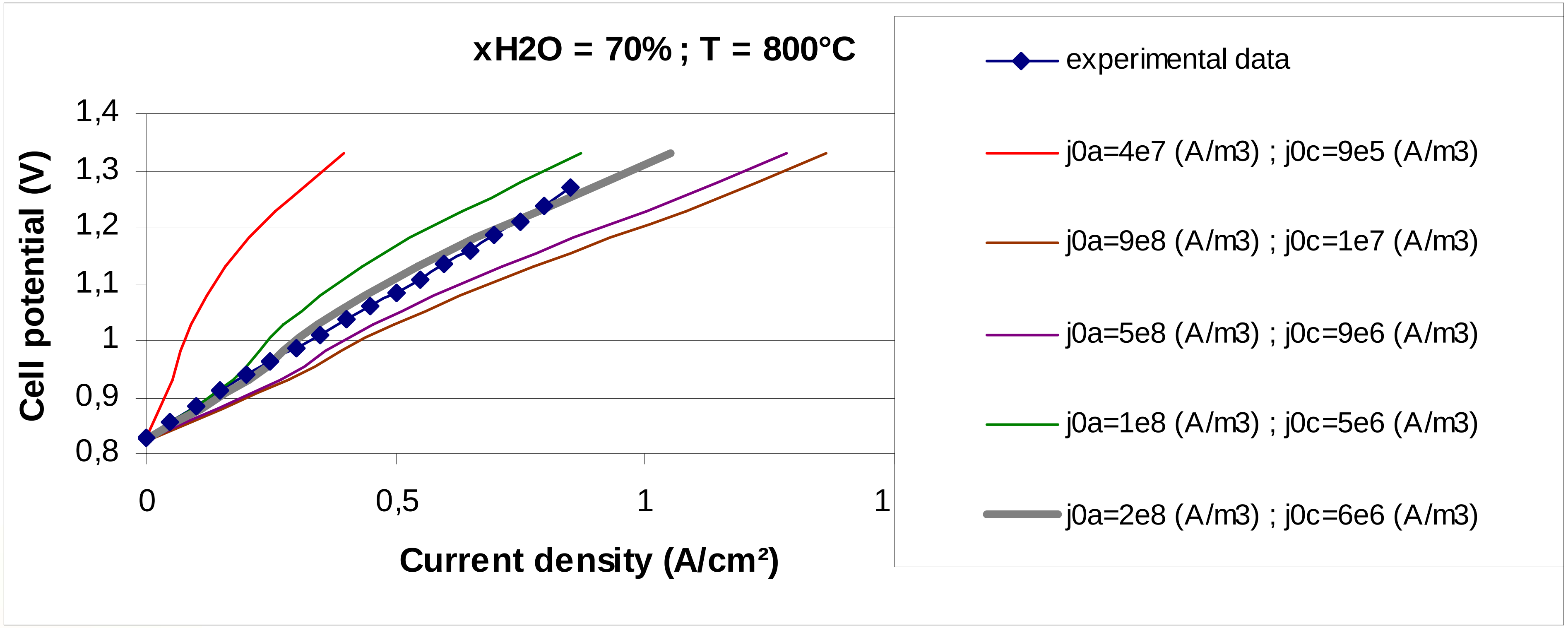
Convection and Conduction

✓Polarisation Curves

✓Temperature distribution

Comparison with experimental data

Electrochemical kinetic descriptions



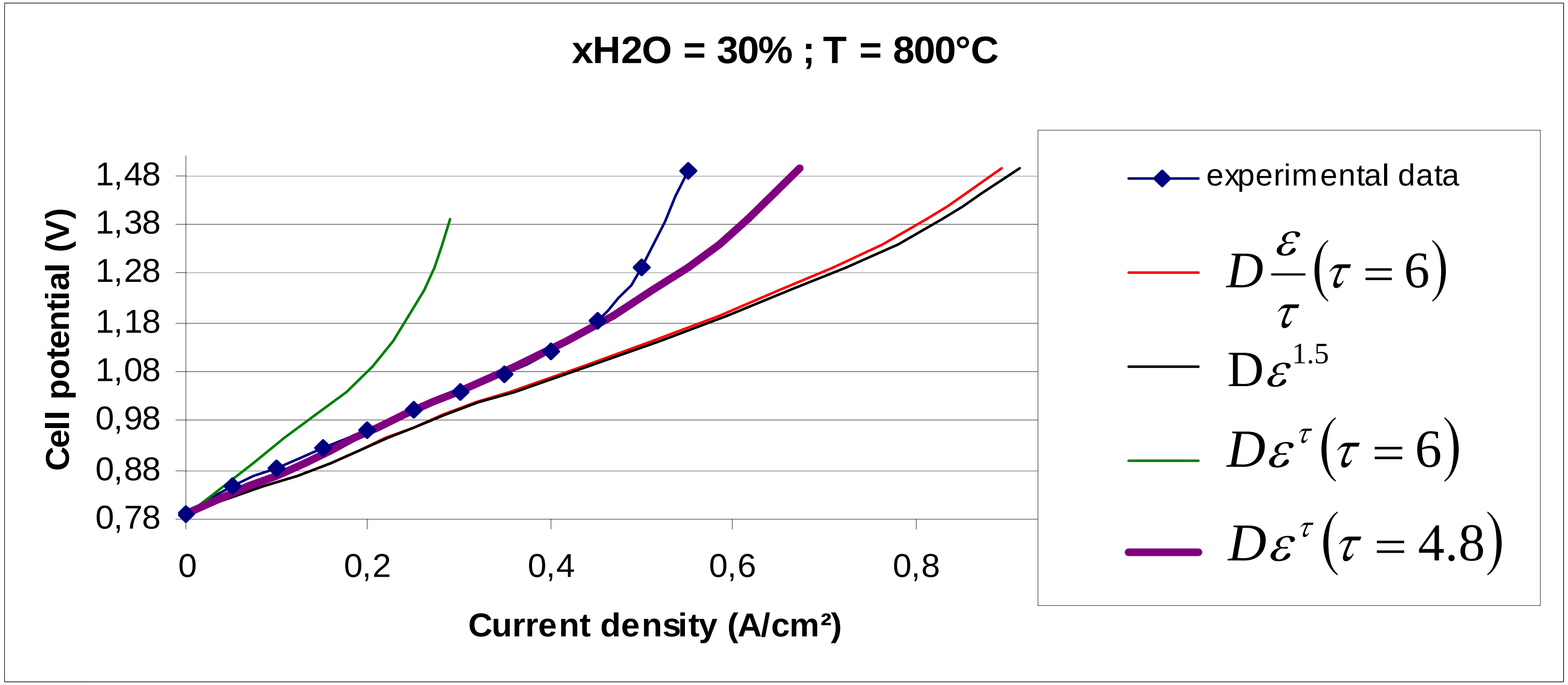
- Good prediction for $xH_20 = 70\%$

- $xH_20 = 30\%$?

- Several relations for effective diffusion coefficient estimation

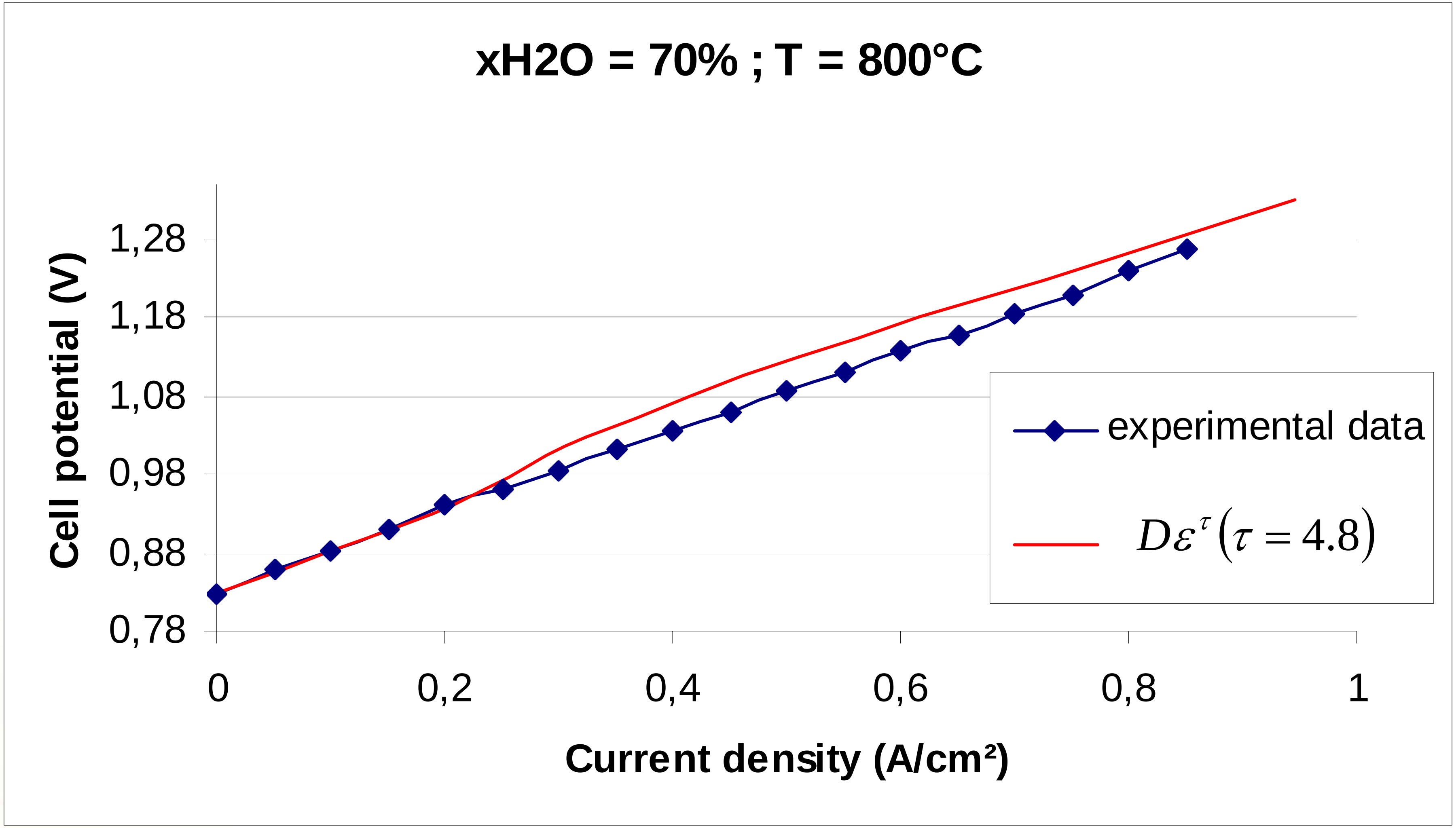
$$\mathbf{D}\varepsilon^{\tau} \qquad \mathbf{D}\frac{\varepsilon}{\tau}$$

Effective Diffusion Coefficient Sensibility



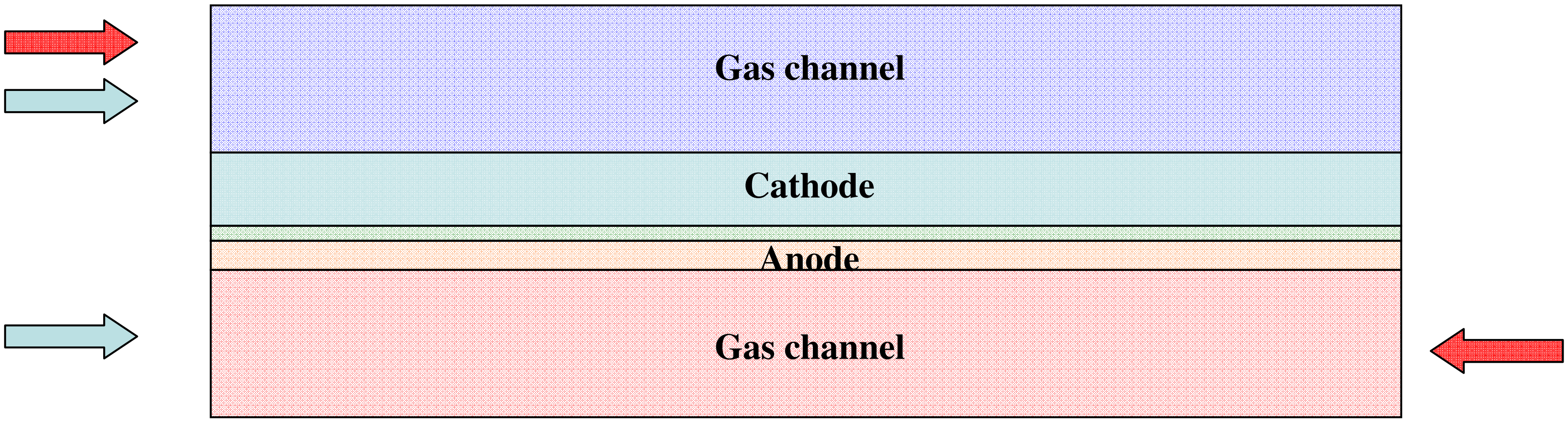
High sensitivity has also been observed for ε and pore diameter

Effective Diffusion Coefficient Sensibility



Feeding Configuration

Co - flow (⇨)
Counter - flow (⇨)



- **Electrical behaviour?**
- **Thermal behaviour?**

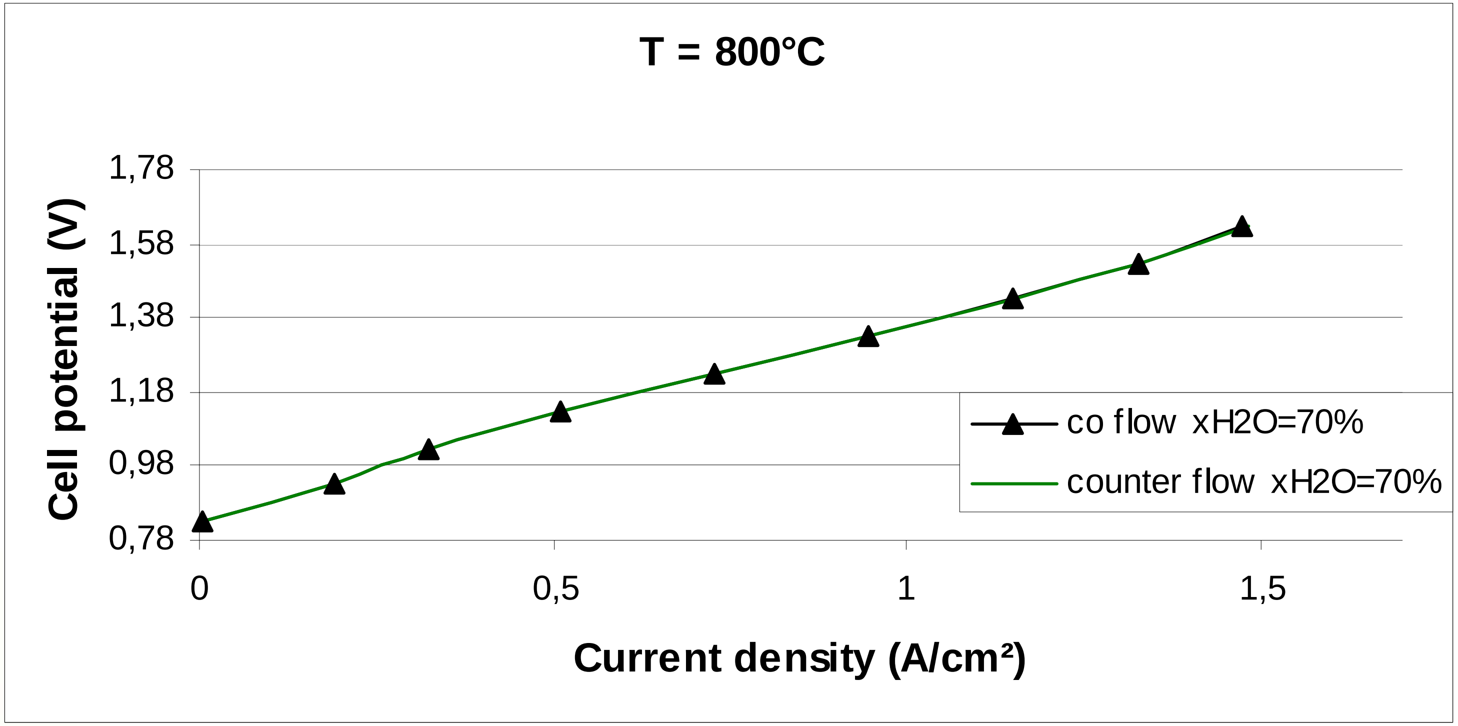
Feeding configuration

- Co flow

Temperature distribution

- Counter flow

Temperature distribution



Conclusions

- Temperature distribution depends on feeding configuration
- High sensitivity to material properties : grain diameters, porosity

  → good estimation is needed
- Butler-Volmer law cannot predict electrical cell behaviour at high current densities

  → a new electro-kinetic description is required

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