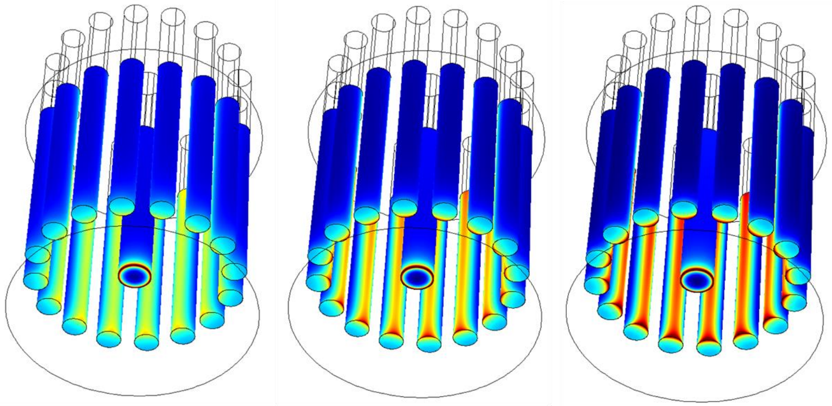
SIMTEC

Numerical modeling

that predicts, optimizes and innovates

Electrical Modeling of Molten Salt Electro-Refining Processes



Alexandre OURY
alexandre.oury@simtecsolution.fr
00 33 (0) 9 53 51 45 60

COMSOL CONFERENCE
2015 GRENOBLE

SIMTEC

Numerical modeling that predicts, optimizes and innovates

SIMTEC, www.simtecsolution.fr

COMSOL Certified Consultant

- French company, founded in 2006, 4 Ph. D. Engineers
- Expert in Modeling, COMSOL Certified Consultants :
    - CFD
    - Structural mechanics
    - Electromagnetism
    - Heat transfer
    - Chemical engineering
- Services:
    - Numerical modeling
    - Custom-made training session
    - Modeling Assistance
- Main Clients:

AIRBUS, AREVA, tronics microsystems, Nexans, cea, Seventh Framework Programme, L'ORÉAL Recherche, dbv technologies, SOLVAY, Schlumberger, faurecia, SAINT-GOBAIN

Content

1. Introduction: about molten salt electrorefining

2. Electrical model implementations

2.1. Primary current model

2.2. Secondary current model

3. Results

3.1. Primary *vs.* secondary approach

3.2. Influence of the prescribed current

1. Introduction: about molten salt electrorefining

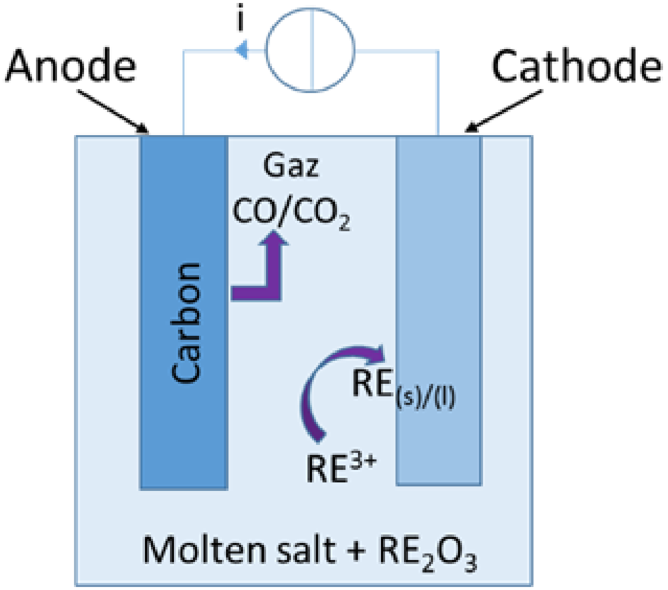
- **Principle**

Molten salt bath
+ rare earth oxide
(neodymium, dysprosium…)

⇒ Current flow between anode and cathode

⇒ Rare earth deposit at the cathode

⇒ Oxide gas evolution at the anode



Reactions:

-Cathode : $RE^{3+} + 3e^- \rightarrow RE_{(s)\ or\ (l)}$

-Anode : $C + O^{2-} \rightarrow CO + 2e^-$

$C + 2O^{2-} \rightarrow CO_2 + 4e^-$

1. Introduction: about molten salt electrorefining

- **Modeling of electrorefining processes: what for?**

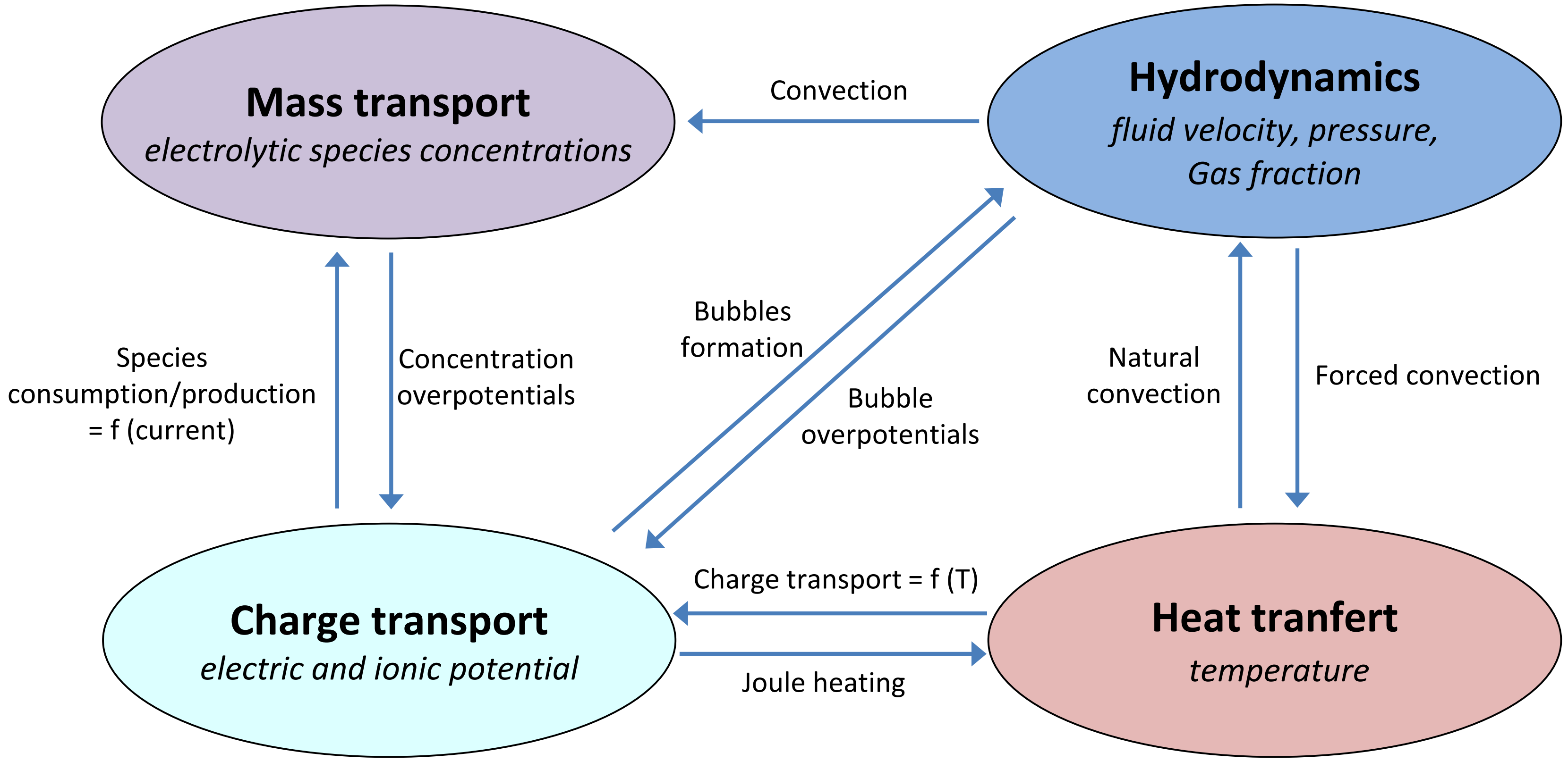
- Prediction of the local **reaction rates** at the electrodes:
  Presence of preferential active zones? of undesirable side reactions?

- Prediction of the **temperature** throughout the reactor/in the electrolyte,
  as a function of the Current/Voltage specifications

→ **Optimizing:** cell design, operating conditions (current, voltage), electrolyte composition…

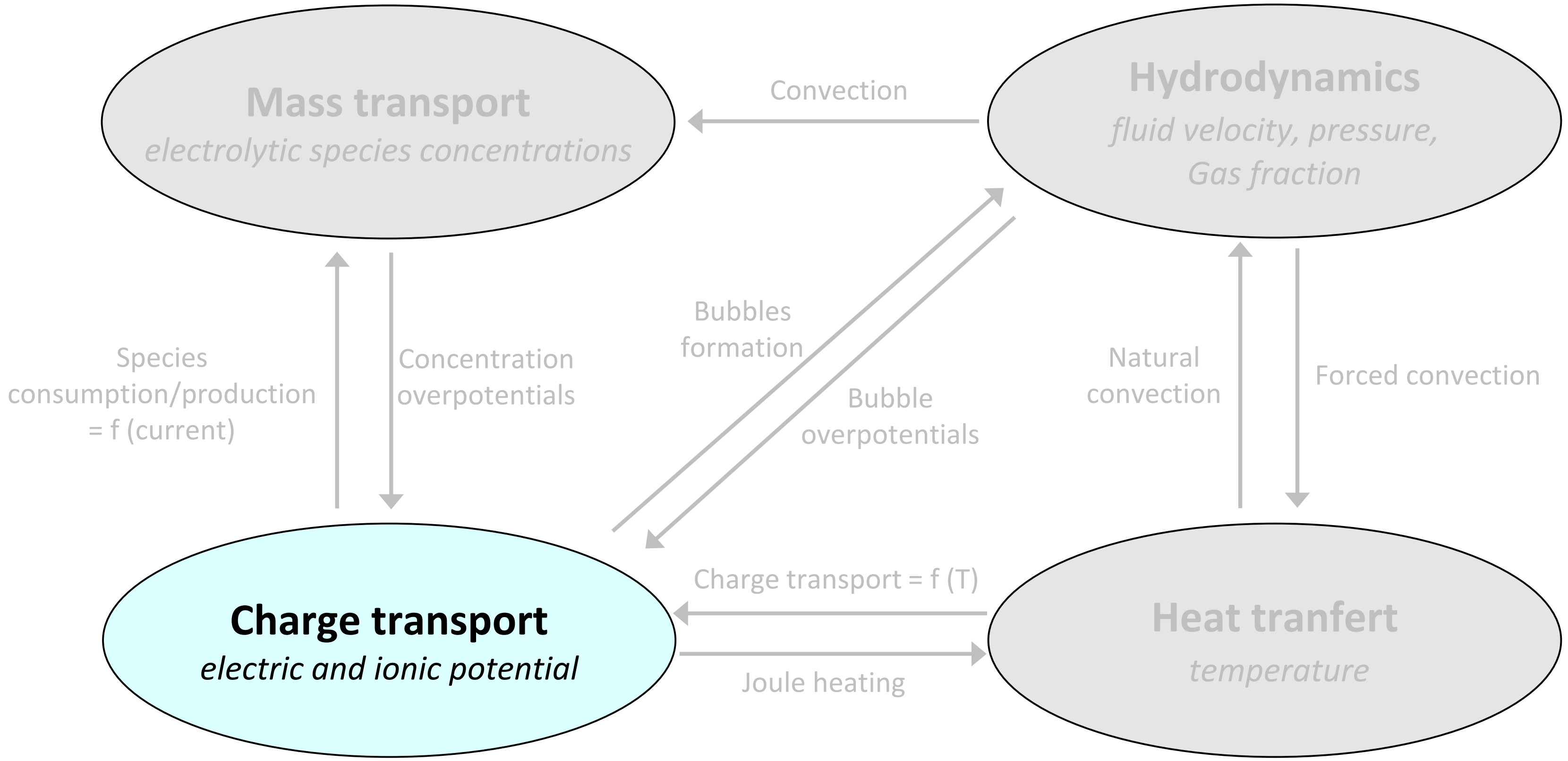
1. Introduction: about molten salt electrorefining

- **Modeling of electrorefining processes: physical interactions**



1. Introduction: about molten salt electrorefining

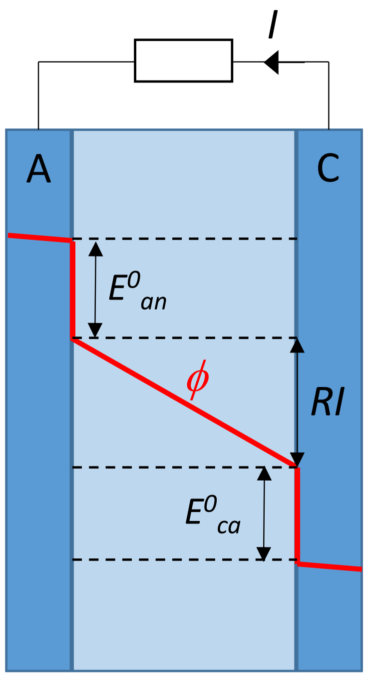
- **Modeling of electrorefining processes: physical interactions**



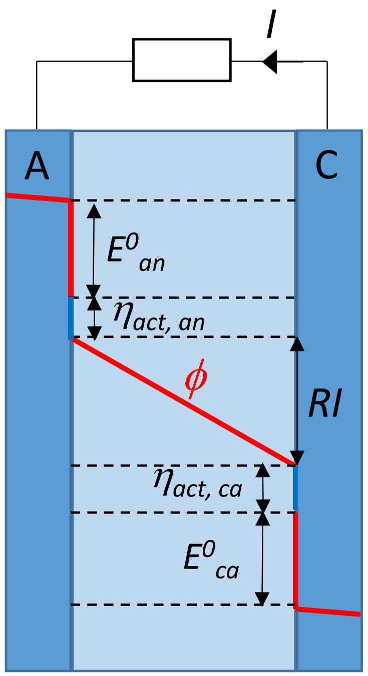
2. Electrical model implementations

- **The 3 current approaches**

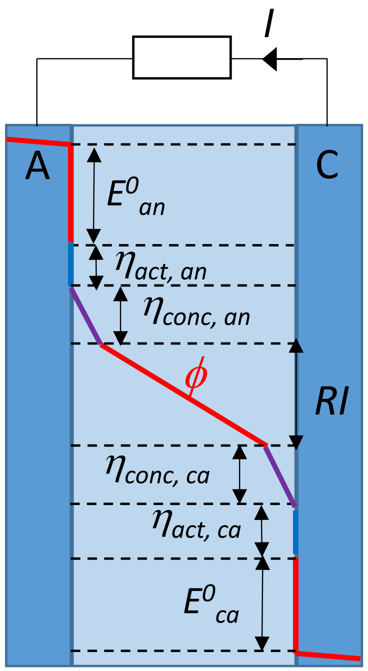
Primary current
No reaction overpotentials



Secondary current
Activation overpotentials

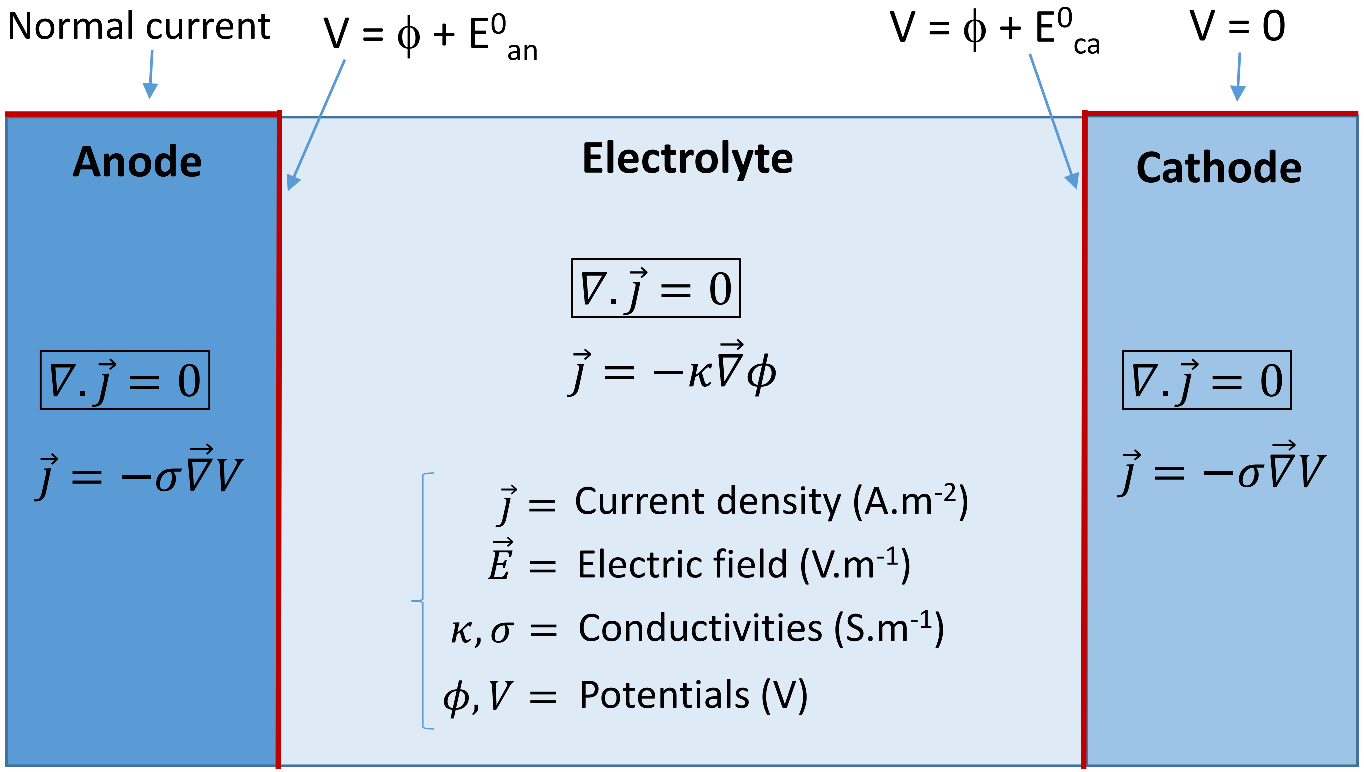


Tertiary current
Activation + concentration overpotentials



2. Electrical model implementations

- **The primary current distribution**



2. Electrical model implementations

- **The secondary current distribution**

Normal current

$$\vec{j}.\vec{n} = i_0\left(e^{\frac{0,5F}{RT}\eta} - e^{-\frac{0,5F}{RT}\eta}\right)$$

with $\eta = V - \phi - E^0$

V = 0

Anode

$$\boxed{\nabla.\vec{j} = 0}$$

$$\vec{j} = -\sigma\vec{\nabla}V$$

Electrolyte

$$\boxed{\nabla.\vec{j} = 0}$$

$$\vec{j} = -\kappa\vec{\nabla}\phi$$

$\vec{j} =$ Current density (A.m^{-2})

$\vec{E} =$ Electric field (V.m^{-1})

$\kappa, \sigma =$ Conductivities (S.m^{-1})

$\phi, V =$ Potentials (V)

Cathode

$$\boxed{\nabla.\vec{j} = 0}$$

$$\vec{j} = -\sigma\vec{\nabla}V$$

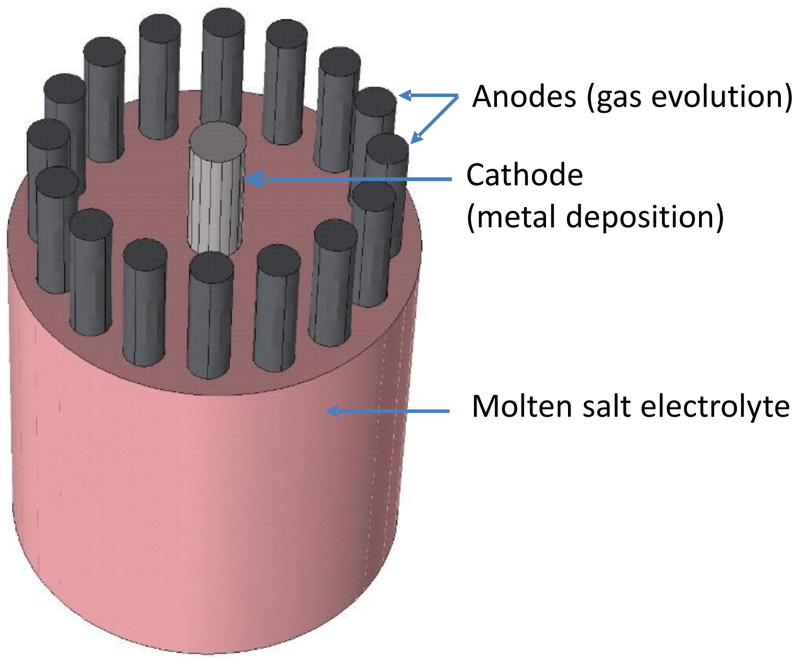
Cathodic process (fast):
$i_{0,C} = 1\ A/cm^2$

Anodic process (slow):
$i_{0,A} = 0.001\ A/cm^2$

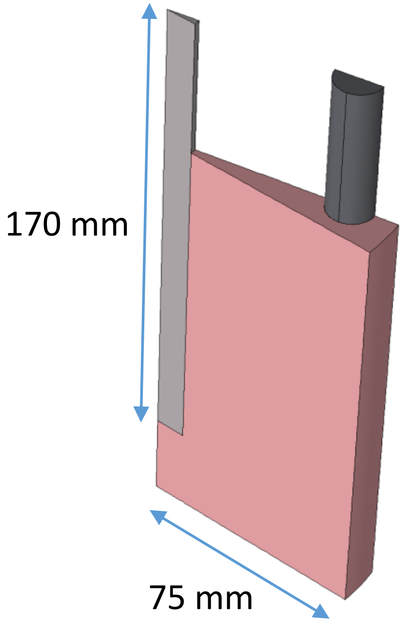
2. Electrical model implementations

- **Model geometry**

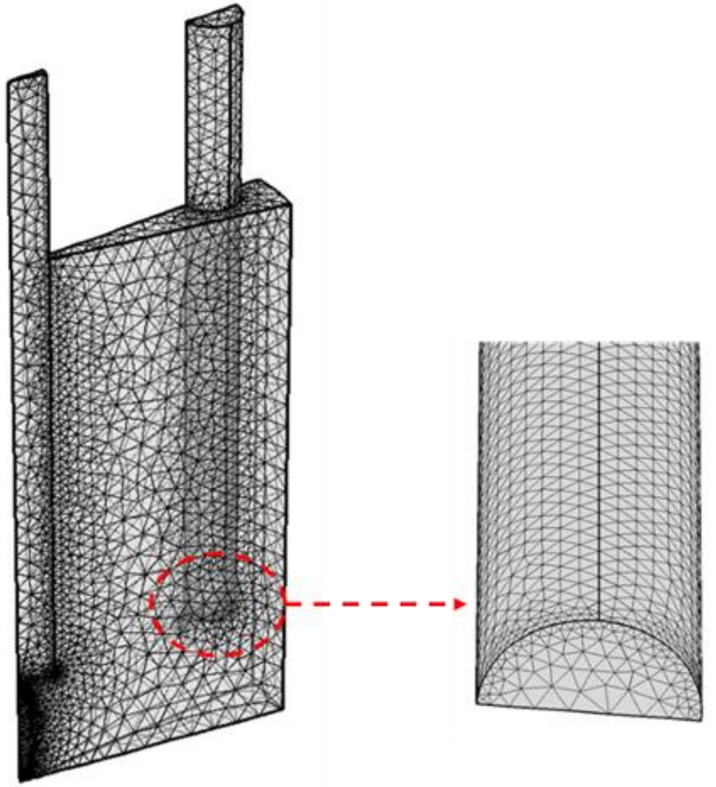
Overall geometry of the electro-refiner



Elementary unit implemented for simulations



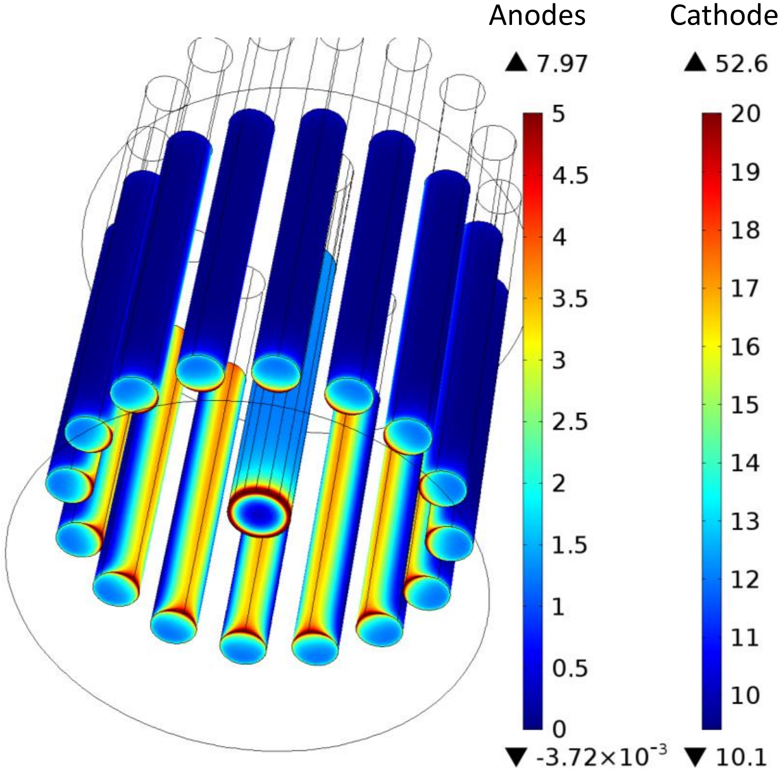
Mesh details



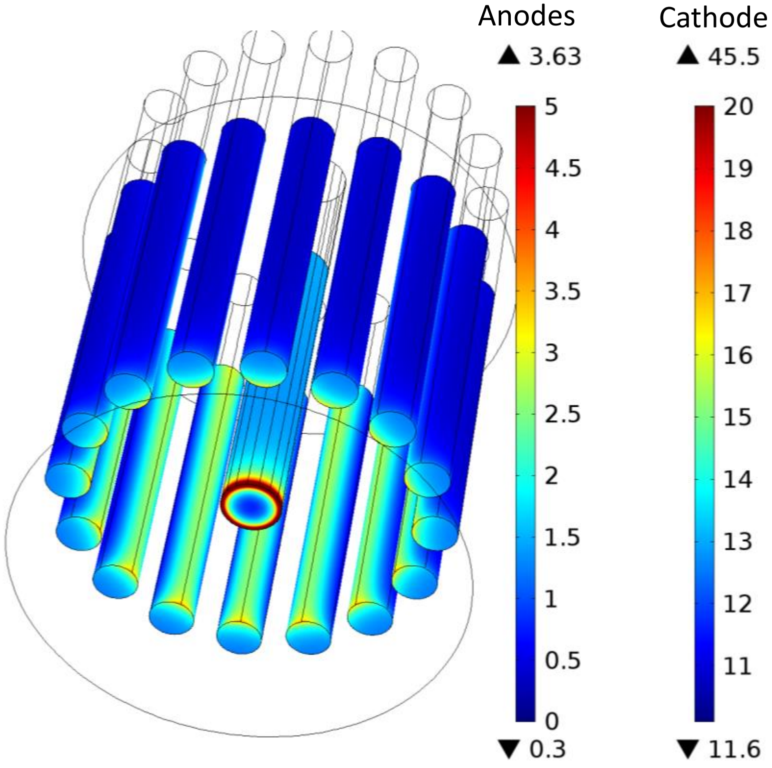
3. Results

- **Primary *vs.* secondary current density**

Primary distribution (A/cm²)



Secondary distribution (A/cm²)



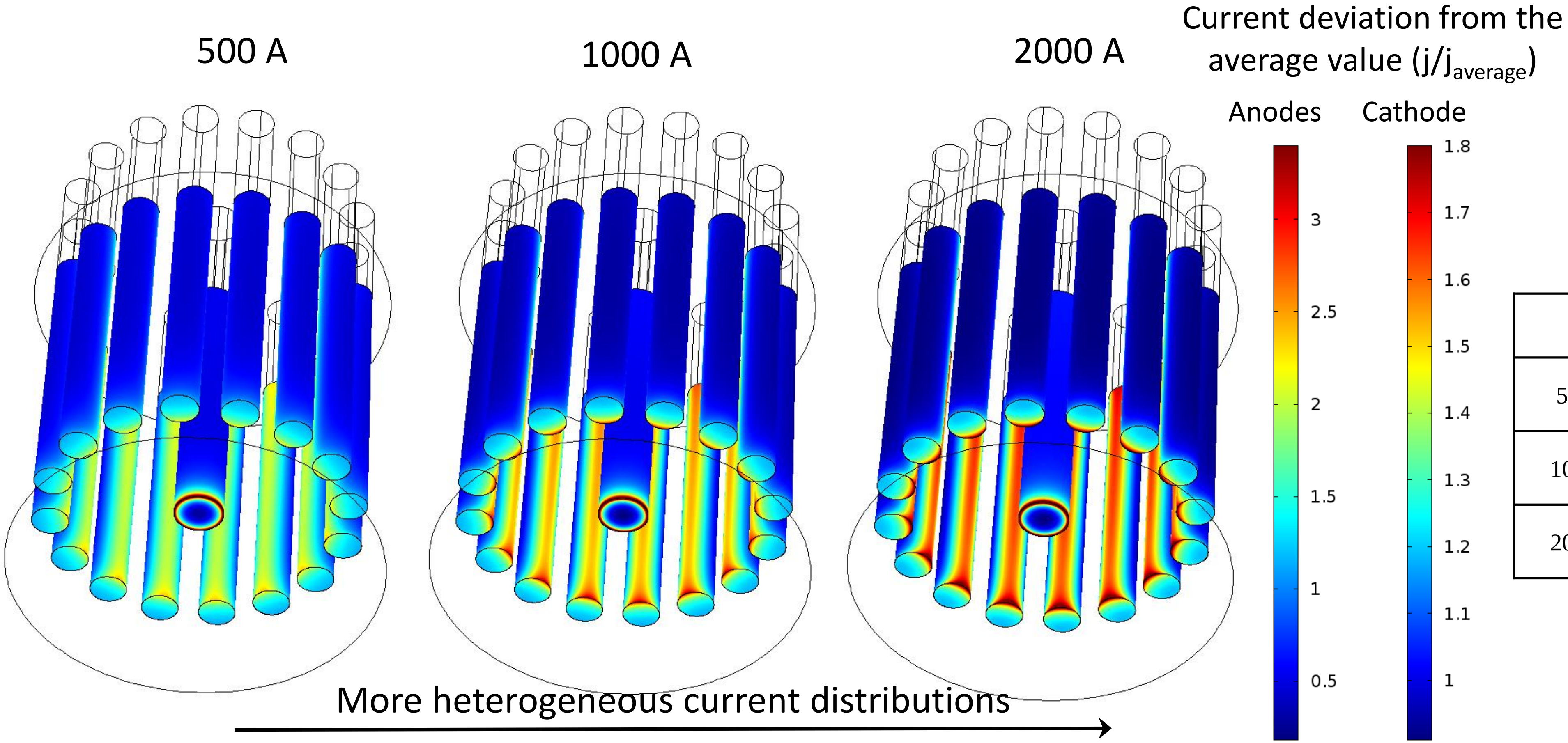
3. Results

- **Primary *vs.* secondary current density**

Current model	Decomposition voltage (V)	Ohmic drops (V)	Activation overpotentials η (V)	Overall cell voltage (V)
Primary distribution	1.7	6.3	0	**8**
Secondary distribution	1.7	6.5	1.5 (anodic) + 0.6 (cathodic)	**10.3**

3. Results

- **Effect of the current prescribed (secondary model)**



	Anodes	**Cathodes**
500 A	Min. 0.42 Max. 2.39	Min. 0.94 Max. 2.7
1000 A	Min. 0.28 Max. 3.4	Min. 0.91 Max. 3.6
2000 A	Min. 0.18 Max. 4.9	Min. 0.91 Max. 4.9

4. Conclusion

- 2 simple current models for describing electro-refining cells: **primary** or **secondary** approaches
- Primary current: only Ohmic drops
  Secondary current: activation overpotentials of reaction taken into account
- More uniform reaction rate distribution obtained with the secondary approach
- Increase of the total current applied to the cell → heterogeneization of the current distribution
- Secondary model → more appropriate for simulating electro-refining processes.
  → simple tool for optimizing the electrode design, the applied current…

Thanks for your attention …and your questions!

Alexandre OURY
alexandre.oury@simtecsolution.fr
00 33 (0) 9 53 51 45 60