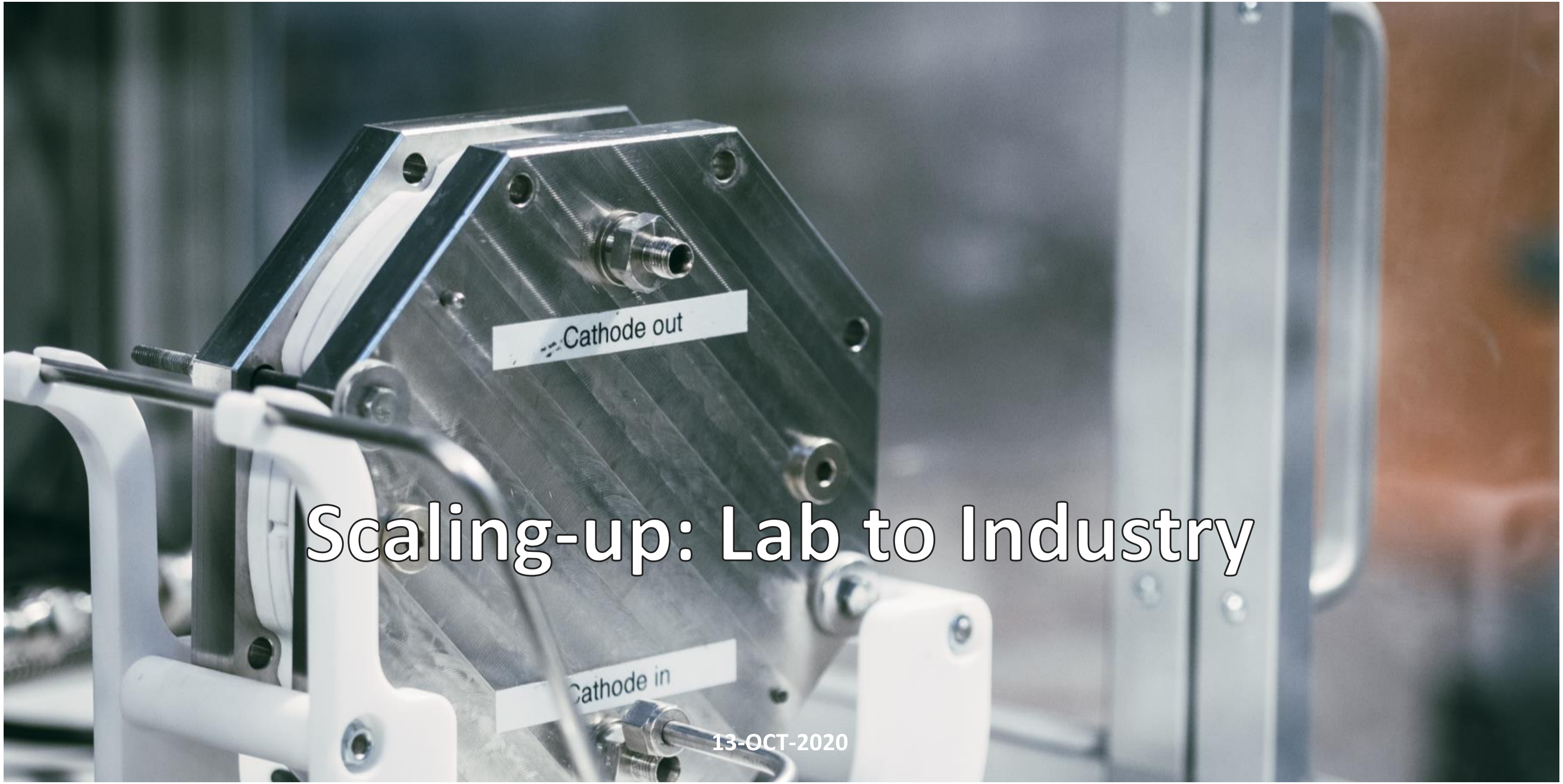
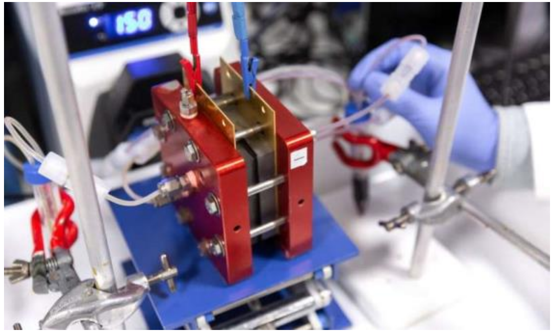


Scaling-up: Lab to Industry

13-OCT-2020

Intro

- The importance of scaling
- Focusing: scaling of the electrochemical reactor
- A little bit about myself



Topics

- Electrochemical cells
- Key factors in scaling
- Electrochemical cell scale-up
  - Geometric
  - Kinematic
  - Thermal
  - Current/potential
- Balance of Plant (BoP)
- Economic impacts

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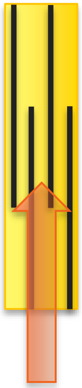
Electrochemical cells - Industrial types

Flow by

Flows by 2D electrodes; possibly separated



Flow cells

2D electrode

One electrolyte

One product

Flow through

Flows through a porous separator or electrode pack

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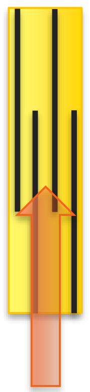

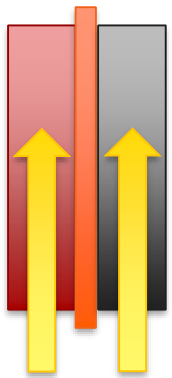

Flow cells

2D electrode

One electrolyte

One product

Membrane

Membrane separation

Pure products

2 possible product streams

Diaphragm

Diaphragm separation

Less pure product

2 possible products

More robust

Electrochemical cells - Industrial types

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Flows by 2D electrodes; possibly separated

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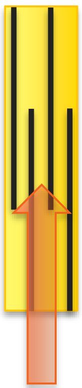

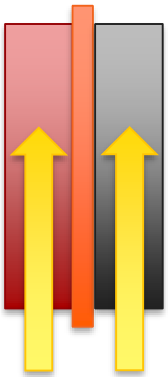

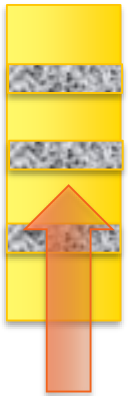

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Plug flow cells

3D electrodes – sponges

One electrolyte

One product

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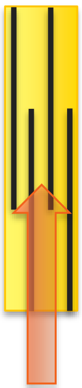
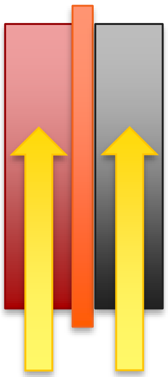
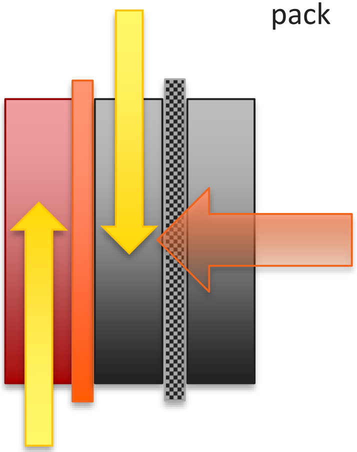
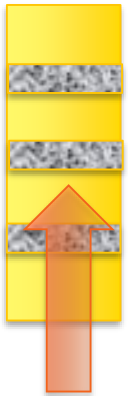








Flow cells

2D electrode
One electrolyte
One product

Membrane

Membrane separation
Pure products
2 possible product streams

Diaphragm

Diaphragm separation
Less pure product
2 possible products
More robust

Gas diffusion

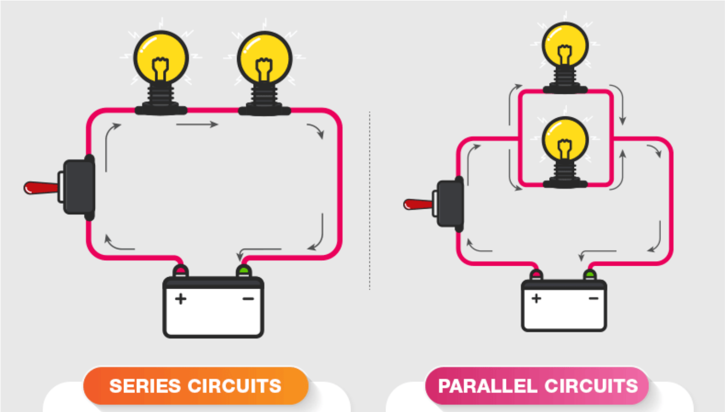
High surface area
Pure products
2 possible product streams

Plug flow cells

3D electrodes – sponges
One electrolyte
One product

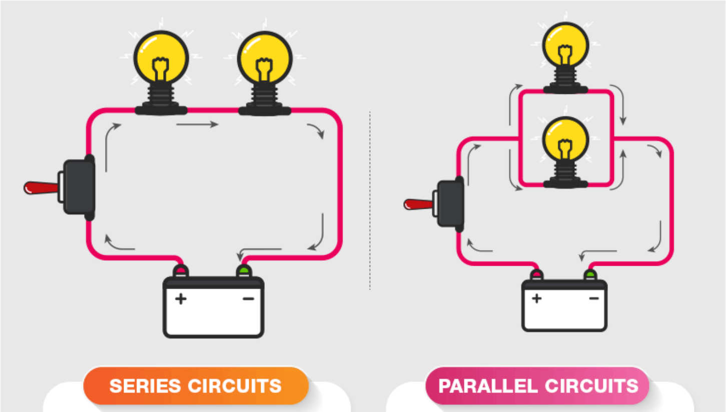
Electrochemical cells - Processing

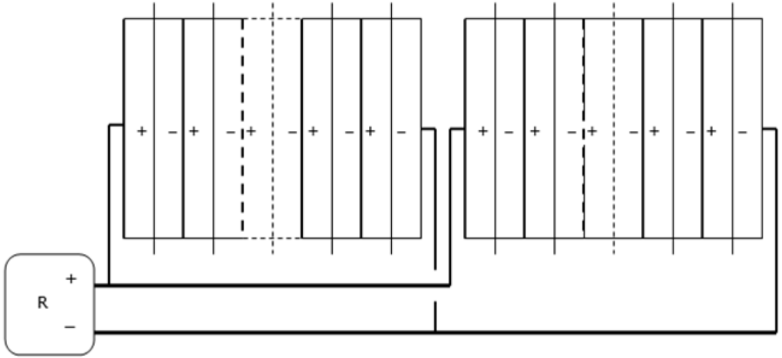
- Batch/Continuous
  - Recycle
- Series/Parallel electrolyte flow



Electrochemical cells - Processing

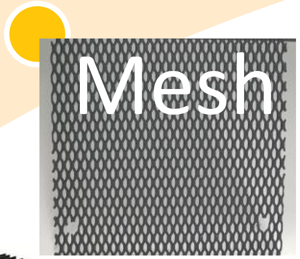
- Batch/Continuous
  - Recycle
- Parallel/series electrolyte flow
- Bipolar/Monopolar electrical connections (ex. 2 cells, 3V/cell at 5kA/m^2, 1.5m^2 cell area)
  - Bipolar – Voltage is added and Amperage stays constant
    - (5*1.5)*(3+3) = 45kW
  - Monopolar: Amperage is added and voltage stays constant
    - ((5+5)*1.5)*3 = 45kW

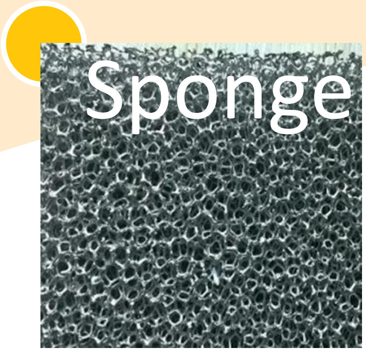


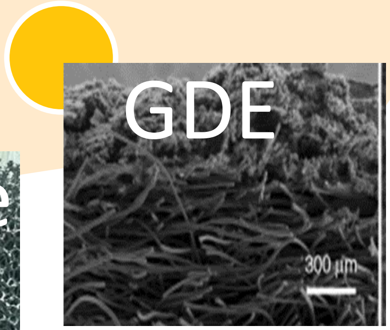


Electrochemical cells - Processing

- 2D/3D electrodes
  - High surface area to compensate for low current density reactions

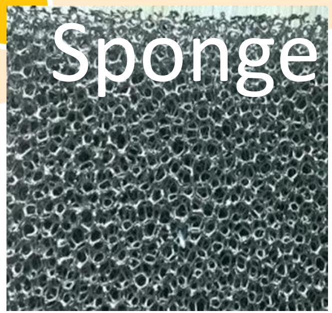


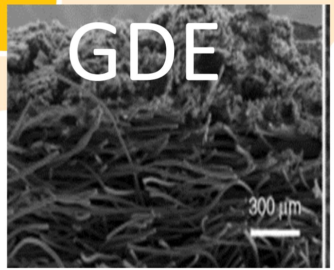




Electrochemical cells - Processing

- 2D/3D electrodes
  - High surface area to compensate for low current density reactions
- Horizontal/ vertical electrodes





Topics

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- **Key factors in scaling**
- Electrochemical cell scale-up
  - Geometric
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Key scale factors

- Transport process theory
  - Heat conduction
  - Fluid flow
  - Molecular diffusion
  - Electrical charge transfer

Key scale factors

- Transport process theory
  - Heat conduction
  - Fluid flow
  - Molecular diffusion
  - Electrical charge transfer
- Chemical reactor theory
  - Rate constants
  - Transfer coefficients
  - Transport properties
  - Reactor dimensions

Topics

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Key Factors

Geometric

Geometric

- It is impossible to directly scale the reactor
- Increased gap between electrodes that increase the voltage
  - In 3D electrodes the potential can be unevenly distributed if the thickness is too large [or secondary reaction can take place]
  - This scaling element is always sacrificed to maintain the potential

Geometric

- It is impossible to directly scale the reactor
- Increased gap between electrodes that increase the voltage
  - In 3D electrodes the potential can be unevenly distributed if the thickness is too large [or secondary reaction can take place]
  - This scaling element is always sacrificed to maintain the potential
- Maintaining active area is most important to maintain the current density
  - Scale-up always utilizes multiple cells
  - A way to calculate this is to fix the current density, production and hours of operation of the electrode, then divide by the area of one cell to obtain the total cells.

where P is the production target, CD is the current density, Hrs is the number of hours of operation in 1day, MW is the molecular weight, ε is the cell efficiency and n is the number of electrons for the formation of one molecule

$$m^2 = \frac{P}{CD * hrs * MW * \frac{\varepsilon}{26.8 * n}}$$

$$\#cells = \frac{m^2}{area\ of\ cell\ (m^2)}$$

Avantium | RNC-VOLTA-ELCOREL

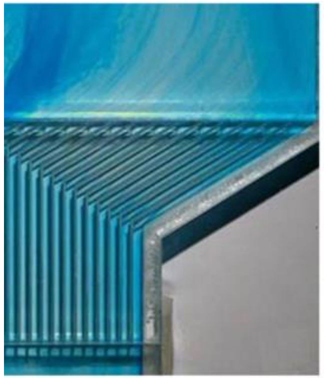

Typical cell room
About 440 cell
~3m wide

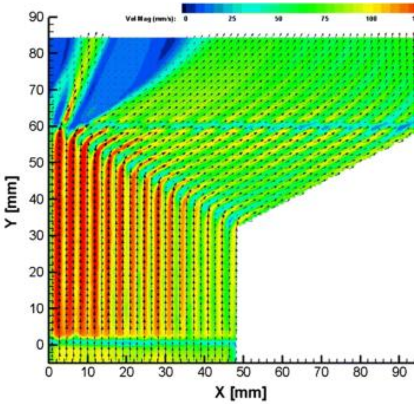
Key Factors

Kinematics

Kinematic

- Flow distribution
  - Velocities in the cell should be maintained: gas/liquid flow loads
    - Pressure drop
    - Fluid hold up
    - Mass transfer capacities





Key Factors

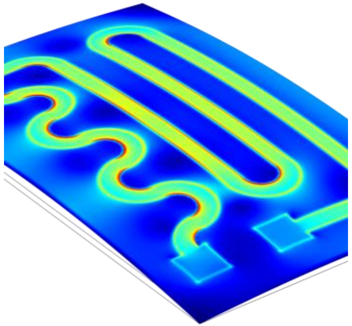
Thermal

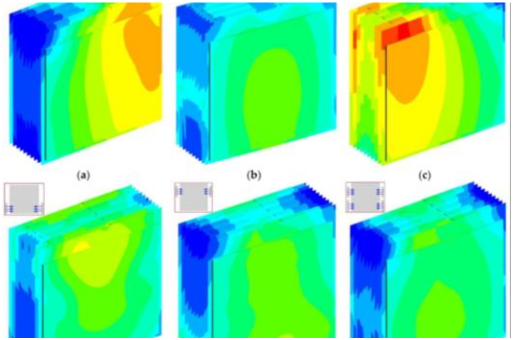
Thermal

- Joule effect heating is a large scale up effect

$$P \propto I^2 R$$

  - Hard to control
  - Cooling channels [fuel cells] are not possible when increasing the cell to 2.5-3m^2
  - Mitigated:
    - standardizing flow rates
    - cell area
    - bulk cooling





Key Factors

Current/Potential

Current/potential

- Constant gap required
- Wagner number will quantify this when scaling
  - $Wa = \left(\frac{k}{L}\right)\left(\frac{dV}{di}\right)$ *L = gap; K = electrolyte conductivity; V = cell potential; i = current density*
  - should be the same throughout the cell
- Better uniformity is attained by:
  - Higher conductivity of the electrolytes
  - Smaller gap
    - Balance between gas release and gap
  - Lower average current density
    - How current is delivered to the current collector

Questions at this time?

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BoP - Materials

- Close attention needed to material compatibility
  - Material compatibility charts – SO MANY!
- Understand what is happening in the whole cell [micro/macro scale]
  - The electrode interface is important when using binder materials
- Test different plastics or rubbers for the system=
  - Place a weighed sample in the same solution at the same temperature and see if it gains or loses weight over different time intervals.

BoP - Cell preparation and equipment

- Mounting the cell
  - Hydraulic press to ensure contact of all pieces of the cell
  - Mounting rigs to ensure the cells are closed and pressure/leak check before mounting into the cell room (some designs do not allow this)
- Electricity to the cell
  - Rectifiers
  - Copper bussing

BoP - Up-stream processing

- Purity is a big deal in electrochemical processing to commodity chemicals.
  - Water
  - Dry chemicals
  - Gases

- When dealing with waste waters this may not be necessary, as it depends on the way you decide to treat them [indirect or direct].

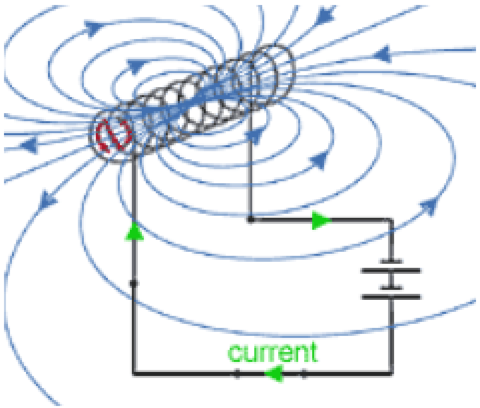
BoP – Down-stream processing

- WATER
  - How much is there?
  - How much needs to be removed?
  - Can it be recycled?

- All DSP should be tested if you are planning on scaling
  - Find partners that are experts in the field of the process
- Always have choices.
  - Pick 2-3 companies in the field and have conversations with them all
  - Just because they are the best doesn't mean they will have the time to give your company the attention you need.

BoP – Safety

- Waste treatment – sending to municipality
- Interlocks for voltages and flows
- Reactions
  - Out of control bulk reaction
  - Side reactions becoming dominate
- Electromagnetic field generation



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Economic impact of choices

- Current efficiency and purity in the electrochemical cell VS cost
  - Economics for more cells vs cheaper downstream processes – is it possible to purify with filters? Or concentrate with RO or filters?

Economic impact of choices

- Current efficiency and purity in the electrochemical cell VS cost
  - Economics for more cells vs cheaper downstream processes – is it possible to purify with filters? Or concentrate with RO or filters?
- Is the direct chemical process cheaper? Why?
  - E-chem will be hard to compete as it is energy intensive, but the produce is more likely to be pure
  - What is the case for this process to be better?
  - What can make it cheaper?

Thank You!!

Presented by:

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