COMSOL CONFERENCE 2016 MUNICH

INVESTIGATION OF REVERSE ELECTRODIALYSIS UNITS BY MULTIPHYSICAL MODELLING

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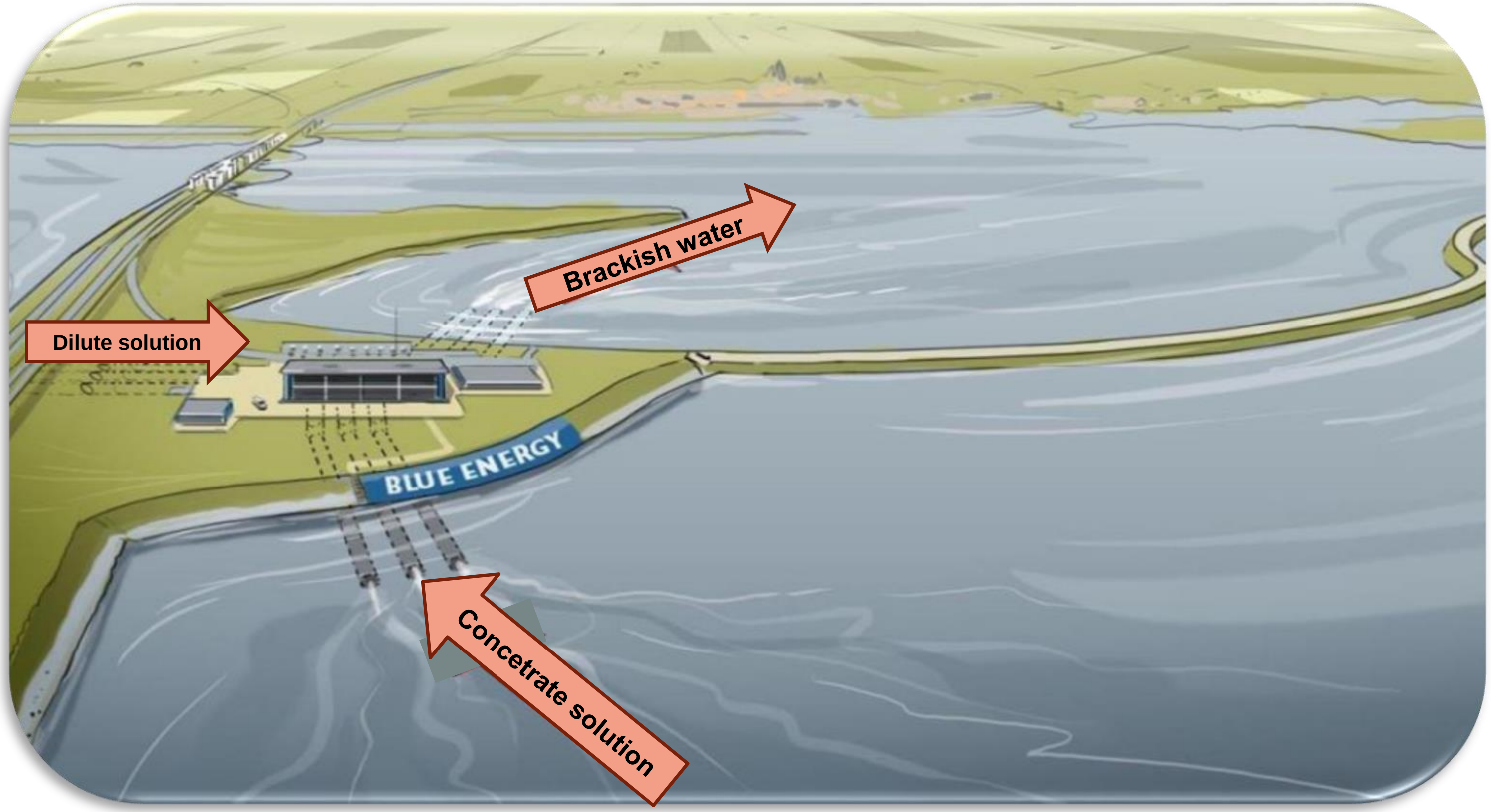
RED HEAT TO POWER

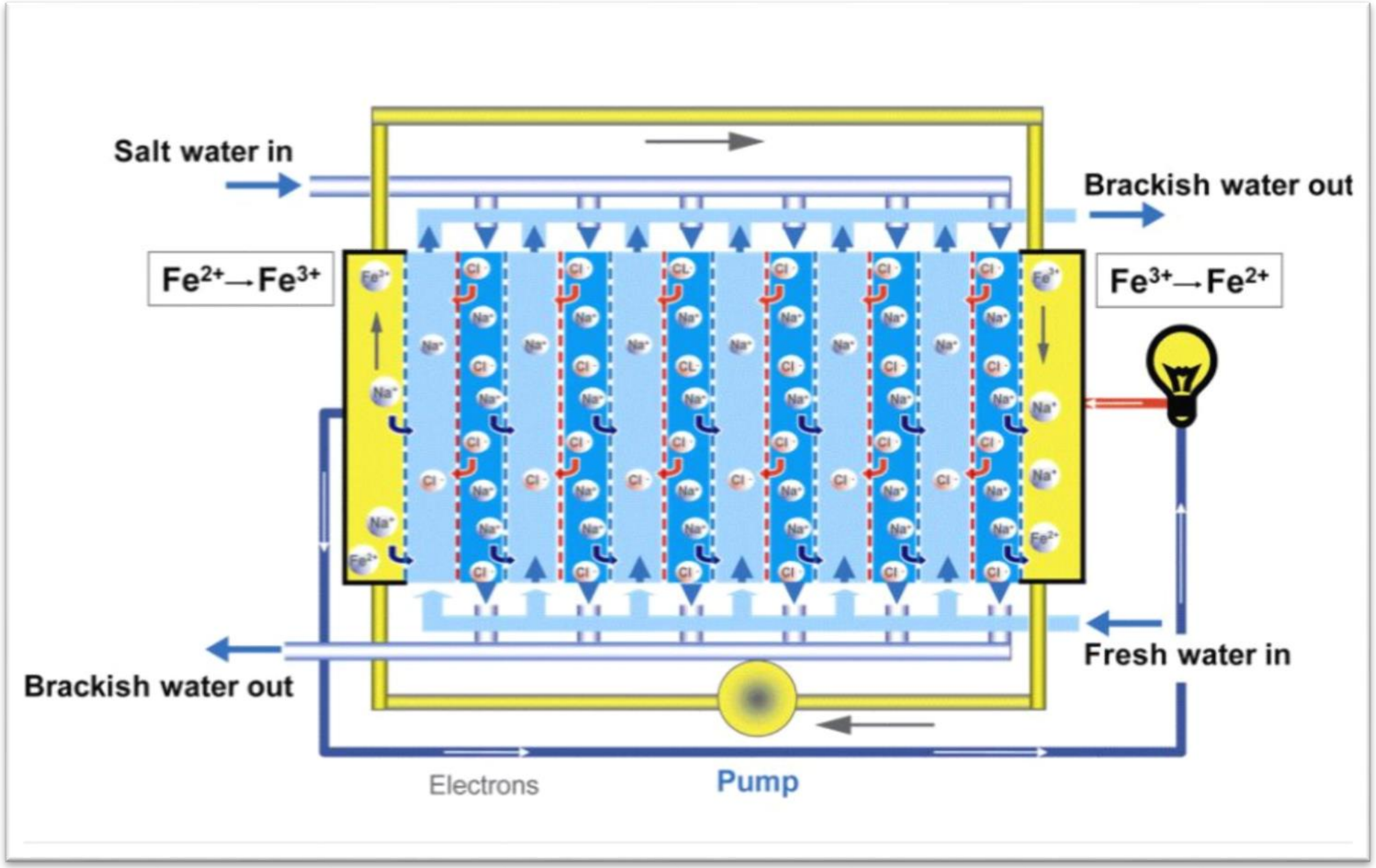
CONTENTS

Reverse Electrodialysis



- Reverse electrodialysis (RED) is a technology to produce electrical energy from the salinity difference between two salt solutions.

RED STACK



- Reverse electrodialysis uses ion-exchange membranes. These present fixed charges in their polymeric structure that allows selectivity transport of ions with opposite charge through the membranes.

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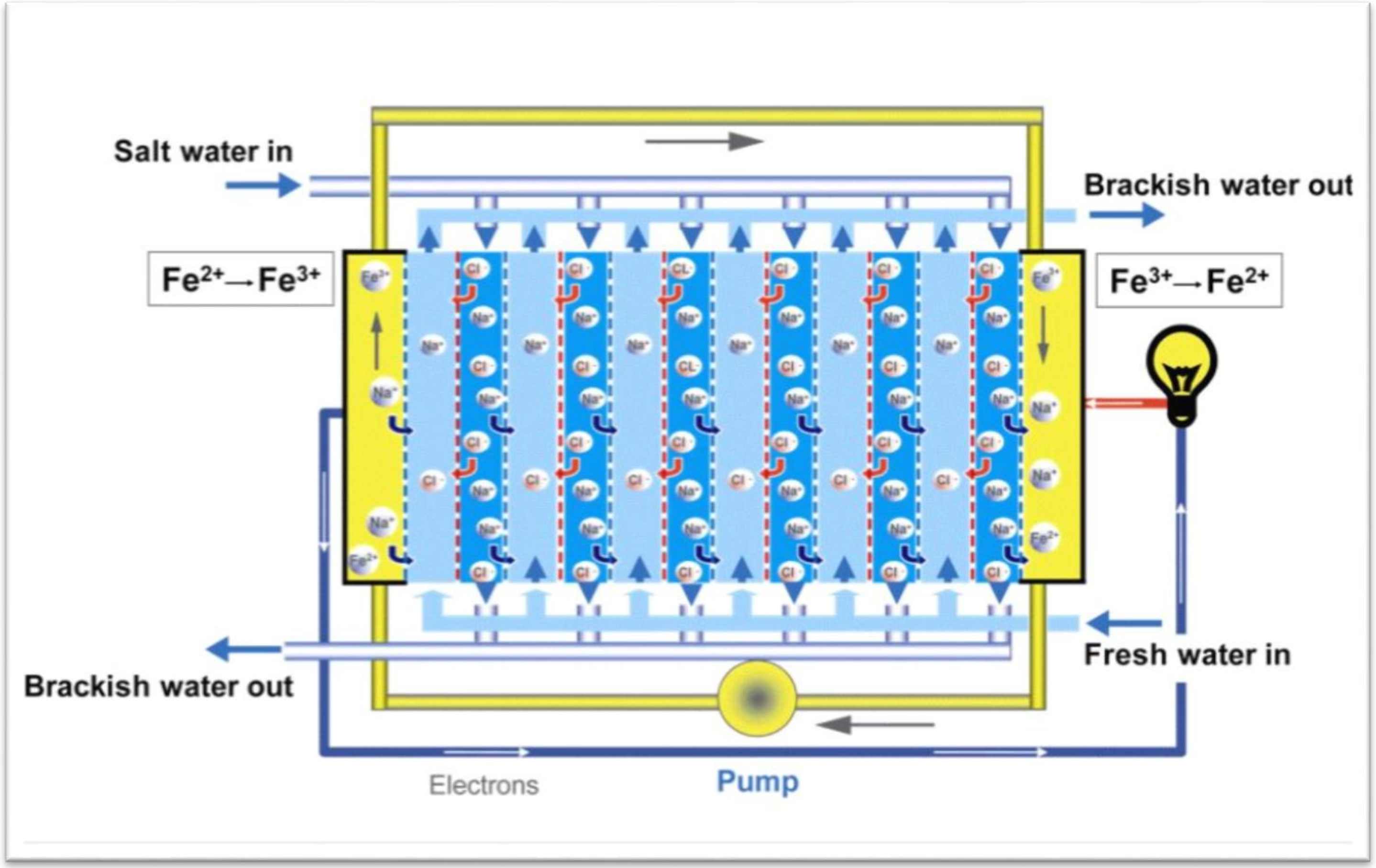
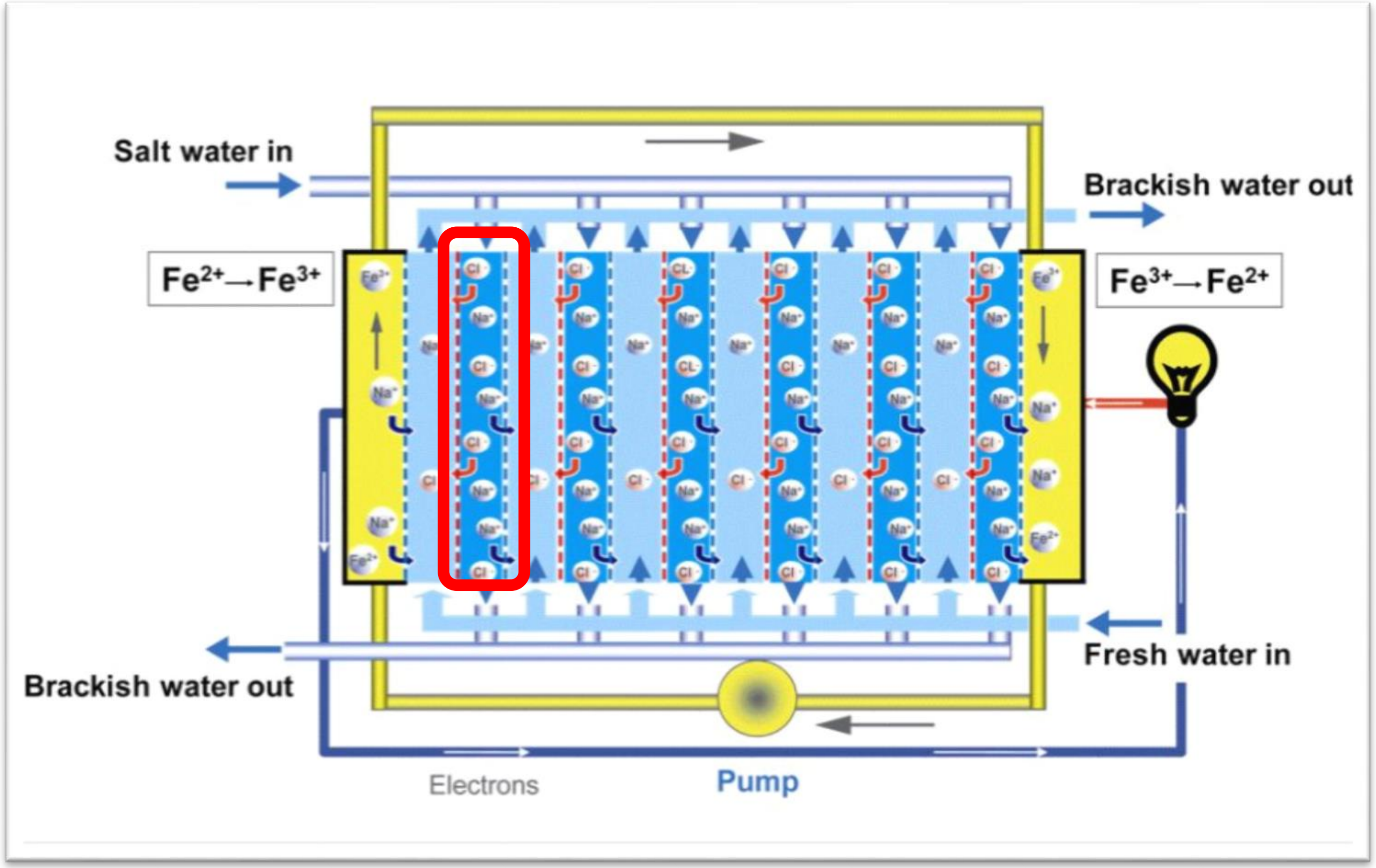


Consists of:

- Concentrate flow compartment
- Dilute flow compartment
- Redox solutions compartment
- Anionic exchange membrane
- Cationic exchange membrane

RED STACK



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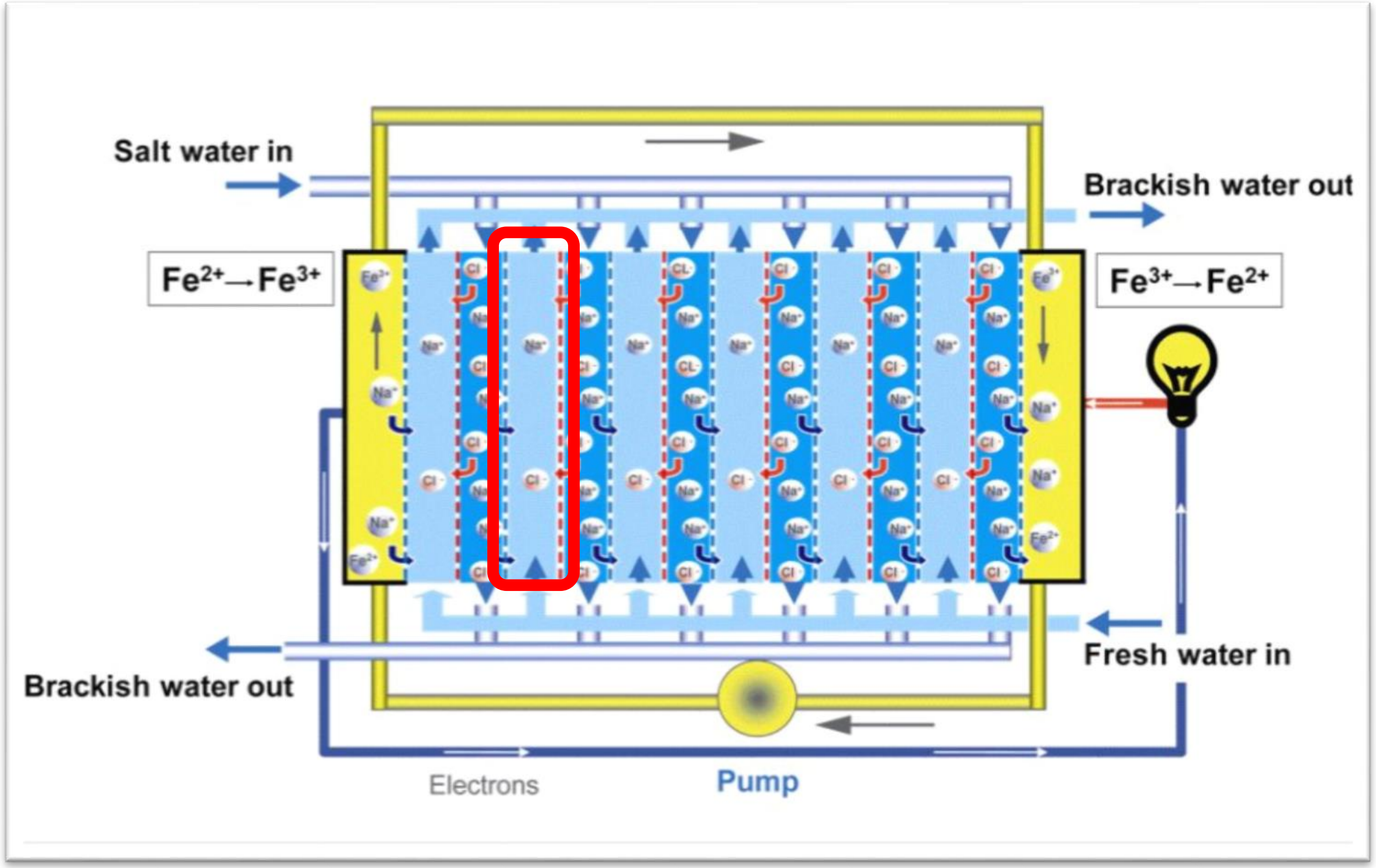

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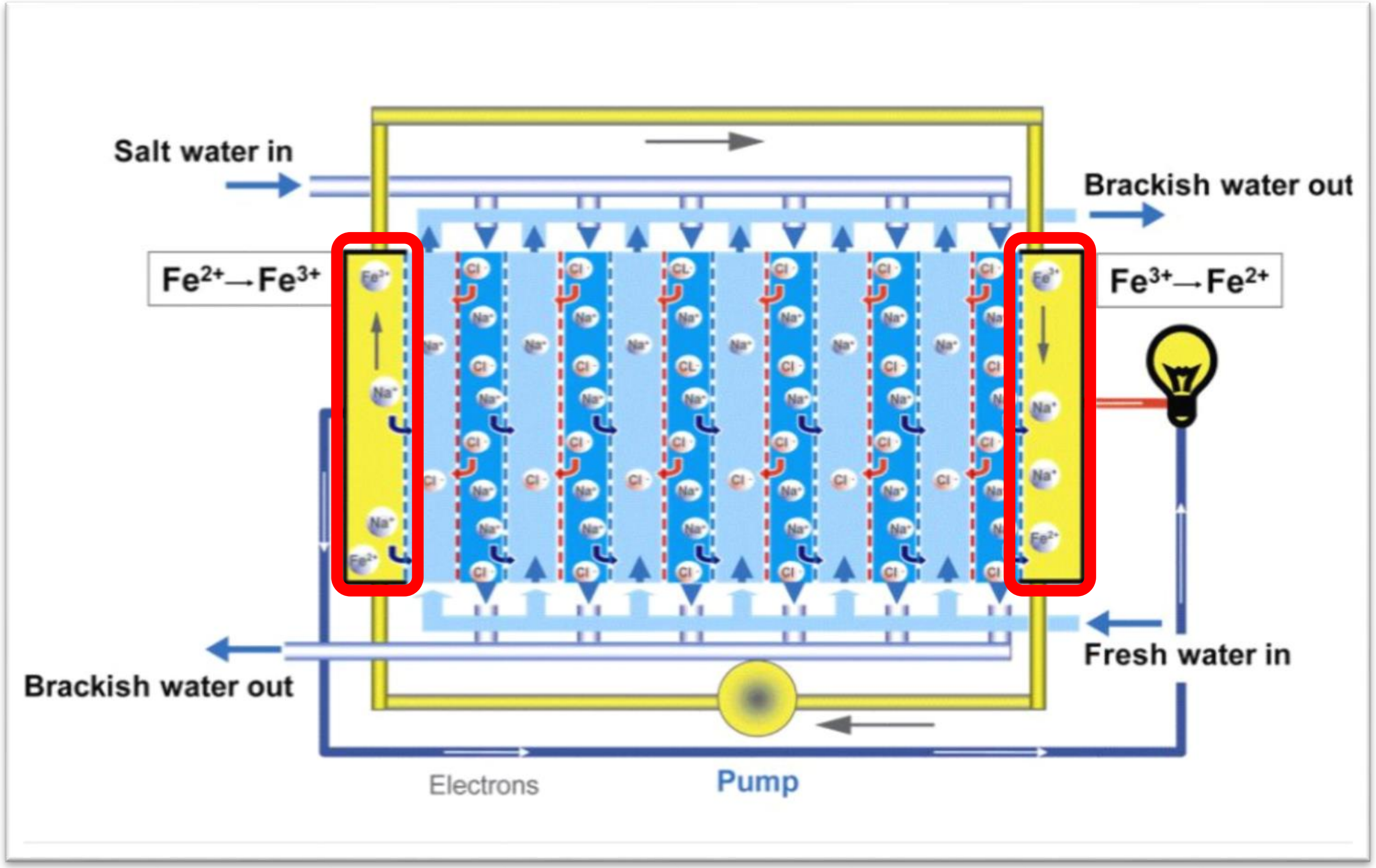

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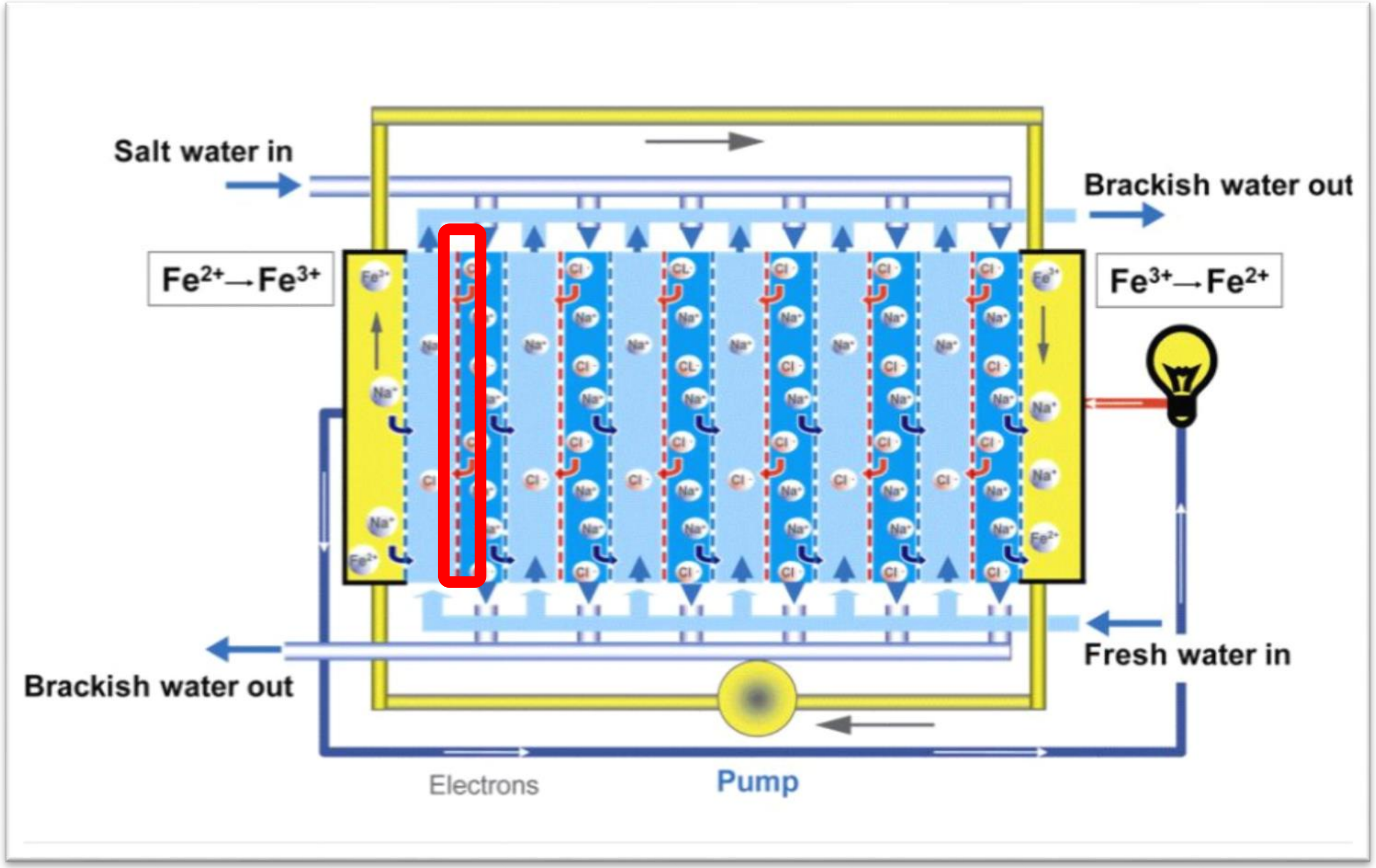

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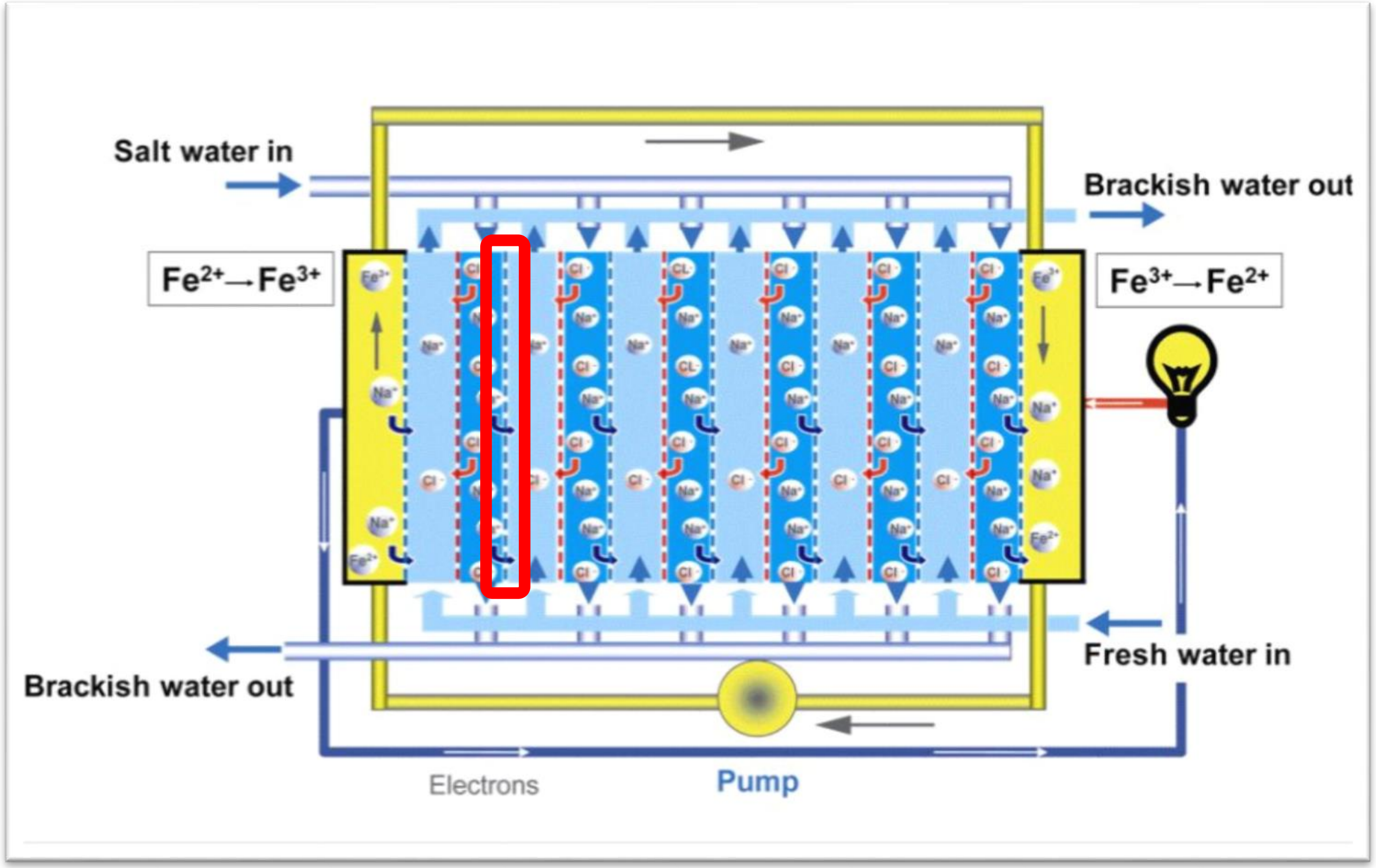

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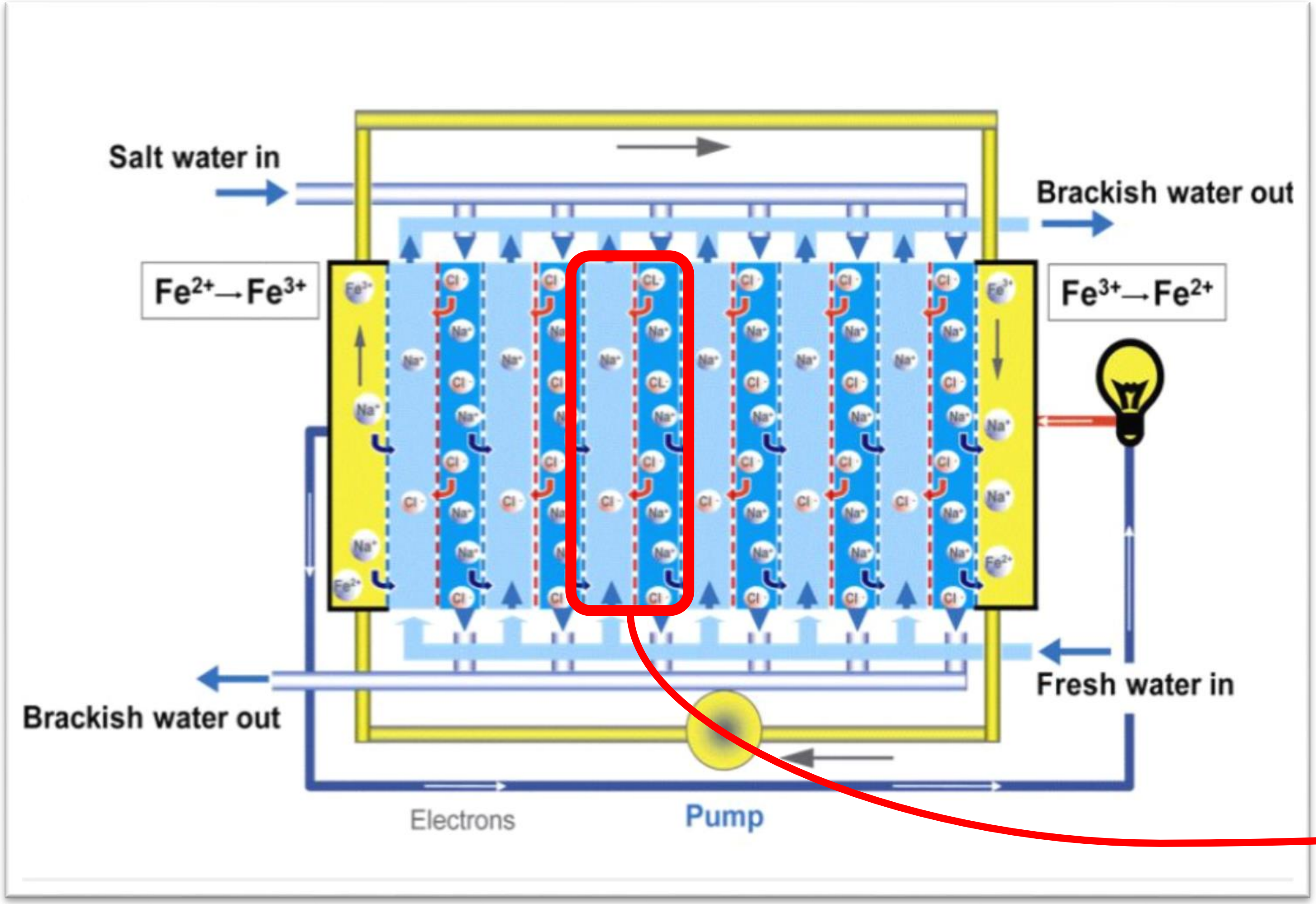
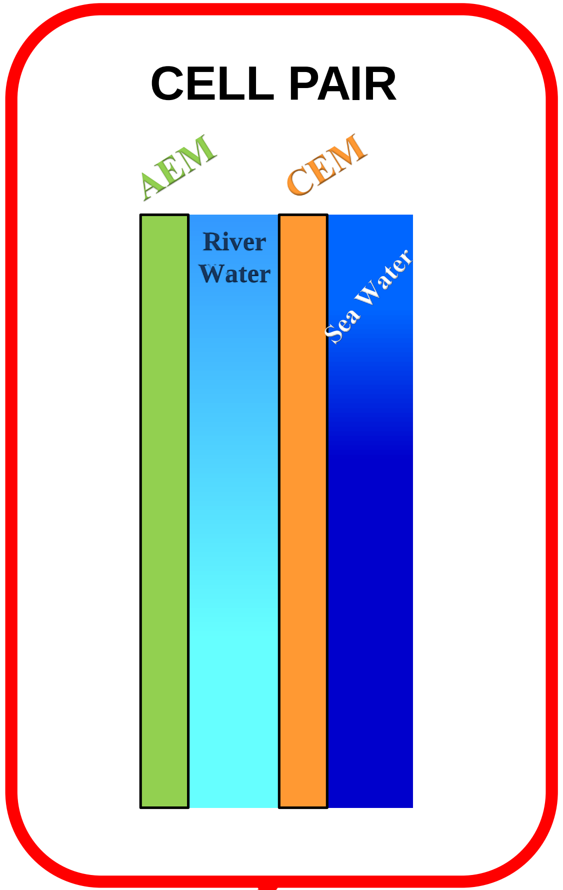

Salt water in
Brackish water out
$Fe^{2+} \rightarrow Fe^{3+}$
$Fe^{3+} \rightarrow Fe^{2+}$
Brackish water out
Fresh water in
Electrons
Pump

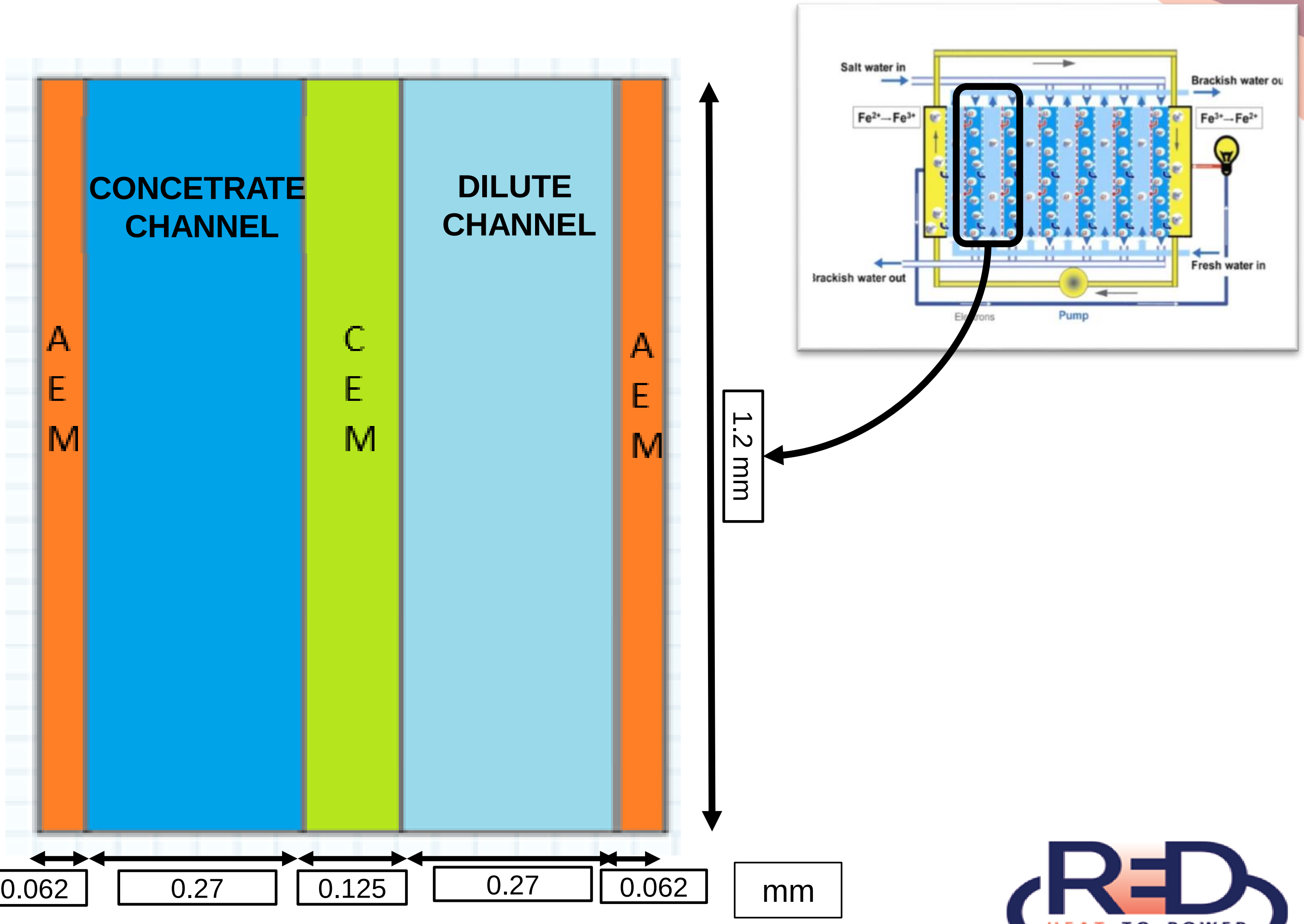

CELL PAIR
AEM
CEM
River Water
Sea Water

RED STACK MODELLING

COMPUTATIONAL DOMAIN

CELL PAIR

- 2-D simulations
- Consists of:
  - Half anionic membrane
  - Concentrate flow compartment
  - Cationic membrane
  - Dilute flow compartment
  - Half anionic membrane
- Cell pair of 1.2 mm instead of 10 cm
- Pure NaCl solutions



MODEL EQUATIONS

- Continuum equation:

$$\rho\nabla(\boldsymbol{u}) = 0$$

- Navier-Stokes:

$$\rho\frac{\delta\boldsymbol{u}}{\delta t} + \rho(\boldsymbol{u}\nabla)\boldsymbol{u} = \nabla[-pI + \mu(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T] + \mathbf{F}$$

- Nernst-Plank :

$$\boldsymbol{N}_i = (-D_i\nabla c_i - z_i u_{mi} F c_i \nabla\Phi_i) + \boldsymbol{u}c_i$$

- Electro-neutrality:

$$\sum z_i c_i = 0$$

- Current density:

$$\boldsymbol{i} = F\sum z_i(-D_i\nabla c_i - z_i u_{mi} F c_i \nabla\Phi_i)$$

- Donnan Potential:

$$\Phi_{Donnan} = \Phi_{Membrane} - \Phi_{Solution} = \frac{RT}{ZF} ln\left(\frac{a_{solution}}{a_{membrane}}\right)$$

- Absorption equilibrium at solution-membrane interface:

$$C_{Co-ion,mem} = \frac{1}{2}\left(\sqrt{C_{fix,mem}^2 + 4C_{counter-ion,solu}C_{Co-ion,solu}} - C_{fix,mem}\right) + \alpha C_{fix,mem}$$

EQUIVALENT ELECTRICAL CIRCUIT

- Cell pair electric potential:

$$E_{cp} = \Phi_{AEM\_right} - \Phi_{AEM\_left}$$

- External current:

$$I = \frac{N\, E_{cp}}{(R_{blanck} + R_{ext})}$$

- Stack electric potential:

$$E_{stack} = I R_{ext}$$

- Total cell pair resistance:

$$R_{cp} = \frac{(E_{OCV,cp} - E_{cp})}{I}$$

- Gross power density:

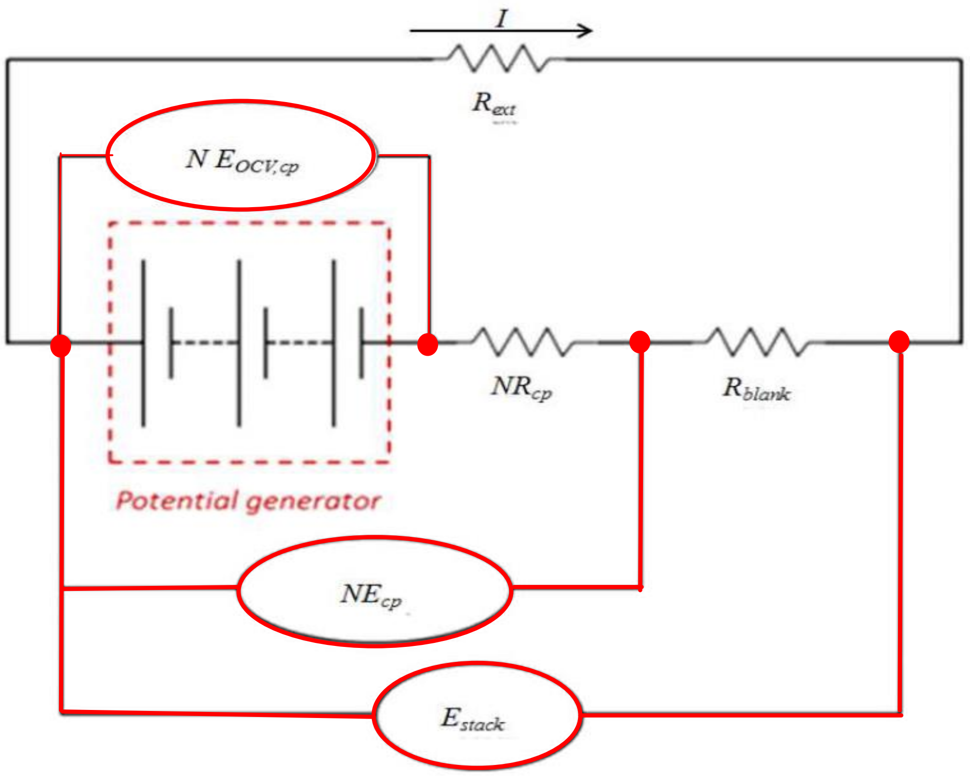
$$\mathrm{P_{Gross}} = \mathrm{E_{stack}} * \mathrm{j}$$

- Pumping power density:

$$\mathrm{P_{pump}} = \frac{(\Delta \mathrm{P_{dil}} * \mathrm{Q_{dil}} + \Delta \mathrm{P_{conc}} * \mathrm{Q_{conc}})}{\mathrm{A_{membrane}}}$$

- Net power density:

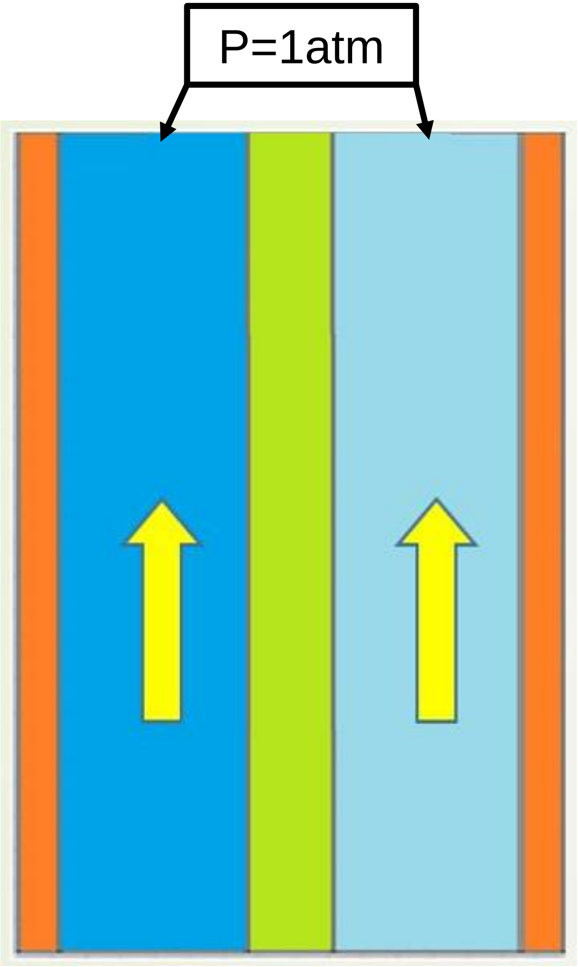
$$\mathrm{P_{Net}} = \mathrm{P_{Gross}} - \mathrm{P_{Pump}}$$



A=9.6*9.6 cm^2 and N=10

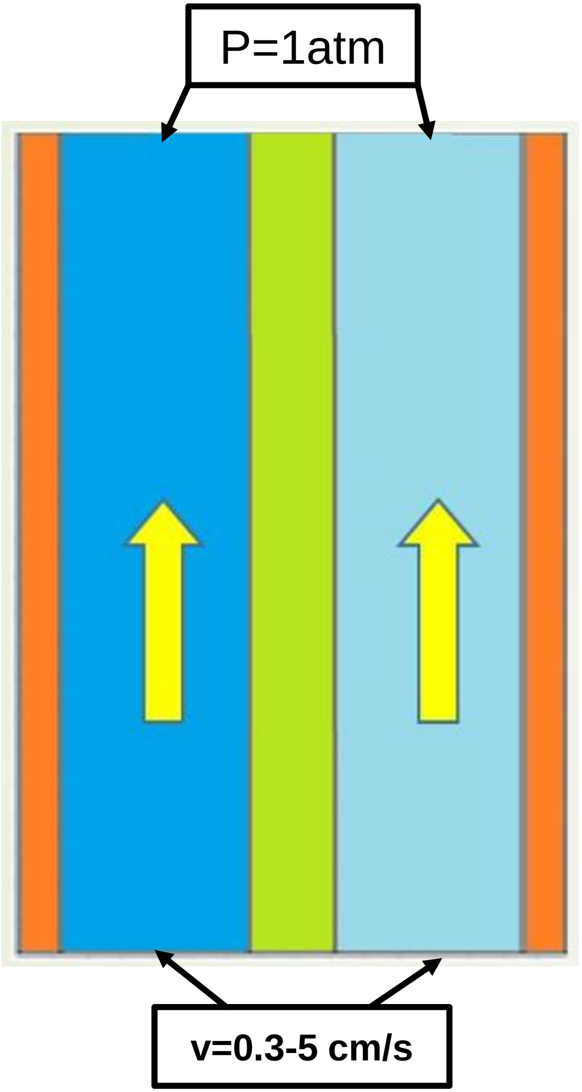
BOUNDARY CONDITIONS

- Outlet Pressure



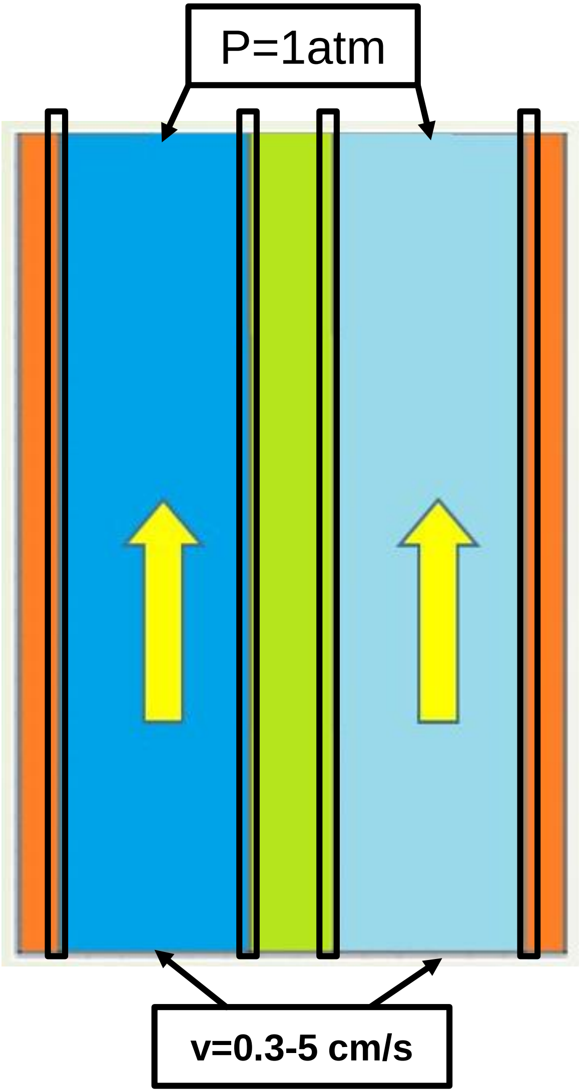
BOUNDARY CONDITIONS

- Outlet Pressure
- Inlet Velocity



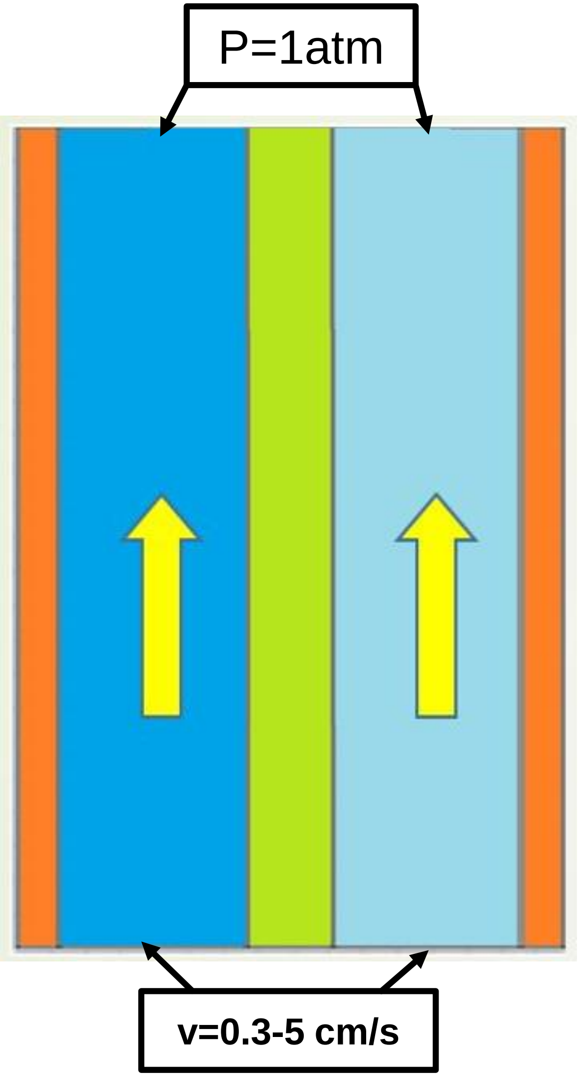
BOUNDARY CONDITIONS

- Outlet Pressure
- Inlet Velocity
- No slip condition at membranes surfaces

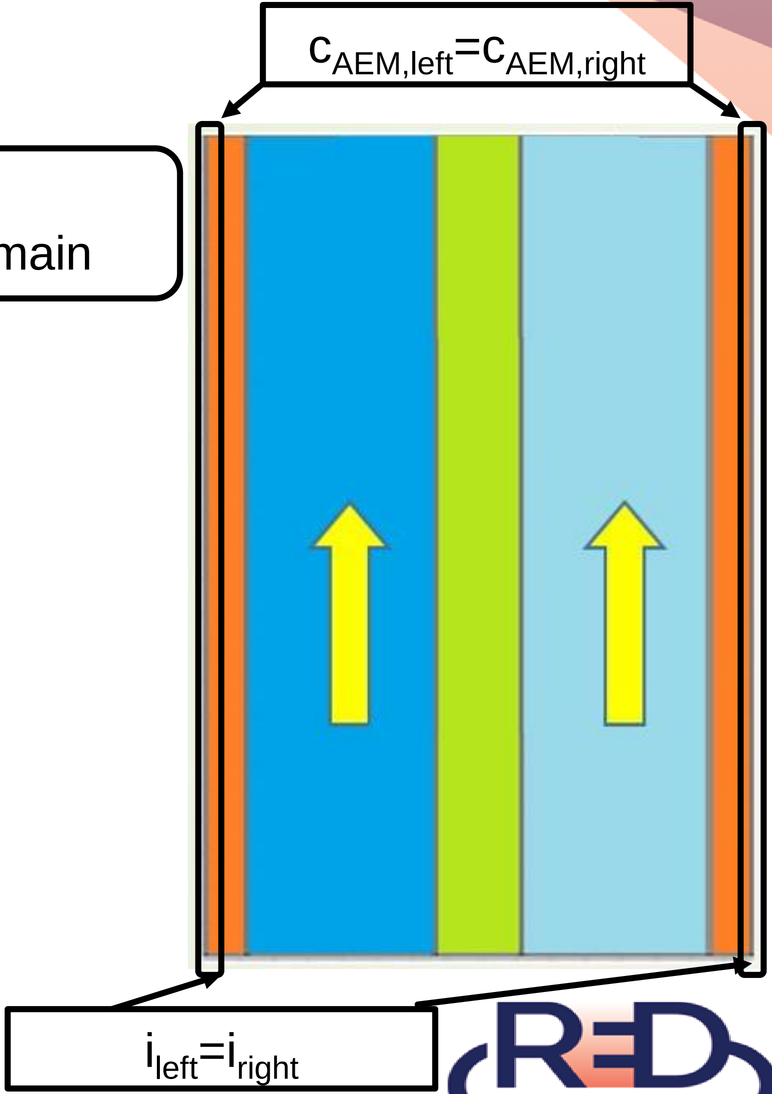


BOUNDARY CONDITIONS

- Outlet Pressure
- Inlet Velocity
- No slip condition at membranes surfaces

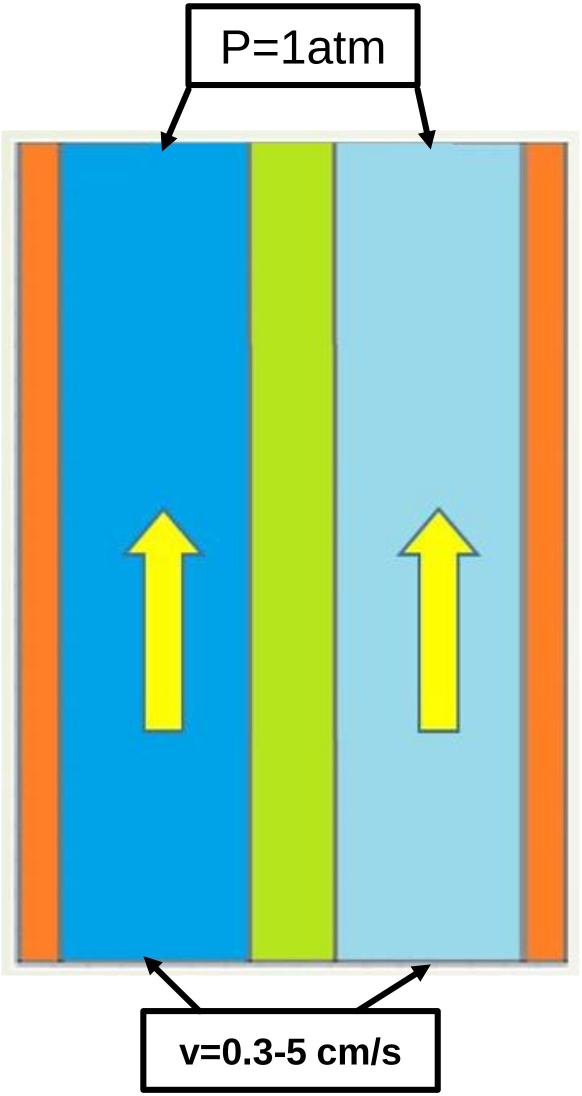


- Periodic concentration at external boundaries of domain
- Current density at external boundaries of domain

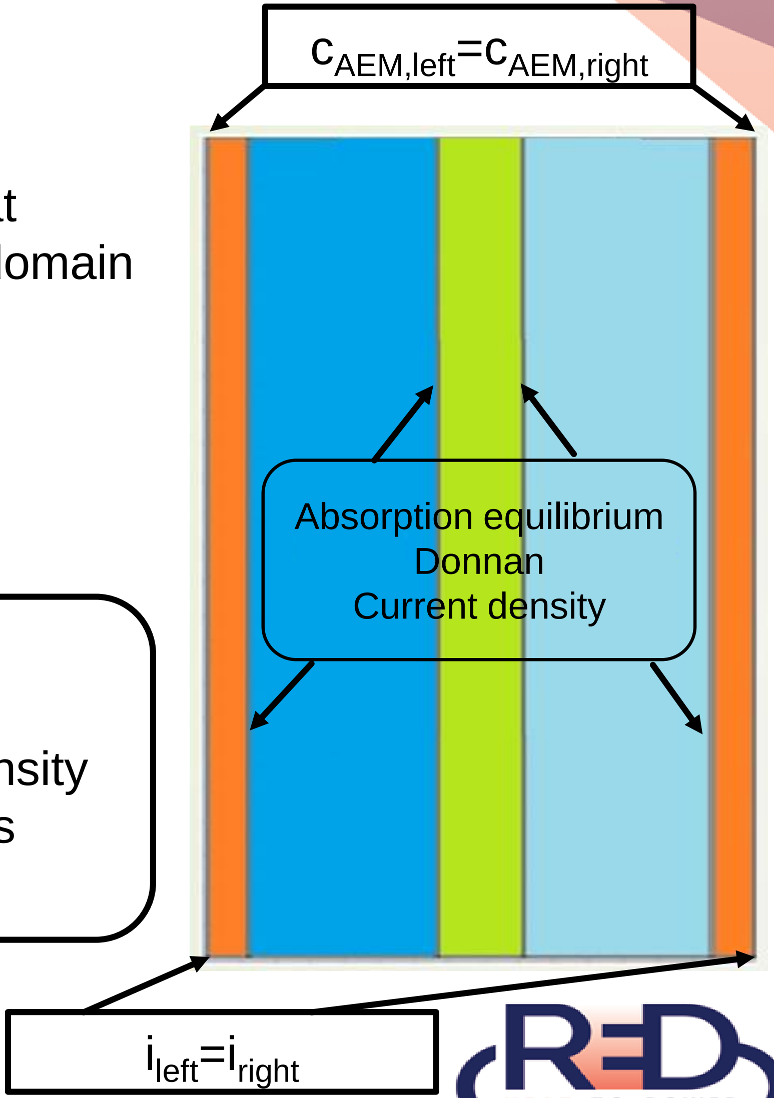


Boundary conditions

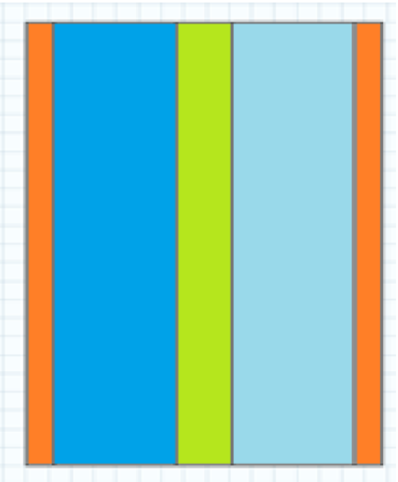
- Outlet Pressure
- Inlet Velocity
- No slip condition at membranes surfaces

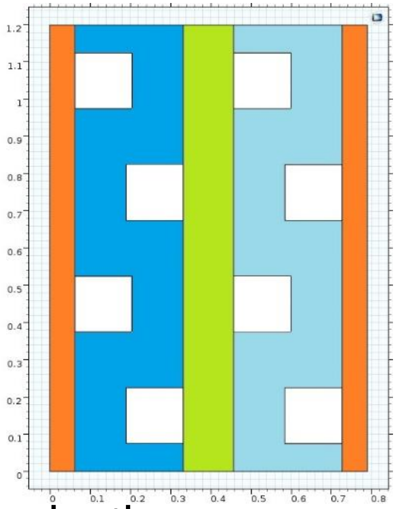


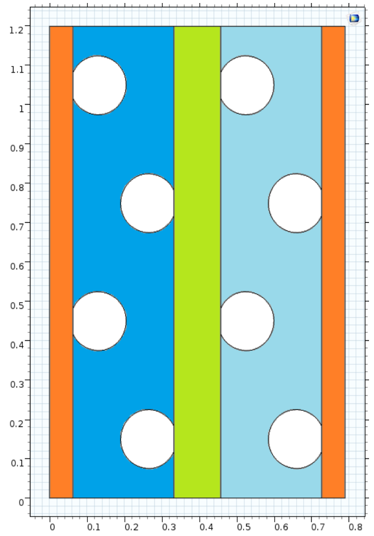
- Periodic concentration at external boundaries of domain
- Current density at external boundaries of domain
- Absorption equilibrium, Donnan potential and continuity of current density at solutions-membranes interfaces

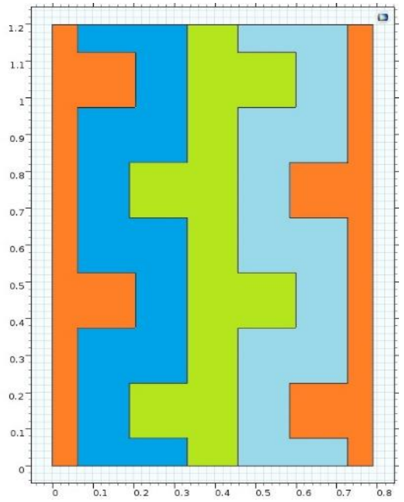


GEOMETRIES

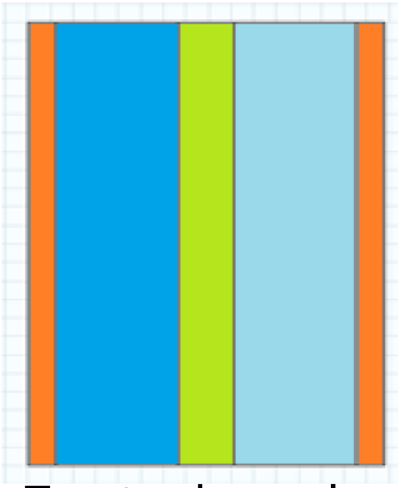

Empty channel


Non conductive square spacers

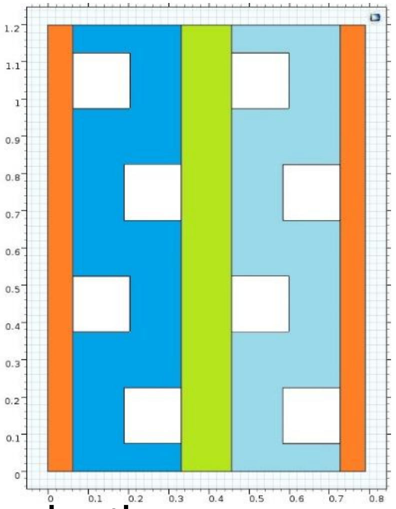

Non conductive round spacers


Profiled Membranes

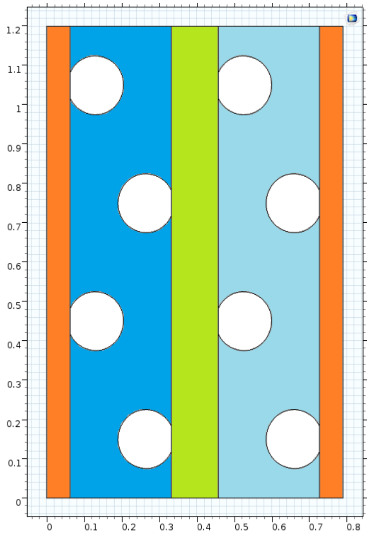
GEOMETRIES



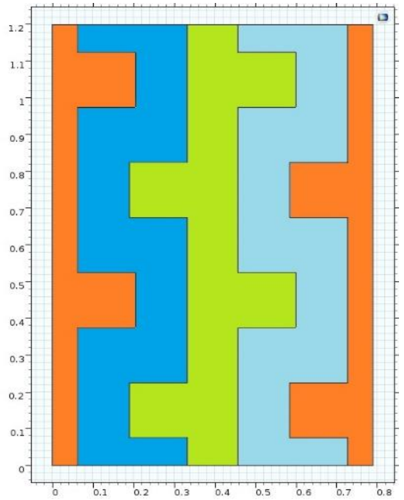
Empty channel



Non conductive square spacers



Non conductive round spacers



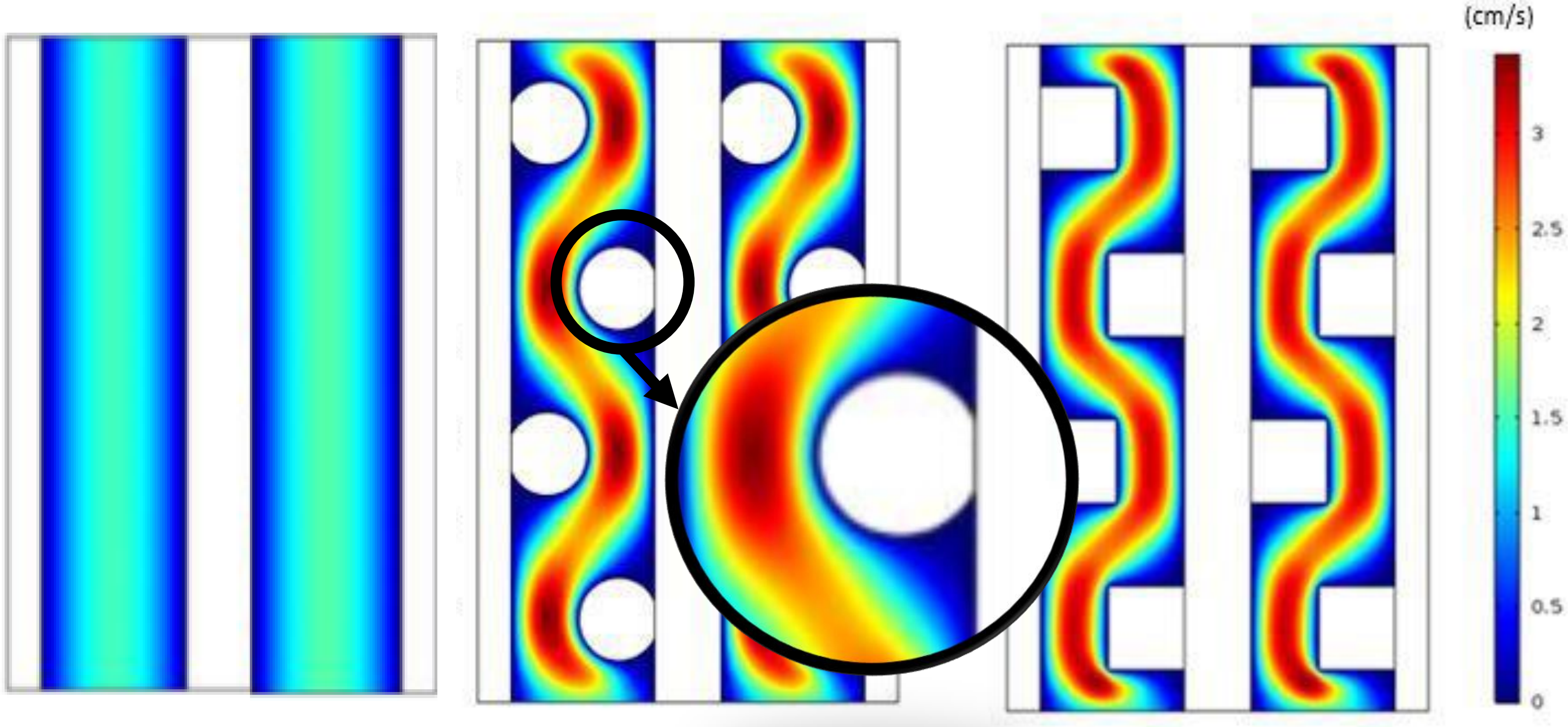
Profiled Membranes

RESULTS

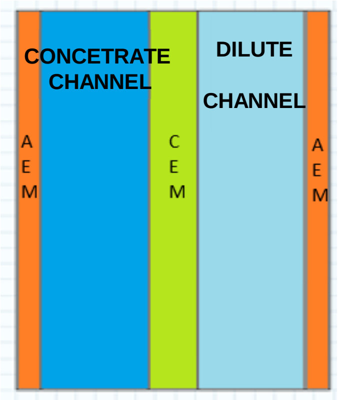
VELOCITY MAPS

Velocity maps:

- Parabolic profile in empty channel
- Dead pocket

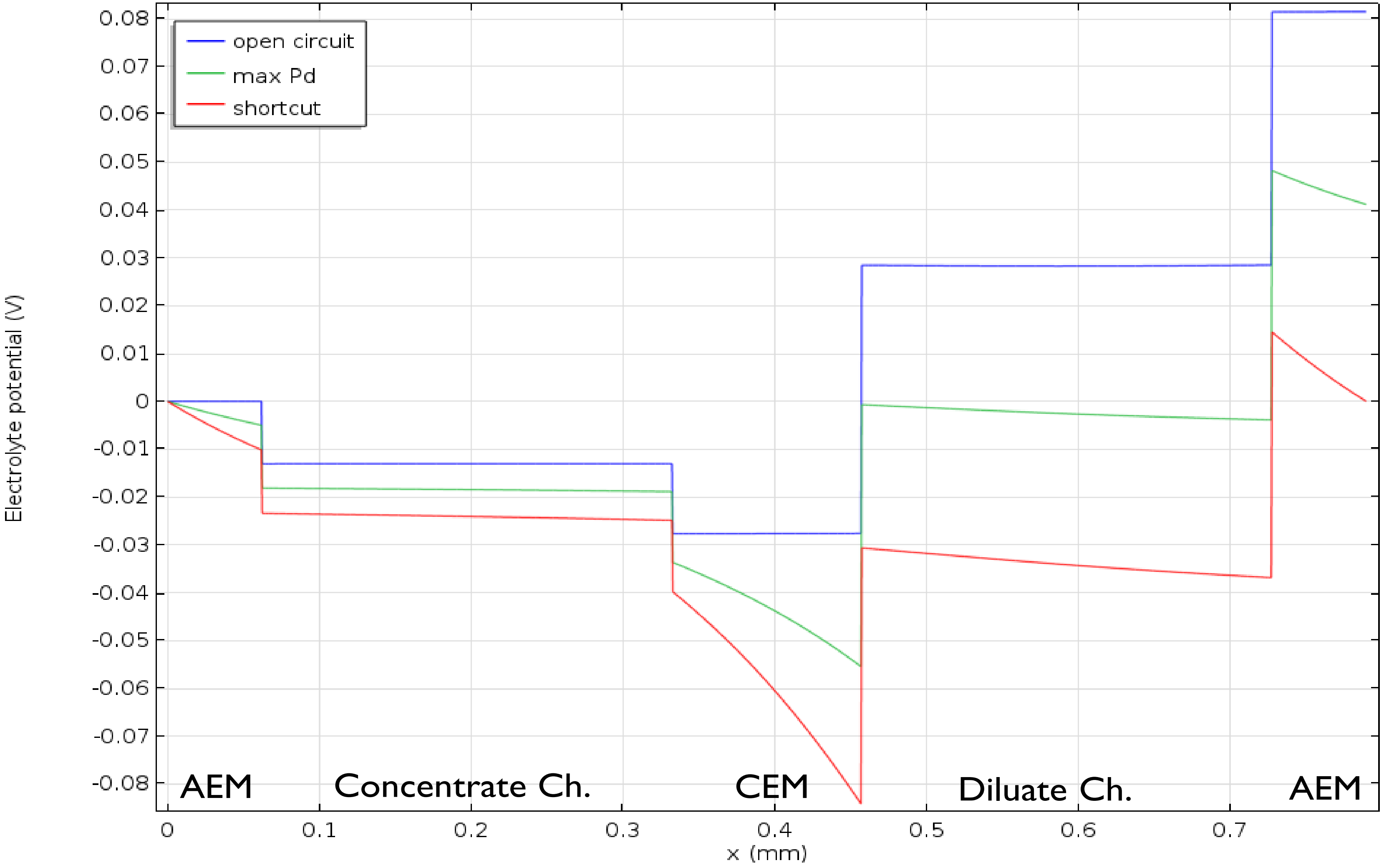


Electric potential



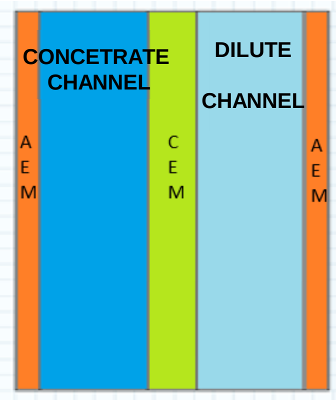
Electric potential:

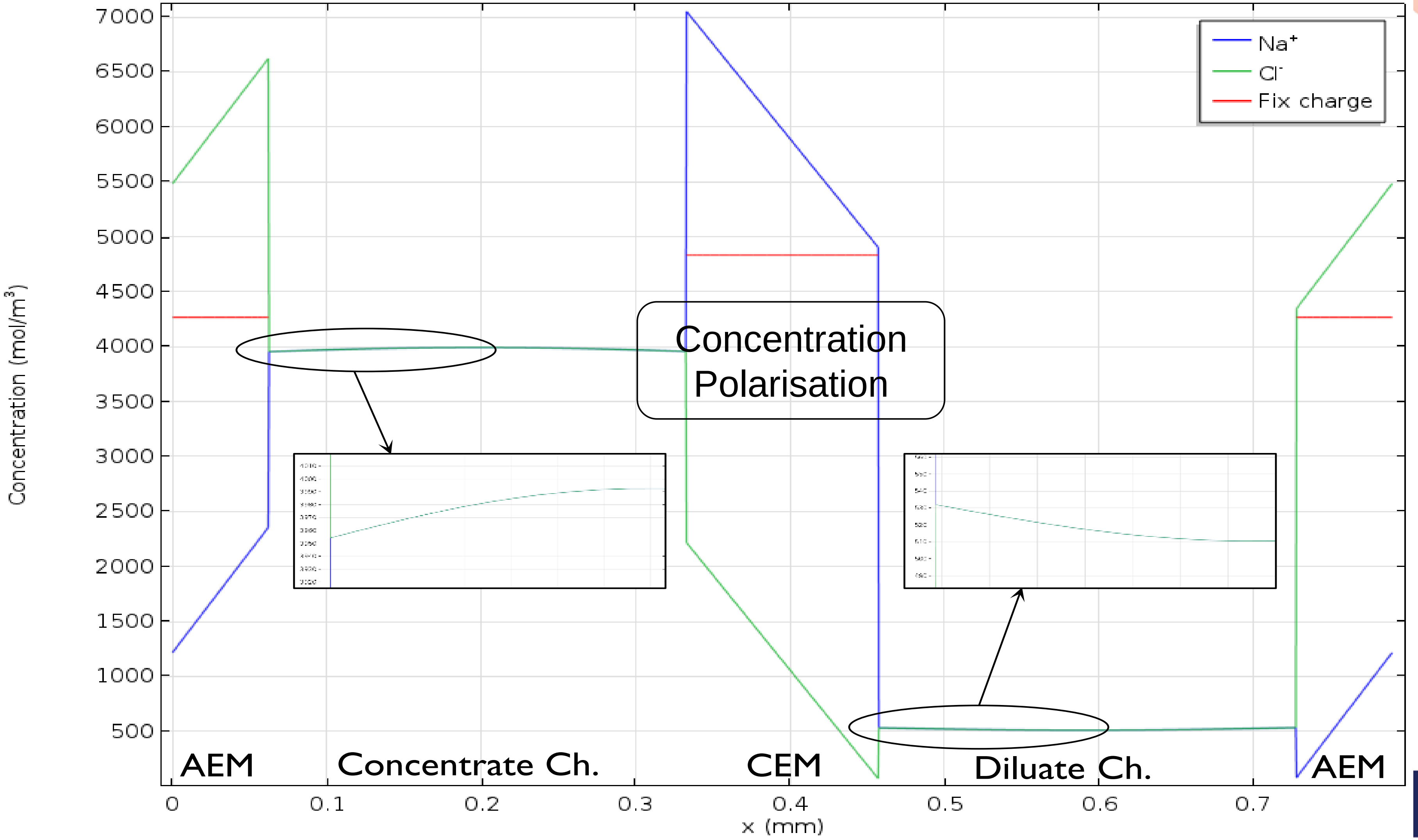
- **Open circuit**
- **Max Gross Power Density**
- **SHORTCUT**



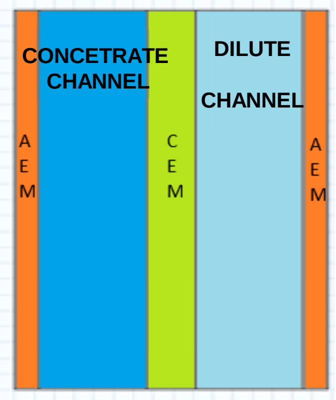
C_con_4M and C_dil_0.5M

CONCENTRATION PROFILES

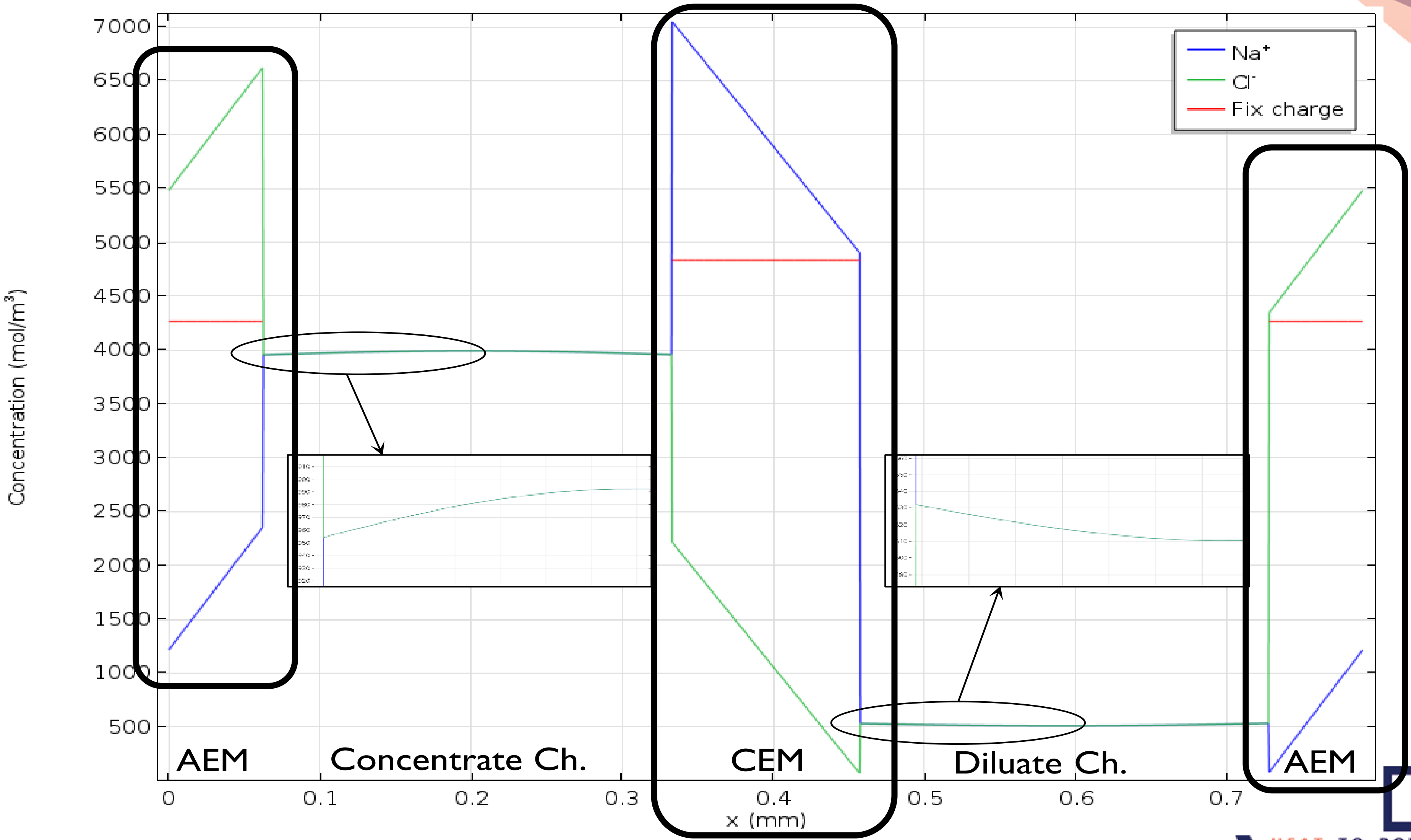




Concentration Profiles



Concentration profiles in membranes



SENSITIVITY ANALYSIS C_CON=4M

A sensitivity analysis was performed in order to investigate the produced Net Power Density studying:

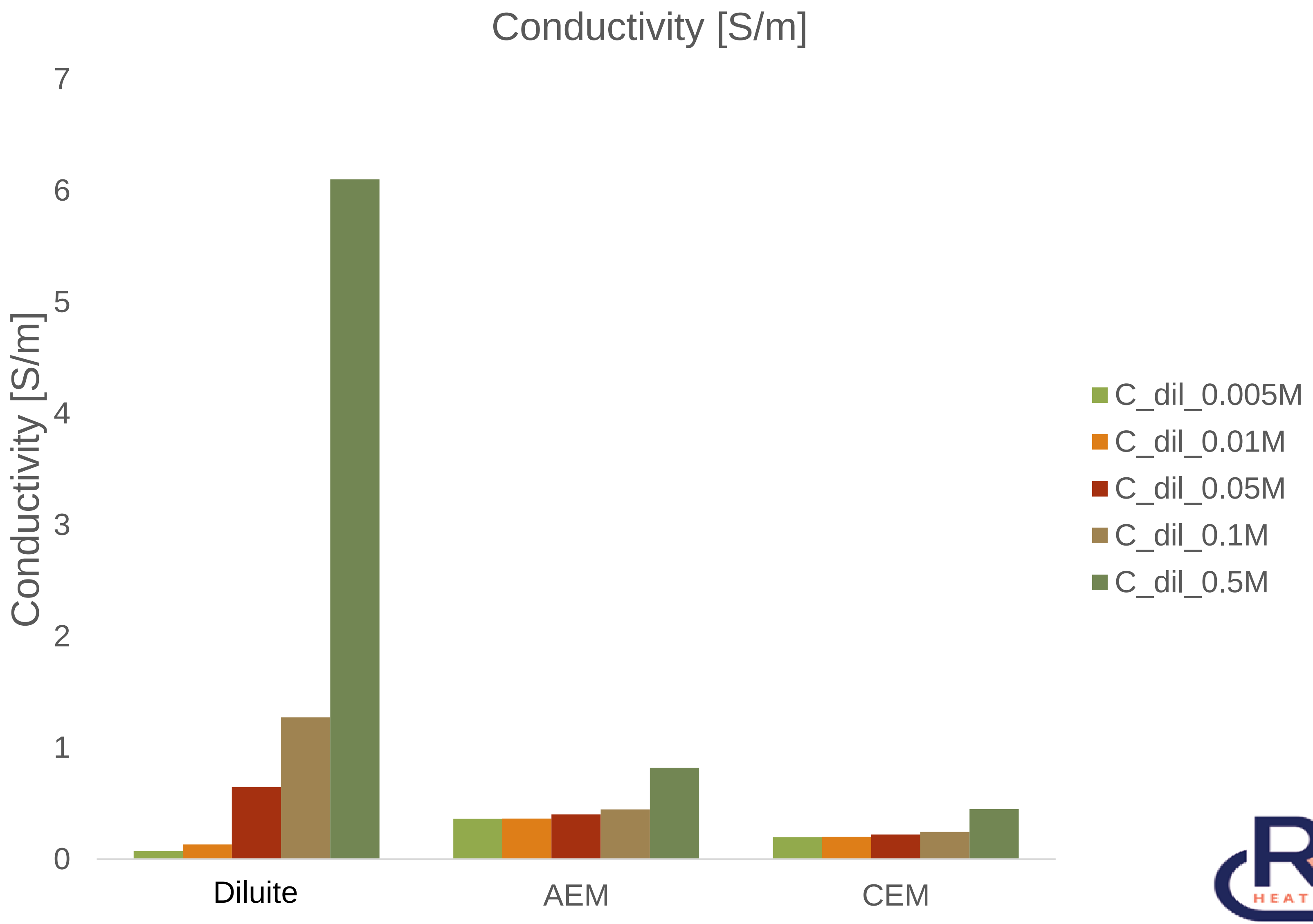
- Previously presented geometries of cell pair:

- Velocity of solutions between 0.3-5 cm/s

- Five dilute solutions:
  - 0.5M
  - 0.1M
  - 0.05M
  - 0.01M
  - 0.005M

SENSITIVITY ANALYSIS C_CON=4M

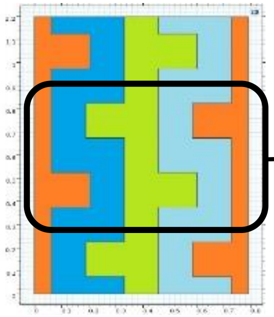
- Less concentrated dilute solutions have less conductivity
- Membranes have higher conductivy than dilute solutions at 0.005-0.01M

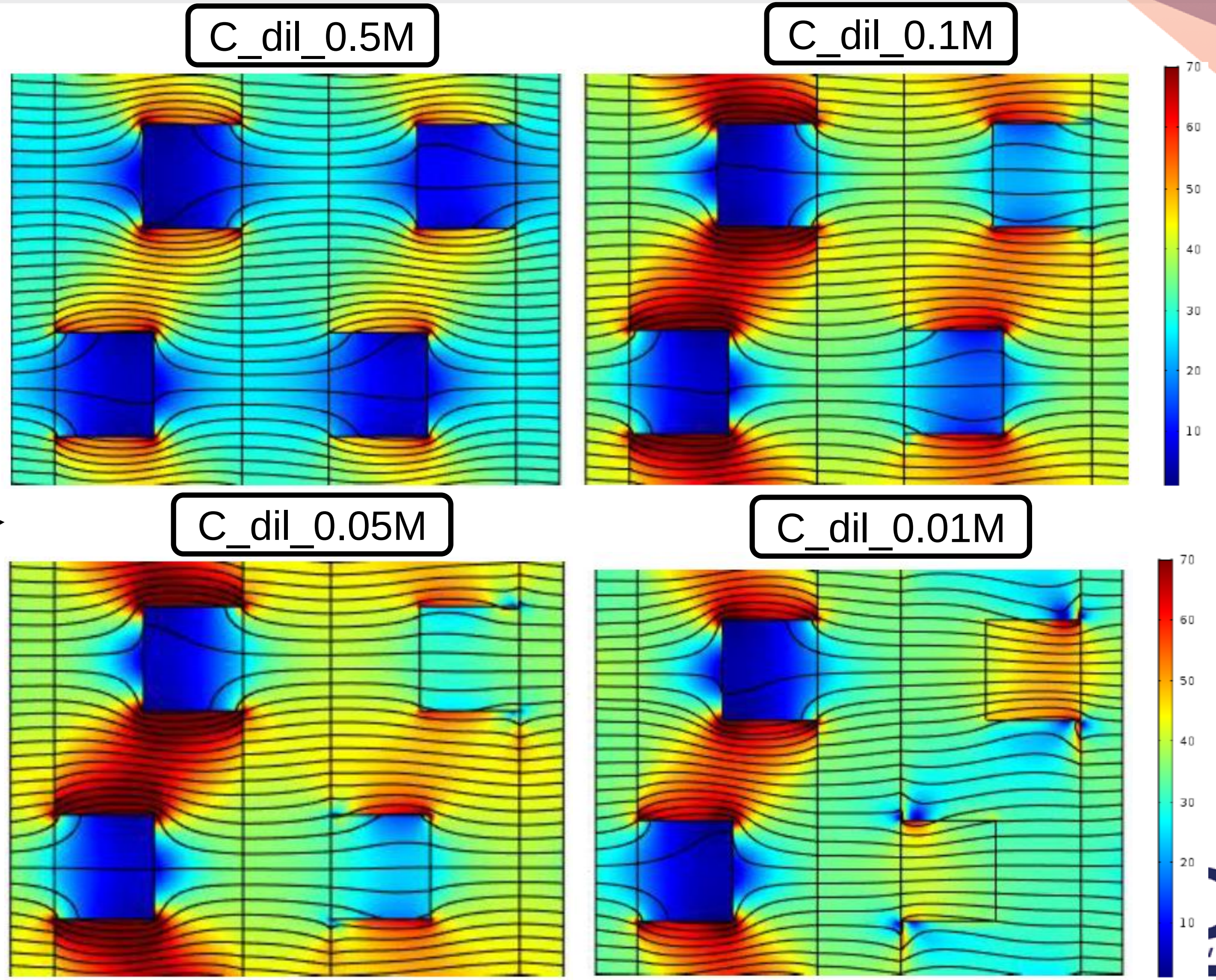


SENSITIVITY ANALYSIS C_CON=4M

CURRENT DENSITY MAPS

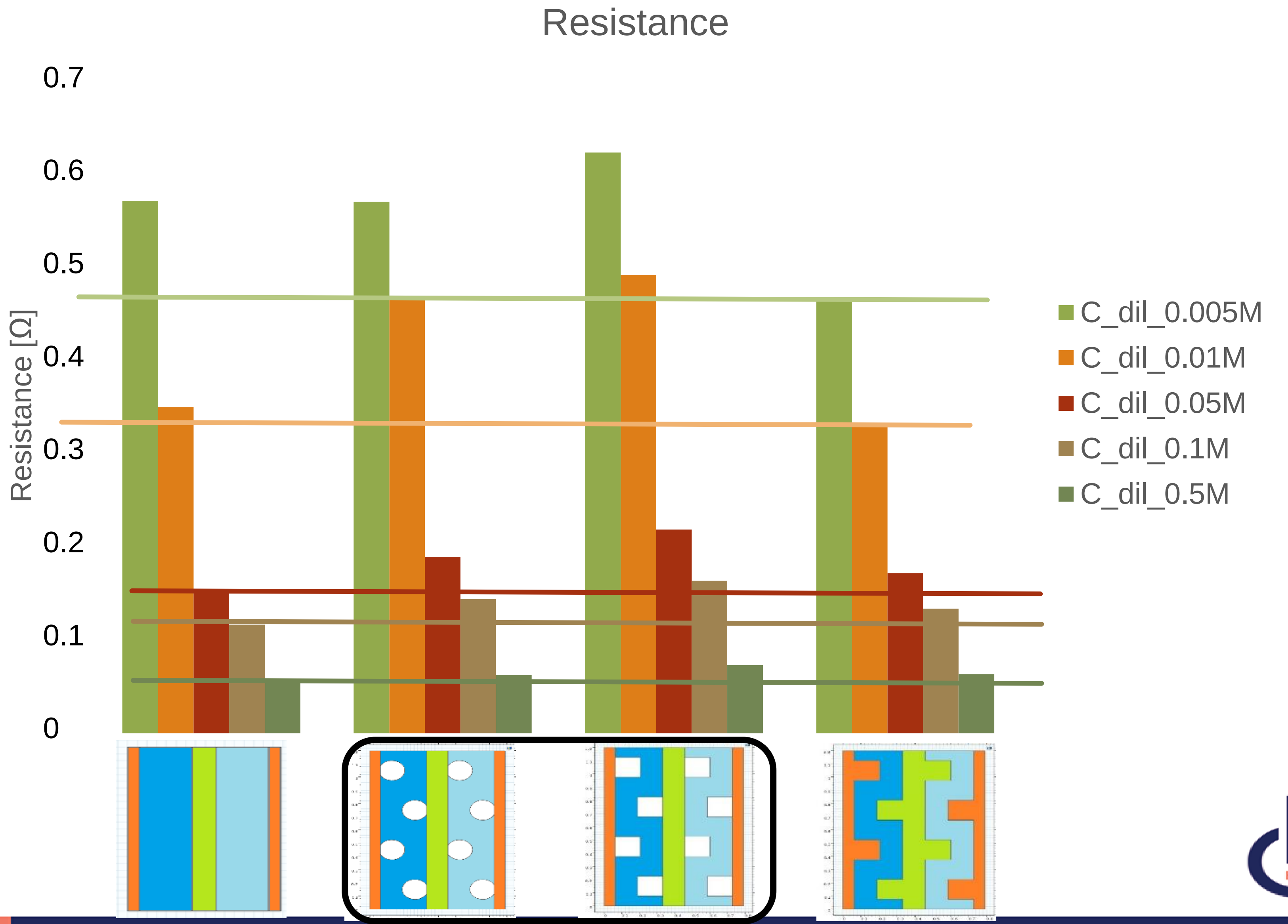
As dilute concentration decreases, the current density flows preferentially through membrane profiles instead of flowing through the solution, due to their higher conductivity.





SENSITIVITY ANALYSIS C_CON=4M

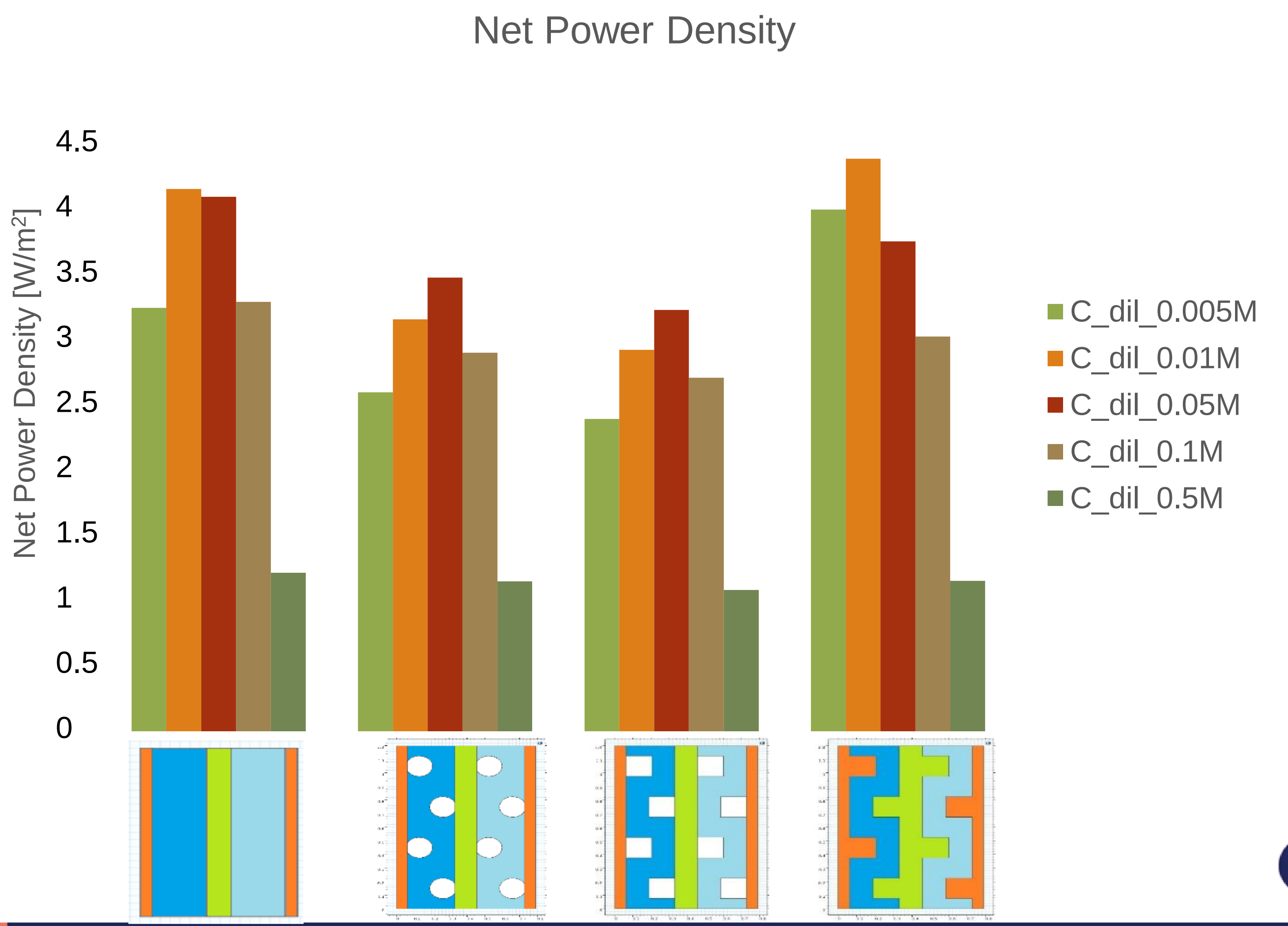
- At C_dil_0.01M and C_dil_0.005M profiled membranes give the lowest resistance
- At higher concentrations the empty channel gives the lowest resistance
- Non conductive spacers give always the highest resistance



SENSITIVITY ANALYSIS C_CON=4M

- The profiled membrane gives the highest net power density with a value of 4.38 W/m^2 at dilute solution of 0.01M

- Empty channel gives higher power density for all other more concentrated diluite solutions



Conclusions

- The model allows:
  - to analyze stacks with different configurations;
  - to study different electric current conditions;
  - to describe the concentration profiles in the membranes.

- The model has shown that profiled membranes less resistive than diluite solution are able to increase Net power density of RED Units.

- 4M-0.01M solutions, with profiled membranes, give the highest net power density with a value of 4.38W/m^2.

- Even if C_dil_0.005M gives the highest driving force to the process, its high dilute solution resistance gives rise to high ohmic losses with less Net power Density production.

THANK YOU FOR YOUR ATTENTION

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