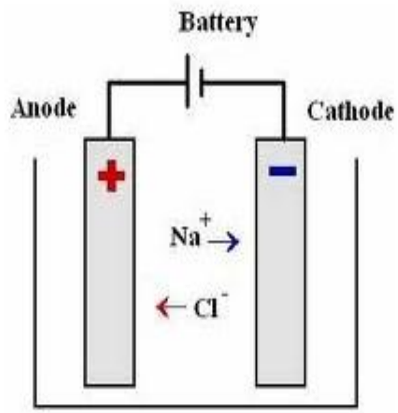
COMSOL CONFERENCE INDIA 2012

Numerical Simulation of Flow Electrolysers: Effect of Various Geometric Parameters



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Presented by Pragati Shukla

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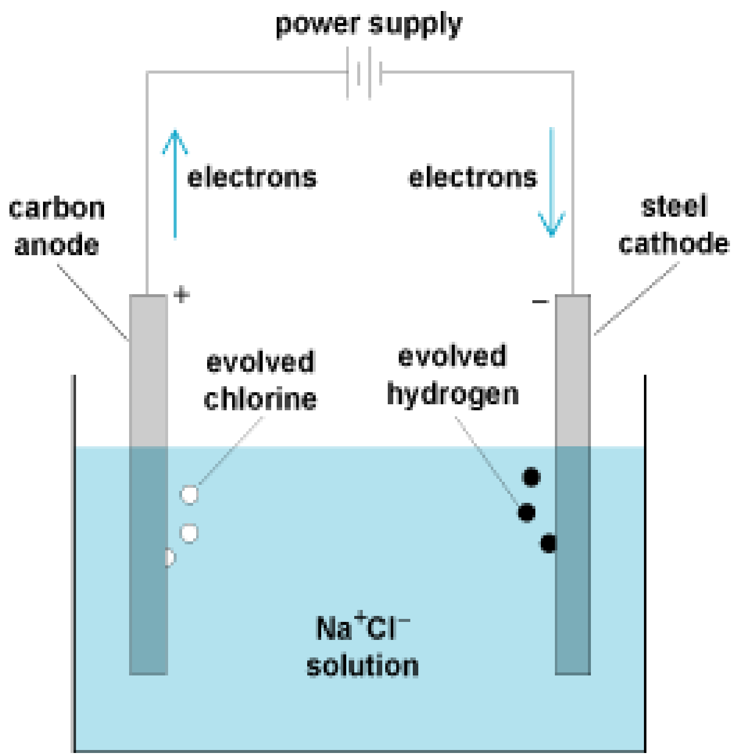
Outline

- Electrolysis and its Industrial applications
- Objective of this work
- Governing equations and boundary conditions
- Validation of the computational approach
- Effect of inlet channel length
- Effect of offset between anode and cathode
- Effect of size of anode
- Conclusion

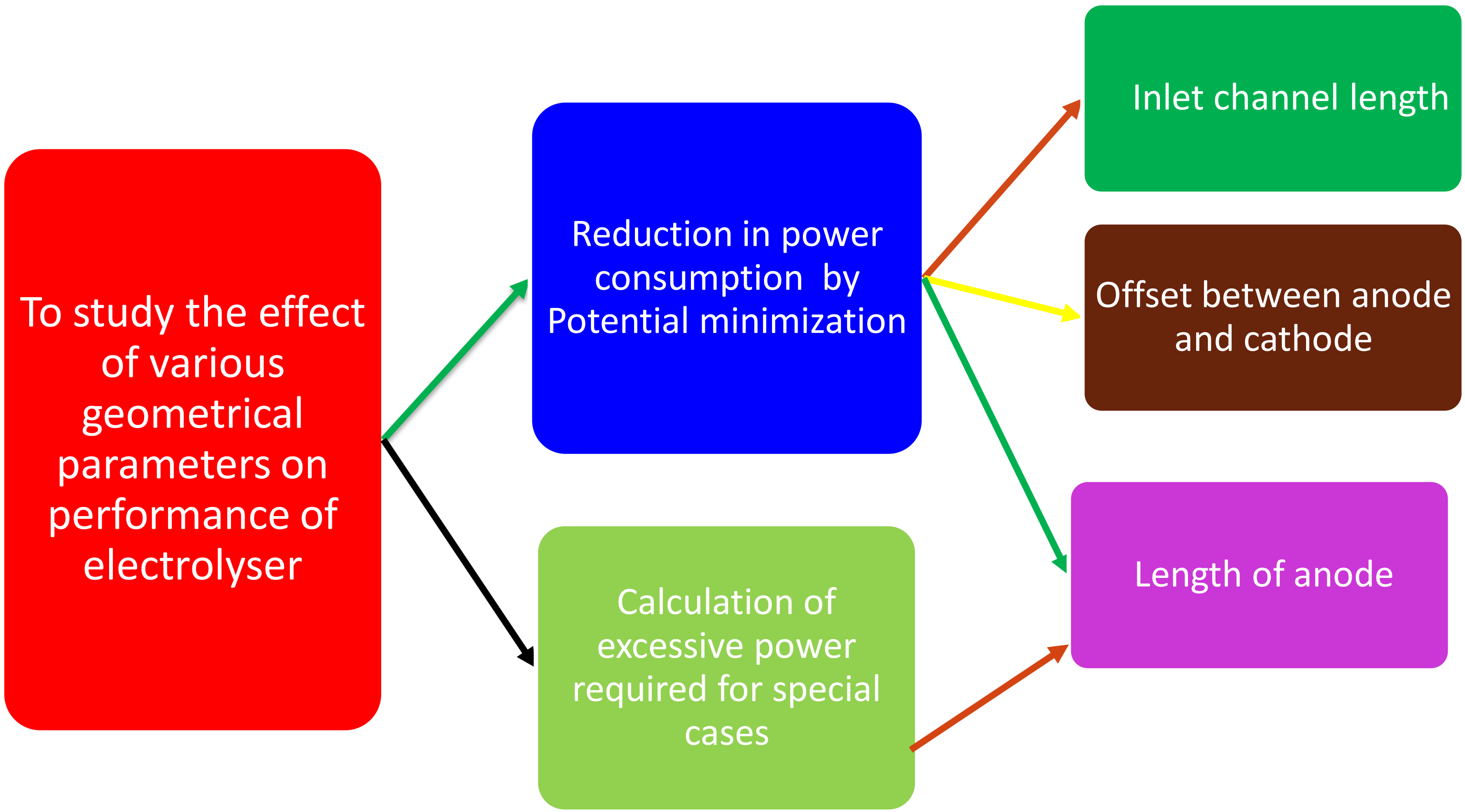
Electrolysis and its Industrial Applications



Schematic diagram of an electrolyser

- Electroplating
- Electrolytic etching of metal surface
- Cleaning and preservation of old artifacts
- Production of aluminium, lithium, sodium, potassium, magnesium
- Production of electrolytic copper as a cathode, from refined copper of lower purity as an anode
- Caustic soda production

Objective of this Work



Li Lianhua, Kong Xiaoying, Sun Yongming, Yuan Zhenhong, Li Ying, Performance of microbial fuel cell in different anode and cathode sizes, *International Conference on Remote Sensing, Environment and Transportation Engineering*, 7707-7710 (2011)

How We Proceed

Applicable governing equations and boundary conditions.

Validation of computational approach

Effect of geometrical parameters (inlet channel length, offset, anode length) on potential

Conclusions

Governing Equations and Boundary Cond.

Navier- Stokes Equations

$$\nabla \bullet \mathbf{u} = 0$$

$$\rho \mathbf{u} \bullet \nabla \mathbf{u} = \mu \nabla^2 \mathbf{u} - \nabla p + \rho \mathbf{g}$$

Nernst-Planck equations

$$\nabla \bullet \mathbf{N}_i = 0$$

Diffusion term

Migration term

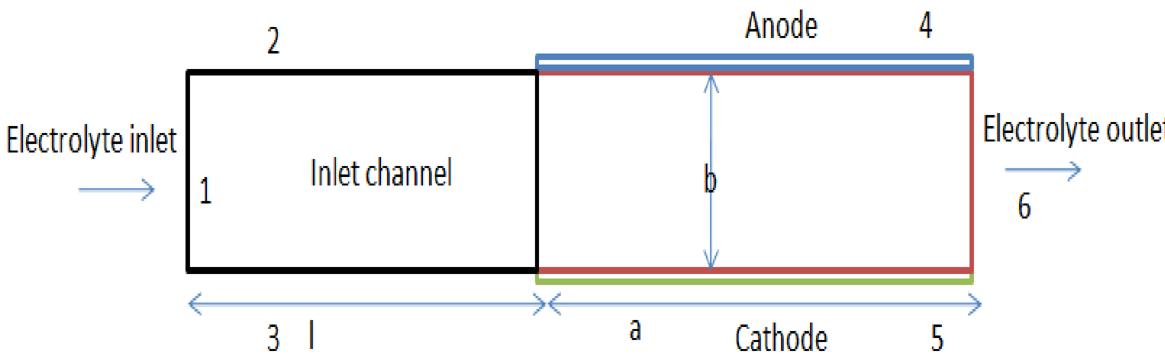
Convection term

$$\mathbf{N}_i = -D_i \nabla c_i - z_i u_{mi} F c_i \nabla V + c_i \mathbf{u}$$

Possible boundary conditions for NP equations

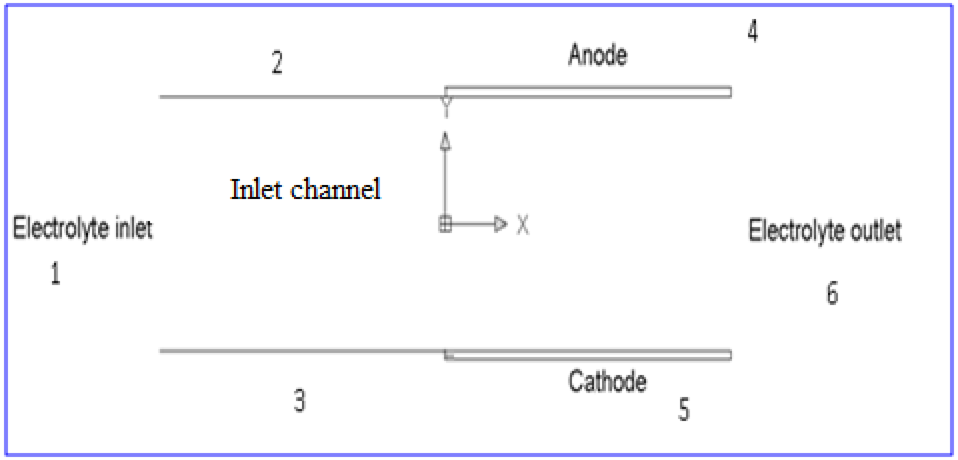
Current/potential BC		Concentration BC	
$n.i = 0$	(Electrical insulation)	$C = C_o$	(Constant concentration)
$i = i_0$	(Constant inward current density)	$-\bar{n}.\bar{N}_i = i_o/F$	(Constant flux)
$i = -i_0$	(Constant outward current density)	$-\bar{n}.\bar{N}_i = 0$	(Zero flux)
$v = v_o$	(Constant potential)	$-\bar{n}.\left(-D_i \nabla C_i - \frac{z_i F}{RT} D_i C_i \nabla \emptyset\right) = 0$	(Convective flux)

Governing Equations and Boundary Cond.



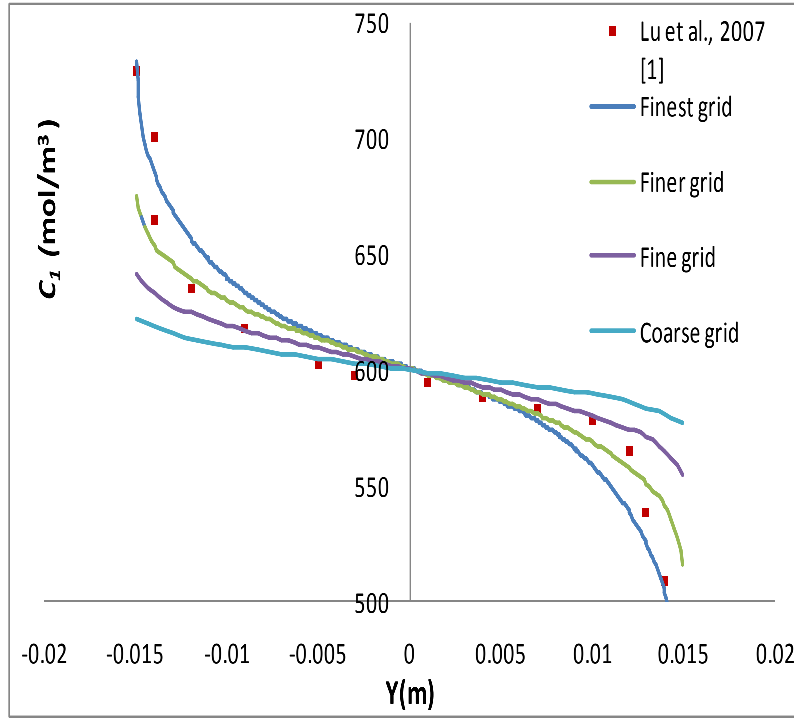
Wall	Current potential boundary cond.		Concentration/flux boundary cond.	
1	Insulation	$\mathbf{n} \bullet \mathbf{i} = 0$	Concentration	$c_2 = c_o$
2	Insulation	$\mathbf{n} \bullet \mathbf{i} = 0$	Zero flux	$-\mathbf{n} \bullet \mathbf{N}_2 = 0$
3	Insulation	$\mathbf{n} \bullet \mathbf{i} = 0$	Zero flux	$-\mathbf{n} \bullet \mathbf{N}_2 = 0$
4	Current density	$\mathbf{i} = i_o$	Faraday's law	$-\mathbf{n} \bullet \mathbf{N}_2 = \pm \frac{i_0}{F}$
5	Voltage	$V = V_o$	Zero flux	$-\mathbf{n} \bullet \mathbf{N}_2 = 0$
6	Insulation	$\mathbf{n} \bullet \mathbf{i} = 0$	Convective flux	$-\mathbf{n} \bullet (-D_2 \nabla c_2 - z_2 u_{mi2} F c_2 \nabla V) = 0$

Validation of the Computational Approach



Reactions:
$2Cl^- \rightarrow Cl_2 \uparrow + 2e$ (at the anode)
$2H_2O + 2e \rightarrow 2OH^- + H_2 \uparrow$ (at the cathode)
Na^+ (species 1, C_1), Cl^- (species 2, C_2) and OH^- (species 3, C_3) are the ions carrying currents.

Size of the domain:
Electrode length-0.1m
Gap between electrodes-.03m
Main channel length-.08m

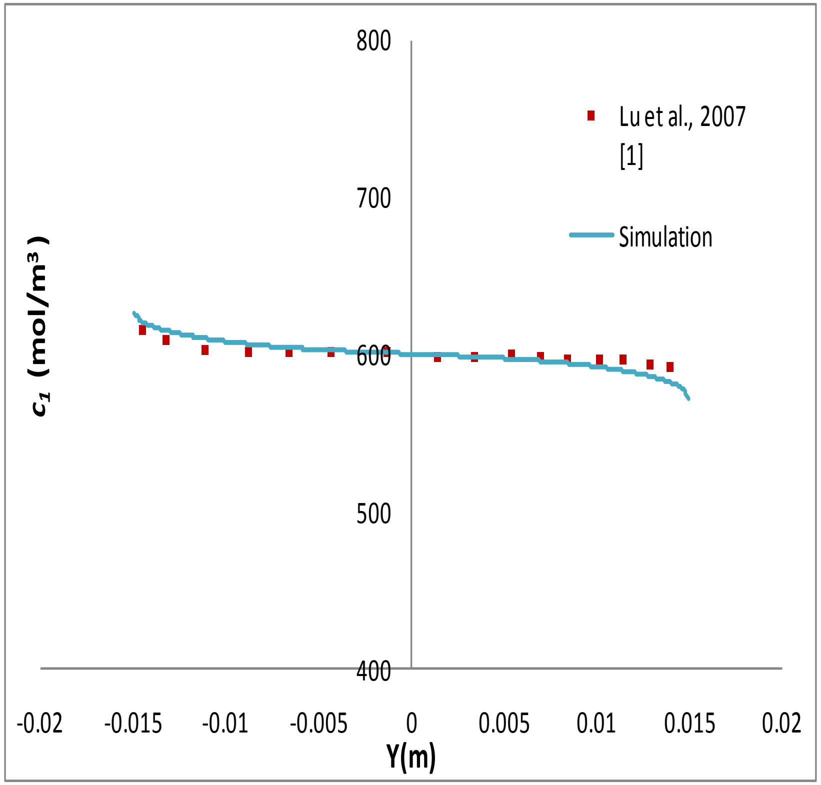


Concentration profile of species 1 at the outlet for i_o =10000A/m², u_o = 0.01m/s, c_o=600mol/m³

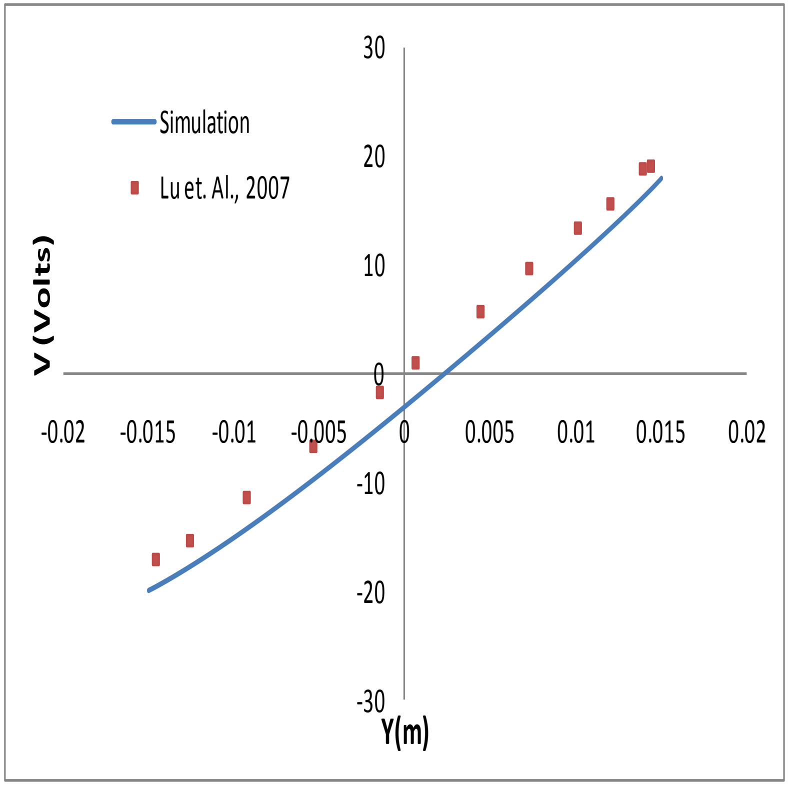
[1] Jun Lu, Dong-Jie Li, Li-Li Zhang, Yu-Xin Wang (2007). Numerical simulation of salt water electrolysis in parallel plate electrode channel under forced convection. Electrochimica Acta, 53 : 768–776.)

*[2] Pragati Shukla, K.K. Singh, P.K. Tewari, P.K. Gupta (2012). Numerical simulation of flow electrolysers: Effect of obstacles, Electrochimica Acta, **79**, 57–66)*

Validation of the Computational Approach

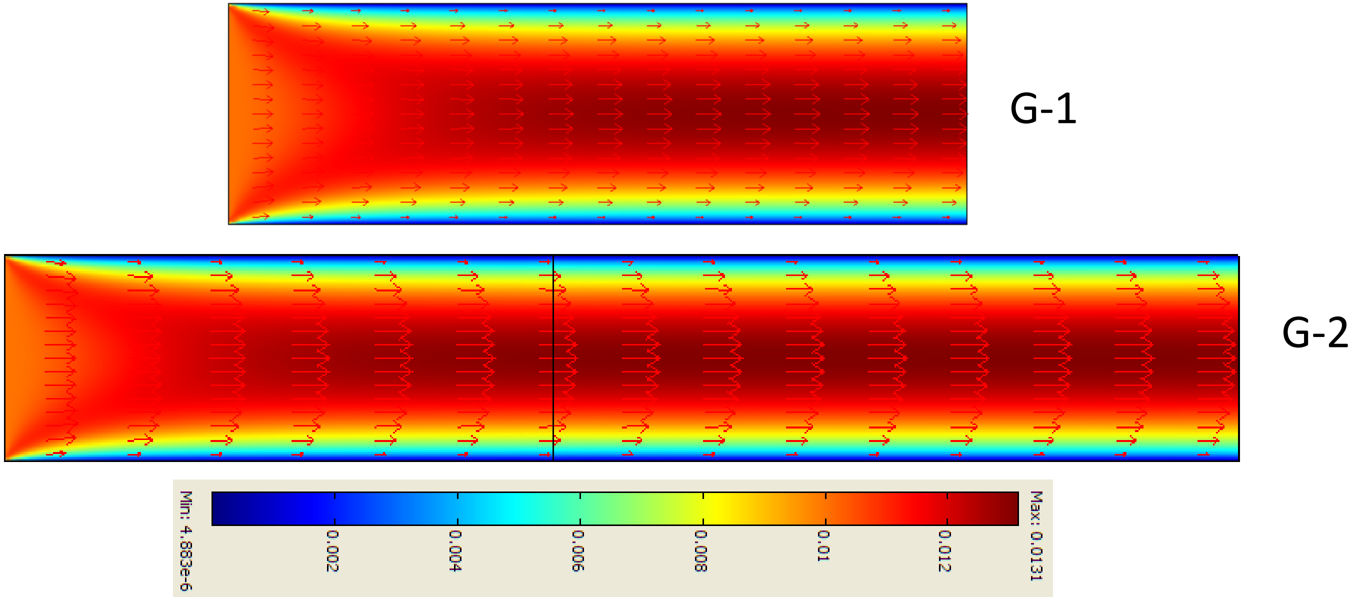


Concentration profile of species 1 at the outlet for u_o = 0.05 m/s, i_o = 10000 A/m^2, c_o = 600 mol/m^3



Potential profile at the outlet for u_o = 0.01m/s, i_o =10000 A/m^2, c_o = 600mol/m3

Effect of Inlet Channel Length



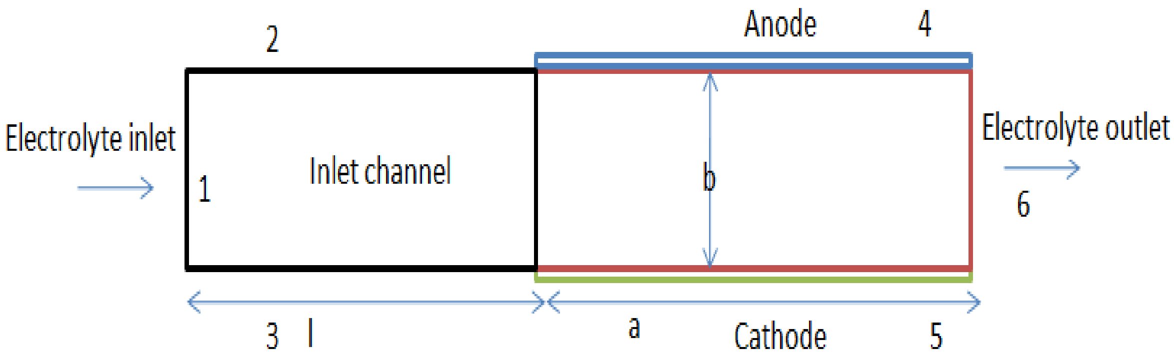
Velocity vector and velocity contours for geometries G-1 to G-2

Comparison of geometries with and without inlet channels

Geometry	**Current density for constant applied voltage**
	J (A/m^2)
G-1	6729.16
G-2	7067.30

Pragati Shukla, K.K. Singh, P.K. Tewari, P.K. Gupta, Numerical simulation of flow electrolysers: Effect of obstacles, Electrochimica Acta, ***79****, 57–66 (2012)*

Effect of Inlet Channel Length



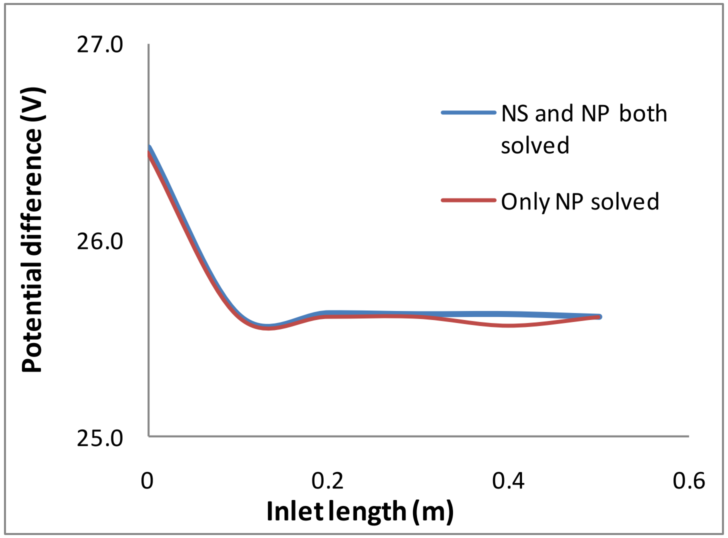
$2Cl^{-} \rightarrow Cl_2 \uparrow +2e^{-}$ (Anodic reaction)

$Na^{+} + e^{-} \rightarrow Na$ (Cathodic reaction)

Range of parameters-

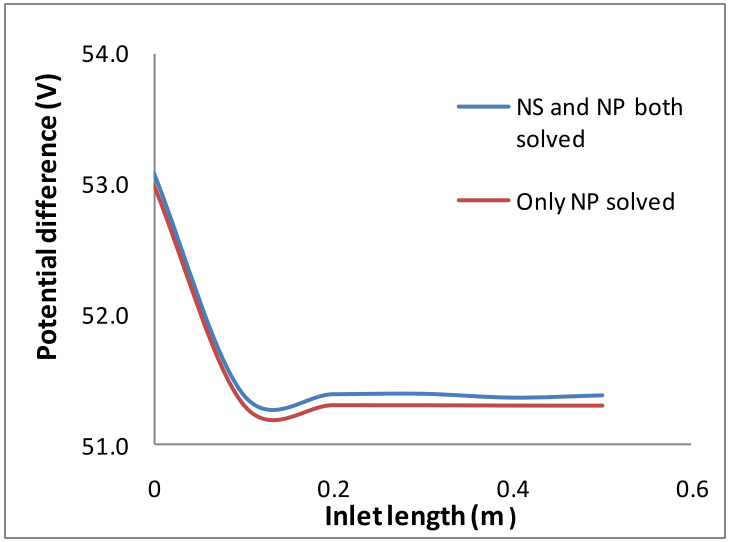
- Two charged species- (Na+ and Cl)
- Current density- (2000 - 10,000A/m^2)
- Base case- No inlet channel.
- Inlet length-(20% to 100% of electrode length)
- Inlet flow velocity -0.03 m/s
- Initial electrolyte concentration -600 mol/m^3

Effect of Inlet Channel Length



2,000 A/ m^2

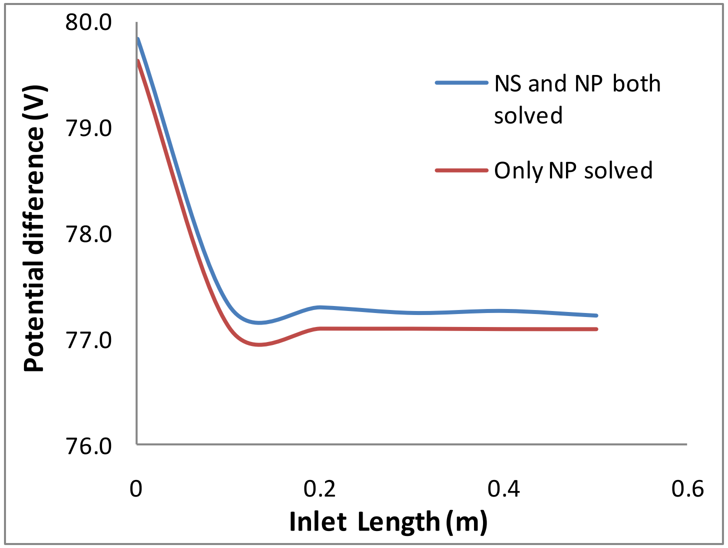
Potential Vs Inlet length Plots



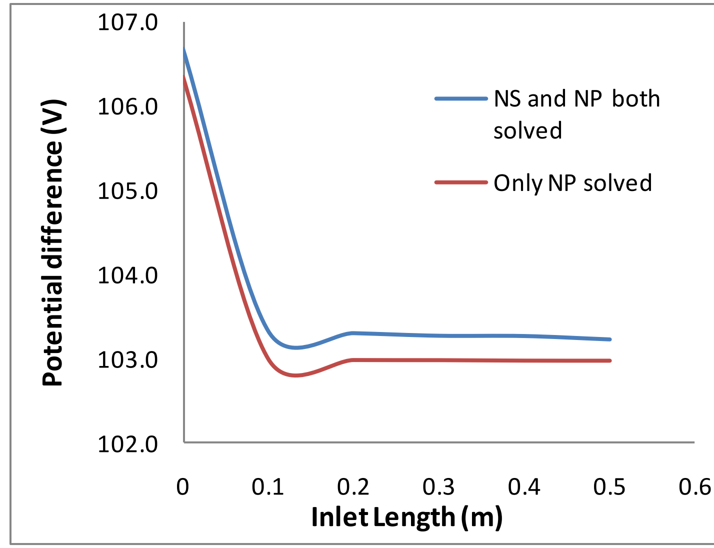
4,000 A /m^2

Effect of Inlet Channel Length

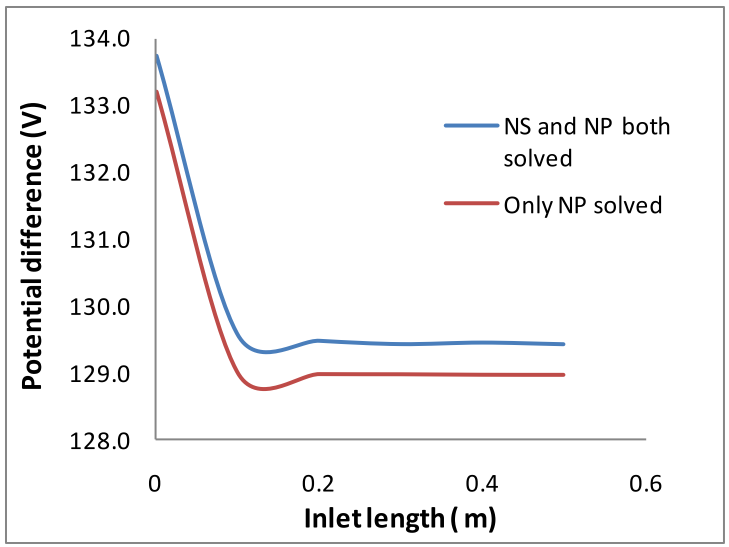
Potential Vs Inlet length Plots



6,000 A/m^2

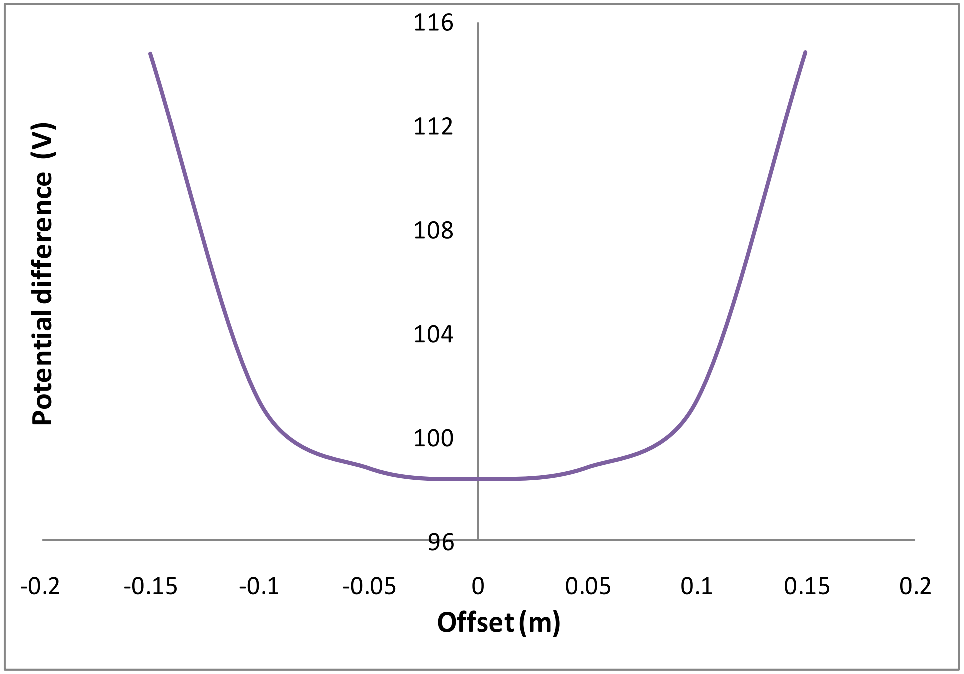


10,000 A/m^2



8,000 A/m^2

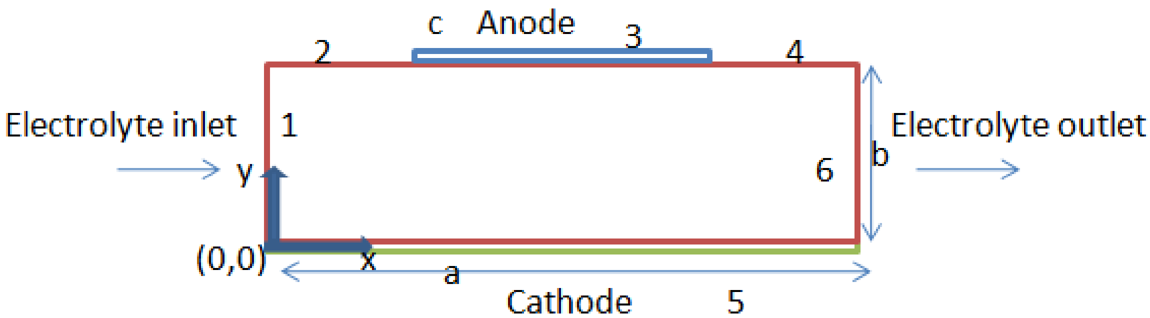
Effect of Offset between Anode and Cathode

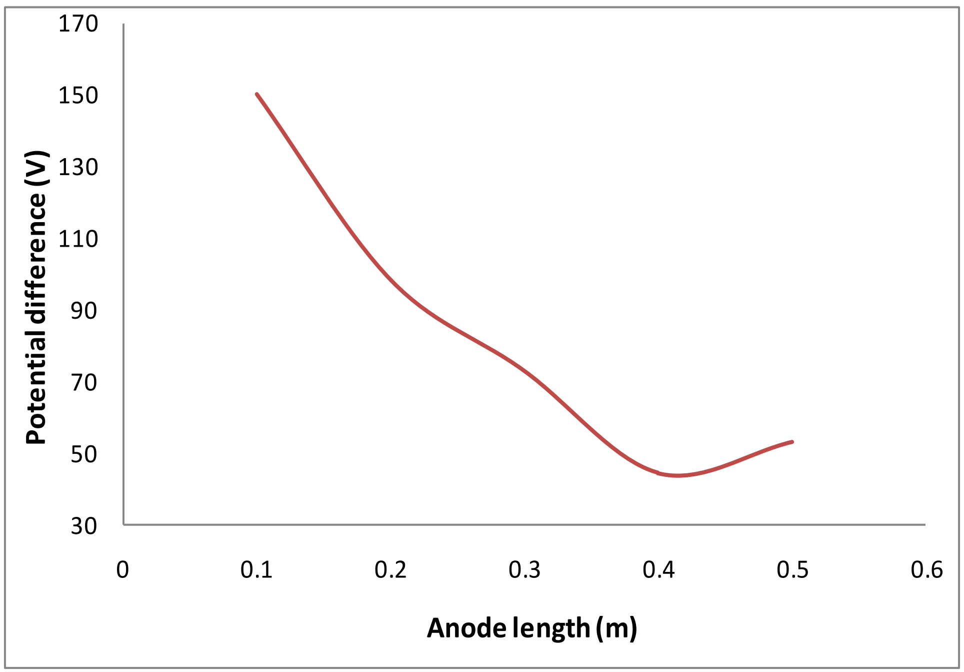


Effect of providing offset between the location of anode and cathode at current density 10,000 A/m^2

- anode length 20 cm and cathode length 50 cm.
- No inlet channel
- As expected, as the offset increases the potential difference across the electrode increases for a given current density.
- It is therefore better to design an electolyser in which anode and cathode are of different length such that the offset between the anode and cathode is kept minimum.

Effect of Size of Anode



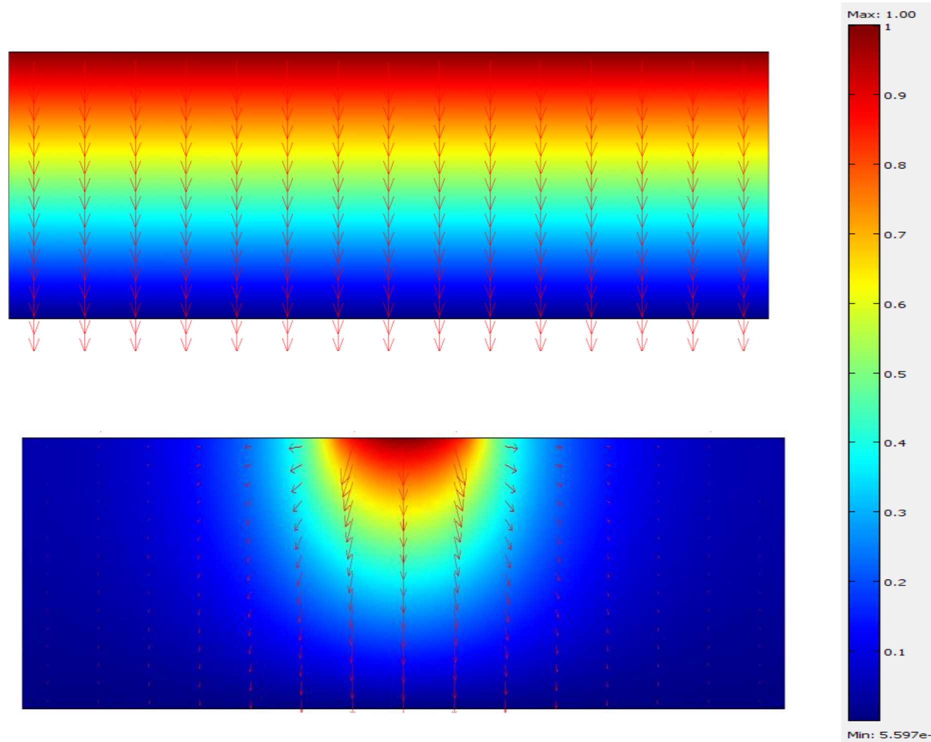


Effect of varying anode length on potential difference at current at current 2000 A

- Constant total current 2000A.
- The offset between the anode and cathode is zero for these simulations.
- As the length of anode reduces , the potential difference between the electrode increases

Effect of Size of Anode

Surface normalized potential and current density vector plots for anode of 50 cm lengths at current 2000 A



Surface normalized potential and current density vector plots for anode of 10cm lengths at current 2000 A

Conclusions

- The simulations reported in this work provide useful insights into how the performance of a flow electrolyser is affected when certain geometric parameters namely inlet channel length, offset between anode and cathode and the length of anode are changed.

- The results also show that providing an inlet channel having length about 20-30% of electrode length improves the performance of electroneutral bulk.

- Results show that providing offset, increases the potential drop for same applied current and hence leads to inefficient electroneutral bulk.

- Simulations also show that as length of one of the electrode reduces, keeping the current same, performance of electroneutral bulk degrades.

- These multiphysics simulations also highlight that it is important to consider both Nernst -Planck and Navier Stokes equations while simulating electroneutral bulk of a flow electrolyser.

THANKS
FOR YOUR ATTENTION!

QUESTIONS, COMMENTS?