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Modeling of Electrochemical Reduction of CO_2 to Methanol in a Micro Flow Cell

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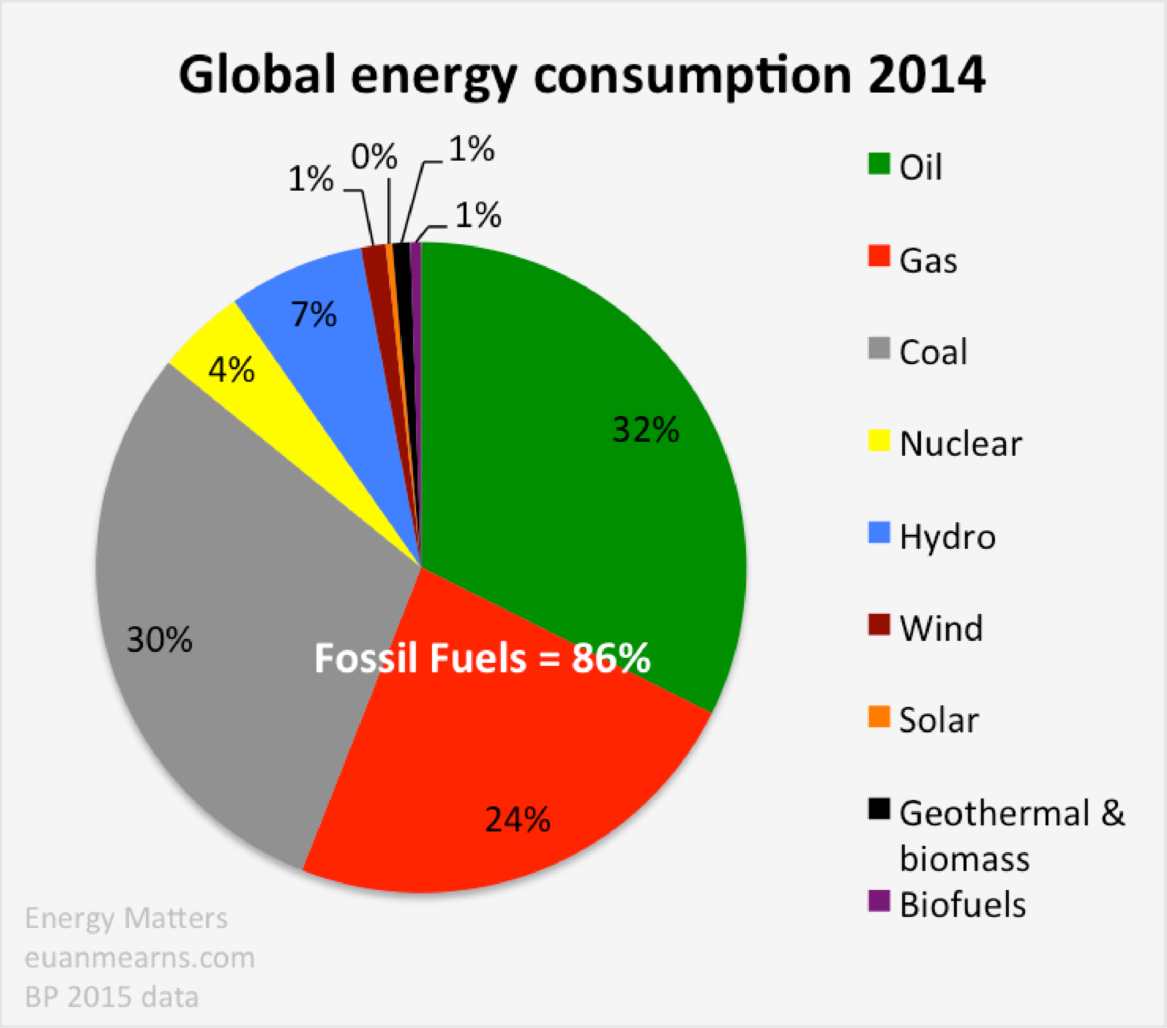
Introduction

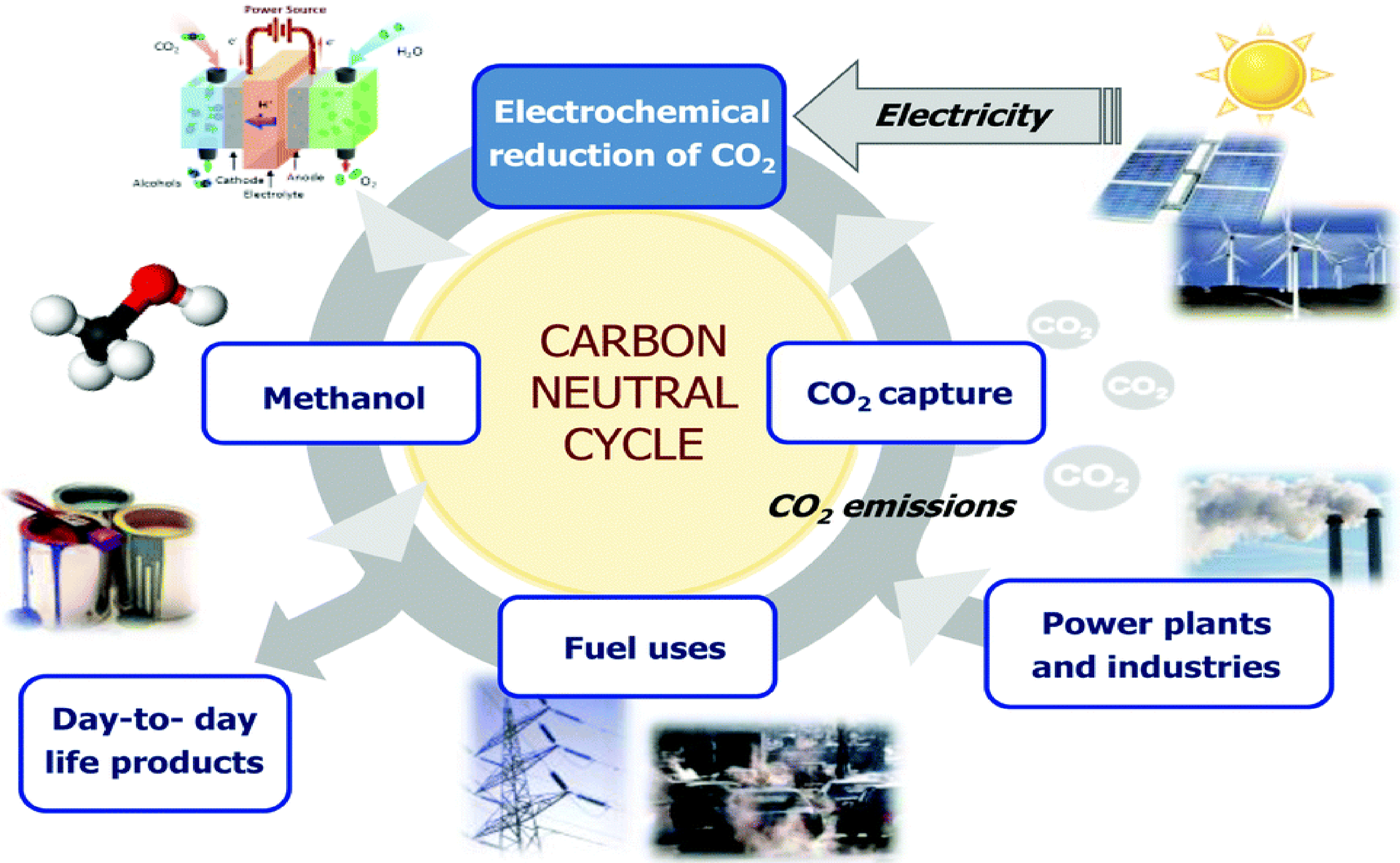
- Fossil fuels depleted at a rate of 4 billion tons a year
- CO_2 levels spiked up from 280 ppm to 400 ppm nowadays
- To reduce climate change effect: decrease the CO_2 emissions by 50% by 2050!



Global Energy Consumption (BP, 2015)

Introduction

- Methanol Based Economy



The methanol-based economy cycle model (J.Albo, M. Alvarez-Guerra, P. Castaño and A. Irabien, 2015)

Scope of Work

1- An electrochemical micro flow cell of CO_2 reduction to methanol modeled using COMSOL Multiphysics

2- Model validated against experimental data

3- Model used to determine different operating conditions effects and optimize the cell performance

Schematic of Cell and Reactions

Cathode

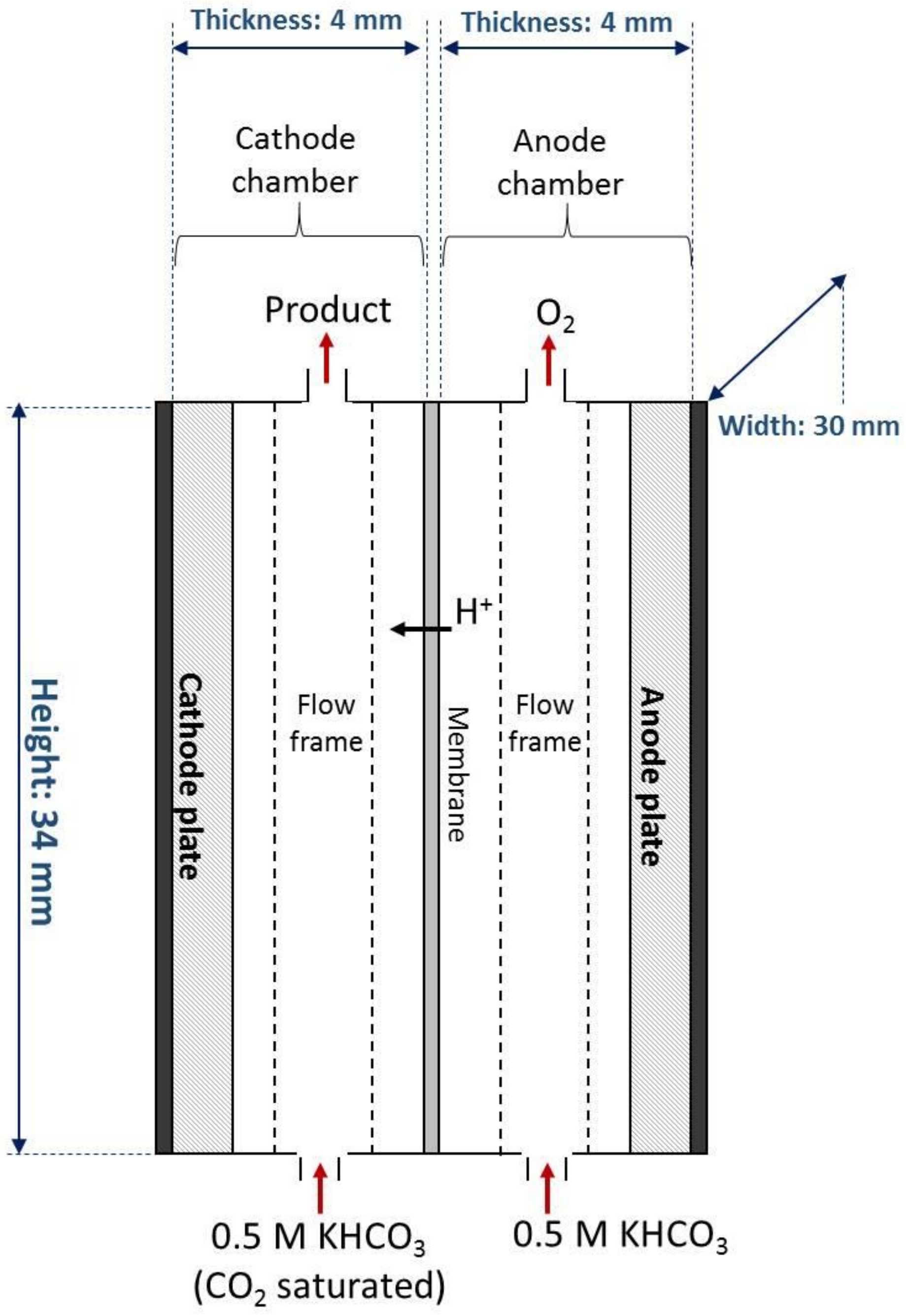
$$CO_2 + 6H^+ + 6e^- \rightleftarrows CH_3OH + H_2O$$

$$CO_2 + 2H^+ + 2e^- \rightleftarrows CO + H_2O$$

$$2H^+ + 2e^- \rightleftarrows H_2$$

Anode

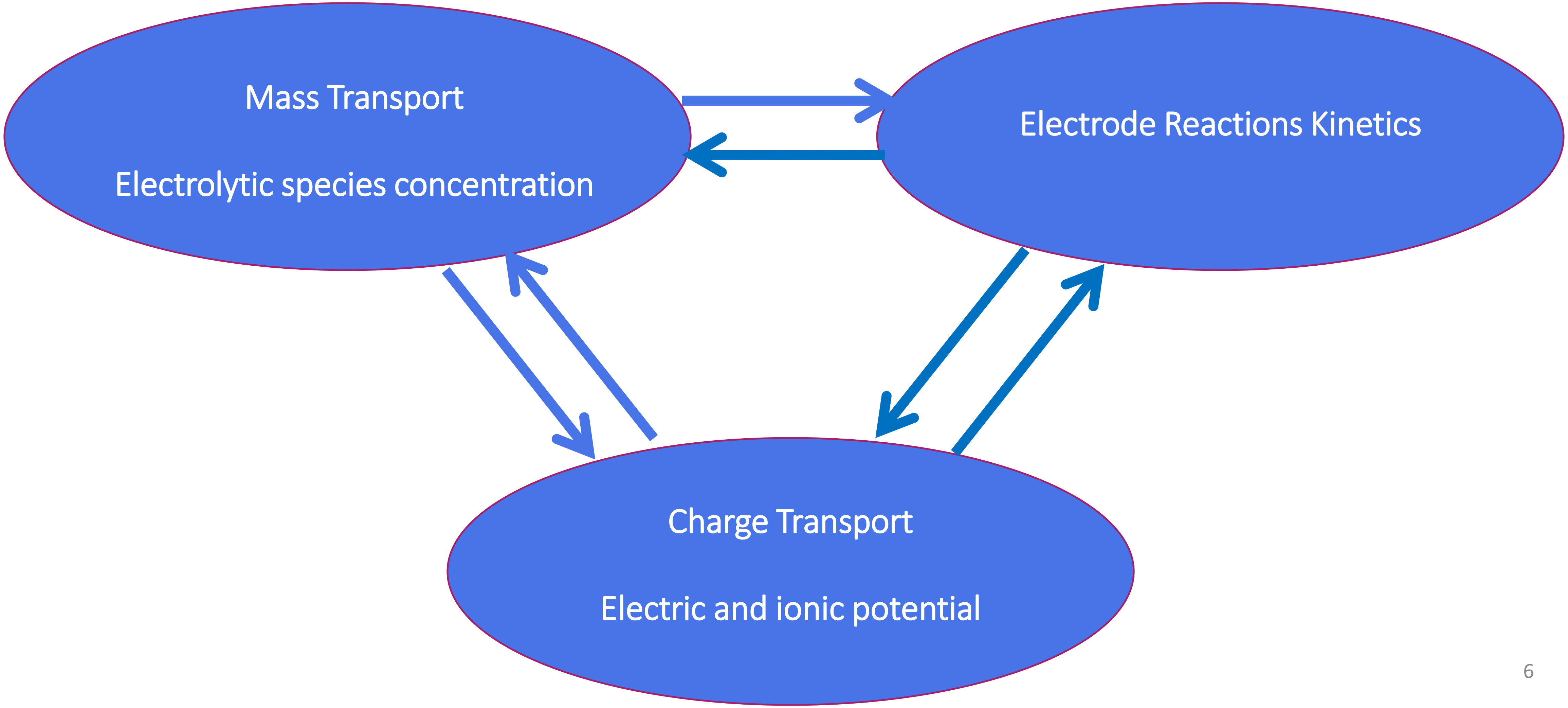
$$5H_2O \rightleftarrows 2.5\ O_2 + 10H^+ + 10e^-$$



Cell configuration and geometry

Methodology

Physical interactions inside the cell



Methodology

Governing Equations

$n. \, i_{l,e} = n. \, i_{l,m}$

$n. \, N_{H+,e} = n. \, \frac{i_{l,m}}{F}$

$\Phi_{l,m} = \Phi_{l,e} + \frac{RT}{F} \ln \frac{aH^{+}{,m}}{aH^{+}{,e}}$

$n. \, i_{l,e} = n. \, i_{l,m}$

$n. \, N_{H+,e} = n. \, \frac{i_{l,m}}{F}$

$\Phi_{l,m} = \Phi_{l,e} - \frac{RT}{F} \ln \frac{aH^{+}{,m}}{aH^{+}{,e}}$

$R_{i,src} = \frac{\nu_i \, i_{loc}}{n_i \, F}$

Catholyte

For: H^+, CO_2, OH^-, K^+, HCO_3^-, CO_3^{2-}, H_2, CH_3OH, CO

$\nabla N_i = R_{i,src}$

$\nabla i_l = F \sum z_i R_{i,src}$

$\sum z_i c_i = 0$

Membrane

H^+

$-\nabla (i_{l,m}) = 0$

Anolyte

For: H^+, CO_2, OH^-, K^+, HCO_3^-, CO_3^{2-}, O_2

$\nabla N_i = R_{i,src}$

$\nabla i_l = F \sum z_i R_{i,src}$

$\sum z_i c_i = 0$

$R_{i,src} = \frac{\nu_i \, i_{loc}}{n_i \, F}$

Methodology
Electrochemical Reaction Kinetics

Cathode	Anode
Methanol and Carbon monoxide reactions $i_{loc}=i_0[C_R\exp(\frac{\alpha_a F \eta}{RT})-C_O\exp(\frac{-\alpha_c F \eta}{RT})]$	OER $i_{loc}= i_0(\frac{(\alpha_a+\alpha_c)F}{RT})\eta$
HER $i_{loc}= i_0(\frac{(\alpha_a+\alpha_c)F}{RT})\eta$	

COMSOL Implementation

- **Module**

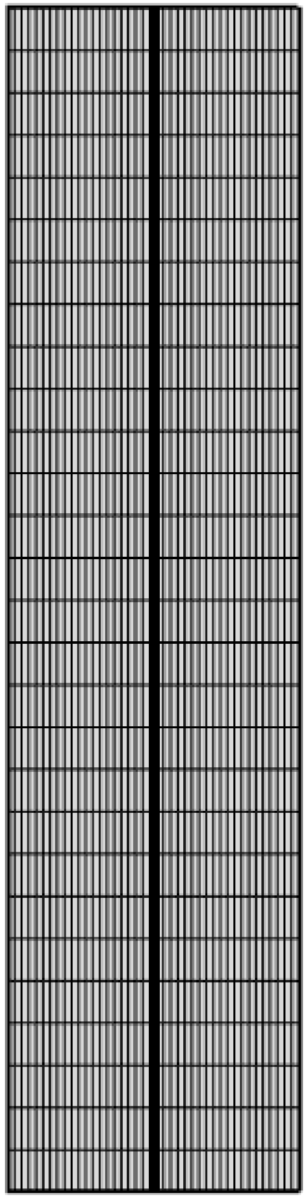
Electrochemistry

- **Interfaces**

Tertiary current distribution for electrolytes channels
Secondary current distribution for membrane

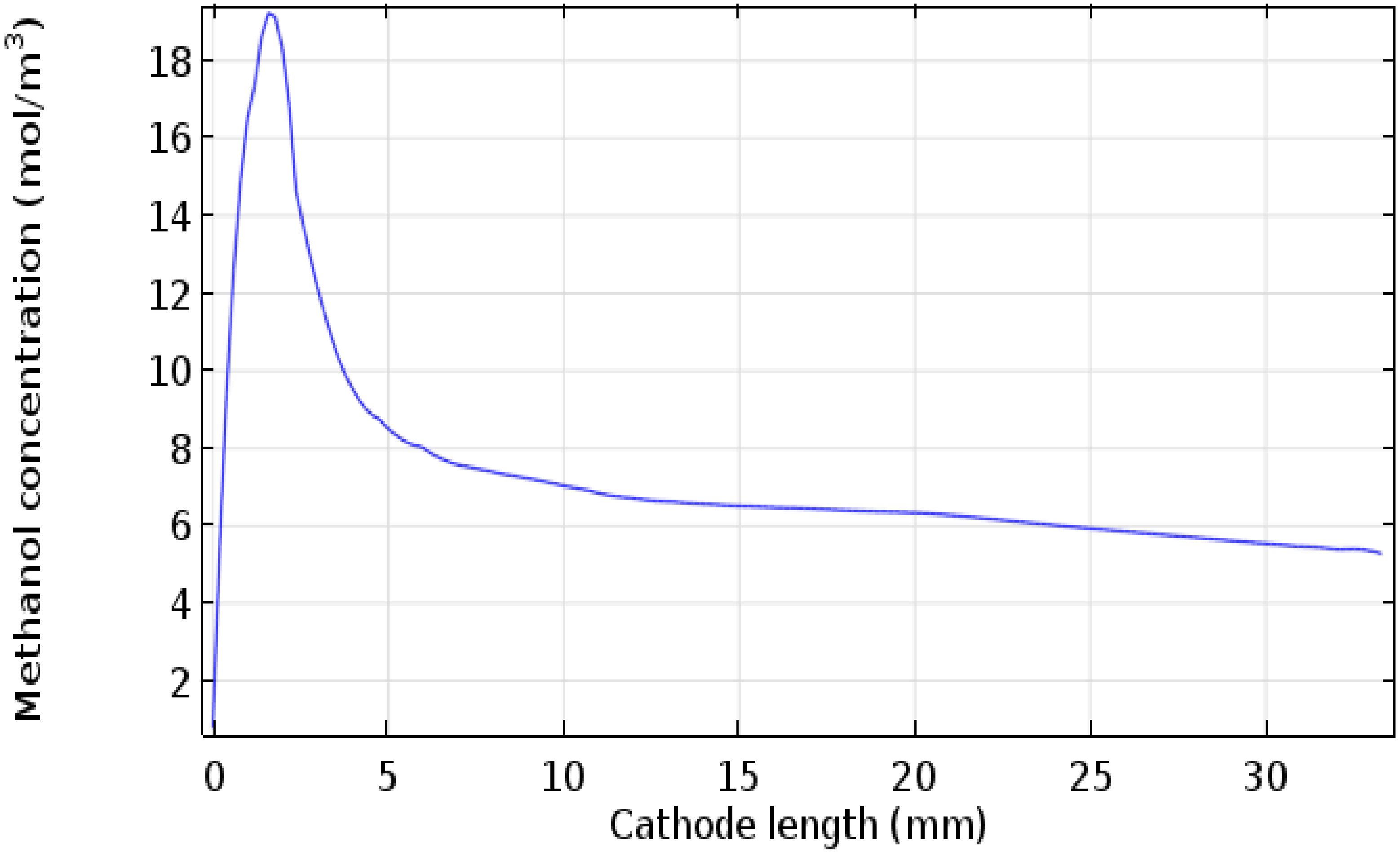
- **Mesh**

User controlled mesh (Mapped Distribution)



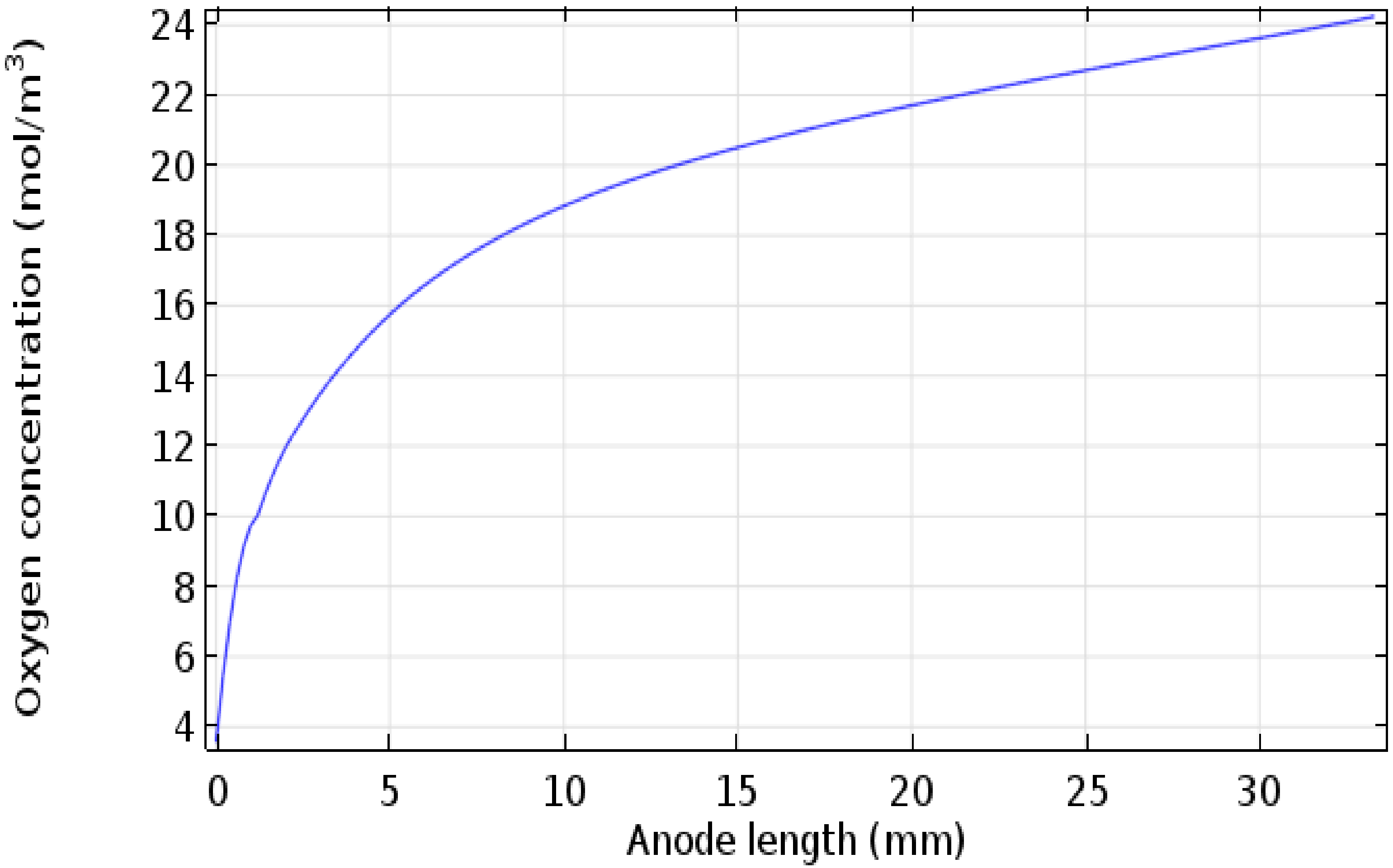
Results and Discussion

- Base Case



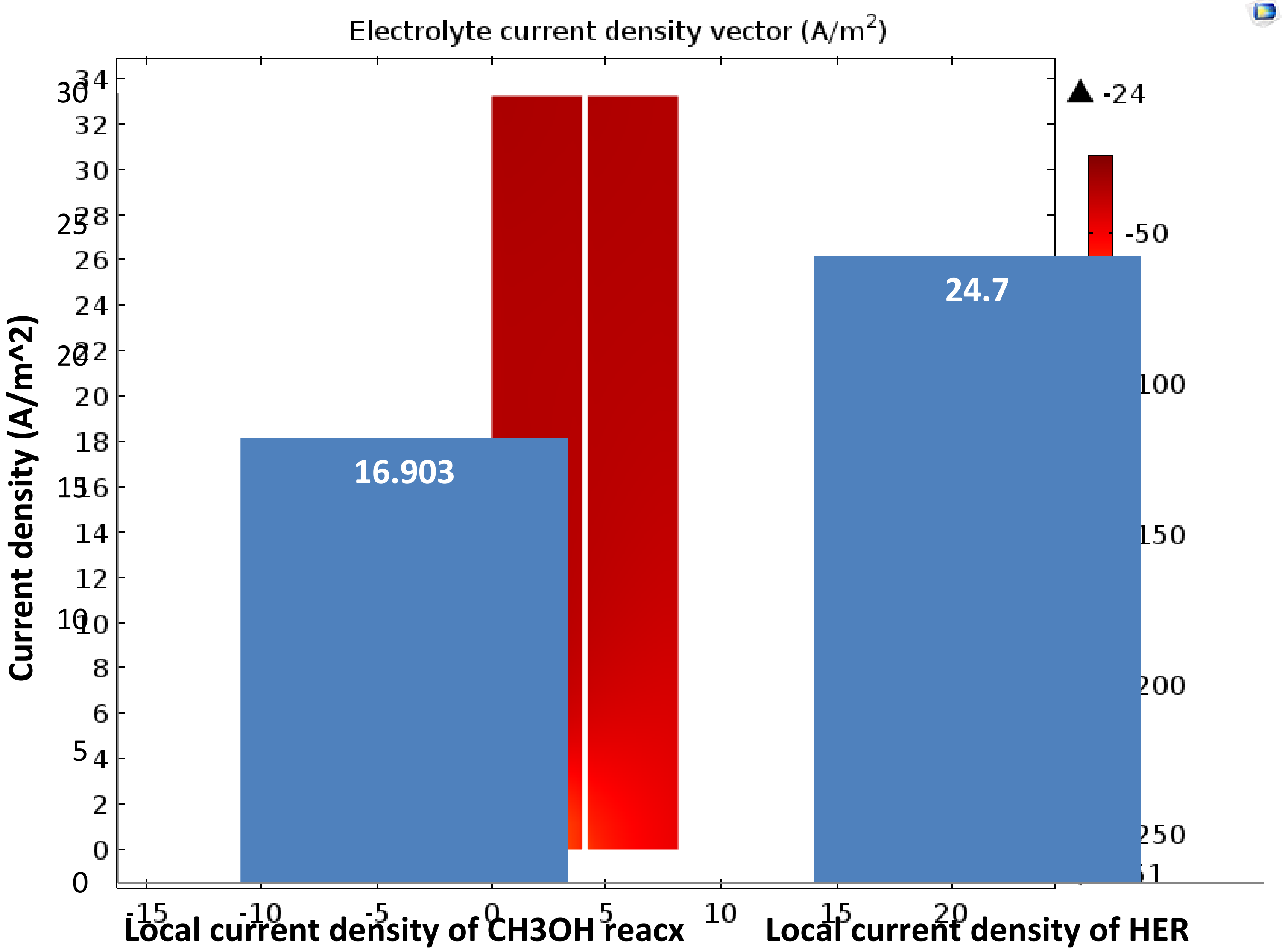
Results and Discussion

- Base Case



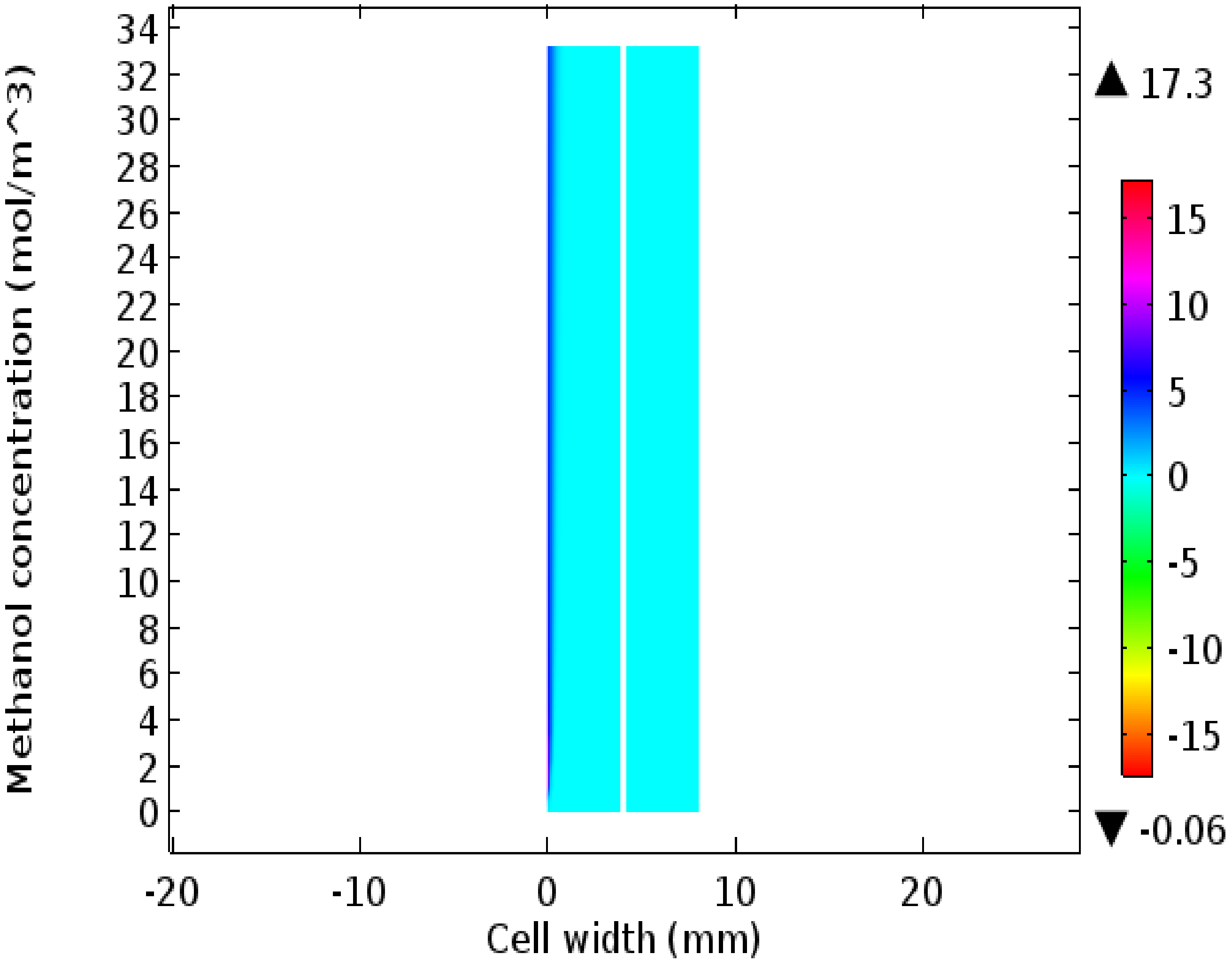
Results and Discussion

- Base Case



Results and Discussion

- Methanol Flow Behavior

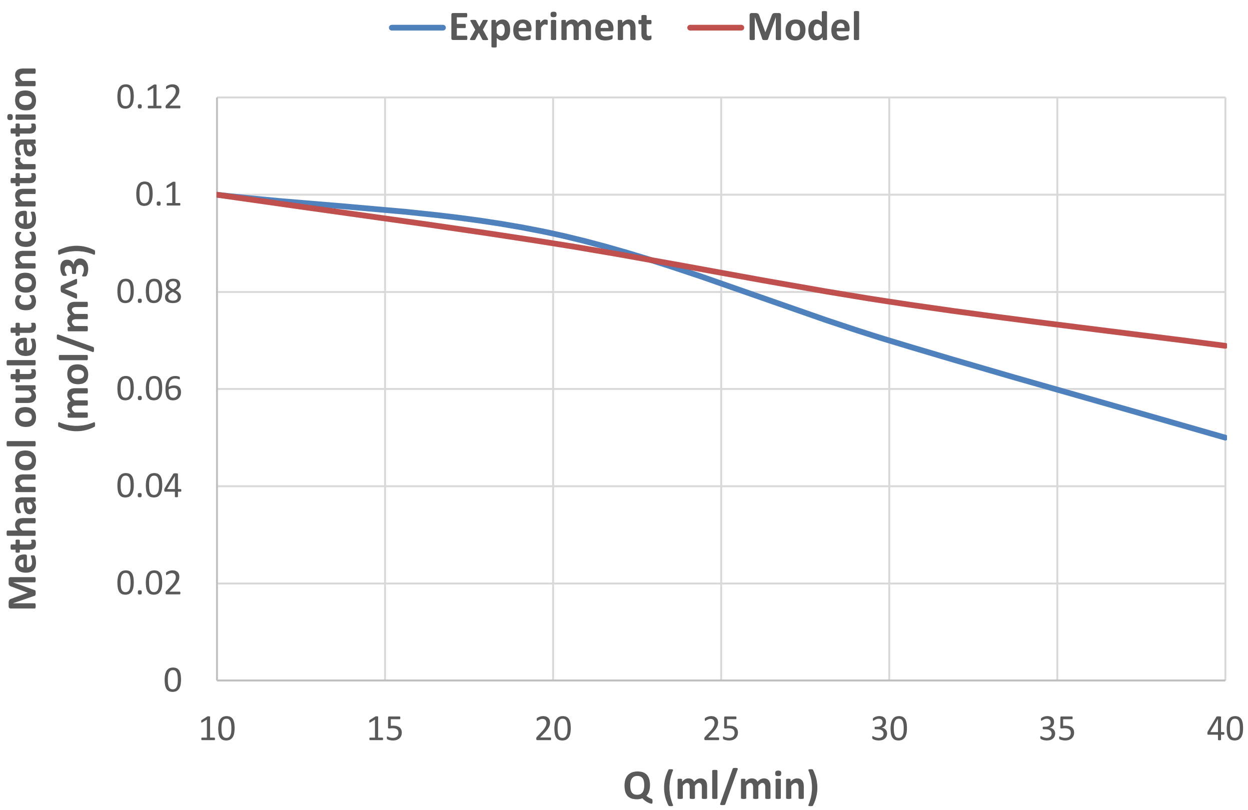


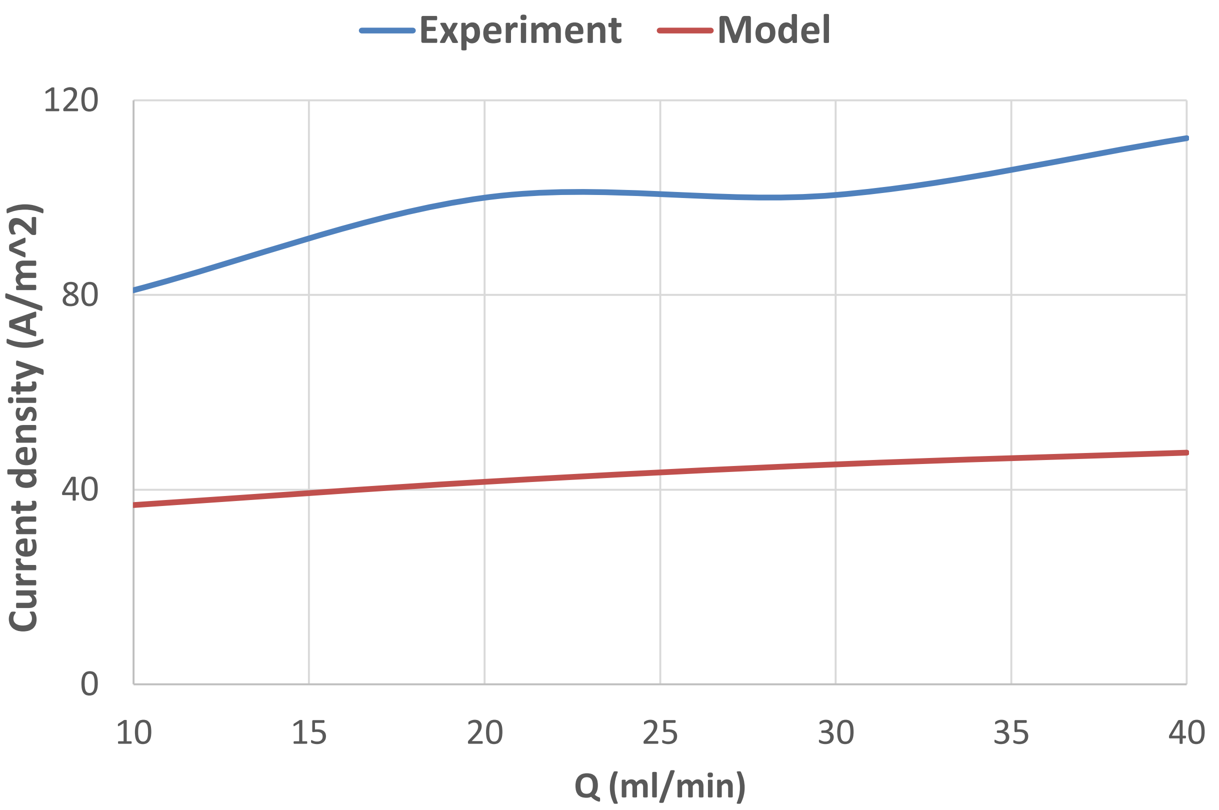
Methanol convective flux is 100 times its diffusive flux

Reconsidering membrane function in the cell

Model Validation

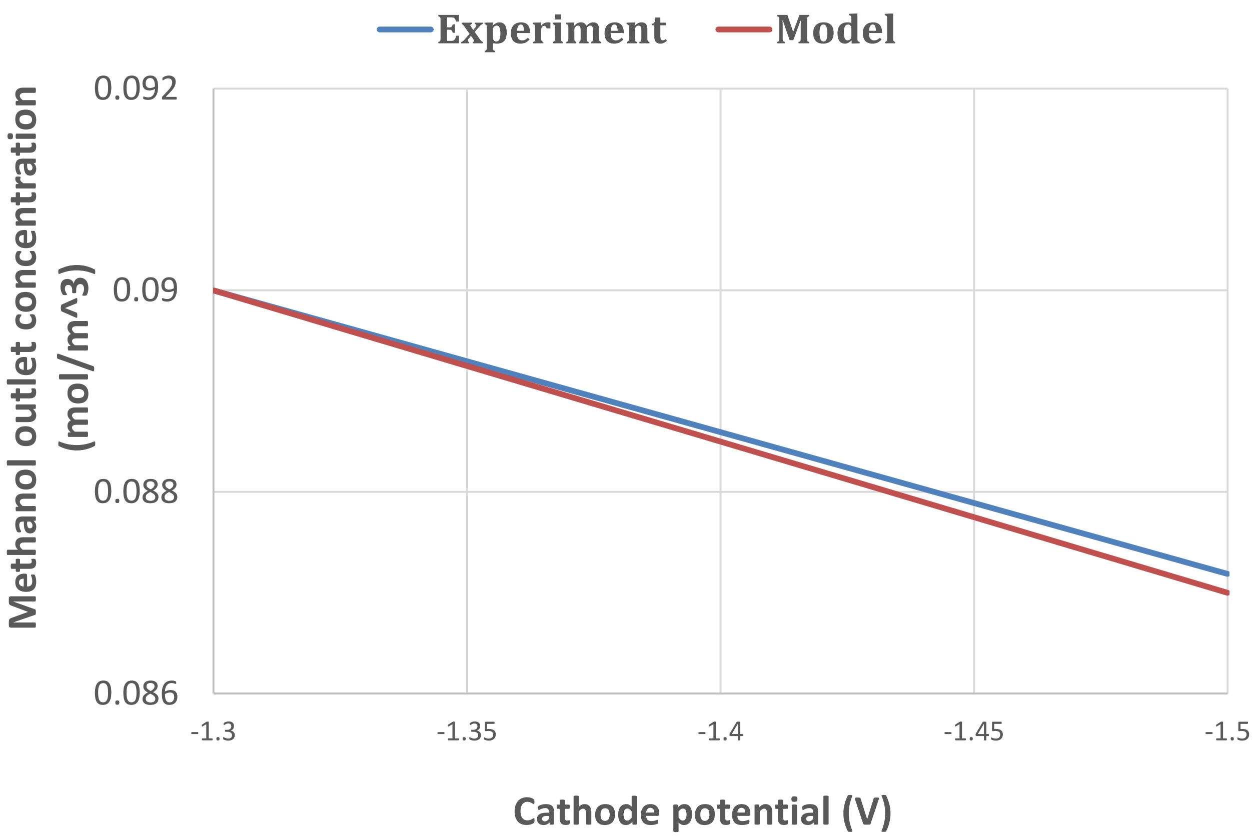
Flowrate Effect

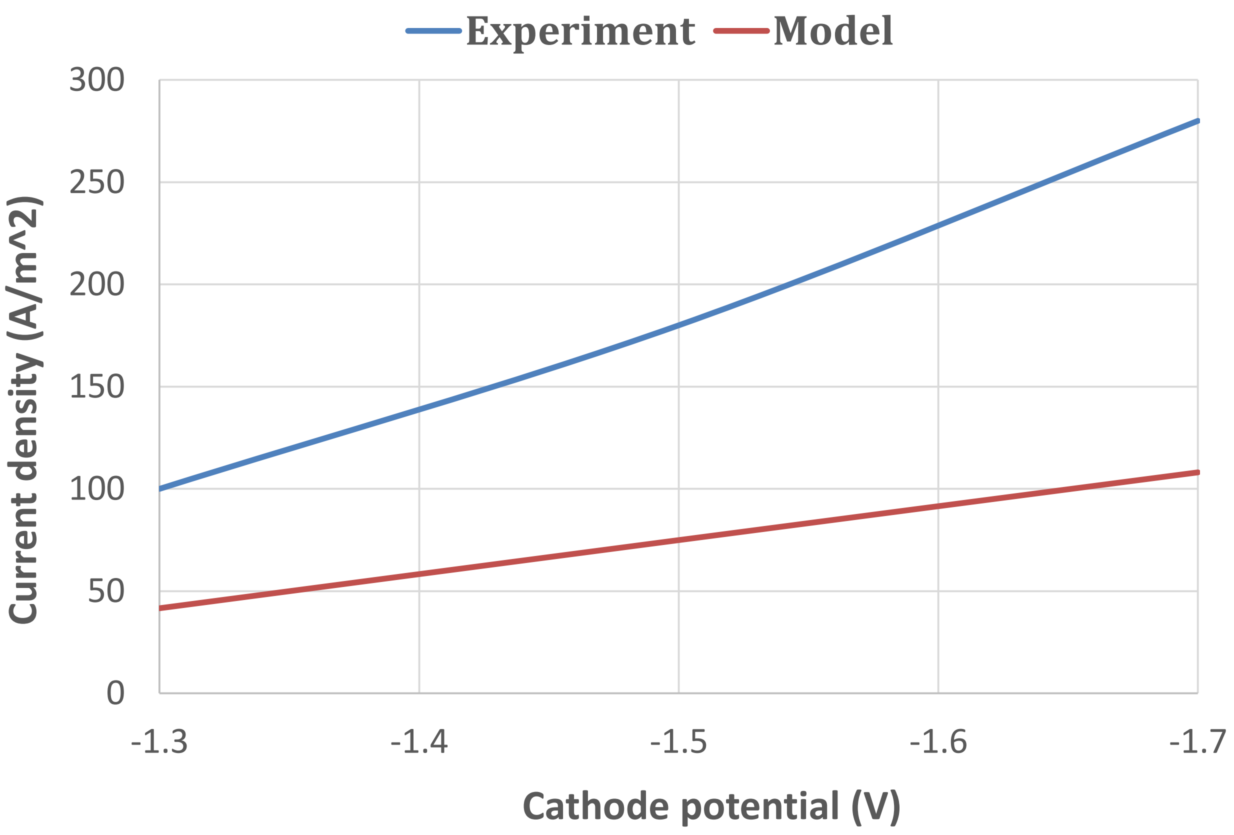




Model Validation

Applied Cathode Potential Effect





Conclusions and Next Steps

- Model showed good agreement with the experimental results
- Other by products reactions to be added at the cathode → decrease the discrepancy in the current density values
- As the model predicted, preliminary experimental results without the membrane proved that the methanol outlet concentration is not greatly reduced → a more effective cell design will be adopted
- Further modeling and experimental studies →enhance process feasibility and decide on the optimum operating conditions
- Thorough thermodynamic analysis → investigate the whole process's energy efficiency and reduce the energy waste

Thank you for you attention!

Questions?