Electrical Field Effect on CO_2 Absorption and Chemisorption in a Rectangular Bubble Column by COMSOL MULTIPHYSICS

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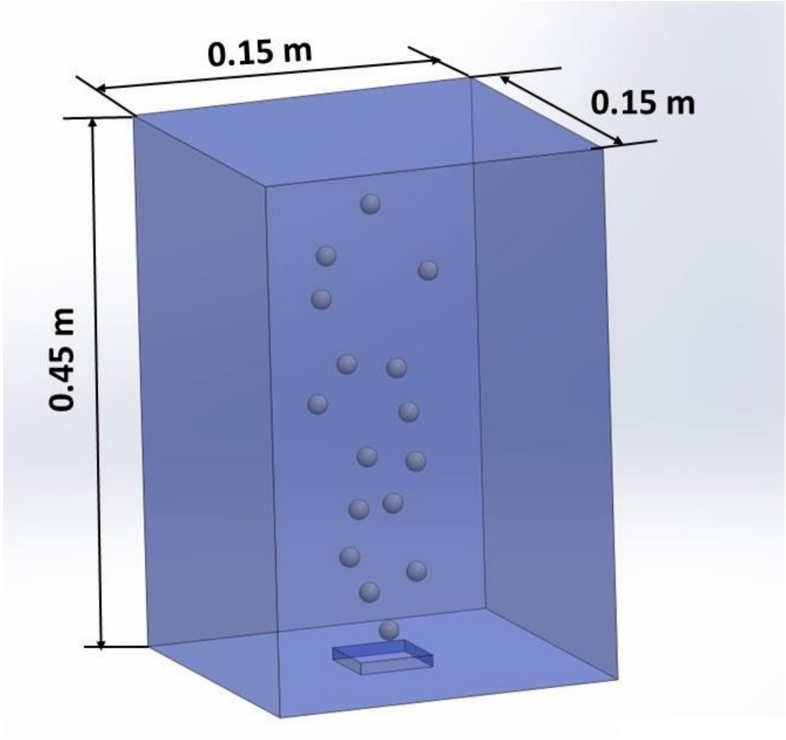
Outline

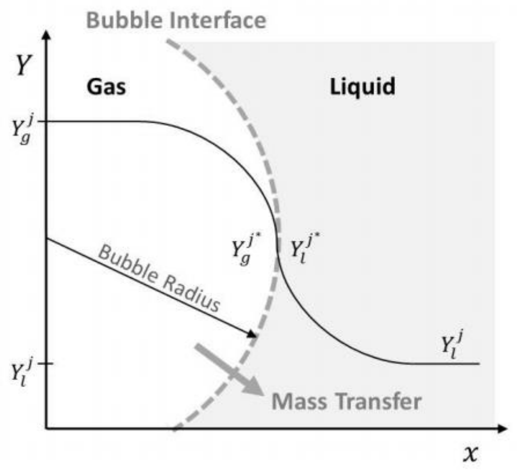
- Introduction
- CO_2 bubble column reaction
- Mathematical model
- Result and discussion
- Conclusion

Introduction

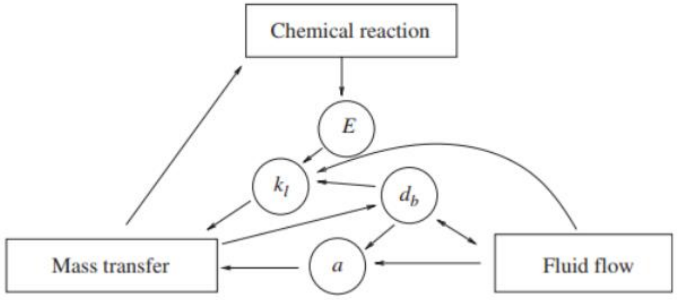
- Used in chemical, petrochemical and biological processes where mass transfer happen between gas and liquid interface
- Different intrinsic phenomena like hydrodynamic, absorption, reaction, coalescence happen in the system
- Commonly two model E-E and E-L model are used
- $\mathrm{OH^-}, \mathrm{CO_3^{2-}}, \mathrm{HCO_3^-}$ and $\mathrm{Na^+}$ or $\mathrm{K^+}$ ions are present
- In the presence of electric field these species are oriented towards one direction



Bubble column



Interface mass transfer



Inter-dependency diagram

- CO_2 gas convert into aqueous CO_2

$$CO_2(g) \rightarrow CO_2(aq)$$

- At higher pH CO_2 (aq) reactions

$$CO_2(aq) + OH^- \leftrightarrow HCO_3^-$$

$$HCO_3^- + OH^- \leftrightarrow CO_3^{2-} + H_2O$$

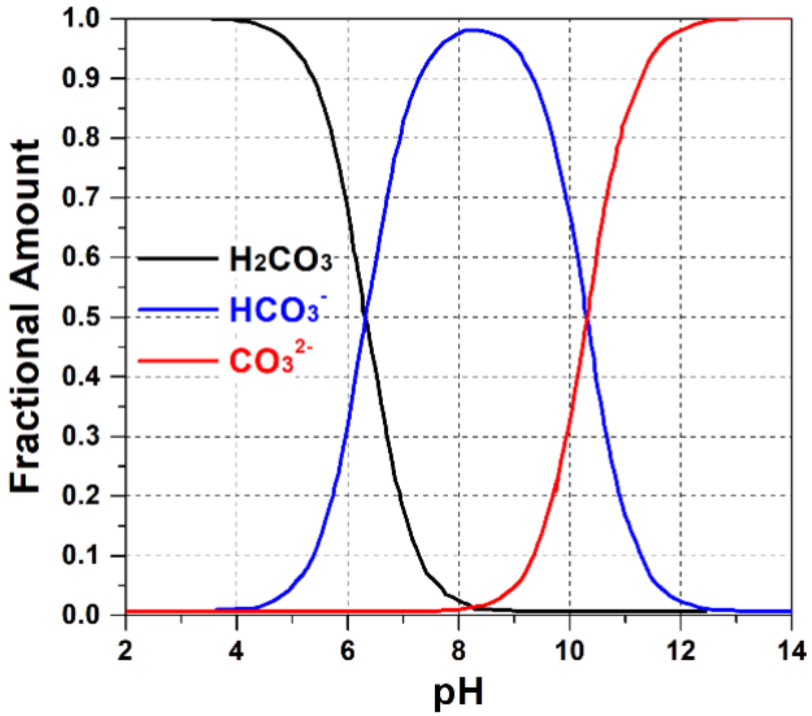
- Reaction rates

$$R_{1f} = k_{1f} c_{CO_2(aq)} c_{OH^-}$$

$$R_{1b} = k_{1b} c_{HCO_3^-}$$

$$R_{2f} = k_{2f} c_{HCO_3^-} c_{OH^-}$$

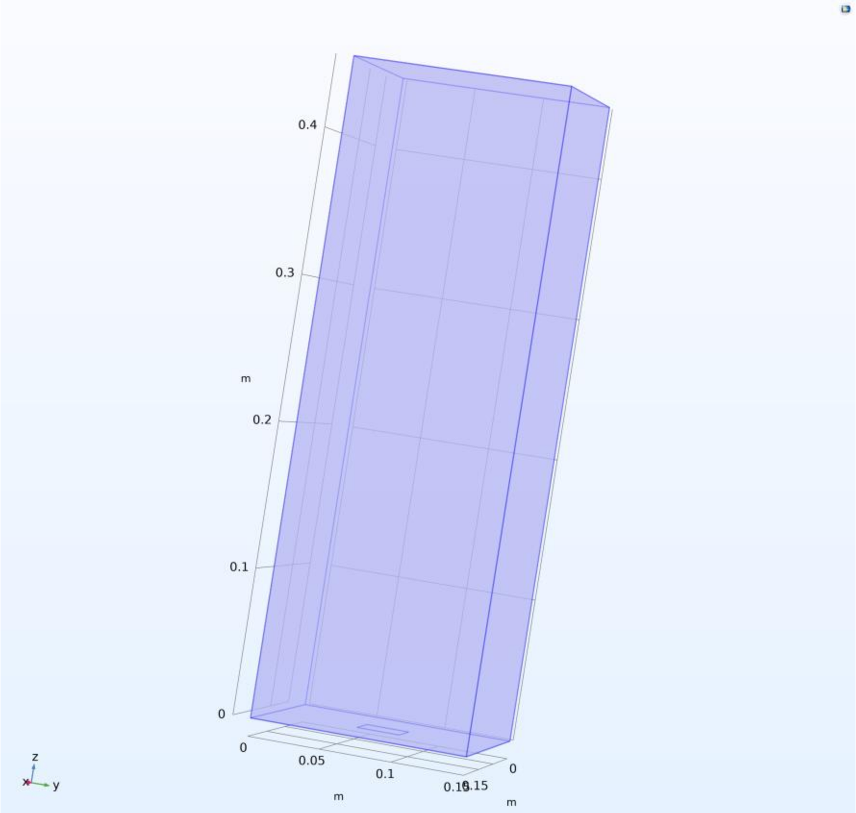
$$R_{2b} = k_{2b} c_{CO_3^{2-}}$$



Mole fraction of the three different carbonate forms

Modelling of the bubble column

- Assumption
  - Constant temperature, flux density, diffusivity and viscosity
  - Flow is laminar for both gas phase and liquid phase
  - No change in bubble diameter



Modelling

- COMSOL Multiphysics 6.1
  - Bubbly flow, laminar flow
  - Tertiary current distribution, Nernst-plank equation, electroneutrality
  - Transport of diluted species
- Momentum transport equation

$$\alpha_l\rho_l\frac{\partial u_l}{\partial t}+\alpha_l\rho_l(u_l.\nabla)u_l=-\nabla.\left[p+\alpha_l\mu_l\left(\nabla u_l+(\nabla u_l)^T-\frac{2}{3}(\nabla.u_l)I\right)\right]+\alpha_l\rho_l g+F$$

- Continuity equation

$$\frac{\partial}{\partial t}(\rho_l\alpha_l+\rho_g\alpha_g)+\nabla.(\rho_l\alpha_l u_l+\rho_g\alpha_g u_g)=0$$

- Mass transfer equation

$$\frac{\partial}{\partial t}(\rho_g\alpha_g)+\nabla.(\rho_g\alpha_g u_g)=-m_{gl},\ Where\ m_{gl}=k_l aE\rho_l(c_l-c_{CO_2})M_{CO_2}$$

Modelling

- Mass transport equation

$$\frac{\partial(\alpha_l c_i)}{\partial t} = -\nabla . N_i + \alpha_l S_i$$

$$N_i = -D_i \nabla c_i - \boxed{\frac{z_i D_i}{RT} F c_i \nabla \phi_l} + u_l c_i$$

- Electroneutrality

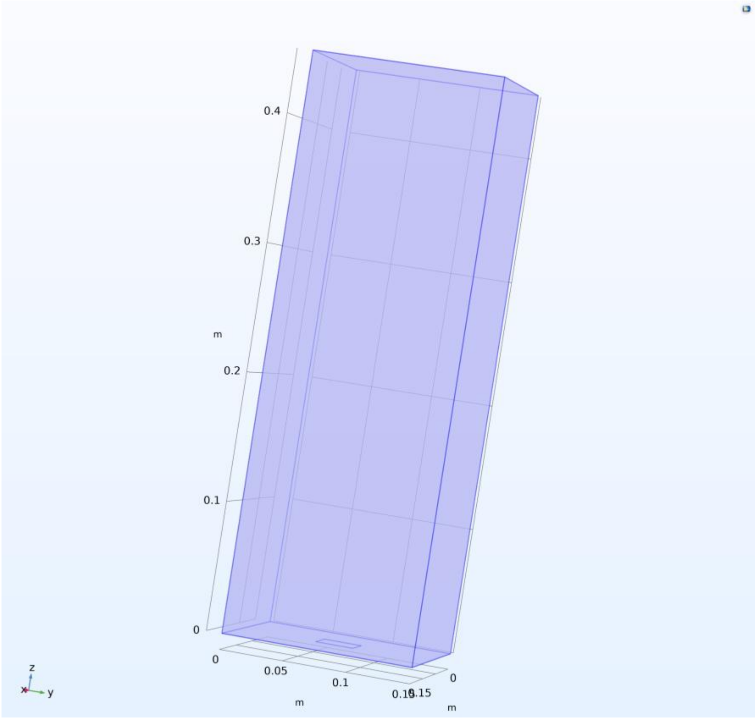
$$\sum z_i c_i = 0$$

$S_{CO_2(aq)}$	$\frac{m_{gl}}{M_{CO_2}} - R_{1f} + R_{1b}$
$S_{CO_3^{2-}}$	$R_{2f} - R_{2b}$
$S_{HCO_3^-}$	$R_{1f} - R_{1b} - R_{2f} + R_{2b}$
S_{OH^-}	$-R_{1f} + R_{1b} - R_{2f} + R_{2b}$

Boundary Conditions

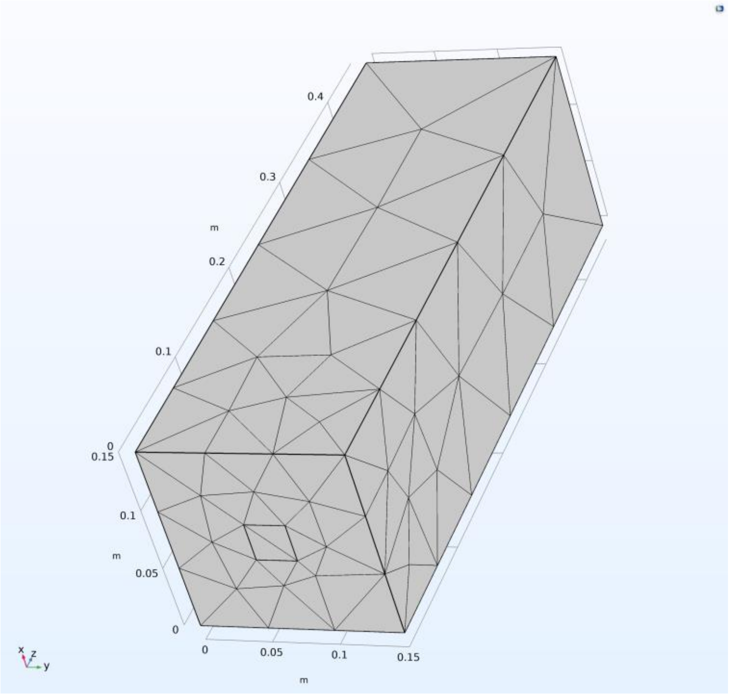
- The pressure at the top surface is 1 atm
- Gas outlet at the top of the column
- At the inlet gas velocity is 0.1125 m s^{-1}
- The potential is along y-axis
- No gas flow or liquid slip at the remaining walls

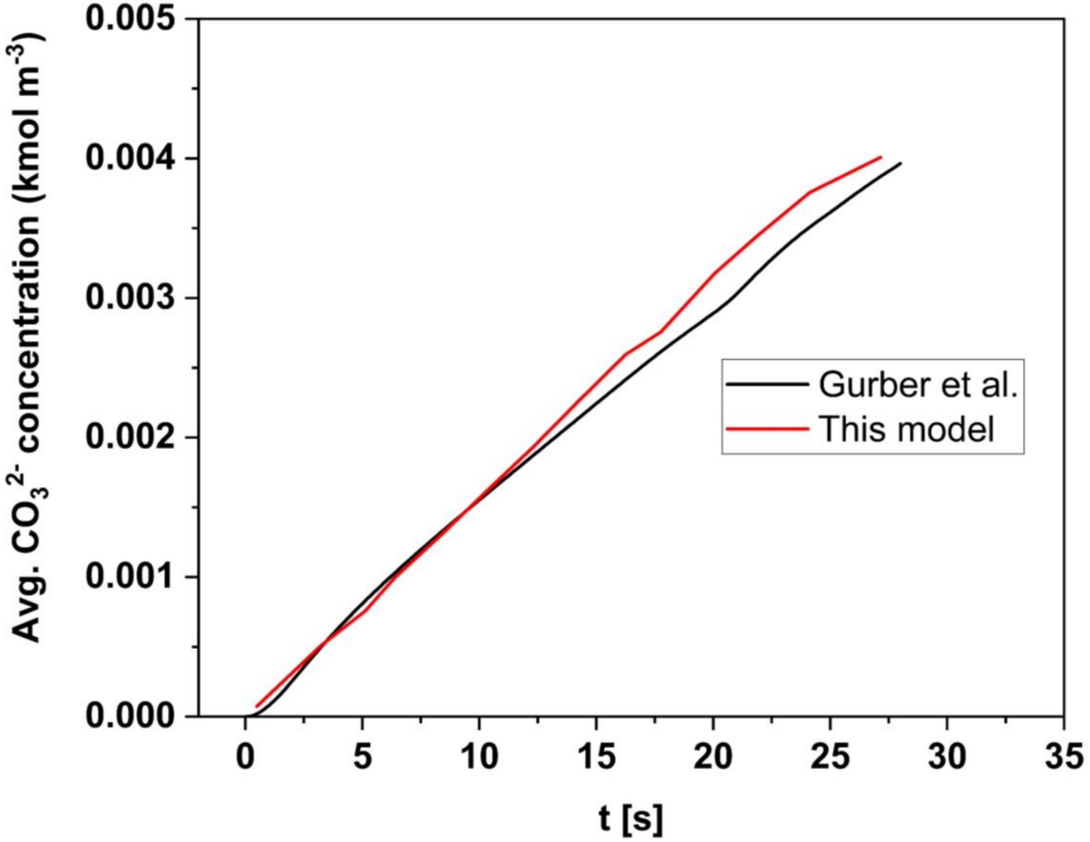
- Initial conditions
  - The pH of aqueous solution is 12
  - The pressure in the column is $-\rho_l g(z-h) + p_{ref}$
  - $c_{\mathrm{Na}^+} = c_{\mathrm{OH}^-} = 0.01\ \mathrm{M}$
  - All other species initial concentration is zero



Validation of the model

- COMSOL 6.1 used
- HCO_3^- ion concentration is calculated from electroneutrality condition
- Applied voltage is 0 V



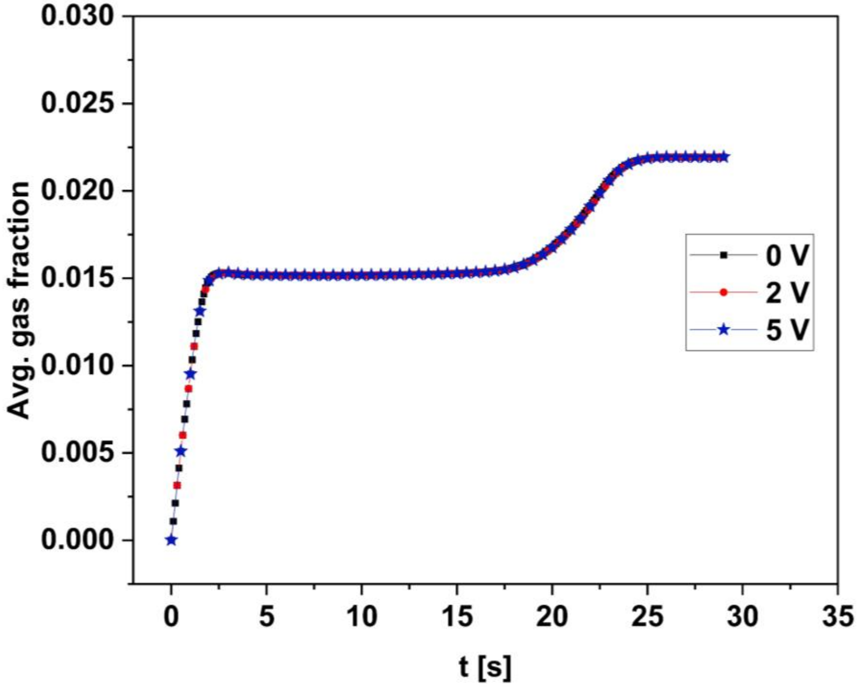


Avg. CO_3^{2-} ion concentration

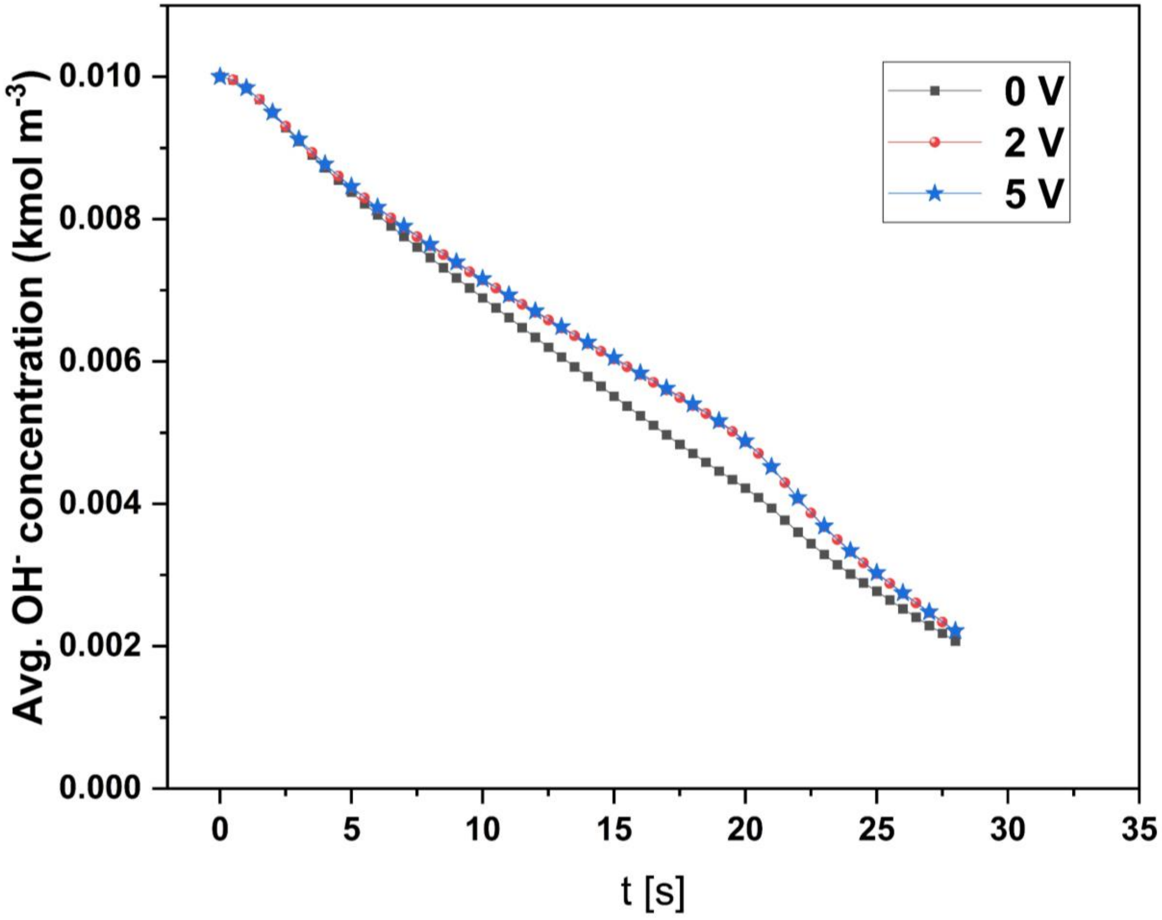
Gruber et al. (2015). *Chemical Engineering Science*, *137*, 188-204.

Physisorption

- Gas volume fraction is changing with applied voltage
- Mass transfer rate: $2.1310 \times 10^{-4}\ \mathrm{m\ s^{-1}}$

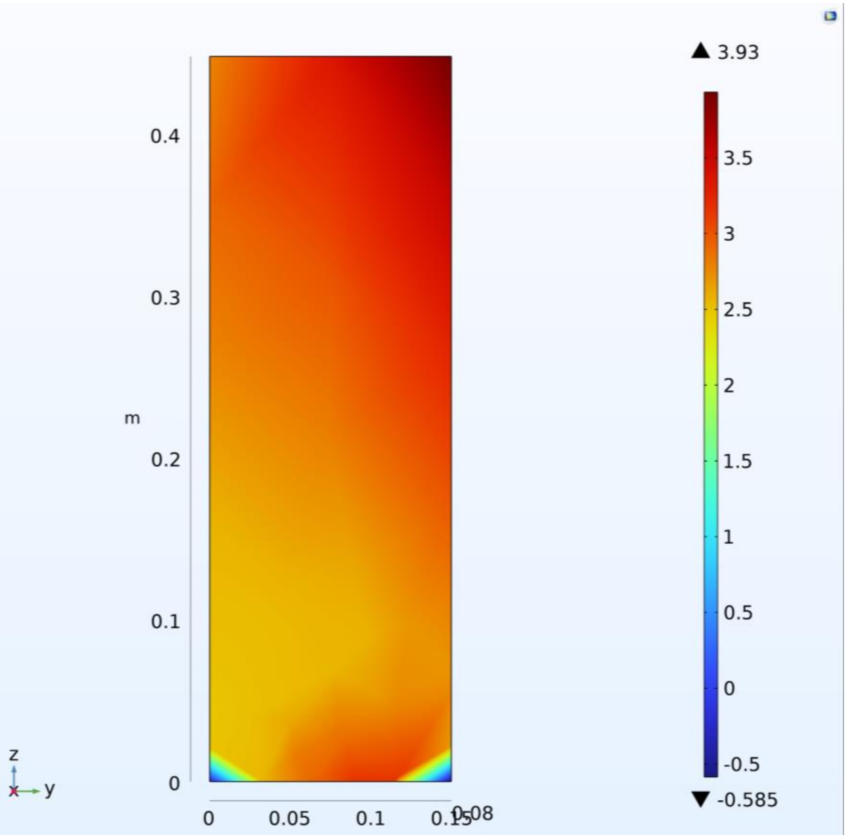


Gas volume fraction

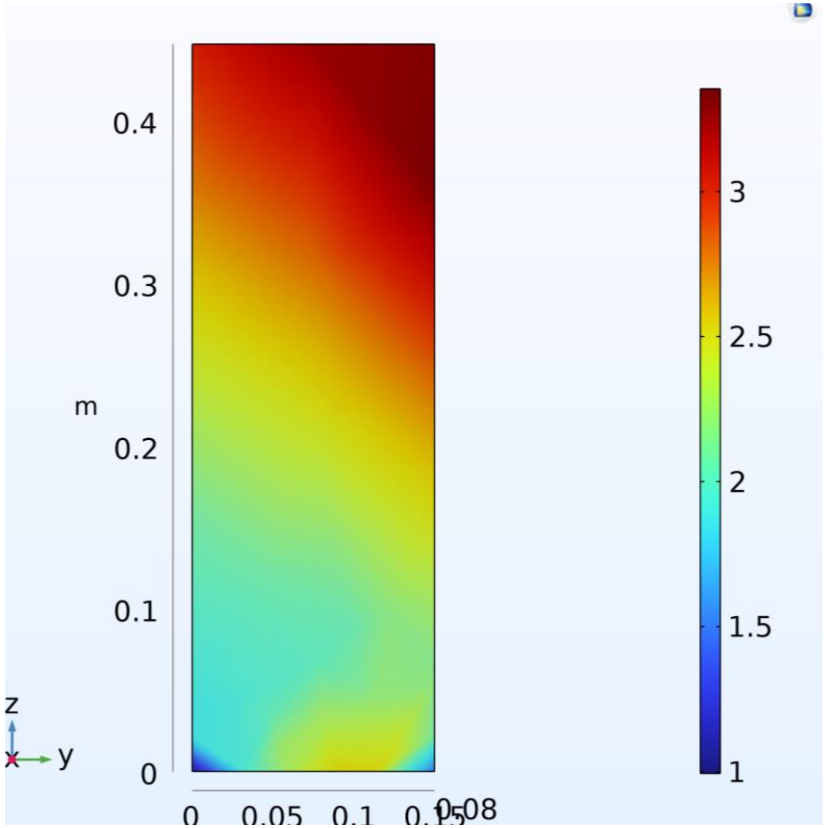


Avg. OH^- ion concentration

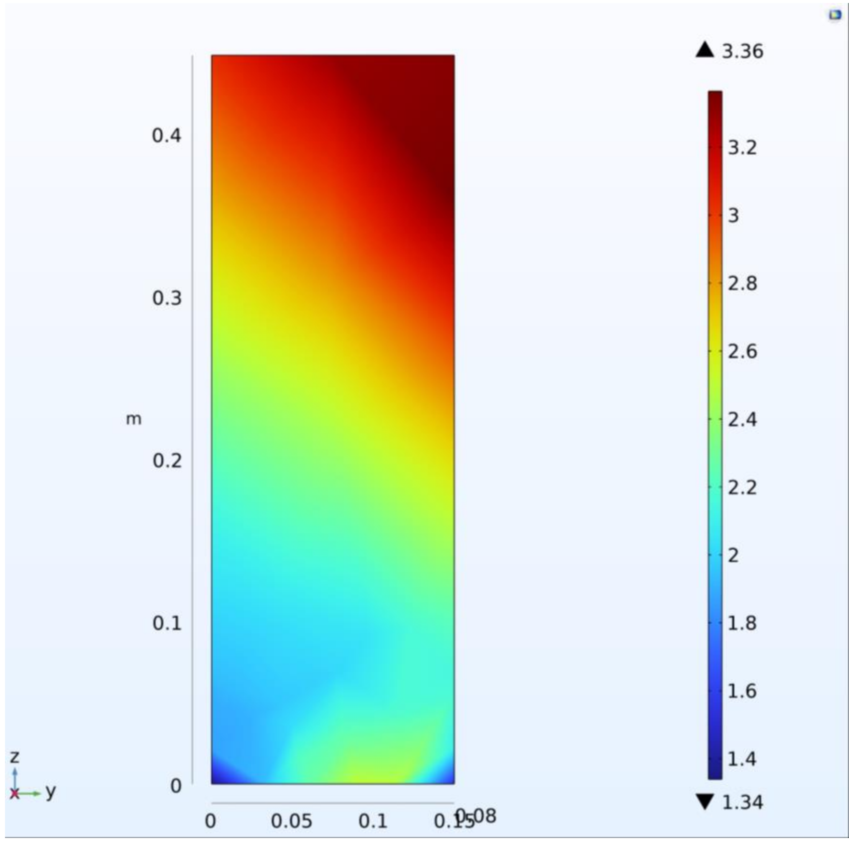
Effect of electric field on the local concentration distribution of CO_3^{2-}



Applied potential is 0 V

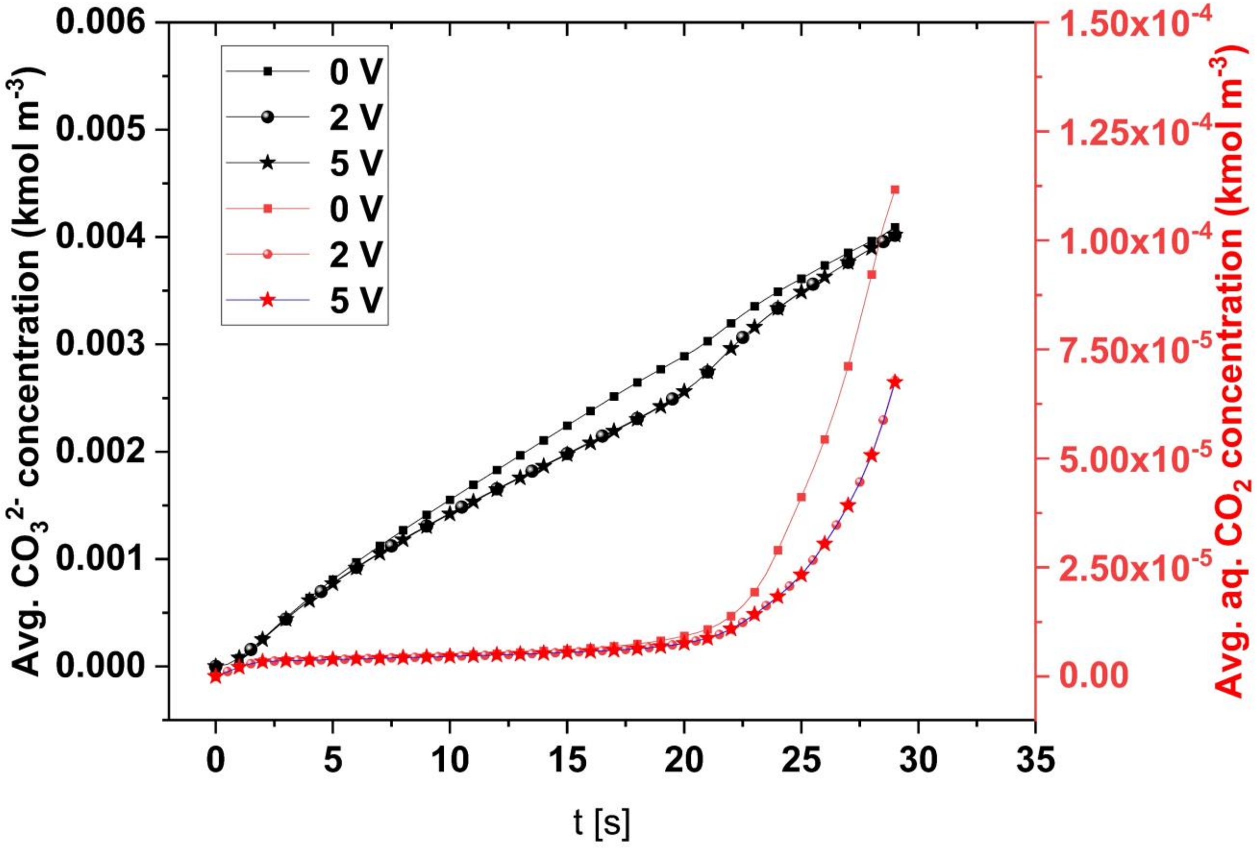


Applied potential is 2 V



Applied potential is 5 V

Volumed average concentration variation of aqueous CO_2 and CO_3^{2-}



Conclusion

- The system was successfully simulated, and it was able to predict the concentration of species under an electric field.
- It has been observed that the mass transfer rate (k_l) remains constant even in the presence of an electric field
- There is less visible change in the concentration at higher potential as compared to lower potential.
- The application of this model can be extended to other electrochemical devices, such as electrochemical CO_2 reduction

Thank You for your attention!