

# High Fidelity Multiphase Modelling Of Hydrogenics In Zero Gap Alkaline Water Electrolyzer

This study focuses on Zero Gap Alkaline Water Electrolysis (ZGAWE) to improve hydrogen production efficiency by reducing internal resistance. It developed a 2D model and conducted comparative and experimental validation studies, enhancing understanding of ZGAWE technology.

 $Prasanth\ S\ M^1$ 

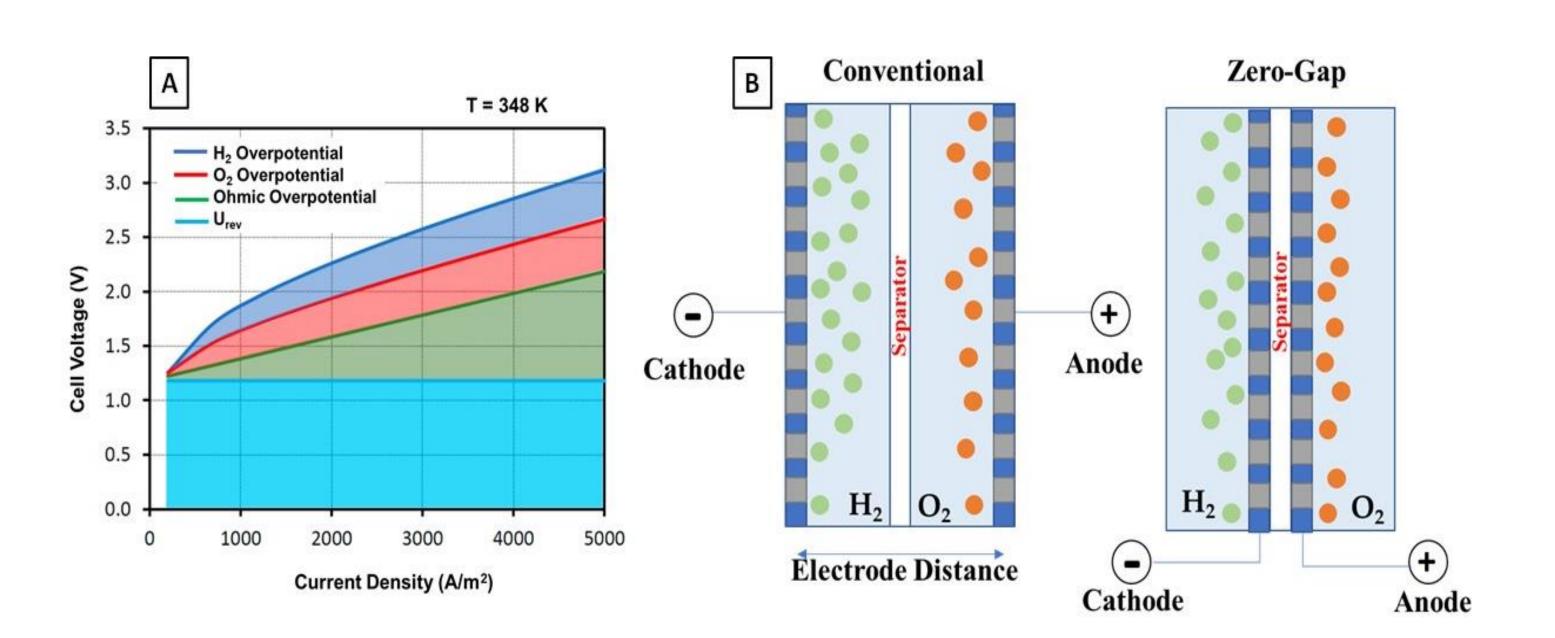
O<sub>2</sub> Separator

1. Department of Chemical Engineering, IISc Bangalore, India

#### Abstract

Electrolytic hydrogen production offers high energy density and long duration storage capabilities. Alkaline Water Electrolysis (AWE) stands out as a cost-effective and mature technology for hydrogen production. Traditional AWE suffers from high internal resistance, limiting operation to low current densities. The Zero Gap configuration of AWE (ZGAWE) overcomes this limitation by reducing ohmic overpotential and enabling higher current densities for improved efficiency. This study developed a 2D, 2Phase

electrochemistry-transport coupled model of the ZGAWE cell using COMSOL Multiphysics. The model simultaneously solved fluid dynamics and electric current conservation equations, incorporating the Euler-Euler approach to describe the two-phase bubbly flow. Comparative studies were conducted between a standard non-zero gap alkaline electrolyzer and a zero-gap alkaline water electrolyzer for the developed model, followed by experimental validation of the same parameters in accordance with the reported literature.



## Equations

Electrical Charge Conservation: Water Electrolyzer Module  $\nabla \cdot \vec{J} = Q_j \Rightarrow -\nabla \cdot \left[ \sigma(\nabla U) - \frac{\partial \vec{D}}{\partial t} - \vec{J}_e \right] \cdot d = Q_j$ 

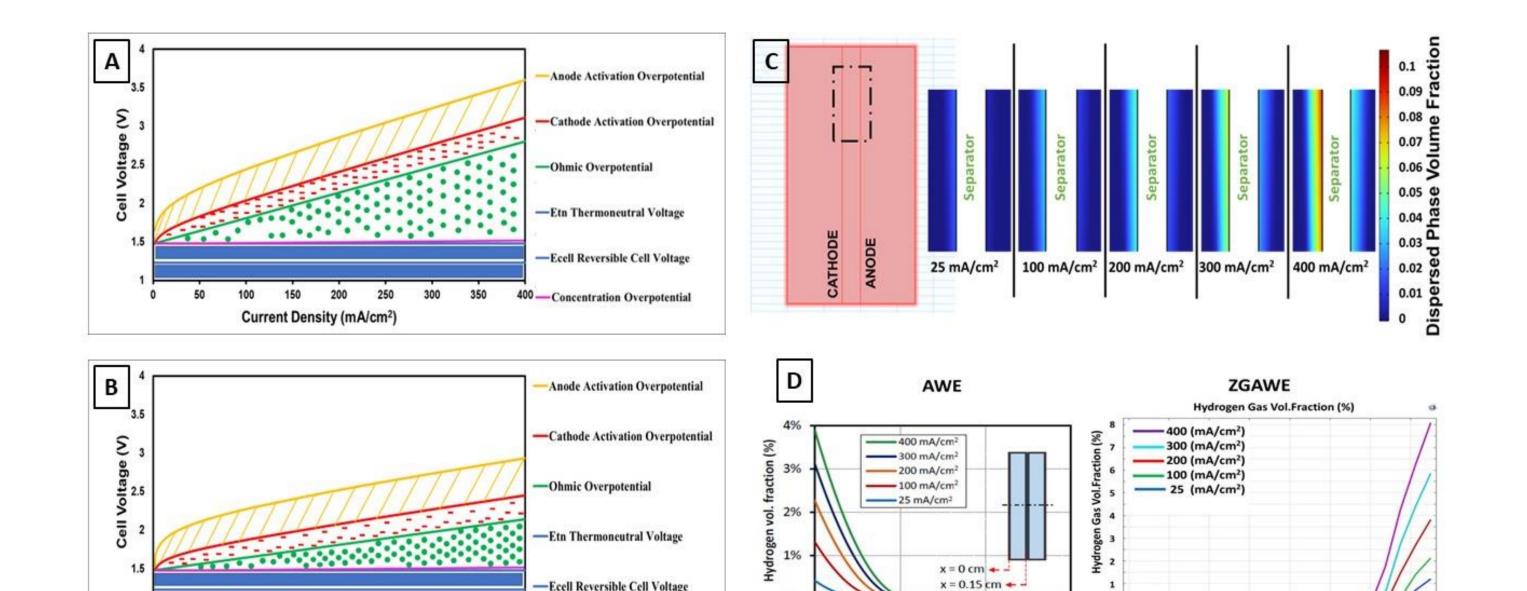
Figure 1 A) Overpotentials in Alkaline Water Electrolyzer

B) AWE Vs ZGAWE

### Results

A 2D two-phase "Electrochemistry-Transport" coupled model for Alkaline Water Electrolysis (AWE) was developed using an inhomogeneous Euler-Euler mixture modeling approach. This model offers versatility for simulating different operating conditions and concurrently analyzing fluid dynamics and electrochemical phenomena. The study confirmed the reduction in ohmic overpotential achieved by the Zero Gap configuration through a comparison with standard AWE.

Faraday Equation for each Current Density  $\dot{m}_{H2} = \frac{M_{H2}}{2 \cdot F} \cdot i$   $\dot{m}_{O2} = \frac{M_{O2}}{4 \cdot F} \cdot i$ Bubble Resistance  $\sigma_{eff-electrolyte} = \sigma_{electrolyte} \cdot (1 - \Phi_g)^{1.5}$   $R_{eff-electrolyte} = \frac{1}{\sigma_{eff-electrolyte}} \left(\frac{d_{am}}{A_a} + \frac{d_{cm}}{A_c}\right)$ 



Additionally, the research investigated the impact of temperature and concentration on AWE performance, revealing that the gases produced during electrolysis create a "curtain profile" within the electrode, increasing the void fraction vertically due to gas accumulation. These findings enhance our understanding of AWE and its potential for efficient hydrogen production.

#### REFERENCES

- A. Zarghami, N.G. Deen, A.W. Vreman, CFD modeling of multiphase flow in an alkaline water electrolyzer, Chem. Eng. Sci. 227 (2020) 115926. <u>https://doi.org/10.1016/j.ces.2020.115926</u>.
- J. Rodríguez, E. Amores, Cfd modeling and experimental validation of an alkaline water electrolysis cell for hydrogen production, Processes. 8 (2020) 1–17. https://doi.org/10.3390/pr8121634.

Excerpt from the Proceedings of the 2023 COMSOL Conference

#### Indian Institute of Science IISc Bangalore



Figure 2 A & B Comparison of Overpotentials, C) Gas Fraction Distribution in ZGAWE D) Hydrogen Quantification