# *Influence of Electrodes Configuration on Fluid Dynamics in an Eletrochemical Reactor*

POSTER
Ph.D. Student: N
Journal: NONE

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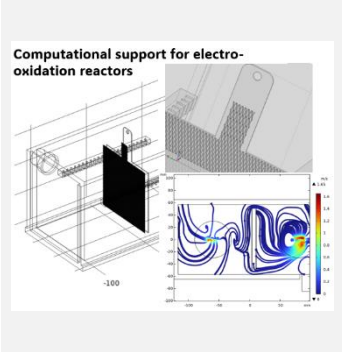


*The efficient degradation of hazardous compounds for the ecosystem is a major challenge. Electro-oxidation process represent an eco-friendly approach to effective environmental remediation. Here, we investigate the dynamic flow behavior in an electrochemical reactor by replacing traditional plate electrode with mesh electrode. Turbulent flow simulation was used to assess the flow behavior in batch operation (stirred system) and recirculated batch system. The theorical analysis provided insights into the effect of mesh electrodes, demonstrating efficient transport of chemical species. The batch system showed the formation of vortices, while in the recirculated batch system, preferential pathways were formed. Both cases have peculiarities that can significantly affect the velocity of electrochemical reactions.*

## *Introduction*

*Electro-oxidation processes rely on the electrochemical generation of strong oxidizing agents, such as •OH radicals in solution, in sufficient quantities for the non-selective reaction with organic compounds, enabling the degradation of even recalcitrant compounds [1]. As a result of the close relationship among different variables in electro-oxidation, experimental design techniques are often employed to optimize the degradation of some compounds [2,3]. Electrode stacking may be employed to increase treated effluent volume, while computational fluid dynamics (CFD) techniques are crucial for refining both electrode and reactor designs, aligning with various electrochemical processes' needs. Efforts to understand the intricate relationship between electrode/effluent reactions, reactor design, and operational parameters are ongoing in environmental studies, with research focusing on strong oxidant formation and emerging pollutant degradation, proposing models to assess reactor performance based on factors like flow rate and applied current. The use of mesh electrodes or plate electrodes operated in batch and recirculated batch mode was explored in this work to address design drawbacks such as short-circuiting, back-mixing, and the presence of dead zones. In this study, the simulations were conducted by COMSOL Multiphysics software by solving the governing equations through finite elements method to assess the understanding about the theorical hydrodynamic behavior of the electrolyte.*

## *Material and Methods*

*The electrochemical system used in the simulation is represented in Fig. 1a, showing the electro-oxidation reactor. The reactor consists of a rectangular vessel (25×10×8 cm) with two electrodes of 85 cm² as area. The overall volume of water simulated was 2000 cm³ and the interelectrode gap was 0.5 cm. The computational fluid domain was created into COMSOL and the computational mesh was generated, which consisted mainly of tetrahedral elements as seen in Fig. 1b. In the case of batch recirculation process, the mass flow was 340 mL min⁻¹. Magnetic stirrers were employed in the stirred batch system, positioned between the wall and the electrodes (Fig. 1c), rotating at 940 rpm. The aperture size of the rhombic mesh electrode (Fig. 1d) was 2 mm. The flow model was based on interacting with Reynolds Navier-Stokes (RANS) equations using the standard k – ε turbulence model [3,4]. Steady-state for an incompressible fluid and isothermal conditions were assumed and the governing equations were 1 and 2:*

$$\rho(u \cdot \nabla u) = -\nabla P + \nabla((\mu + \mu_T)(\nabla u + (\nabla u^T)) \quad (1)$$

$$\nabla u = 0 \quad (2)$$

*The RANS equation involves molecular forces including dynamic viscosity ($\mu$), pressure ($P$), fluid density ($\rho$), and the applied velocity vector ($u$). The turbulent viscosity ($\mu_T$) is described by means of equations 3 to 5:*

$$\mu_T = \rho C_\mu \frac{K^2}{\varepsilon} \quad (3)$$

$$\rho(u \cdot \nabla)K = \nabla \cdot \left(\left(\mu + \frac{\mu_T}{\sigma_K}\right)\nabla K\right) + P_K - \rho\varepsilon \quad (4)$$

$$\rho(u \cdot \nabla)\varepsilon = \nabla \cdot \left(\left(\mu + \frac{\mu_T}{\sigma_\varepsilon}\right)\nabla \varepsilon\right) + C_{\varepsilon 1}\frac{\varepsilon}{K}P_K - C_{\varepsilon 2}\rho\frac{\varepsilon^2}{K} \quad (5)$$

*In the equations, $K$ represents the turbulent kinetic energy, $\varepsilon$ denotes the velocity of turbulent energy dissipation, and $P_K$ stands for an energy production term. These equations incorporate dimensionless model constants, including $C_{\varepsilon 1}$ (1.44), $C_{\varepsilon 2}$ (1.92), $\sigma_K$ (1) and $\sigma_\varepsilon$ (1.3). To solve these equations, boundaries were established: a) the input velocity value was $u = -V_0 n$. This specifies that velocity is equivalent to a specified vector. b) a non-slip condition was applied to the wall ($u = 0$). c) a constant pressure value at the outlet. The convergence criterion of $< 10^{-5}$ was employed for all the simulations.*

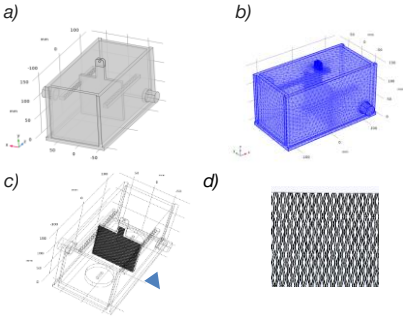


***Figure 1.*** *a) electro-oxidation configuration reactor. b) computational mesh. c) reactor with rhombic mesh electrode. d) zoom of the rhombic aperture of the electrode.*

## *Results and Discussion*

*The results shown in Fig. 2 are related to the stirred batch system. The use of the mesh electrode (Fig. 2b) maximizes surface area and distributes fluid flow more uniformly around the anodic electrode surface (mesh) compared to the use of plate electrodes (Fig. 2a). The mesh electrode can enhance both the likelihood of electrode-electrolyte contact and the local mass transfer rates of pollutants. The formation of vortices can be observed at points within the reactors. Their occurrence may be beneficial for enhancing system mixing and facilitating the diffusion of chemical species at certain points; however, they can lead to undesirable flow patterns and complexity in maintaining proper operational conditions. In the recirculated reactor (Fig. 3) with plate electrodes it is possible to observe the layers of fluid moving parallel to each other in an orderly manner. In this specific case, the flow passes more intensively over the electrodes, and between the electrodes, there is almost no electrolyte flow, which hinders the transport of species across both sides of the electrode, potentially making the oxidation process less effective, despite the more uniform distribution of chemical species.*

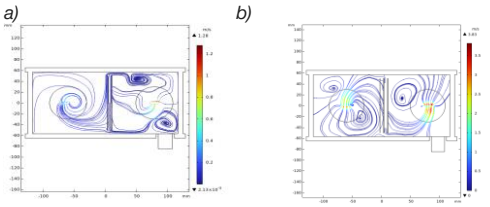


***Figure 2.*** *Reactor operating in batch mode: velocity stremlines a) plate electrodes b) mesh electrode and plate electrodes.*

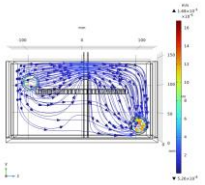

***Figure 3.*** *Velocity stremlines of the reactor operating in recirculating batch mode.*

## *Conclusions*

*In this study, different system configurations reveal peculiarities that can significantly impact electrochemical reactions. Mesh electrodes can enhance electrode-electrolyte contact, while batch reactor demonstrate vortex formation. Additionaly, in recirculated batch system, preferential pathways are formed. These results highlight the important role of CFD in optimizing reactor configuration and understanding fluid flow behavior in electrochemical process.*


### *Acknowledgments*

*We would like to thank PETROBRAS [2023/00226 0] for financial support and LEMA-UFSC for the infrastructure.*


### *References*


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