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Use of CFD Tools to Design and Evaluate Tubular Baffles in an Electrochemical Reactor for the Removal of Hexavalent Chromium

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This study evaluates the effect of mixing conditions on the electrochemical reduction of hexavalent chromium (Cr(VI)) using Computational Fluid Dynamics (CFD) simulations. The research focuses on optimizing the internal geometry of the reactor, particularly the arrangement of tubular baffles, to improve flow patterns and minimize energy consumption. CFD simulations indicate that the configuration with eight tubular baffles provides the best hydrodynamic performance by promoting axial flow, improving mixing efficiency, and reducing homogenization energy by up to 50 % compared to the case with four baffles. Experimental results confirm that Cr(VI) removal efficiency exceeds the predictions of Faraday's law, with treatment times decreasing by up to 20 min as agitation speed increases. Energy consumption analysis shows that the optimum balance between mixing energy and electrode power consumption is achieved at 300 rpm, resulting in a 13 % reduction in total energy consumption compared to previous studies. These results highlight the critical role of reactor geometry in electrochemical processes and provide a more energy efficient approach for wastewater treatment applications.

1. Introduction

Water is an essential resource that must be protected to ensure its availability for various human activities. Among these, industrial processes such as electroplating produce wastewater that is contaminated with hexavalent chromium (Cr(VI)) (Téllez et al., 2004), a highly toxic and persistent pollutant that poses a significant risk to the environment and human health (Saha et al., 2011).
Conventional Cr(VI) removal methods include chemical precipitation, where $FeSO_4$ reduces Cr(VI) to Cr(III), a less toxic species (Sarria-Villa et al., 2020). However, this process results in large volumes of sludge that are in need of further treatment and special disposal. Adsorption onto various materials is another alternative (Gill et al., 2025), but its efficiency declines over time and Cr(VI) is not reduced to Cr(III), making complete removal difficult.
Electrochemical reduction has emerged as a promising alternative (Calma et al., 2024). In this process, under acidic conditions (pH <2) results in several reactions as shown in Figure 1 (Martínez et al., 2004). The sacrificial iron electrodes release of ferrous ions (Fe(II)) into the liquid (R1). The Fe(II) then reacts with Cr(VI), reducing it to Cr(III), which is the primary reaction (R2). In addition, the reduction of Fe(III) to Fe(II) (R3) and the direct reduction of Cr(VI) to Cr(III) (R4) also occur at the cathode, both contributing to the overall reduction of Cr(VI. Subsequent pH adjustment leads to the precipitation of the reduced species, producing a treated effluent with

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low metal content. Despite its effectiveness, this method is limited by high energy demands and passivation of the electrodes, which reduce reaction efficiency (Yáñez-Varela et al., 2018). Effective mixing is critical to prevent passivation and ensure uniform mass transfer across the reactor volume (Ibrahim et al., 2020).

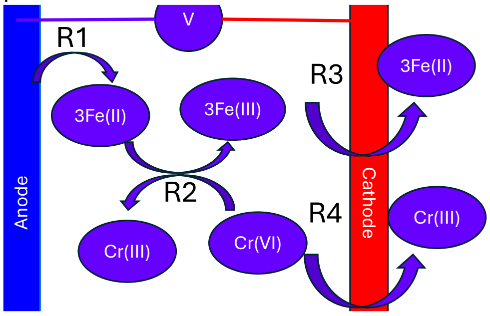

Figure 1: Main reactions involved in the reduction of Cr(VI).

Computational Fluid Dynamics (CFD) has become an essential tool for optimising reactor design prior to physical implementation, allowing hydrodynamic performance to be assessed while reducing experimental cost and time (Lugo-Hinojosa et al., 2024). CFD helps to identify areas for improvement in system geometry and operating kinematics, which can help to develop an electrochemical process under improved conditions, by simulating flow patterns and turbulence effects (Catañeda et al., 2019). In this study, CFD simulations are used to evaluate the effect of tubular baffles on the flow behaviour in an electrochemical reactor for Cr(VI) reduction. The results aim to identify an optimal reactor configuration that maximises mixing efficiency while minimising energy consumption.

This study introduces a novel approach that integrates advanced computational fluid dynamics (CFD) modelling with experimental analysis of electrochemical reactors. This approach was used to optimise the geometric configuration and operational parameters for efficiently removing Cr(VI). Previous research (Major-Godlewska and Karcz, 2018) has revealed that increasing the number of tubular baffles and identifying an optimal stirring speed can significantly reduce energy consumption while enhancing treatment efficiency. This method not only improves reactor design but also provides scalable solutions for industrial wastewater treatment processes, where energy-intensive mixing and pollutant removal present major challenges. The results support the development of sustainable water treatment technologies that align with global environmental objectives, thereby fostering the transition to more resource-efficient, environmentally friendly industrial practices worldwide.

2. Methodology

2.1 Configurations of the stirred tank

A cylindrical electrochemical reactor (12 L) with an internal diameter of 0.25 m and height of 0.25 m was used. Agitation was provided by a four-bladed PBT impeller (0.08 m diameter), positioned at 0.08 m from the reactor bottom and operated at 500 rpm. The electrodes consisted of 6 mm iron rods arranged as tubular baffles (TB) to act as sacrificial anodes, as shown in Figure 2. Three configurations were evaluated: four, eight and twelve tubular baffles (4 TB, 8 TB, 12 TB), designed to improve both mass transfer and Cr(VI) reduction efficiency.

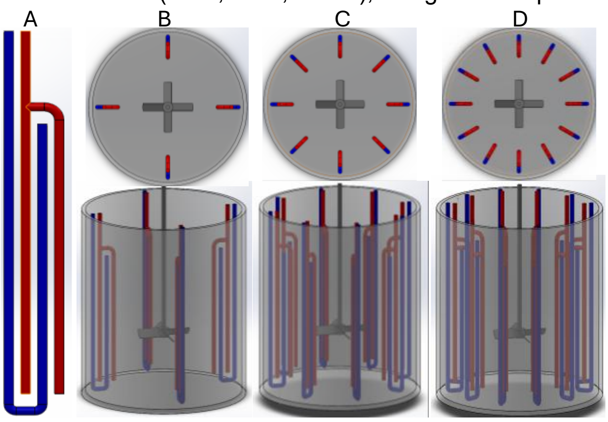

Figure 2: A) Single electrode anode (blue) and cathode (red), B) Case 4 TB, C) Case 8 TB, and D) Case 12 TB.

2.2 Details of the numerical solution

The numerical simulation was carried out using ANSYS. It started with a geometry created in Design Modeler, to which a tetrahedral unstructured mesh was added using ANSYS Meshing. To accurately and efficiently capture the impeller's rotational motion, the Multiple Reference Frame (MRF) technique was employed. This technique divides the computational domain into a rotating region (MRF) and a stationary region (SRF). In the MRF zone, which contains the impeller, the mesh remains fixed but is assigned to a constant angular velocity. This enables the rotational effect to be reproduced without the need for remeshing, which significantly reduces the computational cost compared to more complex methods while delivering reliable results for steady-state flows in stirred tanks. The remainder of the domain, corresponding to the tank and baffles, was modelled in a stationary reference frame. All tank and baffle walls were assigned to a no-slip condition, while the free surface of the fluid was given a symmetrical boundary condition (zero shear stress). The impeller and shaft walls were modelled as moving using standard wall functions. Second-order discretization schemes were applied to all variables with a convergence criterion set at residuals of 1×10^{-6} and the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm was employed for pressure–velocity coupling. Local mesh refinements were introduced in critical regions, particularly at the impeller discharge and around the baffles. Mesh sizes ranged from one to four million elements, and a mesh independence analysis concluded that two million elements provided the optimal balance between accuracy and computational cost.

2.3 Electrochemical reduction

The reactor was filled with synthetic wastewater treated with potassium dichromate ($K_2Cr_2O_7$) to achieve an initial Cr(VI) concentration of 100 mg/L. Prior to each experiment, the electrodes were mechanically polished and immersed in 1 M sulphuric acid to remove oxide layers and ensure uniform initial conditions. The system was connected to a DC power supply set at 5 A (Figure 3A).
Samples were collected every 5 min and immediately treated with NaOH to precipitate Cr(III). Cr(VI) concentration was determined spectrophotometrically using 1,5-diphenylcarbazide at a wavelength of 540 nm (Doria Herrera et al., 2013), as shown in Figure 3B.

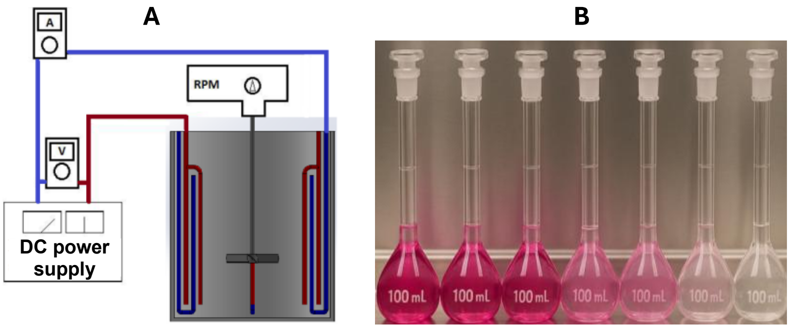

Figure 3: A) Experimental setup of the electrochemical reactor and B) Reactor samples at different time intervals showing the evolution of Cr(VI).

2.4 Energy Consumption Analysis

The total energy consumption of the process (E_t) was obtained by summing the energy consumed by stirring and electrochemical reaction.
Stirring power (P_A) was measured using a FUTEK torque sensor mounted on the impeller shaft. Data was recorded for 3 min, yielding approximately 12,000 readings, which were processed in SENSIT software. The average torque was used to compute P_A using:

$$P_A = 2\pi N\tau \quad (1)$$

where N is the impeller speed (RPM) and τ is the measured torque (Nm).
Electrode power (P_E) was determined by continuously monitoring voltage (V) and current (I) during treatment:

$$P_E = I * \mathrm{V} \quad (2)$$

where V is the applied voltage (V) and I is the current (A).
The specific energy consumption was then calculated as:

$$E_t = \frac{(P_A + P_E)\cdot t}{m_{(Cr(VI),removed)}} \quad (3)$$

where t is the treatment duration and $m_{(Cr(VI),removed)}$ is the mass of Cr(VI) removed (kg).

3. Results and discussions

3.1 CFD Model Results

CFD models provide valuable insight into the hydrodynamic changes that occur within the reactor when geometric modifications are made to the vessel. This study focuses on evaluating the effect of increasing the number of tubular baffles within the reactor on flow patterns, mixing efficiency and energy consumption. The aim is to identify the most effective configuration, construct the optimized design and evaluate its efficiency in Cr(VI) removal (Yáñez-Varela et al., 2020).
Table 1 shows that increasing the number of baffles from four to eight results in a 20 % increase in energy consumption. In terms of the pumping effect generated by the interaction between the impeller and the baffles, a slight increase of up to 7 % is observed, indicating that the fluid flow is improved with additional baffles.
Considering these parameters in the pumping efficiency (η_E), the 4 TB configuration achieves the highest efficiency, requiring less energy to circulate a greater volume of fluid within the impeller's area of influence. However, as this parameter only considers the immediate impeller area, additional metrics that take into account the entire tank volume are essential.
To this end, the mixing time ($T_{M_{95}}$) and the energy dissipation rate ($\bar{\varepsilon_\tau}$) through the impeller were evaluated to assess the overall mixing performance. These values were then used to calculate the homogenization energy (η).
The results show that the 8 TB configuration requires the least energy while achieving the shortest mixing time. This suggests that the impeller efficiently use the energy supplied to create homogeneous conditions throughout the tank. Conversely, the 4 TB configuration requires almost twice the energy to achieve similar mixing conditions due to the reduced interaction between the impeller and the top of the reactor, significantly increasing the mixing time.

Table 1: Global hydrodynamic parameters of the different CFD models

case	P [W]	$N_P = \frac{P}{\rho N^3 D^5}$	$N_Q = \frac{Q}{ND^3}$	$\eta_E = \frac{N_Q}{N_P}$	$T_{M_{95}}$ [s]	$\bar{\varepsilon_\tau} = \frac{P}{V_T \rho}$ [W/kg]	$\eta = \bar{\varepsilon_\tau} T_{M_{95}}$
4 TB	2.4	1.02	0.84	0.82	6.95	0.194	1.35
8 TB	2.6	1.13	0.87	0.77	3.35	0.218	0.73
12 TB	2.9	1.23	0.90	0.73	3.79	0.239	0.90

Figure 4 shows the axial and radial velocity contours obtained from the CFD simulations for the different cases. The flow at the impeller outlet remains constant in all scenarios due to the high flow rate generated by the impeller motion. However, in the upper region of the tank (y = 0.2 m), increasing the number of baffles increases the axial circulation (dotted line). In addition, the velocity contours in the upper part of the tank show that eight tubular baffles effectively direct the flow towards the center of the reactor, improving mixing performance and reducing mixing time, as shown in Table 1.

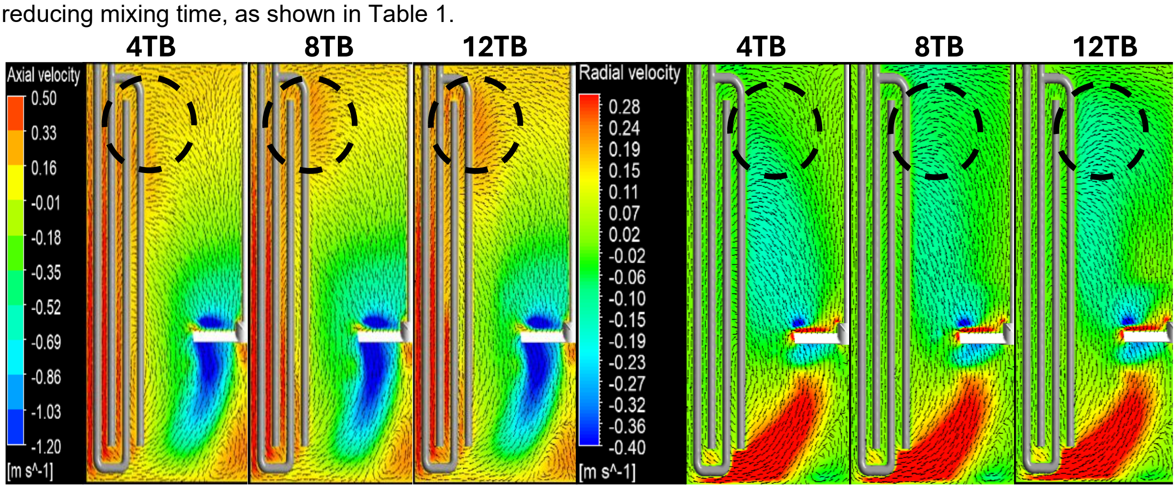

Figure 4: CFD axial and radial velocity maps obtained in the middle plane for the evaluated cases.

3.2 Experimental evaluation of hexavalent chromium reduction

Figure 5 shows the reduction of Cr(VI) in the reactor equipped with eight tubular baffles at different agitation speeds. The results show that increasing the agitation speed accelerates Cr(VI) removal, reducing the treatment time from 28 min at 100 rpm to 17 min at 500 rpm. The removal process follows a linear trend as the agitation system provides optimal mixing conditions within the reactor, in agreement with numerical simulations.
Experimental data showed that the required treatment time is shorter than predicted by Faraday's law for electrolysis. This suggests two key factors: (1) secondary reactions at the cathode, such as Fe(III) reduction and direct Cr(VI) reduction at the electrode surface, enhance Cr(VI) removal; and (2) under acidic conditions and intense mixing, the electrode undergoes accelerated corrosion, releasing more iron into the fluid and further facilitating Cr(VI) reduction, significantly reducing treatment times (Figure 3).

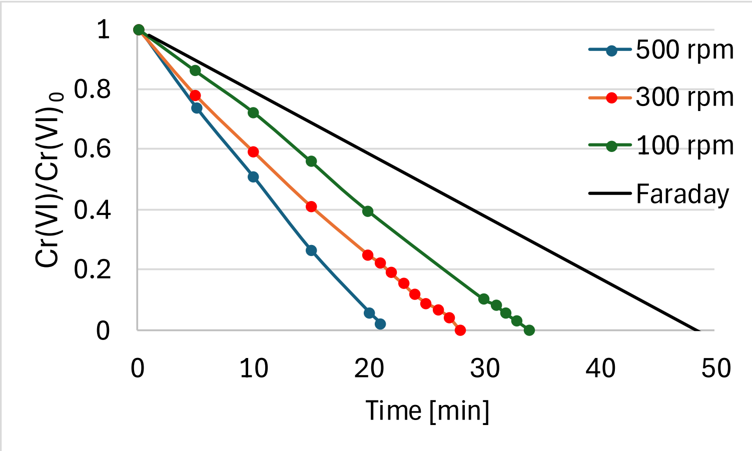

Figure 5: Cr(VI) reduction rate at different stirring speeds in the reactor with eight tubular baffles.

Figure 6 shows the total energy consumption for the case with eight tubular baffles. The results show that operating the reactor at 300 rpm gives the lowest energy consumption, with a value of 2.8 kWh/kg Cr(VI), which is 17 % lower than the value obtained at 100 rpm and 13 % lower than that reported in similar studies (3.32 kWh/kg Cr(VI)) (Yáñez-Varela et al., 2024).
At a stirring speed of 100 rpm, the electrodes consume more than 99 % of the total energy. However, at 500 rpm, the energy consumed by the electrodes drops to 70 %. Nevertheless, it is important to balance the contributions of mixing energy and electrode energy consumption. The 300 rpm configuration achieves the optimum balance by minimizing both energy inputs. Although this increase in speed results in a slight 5 % increase in total energy consumption, it remains a viable option for achieving faster Cr(VI) removal.

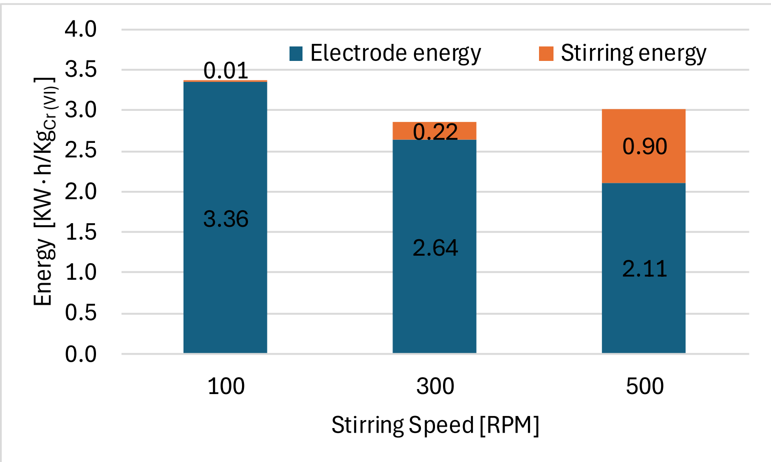

Figure 6: Characteristic energy for Cr(VI) removal using a reactor equipped with eight tubular baffles at different agitation speeds.

4. Conclusions

This study shows that targeted geometric optimization and hydrodynamic analysis can significantly improve the sustainability of stirred tank electrochemical reactors used for hazardous wastewater treatment. The eight-baffle configuration enhances whole-tank mixing efficiency, reducing homogenization energy by almost 50 % compared to the more conventional four-baffle design. This improvement accelerates the removal of toxic Cr(VI) and lowers the process's overall energy demand.

Identifying 300 rpm as the optimal operating speed enables the system to strike a balance between rapid contaminant removal and reduced resource consumption, minimizing both electrode and mixing energy inputs. This directly contributes to environmental sustainability by decreasing operational energy use and associated greenhouse gas emissions.

Furthermore, integrating CFD-based hydrodynamic optimization with electrochemical performance evaluation paves the way for the development of cleaner, more resource-efficient technologies. The resulting design reduces the environmental footprint of industrial water treatment while maintaining high treatment effectiveness. This aligns with global efforts to promote the principles of the circular economy, conserve resources, and encourage the adoption of greener industrial practices.

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