

# **Evaluation of the Hydrodynamic Performance of an Electrochemical Reactor with Rotating Ring Electrodes using CFD Analysis**

Sergio A. Martínez-Delgadillo<sup>1\*</sup>, Helvio Mollinedo-P<sup>2</sup>, Víctor X. Mendoza-Escamilla<sup>3</sup>, Oliver Huerta<sup>4</sup>

<sup>1</sup>Depto. Ciencias Básicas. Universidad Autónoma Metropolitana Azcapotzalco. Av. San Pablo 180. Azcapotzalco. CP 07740, México D.F. México. [samd@correo.azc.uam.mx](mailto:samd@correo.azc.uam.mx).

<sup>2</sup>Academia de Mecánica. UPIITA, Instituto Politécnico Nacional. Av. IPN 2580, Ticoman. México D.F., México

<sup>3</sup>Depto. Electrónica. Universidad Autónoma Metropolitana –Azcapotzalco. Av. San Pablo 180. Azcapotzalco. CP 07740, México D.F. México.

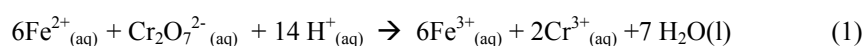
<sup>4</sup>SEPI-ESIME-Zacatenco IPN. Av. IPN s/n Unidad Profesional Adolfo López Mateos, México D.F., México

Chemical precipitation, ion exchange, evaporation and reverse osmosis processes have been applied to remove hexavalent chromium Cr(VI) from industrial wastewaters. However, some of chemical precipitation methods use great quantities of chemical and flocculating that produce elevated quantities of sludge that must be treated, handled and disposed, increasing the process costs. The other methods require high capital and operating costs. The electrochemical process is an alternative method to remove Cr(VI) from industrial wastewaters process. However, in electrochemical plug flow reactors with no liquid mixing or static electrodes, iron salt film is formed on the electrodes surface (electrode passivation) because of the poor diffusion and mass transfer that reduces the Cr (VI) removal efficiency and causes greater energy consumption. Therefore, the electrochemical reactors require to be designed to provide high mass transfer between the bulk liquid and the electrodes. However, their performance generally has been evaluated as if they were a “black box”. In this work, the performance of an electrochemical reactor with rotating ring electrodes was evaluated using state-of-the-art computational fluid dynamics (CFD) tools at different rotational speeds to evaluate their effect on the electrochemical process to remove Cr(VI) from wastewater.

## **1. Introduction**

Hexavalent chromium Cr(VI) is one of the most hazardous pollutants discharged into the wastewaters from the electroplating and other industrial plants. Cr(VI) is generally considered 1000 times more toxic than Cr(III), so it is highly dangerous to human health. In addition, wastewaters with Cr(VI) are sources of groundwater contamination, then this hazardous heavy metal must be removed to reach acceptable concentration level (less than 0.1mg/L) and comply with the environmental regulations for wastewater disposal. A number of processes including chemical precipitation, ion exchange,

evaporation and reverse osmosis have been applied to industrial wastewater containing Cr(VI). Traditional methods to remove chromium from industrial wastewater use chemical and flocculating agents producing high quantities of sludge and expend a lot of chemical reagents, increasing the process costs. Alternative electrochemical methods have been carried out using polypyrrole deposits on porous, high area three-dimensional carbon electrodes. Unfortunately, 80% overall removal was obtained. (Alatorre, et al., 1998). The electrochemical treatment to remove Cr(VI) using the proposed iron rotating electrodes is an alternative process, and a 99.9 % removal of Cr (VI) can be achieved. In this process, the Cr(VI) is reduced to Cr(III), mainly because of the ferrous ions Fe (II) which are released from the anode to the solution, when a direct electrical current is applied to an iron sacrificial anode. The reaction (1) that takes place into the solution.



However, during the process, an oxides film is formed on the electrodes (passivation effect) in electrochemical reactors with no liquid mixing or static electrodes because the poor diffusion and mass transfer, reducing the process efficiency and increasing the energy consumption (Martinez et al., 2000). In this work, the performance of an electrochemical reactor with rotating ring electrodes (Rodriguez et al, 2003) was evaluated experimentally and its hydrodynamic behavior was analyzed using state-of-the-art computational fluid dynamics (CFD) tools at different rotational speeds to evaluate their effect on the electrochemical process to remove Cr(VI) from wastewater. The CFD analysis has proven to be a useful tool to simulate and evaluate the performance in reactors and mixers (Martinez et al., 2010 and Hosseini et al., 2010), used to simulate a solid – liquid mixing in a cylindrical tank, evaluating the type of impeller, impeller off-bottom clearance, speed, particle size and other parameters. Rahimi and Parvareh (2005), studied the flow generated and mixing time in a semi-industrial tank equipped with a side entry jet mixer. They tested a family of k-ε turbulence models including: standard, RNG and realizable models and the effect of these models on the predicted results was investigated. The results show that there are considerable differences between the predicted mixing progresses using the three versions of the k-ε family models.

## 2. Experimental methods

The tests were performed in an electrochemical batch reactor with a synthetic wastewater prepared with potassium dichromate. The electrochemical reactor capacity was 8.5 L (Fig. 1). In order to produce turbulence in the reactor, a rotating iron ring electrode was used during the electrochemical chromium removal process. The rotating iron electrodes contained 14 iron steel rings allocated as a sequence of one cathode and one anode. Each ring has an 11.5 cm diameter, 7 rings function as cathodes and the other 7 as anodes. The liquid high in the reactor was 22.0 cm and the tank diameter was 21.5 cm. Gap among ring electrodes was 1.0 cm. The superficial area of each iron ring was 75.0 cm<sup>2</sup>. A constant electric current of 5.0 A was applied during the process, using a direct current power supply.

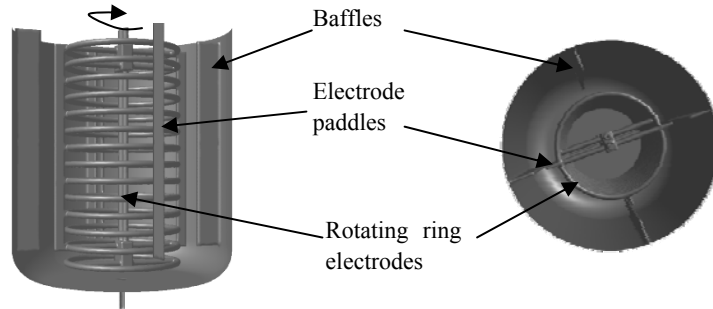


Figure 1:- Electrochemical reactor with rotating ring iron electrodes.

A shaft was used to support ring arrangement and was connected to a variable speed motor to control the electrode revolutions per minute (rpm). The pH in the reactor solution was maintained at 2.0 units during electrochemical process by the addition of sulfuric acid. In order to evaluate chromium reduction, samples were taken out from the electrochemical reactor at different times during the process. To each sample the pH was risen up to 8.5 units (under this condition chromium hydroxide and ferric hydroxide are formed and precipitated) by the addition of sodium hydroxide. After the precipitation, the Cr(VI) concentration in supernatant liquid was measured by the diphenylcarbazide method. To obtain the processing theoretical time, the Faraday constant was used to calculate the time required to release in the solution, the stoichiometric amount of iron ions to react with the Cr(VI). Also it was assumed that reaction takes place instantaneously.

### 3. CFD Modeling and simulation

To analyze the performance of mixed stirred tanks is necessary to know the flow field. There have been some important parameters that provide information on the hydrodynamic behaviour of the reactor and velocity, vorticity, turbulence intensity, etc. Besides this, the geometric configuration of the reactor can determine its efficiency as impeller-type, number of blades, power input, and number of baffles (Rammohan, et. al 2001). A CFD computational model of the reactor was prepared to analyze the performance of the reactor at different steady state operational velocities: 75, 150 and 230 revolutions per minute (rpm). The conservation equations can be set to a rotating reference system, expressing the governing equations of fluid flow for a steadily rotating frame in terms of the relative velocity  $\vec{v}_r$ . The steady state continuity equation (mass conservation) for incompressible fluid can be written as follows:

$$\nabla \cdot \vec{v}_r = 0 \quad (1)$$

where:  $\vec{v}_r$  = relative velocity vector

The conservation of momentum for a rotating reference frame is given by:

$$\frac{\partial}{\partial t}(\rho \vec{v}_r) + \nabla \cdot (\rho \vec{v}_r \vec{v}_r) + \rho(2\vec{\omega} \times \vec{v}_r + \vec{\omega} \times \vec{\omega} \times \vec{r}) = -\nabla p + \nabla \cdot (\vec{\tau}) + \rho \vec{g} + \vec{F} \quad (2)$$

Where:  $\rho$  = density,  $\bar{\tau}$  = stress tensor,  $\rho\vec{g}$  = gravitational body force,  $\vec{F}$  = external force vector, the momentum equation contains two additional acceleration terms: the Coriolis acceleration  $2\vec{\omega}\times\vec{v}_r$ , and the centripetal acceleration  $2\vec{\omega}\times\vec{\omega}\times\vec{r}$ .

The CFD simulations was performed using the commercial software Fluent. Due to the unsymmetrical configuration of the blades, a complete three dimensional model reactor was used. The reactor model was meshed using tetrahedral cells. A pressure-based segregated algorithm solver has been used, where the governing equations are solved sequentially. For the pressure–velocity coupling the semi-implicit pressure-linked equation (SIMPLE) algorithm was used, the Standard scheme was selected for pressure discretization, and for the momentum discretization, the first order upwind scheme. The standard  $\kappa$ - $\epsilon$  model of turbulence model was used. Finally, a 0.001 tolerance was chosen for the convergence criterion in the modeling.

#### 4. Results and discussion

Figure 2 shows the experimental results obtained to reduce chromium concentrations from 130 mg/L to less than 0.5 mg/L, at the different rpms. Processing theoretical time was calculated considering that the Cr (VI) is reduced to Cr (III) only by means of anodically generated  $\text{Fe}^{2+}$  and the reaction (1) was instantaneous.

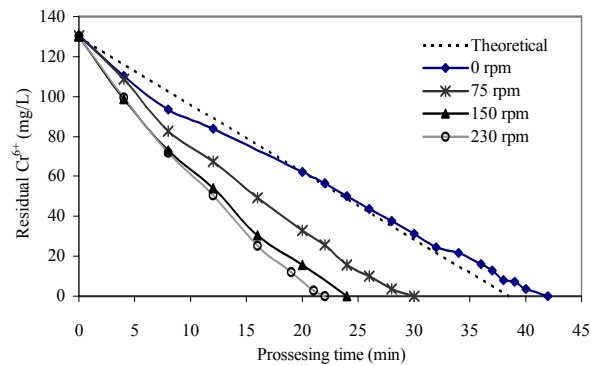


Figure 2: Residual Cr (VI) concentration as a function of processing time at different electrode rotation rates.

The experimental results obtained, show that the processing experimental time is less than the theoretical processing time, and decreases as the rotation electrodes rate increases, only when the electrodes were static (0 rpm), this time was almost the same. Comparing with the theoretical processing time, the processing time reduction at 230 150 and 75 rpm were a 42%, 38% and 22%, respectively. As shown, the processing time reduction between and 230 and 150 rpm was only two minutes, but the power consumption increase almost twice (Martinez et al. 2003). Analyzing the effect of rpm on the processing time inside the reactor, it may find appropriate criteria to set up the speed for this particular reactor. From the point of view of the fluid dynamics, in general, when a force is applied on an infinitesimal fluid element, this not only will move at a certain speed, it also deforms and rotate, generating vorticity fields to along

its path. Vorticity is a natural tendency to rotate in the majority of fluids moving within a pipeline and in this case, inside the reactor, this behavior improves the mixing and movement of the flow that is circulating near the walls, so inducing the increment of vorticity through the rotation of paddles mounted on the rings, which increases the dynamism of the vorticity fields, and then it causes that the mass transfer rate between the ring electrodes walls and the bulk liquid increases. Figure 3 shows the effects of the increment in rpm over the vorticity field, where it is possible to observe that the increase in the dynamism of the particles is directly proportional to the increase in rpm.

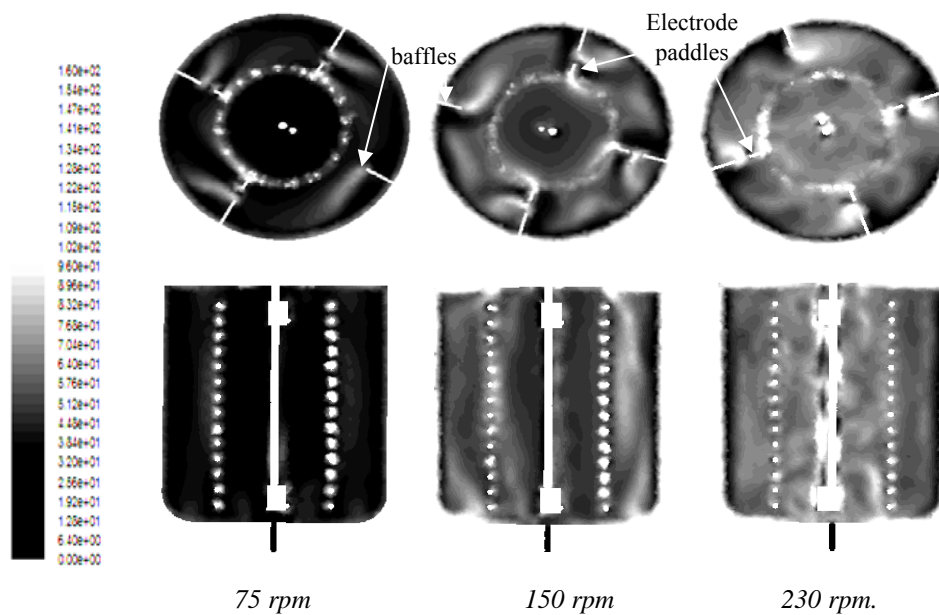


Figure 3: Vorticity into the liquid zone at the different rpm.

As seen, as the rpm increases, the liquid zones with high vorticity (with zones) increase. In addition, high vorticity occur on the electrode walls, which improves the mass transfer rate between the electrodes and the liquid. The vorticity volume-weighted average into the liquid at 75 rpm ( $17.2 \text{ s}^{-1}$ ) is about the half of 150 and 230 rpm,  $34.46$  and  $41.84 \text{ s}^{-1}$ , respectively. On the other hand, the difference of the vorticity average in the liquid, between 150 and 230 rpm is about 7%. The percentage of elements at different vorticity ranges in the liquid, are shown in figure 3. As seen, for 75 rpm the majority of elements (86.28%) are in the range of 0 to  $40 \text{ s}^{-1}$ , while at 150 and 250 rpm 68% and 45%, respectively. On the other hand, at higher vorticity ranges, from 20 to  $100 \text{ s}^{-1}$ ; only 36% of the elements are in this range when the electrochemical reactor was operated at 75 rpm, while at 150 and 230 rpm, the majority of elements (85.8 and 91.1 %, respectively) are in the range. As seen, the differences in vorticity between 150 and 230 rpm is small, then the hydrodynamic behaviour into the electrochemical reactor at that rpm is very similar, and then this can explain why the processing times to reduce

the Cr(VI) from 130 mg/L to less than 0.1 mg/L, is only 2 minutes as shown in figure 2. Therefore, the rotational movement of the paddles mounted on the rings have a twofold benefit: first, because it increases the fluid dynamics, reflected in the increased intensity of the vorticity fields (with zones in figure 3) to improve mass transfer, and secondly because centrifugal force helps to reduce the build-up of oxides film on the electrodes, reducing the passivation effect and maintaining a consistent performance for longer than if the electrodes did not rotate. However, the rotational movement of the reactor has an energy cost that is not always justifiable, when we change from 75 to 150 rpm the trend in reducing the processing time is not linear, therefore only earn 6 min, and from 150 to

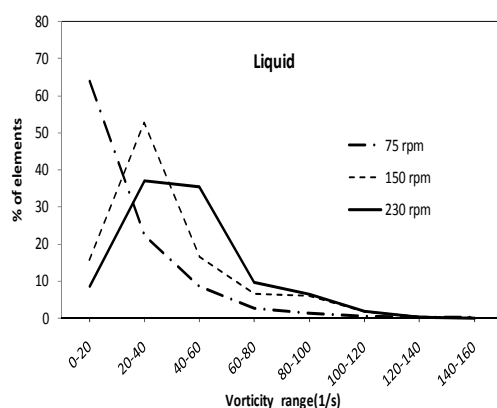


Figure 3: Distribution of the % of elements at different vorticity ranges into the liquid zone at the different rpm.

230 rpm the energy increases twice, but the savings is only 2 minutes. Then, operate the reactor at 150 rpm would be better option.

## 5. Conclusions

The electrochemical reactor with rotating ring electrode mixes the liquid, creates turbulence, promotes the reaction and diminishes the electrode passivation. The hydrodynamic behavior at 150 and 230 rpm is very similar, however at the highest rpm the energy consumption increases twice.

## References

- Hosseini S., Patel D., Mozaffari F. E., and Mehrvar M., 2010, Study of Solid-Liquid Mixing in Agitated Tanks through Computational Fluid Dynamics Modeling. *Industrial and Engineering Chemistry Research*, 49, 4426–4435.
- Martínez S., Rodríguez M. and Aguilar R., 2003, Electrochemical Process to Remove Hexavalent Chromium From Industrial Wastewater in a Rotating Electrode Reactor. *Water Intelligence* <[www.iwaponline.com/wio/2003/09/wio200309015.htm](http://www.iwaponline.com/wio/2003/09/wio200309015.htm)> accessed 17.3.2011.
- Martínez S.A., Helvio Mollinedo-Ponce, Victor Mendoza-Escamilla and Carlos Barrera-Díaz, 2010, Residence time Distribution and back-mixing in a tubular electrochemical reactor operated with different inlet flow velocities, to remove Cr (VI) from wastewater. *Chemical Engineering Journal*, 165, 776–783.
- Rahimi M. and Parvareh A., 2005, Experimental and CFD investigation on mixing by a jet in a semi-industrial stirred tank, *Chemical Engineering Journal*, 115, 85–92
- Rammohan A. R., Kemoun A., Al-Dahhan M. H., and Dudukovic M. P., 2001, A Lagrangian description of flows in stirred tanks via computer-automated radioactive particle tracking (CARPT) *Chemical Engineering Science*, 56, 2629-2639
- Rodríguez, M. G., Aguilar, R., Soto G. and Martínez, S. A., 2003, Modeling an electrochemical process to remove Cr(VI) from rinse-water in a stirred reactor, *Journal of Chemical Technology and Biotechnology*, 78, 371–376.