ABSTRACT
A limitation for the use of electrocoagulation for wastewater treatment is its complexity, since the process is affected by many variables, including the hydrodynamics in the reactor. This paper aimed to present a simulation, through Computational Fluid Dynamics (CFD), of the flow and velocity field of a bench scale electrocoagulation reactor for textile wastewater treatment, with the goal of selecting the best design for the cell, which consists in a continuous, multiple parallel plate reactor. Six scenarios were proposed combining the different values for the two studied variables: electrode width (7 cm, 9 cm and 11 cm) and number of electrodes (5 pairs or 6 pairs). The CFD simulations were carried out within the software COMSOL Multiphysics®, which solved the Navier-Stokes equations for the incompressible, laminar, steady-state conditions. The results showed that from the scenarios, the best for the desirable conditions within the reactor (good mixture, low velocity profile and few stagnant zones) were the configurations with 5 pairs of 7 cm wide and 6 pairs of 9 cm wide electrodes. A definitive design for the reactor will possibly be achieved in future studies which will include simulations for the concentration profile.

KEY WORDS
Environment; Computing; Electrocoagulation; Computational Fluid Dynamics.

1. Introduction
The large amount of wastewater generated by the textile industry often presents itself as an environmental issue, due to the presence of dyes, which are difficult to degrade [1]. The usual treatment techniques applied, such as coagulation and flocculation, require large areas to place the reactors and make use of great amounts of iron and aluminum salts. These chemicals, in turn, endanger the ecosystems and human health, making the use of alternative treatment technologies greatly advantageous. The potential of electrocoagulation for textile wastewater treatment has been discussed in various papers [2] [3]. It consists in a complicated process that involve chemical and physical phenomena, based on the production in situ of coagulants (ions) from sacrificial electrodes [4]. Despite the proven effectiveness of the technology, literature does not present a systematic approach to the design and operation of electrochemical reactors, due to the lack of a quantititative understanding of the interactions that occur within them, as well as the inability to predict their relative importance in a situation [5].

In this scenario, modelling and simulation studies may be very resourceful tools in the project of electrochemical reactors. A model or numerical tool that could allow predicting the resulting concentration profile of such a reactor for each change in configuration, dimensions or operational conditions, would make it easier to obtain a better design without the need for adaptations and experimental studies after the reactor is built.

Previous papers [6] highlight the importance of having a preliminary hydrodynamic characterization analysis of the electrochemical cell, despite most of the research devoted to electrocoagulation processes not presenting one. Thus, the aim of this paper is to present a simulation, through Computational Fluid Dynamics (CFD), of the flow and velocity field of a bench scale single channel, parallel plate electrocoagulation reactor for dye removal from a synthetic textile wastewater treatment. The study will allow to select the best design for the cell, and as a preliminary study for a posterior simulation study of the reactor’s concentration profile.

2. Process description
Briefly stated, electrocoagulation consists in applying an electrical current to sacrifice electrodes (a cathode and an anode) that oxidate, thus producing coagulants in the form of ions. These ions cause the destabilization and posterior coagulation and flocculation of the pollutants [4]. Simultaneously, the electrical current provokes water electrolysis, producing microbubbles of oxygen and hydrogen. The bubbles cause the flotation of the contaminants, which are then removed in the form of sludge [2]. This is why the process success is determined,
velocity profiles between the electrodes, and that the low turbulence intensity and velocity field inside the electrodes zone, thus providing aids to optimize the electrode design and operational advantage of fixed coagulant requirements [5].

The configuration also allows a serpentine flow, which is advantageous since the solution, by having opportunity to approach both anode and cathode, suffers from multiple changes in polarity along the path, thus making possible for a complete treatment in a single pass [4]. The reactor’s dimensions and operational conditions are presented in Table 1.

3. Previous studies

There have been successful studies presenting predictions of the flow profile of electrochemical reactors by CFD models, however few papers have studied configurations with multichannel multiple parallel plate electrodes [8]. CFD simulations of a rotating batch reactor for industrial wastewater treatment were used to analyze variations in the reaction time due to changes in the angular speed, and its relations to turbulence intensity and velocity field inside the electrodes zone, thus providing aids to optimize the impeller design and operation parameters [9].

A different paper regarding an electrochemical reactor with rotating ring electrodes proposed three different reactor configurations in order to study their performances in the mixing time and process costs through CFD simulations. The different arrays consisted in: without impellers; with a pitched blade central impeller; and with four internal vertical fins. It was found the latter was the best configuration [11].

The hydrodynamic behavior of a parallel plate multichannel electrocoagulation reactor and the effects on its performance were evaluated by means of a CFD software using a turbulent model (k-e). The CFD analysis indicated that the cell geometry arrangement generated low velocity profiles between the electrodes, and that the low velocity improved EC performance. Also, the study showed the impact of hydrodynamic behaviour in the removal of sludge and in the formation of clots [8].

Another hydrodynamics study for a parallel plate multichannel reactor was carried out through both CFD and Residence Time Distribution (RTD), and the latter was used to describe the flow path. The results showed an accurate description of channeling sections and stagnant zones that, according to the authors, should be taken into account [6].

4. Characterization of the electrocoagulation reactor

The reactor configuration as continuous, single channel with multiple parallel plate electrodes was defined based on guidance found in the literature. Continuous flow reactors, for instance, are more widely used and present the design and operational advantage of fixed coagulant requirements [5].

The configuration also allows a serpentine flow, which is advantageous since the solution, by having opportunity to approach both anode and cathode, suffers from multiple changes in polarity along the path, thus making possible for a complete treatment in a single pass [4]. The reactor’s dimensions and operational conditions are presented in Table 1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length (cm)</td>
<td>65</td>
</tr>
<tr>
<td>Width (cm)</td>
<td>12</td>
</tr>
<tr>
<td>Height (utile) (cm)</td>
<td>7.45</td>
</tr>
<tr>
<td>Electrode distance (cm)</td>
<td>5 (5 pairs configuration)</td>
</tr>
<tr>
<td>Volume (L)</td>
<td>9.5</td>
</tr>
<tr>
<td>Flow rate (L.s⁻¹)</td>
<td>7.916x10⁻³</td>
</tr>
<tr>
<td>Inlet velocity (cm.s⁻¹)</td>
<td>1.644</td>
</tr>
</tbody>
</table>

Since the object of study consists in a bench scale reactor, a low flow rate and inlet velocity as the ones adopted are to be expected, which is not a drawback to the project, since this condition also allows increasing retention time [4]. Six scenarios for the reactor design were proposed by testing different conditions for two variables: electrode width and number of pairs of electrodes (each pair consists of one anode and one cathode). The conditions for the tests are presented in Table 2.
## Table 2

<table>
<thead>
<tr>
<th>Test</th>
<th>Number of electrodes</th>
<th>Electrode width (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>7</td>
</tr>
<tr>
<td>2</td>
<td>5</td>
<td>9</td>
</tr>
<tr>
<td>3</td>
<td>5</td>
<td>11</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td>5</td>
<td>6</td>
<td>9</td>
</tr>
<tr>
<td>6</td>
<td>6</td>
<td>1</td>
</tr>
</tbody>
</table>

For illustration of the geometry of the reactor, since it is not possible to present all scenarios, the configuration for Test 4 is presented in Figure 1.

The fluid dynamics simulations were performed in the software COMSOL Multiphysics®, which applies the Finite Elements Method (FEM) in order to solve the partial differential equations of the fluid flow model. The result variable considered was the flow velocity. The procedure to build the geometry was based on a pre-existing tutorial application from the software [12]. Preliminary simulations were carried out using the laminar flow and the Turbulent flow (k-ε model) interfaces, both of which are based on the Navier-Stokes equations to model the fluid flow. Due to the low velocity profile resulting of both models, in the order of $10^{-2}$ m.s$^{-1}$ the laminar was chosen as the most likely to predict accurately the fluid flow in the reactor.

A few simplifications were made to perform the simulations, so that it was considered: the same density and viscosity as those of water for the effluent, since it is synthetic; an incompressible fluid; a steady-state flow; and a constant temperature of 293.15K.

To solve the Navier-Stokes equations for these conditions (incompressible, laminar, steady-state), the following conditions were imposed: a constant normal influx velocity at the inlet (value presented on Table 1); a constant pressure at the outlet of 1 atm; a no-slip condition to the walls (by which the fluid at the wall is not moving); and a symmetry condition in the top domain. The relative tolerance adopted was 0.001.

The mesh was generated automatically by COMSOL Multiphysics®, which self-adjusts to provide better refinement when there is a higher gradient. The predefined size of elements was set at “coarser”, and the element type setting was set at “All elements”, so that the final mesh was constituted by tetrahedral, pyramid, prism, triangular, quadrilateral, edge and vertex elements.

The resulting mesh varied from one Test to another, due to the different geometries of each, and the number of elements varied from approximately $1.6x10^5$ to $1.9x10^5$. For illustration, the resulting mesh for Test 4 is presented in Figure 2.

After computing the stationary study for each Test, the results for the velocity magnitude and velocity field were plotted in a 2D graph of the top surface of the reactor. The values for minimum, maximum and average velocities for each Test also were extracted from the simulations and discriminated in tables.

### 5. Results and discussion

In Table 3, the values for maximum, minimum and average velocities for the simulations are presented.

<table>
<thead>
<tr>
<th>Test</th>
<th>Maximum velocity$^a$ (cm/s)</th>
<th>Minimum velocity$^b$ (cm/s)</th>
<th>Average velocity$^c$ (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.23466</td>
<td>0.00000</td>
<td>0.32345</td>
</tr>
<tr>
<td>2</td>
<td>2.24591</td>
<td>0.00000</td>
<td>0.34504</td>
</tr>
<tr>
<td>3</td>
<td>2.23232</td>
<td>0.00000</td>
<td>0.41741</td>
</tr>
<tr>
<td>4</td>
<td>2.20596</td>
<td>0.00000</td>
<td>0.32150</td>
</tr>
<tr>
<td>5</td>
<td>2.21969</td>
<td>0.00000</td>
<td>0.34067</td>
</tr>
<tr>
<td>6</td>
<td>2.21324</td>
<td>0.00000</td>
<td>0.43308</td>
</tr>
</tbody>
</table>

Standard deviation: $^a0.0149; ^b0.000; ^c0.0489$

Firstly, the results displayed in Table 3 illustrate what was previous mentioned regarding the choice for the laminar model over the turbulent one. It is important to note that this configuration would indeed be interesting since researches show that a laminar regime in the reactor
chamber allows the formation of larger flocks, which are easier to remove [13].
The results show that there is not a pronounced difference for these parameters among the results. However, the average velocity does present a more apparent influence of the geometry, with a standard deviation close to 5%.
An important information obtained from Table 3 is that the minimum velocity for all the tests is zero, which means that all the configurations presented stagnant zones. From these data, however, it is not possible to determine how spread these zones are.
To better understand the fluid dynamics in the reactor, it is important to analyze the resulting velocity magnitude and velocity field graphs for the six simulations, which are presented in Figure 2.

(a) Velocity magnitude (m/s) and velocity field (arrow surface) for Test 1 (5 pairs of 7 cm-width electrodes)

(b) Velocity magnitude (m/s) and velocity field (arrow surface) for Test 2 (5 pairs of 9 cm-width electrodes)

(c) Velocity magnitude (m/s) and velocity field (arrow surface) for Test 3 (5 pairs of 11 cm-width electrodes)

(d) Velocity magnitude (m/s) and velocity field (arrow surface) for Test 4 (6 pairs of 7 cm-width electrodes)
The results analysis show that, as for the electrode size, both the 7 cm and 9 cm widths promoted a good mixture in the fluid, since the velocity profile was found to be more evenly distributed along the reactor. Besides the 11 cm width configuration allowing for an increase in the maximum fluid speed, it led to a straining in the velocity profile as well as to a spreading of the stagnant zones. This would possibly cause a decrease in the treatment efficiency and entrapment of sludge.

Also, it should be noted that an increment in velocity is not always advantageous, since it reduces retention time [4] and an excessive agitation may cause the agglutinated flocks to separate [10]. Indeed, studies [8] found that the better results for flock formation were obtained with the lowest flow rates (and consequent inlet velocities) among the tested conditions.

Regarding the definition of the number of electrodes, it is perceived that, as for the 7 cm width Tests, a raise in this variable (and consequent decrease in the distance between electrodes) led to a worse mixture in the fluid, and spreading of stagnant zones as well. For the 9 cm width configuration, an increase in the parameter allowed a desirable better flux distribution.

6. Conclusions

In order to achieve a definitive judgement for the best configuration of an electrocoagulation reactor, it is required to evaluate the concentration profile for each proposed design, which can be generated by including the mass balance for the studied component (in this case, dye) in the simulations. This implicates in knowing the reaction kinetics. However, the results obtained in this study allowed to obtain a preliminary knowledge of the fluid dynamics in the proposed reactor, which have great impact in the treatment success, hence saving resources in experimental tests that will not be needed.

The velocity magnitude profiles and velocity field for the tested configurations show that an electrode width of 11 cm is not an interesting option. For the 7 cm width configuration, the most adequate number of electrodes among the tested would be 10 (5 pairs), while for electrodes 9 cm width an increase to 12 electrodes could be better.

It is important to notice that the latter configuration, which presents both a larger width and greater number of electrodes, promotes an increment in the reactor treatment potential, once the contact surface also is increased.

By evaluating the concentration profile for the dye along the reactor, in future studies, it is believed that it will be possible to reach a consensus regarding the best configuration for the reactor.

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References


