Initial Approximation to the Design and Construction of a Photocatalysis Reactor for Phenol Degradation with TiO$_2$ Nanoparticles

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ABSTRACT: A photoreactor was designed, built, and optimized to carry out the degradation of phenol. To achieve this, phenol concentration was used as the reference to compare the photocatalysis reaction efficiency obtained through this research with results from other studies. Additionally, during the building process, different types of glass were evaluated with the objective of finding a functional and economic material to build the photoreactor. It was found that Pyrex glass was the most suitable material to work with. As a UV light source to build the photoreactor, a dry gel nail lamp was used with 9 W, $\lambda = 365$ nm bulbs. On the other hand, the effects of different parameters (such as the catalyst mass (TiO$_2$ Degussa P-25), stirring speed (RPM), UV lamps, and temperature) over the photocatalysis reaction rate were analyzed. Also, the reaction’s thermodynamic parameters were determined and found to be similar to those found in other investigations. Finally, the homogeneity in the distribution of TiO$_2$ particles inside the reactor when stirred at 475 rpm was verified using a COMSOL Multiphysics computer fluid dynamics simulation, which showed the theoretical trajectory of particles inside the reactor depending on the stirring rate of the reactor.

1. INTRODUCTION

Currently, heterogeneous photocatalysis is considered as one of the research areas among advanced oxidation processes of greater interest. In this process, a semiconductor material is irradiated with UV light to produce highly reactive oxygen species (e.g., hydroxyl radicals), which can carry out the degradation of organic compounds that are difficult to eliminate via traditional wastewater treatment methods.

Now, photocatalysis reactions require reactors with specific optic characteristics, such as a high transmittance and reflectance, using mostly clear materials, such as fluoropolymers (FP) and glass, which allow a high transmittance of UV rays to the sample. However, the main issue with fluoropolymers is their low mechanic resistance. Because of this, while using this material, it is necessary to increase the photoreactor’s wall thickness, thus decreasing the transmittance of UV rays.

Therefore, the most common material in photoreactor design and construction is glass, but its efficiency depends on the type of glass that is used. For example, common glass has a variable iron concentration in its composition, allowing different grades of UV light absorption. Compared to common glass, borosilicate glass (Pyrex) has a higher transmittance at wavelengths between 300 and 400 nm. However, the main disadvantage of this material is its high cost.

Additionally, to maximize the yield of the photocatalysis reaction, it is necessary to use materials that allow a high reflectance of UV radiation; in a photoreactor design, it is vital to consider various material characteristics to optimize the UV radiation that irradiates the catalyst. Among some of the materials used, silver mirrors are preferred for their high reflectivity in the visible spectrum, although their reflective capacity is poor for wavelengths between 300 and 400 nm; during the manufacturing process of these mirrors, common

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glass is used as a protective cover, diminishing the material’s capability to absorb UV radiation. On the other hand, aluminum is also used to fabricate various photoreactors. Nevertheless, when this material is oxidized, it loses its highly reflective characteristics.7

Currently, there are many UV lamp types available in the market. Those most commonly used in photoreactors are high-pressure mercury vapor, low-pressure mercury vapor, and fluorescent and xenon lamps, among others.6 Furthermore, other UV lamps with more specific applications can be easily found in common markets, as they are used to disinfect surfaces or even dry gel nail polish.

Regarding photocatalysts, titanium dioxide (TiO₂, Degussa P-25) is commonly used because of its physicochemical characteristics and high photocatalytic activity.5,6 This material’s characteristics of interest are the crystal size, specific surface area, pore structure, and high adsorption capacity.9 Phenol is considered as a priority pollutant (at concentrations over 1 mg L⁻¹) according to the United States of America Environmental Protection Agency (EPA). Therefore, it has been widely studied in photocatalytic reactions and used as a reference molecule for the evaluation and design of photoreactors.10,11

Now, there are aspects such as particle distribution that are not easily seen by the naked eye during experiments, but should be understood as they can explain how important parameters affect a reaction, such as the stirring speed. For this purpose, computational resources have become useful, by providing a mathematic environment where realistic approaches to phenomena can be modeled, without the need for specific and complex experimentation. When used effectively, computational resources such as COMSOL Multiphysics give accurate representations of the physical characteristics of a model, such as the temperature, pressure, and velocity profile of a continuously stirred fluid in a defined vessel or even the trajectory of a solid particle that interacts with a continuously stirred fluid inside a reactor.

The objective of this research is to (1) present the design of a photoreactor,12 (2) evaluate the effect of different reaction parameters over the photodegradation process13,14 and (3) verify the effect of stirring inside the reactor using simulation environments. For the reactor’s construction, economic and easy-to-access materials were used seeking to take advantage of the greatest amount of UV radiation possible. Finally, the phenol concentration was followed to determine optimum photoreactor design parameters. Thus, the reactor presented in this research can be used to study the degradation of different organic pollutants in an aqueous phase.

2. EXPERIMENTAL SECTION

2.1. Reactants.

- Photocatalyst: titanium(IV) oxide nanopowder; primary particle size: 21 nm (TEM); ≥99.5% trace metal basis (Aeroxide Degussa P-25, Sigma Aldrich).

- Phenol solutions: crystallized phenol, 99% (detached crystals), PS (pancreac), and distilled (type 1) water. A stock solution (1000 ppm) was prepared by weighing 1 g of phenol and dissolving it into a 1 L volumetric flask. After this, small amounts of stock solution were diluted in a 250 mL volumetric flask to obtain concentrations of 5, 10, 25, 33, 50, 75, and 100 ppm. The dilutions were evaluated under a UV−vis spectrophotometry (Thermo Spectronic Genesys S). Table 1 shows the physical properties of dyes and chemicals used in this work.

2.2. Equipment.

- Digital hotplate MaXtir 500 with an external/direct contact temperature probe. A temperature sensor is used inside the solution to verify that the temperature is always at the constant, desired value (298, 308, 318, and 326 K) when the reaction is taking place.

- Additionally, a magnetic stirrer (length 5 cm and Ø = 1 cm) was used at different stirring rates (0, 200, 400, 475, and 800 rpm).

3. RESULTS AND DISCUSSION

3.1. Photoreactor Construction. Seeking to use common, nonexpensive materials, a commercial lamp used to dry gel nail polish was used as a UV light source.10 This apparatus consisted of four 9 W lamps with a maximum wavelength peak of 365 nm each, an electronic circuit (used to toggle the device on and off), a piece of aluminum adhesive, and a plastic case. Almost all parts were used to design the photoreactor, only leaving the plastic case behind (Figures 1 and 2).

Figure 1. UV lamp used to dry the gel nail polish (picture taken by authors).

Regarding the reactor’s structure, it was important to evaluate how the glass type used for its construction affected the reaction’s efficiency; three types of glass were evaluated: common glass, Pyrex, and quartz. These materials were evaluated under a UV−vis spectrophotometer (Genesys S) to determine the materials’ transmittance in a wavelength range between 300 and 500 nm.

The results obtained during this test are shown below in Figure 3, where it is evident that in the visible range, between...
example, the quartz glass that was used had an iron percentage of 40 and 1.3%, respectively, at 300 nm. Quartz glass was chosen to build the photoreactor because of its high cost and the fact that, at a wavelength of 365 nm, all three materials have a transmittance of 100%. However, for wavelengths in the UV-A range (315−380 nm), common glass exhibits reduced transmittances inversely proportional to iron concentration in the sample (in an inversely proportional manner). Taking this into account, it is possible to infer that the material’s transmittance decreases as a function of iron concentration in the sample (in an inversely proportional manner). Taking this into account, Pyrex glass was chosen to build the photoreactor because of quartz’s high cost and the fact that, at a wavelength of 365 nm, Pyrex glass shows a transmittance of 99.7%.

### 3.2. Photoreactor Design

In a photocatalytic reaction, just like in other reactions, many variables must be controlled. In this case, the most important variables include the pH, temperature, stirring speed, UV lamp placement and wavelength, radiant flux, and initial concentration. Therefore, the instrumentation needed to control these variables must be included in the design of the reactor, as the control of the main variables that determine the reaction will ensure that the pollutant is being degraded and also give a better understanding of the degradation mechanism. The photon flux was determined by potassium ferrioxalate actinometry, and the obtained value was $9.37 \times 10^{15}$ photons/cm²/min.

Taking the need for instrumentation and control into account, the following design was proposed (Figure 4).

Figure 4 shows the reactor and the main parts that compose it, which are identified using the numbers in parentheses. A description of its functionality as well as every part’s measurements can be seen below. First, tube (1) (12.5 cm high, $\Omega = 0.6$ cm) is used for sample extraction. In this tube, a 5 mL syringe is connected and used to extract and retain small samples. Next, an L-shaped tube (2) (inner section: 5.7 cm, $\Omega = 0.6$ cm) is used as a gas inlet for the reaction to insert $N_2$, $O_2$, or air, if necessary. However, it is important to know that the reactor can function without the need of a gas inlet. Now, the photoreactor body (6) consists of two concentric cylinders ($\Omega = 6.6$ and $\Omega = 8.7$ cm). Inside the first cylinder, the reaction occurs, while between the boundaries of the two cylinders is the reactor’s jacket, which is used to control the reaction temperature, maintaining it at the desired temperature. The heating fluid used inside the jacket is water, which enters the jacket on tube (3) and exits the jacket on tube (4), and is recirculated constantly. Moreover, tube (5) is used as a gas outlet, where the concentration of $CO_2$ in the reactor can be analyzed, as $CO_2$ is one of the main products of the mineralization of organic compounds. Next, both the photoreactor body (6) and its lid (7) are made of Pyrex glass and reinforced with Teflon clamps as well as metal clamps. Finally, the top box (8) contains two UV, 9 W lamps, which operate at a maximum wavelength of 365 nm and a voltage of 120 V.

The photoreactor lid is manufactured using Pyrex glass. The reactor’s top view is shown in Figure 5.

Figure 5 depicts the following features: (1) is the tube used for taking the sample, (9) is a hole ($\Omega = 0.6$ cm) and a GL 25 screw cap, which is open at the top with an adjustable septum and is used to insert several instruments (Thermometer, Titrator, Thermocouple), and (10) is a hole ($\Omega = 1.2$ cm), which connects to a pH-meter. All of these holes are designed with shut-off valves or screw caps, which allow the analysis of the different variables necessary to evaluate the reaction at a certain time. Every hole can be sealed to eliminate environmental interference when the samples are evaluated.

### 3.3. Determination of Optimal Reaction Parameters

To successfully determine the photocatalysis reaction rate, it was modeled under a pseudo-first-order kinetic model with an apparent rate constant, which represents both the adsorption and reaction phenomena (eq 1).

$$\ln \frac{C_0}{C} = k_{app}t$$

where $C_0$ is the reactant’s initial concentration, while $C$ corresponds to its concentration at any moment of time ($t$). If the experiments adjust correctly to a pseudo-first-order kinetic model, then a linear function is obtained by plotting $\ln \left(\frac{C_0}{C}\right)$ vs $t$.

#### 3.3.1. Determination of the Optimum Weight of the Catalyst

To determine the optimum amount of the catalyst to be used in the photocatalysis reaction, the reaction’s degradation rate was evaluated for different amounts of the catalyst (10, 50, 77, 100, 150, and 200 mg). The results from these experiments are shown in Figure 6, where it is observed that for weights lower than 100 mg, the reaction rate is 33% lower than that for amounts larger than 100 mg; however,
further increase in the amount does not cause a significant increase of the reaction rate. In other words, once the mass of Degussa P-25 is greater than 100 mg, a screening effect occurs between the catalyst particles, giving rise to a photon barrier as a product of UV radiation. Therefore, to obtain a maximum degradation rate (equal to 0.07 h⁻¹), it is necessary to use 100 mg of the photocatalyst.

3.3.2. Influence of the Stirring Speed. Regarding the effect of stirring speed over the reaction rate, various stirring rates, between 0 and 1000 rpm, were evaluated to understand the effect of turbulence and catalyst distribution inside the reactor. According to the results shown in Figure 7, the degradation rate presents an upright increase between 200 and 400 rpm, reaching its maximum at a value near 500 rpm (475 rpm). In this case, when the maximum value of the apparent reaction rate \( k_{app} \) is equal to 0.44 h⁻¹, the particles are totally irradiated and homogeneously distributed inside the reactor.

On the other hand, at low stirring speeds, the particles settle at the bottom, while (Figure 4a) rates higher than 475 rpm create a concentration gradient by pushing most catalyst particles to the walls of the reactor away from the light by centrifugal forces (Figure 4b).

3.3.3. Effect of the Wavelength of UV Light. Besides the catalyst’s mass and stirring speed, the reaction rate also varies

Figure 4. (a) Frontal view of the reactor with the following main parts: (1) opening for taking the sample, (2) gas inlet (for N₂, O₂, or air, although the photoreactor may work without the insertion of gas into the system), (3) water inlet for the reactor’s jacket, (4) water outlet of the reactor’s jacket, (5) gas outlet for the main reaction’s products, (6) reactor body, (7) reactor lid, and (8) UV lamp vessel. (b) Frontal view of the reactor with its main dimensions in millimeters. (c) Frontal view of the reactor with the main dimensions of the inlet and outlet tubes in millimeters.

Figure 5. (a) Reactor’s top view. The main components shown are (1) tube for taking the sample, (9) connection to other instruments, and (10) connection to a pH-meter. (B) Reactor’s top view with the lid’s main dimensions in millimeters.

Figure 6. Influence of the catalyst’s mass over the reaction rate \( k_{app} \). These experiments were conducted under the following conditions: an initial phenol concentration of 100 ppm, a stirring rate of 800 rpm, and a temperature of 293 K. Each dot represents a different experiment, while the red and black dotted lines represent the maximum amount of catalyst and the data’s mathematical fit.
as a function of the light source used to stimulate the particles. To start a photocatalytic reaction, it is necessary to stimulate the catalyst with enough energy so that its photogenerated holes (h+) react and produce reactive oxygen species.\textsuperscript{19} For example, the energetic requirement for TiO\textsubscript{2} is equal to 3.02 eV, usually provided by wavelengths that are lower than 400 nm. Now, to ensure that the catalytic reaction is taking place, the light source must not only react with the pollutants. If the pollutant reacts with the light source, it will absorb radiation and produce specific reactions; this is a process known as photolysis.

Figure 8 shows that phenol’s photolysis occurs at a wavelength of 254 nm (using 9 W Phillips TUV bulbs). On the other hand, at 365 nm, there is no interaction between the UV light source and the molecule, maintaining a constant phenol concentration over time.

3.3.4. Effect of Temperature over the Reaction Kinetics. To test the effect of temperature over the reaction rate, this parameter was varied between 298 and 326 K under the following reaction conditions: an initial phenol concentration (C\textsubscript{0}) of 100 parts per million (ppm), 100 mg of TiO\textsubscript{2} Degussa P-25, and a stirring speed of 475 rpm. Figure 9 shows that the reaction rate increases proportionally with the temperature, achieving its maximum at 326 K. Additionally, the experimental data fit a first-order kinetic model in which the reaction’s efficiency depends on the temperature. Regarding the results in Figure 9, adsorption kinetics are exothermic;\textsuperscript{1} therefore, at low temperatures, the adsorption of pollutants onto the catalyst’s surface is favored, while product desorption increases with temperature.

Next, the Arrhenius expression (eq 2) was used to determine the reaction’s activation energy:\textsuperscript{20}

$$k_{\text{app}} = A e^{-E_a/RT}$$

where $k_{\text{app}}$ is equal to the apparent reaction rate, $A$ is the Arrhenius factor, $E_a$ corresponds to the reaction’s activation energy, $R$ is the constant for ideal gases (8.3144 J K\textsuperscript{-1} mol\textsuperscript{-1}), and $T$ is the reaction’s temperature (K). Now, the linear form of Arrhenius’s expression is as follows (eq 3):

$$\ln k_{\text{app}} = \ln A - \frac{E_a}{RT}$$

The activation energy ($E_a$) may be obtained by plotting $\ln k_{\text{app}}$ vs $1/T$, where the slope is equal to $-E_a/R$, while the y intercept corresponds to $\ln A$ (Figure 10). In this case, the experimental data approximate to a linear fit with a correlation coefficient ($R^2$) of 0.9975. This means that 99.75% of the data can be expressed by the equation obtained from the linear fit. In this case, the calculated value of the reaction’s activation energy corresponds to 21.95 kJ/mol, which is similar to the value of 21.44 kJ/mol reported in the literature.\textsuperscript{20}

Then, the thermodynamic parameters were determined using Henry Eyring’s linear equation (eq 4):\textsuperscript{21}

$$\ln \left( \frac{k_{\text{app}}}{T} \right) = \ln \left( \frac{K_h}{h} \right) + \frac{\Delta \approx \Delta^0}{R} - \frac{\Delta \approx H^0}{RT}$$
The values of $\Delta \approx S^0$ and $\Delta \approx H^0$ were obtained by plotting $\ln(k_{\text{app}}/T)$ vs $1/T$, where the slope corresponds to $-\frac{\Delta \approx H^0}{R}$ and the y-intercept corresponds to $\frac{\Delta \approx S^0}{R}$. These parameters can be calculated knowing that $K_0$ is Boltzmann’s constant ($1.3805 \times 10^{-23}$ J/K) and $h$ is Planck’s constant ($6.6261 \times 10^{-34}$ J/s). This plot can be seen below in Figure 11:

![Eyring plot](image)

Figure 11. Eyring plot.

After obtaining $\Delta \approx S^0$ and $\Delta \approx H^0$, it was possible to determine the standard Gibb’s free energy by using eq 5

$$\Delta \approx G^0 = \Delta \approx H^0 - T\Delta \approx S^0$$

Finally, after calculating all of the reaction and thermodynamic parameters, they were sorted into the following table:

As can be seen in Table 2, $k_{\text{app}}$ increases as the temperature increases. This can be explained by different processes that occur: (1) the temperature might affect the interfacial rate of electron transfer to oxygen due to the recombination rate slowly increasing with the temperature;22 (2) however, the holes localized on surface oxygen atoms are stabilized due to the adsorption of water;23 and (3) the temperature induces a faster rate of pollutant/product desorption, which might lead to a higher availability of active sites for surface reactions.

On the other hand, the enthalpy value of $\Delta \approx H^0 = 20.57$ kJ/mol shows that the photodegradation reaction is an endothermic process. Because of this, the overall reaction requires an initial stage of photon absorption on the catalyst’s surface to generate the electron–hole pairs, but the amount of energy is specific for each photocatalyst (TiO$_2$ Degussa P-25 uses a wavelength lower than 400 nm). This is also explained by the fact that the values obtained for the Gibb’s free energy indicate a nonspontaneous process. Finally, mechanisms that do not encompass photocatalysis are responsible for the negative entropy value.

### 3.4. CFD Simulations

After analyzing the effect of the stirring speed over the reaction rate, a group of computational models were developed to observe and compare this parameter’s effect over the velocity profile and particle distribution inside the designed reactor. This was achieved using COMSOL Multiphysics 5.2 implementing, first, a rotating machinery laminar flow model (rmspf) to determine the velocity profile of the fluid inside the reactor, with which it is possible to compute a particle tracing for fluid flow (fpt) model to identify the appearance of “dead” stirring zones with low to no particle movement. The model’s geometry and mesh are shown in Figure 12.

Regarding the model’s assumptions and inputs, first, it is assumed that after a short moment, the stirring speed reaches a constant value; therefore, it is possible to carry out a steady-state simulation with a constant stirring speed. Additionally, the reactor’s walls have a non-slip boundary condition, and water was modeled as an isothermal incompressible flow. Also, water was used as the reference fluid as the concentration of phenol in the reactor is very low, and so the fluid’s properties approximate very closely to those of water. Now, regarding the input parameters, the fluid is at a temperature of 318 K, with 1 atm reference pressure and an initial velocity field of 0 m/s, and is subject to a rotational speed of 475 rpm.

To observe the manner in which the particle’s velocity and distribution inside the reactor changed, the stirring speed was subjected to a parametric sweep, analyzing speeds of 100, 300, and 475 rpm. Stirring speeds higher than these were evaluated but not included because they failed to converge successfully. At higher speeds, a transition from a laminar flow regime to a turbulent flow regime appears. Because the reactor was modeled using a rotating machinery laminar flow model, changing the system’s physics requires new governing equations to fully characterize the system and this in turn

![Graph](image)

Figure 10. Arrhenius plot.

### Table 2. Phenol Photocatalysis Reaction Thermodynamic Parameters

| $T$ (K) | $k_{\text{app}}$ (min$^{-1}$) | $\ln(k_{\text{app}}/T)$ | $E_r$ (kJ/mol) | $A$ | $R^2$ | $\Delta \approx H^0$ (kJ/mol) | $\Delta \approx S^0$ (kJ/mol) | $\Delta \approx G^0$ (kJ/mol) | $R^2$ |
|--------|----------------|-----------------|---------------|-----|------|-----------------------------|-----------------------------|-----------------------------|------|
| 298    | 0.0013         | -17.09          | 21.95         | 0.15| 0.9975| 20.57                        | -0.270                     | 101.2                        | 0.9970|
| 308    | 0.0018         | -16.78          | 21.58         | 0.16| 0.9980| 20.37                        | -0.300                     | 101.2                        | 0.9970|
| 318    | 0.0023         | -16.55          | 21.79         | 0.20| 0.9985| 20.42                        | -0.280                     | 101.3                        | 0.9970|
| 326    | 0.0028         | -16.37          | 21.93         | 0.22| 0.9988| 20.55                        | -0.260                     | 101.4                        | 0.9970|
entails the input of new model parameters, which were not necessary to achieve the objectives of this study.

Figure 13 shows how particles change their velocity proportionally with the reactor’s stirring rate. First, it can be observed that because the designed reactor uses a radial stirring system, a dead or zero-velocity stirring zone is always present at the center of the reactor’s geometry. Additionally, this stirring mechanism is associated with low-turbulence regimes as the particles are homogeneously distributed among different velocity profiles across the x−y planes. Furthermore, these results match with those of Figure 7. For example, most particles in Figure 13a have a velocity ranging from 0 to 0.2 m/s, causing their sedimentation at the bottom of the reactor.

After obtaining the results for these simulations, it can be observed that because a radial stirring system is used, a dead stirring zone is always present at the center of the reactor’s geometry. This type of stirring mechanism is related to low-turbulence regimes as the particles are homogeneously organized among different velocity profiles across the x−y planes, explaining the UV screening effect observed for high stirring rates, when vortexes are formed. Furthermore, by analyzing the y−z velocity profiles, it is possible to observe that at higher stirring speeds, the average velocity inside the reactor increases, ensuring a homogeneous distribution of catalyst particles.

As evidence of this statement, it is possible to observe the velocity profile of the liquid inside the reactor across the x−z plane as this plane allows one to observe the behavior of the vortex and the streamlines generated by the magnetic stirrer’s movement.

In the case of Figure 14, the most representative differences between the velocity profiles may be observed in the diagonal and upper streamlines. For example, for a stirring speed of 100 rpm, the average speed of these regions is represented by a
dark blue color, which corresponds to a velocity of approximately 0.02 m/s. As stated before, this means that at low stirring speeds, the momentum transport inside the reactor occurs at the bottom of the flask. Therefore, there is not enough energy for the liquid to form a well-defined vortex capable of conferring enough vertical motion to the nanoparticles. On the other hand, for a speed of 475 rpm, these low-velocity dead zones are replaced by a more homogeneous velocity profile along the vertical axis. This can be seen in Figure 14c, as the velocity of the diagonal and superior streamlines resembles that at the bottom, at approximately 0.64 m/s.

Thanks to these simulations, it is possible to understand the effect of the stirring speed over the catalyst’s distribution inside a reactor and, therefore, on the reaction. This is extremely important because it ensures effective collisions between the catalyst and the pollutant, which, in turn, make sure that the reaction occurs. Also, regarding the simulation, considering that the results resemble what is seen in Figure 7, it is possible to say that the simulation is accurate and effective in showing a phenomenon that would need costly experimentation. Therefore, future works could use it as a predictor of how the reaction kinetics will be affected.

**CONCLUSIONS**

A photoreactor was effectively designed to evaluate the effect of different variables, such as temperature and stirring speed, on the photocatalytic degradation of phenol. The results obtained show that depending on the characteristics of the available UV lamp such as its wavelength, it is possible to select the correct glass material to use in the photoreactor’s design. In this case, the concentration of iron in Pyrex glass, which is a low-cost material, allows a high light transmittance at the used wavelength (365 nm UV-A). Using this type of glass, it was possible to obtain effective kinetic reaction parameters for the photodegradation of phenol. The optimal reaction parameters were a temperature of 318 K, a weight of 100 mg TiO₂ (Degussa P-25), and a stirring rate of 475 rpm, which allowed one to obtain a reaction rate of 0.0023 min⁻¹. Finally, the effect of stirring the reactor was explained through the computer fluid dynamics simulation of a stirred static reactor with solid particles using COMSOL multiphysics laminar flow and particle tracing models, which show that when the reactor presents a laminar mixing regime (stirring speeds lower than and equal to 475 rpm), as the stirring speed increases, the homogeneous distribution of particles is ensured; however, when the stirring speed is higher than 475 rpm and a turbulent regime is introduced into the system, the distribution will not be homogeneous, thus explaining the screening effect observed at high stirring speeds in the experimental data.

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**Figure 14.** Velocity profiles of the liquid inside the reactor for stirring speeds of (a) 100, (b) 300, and (c) 475 rpm.
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