Development and numerical modelling of a novel UV/H₂O₂ rotating flow reactor for water treatment

Minghan Luo, Wenjie Xu and Taeseop Jeong

ABSTRACT

The ultraviolet photochemical degradation process is widely applied in wastewater treatment due to its low cost, high efficiency and sustainability. In this study, a novel rotating flow reactor was developed for UV-initiated photochemical reactions. The reactor was run in a continuous flow mode, and the tangential installation of the inlet and outlet on the annular reactor improved reaction rates. Numerical modelling, which combined solute transport, radiation transfer and photochemical kinetic degradation processes, was conducted to evaluate improvement compared to current reactor designs. Methylene Blue (MB) decomposition efficiency from the modelling results and the experimental data agreed well with each other. The model results showed that a rotational motion of fluid was well developed inside the designed reactor for a wide range of inflow rates; the generation of ·OH radicals significantly depended on UV irradiation dose, and thus the degradation ratio of MB showed a strong correlation with the UV irradiation distribution. In addition, the comprehensive numerical modelling showed promising potential for the simulation of UV/H₂O₂ processes in rotating flow reactors.

Key words | advanced oxidation process, CFD, MB, photoreactor, UV/H₂O₂, water treatment

HIGHLIGHTS

- A novel efficient rotating annular reactor is applied to UV-initiated photo-reactor.
- The simulation of the UV-reactor is performed considering a 3D and continuous flow.
- CFD and photochemical kinetic models were applied to UV/H₂O₂ for wastewater treatment.
- Good correlation between experimental and CFD simulation results for flow rates.

INTRODUCTION

Advanced oxidation processes (AOPs) such as photochemical oxidation, Fenton oxidation and ozone oxidation have unique superiority in degrading refractory organic contaminants in wastewater. Addition of UV energy in the presence of H₂O₂ is an advanced oxidation process (AOP); when UV radiation is absorbed by H₂O₂, the molecule splits apart into two OH radicals, which makes much of the micropollutant oxidation occur. Among all the AOPs, the ultraviolet (UV)/hydrogen peroxide (H₂O₂) technique, which combines the advantages of UV and H₂O₂ methods, is becoming an attractive alternative for the degradation of organic contaminants that are difficult to remove by conventional water treatment processes. The UV-type AOPs have been widely applied in the disinfection process of drinking water, and research is being conducted to optimize the reactors for the disinfection procedure, some of which have been commercialized. However, few studies report optimization of the reactor design for wastewater treatment. Treatment of wastewater normally requires a long residence time for removing relatively high concentrations of pollutant species, and therefore a suitable reactor shape enabling
sufficient mixing, as well as matching fluid analysis (Sharpless & Linden 2005). In addition, the chemical reaction mechanism and kinetic rate constants are also required for the structural design of the reactor to enhance degradation performance.

Numerical models are widely employed in the analysis of UV based AOPs. For example, hydrodynamic models, UV radiation models and chemical reaction rate models of UV-AOPs systems (Sharpless & Linden 2003; Subramanian & Kannan 2010; Luo et al. 2017). Alpert et al. (2010) assessed the degradation performance for organic contaminants of the UV/H₂O₂ system through combined computational fluid dynamics (CFD)/UV/AOPs models which integrate UV radiation sub models, turbulence sub models and kinetic rate constants. The system parameters such as inlet flow rate, hydrogen peroxide capacity and the radical scavenger sensitivity analysis were also analyzed. This study indicated that the CFD model underestimated the experimental removal performance of Methylene blue in comparison with the results from pilot reactors. Besides, the reaction mechanisms of the degradation of organic contaminants by UV-AOPs consist of typical and complex radical chain reactions. Generally, the intermediates and final products resulting from the UV-assisted AOPs are sensitive to UV irradiation rates in the reactor as well as turbulence and mixing levels (Marchisio & Barresi 2005). Many studies have emphasized the important role of fluid dynamics and irradiation models of UV reactors in predicting the efficiency of disinfection processes (Domenico et al. 2010; Kumar & Bansal 2012; Boyjoo et al. 2013; Bagheri & Mohseni 2014; Li et al. 2016; Yu et al. 2016). Thus, effective CFD simulations should include turbulence models, UV irradiation models and reaction mechanisms that accurately describe the oxidation of contaminants. Similarly, the performance evaluation of the degradation process of organic contaminants by UV-AOPs should include the estimation of reactor characteristics such as hydrodynamic properties and UV irradiation rates.

Studies have been conducted to investigate the design of reactors (Hofman-Caris et al. 2012; Boyjoo et al. 2013; Li et al. 2016; Yu et al. 2016; Sanaa et al. 2020), the hydrodynamics involved (Casado et al. 2017) and the chemical reactions (Crittenden et al. 1999; Alpert et al. 2010; Domenico et al. 2010; Wols & Hofman-Caris 2012; Wols et al. 2015; Mouussavi et al. 2018; Gu et al. 2019). In order for contaminants in wastewater to be effectively treated by UV reactions, the target species should have as much contact as possible with the radicals generated by UV radiation. Hence, the wall surface of the UV reactor is normally designed to be close to the lamp, as the reaction is more active in the nearer region of the lamp. Most of the photochemical reactors in previous studies were designed as a long pipe type considering the UV irradiation distance and contact time for treatment. On the other hand, some other types of reactors were also developed in recent years. For example, Hofman-Caris et al. (2012) investigated the flow characteristics and treatment performances of UV-AOPs reactors in various shapes and equipped with different UV lamps of low pressure (LP) type, medium pressure (MP) type and dielectric barrier discharge (DBD) type. The hydrodynamics and chemical reactions in reactors were usually studied through dynamic models. Crittenden et al. (1999) developed a kinetic model for UV/H₂O₂ AOPs in a completely mixed batch reactor to predict the degradation of organic contaminant, demonstrating consistency between the predicted and experimental data. Recently, Casado et al. (2017) performed numerical computations for hydrodynamics, radiation transfer, mass transport and chemical reaction rates in an annular laboratory scale photo-reactor (ALSPR) based on a comprehensive multiphysics kinetic model. The results of photocatalytic activity from model predictions corresponded well to the experimental data, with errors in the range of 2% to 10% depending on the catalyst concentrations.

This work aims to promote the application of UV-based AOPs in the wastewater treatment field by developing a UV reactor with increased retention time as well as enhanced mixing effect. The numerical modelling method was used to evaluate the performances of the designed reactor, and the differences between the experimental and CFD results were analysed. Moreover, the turbulence models, irradiation models and chemical kinetics (reaction mechanisms and kinetic rate constants) were combined to simulate the chemical reactions that occurred in the reactor for optimization of the reactor.

**METHODS**

**Hydrodynamic and mass transfer model**

The hydrodynamic calculation is an important tool to understand the distribution of various species in the reactor. In this study, the simulation of the rotating annular UV-reactor (RUR) was conducted based on the assumption of a three-dimensional steady state. The fluid in the reactor is assumed to be Newtonian fluid – incompressible, isothermal with
constant physical properties and under turbulent steady state flow. The hydrodynamic and species transport equations are listed as follows:

The mass conservation equation:
\[ \nabla \cdot (\rho V) = 0 \]  
(1)

The momentum conservation equation:
\[ \nabla \cdot (\rho V V) = -\nabla P - \nabla \cdot \tau \]  
(2)

where, the stress tensor is calculated from
\[ \tau = \mu (\nabla V + \nabla V^T) - \frac{2}{3} \mu \nabla \cdot V U \]  
(3)

The species transfer equation:
\[ \nabla \cdot (\rho V m_i) = -\nabla \cdot J_i + R_i, \quad i = 1, 2, \ldots, N \]  
(4)

where the diffusive flux of species \( i \) is estimated using Fick’s first law of diffusion:
\[ J_i = -D_m \nabla (\rho m_i) \]  
(5)

In Equations (1)–(5), \( \rho, V, P \) and \( \tau \) are fluid density, velocity vector, pressure and the viscous stress tensor respectively. These equations related the stress tensor to the kinetic energy of the continuous fluid through computing the velocity field within the reactor based on the Newton’s law of viscosity. In addition, \( \mu \) is molecular viscosity, \( m_i \) is mass fraction of species \( i \), \( J_i \) is diffusive flux of species \( i \), \( R_i \) is the source rate of species \( i \) (net reaction rate per unit volume) and \( D_m \) is the molecular diffusivity of species \( i \) in the mixture.

**Radiative transfer model**

The radiative transfer equation (RTE) for an absorbing, emitting, and scattering medium at position \( \vec{r} \) in the direction \( \vec{s} \) is described as:
\[ \frac{dI(\vec{r}, \vec{s})}{ds} + (\alpha + \sigma_s) I(\vec{r}, \vec{s}) = an^2 \sigma T^4 \pi \]
\[ + \frac{\sigma_s}{4\pi} \int_0^4 I(\vec{r}, \vec{s}') \Theta(\vec{s}', \vec{s}) d\Omega' \]
(6)

where \( \vec{r} \) and \( \vec{s} \) are position and direction vectors, respectively. The \( I \) is the radiation intensity, which depends on position and direction, \( n \) is the refractive index, \( \sigma \) is the Stefan-Boltzmann constant (5.67 × 10^(-8) Wm^(-2) K^(-4)), \( \alpha \) is the absorption coefficient, \( \sigma_s \) is the scattering coefficient, \( \Theta \) is the phase function, and \( \Omega' \) is the solid angle. Additionally, \( (\alpha + \sigma_s) \) is the optical thickness or opacity of the fluid. The refractive index \( n \) is important when considering the radiation in semi-transparent media.

**The RUR system setup**

A flow through continuously operating the RUR was used for experimentally evaluating the CFD results, the RUR system is presented in Figure 1. The reactor has a tangential inlet and outlet, with an annular and rotation flow configuration, operated with an electrical power output of 17 W (UV-C, efficiency = 35%) low-pressure mercury lamp (G10T5 L, Light Sources Inc.), and longitudinally placed at the axial center of the reactor. The effective length of the lamp (20 mm outer diameter) and associated quartz sleeve (23 mm outer diameter, >98% transmittance at 254 nm) was in fact 300 mm. The internal diameter and length of the reactor are 100 and 500 mm, respectively. The internal diameter of the lamp (20 mm inner diameter) and associated quartz sleeve (23 mm outer diameter, >98% transmittance at 254 nm) was in fact 300 mm. The internal diameter and length of the reactor are 100 and 500 mm, respectively. The internal diameter of the inlet and outlet is 20 and 30 mm, respectively, and the length is 100 mm. The inlet flow rate was adjusted to the range of 1.963–23.550 L/min by setting the appropriate concentration of methylene blue and H_{2}O_{2}, and the hydraulic retention time varied from 10 to 120s. Flow rates of the MB and H_{2}O_{2} solutions were controlled by two peristaltic pumps.

**Figure 1 | Scheme of the UV/H_{2}O_{2} reactor system.**
Kinetic model

In this study, the degradation of Methylene blue (MB) was selected to determine the properties of designed reactor and to verify the suitability of the selected model. Methylene blue cannot be directly photolyzed by UV light nor react with $\text{H}_2\text{O}_2$ alone, only decolorized by ·OH generated in the reaction system. Thus, MB is a good indicator for the performance evaluation of UV/ $\text{H}_2\text{O}_2$ AOPs. The detailed kinetic models for UV/$\text{H}_2\text{O}_2$ systems have been reported in previous researches, particularly in the studies of (Crittenden et al. 1999) for continuous flow stirred tank reactors and Alpert et al. (2010).

Table 1 summarized the involved reaction equations and kinetic rate constants in the UV/$\text{H}_2\text{O}_2$ system to describe the production of the ·OH from $\text{H}_2\text{O}_2$ and the degradation of MB. In addition, the kinetic models were incorporated into the CFD model using the User Defined Function (UDF) of FLUENT Software to prescribe the net rate of each species in equations No.1 to No. 7 via $R_i$.

Geometry and mesh structure

A simple 3D geometry and mesh structure developed for the RUR were shown in Figure 2. The geometry was created in ANSYS Design Modeler software. RUR consists of a reactor with a total length of 500 mm, a 20 mm internal diameter inlet, a 30 mm internal diameter exit tube and a 5 mm wall thickness. The inlet exit tube was attached to the reactor in a tangential direction to increase the mixing and reactivity of the reactor. The inlet and outlet tubes were 100 mm in length to induce a rotating flow of the reactor. The RUR

<table>
<thead>
<tr>
<th>No.</th>
<th>Reaction equation</th>
<th>Rate constant, $M \cdot s^{-1}$</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\text{H}_2\text{O}_2 + h\nu \rightarrow 2 \cdot \text{OH}$</td>
<td>$\varnothing_{\text{H}_2\text{O}_2} = 0.5$</td>
<td>Alpert et al. (2010)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$\varepsilon_{\text{H}_2\text{O}_2} = 19.6 , M^{-1} \cdot \text{cm}^{-1}$</td>
<td>Alpert et al. (2010)</td>
</tr>
<tr>
<td>2</td>
<td>$\text{H}_2\text{O}_2 + \cdot \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2 \cdot (\rightarrow \text{H}^+ + \text{O}_2^-)$</td>
<td>$k1 = 2.7 \times 10^7$</td>
<td>Buxton et al. (1988)</td>
</tr>
<tr>
<td>3</td>
<td>$\text{H}_2\text{O}_2 + \cdot \text{O}_2 \rightarrow \cdot \text{OH} + \text{O}_2 + \cdot \text{OH}^{-}$</td>
<td>$k2 = 0.13$</td>
<td>Alpert et al. (2010)</td>
</tr>
<tr>
<td>4</td>
<td>$\cdot \text{OH} + \cdot \text{OH} \rightarrow \text{H}_2\text{O}_2$</td>
<td>$k3 = 5.5 \times 10^9$</td>
<td>Buxton et al. (1988)</td>
</tr>
<tr>
<td>5</td>
<td>$\cdot \text{OH} + \cdot \text{O}_2^- \rightarrow \text{O}_2 + \cdot \text{OH}^{-}$</td>
<td>$k4 = 7.0 \times 10^9$</td>
<td>Alpert et al. (2010)</td>
</tr>
<tr>
<td>6</td>
<td>$\cdot \text{OH} + \cdot \text{MB} \rightarrow \text{Products}$</td>
<td>$k_{\text{MB, OH}} = 2.1 \times 10^{10}$</td>
<td>Buxton et al. (1988)</td>
</tr>
<tr>
<td>7</td>
<td>$\text{HCO}_3^- + \cdot \text{OH} \rightarrow \text{CO}_3^- + \text{H}_2\text{O}$</td>
<td>$k_{\text{HCO}_3^- , \text{OH}} = 8.5 \times 10^6$</td>
<td>Buxton et al. (1988)</td>
</tr>
</tbody>
</table>

Composite

$$R_{\text{OH}} = 2\varnothing_{\text{H}_2\text{O}_2} \varepsilon_{\text{H}_2\text{O}_2} \text{E}_{\text{CFD}} - k_1[\text{H}_2\text{O}_2][\cdot \text{OH}] + k_2[\text{H}_2\text{O}_2][\cdot \text{O}_2^-] - k_3[\cdot \text{OH}][\cdot \text{OH}] - k_4[\cdot \text{OH}][\cdot \text{O}_2^-] - k_{\text{MB, OH}}[\cdot \text{OH}][\cdot \text{MB}] - k_{\text{HCO}_3^- , \cdot \text{OH}}[\cdot \text{OH}][\text{HCO}_3^-]$$

$$R_{\text{O}_2^-} = k_1[\cdot \text{OH}][\cdot \text{O}_2^-] - k_2[\cdot \text{H}_2\text{O}_2][\cdot \text{O}_2^-] - k_5[\cdot \text{OH}][\cdot \text{O}_2^-]$$

$$R_{\text{H}_2\text{O}_2} = -\varnothing_{\text{H}_2\text{O}_2} \varepsilon_{\text{H}_2\text{O}_2} \text{E}_{\text{CFD}} - k_1[\cdot \text{OH}][\cdot \text{OH}] + k_2[\cdot \text{H}_2\text{O}_2][\cdot \text{O}_2^-] - k_3[\cdot \text{OH}][\cdot \text{OH}] - k_5[\cdot \text{OH}][\cdot \text{O}_2^-]$$

$$R_{\text{MB, OH}} = -k_{\text{MB, OH}}[\cdot \text{OH}][\cdot \text{MB}]$$
volume was discretized into 132,529 structured and unstructured volume cells using ANSYS Meshing software.

Boundary conditions

The inlet velocity was in the range of 0.104–1.250 m/s, equivalent to a flow rate of 1.963 to 23.550 L/min. The inlet MB concentration as model contaminant equalled 0.5 ppm, and the inlet H2O2 concentration was set to 10 ppm. A no-slip boundary condition was imposed on the walls. In addition, zero diffusive flux of species was specified at the walls. As per radiation field boundary conditions, the radiation of lamp was defined as a zero-thickness wall semi-transparent, no-reflecting walls. The density and viscosity of water were considered 998.2 kg/m^3 and 1.003 × 10^3 Pa, respectively, the refractive index was assigned at 1.376 and absorption coefficient 12.78 (m^3/C0, UVT = 88%).

Numerical solution

ANSYS 16.2 Fluent was employed to read the mesh and perform the CFD computations. The segregated steady state solver was used to solve the governing equations. Second order upwind discretization scheme was applied except for pressure for which the standard scheme was selected. The SIMPLE algorithm was chosen for the pressure-velocity coupling. The variation of velocity magnitude, model contaminant concentration, and irradiation flux at several points of the computational domain were used as indicators of convergence (at least 20 iterations). Additionally, convergence of the numerical solution was assured by monitoring the scaled residuals to a criterion of at least 10^-4 for the concentration of MB. While the simulation was always tracked with time, the solution algorithm has been run with both steady and transient flow simulations.

Chemicals and analytical methods

For the UV-reactor experiments, chemicals used for the experiments were reagent grade or higher, supplied by Sigma-Aldrich. MB powder and H2O2 solution (30% w/v) were used. The MB and H2O2 were diluted separately with ultrapure laboratory water. Distilled water was used in all experiments and analytical determinations. The concentration of MB in the UV-reactor effluent was determined spectrophotometrically following the peak at 664 nm using a UV spectrophotometric probe (UV1800, Shimadzu Co., Japan spectrophotometer). The concentration of hydrogen peroxide was determined via UV spectrophotometry utilizing the I3^- method (Normal et al. 1994).

During this research, four combinations of flow rates were evaluated using MB in the RUR with stable state conditions. When the concentration of the treated MB did not change during 30 seconds, it would be determined as the final result data. A sensitivity analysis was also conducted to ensure that the model predictions were insensitive to small variations within the reported accuracy of the kinetic rate constants (Bagheri & Mohseni 2015).

RESULTS AND DISCUSSION

Hydrodynamics

Figure 3 displayed the streamlines of velocity magnitude (Figure 4(a)) calculated for the rotating annular UV-reactor (RUR). As can be seen from the stream line, the fluid from the inlet to the outlet of the reactor maintained the rotational force and showed a rotating flow. It was found that, without supplying additional rotational energy, the strong rotational flow was maintained at the center axis of the reactor due to the momentum of the fluid entering the inlet. This rotating flow around the UV lamp in the whole reactor plays a mixing role and extends water retention time without a dead zone.

For a better understanding of flow characteristics, velocity vectors were obtained at different distances from the bottom of the reactor (Figure 4(b)). As can be seen from Figure 4, the fluid velocity at the inlet of the reactor is larger, and then gradually decreases until the outlet is reached and flows out of the reactor. From the radial velocity vector distribution, the larger fluid velocity on the wall gradually decreases to the light source, which is due to the decrease of kinetic energy of swirling flow. The rotating fluid surrounds the UV lamp and inner reactor until it
reaches the exit of the reactor and leaves it. This kind of rotation flow helped to UV irradiate the chemical species in the water more uniformly, and extended the residence time of the species in the reactor. On the other hand, there is not only upward rotating flow but also downward rotating flow in the rotating reactor, which will play a positive role in the mixing effect in the reactor.

Figure 5 shows the horizontal (rotational force) velocity and the vertical (upward force) velocity according to the height of the reactor, respectively. As shown in Figure 5, the radius velocity in the reactor was about 10 times higher than the vertical velocity. This means that the fluid rose slowly while rotating quickly when moving from the inlet to the outlet, presenting more opportunities to react.
with UV or radicals. Therefore, compared to other same-scale pipe type reactors, this reactor can attain a more efficient treatment without extra energy and equipment because of increased chance of reaction in this reactor.

The results showed that the vertical velocity ($W$) was smaller compared to the radius velocity ($U$) under all flow conditions. As can be seen from Table 2, in the case where the inlet flow rate was highest (the shortest residence time), $U$ at the inlet of the reactor was 1.270 m/sec at the outlet of 0.209 m/sec, $W$ was 0.132 m/sec and 0.035 m/sec at the outlet, the velocity ($U$ and $W$) multiplied by about 9.6–5.8 times. In the case of the smallest influent flow rate (long residence time), the $U$ of the reactor inlet was 0.103 m/sec, the $U$ of the outlet was 0.009 m/sec, and the $W$ was 0.010 m/sec and 0.002 m/sec, respectively. The velocity component ($U$ and $W$) increased 10.3–4.9 fold. The results matched the flow characteristics in the reactor, which rose slowly while rotating at the inlet to the outlet of the reactor. Species rose slowly while rotating along the streamline, which increased the chance of contact with UV, therefore increasing the reaction rate. By maintaining the geometry of the inlet and outlet in the tangential direction of the reactor, a high reaction rate was achieved without additional mixing devices.

### Table 2 | Velocity component in the reactor due to the change in flow rate

<table>
<thead>
<tr>
<th>Flow rates</th>
<th>23.550 L/min</th>
<th>7.850 L/min</th>
<th>3.925 L/min</th>
<th>1.963 L/min</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max.</td>
<td>1.270</td>
<td>0.132</td>
<td>0.421</td>
<td>0.044</td>
</tr>
<tr>
<td>Min.</td>
<td>0.209</td>
<td>0.035</td>
<td>0.064</td>
<td>0.011</td>
</tr>
</tbody>
</table>
Radiation and reaction

Figure 6 shows the radiation intensity of the UV lamp along a perpendicular axis or bisecting the longitudinal axis of the UV/H\textsubscript{2}O\textsubscript{2} photoreactors, respectively. The radiation decreased with increasing radial distance from the lamp as a result of absorption in water (UVT = 88%, resulting in negligible effect) and the increasing circumferential area.

RUR performance was simulated based on the resolution of the CFD model, including the specific kinetics for the chemical reaction in the mass balance of the species. Using the dependence of the hydrodynamic distribution of RUR, the kinetic responses of the UV/H\textsubscript{2}O\textsubscript{2}/MB in Table 1 are represented in Figure 7 as the chemical reaction rates calculated by UDF.

The radius profile of the reaction rate showed that H\textsubscript{2}O\textsubscript{2} absorbed UV closer to the UV lamp and generated OH radicals, so its concentration was low. By contrast, the H\textsubscript{2}O\textsubscript{2} concentration was high near the wall of the reactor. Closer to the UV lamp, more OH radicals were generated to degrade MB. In other words, OH radicals increased around the lamp and with increasing UV intensity, while H\textsubscript{2}O\textsubscript{2} and MB concentrations decreased closer to UV lamp.

On the other hand, since UV was barely irradiated at the inlet (P-1) of the reactor, H\textsubscript{2}O\textsubscript{2} was hardly decomposed, so the radial profile imparted a high concentration from the central location (P-2, P-3, P-4) of the reactor to the wall almost uniformly, the OH radical concentration was low, thus the MB maintained a high concentration at each position. However, the concentration profile of the outlet cross section (P-5) without irradiation with UV had a tendency similar to that of the central location (P-2, P-3, P-4) compared with the central location of the reactor (strong UV irradiation). The flow pattern of the reactor showed the plug flow shape. These results demonstrate that the most efficient way to increase the photolysis reaction efficiency was to increase the chance of contact between UV light and the target reactant.

Ultimately, the two most important considerations in the photochemical reaction processing of UV/H\textsubscript{2}O\textsubscript{2} were: (i) the H\textsubscript{2}O\textsubscript{2} concentration should be kept at high concentration near the irradiating UV lamp, because H\textsubscript{2}O\textsubscript{2} and UV irradiation were indispensable to produce OH radicals; (ii) reaction efficiency can be increased by increasing contact opportunity between the generated OH radicals and the species (MB). This can be achieved in various ways.
One was maximizing UV light intensity, for which a pipe type reactor with a small diameter can be considered (Hofman-Caris et al. 2012; Kumar & Bansal 2012; Wols et al. 2015; Li et al. 2016). However, this method’s disadvantage is that the contact time (residence time) required for the reaction can be obtained only with a long reaction pipe (pipe).
Figure 8 | Molar concentration of species at different flow rates (a, b, c and d corresponds to H$_2$O$_2$, OH, O$_2$ and MB, respectively).
length. Another one was to install a baffle to increase vortex inside the reactor (Alpert et al. 2010; Bagheri & Mohseni 2015; Yu et al. 2016). It was possible here on a small-scale reactor (lab scale), but is infeasible on an industrial scale. Another method is to use an adsorption medium (catalyst) for adsorption (Casado et al. 2017). However, the catalyst reduces the penetration of UV irradiation. In conclusion, reactor design is a key variable for water or wastewater treatment of photochemical reaction process using OH radicals. In this study, we propose a method to maximize the rotational force of the fluid by adapting the inflow water velocity.

The calculated contours of hydrogen peroxide for the RUR with different flow rates are presented in Figure 8(a). Only minor changes in H2O2 concentration occurred in high flow rates, where the hydraulic retention times were rather low when a considerable spatial variation in H2O2 photolysis took place in the position of the lamp installed. Contours of hydroxyl radical concentrations along the RUR with different flow rates are presented in Figure 8(b). Given the key role of ·OH concentration, it was important to investigate the profile and distribution of ·OH within the reactors. As displayed in Figure 8(b), ·OH was densely concentrated around the UV lamp, varying from $2.594 \times 10^{-2}$ to $2.854 \times 10^{-1} \text{mol/m}^3$. Regions of high hydroxyl radical concentration resulted from both the complex generation and termination reactions and from the transport phenomena occurring in the UV/H2O2 photoreactors with significant concentration gradients displayed in the radial direction. Obviously, the longer the retention time, the higher the concentration of OH radicals from direct photolysis of H2O2. Considerable OH radical concentration was still present at lower flow rate. This underscored the determining role of mass transfer on the performance of the UV reactor.

In order to gain a better understanding of the efficacy of the UV/H2O2 process at different flow rates in the RUR, local concentration contours of MB along the reactor are presented in Figure 8(d). The concentration of MB in the steady state gradually decreased from the entrance towards the exit: the higher the flow rates, the smaller the dose of radiation and ·OH concentration (Bagheri & Mohseni 2014). As shown in Figure 8, decreasing the flow rate rapidly incremented active reactor volume along the annular reactor passing in the proximity of the UV lamp.

The results of each flow rate through a certain time is shown in Figure 9. The degradation efficiency of MB increased as the flow rate decreased and achieved a stable state after 80–200 seconds. This is because, as the flow rate became smaller, the retention time of the species was longer, resulting in an increased opportunity for photo-degradation. However, after a period of active photolysis, the balance between supply and demand in each species no longer changed. This continuous flow experiment was different from the batch reactor, as the treatment efficiency of pollutants was not a function of time.

Figure 10 displays methylene blue conversion percentages obtained when using the same experimental parameters with four different flow rates. As shown in Figure 10, it was evident that low flow rate conditions produced a good degradation of the MB. Indeed, low flow rates can also get more UV dose and promote reaction between species. Overall, the CFD model fitted experimental data very well, and the discrepancy may be attributed to higher scavenging contribution by MB degradation by-products.

**CONCLUSIONS**

To evaluate the reaction characteristics of the rotating annular UV-reactor, the kinetic and CFD models of the species
were simulated. In the radial profile of the reaction rate, H₂O₂ absorbed UV closer to the lamp and generated OH radicals, so their concentration was low and H₂O₂ concentration was high near the wall. More OH radicals were produced closer to the UV lamp, which resulted in a higher rate of MB degradation due to OH radicals. The OH radical concentration showed an opposite trend compared to H₂O₂, whereas the MB showed the same concentration profile as H₂O₂. Two of the most important considerations in UV/H₂O₂ photochemical reaction processes were that first, a high H₂O₂ concentration should be kept around the UV radiation lamp. Second, the efficiency of the reaction can be increased by increasing contact opportunity of the generated OH radicals with MB. In this study, inflow velocity of the inflow water was used to maximize the utilization of the rotational force of the fluid.

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**DATA AVAILABILITY STATEMENT**

All relevant data are included in the paper or its Supplementary Information.

**REFERENCES**


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