CFD modeling of annular photoreactor hydrodynamics: Evaluation of alternative turbulence models

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Abstract: The hydrodynamics of an annular reactor is characteristic of its overall performance and it helps to evaluate the nature of flow patterns in the reactor. In the present study, the influence of three turbulence models: Standard K-ε, Realizable K-ε, and Reynolds stress model (RSM), on the simulation results were evaluated in two annular UV reactor configurations through computational fluid dynamic (CFD). The velocity distribution was characterized to assess the flow structures within the reactors. The CFD simulations performed in both annular reactors revealed that the inlet region plays an important role in the reactor hydrodynamics and consequently on its performance.

Keywords: Hydrodynamic, Annular UV reactor, Turbulence models, Simulation, Computational fluid dynamic.

I. INTRODUCTION

The use of photoreactors in water treatment applications has increased substantially over the past few years, they are commonly employed in ultraviolet (UV) disinfection and UV-based advanced oxidation processes (AOPs). These UV technologies are innovative, reliable, and cost-effective solutions for treating enormous diversity of toxic and emerging pollutant components which are continuously released into the environment after little or no treatment.

Recently, the modeling of UV photoreactors experienced a great intention because it can contribute to our understanding of UV technology for water treatment, allowing for the full benefit of UV photoreactors and can help the designer to obtain the main parameters to meet the best performance and the least energy consumption. As it is well known that the performance of ultraviolet reactors used for water treatment is greatly influenced by hydrodynamics, reliable modeling of the reactor flow structure is therefore crucial for the design process. A very effective approach to tackle this challenge is computational fluid dynamics (CFD). This tool is a well-established technique for the analysis of systems involving fluid flow, radiation transfer, mass transfer, reaction and associated phenomena.

Among the factors that may influence the CFD results are the discretization of the domain (structure and size of the cells), and the type of modeling approach employed (turbulence model). The quality of the grid has a direct influence on the quality of the analysis, regardless of the flow solver used. Additionally, the solver will be more robust and efficient when using a well-constructed mesh.

Although several researchers have used turbulence models to analyze and improve the hydraulics through UV systems (Liu et al. 2007; Wols et al. 2010; Chen et al. 2011), few of them used structured grid (Sozzi and Taghipour 2006; Duran et al.
In this study, the influence of three turbulence models: Standard K-\(\varepsilon\), Realizable K-\(\varepsilon\) and Reynolds Stress Model (RSM) on the simulation results of two annular reactors, was evaluated by CFD, using hexahedral meshes in three-dimensional geometries. Structured grids generally lead to fast and accurate flow solvers and are therefore preferred where the cost of generating the grid is not excessive. Both mesh quality and grid independence of the solution, were ensured.

II. PHOTOREACTORS GEOMETRY

The schematic diagram of the two photoreactors used in this study is depicted in Figure 1, (a) for U-shape and (b) for tubular reactors. The geometries were created in commercial software Gambit (Gambit® 2.4.6). The photoreactors are composed of two concentric cylinders.

In the U-shape photoreactor, the aqueous solution to be treated enters the system from the top, flows through the annular space between the inner shell of the reactor and the quartz sleeve, containing the UV lamp that radiates the circulating water, and exits through the outlet. The inlet and outlet tubes were placed 0.025 m from each respective end to form a U-shape annular reactor. The inlet tube length was chosen to be 45 diameters in length to ensure that a fully developed flow was established at the entrance of the reactor.

In the tubular photoreactor, as the water flows into the system, it circulates in the annular space, before exiting through the outlet along the reactor body. In this system, two equal-sized UV lamps in series with a total length equal to that of the reactor were considered.

The photoreactors descriptions and operating conditions are summarized in Table 1.
Table n° 1, Photoreactors descriptions and operating conditions

<table>
<thead>
<tr>
<th>Parameters</th>
<th>U-shape reactor</th>
<th>Tubular reactor</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Reactors body</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Length (m)</td>
<td>0.94</td>
<td>1.68</td>
</tr>
<tr>
<td>Diameter (m)</td>
<td>0.089</td>
<td>0.089</td>
</tr>
<tr>
<td>Inlet/outlet diameter (m)</td>
<td>0.022</td>
<td>/</td>
</tr>
<tr>
<td><strong>Quartz sleeve</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Length (m)</td>
<td>0.94</td>
<td>1.68</td>
</tr>
<tr>
<td>Diameter (m)</td>
<td>0.02</td>
<td>0.02</td>
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<tr>
<td><strong>UV lamp</strong></td>
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<td></td>
</tr>
<tr>
<td>Type</td>
<td>Low pressure</td>
<td>Low pressure</td>
</tr>
<tr>
<td>Number</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>Length (m)</td>
<td>0.84</td>
<td>0.84</td>
</tr>
<tr>
<td>Output power (W)</td>
<td>39</td>
<td>39</td>
</tr>
<tr>
<td><strong>Operating conditions</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Flow rate (m³/s)</td>
<td>1.82×10⁻³</td>
<td>1.82×10⁻³</td>
</tr>
<tr>
<td>Inlet velocity (m/s)</td>
<td>4.789</td>
<td>0.308</td>
</tr>
<tr>
<td>hydraulic diameter (m)</td>
<td>0.069</td>
<td>0.069</td>
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<tr>
<td>Re</td>
<td>21167</td>
<td>21167</td>
</tr>
<tr>
<td>Turbulent intensity %</td>
<td>5</td>
<td>5</td>
</tr>
</tbody>
</table>

III. MESH STRUCTURE

The mesh generator Gambit was used to create the grid. The hexahedral cells were used to discretize the reactors domains. In order to generate structured mesh for U-shape reactor, the domain was split into several subvolumes. The utilized grid for the reactors has 1474000 and 201600 elements for U-shape and tubular reactors respectively, and they were verified to give mesh independent results.

IV. BOUNDARY CONDITIONS

The boundary conditions for the CFD model were defined as follows. Water (liquid H₂O) was utilized as the main primary fluid in the system. At the inlet, the velocity of the fluid was specified (Table 1). The direction of the flow was defined normal to the boundary. At the outlet, a fully developed flow condition was considered. At all the walls, a no-slip boundary condition was imposed.

V. CFD SOLUTION: METHOD AND STRATEGY

Commercial CFD code Fluent (Fluent® 6.3.26) was used to perform simulations. The governing equations were solved using pressure based three-dimensional solver. Since flow in this system is found to be turbulent, three turbulent models were used; Standard k-ε, Realizable k-ε and Reynolds stress model (RSM), with standard wall functions. First order upwind discretization scheme was employed except for the pressure where STANDARD was selected. The SIMPLE algorithm was chosen for the
pressure-velocity coupling. Convergence of numerical solution was ensured by monitoring the scaled residuals to a criterion of $10^{-5}$ for the continuity, momentum variables and the turbulence parameters.

VI. RESULTS AND DISCUSSION

VI.1 U-shape reactor

Figure 2 (a), (b) and (c) shows the contours of velocity magnitude in cross sections along the U-shape reactor, computed using the Standard K-ε, Realizable K-ε, and RSM turbulence models, respectively. Clearly, the highest velocity magnitude can be found at the inlet and the outlet.

It can be seen that the fluid enters the reactor body from the top with a steep velocity gradient. When the flow reaches the lamp surface, it is diverted, then recombines below the lamp and detaches as a jet in an upward movement towards the entry along and parallel to the reactor walls. This fluid motion generates two symmetric recirculation zones confining stagnation regions characterized by low velocity. The generation and location of such zones at the entrance of the annular region in similar reactor geometry were observed numerically and experimentally using PIV techniques by Sozzi and Taghipour (2006) and numerically by Duran et al (2009).

Furthermore, it can be perceived (Figure 3) that there is non-uniformity in the flow at the entrance of the annulus region due to separation, recirculation, and reattachment of the flow at this area. Then, the motion dissipates and the fluid starts flowing in parallel direction of the length of the chamber towards the outlet with small velocity gradients.

Clearly, the velocity fields computed using different turbulence models don’t predict similar distributions for the fluid recirculation zones located at the entrance of the annular region (between the inner tube and the outer wall).

We can also notice that the Standard K-ε model shows an important stagnation zone in the lower region of the first third of the reactor, while the Realizable K-ε and RSM models display significant stagnation zones in the upper region of the last two thirds of the reactor.
Figure 2: Radial cross sections of velocity magnitude along the U-shape reactor obtained using Standard k-ε model (a), Realizable k-ε model (b) and RSM model (c)
Figure 3: Contours of velocity magnitude along the U-shape reactor obtained using Standard k-ε model (a), Realizable k-ε model (b) and RSM model (c)
VI.2 Tubular reactor

Figure 4 shows the contours of velocity magnitude for tubular reactor using similar turbulent models as for the U-shaped reactor. The analyzed results, for the tubular geometry, indicate that the velocity along the reactor is almost uniform, a higher velocity magnitude is observed at the middle of the annular region in comparison to the walls. Clearly, the turbulence models used (Standard K-\(\varepsilon\), Realizable K-\(\varepsilon\) and RSM) predict accurately the velocity distribution within the reactor and give similar results.

(a)  

(b)
VII. CONCLUSION

In this study, CFD simulations were carried out in order to evaluate the accuracy of different hydrodynamic models for the prediction of fluid flow in two annular reactors operating at the same flow rates and conditions. The investigation focused on the effect of turbulence models on the numerical solution for both reactor geometries.

The velocity fields computed within the tubular reactor are shown to be almost uniform, and therefore not affected by the turbulence model used. Whereas, the influence of these models on the velocity distribution is seen to be significant within the U-shape reactor. This is due to the complexity of the fluid flow in this type of reactor especially at the inlet region where high velocity gradients and flow separation are encountered.

The CFD simulations performed in both annular reactors revealed that the inlet region plays an important role in the reactor hydrodynamics and consequently on its performance.

These CFD models represent the flow structure that could be used for UV reactor performance simulation by integrating radiation distribution and reaction kinetics models.

References


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