Simulation Design and Optimization of UV-LED Water Purification System Based on Fluid Dynamics and Radiometry

Rui Liu, Chao Zhou, Rucong Lu and Jiang Zhang*
Department of Physics, South China University of Technology, Guangzhou, China

*Corresponding author email: jonney@scut.edu.cn

Abstract. In this paper, we established the flow field and radiation intensity distribution models of water purification equipment based on computational fluid dynamics (CFD) technology and radiometric principles. From geometric shape to hydraulic state and radiation intensity distribution, we fully simulated the real scene of the Ultraviolet LED (UV-LED) water purification system, and provided the reliable data for the UV-LED in the water purification field. Compared with mercury lamp, UV-LEDs have a more flexible layout to produce a variety of radiation intensity distributions. UV dose (the product of radiation intensity over time) is an important indicator. We used a discrete phase model (DPM) to track the path of microbial particles, and found that the residence time of microorganisms in different parts of the model was different. By optimizing the UV-LED layout, the radiation intensity was increased in the sites where the microbes resided longer. The results show that we can improve the efficiency of the water purification equipment by simply adjusting the UV-LED layout without increasing the power, and make the UV dose achieves the national standard.

Keywords: Computational fluid dynamics; Water purification model; UV-LED; UV disinfection.

1. Introduction

Fresh water resources on the earth account for only 2.53% of the total\(^1\), in recent years, the reserves and quality of fresh water have decreased\(^2\). The World Health Organization (WHO) survey pointed out\(^3\), one in six people in the world have difficulty in obtaining stable and clean water in their lives. Therefore, it is meaningful to purify domestic water. UV sterilization method is easy to operate, safe and stable, and has higher efficiency, doesn’t produce toxic by-products and secondary pollution\(^4\). UV disinfection technology is widely concerned because of its energy saving and environmental protection. At present, most UV water purification equipment uses mercury lamps to emit ultraviolet light\(^5\). However, mercury lamps still have some disadvantages, such as their efficiency being affected by temperature and glass tubes being easily broken, resulting in mercury contamination\(^6\). In 2016, China ratified the Minamata Convention on mercury, the Convention requires us to gradually restrict the import, export and production of mercury-containing products starting in 2020\(^7\). Compared with the mercury lamp, UV-LED has many advantages, such as its fast start-up, narrow half-peak width and small size\(^8\). Moreover, we can control the distribution of radiation intensity by changing the layout of the UV-LED. It’s inevitable that UV-LED will gradually replace mercury lamps, therefore, the research on UV-LED water purification system has important scientific and practical significance.

We first established a 3D model of the water purification equipment, and then constructed a calculation model based on the physical properties of the fluid and radiation. We track the motion trajectory of microbial micelles through the discrete phase model (DPM) in Ansys Fluent. The movement process...
showed that microorganisms stayed longer in the upper part of the water purification model, so we moved some UV-LEDs installed in the lower part to the upper part of the model. Through this operation, we increased the UV dose without increasing the power. However, the mercury lamp as a whole cannot achieve such a flexible design. At present, there are very few studies on the effect of UV-LED layout on equipment efficiency. Therefore, the results of this article have important scientific and practical significance for the related design and research of UV-LED water purification equipment.

In our work, we first established a 3D geometric model, then set the relevant parameters to establish a calculation model, and finally analyzed the results according to the calculation method of the ultraviolet dose, and evaluated the optimization effect. In the second part, we briefly explained the principle of the calculation model and the calculation method of the effective ultraviolet dose. The third part showed our model and analyzed the results. Finally, we put forward conclusions and prospects.

2. Method

2.1. CFD Model

Computational fluid dynamics (CFD) is an independent subject based on numerical calculation methods and classical fluid dynamics. The principle of CFD is to replace the continuous physical quantity with a series of finite discrete points, establish the relationship between the variables on the discrete points, obtain a set of algebraic equations, and then solve the algebraic equations to obtain the approximate values of the variables. Usually, the finite volume method is used [9].

The CFD calculation process includes [10]: establish geometric models, establish control equations, mesh division, parameter settings, simulation calculations, and display results. The choice of governing equation is a fundamental issue. The water purification system in this paper works in a turbulent environment. So we used the standard \( k - \varepsilon \) two-equation model. The transport equation of turbulent kinetic energy \( k \) and turbulent energy dissipation \( \varepsilon \) are:

\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho ku_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left[ (\mu + \frac{\mu_t}{\sigma_k}) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k
\]  

(1)

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho \varepsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left[ (\mu + \frac{\mu_t}{\sigma_\varepsilon}) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_{3\varepsilon} G_b) + G_b - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} + S_\varepsilon
\]  

(2)

\[G_k = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} \]  

(3)

\[\mu_t = \rho C_{\mu} \frac{k^2}{\varepsilon} \]  

(4)

The above formulas are expressed in the form of a tensor index. Among them, \( \rho \) is the fluid density; \( \mu \) is the dynamic viscosity; \( \mu_t \) is the turbulent viscosity; \( u_i, u_j \) are the time average speed, the values of \( i \) and \( j \) are (1,2,3); \( S_k, S_\varepsilon \) are the source terms; \( G_k \) is the production term of turbulent kinetic energy \( k \) caused by the average velocity gradient; \( G_b \) is the production term of turbulent kinetic energy \( k \) caused by buoyancy; \( Y_M \) is the fluctuation caused by the pulse expansion of the compressible fluid in the turbulent state; \( C_{1\varepsilon}, C_{2\varepsilon} \) and \( C_{3\varepsilon} \) are all experience coefficients.

2.2. Radiative Transfer Equation

Ultraviolet is a type of electromagnetic radiation. During the transmission process, radiation is affected by both enhancement and attenuation. The transmission equation is [11].
\[-\mu \frac{dI(\tau, \Omega)}{d\tau} = -I(\tau, \Omega) + \frac{\sigma}{4\pi} I_0 e^{-\tau/\mu_0} P(\Omega, \Omega_0) + \frac{\sigma}{4\pi} \int_{4\pi} I(\tau, \Omega') P(\Omega, \Omega') d\Omega' \quad (5)\]

Among them, \(\mu = \cos \theta\), \(\theta\) is the Angle between the direction of radiation and the normal of the dielectric layer; \(\mu_0\) is the cosine value of the initial incident direction; \(I_0\) is the initial radiation intensity; \(\Omega_0\) is the initial transmission direction; \(\tau\) is the optical thickness, the optical thickness between any two points \(s_1\) and \(s_2\) is \(\tau = -\int_{s_1}^{s_2} k \rho ds\); \(\sigma\) is the scattering reflectance; \(I(\tau, \Omega')\) is the radiant intensity of the propagation direction \(\Omega'\) at the optical thickness \(\tau\); \(I(\tau, \Omega)\) is the radiation intensity in the \(\Omega\) direction at the optical thickness \(\tau\); \(P(\Omega, \Omega')\) is the proportion of radiation in the \(\Omega'\) direction that is scattered to the \(\Omega\) direction; \(P(\Omega, \Omega_0)\) is the proportion of radiation in the \(\Omega_0\) direction that is scattered to the \(\Omega\) direction.

2.3. Calculation of UV Dose

We used DPM model to obtain the movement path data of microbial particles, and then integrated the product of radiation intensity and time along the path. We supposed the time taken by the particle to move a short distance is \(dt\), so the ultraviolet dose \(D\) obtained by this particle is:

\[D = \int [I(x(t), y(t), z(t))] dt \quad (6)\]

The value of radiation intensity \(I\) depends on the position, and the position coordinates will change with time. \([x(t), y(t), z(t)]\) is the coordinates at time \(t\).

The intensity of UV radiation at position \(l_1\) and position \(l_2\) is \(I_1\) and \(I_2\), the movement time is \(\Delta t\). Accumulate the values at all position, the UV dose obtained by the microbial particles on the entire path is:

\[\sum \Delta D = \sum (\Delta I_i \times \Delta t_i) \quad (7)\]

\[\Delta I_i = \frac{I_i + I_{i+1}}{2} \quad (8)\]

3. Results and Discussion

We arranged 16 UV-LEDs at equal intervals length-wise in the shape of mercury lamps. The starting point is 2 cm from the bottom, and the spacing is 3 cm, each UV-LED has a power of 30 mW, the wavelength of light is 165 nm. The water flow velocity at the inlet is 0.4 m/s. The outlet is connected to the atmosphere. Set the reflection of ultraviolet rays on the wall to Lambertian scattering, for other parameters such as absorption coefficient and refractive index, we can directly import the parameters related to liquid water from the material library of the software. The model of water purification equipment and the UV-LED layout are shown in Figure 1. The motion path of the microbial particles is shown in Figure 2.
Figure 1. Water purification equipment model and UV-LED layout

Figure 2. Microbial particle motion path

Figure 3. The relationship between particle velocity and movement time

Figure 4. The time the particle travels along the vertical axis

We selected ten particles and analysed their movements. As can be seen from the figure 3 and 4 above, microorganisms stayed longer in the upper half of the water purification model. The closer a point is to the UV-LED, the stronger the radiation intensity at this point. Therefore, we can move some UV-LEDs up, to increase the radiation intensity in the upper part of the model, thereby increasing the UV dose.

We chose two places, 5cm from the bottom and 5cm from the top, then got two cross sections. In the initial arrangement of the UV-LEDs, the average radiation intensity of the two sections is 6.2607 mW/cm^2 and 6.1008 mW/cm^2, respectively.

Then, We optimized the UV-LED layout, inserted \( L_4 \) between \( L_{41} \) and \( L_{42} \), inserted \( L_3 \) between \( L_{42} \) and \( L_{43} \), inserted \( L_3 \) between \( L_{43} \) and \( L_{44} \). This is shown in Figure 5:

Figure 5. Optimized UV-LED layout
The average radiation intensity of the lower and upper sections changes to 5.8340 \text{mW/cm}^2 and 6.4524 \text{mW/cm}^2, respectively. It indicates that the radiation intensity has shifted upwards. After optimizing the layout, the changes in the UV dose of ten particles are shown in Figure 6:

![Figure 6. Changes in UV dose of each particle](image)

It can be seen from the figure 6 that we have improved the UV dose without increasing the power by optimizing the UV-LED layout. The UV dose of these 10 particles has been increased by 2.812, 1.4298, 5.7602, 2.1344, 3.2455, 2.3364, -0.801, 0.397, 1.0955, 7.7313 \text{mJ/cm}^2.

4. Conclusion

In summary, by analysing the particle flow, we learned that microorganisms would stay longer in the upper part of the model, so we optimized the UV-LED layout, then found that the average radiation intensity of the upper section has increased by 0.3518 \text{mW/cm}^2 and the radiation intensity of the lower section is reduced by 0.4267 \text{mW/cm}^2. In other words, the radiation intensity of the lower part is transferred to the upper part. The UV dose obtained by ten particles totally increased by an average of 2.3329 \text{mJ/cm}^2. Therefore, by optimizing the UV-LED layout in conjunction with the microbial flow state, we can increase the UV dose without increasing the power.

Compared with mercury lamps, UV-LED has a more flexible layout. When designing and arranging the light source, this paper adopts a one-dimensional arrangement that imitates the mercury lamp. Therefore, in future work, we can consider the three-dimensional arrangement of UV-LEDs, so as to develop a layout scheme with lower cost and better efficiency.

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