Research on the sterilization effect of hydrogen peroxide and equipment optimization

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Abstract. Hydrogen peroxide sterilization is widely used in food packaging, public health and other fields. The sterilization effect is related to the vaporization spray time and nozzle parameters. This paper uses AnsysFluent software to mathematically simulate the flow field and concentration distribution of vaporized hydrogen peroxide in the sterilization space; and verify the correctness of the numerical simulation results through field experiments. UDF module is used to describe the component concentration of the nozzle, and the distribution of vaporized hydrogen peroxide is analyzed by changing the nozzle spray angle and spray speed of the equipment, and the spray time T required to reach the standard concentration in the sterilization space is the shortest and the hydrogen peroxide dosage Q is the minimum For the goal, optimize the design parameters. The results show that when the spray speed is 4.8 m/s and the spray angle is -18°, the spray time required to reach the sterilization standard is the shortest, and the amount of hydrogen peroxide is the least. This article provides a theoretical basis for the improvement of vaporized hydrogen peroxide sterilization equipment.

1. Introduction
The vaporized hydrogen peroxide has great bactericidal ability [1]. With its free hydroxyl group, it can kill bacterial spores in a short time and decompose into water and oxygen without pollution to the environment [2]. Therefore, it is widely used in many fields such as epidemic prevention and control, medical and health, pharmaceutical manufacturing, food packaging, and public health [3] [4]. Although vaporized hydrogen peroxide has been studied as early as the last century. But now its research results are only for the sterilization effect, sterilization process and equipment. Ren Zhe [5] and others found that bacteria on stainless steel and plastic are more difficult to kill than bacteria on glass, indicating that the sterilization effect will be affected by the material. Qi Jiancheng [6] and others invented a flash vaporization method that can uniformly diffuse vaporized hydrogen peroxide. Ye Kaixue [7] uses a high-frequency resonance vibration plate to separate gaseous hydrogen peroxide at a temperature of only about 40 degrees Celsius. Zeng Shiqing [8] used a high-frequency acoustic wave generator to generate micron-level suspendable hydrogen peroxide particles.

Although there are many researches on hydrogen peroxide equipment, there are very few researches on its flow field distribution in the sterilization space combined with field experiments to verify numerical simulations. However, the nozzle of the vaporized hydrogen peroxide device is an important structure of the entire device, and the flow field of the vaporized hydrogen peroxide in the sterilized space is directly affected by its design parameters, which determines the sterilization efficiency and effect. In this paper, a symmetrically distributed nozzle device with 6 openings with a diameter of 14 cm is used as a model to numerically simulate a space to be sterilized with a height of 3.5 m, a length of 4 m and a width of 5 m, and analyze the effect of different injection speeds and
angles on the distribution of vaporized hydrogen peroxide. Impact. In order to obtain the best injection speed and angle, an optimization scheme for the nozzle of the vaporized hydrogen peroxide equipment is proposed. It is of great significance to improve the efficiency of sterilization.

2. Numerical simulation method and its experimental verification.

2.1. Simulation method
The room to be sterilized is 3.5m high, 4m long, 5m wide, the total height of the equipment is 1.043m, the length and width are 0.5m, the nozzle shape is circular and the diameter is 10cm. The three-dimensional simulation model is established according to the size 1:1 in the experiment.

![Figure 1 Grid](image1)

2.2. Simulation results
Through the sterilization simulation of the equipment used by the company (hydrogen peroxide solution with a mass fraction of 35%, the spray speed is 3.5m/s, and the angle is 0°), the total sterilization time is 20 minutes. The velocity vector diagram of the sterilization space (part), the vaporized hydrogen peroxide concentration cloud diagram 3m from the ground and 1.5m from the symmetry plane (sym) are obtained as shown in the figure.

![Figure 2 Simulation results](image2)

Figure 2 shows that the gas floats up after being ejected from the nozzle. When the gas movement hits the wall, a part of the gas will continue to move forward until a large vortex area appears on the vertical wall of the room to be sterilized. Part of the gas will move downwards with the spray nozzle to the vertical wall, forming a small vortex area with the bottom of the room, and the other part will form a vortex between the vertical walls, and finally move to the bottom and be sucked in by the suction port of the equipment. At a distance of 3m from the ground, there will be a larger area and a slightly lower concentration than the surrounding "jet dead zone". Due to the larger disturbance of the vortex area to the flow field and the upward movement of the gas, the "jet dead zone" and the same plane The concentration difference is not obvious. At a plane that is 1.5m away from the symmetry plane, the concentration difference between the top and bottom of the room to be sterilized is the largest, the concentration at the top of the room in the room to be sterilized is the highest, and the concentration at the bottom is the lowest.
2.3. Simulation result verification

2.3.1. Experimental method
In order to verify the credibility of the Fluent numerical simulation, the concentration of vaporized hydrogen peroxide measured through on-site sterilization was compared with the simulation results. The field test is shown in Figure 3. During the 20-minute sterilization process, data was recorded every 2 minutes. After the test data is acquired at each detection point, the room is immediately de-residualized to prevent the previous experiment from affecting the data of the next experiment. The test is repeated 3 times for each measuring point, and the average value is taken as the final test data.

![Figure 3 Spatial measurement points and field test](image)

Formula (1) is the conversion relationship between volume fraction and ppm, $c_{wt}$ is mass fraction, $\rho_w$ is mixing density, $\rho_i$ is the density of $i$ component, and $C$ is a constant.

2.3.2. Field experiment verification
The vaporized hydrogen peroxide concentration at the measuring point obtained through numerical simulation is substituted into the formula and converted into a concentration in ppm and the actual concentration measured on site are shown in Table 1.

| Measuring point | Concentration ppm | t (min) |
|-----------------|-------------------|---------|
|                 | On-site measurement |     | Using UDF |
| Measuring point 1 | 0 | 0 | 0 | 16.5 | 27.1 | 39.7 | 57.4 | 73.8 | 87.9 | 101.0 | 118.0 |
|                  | 0.3 | 2.8 | 11.8 | 23.9 | 31.6 | 50.4 | 67.0 | 81.8 | 92.3 | 110.2 |
| Measuring point 2 | 0 | 5 | 14.7 | 29.5 | 41.8 | 58.3 | 76.9 | 90.7 | 109.4 | 123.7 | 139.7 |
|                  | 0 | 15.1 | 24.6 | 36.3 | 45.1 | 56.8 | 75.4 | 89.3 | 103.2 | 116.5 | 130.8 |
| Measuring point 3 | 0 | 0 | 57.3 | 99.9 | 145.4 | 194.6 | 246.4 | 292.1 | 331.5 | 360.3 | 380.8 |
|                  | 0 | 37.7 | 79.1 | 121.0 | 161.5 | 203.6 | 242.8 | 281.8 | 320.8 | 347.9 | 368.4 |

Table 1 shows that the simulation results of the measurement points are basically consistent with the trend of the concentration changes over time measured on site, and the concentration error of each measurement point is within 7%. In the actual sterilization, the microorganisms in the room and the...
vaporization process will cause a small amount of decomposition of hydrogen peroxide, and the use of UDF to describe the inlet injection condition is the change of the vaporized hydrogen peroxide concentration at the outlet with the original nozzle concentration as a constant. The curve is calculated by superimposing the concentration of the nozzle. Therefore, in the early stage of sterilization, the simulated data will be higher than the actual measured value, and the simulated value in the later stage of sterilization will be lower than the actual value. In summary, UDF compiled nozzle vaporized hydrogen peroxide concentration can accurately reflect the actual injection conditions, and the experiment can verify the correctness of the numerical simulation results.

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### 3. Optimization plan

When the concentration of vaporized hydrogen peroxide reaches the minimum standard value (100ppm) in the sterilization room, it can fully combine with bacteria to achieve the sterilization effect. Therefore, in order to shorten the time T and the amount of hydrogen peroxide required for the minimum concentration in the room to be sterilized to reach the standard value, keep the angle between the nozzle and the horizontal plane unchanged, change the nozzle rate, and analyze the T and Q values by comparison, To get the best spray speed. Then keep the rate of fire constant, change the nozzle angle, get the T and Q values at different angles, and get the best injection angle through comparative analysis.

Q indicates the amount of hydrogen peroxide used when the room reaches the standard sterilization concentration. The formula is as follows:

$$Q = \int_{t_0}^{t} n S V c_{wt} \rho dt \tag{2}$$

In the formula: Q is the amount of hydrogen peroxide solution (g); n is the number of nozzles; S is the cross-sectional area of the nozzles; V is the injection velocity; c_{wt} is the mass fraction of volume vaporized hydrogen peroxide; ρ is the mixed gas density; t is time.

### 4. Analysis and results

#### 4.1. Numerical analysis of the influence of nozzle jet velocity V on the flow field

In order to analyze the influence of the injection speed on the charging efficiency of vaporized hydrogen peroxide and the standard dosage and obtain the best injection speed, the nozzle injection angle was kept unchanged, and the horizontal angle was 0°. The inlet speed of the system is 5.5m/s, 4.5m/s, 3.5m/s, 2.5m/s, 1.5m/s. Use ANSYS Fluent to simulate the spatial distribution of vaporized hydrogen peroxide with different injection speeds. The time it takes for hydrogen peroxide to reach the standard value at different speeds is shown in the figure:

![Figure 4](image)

Figure 4 The injection speed and the time it takes for the hydrogen peroxide concentration in the room to reach the standard value (100ppm)
Figure 4 shows that as the injection speed V increases, the time it takes for the hydrogen peroxide concentration to reach the standard value (100 ppm) decreases. Compared with the time-consuming T reduction when the injection speed is 1.5m/s-3.5m/s, the time-consuming T reduction when the injection speed is 3.5m/s-5.5m/s is significantly smaller. Substituting the T value at each spray speed into formula (2) to obtain the amount of hydrogen peroxide at different spray speeds is plotted as a curve as shown in the figure below:

![Figure 5 Injection speed and hydrogen peroxide consumption](image)

It can be seen from Figure 5 that there are two minimum points in the curve at 2.4m/s and 4.8m/s. When the injection speed increases, the T value will decrease, but the mass fraction of hydrogen peroxide increases with the injection speed. When the injection velocity is between 1.5m/s-2.4m/s and 3.4m/s-4.9m/s, the amount of hydrogen peroxide Q is greatly affected by the time T, so the amount of hydrogen peroxide Q increases with the rate of injection Shows a decreasing trend; the rate of fire is between 2.4m/s—3.4m/s and 4.9m/s—5.5m/s. The amount of hydrogen peroxide Q is greatly affected, so the amount of hydrogen peroxide Q increases with the rate of fire. Shows an increasing trend.

From Table 5 and Figure 6, it can be seen that the highest Q value when the injection velocity is 1.5m/s, the maximum vaporized hydrogen peroxide material is 87.8g, and the T is 3216s; when the injection velocity is 4.8m/s, the minimum Q value is 61.8g, The time required for the room to reach the standard concentration is 748s; the minimum T value of 5.5 m/s is a 2% decrease from the T value of 4.8 m/s, but the Q value increases by 8%. Therefore, the comprehensive index is better when the injection velocity is 4.8m/s.

4.2. Numerical analysis of the influence of nozzle injection angle on vaporized hydrogen peroxide

In order to study the influence of the spray angle of the nozzle on the sterilization of vaporized hydrogen peroxide, the spray speed of the nozzle was set to 4.8m/s and kept unchanged, with the horizontal plane as the boundary, the angle between the system entrance and the horizontal plane was -45° and -30°, respectively, -15°, 0°, 15°, 30°, 45°. Using ANSYS Fluent to simulate the spatial distribution of vaporized hydrogen peroxide at different injection speeds, it is obtained that the mass fraction of vaporized hydrogen peroxide on the center line 1.5m from the symmetry plane at different injection angles after 30 minutes of injection is distributed with the room height Z. The graph is as shown

It can be seen from Figure 7 that the distribution of vaporized hydrogen peroxide at different injection angles is basically consistent with the height of the room. As the height of the room increases, the mass fraction of vaporized hydrogen peroxide also increases. The mass fraction of vaporized hydrogen peroxide is the lowest when the height is 0m (bottom of the room). Therefore, when the bottom of the room reaches the standard sterilization concentration of 100 ppm, the spray time is T. The duration T corresponding to different injection angles is shown in the following figure:
Figure 6 The time it takes for the spray angle and room concentration to reach the standard value

Hydrogen peroxide consumption Q at different injection angles is obtained by substituting cwt and T (required for the concentration of vaporized hydrogen peroxide at different injection angles to reach the standard value) into the formula (1). As shown below:

Figure 7 Hydrogen peroxide consumption Q at different injection angles

It can be seen from Table 6 and Figure 7 that when the angle Θ is greater than 0, as the angle Θ between the injection port and the horizontal plane increases, the amount of hydrogen peroxide in the Q and T values tends to increase. When Θ is +45°, the maximum Q is 94.8g, and the T value also reaches the maximum 1138s. When Θ is -18°, the minimum Q value and T are 57.2g and 725s. When Θ is less than -30°, the material ejected from the nozzle near the suction port is sucked into the equipment, making the room concentration reach the standard. The time used for the value increases significantly, and the amount of hydrogen peroxide also increases significantly, so the spray angle should not be too small.

5. Conclusion
Using fluent15.0 software for numerical simulation research combined with field tests, the sterilization equipment was optimized from two aspects: the spray speed and spray angle of different equipment. By comparing the Q value and T value under different parameters, the following conclusions are obtained:

1. Using UDF to compile and simulate the change trend of vaporized hydrogen peroxide concentration over time and the measured value error is 7%. It can be seen that using UDF to compile the nozzle concentration can accurately reflect the actual working conditions.

2. Spray speed The spray and spray angle have a great influence on the sterilization efficiency and effect of vaporized hydrogen peroxide. The Q value and T are the lowest when the shooting speed is 4.8m/s and the angle is -18°. Compared with the company’s existing equipment (the shooting speed is
3.5 m/s, the injection angle is 0°), the optimized T value (the injection speed is 4.8 m/s, the injection angle is -18°) decreases by 34% and the Q value A decline of 22%. In summary, the most suitable rate of fire for the equipment is 4.8 m/s and the angle is -18°.

3. The suction port of the equipment should be designed at the bottom position to prevent the ejected materials from being sucked directly from the suction port and affecting the sterilized fruit.

Acknowledgments
This work was supported by R&D of vaporized hydrogen peroxide sterilization equipment based on big data (Shanghai Alliance Program LM2018190)

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