The Simulative Optimization of Aerosol Micro Atomizer for Pulmonary Delivery Device

Zhen Zhang\textsuperscript{1,2,*}, Wenhui Yang\textsuperscript{3}, Jun Chen\textsuperscript{2}, Yujie Liu\textsuperscript{4} and Xudong Wang\textsuperscript{2}

\textsuperscript{1}School of Mechanical, Electronic and Control Engineering, Beijing Jiaotong University, 100044, Beijing, China
\textsuperscript{2}Beijing Institute of Control Engineering, 100190, Beijing, China
\textsuperscript{3}State Key Laboratory of Pathogen and Biosecurity, Beijing Institute of Microbiology and Epidemiology, 100071, Beijing, China
\textsuperscript{4}Beijing Huironghe Technology Co. Ltd, 101102, Beijing, China

*Corresponding author email: cning@mail.cgs.gov.cn

Abstract. The present study investigated the design optimization of aerosol micro atomizer for liquid pulmonary device. Pulmonary delivery device with a micro atomizer at the tip is commonly used to penetrate into a small animal’s trachea, and directly quantitatively spray the infected dosing aerosol samples to animal’s lung. In order for no damage to animal’s trachea, a long capillary with a diameter of 0.5-0.6 mm is used for flow diversion. Therefore, the swirl atomizer size of the head is required to be adequately tiny with uniformity and penetration of aerosol spray. Due to structural limitation without adequate rotational space, it is highly challenging to provide the fine atomization with high quality. Therefore, based on the simulation analysis in Simspray software, the optimization design of the micro atomizer is conducted, aiming to improve the atomization quality with a certain spray angle. Parametric study on swirl atomizer structure, including swirl pitch, nozzle diameter and size of swirl channel, realized an excellent combination of parameters to meet requirement of fine spray. The experiment testifies that the 3-5μm aerodynamic diameter of droplets in spray is available.

Keywords: Micro atomizer; Swirl microchannel; Design optimization; Large eddy simulation; Laser femtosecond processing.

1. Introduction
The hand-held aerosol injector, which is a type of pulmonary delivery device, can directly penetrate into the trachea of small animals in the biological experiment [1, 2]. Thus, the aerosol micro atomizer at the injector tip can quantitatively generate aerosols with tiny droplets size and uniform distribution. In this way, atomized liquid samples can effectively work in lungs of small animals. The objective of aerosol toxicity test can be achieved, as shown in figure 1.

Aerosol micro atomizer is concerned to play a significant role in pulmonary delivery device, which directly affects the aerosols atomization quality in the bioresearch. The structural design, parameter combination and nozzle size of micro atomizer significantly determine droplets size, distribution, uniformity and penetration distance of aerosols. In this paper, based on the simulation analysis and experimental verification, the parameters of micro atomizer were optimized to effectively improve the spray quality. The optimized aerosol-generating head realizes the uniform spray, and ultimately control aerosols with 3 to 5 μm in mean aerodynamic diameter, targeting promising delivery effects. Precision machining of fine dimensions is achieved by laser femtosecond technology. Therefore, complexity and efficiency in manufacturing of swirl microchannel and tiny nozzle can be achieved.
2. Structural Design
As shown in figure 2, the micro atomizer provides injection spray with a spinning centrifugal structure at the nozzle tip. User pushes a small cross-section plunger through a hand-held syringe in the test. When the plunger is pushed, a high-pressure flow can be downstream generated through a very thin capillary to form a high-speed flow. As the liquid fluid flows through the end of the capillary with inner diameter of 0.6mm, a small swirl atomizer is used to change the high-speed flow into a rotating flow, which is then sprayed out through a jet hole 50 to 60 μm in diameter, as shown in figure 3. The fluid is ejected in the form of a circular cone film. Under the combinative influence of centrifugal force, aerodynamic force, liquid viscosity force and surface tension force, the liquid film expands outward after spraying out from the atomizer, then forming conical liquid film with strong fluctuation on the surface. As the thickness of the liquid film decreases and gradually becomes unstable, it tends to primarily breakup into liquid ligaments. The liquid ligaments formed by the conical liquid film can be further broken into large liquid droplets in the movement, and then develop into smaller liquid droplets [3,4]. When downstream breakup is developed to a certain extent, the formed aerosols can meet the experimental requirement.

Figure 2. Hand-held injector and its swirl micro atomizer.
Different from ordinary centrifugal atomizers limited by the size of the capillary structure, the swirling radius is too small. That results in insufficient centrifugal force in spray process [5,6]. Being lack of centrifugal force is easy to form a micro hole jet flow. This jet flow easily causes the local high concentration with big droplets, sequentially resulting in the failure of toxicity test for small animals.
3. Simulation Discussion

In order to form a wide range of uniform atomization and avoid concentration of jets, it is necessary to make the centrifugal effect of the swirl atomizer fully effective. Due to difficult manufacturing, simulation study is considered to be the best way in optimization.

3.1. Simulation Method

Based on the Simspray software, several simulation comparisons were conducted through the mesh discretization method and piecewise linear volume tracking algorithm. Parametric study was used to simulate two-phase liquid spray field in three dimensions, using the VOF (volume of fluid) method and LES (large eddy simulation) turbulence model. The VOF method was used to capture the gas-liquid interface for two-phase flow [7]. In order to accurately consider the influence of turbulence, the LES method was used to solve the governing equations. LES is a turbulent model between DNS (Direct Numerical Simulation) and RANS (Reynolds Mean Equation Simulation). The direct numerical solution of large-scale turbulence and the modeling of small-scale turbulence pulsation can capture many large-scale effects and quasi-ordered structures in unsteady and non-equilibrium processes, which are unable to be obtained by RANS method. Therefore, it can effectively simulate the gas-liquid flow process and the formation mechanism of atomization in the complex atomizer structure [8].

PIMPLE algorithm, which is a combination of SIMPLE (semi-implicit method for pressure linked equations) algorithm and PISO (pressure-implicit with splitting of operators) algorithm, is adopted in this paper. The basic idea is that the SIMPLE steady-state algorithm is used to solve each timestep, and the PISO algorithm is used to complete the timestep. Each timestep can be regarded as a steady-state flow. When the solution reaches a certain point in accordance with the steady-state solver, the standard PISO algorithm can solve the final step.

The flow rate inlet boundary was set at the inlet, so that the injection flowrate was constant 50 mg/min. The simulation domain of 5 mm×5 mm and the ambient pressure of 0.1 MPa were set to observe the atomization differences under different design parameters.

3.2. Simulation Results

In figure 4, it is evident to see that a jet flow is the mainstream when swirl channel is set to be larger with nozzle diameter of 0.05 mm. Obviously, swirl channel in these two cases affects slightly on the spray without spinning acceleration. Swirling force does not work, no matter how fine or coarse the swirl pitch is. Even so, we can also see that as the pitch of swirl channel increases, the pressure drop also goes up with higher tangential velocity. Under the disturbance of aerodynamic interaction, the jet flow becomes more unstable, and a few small droplets form around the jet.
Figure 4. Simulative spray with larger swirl channel at fine pitch (left) and coarse pitch (right). When flow area of swirl channel is decreased with larger nozzle diameter of 0.06 mm, the pressure drop can be relatively higher with most in the swirl microchannel, as shown in figure 5. That means tangential velocity of flow is enhanced with lower discharge coefficient. However, spinning influence is still not significant, when jet flow ejected from the nozzle.

Figure 5. Simulative spray with larger nozzle diameter and smaller swirl channel at fine pitch.

Figure 6. Simulative spray with smaller nozzle diameter and smaller swirl channel at fine pitch.

In order to sequentially strengthen the expanding energy to trigger the spinning effect, we decreased the nozzle diameter from 0.06 mm to 0.05 mm. In figure 6, tangential velocity continues to increase under the condition of 0.24 MPa pressure drop. At this moment, swirl channel starts to take a certain effect, and the jet showed signs of slight rotation process. As mentioned in figure 4, it is concluded that increasing pitch indicates higher pressure drop with higher tangential velocity. Therefore, based on the case in figure 6, we further increased the pitch of swirl channel, hence, the pressure drop increases by three times. More potential energy can be converted into kinetic energy, then into surface energy of droplets. The key underlying mechanism of droplets breakup in micro atomizer is to enhance the dynamic interaction between the jet flow and the incoming ambient gas flow. Therefore, in figure 7, when the discharge coefficient of the atomizer is reduced with higher pressure drop, more potential energy is provided and greater tangential velocity is formed. At this moment, Kelvin-Helmholtz instability produces waves on the surface of stratified two-fluid flows if the relative velocity difference is larger than a critical value [9]. The surface waves grow unstably and form ligaments. As the ligaments eject into the surrounding gas, the aerodynamic interaction causes the liquid-gas interface to deform. Combining with the effect of the thinning process on the wavy surface of the liquid ligament, a pinch-off droplet formation mechanism is identified [10]. Accordingly, coarse pitch, smaller swirl channel and smaller nozzle are a better combination of parameters, resulting in adequate swirling effect.
Figure 7. Simulative spray with smaller nozzle diameter and swirl channel at coarse pitch.

4. Manufacturing and Test
For the micro atomizer, its nozzle diameter is only 0.05 mm, and its swirling microchannel is on the thin rod with the length of 0.6 mm and the diameter of 0.6 mm. It is difficult to meet the accurate requirements in realizability with traditional machining or electric machining. Therefore, femtosecond laser processing without recasting layer, microcrack, heat affected zone, contact stress and deformation, has a very significant machining advantage. As shown in left image of figure 8, femtosecond laser source is used to etch nozzle hole and equilateral triangular spiral groove on the cylindrical surface of fine manganese steel wire. This spiral groove pitch is only 0.2 mm and its side length of triangle is just 0.08 mm, as shown in right image of figure 8. Because the swirl microchannel is too small, special fixture is needed to ensure that when the swirl channel is rotated and etched, the rotation axis of the machine is coaxial with the axis of the workpiece, and the coaxiality must be less than 5 μm.

Figure 8. Femtosecond laser processing (Left) and the photo of manufactured swirl channel (Right). The aerosol micro atomizer, which was optimized in parametric simulation and manufactured through femtosecond laser processing, was tested as shown in figure 9. The atomizing angle of droplets is around 80 degrees with great dispersion effect, under the condition of limited swirling diameter. The atomization quality measured by Aerodynamic Particle Sizer Spectrometer (TSI, APS-3321) can achieve high quality atomization of 3 to 5 μm, as shown in the right image of figure 9. The spray distribution is also fine with geometric standard deviation of only 1.61. The test results show expected effectiveness of pulmonary delivery in bioresearch.
5. Conclusion
The present research focused on the design of aerosol micro atomizer for liquid pulmonary delivery device. Limited by the tiny size of atomizer, droplets atomization of 3 to 5 μm with uniform distribution over a large area requires optimization in parametric design and manufacturing. LES simulation shows that smaller discharge coefficient and higher pressure drop are more conducive to providing more expanding energy under the same injection flowrate. After parametric comparison in simulation, coarse pitch, smaller swirl channel and smaller nozzle diameter are testified to be the optimal group for high-quality atomization. Femtosecond laser technology without recasting layer, microcrack, heat affected zone, contact stress and deformation is used to process the micro atomizer. The micro atomizer shows a good atomization quality with small droplets size and uniform distribution over a large atomizing angel.

Acknowledgments
This work is supported by the scholarship from China Scholarship Council (CSC) under the Grant CSC 201804980052.

References
[1] Wang Z D, Deng J H, Zhou J P, Jin F. Pulmonary delivery drugs: developments in nebulizers. World Clinical Drugs, 2011, 32(5), pp:64-70.
[2] SUN W W, WANG H, YANG H Y, CAO L L, MA Z. Development of New Pulmonary Miniaturized Nebulization Device. Chinese Medical Equipment Journal, 2011, 32(5), pp:28-29.
[3] Ding J W, Li G X, Yu Y S. The influence of injector structure on turbulence and fuel atomization based on large eddy simulation. Beijing: 2012 Chinese Society for Engineering Thermophysics Combustion Academic Conference, 2012.
[4] Sheng L Y, Li Q L, Bai X, etal. Review on spray process of liquid-liquid coaxial swirl injector. Journal of Rocket Propulsion, 2020, 46 (3), pp: 4-13.
[5] Sarker M, Rahman S, Mandal S, et al. A Study on Aerosol Spray Characteristics of Different Size Atomizers[J]. Aerosol Science and Technology, 2020, 4(4), pp:1-14.
[6] Chen S K, Lefebvre A H, Rollbuhler J. Factors influencing the effective spray cone angle of pressure-swirl atomizers[J]. Asme Transactions Journal of Engineering Gas Turbines & Power, 1992, 114(1), pp:97-103.
[7] Gurakov N I, Zubrilin I A, Abrashkin V Y, et al. Validation of the VOF method for liquid spray process simulation from a pressure-swirl atomizer[C]. International Conference on Physics and Chemistry of Combustion and Processes in Extreme Environment, 2020.
[8] Vinkovic I, Aguirre C, Simoens S, etal. Large eddy simulation of droplet dispersion for inhomogeneous turbulent wall flow. International Journal of Multiphase Flow, 2006, 32(3), pp:344-364.
[9] Štrubelj L and Tiselj I. CFD Simulation of Kelvin-Helmholtz instability. Bled: Nuclear Energy for New Europe 2005 International Conference, 2005.
[10] Zhang Z, Shin D H. Effect of ambient pressure oscillation on the primary breakup of cylindrical liquid jet spray. International Journal of Spray and Combustion Dynamics, 2020, 12:175682772093555.