The Multiphysics Modeling of droplet generation in the ultrasonic nebulization

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Abstract

Ultrasonic nebulizers are widely used for inhalation drug therapy. They can be generating aerosol when ultrasonic frequency around 1-3 MHz is supplied. In order to improve the drug delivery efficiency of the ultrasonic nebulizers, in this study, minimizing droplet size will be chosen out of several possible parameters. The purpose of this work is to understand how droplet is generated in the ultrasonic nebulizers by using finite element modeling in Comsol Multiphysics program.

There are three modules used in modeling: piezoelectric actuator module, pressure acoustic module, and laminar two phase flow module. The results reveal not only the relationships between the vibration of the piezoelectric disk, the pressure acoustic of the liquid, and the liquid dispersion in the chamber, but also the understandings of the relationships between the excitation frequency, surface wavelength, and droplets size. The results of this work open an opportunity to redesign the ultrasonic nebulization device with a smaller droplets size for better drug delivery performance.

Keywords: Ultrasonic nebulization, Droplets size, Piezoelectric actuator and Liquid film surface.

1. Introduction

Ultrasonic nebulizers are used for inhalation drug therapy in patients with respiratory diseases. They are suitable for young, elderly, and unconscious patients who are not able to use other devices such as Metered Dose Inhaler (MDI) and Dry Powder Inhaler (DPI). In addition, ultrasonic nebulizers are able to deliver variety of drugs such as proteins, antibiotics, enzymes or mucolytic drugs, while neither MDI nor DPI are not, [1],[2],[3],[4].

An ultrasonic nebulizer system, composed of many components: an electric generator, drug or liquid chamber, piezoelectric disk at the bottom of the drug chamber, and a baffle. In order to generate aerosol, three steps will be described as the following. First, the ultrasonic frequency around 1-3 MHz supplied by the electric generator to excite the piezoelectric disk. Second, the piezoelectric disk converts electrical energy to mechanical energy that cause vibration to the liquid in the chamber. Finally, when the kinetic energy of the liquid is accumulated enough, a fountain will be formed at the surface. At the crest of the fountain, due to the intensive energy, the droplets are formed and flown out as aerosol,[2],[5],[6],[7].

The efficiency factors of ultrasonic nebulizers are droplet size distribution, aerosol flow rate, solution characteristics after nebulization, etc. Only droplet size minimization is interested in this study. Even though, the particle size of 1-5 µm can deliver drug to the alveolar, however, only the particle size smaller than 1 µm penetrate to the alveolar cell when patients inhale and momentary hold their breath, [1],[2],[5],[8].

To produce the droplets size smaller than 1 µm in ultrasonic nebulizers, three modules of the finite element modeling in Comsol Multiphysics program was used. The results are verified by other experimental works,[2],[15],[16].

2. Theory and governing equations

The ultrasonic nebulization droplet is generated when the liquid surface is accumulated enough energy, transmitted by piezoelectric disk, to overcome the surface tension at the crests of the capillary waves of the fountain peak,[2],[9]. Kelvin established the expression of wavelength in capillary waves as below, [9],[10]:

\[
\lambda_s, f_s = \sqrt{\lambda_s g \frac{2\pi \sigma}{\rho \lambda_s \tan h \left(\frac{2\pi h}{\lambda_s}\right)}}
\]  

(1)

where \(\lambda_s\) (m) is the capillary wave length of surface waves, \(f_s\) (Hz) is the frequency of liquid surface, \(g\) (m/s^2) is the gravity acceleration, \(\rho\) (kg/m^3) is the density of liquid, \(\sigma\) (N/m) is the surface tension coefficient, and \(h\) (m) is the liquid film thickness.

Lang has simplified some terms in eq.(1) as follows: the liquid film is thin so that \(\tan h(2\pi h/\lambda_s) = 1\). and due to the fact that the influence of gravity forces has such a less significant compared to capillary forces that \((\lambda_s g / 2\pi) << (2\pi \sigma / \rho \lambda)\),[9]:

\[
\lambda_s = \left(\frac{2\pi \sigma}{\rho f_s^2}\right)^{\frac{1}{3}}
\]  

(2)
He found that the droplet size is proportional to the capillary wave length, [6],[11]:
\[
D_{nm} = 0.34\lambda_s
\]
(3)
where \(D_{nm}\) (m) is the droplet diameter, see Figure 1.

Figure 1. Disintegration mechanism

In order to find the droplet size, the frequency of the liquid surface, \(f_s\), must be determined. There are three modules involved in this study: piezoelectric actuator module, pressure acoustic module, and laminar two-phase flow module.

2.1. The effect of the piezoelectric actuator

The relationship between electrical and mechanical energy of the piezoelectric effect is described in terms of stress, strain, electric field, and electrical displacement. It can be written in the stress-charge representation as:
\[
\sigma = C_{el}\varepsilon - e^{eff}E
\]
(4)
\[
D = e\varepsilon + \varepsilon_sE
\]
(5)
where \(\sigma\) (N/m²) is the stress, \(C_{el}\) (Pa) is the elasticity matrix, \(\varepsilon\) (unitless) is the strain, \(e\) (C/m²) is the coupling matrix, \(E\) (N/C) is the electric field defined as the electric force per unit charge, \(D\) (C/m²) is the electrical displacement, and \(\varepsilon_s\) (F/m) is the dielectric matrix, [12],[13],[17].

When the piezoelectric actuator is actuated by alternating current (AC: \(E = -\nabla V\)) where \(V\) (V) is electric potential) that causes the vibration energy transmits in to the liquid, the harmonic analysis for steady state and the transient analysis of piezoelectric actuator module are used to determine the displacement response (u,v,w) as the following:
\[
-\rho_0\frac{\partial^2 u}{\partial t^2} - \nabla \sigma = F_r e^{i\omega t}
\]
(6)
\[
\frac{\partial^2 v}{\partial t^2} - \nabla \sigma = F_r
\]
(7)
\[
\nabla D = \rho_t
\]
(8)
where \(\rho\) (kg/m³) is the density of the piezoelectric material, \(\omega\) (Hz) is the resonance frequency, \(u\) (m) is the displacement response (u,v,w), \(F_r\) (N) is the volume force, \(\rho_t\) (kg/m³) is the volume density, and \(t\) (s) is the time.

Next, the displacement response is set as the boundary condition value in the pressure acoustic module to determine the liquid acoustic pressure in the system, as discussed next.

2.2. The effect of the pressure acoustic

The acoustic pressure, the summation of background and scattered pressure from the boundary effect, is analyzed by the pressure acoustic module.

There are three boundary condition used in this module: the piezoelectric displacement response is converted to the liquid normal acceleration at the interface between the piezoelectric disk and the liquid as in eqs.(9) and (10), the acoustic pressure is zero, \(p=0\), at the air-liquid interface, and the sound hard boundary condition at the chamber wall as in eq.(11):
\[
-n\left(\frac{\nabla p - q}{\rho_1}\right) = n u_u
\]
(9)
\[
\sigma_n = p n
\]
(10)
\[
-n\left(\frac{\nabla p - q}{\rho_1}\right) = 0
\]
(11)
where \(p\) (Pa) is the acoustic pressure, \(q\) (N/m³) is the dipole source that radiates a sound field in two opposite directions, and \(u_u\) (m/s) is the second time derivative of the displacement.

The governing equations of this module is used to determine the acoustic pressure, \(p\), in the frequency and time domains are respectively written as follows:
\[
\frac{\nabla p}{\rho_1\omega^2} - \frac{1}{\rho_1} \frac{\partial^2 p}{\partial t^2} = Q
\]
(12)
\[
\frac{1}{\rho_1\omega^2} \frac{\partial^2 p}{\partial t^2} + \nabla - \frac{1}{\rho_1} \left(\nabla p - q\right) = Q
\]
(13)
where \(k_{eq}\) (1/m) is the wave number, \(Q\) (1/s²) is the monopole source, and \(c\) (m/s) is the speed of sound. After that, the acoustic pressure is used to deliver the boundary condition value to laminar two-phase flow module to determine three parameters at the liquid surface: the volume fraction, the velocity, and the frequency, as described next.[8]

2.3. The effect of the laminar two-phase flow

The laminar two-phase flow module is based on the Navier-Stokes equation which was developed from the compressible formulation of the continuity:
\[
\frac{\partial \rho}{\partial t} + \nabla (\rho \mathbf{u}) = 0
\]
(14)
and the momentum equation:
\[
\rho_t \frac{\partial \mathbf{u}}{\partial t} + \rho_0 \mathbf{u} \nabla \mathbf{u} = - \nabla p + \nabla (\mu \nabla \mathbf{u}) + \mathbf{F}...
\]
(15)
where \(\mathbf{u}\) (m/s) is the surface wave velocity, \(\mu\) (Pa.s) is the fluid dynamic viscosity, and \(F\) (N/m³) is the volume force vector. By assuming that the fluid is Newtonian and incompressible (both \(\mu\) and \(\rho\) are constant), the continuity equation becomes \(\nabla \mathbf{u}_i = 0\), and the momentum equation can be reduced to
\[
\frac{\partial \mathbf{u}_i}{\partial t} + \rho_0 \mathbf{u} \nabla \mathbf{u}_i = \left[ -\nabla p + \rho_0 \nabla (\mathbf{u}_i + (\mathbf{u}_i)^T) \right] + \mathbf{F}
\]
(16)
Then the surface wave velocity can be determined and lead to find the value of liquid surface frequency which can be substituted into the droplet equations (2) and (3).
In order to describe the aerosol phenomena, the volume fraction at the liquid surface needs to be determined by using the following equations:
\[
\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = \nabla \cdot \left( \frac{\lambda}{\varepsilon_{\phi}} \nabla \phi \right)
\]
when the governing equation, \( \psi \), is:
\[
\psi = -\nabla \cdot \varepsilon_{\phi} \nabla \phi + (\phi - 1) \phi + \frac{\varepsilon_{\phi}^3}{\lambda} \frac{\partial \phi}{\partial t}
\]
where \( \gamma \) (m/s) is the reutilization parameter, \( \lambda \) (N) is the mixing energy density, \( \varepsilon_{\phi} \) (m) is the parameter controlling interface thickness, and \( x \) (m/s/kg) is the mobility turning parameter.[19]

3. Simulation models and boundary conditions

The two-dimensional axisymmetric model of ultrasonic nebulizer consists of piezoelectric and two fluid domains is shown in Figure 2. Cylindrical coordinate system is chosen where the bottom left corner is an origin.

The geometry of piezoelectric domain or disk has diameter of \( d_1 = 0.008 \) m and thickness of \( t = 0.0011 \) m. The chamber with diameter of \( d_2 = 0.03 \) m and height of \( h = 0.1 \) m contains one-eighth height filled with water. The fluid and the piezoelectric properties are shown in Table 1 and 2.

When the top of a piezoelectric disk is ground, the bottom is given 12 V of harmonic electrical signal causing change in the normal acceleration that lead to an occurrence of acoustic pressure at the interface between the piezoelectric and the fluid domain. At the chamber wall, both the fluid velocity and the normal component of acceleration are assigned to be zero (\( u_i = 0 \) and \( a_n = 0 \)). The atmospheric pressure is assigned at the two-fluid interface and at the top of the chamber.

The Triangular mesh, total of 3,805 elements, is chosen in the finite element model. The MUMPS (MUltifrontal Massively Parallel sparse direct Solver) is used as a calculation solver since it has several preordering algorithms to permute the columns and there by minimize the fill-in.

### Table 2 Piezoelectric material properties.

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<td></td>
<td>( C_{E2} )</td>
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<td>Loss factor</td>
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</tr>
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</table>

![Figure 2. A 2D Axisymmetric model of ultrasonic nebulizer.](image)

![Figure 3. The finite element mesh and boundary condition](image)
4. Results and discussion

When the harmonic electrical potential with amplitude is excited, a few harmonic displacement peaks appear at the disk center, shown in Figure 4. The one with a natural frequency of 1.77 MHz is chosen in this study because the frequency corresponds to other experimental works. Then the harmonic displacement of $5.226 \times 10^{-7}$ m is used to calculate the setting time to be of $2.5 \times 10^{-4}$ second, shown in Figure 5 and 6.

Figure 4. Vibration shape of piezoelectric disk.

Figure 5. Displacement amplitude, Z component (m) from harmonic analysis.

Figure 6. The transient response of the piezoelectric disk at the center point.

Due to the piezoelectric excitation, the acoustic pressure about 24.5 MPa is increased at the center of the liquid chamber, as shown in Figure 7, which is enough to cause droplets generation, [14]

Figure 7. Acoustic pressure when piezoelectric disk was actuated.

Figure 8 shows steps of how the fountain is generated which can be seen and distinguished by the color of air and liquid volume fraction. It is found that the liquid begins to break free at the bottom surface after 0.30 ms, and then expand to the top surface at 0.38 ms. After that, the mixture splash the whole chamber.

Figure 8. Volume fraction of Air.

The transverse velocity of the liquid surface is plotted in Figure 9. The magnitude is about 0.4 m/s and the frequency of the surface oscillation is 1.33 MHz. According to the eq.(2) and (3), the wavelength of the surface is 6.35 µm and the droplet diameter is 2.7 µm. This simulation results are verified by previous experiments,[2],[15],[16].

Figure 9. The normal velocity component of the liquid surface.
5. Summary

The results of this study, according to the three steps simulation, show the following. Firstly, the piezoelectric actuator module is best to perform at the operating frequency of 1.77 MHz (0-3 MHz) which given 0.57 $\mu$m of the transverse displacement of the piezoelectric disk center that lead to provide the setting time of $2.5 \times 10^{-4}$ second. Secondly, the pressure acoustic module has shown that the droplet can be generated at 24.5 MPa. Thirdly, the transverse velocity of the liquid surface is 0.4 m/s at 1.33 MHz. Finally, the droplet size of 2.7 $\mu$m where is generated.

The simulation results in this study are agree with the previous experimental works. Therefore, this finite element model designed for this study can be further developed to achieve the point where submicron droplet size is generated.

Acknowledgments

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