Numerical Simulation of Multi-puffing Process of Electronic Atomizer

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Abstract. The thermodynamic behaviors of electronic atomizer during the multi-puffing process have an important influence on the product performances. Exploring the thermodynamic mechanisms behind the vaporization phenomena is helpful for engineers and consumers to understand electronic atomizer. The theoretical modelling and simulation of the multi-puffing process for the electronic atomizer were carried out in this study. During 1~10 puffing number, the mass fraction of propylene glycol in the residual e-liquid reduced when the puffing number increased. Meanwhile, the mass fraction of vegetable glycerin in the residual e-liquid increased gradually. The total particulate matter of aerosol generated from the electronic atomizer decreased with the puffing number increasing. The maximum vaporization temperatures of the residual e-liquid rose gradually in the multi-puffing process.

1. Introduction

Electronic atomization technology is widely used in the electronic atomizer products [1]. The electronic atomizer heats and vaporizes the liquid by the way of electric heating to generate colorless vapor. After mixing with the puffing airflow, the high-temperature vapor condenses and forms aerosol [2]. The main components of electronic atomizer include mouthpiece, wick, coil, tank, battery, etc. E-liquids are mainly composed of two kinds of solvents: propylene glycol (PG) and vegetable glycerin (VG) [3].

At present, the scientific researches on the electronic atomization technology are mainly involved in toxicology. While, the scientific reports about the thermodynamic characteristics of electronic atomizer are few. Talih et al. [4] studied on the release characteristics of the key components of e-liquid in the single puffing process for electronic atomizer by theoretical simulation. A lumped-parameter mathematical model for the vaporization process of e-liquid was established. The theoretical model assumed that the refilling velocity of e-liquid in the heating section of wick is equal to the vaporization rate. The model was established for the single-puffing process and could not be used to simulate the multi-puffing process. The experimental results about the electronic atomizer products tested with variable heating powers showed that the consumption of e-liquid increased when the heating powers improved [5].

The working characteristics of electronic atomizer have an important influence on product performance and safety. To the best of our knowledge, the theoretical simulation on the multi-puffing process for electronic atomizer has not been reported in the field of electronic atomization technology. In this paper, the multi-puffing process of the electronic atomizer was modelled. The atomization
characteristics of the electronic atomizer are analyzed and discussed. The results can provide more information for us to understand the thermodynamic behaviors behind the multi-puffing process for electronic atomizer.

2. Theoretical Model

The schematic diagram of electronic atomizer is shown in Figure 1. The heating section of wick refers to the area which is wound by the coil (i.e. the red area). Two sides of the heating section are the transport section of wick. The material of wick is organic cotton. The e-liquids driven by the capillary force are transported from the tank to the heating section of the wick. The e-liquids in the heating section vaporize after being heated by the coil. The vapor is carried away by the puffing airflow and condenses into aerosol particles. The reasonable hypotheses about the physical processes of electronic atomizer are proposed. (1) The thermal inertia in the multi-puffing process is not considered. The wick is heated from the ambient temperature for each puffing. (2) The e-liquids in the heating section are supplied fast enough to avoid drying out. The refilling velocity of e-liquid in the heating section is equal to the vaporization rate. (3) In the multi-puffing process, the component concentrations of the residual e-liquid in the wick and tank have been fully diffused and uniform before each puffing.

![Figure 1. Schematic diagram of electronic atomizer.](image)

Based on the lumped-parameter model [4], a theoretical model for multi-puffing process of electronic atomizer is established in this study. The energy conservation equation for the heating section of wick is as follows.

\[ C \frac{dT}{dt} = \dot{E}_c - (\dot{Q}_{\text{conv}} + \dot{Q}_{\text{cond}} + \dot{Q}_{\text{lat}} + \dot{Q}_{\text{liq}}) \]

Where \( C \) is the heat capacity of heating section, J/°C; \( T \) is temperature, °C; \( t \) is time, s; \( \dot{E}_c \) is the power input, W; \( \dot{Q}_{\text{conv}} \) is the convective heat transfer, W; \( \dot{Q}_{\text{cond}} \) is the heat conduction, W; \( \dot{Q}_{\text{lat}} \) is the latent heat of vaporization for e-liquid, W; \( \dot{Q}_{\text{liq}} \) is the sensible heat consumed by temperature rising process for e-liquid, W.

The vaporization process of e-liquid in the wick can be divided into two stages: evaporation stage and boiling stage. When the average temperature of the heating section is lower than the boiling point of e-liquid (i.e., evaporation stage), the convective evaporation rate for component \( i \) of e-liquid is calculated by the following equation.
\[ m_i = h_{m,i} A \frac{M_i}{R_u} \frac{P_i}{T} \] (2)

Where \( m_i \) is the evaporation rate of component i, kg/s; \( h_{m,i} \) is the convective mass transfer coefficient, m/s; \( A \) is the surface area of heating section, m\(^2\); \( M_i \) is molar mass of component i, kg/mol; \( R_u \) is universal gas constant, 8.314 J/(mol·K); \( P_i \) is the partial pressure of component i, Pa.

In the evaporation stage, the total vaporization rate is equal to the sum of evaporation rates of each component i.

\[ \dot{m}_v = \sum \dot{m}_i \] (3)

Where \( \dot{m}_v \) is the total vaporization rate of e-liquid, kg/s.

When the average vaporization temperature in the heating section reaches the boiling point, the vaporization process of e-liquid switches to the boiling stage. In the iterative calculation for the slipping process of boiling point, the total vaporization rate of e-liquid (i.e., non-azeotropic mixed solution) in each iteration step is calculated by the energy conservation equation.

\[ \dot{E}_v = (\dot{Q}_{\text{conv}} + \dot{Q}_{\text{cond}} + \dot{Q}_{\text{liq}}) / h_{fg,liq} \] (4)

The slipping phenomena of boiling point for the mixed solution with different PG/VG ratios were calculated through Antoine equation, Raoult's law and Dalton's law. It is assumed that the e-liquids composed of PG and VG are ideal solutions.

At the evaporation or boiling stage, the ratio variation for the composition i of e-liquid in the heating section is calculated by the mass conservation equation.

\[ \frac{dm_i}{dt} = m_{liq} \frac{dw_i}{dt} = w_{i,p} \dot{m}_v - \dot{m}_i \] (5)

Where \( m_i \) is the mass of component i in the heating section, kg; \( w_i \) is the mass fraction of component i of e-liquid in the heating section; \( m_{liq} \) is the mass of e-liquid in the heating section, kg.

In the multi-puffing process, the vaporization amounts of e-liquid (i.e., total particulate matter) per puff are as follows.

\[ m_{i-vap,n} = \int_0^{t_{\text{heat}}} \dot{m}_{i-vap,n} dt \] (6)

\[ m_{vap,n} = \sum m_{i-vap,n} \] (7)

Where \( m_{i-vap,n} \) is the total mass of component i in vapor generated at the n-th puffing process, kg; \( \dot{m}_{i-vap,n} \) is the instantaneous vaporization rate of component i during the n-th puffing process, kg/s; \( t_{\text{heat}} \) is the heating time for single-puffing process, s; \( m_{vap,n} \) is the total mass of vapor generated at the n-th puffing process, kg.

The residual mass of e-liquid in the electronic atomizer and the mass fraction of component i in the residual e-liquid are calculated by the following equations.

\[ M_{liq,n+1} = M_{liq,n} - m_{vap,n+1} \] (8)

\[ M_{i-\text{liq},n+1} = M_{i-\text{liq},n} - m_{i-vap,n+1} \] (9)

\[ w_{i,n} = \frac{M_{i-\text{liq},n}}{M_{liq,n}} \] (10)
Where \( n \) is the puffing number; \( M_{\text{liq},n+1} \) is the residual mass of e-liquid in the electronic atomizer after \( n+1 \) puffing processes, kg; \( M_{\text{liq},n} \) is the residual mass of e-liquid in the electronic atomizer after \( n \) puffing processes, kg; \( m_{\text{vap},n+1} \) is the vaporization amount of e-liquid at the \((n+1)\)-th puffing process, kg; \( M_{i-\text{liq},n+1} \) is the mass of component \( i \) in the residual e-liquid for the electronic atomizer after \( n+1 \) puffing processes, kg; \( M_{i-\text{liq},n} \) is the mass of component \( i \) in the residual e-liquid for the electronic atomizer after \( n \) puffing processes, kg; \( m_{i-\text{vap},n+1} \) is the mass of component \( i \) in the vapor generated from e-liquid at the \((n+1)\)-th puffing process, kg; \( w_{i,n} \) is the mass fraction of component \( i \) in the residual e-liquid for electronic atomizer after \( n \) puffing processes.

In this study, MATLAB software was used to solve the theoretical model. The time step for iterative calculation is 0.01 s. The diameter of wick in the electronic atomizer is 3 mm. The length of heating section is 4 mm. The diameter of airflow passage is 8 mm. The ambient temperature is 27 °C. The heating time for each puff is 3 s. The puffing flow is 18.33 ml/s.

### 3. Results and Discussion

The variation characteristics of the residual mass and PG/VG proportion for the e-liquid in the electronic atomizer are shown in Fig.2. The formulation of e-liquid is 50%PG+50%VG (wt). The initial additive amount of e-liquid is 1371.48 mg. The heating power of coil is 10 W. The residual masses of e-liquid decreased from 1371.48 mg to 1238.12 mg after 10 puffing processes. The mass fractions of PG in the residual e-liquid gradually decreased from 50.00% to about 46.21%. The mass fractions of VG in the residual e-liquid gradually increased from 50.00% to about 53.79%. At the same temperature condition, the saturation pressure of PG is much larger than that of VG. The volatility of PG is relatively stronger. Therefore, the vaporization rate of PG in the e-liquid is relatively fast. The proportion of volatile PG in the residual e-liquid for the electronic atomizer decreases. The content of involatile VG in the residual e-liquid continuously enriches. It leads to the weakening of the volatility for the residual e-liquid with the increase of puffing number. The variation characteristics of total particulate matter of aerosol during the multi-puffing process are shown in Fig.3. The total particulate matters generated at the 1th and 10th puffing processes are about 13.46 mg and 13.21 mg, respectively. With the increase of puffing number, the total particulate matter of aerosol for electronic atomizer reduces.

![Figure 2](image-url)

**Figure 2.** The variation characteristics of the residual mass and PG/VG proportion for the e-liquid.
Figure 3. The variation characteristics of total particulate matter of aerosol during the multi-puffing process.

The variation characteristics of maximum vaporization temperature for the residual e-liquid with puffing number are shown in Fig.4. During the 1th to 10th puffing processes, the maximum vaporization temperature of e-liquid rose from 244.69 ℃ to 250.52 ℃, approximately. The boiling points of PG and VG are about 188 ℃ and 287 ℃, respectively [6]. The boiling point of e-liquid composed of a higher VG content increases. During the multi-puffing process, the maximum vaporization temperature of the e-liquid for each puff gradually increases since the content of VG in the residual e-liquid enriches.

Figure 4. The variation characteristics of maximum vaporization temperature for the residual e-liquid with puffing number.
4. Conclusion
Based on the theoretical model of the multi-puffing process for electronic atomizer, the following conclusions could be drawn from the results. During the first to tenth puffing number, the mass fraction of PG in the residual e-liquid reduced when the puffing number increased. Meanwhile, the mass fraction of VG in the residual e-liquid increased gradually. The total particulate matter of aerosol generated from the electronic atomizer decreased with the puffing number increasing. The maximum vaporization temperatures of the residual e-liquid rose gradually in the multi-puffing process.

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