Volatile Property of Electronic Cigarette Composition by ATR-FTIR

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Abstract. Electronic cigarette has been said to be a less harmful substitute for traditional tobacco cigarette, customized cigarette e-liquid offers various flavors and unique experience for smokers. Different from traditional tobacco cigarette, electronic cigarette uses a heater and atomizer to heat and aerosolize the cigarette e-liquid. The study for the composition and its combustion product are flourishing thanks to the developing analysis instruments and methods. However, the volatile property, and the influence of e-cigarette smoke on environment and human health still remain unclear. In this study, we choose the RELX P53a electronic cigarette with a watermelon-flavor pod to analyse its composition by ATR-FTIR, study its volatility and discuss its influence on environment and human health. We find that propylene glycol(PG) and vegetable glycercin(VG) are the two main composition of the electronic cigarette emission, and a small amount of nicotine is added with benzoic acid to form nicotine salt, which is said to have less negative effect than pure nicotine in traditional tobacco cigarette. One of the main composition propylene glycol(PG) follows a exponential volatile process and its volatile rate falls with the increase of RH. The flow rate of air is then increased to test whether these deposited emissions could be removed. The result shows that these emissions will stay in human body and atmosphere and not easily cleared. Further studies are required to analyse the influence of small amount of compositions such as flavor essence on environment and human health and seek for reasonable regulation on the formula of electronic cigarette e-liquid.

1. Introduction

Electronic cigarette has undergone a rapid emergence and gained widespread popularity in the past decades to serve as a less harmful substitute for traditional tobacco cigarette. Hon Lik is said to be the first person to invent electronic cigarette in early 2000s.[1] Shaped similarly to conventional tobacco cigarette, electronic cigarette has three main components, the heater to heat the cigarette e-liquid at specific temperature, the atomizer to create smoke, and a pod to store cigarette e-liquid. The e-liquid is usually a mixed viscous solution of propylene glycol(PG), vegetable glycerin(VG), nicotine, flavor essence and water, etc. PG and VG usually accounts for more than 90% of the e-liquid mass, and the general content range of nicotine is 0–60 mg/mL. Flavors essences may contain menthol, sugars, esters and pyrazines,[2] it is used to create various flavors. When the users smoke, the battery controlled by an internal chip and sensor starts, the electric heating wire heats the heating element soaked in electronic cigarette liquid, and then the e-liquid is heated and evaporated, meanwhile, the air passes through the atomizer to cool the evaporated gas, and the evaporated gas is thus condensed into aerosol. With the further understanding of electronic cigarette and its influence, the regulation on it becomes more strict these years. China has recently introduced national standards to strictly ask electronic cigarette producers to manufacture cigarette e-liquid with flavors limited only to cigarette flavor. [3] United States and European Union have also strengthened its regulation on electronic cigarette. [4-6]

As a substitute of conventional tobacco cigarette, the electronic cigarette is said to be less harmful, but the long-term research of electronic cigarette on human health and environment is still unclear. Recent studies have found that compared with clean air, the second-hand aerosol produced by e-cigarette heating solution exceeds the general PM1.0 standard by 14 to 40 times, the PM2.5 more than 20% of the standard, 2 to 8 times the standard for acetaldehyde, and 10 to 115 times the standard for nicotine.[7] Therefore, it is of great significance to further discuss the environmental influence of electronic cigarette emission, the research on the process of volatility becomes important. In this work, ATR-FTIR is used to identify the composition of electronic cigarette emissions and collect the real-time spectra of emissions to study its volatility. These data are useful for further investigation and regulation of electronic cigarette production and protection of environment and human health.

2. Conclusion

2.1. Experiment

Sample Preparation. RELX P53a is the electronic cigarette atomizer purchased from Shenzhen Wuxin Technology Co., Ltd. The watermelon flavor pod is...
purchased from Shenzhen Wuxin Technology Co., Ltd. Zero air was purchased from Beijing Huatong Jingke Gas Co., Ltd. Aerosol aqueous droplets were atomized by the electronic cigarette onto a diamond substrate.

Experiment instrument. The Bruker-Alpha Infrared spectrometer paired with a gas flow system is the experimental setup used in this experiment. Consisting of two lines, the gas flow system allows dry and humid gas to pass so that relative humidity (RH) can be controlled. The total gas flow rate was set to be 400 mL·min⁻¹. A deuterated triglycine sulfate (DTGS) detector is used to collect high signal-to-noise IR spectra of aerosols deposited onto diamond substrate. An imitation of real cigarette inhaling and exhaling gadget was self made by 3D printing and shown in Figure 1.(left). The sample cell is customized by computer model constructing and then 3D-printed and it is shown in Figure 1.(right). A set ratio of dry and humid air was introduced to create a stabilized RH atmosphere, and the electronic cigarette emission was then sprayed onto the diamond substrate. Then the spectra was collected every 15 seconds to obtain the real-time change in situ. The spectra was obtained by 12 scans with a resolution of 8 cm⁻¹ in the spectral range of 600~4000 cm⁻¹. The 3D-printer used is JG AURORA Z-603S and the printing material is polylactic acid (PLA). All experiments were performed around 25°C.

Data processing. The obtained infrared was first processed with OMNIC, the peak value of the corresponding characteristic band in the infrared spectra was used to calculate the amount of the specified content. The peak value of 867 cm⁻¹, 1138 cm⁻¹ and 670 cm⁻¹ is attributed to vegetable glycerine (VG), propylene glycol (PG), and nicotine respectively.[8,9]

2.2. Conclusion and discussion

Identification of compositions of e-liquid and atomized emissions. IR spectra of RELX electronic cigarette electronic liquid and electronic cigarette smoke is shown in Figure 2. The band at 3294 cm⁻¹, 1034 cm⁻¹, 922 cm⁻¹ is attributed to O-H stretching mode, C-O stretching mode and O-H bending mode respectively. The intensity at 1138 cm⁻¹ is selected to represent propylene glycol. The intensity at 867 cm⁻¹ is used to represent vegetable glycerin. There is no obvious difference from the spectra of e-liquid and spectra of emissions, so it can be considered that there was no change of chemicals from e-liquid to emissions by heating and atomizing.

Fig. 2. ATR-FTIR spectra of e-cigarette smoke and e-cigarette liquid oil.

Volatility Property of VG. Different proportion of dry and humid air was first introduced to control the RH of the sample cell, after the RH was stabilized, the electronic cigarette smoke was inhaled by a 100mL syringe and then sprayed onto the diamond substrate, the ATR-FTIR started to collect spectra immediately every 15 seconds one spectra. After 30 minutes of collection, the spectra was processed. From Figure 3(a) there is a fitted time-intensity line of propylene glycol (PG) under 80% RH. It shows a perfect fit using the equation as follows:

\[ y = 0.46687 + 0.59928 \times e^{-0.14273x} \]  

(1)

As we can see from the slope that with the increase of RH the rate of volatility falls. According to the Maxwell steady-state diffusion formula, the partial pressure difference between the surface of the droplet and the volatile component at infinity from the center of the droplet is the driving force leading to the volatilization of the component, and the partial pressure is proportional to the molar concentration of the component. With the gradual decrease, the water volatilizes more and more, causing the concentration to gradually increase, thereby accelerating the volatilization of components.[10]
Influence of gas flow rate on the remains of electronic cigarette emissions. After the experiment of volatility, it was obvious that there still remained a proportion of emission upon the substrate, approximately 30%. If the remains of the emission was not easily removed, it might be harmful to environment and human health. So we adjusted the flow rate of air and tried to remove it as much as possible, the flow rate was increased from 200 mL·min⁻¹ to 800 mL·min⁻¹ with the RH set to 40%. After 60 minutes of flushing, it is identified that propylene glycol and vegetable glycerin still remains and nicotine is gone. Keep increasing the flow rate of air, it made little difference on the remains of emissions. It could be concluded that even after long time and high flow rate of flushing, it was still hard to get rid of the remains of emission. Further investigation on the remains of emission on human health and environment is needed.

Conclusion. The composition of RELX P53a electronic cigarette e-liquid and emissions were analyzed by ATR-FTIR. Under the set heating temperature, no obvious change happened during heating and atomizing from ATR-FTIR spectra. The volatility of propylene glycol follows an exponential trend and eventually keeps unchanged with remains of approximately 30%. The rate of volatility process drops with the increase of relative humidity. The elevation of air flow rate makes little difference to the remains of the emissions. These results can be used to deeper understand the and provide significant support for regulation of electronic cigarette in China.

References
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