A Multifaceted Approach for the Analysis of Electronic Cigarettes using DSA-TOF and Headspace GC-MS

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1 Introduction

- Electronic cigarettes have become increasingly popular as a proposed safer and cleaner alternative to conventional cigarettes.
- Electronic cigarette companies claim the produced aerosol is harmless; however, with the lack of FDA regulation and research in this area, more experiments are needed to conclusively refute or support this claim.
- DSA, an ambient ionization source, easily detects compounds in the aerosol that is produced.
- Headspace GC-MS will detect any volatile organic compounds present, helping to identify what is in the sample.
- The goal of this research is to analyze differences between the electronic cigarette aerosol and the liquid itself.

2 Electronic Cigarette

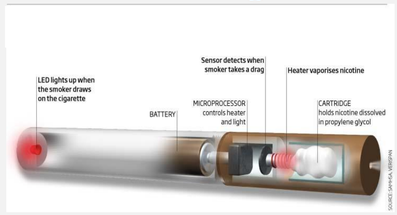

Figure I. Schema of an electronic cigarette[1]

The electronic cigarettes were purchased from a local convenience store. After mass spectra of the aerosol produced by the electronic cigarette was collected, the cigarette was carefully disassembled to remove the filter containing the cigarette liquid. By using pressure to extract the liquid, the liquid analyzed.

3 Sampling Process

Sampling the electronic cigarettes required the use of a puffer. Using a 5 mL syringe and a prototype cigarette sampling apparatus, the cigarettes were puffed and a 5 mL sample was taken. The sample was applied to the DSA directly immediately after being puffed. For headspace analysis, the sample was injected into a sealed headspace vial.

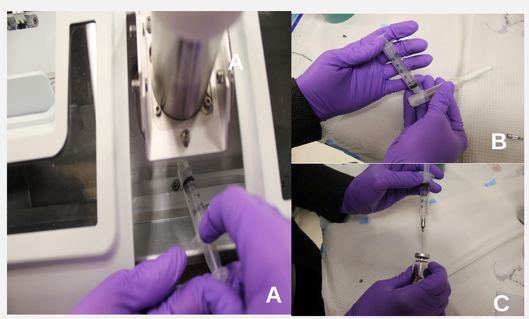

Figure II. A) Introduction of vapor into DSA. **B)** Use of Ecig sampling apparatus **C)** Introduction of sample into headspace vial.

4 DSA- TOF

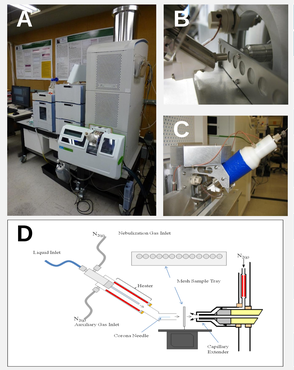

TABLE I: DSA-TOF PARAMETERS	
Parameter	DSA-TOF
Capillary Exit (Volts)	100.00
Low m/z	100
High m/z	3000
Ion Polarity	Positive
Ion Source Type	DSA
Cylinder Lens (Volts)	400
Endplate (Volts)	-400
APCI voltage (Volts)	-2500
APCI Vaporizer Temperature (ºC)	300
Drying Gas Flow Rate (L/m)	0
Nebulizer Gas Pressure (PSI)	80

Figure III. A) Overall view of the DSA attached to the AxION TOF. **B)** Close up view of the DSA sample tray inlet to the AxION TOF. **C)** Close up view of the DSA. **D)** Schematic of the DSA ionization source.

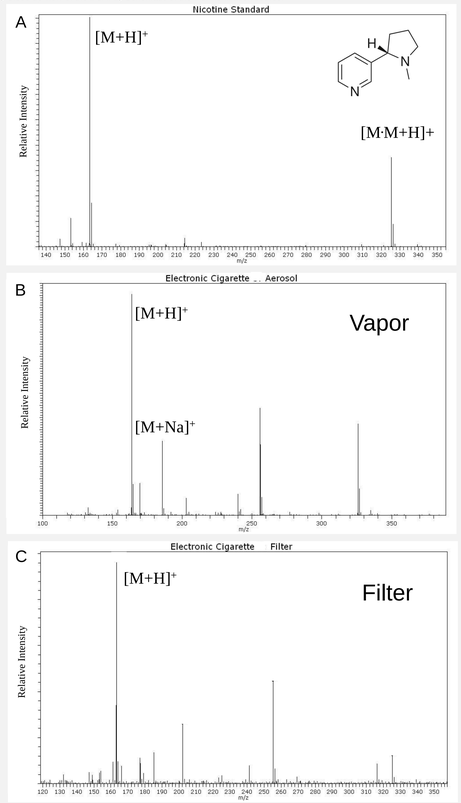

Figure IV. A) Spectrum of the nicotine standard **B)** Spectrum of the electronic cigarette aerosol **C)** Spectrum of the electronic cigarette filter

5 Headspace GC-MS

Figure V. A) Image of PerkinElmer ClarusGC with headspace autosampler. **B)** Diagram of headspace mechanism

TABLE II: HS-GC-MS Parameters	
Parameter	HS-GC-MS
Sample Injector	Headspace
Mode	Trap
Oven Ramp	40º C hold for 3.00 minutes 6ºC/min to 300ºC hold for 3.00 minutes
Column name	PerkinElmer COL-VELOCITY-5 Cat.# N9306311
Gas type	Helium
Column Length (m)	30.00
Column Diameter (µm)	250
Oven Ramp	40º C hold for 3.00 minutes 6ºC/min to 300ºC hold for 3.00 minutes
Ion Source	EI
Ion Polarity	Positive
Low m/z	40
High m/z	600
Solvent Delay (min)	1.5
MS scan time (min)	1.5-50
Inlet Line Temperature (ºC)	200
Electron Energy (V)	70
Repeller (V)	200
Lens 1 (V)	12.0
Lens 2 (V)	159.7
Source Temp (ºC)	150

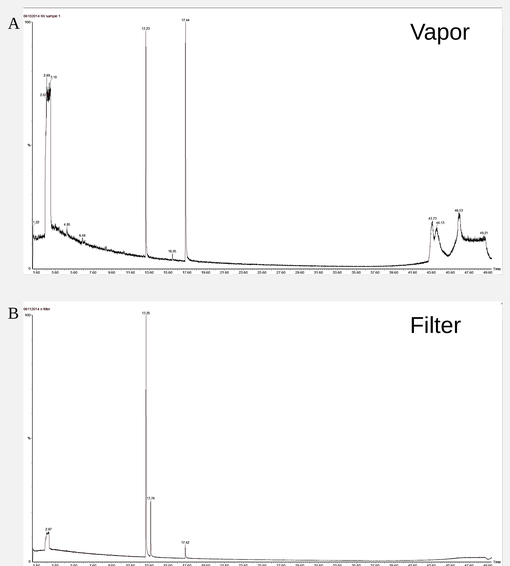

Figure VI. A) Chromatogram of the electronic cigarette aerosol **B)** Chromatogram of the electronic cigarette filter

6 Results

Table III: Peak Identification from Aerosol	
Retention Time	Peak Identity
2.69	Propylene Glycol
4.85	Butanoic acid, 3-methyl-*
6.48	Milbemycin B*
13.23	Levomenthol
16.05	Butanoic acid*
17.44	Nicotine
43.73	Unidentified
44.13	Unidentified
46.53	Unidentified

Table III: Peak Identification from Filter	
Retention Time	Peak Identity
2.87	Propylene Glycol
13.25	Levomenthol
13.74	Unidentified
17.42	Nicotine

***most correlated library result (unconfirmed identity)**

7 Future Direction

- Quantification of compounds
- Further analysis of mass spectrum peaks
- Analysis of different flavors
- Creation of a more efficient GC method

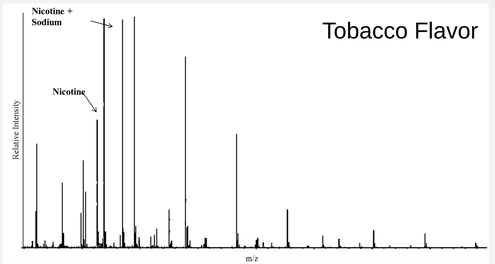

Figure VII. Spectra of produced tobacco electronic cigarette aerosol analyzed by DSA

8 Conclusion

- Nicotine and menthol were detected from the analysis of both the aerosol and liquid of electronic cigarettes.
- The aerosol was able to be directly analyzed without the need for pre-concentration methods or extracting solvents.
- There are notable differences between the liquid and electronic cigarette aerosol across both platforms which will require further study.
- Future research will allow for the detection of various additional compounds in flavored electronic cigarettes.

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Reference: 1) http://static.businessinsider.com/image/5182cf45ecad04a41c000001/image.jpg