Assessment of Flavor Transfer to Aerosols of Electronic Nicotine Delivery Systems

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Purpose

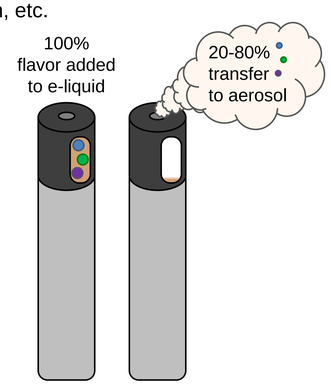
The purpose of this study is to provide a new method for determining the flavor transfer from e-liquid to aerosol for use in risk assessment of ENDS devices. A semiquantitative method is a suitable alternative that is less resource intensive than a quantitative method in facilitating consumer exposure assessments.

Introduction

- In the evaluation of electronic nicotine delivery systems (ENDS), reliable analytical methods are useful for acquiring flavor data for consumer exposure risk assessment calculations.
- Without accurate transfer data, the conservative default assumption that 100% of the flavor added to the e-liquid is being transferred to the aerosol may be an overestimation.
- Flavor transfer values can be calculated by comparing the amount of a flavor in an e-liquid to the amount observed in a generated aerosol.

$$\frac{\left(\frac{\mu g\ flavor\ compound}{g\ whole\ aerosol}\right)}{\left(\frac{\mu g\ flavor\ compound}{g\ eliquid}\right)} \times 100\% = \%\ Flavor\ Transfer$$

- Flavor amounts can be determined using both quantitative and semiquantitative gas chromatography mass spectrometry (GC-MS) methods.
  - In the quantitative method, absolute flavor amounts are calculated using known standards.
  - A semiquantitative approach estimates the amount of flavor by comparing to an internal standard.
- Because the inherent error associated with semiquantitation of flavors in both e-liquids and aerosols is expected to be similar, the semiquantitated flavor transfer values would also be expected to be similar to the quantitated flavor transfer values.
- Flavor transfer from e-liquid to aerosol is expected to be less than 100% due to absorption into cartridge materials, volatilization, etc.



Results

Semiquantitative vs Quantitative Comparison

- Although semiquantitation may over or underestimate absolute flavor concentrations, the ratio between e-liquid and aerosol is the same for both quantitative and semiquantitative methods.

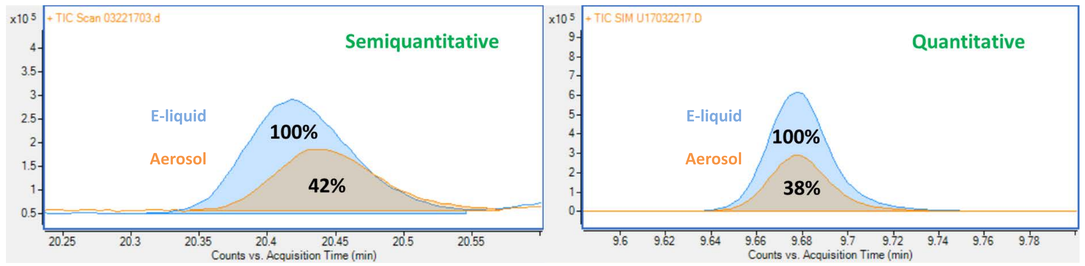
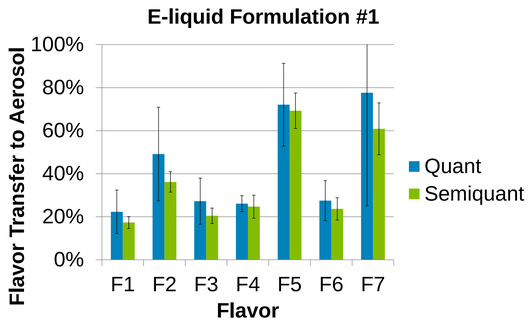
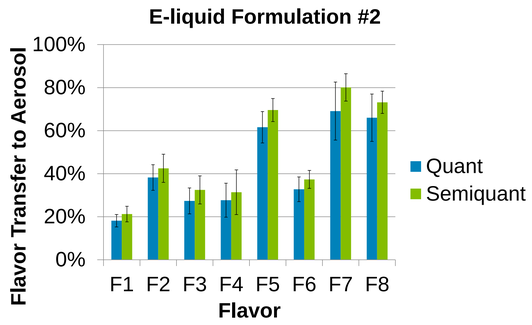


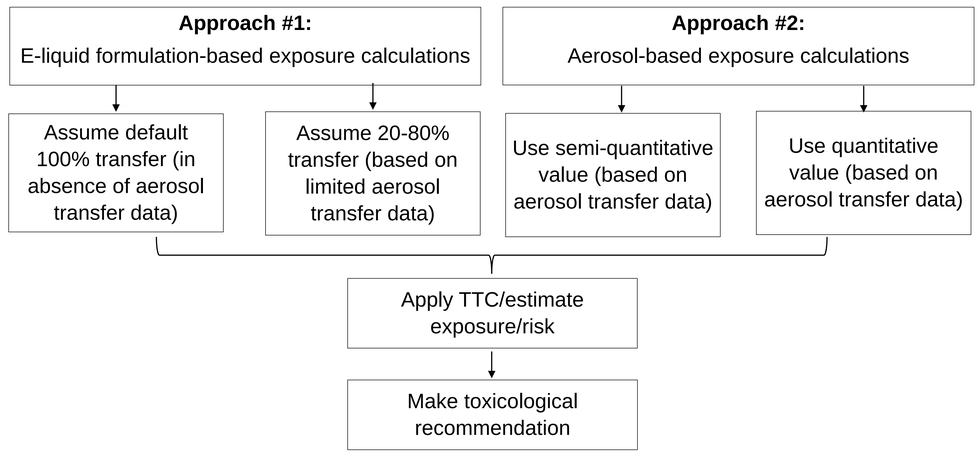
Figure 1. Overlaid e-liquid and aerosol chromatograms for semiquantitative and quantitative analyses (Flavor F2)

Flavor Transfer Values





Risk Assessment Approaches



Methods

E-liquid Samples

- 2 e-liquid formulations tested
- 8 flavor compounds selected for analysis
- 5 replicates, e-liquid analyzed directly from bottle

Aerosol Samples

- Cig-a-like ENDS devices containing the 2 e-liquid formulations
- 5 replicates, 180 puffs
- 55 mL puff volume, 30 second puff interval, 3 second puff duration, square wave puff profile
- Cerulean SM 450 Linear Smoke Machine
- Cambridge pad extracted in impinger for whole aerosol sample collection

Quantitative Analysis

- Calibration with neat flavor standards
- DB-WaxEtr Column (30 m x 0.32 mm i.d. x 0.50 mm film thickness)
- Agilent 6890N-5973 GC-MSD
- Selective Ion Monitoring (SIM)

Semiquantitative Analysis

- Semiquantitation using internal standard

$$\frac{Compound\ Peak\ Area \times \mu g\ Internal\ Standard}{Internal\ Standard\ Peak\ Area} = \mu g\ Compound$$

- DB-WaxEtr Column (30m x 0.25 mm i.d. x 0.25 mm film thickness)
- Agilent 7890B-5977A GC-MSD
- Scan 15-550 amu

Conclusions

- Quantitative and semiquantitative flavor transfer to aerosol was compared.
  - Lowest flavor transfer between e-liquid and aerosol:
    - 18% by quantitation
    - 17% by semiquantitation
  - Highest flavor transfer between e-liquid and aerosol:
    - 78% by quantitation
    - 80% by semiquantitation
  - Flavor transfer values from both methods demonstrate good agreement across all flavors.
- Flavor transfer data from semiquantitative analysis is predictive of a full quantitative analysis.
- Semiquantitation of flavor transfer values provides a more cost effective and less labor intensive method for the evaluation of ENDS flavors and consumer exposure.
- Data driven flavor transfer approach provides a more suitable approach to risk assessment of flavor ingredients than the over-conservative 100% transfer assumption.