Supplemental Information

**Influence of puff topographies on e-liquid heating temperature, emission characteristics and modeled lung deposition of Puff Bar™**

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**Keywords:** Electronic cigarette, Puff Bar™, Particle size distributions, Respiratory deposition, Secondhand exposure estimates, Chemical characterization

# **Graphical abstract**

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# **Graphical abstract**

This study assessed the effect of puff volumes (mL: 55, 65, and 75) on heating temperature from seven different Puff Bar™ e-liquids on the corresponding aerosol emissions. Increasing puff volumes from 55-mL to 75-mL increased e-liquid heating temperature by approximately 50 °C, which in turn, increased masses of emitted particles and VCCs. Dose modeling indicated that an abundance of small particles (~1 µm) emitted by Puff Bar™ presents an exposure risk for users and bystanders, which could pose respiratory health concerns to both (and especially for vulnerable bystanders who cannot easily remove themselves from the exposure). ****

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Supplemental Figure S1A). Sensitivity analysis for chemical characterization of Puff Bar™ emissions at different number (i.e., 2, 3, 4, and 5) of puffs within 3 minutes



Supplemental Figure S1B). Sensitivity analysis for chemical characterization of Puff Bar™ emissions at different puffing duration (minutes: 5, 6, 7, and 8)

Figure S2. Total mass (average (µg/ml/puff)) of VCCs emitted by different flavor types of Puff Bar™ on aerosolizing at puff volumes (mL: 55, 65, and 75) for n = 3 per puff volume. \*Puff Bar™ flavor types significantly influence (at p<0.05) total mass of VCCs.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Puff Bar™ Flavors | Trial # | Total mass of aerosol | Mass based PSD | Inhaled deposition fraction | Exhaled fraction (%) |
| Average(mg/puff)  | MMAD (μm) | GSD | Head (%) | TB (%) | Pulmonary (%) | Total (%) |
| Cucumber | 1 | 5.7 | 1.06 | 1.56 | 37 | 20 | 42 | 30 | 70 |
| 2 | 5.2 | 0.99 | 1.47 | 37 | 20 | 42 | 30 | 70 |
| 3 | 5.2 | 0.99 | 1.45 | 36 | 21 | 43 | 27 | 73 |
| Grape | 1 | 5.1 | 1.12 | 1.71 | 39 | 20 | 41 | 33 | 67 |
| 2 | 5.1 | 1.14 | 1.71 | 40 | 20 | 41 | 33 | 67 |
| 3 | 4.5 | 1.10 | 1.66 | 39 | 20 | 41 | 32 | 68 |
| Melon Ice | 1 | 4.5 | 1.01 | 1.53 | 36 | 21 | 43 | 28 | 72 |
| 2 | 4.4 | 0.97 | 1.49 | 35 | 22 | 43 | 27 | 73 |
| 3 | 4.4 | 0.97 | 1.51 | 36 | 22 | 43 | 27 | 73 |
| OMG | 1 | 4.3 | 1.01 | 1.49 | 36 | 21 | 43 | 28 | 72 |
| 2 | 4.3 | 1.06 | 1.56 | 38 | 20 | 42 | 31 | 69 |
| 3 | 3.9 | 1.06 | 1.58 | 38 | 20 | 42 | 31 | 69 |
| Pomegranate | 1 | 5.1 | 1.01 | 1.47 | 36 | 21 | 43 | 28 | 72 |
| 2 | 5.1 | 1.06 | 1.49 | 37 | 21 | 43 | 29 | 71 |
| 3 | 5.0 | 1.01 | 1.49 | 36 | 21 | 43 | 28 | 72 |
| Sour Apple | 1 | 6.0 | 0.99 | 1.43 | 35 | 22 | 43 | 27 | 73 |
| 2 | 6.2 | 0.95 | 1.32 | 34 | 22 | 44 | 25 | 75 |
| 3 | 6.0 | 0.97 | 1.40 | 35 | 22 | 43 | 26 | 74 |
| Strawberry | 1 | 2.2 | 0.99 | 1.45 | 35 | 22 | 43 | 27 | 73 |
| 2 | 1.8 | 0.97 | 1.40 | 34 | 22 | 44 | 27 | 73 |
| 3 | 2.0 | 0.99 | 1.40 | 35 | 22 | 43 | 27 | 73 |

 Table S1. Total mass, PSD, and lung deposition of all trials with Puff Bar™ for puff volume 55 mL

OMG – orange, mango, guava; PSD – particle size distribution; MMAD – mass median aerodynamic diameter; GSD – geometric standard deviation; TB – tracheobronchial

Table S2. Total mass, PSD, and lung deposition of all trials with Puff Bar™ for puff volume 65 mL

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Puff Bar™ Flavors | Trial # | Total mass of aerosol | Mass based PSD | Inhaled deposition fraction | Exhaled fraction (%) |
| Average(mg/puff) | MMAD (μm) | GSD | Head(%) | TB(%) | Pulmonary (%) | Total (%) |
| Cucumber | 1 | 6.5 | 1.01 | 1.47 | 36 | 21 | 43 | 28 | 72 |
| 2 | 6.6 | 1.03 | 1.49 | 36 | 21 | 43 | 28 | 72 |
| 3 | 6.7 | 1.03 | 1.53 | 37 | 21 | 42 | 29 | 71 |
| Grape | 1 | 5.7 | 1.10 | 1.62 | 38 | 20 | 42 | 31 | 69 |
| 2 | 5.9 | 0.97 | 1.49 | 35 | 22 | 43 | 27 | 73 |
| 3 | 5.9 | 0.95 | 1.40 | 35 | 22 | 43 | 26 | 74 |
| Melon Ice | 1 | 4.9 | 0.97 | 1.38 | 35 | 22 | 43 | 26 | 74 |
| 2 | 5.0 | 0.99 | 1.45 | 35 | 21 | 43 | 27 | 73 |
| 3 | 5.4 | 0.95 | 1.38 | 34 | 22 | 43 | 25 | 75 |
| OMG | 1 | 4.3 | 1.01 | 1.45 | 36 | 21 | 43 | 28 | 72 |
| 2 | 4.8 | 1.03 | 1.45 | 36 | 21 | 43 | 28 | 72 |
| 3 | 4.9 | 1.01 | 1.56 | 37 | 21 | 42 | 29 | 71 |
| Pomegranate | 1 | 6.0 | 0.99 | 1.43 | 35 | 22 | 43 | 27 | 73 |
| 2 | 6.1 | 1.01 | 1.43 | 36 | 21 | 43 | 27 | 73 |
| 3 | 6.1 | 1.01 | 1.43 | 36 | 21 | 43 | 27 | 73 |
| Sour Apple | 1 | 6.4 | 0.97 | 1.40 | 35 | 22 | 43 | 26 | 74 |
| 2 | 7.3 | 0.95 | 1.34 | 34 | 22 | 44 | 25 | 75 |
| 3 | 8.6 | 0.86 | 1.12 | 31 | 24 | 44 | 22 | 78 |
| Strawberry | 1 | 3.5 | 0.93 | 1.32 | 33 | 23 | 44 | 25 | 75 |
| 2 | 3.7 | 0.95 | 1.36 | 34 | 22 | 44 | 26 | 74 |
| 3 | 3.7 | 0.99 | 1.40 | 35 | 22 | 43 | 27 | 73 |

OMG – orange, mango, guava; PSD – particle size distribution; MMAD – mass median aerodynamic diameter; GSD – geometric standard deviation; TB – tracheobronchial

Table S3. Total mass, PSD, and lung deposition of all trials with Puff Bar™ for puff volume 75 mL

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Puff Bar™ Flavors | Trial # | Total mass of aerosol | Mass based PSD | Inhaled deposition fraction | Exhaled fraction (%) |
| Average(mg/puff) | MMAD (μm) | GSD | Head(%) | TB(%) | Pulmonary (%) | Total (%) |
| Cucumber | 1 | 6.7 | 0.99 | 1.40 | 35 | 22 | 43 | 27 | 73 |
| 2 | 6.7 | 0.99 | 1.38 | 35 | 22 | 43 | 26 | 74 |
| 3 | 6.8 | 0.99 | 1.43 | 35 | 21 | 43 | 27 | 73 |
| Grape | 1 | 6.1 | 1.08 | 1.60 | 38 | 20 | 42 | 31 | 69 |
| 2 | 6.4 | 1.10 | 1.51 | 38 | 20 | 42 | 30 | 70 |
| 3 | 6.7 | 1.06 | 1.53 | 37 | 21 | 42 | 30 | 70 |
| Melon Ice | 1 | 7.1 | 0.86 | 1.19 | 32 | 24 | 44 | 22 | 78 |
| 2 | 7.9 | 0.90 | 1.27 | 33 | 23 | 44 | 23 | 77 |
| 3 | 8.2 | 0.86 | 1.23 | 32 | 24 | 44 | 22 | 78 |
| OMG | 1 | 3.9 | 1.01 | 1.43 | 35 | 22 | 43 | 27 | 73 |
| 2 | 3.9 | 1.03 | 1.53 | 36 | 21 | 43 | 28 | 72 |
| 3 | 5.2 | 1.06 | 1.49 | 37 | 20 | 42 | 30 | 70 |
| Pomegranate | 1 | 6.1 | 0.97 | 1.40 | 35 | 22 | 43 | 26 | 74 |
| 2 | 6.1 | 1.01 | 1.47 | 36 | 21 | 43 | 28 | 72 |
| 3 | 6.4 | 0.97 | 1.40 | 35 | 22 | 43 | 26 | 74 |
| Sour Apple | 1 | 7.8 | 0.95 | 1.32 | 34 | 22 | 44 | 25 | 75 |
| 2 | 7.8 | 0.95 | 1.36 | 34 | 22 | 44 | 25 | 75 |
| 3 | 8.2 | 0.95 | 1.36 | 34 | 22 | 44 | 25 | 75 |
| Strawberry | 1 | 4.0 | 0.93 | 1.25 | 33 | 23 | 44 | 24 | 76 |
| 2 | 4.1 | 0.93 | 1.32 | 33 | 23 | 44 | 25 | 75 |
| 3 | 4.2 | 0.93 | 1.32 | 33 | 23 | 44 | 25 | 75 |

OMG – orange, mango, guava; PSD – particle size distribution; MMAD – mass median aerodynamic diameter;

GSD – geometric standard deviation; TB – tracheobronchial

Table S4. Volatile carbonyl compounds (VCCs) emission of all trials with Puff Bar™ for puff volume 55 mL

|  |  |  |  |
| --- | --- | --- | --- |
| Puff Bar™ Flavors | Trial # | Total mass of VCCs (μg/puff) | Mass (μg/puff) |
| Acetaldehyde | Acetone | Acrolein | Formaldehyde | Isovaleraldehyde |
| Cucumber | 1 | 1.31 | 0.10 (7.7%) | 0.33 (25.5%) | 0.01 (1.1%) | 0.60 (45.9%) | 0.21 (16.3%) |
| 2 | 1.25 | 0.08 (6.4%) | 0.33 (26.6%) | 0.01 (1.1%) | 0.57 (45.3%) | 0.23 (18.6%) |
| 3 | 1.24 | 0.07 (5.4%) | 0.33 (26.9%) | 0.01 (1.0%) | 0.57 (45.8%) | 0.24 (19.1%) |
| Grape | 1 | 2.14 | 0.77 (35.9%) | 0.53 (24.9%) | 0.11 (5.0%) | 0.57 (26.5%) | 0.00 (0.0%) |
| 2 | 1.90 | 0.67 (35.1%) | 0.47 (24.6%) | 0.00 (0.0%) | 0.53 (28.1%) | 0.02 (1.2%) |
| 3 | 1.85 | 0.67 (36.1%) | 0.50 (27.0%) | 0.00 (0.0%) | 0.53 (28.8%) | 0.03 (1.4%) |
| Melon Ice | 1 | 2.22 | 0.63 (28.5%) | 0.60 (27.0%) | 0.04 (1.6%) | 0.33 (15.0%) | 0.23 (10.3%) |
| 2 | 2.05 | 0.60 (29.2%) | 0.60 (29.2%) | 0.03 (1.6%) | 0.33 (16.2%) | 0.26 (12.8%) |
| 3 | 1.79 | 0.53 (29.9%) | 0.53 (29.9%) | 0.03 (1.8%) | 0.33 (18.7%) | 0.22 (12.5%) |
| OMG | 1 | 0.66 | 0.07 (11.1%) | 0.26 (39.5%) | 0.01 (0.9%) | 0.11 (17.2%) | 0.21 (31.4%) |
| 2 | 0.82 | 0.06 (7.8%) | 0.30 (36.7%) | 0.01 (0.8%) | 0.09 (11.4%) | 0.22 (27.3%) |
| 3 | 0.80 | 0.08 (10.0%) | 0.30 (37.2%) | 0.01 (0.8%) | 0.12 (15.1%) | 0.22 (28.0%) |
| Pomegranate | 1 | 5.01 | 1.40 (27.9%) | 0.63 (12.6%) | 0.70 (14.0%) | 1.07 (21.3%) | 0.27 (5.4%) |
| 2 | 4.38 | 1.20 (27.4%) | 0.57 (12.9%) | 0.60 (13.7%) | 0.90 (20.5%) | 0.26 (6.0%) |
| 3 | 3.99 | 1.10 (27.6%) | 0.53 (13.4%) | 0.53 (13.4%) | 0.83 (20.9%) | 0.24 (6.1%) |
| Sour Apple | 1 | 1.17 | 0.12 (10.3%) | 0.37 (31.4%) | 0.02 (1.6%) | 0.37 (31.4%) | 0.25 (21.1%) |
| 2 | 1.27 | 0.11 (8.6%) | 0.33 (26.2%) | 0.02 (1.5%) | 0.37 (28.8%) | 0.21 (16.8%) |
| 3 | 1.20 | 0.11 (9.4%) | 0.33 (27.2%) | 0.02 (1.6%) | 0.33 (27.8%) | 0.21 (17.8%) |
| Strawberry | 1 | 3.79 | 0.93 (24.7%) | 0.57 (15.0%) | 0.47 (12.3%) | 0.77 (20.2%) | 0.26 (7.0%) |
| 2 | 3.25 | 0.80 (24.6%) | 0.50 (15.4%) | 0.40 (12.3%) | 0.67 (20.5%) | 0.24 (7.3%) |
| 3 | 3.10 | 0.77 (24.7%) | 0.50 (16.1%) | 0.37 (11.8%) | 0.60 (19.3%) | 0.22 (7.0%) |

 OMG – orange, mango, guava.

(%) – Mass proportion of VCCs

Table S5. Volatile carbonyl compounds (VCCs) emission of all trials with Puff Bar™ for puff volume 65 mL

|  |  |  |  |
| --- | --- | --- | --- |
| Puff Bar™ Flavors | Trial# | Total mass of VCCs (μg/puff) | Mass (μg/puff) |
| Acetaldehyde | Acetone | Acrolein | Formaldehyde | Isovaleraldehyde |
| Cucumber | 1 | 1.63 | 0.09 (5.7%) | 0.26 (15.9%) | 0.04 (2.5%) | 0.90 (55.2%) | 0.21 (12.7%) |
| 2 | 1.45 | 0.09 (6.2%) | 0.29 (19.7%) | 0.04 (2.5%) | 0.80 (55.1%) | 0.21 (14.2%) |
| 3 | 1.56 | 0.10 (6.2%) | 0.30 (19.4%) | 0.04 (2.6%) | 0.83 (53.3%) | 0.22 (13.9%) |
| Grape | 1 | 1.52 | 0.15 (10.1%) | 0.28 (18.3%) | 0.09 (5.7%) | 0.73 (48.4%) | 0.20 (13.2%) |
| 2 | 1.89 | 0.20 (10.7%) | 0.30 (15.7%) | 0.15 (8.1%) | 0.83 (44.0%) | 0.21 (10.9%) |
| 3 | 1.66 | 0.19 (11.3%) | 0.31 (18.7%) | 0.15 (8.9%) | 0.73 (44.3%) | 0.19 (11.5%) |
| Melon Ice | 1 | 1.06 | 0.11 (10.7%) | 0.37 (34.5%) | 0.01 (1.2%) | 0.27 (25.1%) | 0.21 (19.4%) |
| 2 | 1.06 | 0.12 (11.0%) | 0.37 (34.5%) | 0.02 (1.6%) | 0.27 (25.4%) | 0.21 (19.7%) |
| 3 | 1.07 | 0.11 (10.6%) | 0.40 (37.4%) | 0.02 (1.6%) | 0.25 (23.7%) | 0.20 (18.7%) |
| OMG | 1 | 0.90 | 0.12 (13.7%) | 0.40 (44.6%) | 0.01 (0.7%) | 0.11 (12.3%) | 0.24 (26.8%) |
| 2 | 0.99 | 0.16 (15.9%) | 0.43 (44.0%) | 0.01 (0.8%) | 0.14 (14.2%) | 0.22 (22.7%) |
| 3 | 0.72 | 0.07 (9.2%) | 0.32 (44.7%) | 0.01 (1.0%) | 0.11 (14.7%) | 0.22 (30.4%) |
| Pomegranate | 1 | 4.89 | 1.30 (26.6%) | 0.70 (14.3%) | 0.60 (12.3%) | 1.03 (21.1%) | 0.27 (5.5%) |
| 2 | 4.50 | 1.20 (26.6%) | 0.70 (15.5%) | 0.50 (11.1%) | 0.90 (20.0%) | 0.27 (6.0%) |
| 3 | 4.51 | 1.23 (27.4%) | 0.67 (14.8%) | 0.53 (11.8%) | 0.90 (20.0%) | 0.25 (5.6%) |
| Sour Apple | 1 | 1.13 | 0.08 (7.4%) | 0.28 (24.9%) | 0.02 (1.5%) | 0.37 (32.6%) | 0.25 (21.9%) |
| 2 | 0.97 | 0.08 (8.2%) | 0.30 (31.2%) | 0.02 (1.6%) | 0.33 (34.3%) | 0.21 (21.9%) |
| 3 | 1.14 | 0.09 (8.2%) | 0.28 (24.5%) | 0.02 (1.4%) | 0.43 (37.9%) | 0.18 (16.0%) |
| Strawberry | 1 | 5.38 | 1.37 (25.4%) | 0.70 (13.0%) | 0.67 (12.4%) | 1.30 (24.1%) | 0.20 (3.7%) |
| 2 | 4.47 | 1.10 (24.6%) | 0.60 (13.4%) | 0.50 (11.2%) | 1.03 (23.1%) | 0.24 (5.3%) |
| 3 | 4.66 | 1.17 (25.1%) | 0.60 (12.9%) | 0.53 (11.5%) | 1.13 (24.3%) | 0.20 (4.2%) |

OMG – orange, mango, guava

(%) – Mass proportion of VCCs

Table S6. Volatile carbonyl compounds (VCCs) emission of all trials with Puff Bar™ for puff volume 75 mL

|  |  |  |  |
| --- | --- | --- | --- |
| Puff Bar™ Flavors | Trial# | Total mass of VCCs (μg/puff) | Mass (μg/puff) |
| Acetaldehyde | Acetone | Acrolein | Formaldehyde | Isovaleraldehyde |
| Cucumber | 1 | 1.83 | 0.17 (9.3%) | 0.37 (20.1%) | 0.03 (1.5%) | 0.83 (45.6%) | 0.25 (13.7%) |
| 2 | 1.63 | 0.14 (8.8%) | 0.30 (18.2%) | 0.03 (2.0%) | 0.87 (53.3%) | 0.25 (15.6%) |
| 3 | 1.71 | 0.15 (8.8%) | 0.33 (19.1%) | 0.03 (2.0%) | 0.90 (52.7%) | 0.25 (14.8%) |
| Grape | 1 | 1.75 | 0.16 (9.2%) | 0.37 (21.0%) | 0.04 (2.3%) | 0.80 (45.8%) | 0.24 (13.9%) |
| 2 | 1.75 | 0.18 (10.1%) | 0.32 (18.3%) | 0.04 (2.5%) | 0.83 (47.6%) | 0.24 (13.5%) |
| 3 | 1.65 | 0.18 (10.7%) | 0.32 (19.6%) | 0.05 (3.0%) | 0.83 (50.6%) | 0.20 (12.3%) |
| Melon Ice | 1 | 1.00 | 0.11 (11.4%) | 0.25 (25.1%) | 0.01 (1.4%) | 0.33 (33.4%) | 0.23 (22.7%) |
| 2 | 1.27 | 0.13 (10.0%) | 0.33 (26.3%) | 0.02 (1.7%) | 0.37 (28.9%) | 0.24 (18.9%) |
| 3 | 1.08 | 0.13 (11.7%) | 0.30 (27.5%) | 0.02 (1.8%) | 0.37 (33.9%) | 0.23 (21.3%) |
| OMG | 1 | 0.81 | 0.10 (12.4%) | 0.28 (34.6%) | 0.01 (0.6%) | 0.17 (21.4%) | 0.25 (30.9%) |
| 2 | 0.83 | 0.11 (12.9%) | 0.31 (37.3%) | 0.01 (0.8%) | 0.17 (20.1%) | 0.24 (28.9%) |
| 3 | 0.89 | 0.13 (15.0%) | 0.33 (37.1%) | 0.01 (0.7%) | 0.16 (18.4%) | 0.26 (28.8%) |
| Pomegranate | 1 | 3.82 | 0.80 (20.9%) | 0.50 (13.1%) | 0.47 (12.2%) | 0.93 (24.4%) | 0.32 (8.4%) |
| 2 | 4.03 | 0.90 (22.4%)  | 0.53 (13.2%) | 0.50 (12.4%) | 0.87 (21.5%) | 0.30 (7.4%) |
| 3 | 4.61 | 1.03 (22.4%) | 0.63 (13.7%) | 0.57 (12.3%) | 0.97 (21.0%) | 0.30 (6.5%) |
| Sour Apple | 1 | 1.09 | 0.14 (12.5%) | 0.33 (30.5%) | 0.01 (1.2%) | 0.33 (30.5%) | 0.25 (22.6%) |
| 2 | 1.19 | 0.14 (12.1%) | 0.37 (30.8%) | 0.01 (1.0%) | 0.37 (30.8%) | 0.26 (21.9%) |
| 3 | 0.97 | 0.10 (10.6%) | 0.28 (29.2%) | 0.01 (1.1%) | 0.32 (33.3%) | 0.23 (24.0%) |
| Strawberry | 1 | 6.02 | 1.53 (25.5%) | 0.67 (11.1%) | 0.80 (13.3%) | 1.43 (23.8%) | 0.24 (4.0%) |
| 2 | 5.26 | 1.27 (24.1%) | 0.57 (10.8%) | 0.70 (13.3%) | 1.30 (24.7%) | 0.23 (4.4%) |
| 3 | 5.15 | 1.30 (25.3%) | 0.57 (11.0%) | 0.70 (13.6%) | 1.33 (25.9%) | 0.20 (4.0%) |

OMG – orange, mango, guava

(%) – Mass proportion of VCCs