SUPPORTING INFORMATION

Emissions from electronic cigarettes: Assessing vapers' intake of toxic compounds, secondhand exposures and the associated health impacts

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Modeling exposures to secondhand vapor

Secondhand vapor in a residential setting

In a recent study, we estimated exposures to second- and thirdhand tobacco smoke generated by conventional cigarettes. The case study considered a non-smoker living with a smoker in a typical US home.[1] In the current study we reproduced the same scenario and home characteristics for secondhand vaping exposures: a 2000 ft^2 home (186 m^2) with an air exchange rate of 0.14 h^{-1}. Exposure levels were modeled using an occupancy pattern based on the National Human Activity Patterns Survey (NHAPS). In this scenario, both the user and the non-user are home most of the time, a condition under which non-user's exposures would be the highest.[2] The model considered equally spaced daily puffing sessions corresponding to the same three regimes described above (frequent short, intermediate and infrequent long). Only puffing sessions that occurred when the user was at home impacted indoor concentrations. The following mass balance equation was used to describe the time varying indoor concentration.

$$\frac{dC_l}{dt} = \frac{S_{i,j,k,l,m}}{V} + A \cdot C_{out,l} - (k_l + A)C_l \qquad (1S)$$

where S is the mass emission rate in the home, A is the air exchange rate, C_{out} is the outdoor concentration, C is the indoor concentration, k is the first order loss rate (e.g., by deposition or adsorption to indoor surfaces), and V is the indoor space volume. (Subscripts are defined in the text below equation (2) of the published article.) It was assumed that $C_{out} = 0$ to predict the incremental impact of secondhand vaping, and that $k = 0$ considering that species are conserved and remain in the gas phase. The latter assumption is reasonable for formaldehyde and other volatile aldehydes that typically do not react or adsorb to indoor surfaces. By contrast, air levels predicted for nicotine should be considered an upper limit, because this compound adsorbs rapidly to indoor surfaces. [3] Equation 1S can be solved recursively for $C_{in,i}$ with any of the nonconcentration parameters held constant within a given time step and allowed to vary from one time step to another. Equation 2S presents the recursive solutions for $C_l(t)$:

$$C_l(t) = C_l(t-\Delta t)\cdot \exp(-A\cdot \Delta t) + \frac{S_{i,j,k,l,m}(t)\cdot[1-\exp(-A\cdot\Delta t)]}{V\cdot A} \tag{2S}$$

The modeled time step is the interval between the start of two consecutive puffs, 18 s. When a puff is not occurring, S=0, and during a puff $S=EXH/\Delta t$. Occupant exposures were calculated by overlaying non-user occupancy patterns with home concentrations.

Exposures to secondhand vapor in a bar

Smoking bans are common in the US hospitality industry. However, e-cigarettes are often allowed in bars, where secondhand vaping has the potential to negatively impact the health of non-vaping patrons and workers. Impacts on employees are likely to be larger due to longer exposure periods. Waring and Siegel assessed differences in indoor air quality and occupancy levels in 17 bars before and after a smoking ban during 2005 in Austin, Texas, by recording the volume, occupancy and average smoking frequency.[4] These statistics were used here to tune our model using a range of values for room volume, occupancy and number of vapers, assuming that there are not significant differences between bars that allowed smoking and vaping. The steady-state indoor air concentrations of compounds emitted in each bar were calculated using the mass balance approach shown in Equations 3S-4S. As with in the residential model, it was assumed C_{out} = 0 to calculate the contribution of an indoor source. Steady-state air concentrations were described as:

$$\frac{dC_l}{dt} = 0 = \frac{SS_{i,j,k,l,m}\cdot Q_n}{V_n} - A_n\cdot C_l \tag{3S}$$

The subscript n refers to each individual bar considered in the analysis, SS is the average steady state emission rate, and Q is the average number of active vapers in a particular bar. The indoor concentration of a particular compound can be expressed as:

$$C_l = \frac{SS_{i,j,k,l,m} \cdot Q_n}{A_n \cdot V_n} \quad (4S)$$

where the steady state emission rate was calculated as the mean mass emission rate per puff normalized by the interval between the start of two consecutive puffs, Δt = 18 s, as follows:

$$SS_{i,j,k,l,m} = \frac{P_i^{initial} \cdot EXH_{i,j,k,l,m}^{initial} + P_i^{st-state} \cdot EXH_{i,j,k,l,m}^{st-state}}{50 \cdot \Delta t} \quad (5S)$$

To determine occupational exposures, it was assumed that bar employees were exposed to average concentrations during 40 hours per week.

***Table S1**. Predicted and experimental respiratory retention (R_R) for compounds found in e-cigarette vapor, and retention factors (R) used in this study.*

Compound	**Log *VP*** (in Pa)	R_R (%)		$R = (1-MS) \times R_R$ (%) [a]
		Predicted	**Experimental**	
Formaldehyde	5.70	99	97 [b] 95-100 [c]	59 – 79
Acetaldehyde	5.00	98	94-100 [c] 99 [d]	58 – 78
Acrolein	4.56	97	97-100 [c]	58 – 78
Diacetyl	3.88	97	NA	58 – 78
Acetol	2.88	96	NA	57 – 77
Glycidol	2.08	95	NA	57 – 76
Nicotine	0.74	94	93.8 [e] >98 [d]	56 – 75
Nicotyrine	0.08	93	NA	56 – 74
Benzene	4.11	97	NA	58 – 78

a: For mouth spill in the range 20 % < *MS* < 40% using equation 1 (in published article)
b: Predicted from results by Spanel et al, 2013 [5]
c: Reported by Moldoveanu et al, 2007 [6]
d: Reported by Feng et al, 2007 [7]
e: Reported by St Helen et al, 2016 [8]
NA: data not available

Figure S1. *Effect of the variability in retention factors on daily intake when vaping CT e-liquid on an EGO device at 3.8V. This prediction is for a high-usage rate of 250 puffs per day distributed in: (A) frequent and short vaping sessions (25 sessions of 10 puffs each); (B) intermediate conditions (10 sessions of 25 puffs each), and (C) infrequent and long vaping sessions (5 sessions of 50 puffs each). The data represent lower and upper bound values for the retention factor, R.*

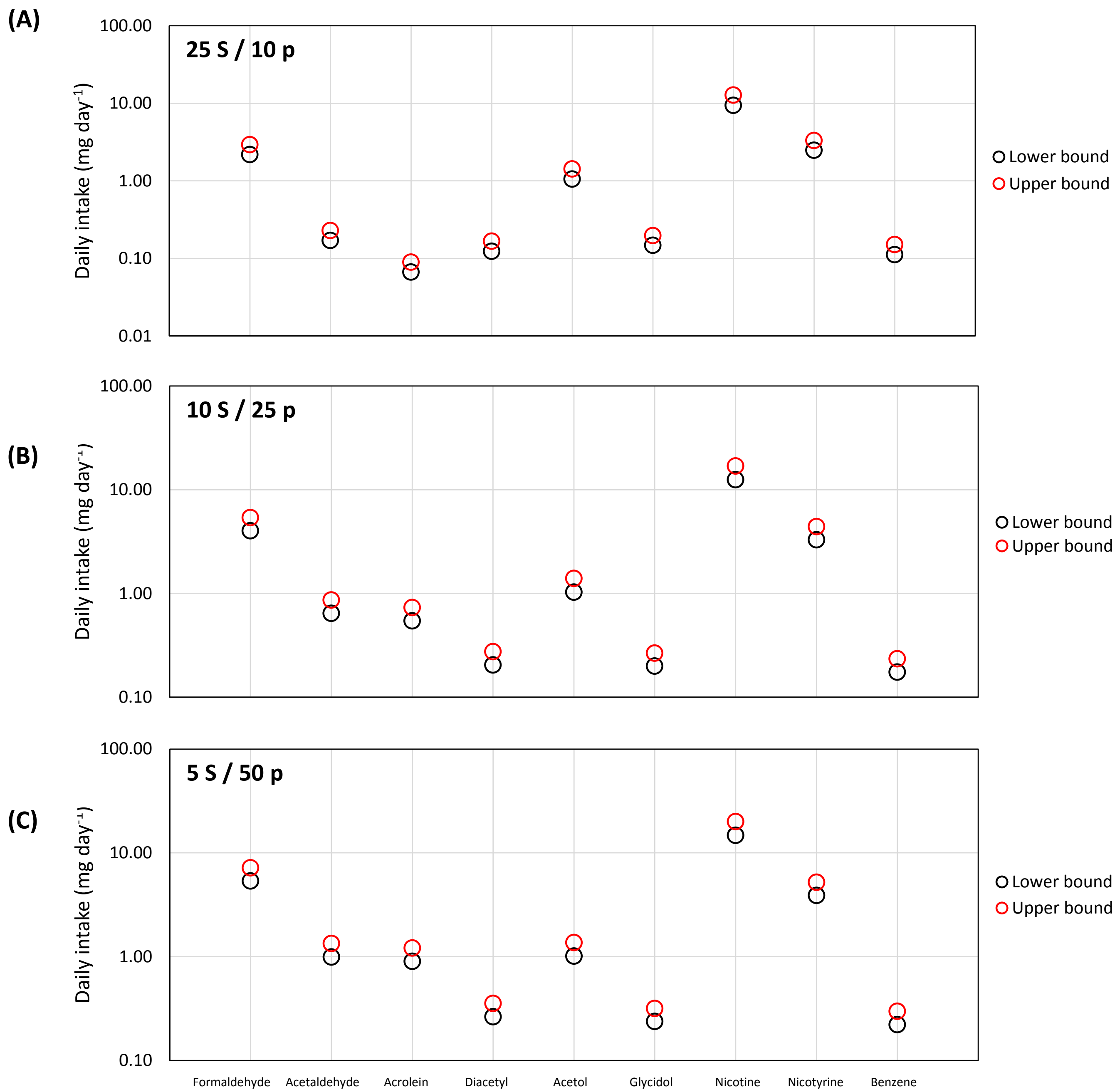


Figure S2. *Impact of the choice of the e-liquid used with the EGO vaporizer at 4.8 V on the intake predicted for a high-usage rate of 250 puffs per day, distributed in: (A) frequent and short vaping sessions (25 sessions of 10 puffs each); (B) intermediate vaping conditions (10 sessions of 25 puffs each), and (C) infrequent long vaping sessions (5 sessions of 50 puffs each). The e-liquids include: Apollo Classic Tobacco (CT), Drip Mojito Mix (MOJ) and Drip Bubblicious (BUB).*

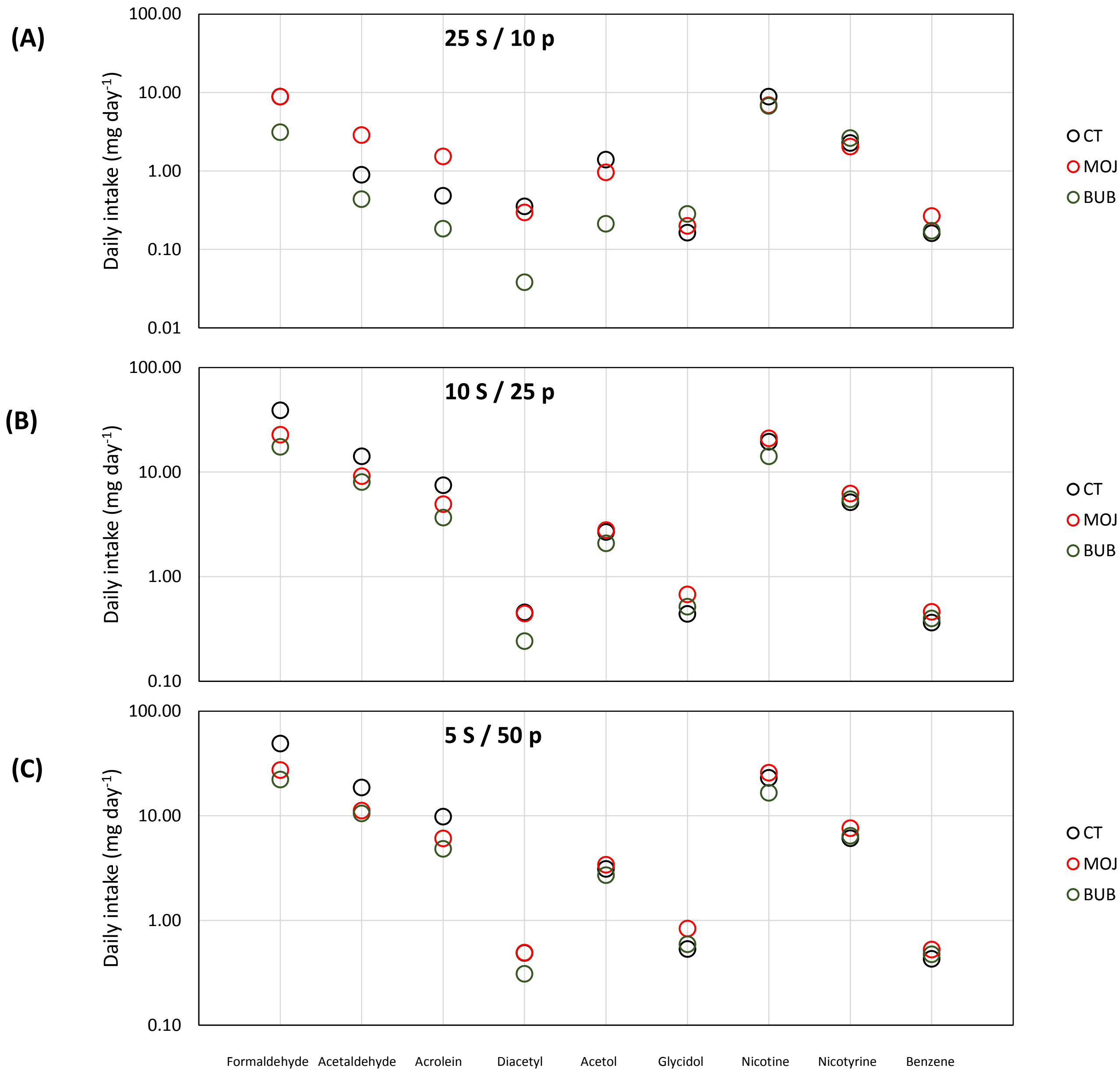


Table S2*. Sensitivity analysis for daily intake reported in Figure 1. Percent increments correspond to changes in toxicant intake due to switching from vaping regime a) to b), and from regime b) to c). The regimes consist on:*

a) ***Frequent short sessions*** *corresponding to 25 puffing sessions of 10 puff each*

b) ***Intermediate (typical) conditions****, with 10 puffing sessions of 25 puffs each, and*

c) ***Infrequent long sessions****, with only 5 puffing sessions daily of 50 puffs each*

Analyte	**Switching from vaping regime (a) to (b)**			**Switching from vaping regime (b) to (c)**		
	AERO 3.8 V	**EGO 3.8 V**	**EGO 4.8 V**	**AERO 3.8 V**	**EGO 3.8 V**	**EGO 4.8 V**
Formaldehyde	-23 %	45 %	77 %	-17 %	34%	26 %
Acetaldehyde	-2 %	73 %	94 %	-1 %	55%	31 %
Acrolein	44 %	88 %	94 %	33 %	66%	31 %
Diacetyl	11 %	39 %	22 %	8 %	30%	7 %
Acetol	-20 %	-2 %	48 %	15 %	-2%	16 %
Glycidol	14 %	26 %	63 %	10 %	19%	21 %
Nicotine	37 %	25 %	54 %	28 %	18%	18 %
Nicotyrine	13 %	25 %	56 %	9 %	18%	19 %
Benzene	20 %	36 %	56 %	15 %	27%	19 %
Average change	**11 %**	**40 %**	**63 %**	**8 %**	**30%**	**21 %**

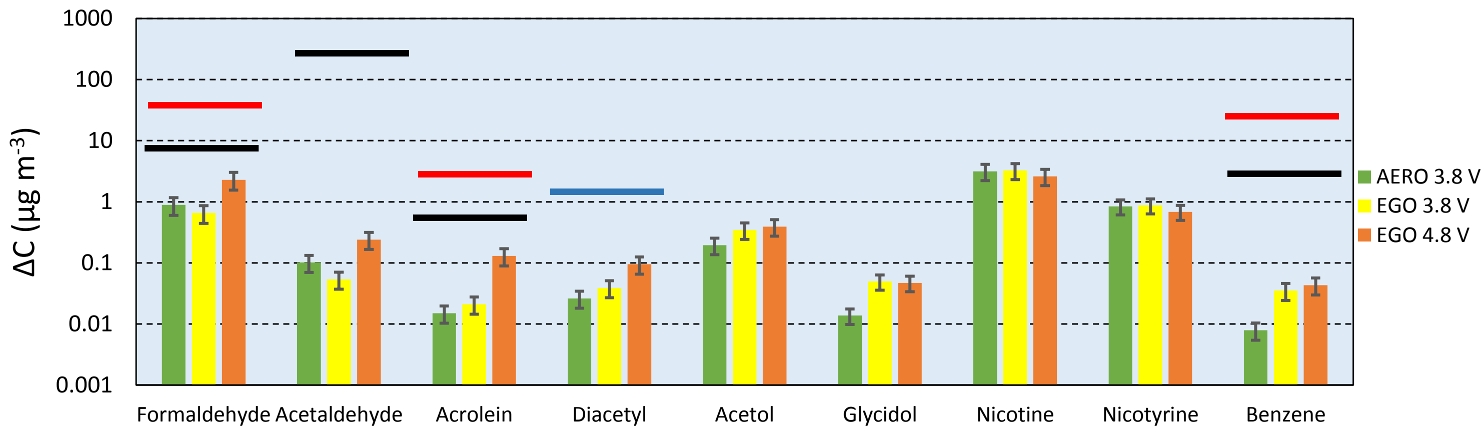
Table S3. *Daily emission rate and intake predicted for smokers consuming 10 conventional cigarettes per day. This information is used to determine intake for combustion cigarettes presented in Figure 2 of the published article.*

Compound	Method	Cigarette	Emission rate (µg/cigarette)	Daily emission rate (mg/day)[a]	Daily intake (mg/day)[a,b]	Reference
Formaldehyde	CRM	various [c]	3 – 43	0.03 – 0.43	0.02 – 0.30	9
	ISO	1R6F	27	0.27	0.19	10
	HCI	1R6F	104	1.04	0.72	10
Acetaldehyde	CRM	various [c]	86 – 651	0.86 – 6.51	0.58 – 4.43	9
	ISO	1R6F	522	5.22	3.55	10
	HCI	1R6F	1552	15.5	10.5	10
	ISO	various [d]	126 – 1143	1.26 – 11.4	0.9 – 8.0	11
	HCL	various [d]	1098 – 2244	11.0 – 22.4	7.7 – 15.7	11
Acrolein	CRM	various [c]	6 – 63	0.06 – 0.63	0.04 – 0.43	9
	ISO	1R6F	43	0.43	0.29	10
	HCI	1R6F	154	1.54	1.05	10
Diacetyl	ad-hoc	various [e]	301 – 433	3.0 – 4.3	2.0 – 2.9	12
	ISO	various [f]	247 – 318	2.5 – 3.2	1.7 – 2.2	13
	MA	various [f]	469 – 705	4.7 – 7.1	3.2 – 4.8	13
	HCI	various [f]	650 – 894	6.5 – 8.9	4.4 – 6.1	13

***a*:** Assuming a smoking rate of 10 cigarettes per day
b: Applying retention factors *R* shown in Table 1S
c: 3R4F, 1R5F, CM6 and five commercial cigarettes
***d*:** 3R4F, 1R5F and 50 filtered cigarette brand varieties corresponding to 89% of the US market share in 2011
e: 2R1F and 14 commercial cigarettes
f: 3R4F and six commercial cigarettes
CRM: CORESTA recommended smoking regime
ISO: Smoking regime defined by International Society for Standardization (ISO) Standard Nr. 3308
HCI: Health Canada Intense smoking regime
MA: Massachusetts Dept. of Public Health smoking regime

***Figure S3**. Change in average indoor air VOC concentration for a residential scenario in which the vaper stays at home most of the time, corresponding to an elevated usage rate of 250 puffs per day. Black and red lines represent California OEHHA Reference Exposure Levels for 8-h and acute 1-h exposures, respectively, for formaldehyde, acetaldehyde, acrolein and benzene. The blue line represents the NIOSH recommended 40-h workweek exposure level for diacetyl. Three different device/voltage combinations using the CT e-liquid were used to determine emission rates corresponding to: (A) frequent short vaping sessions (25 sessions of 10 puffs each), and (B) infrequent long vaping sessions (5 sessions of 50 puffs each).*

(A)



(B)

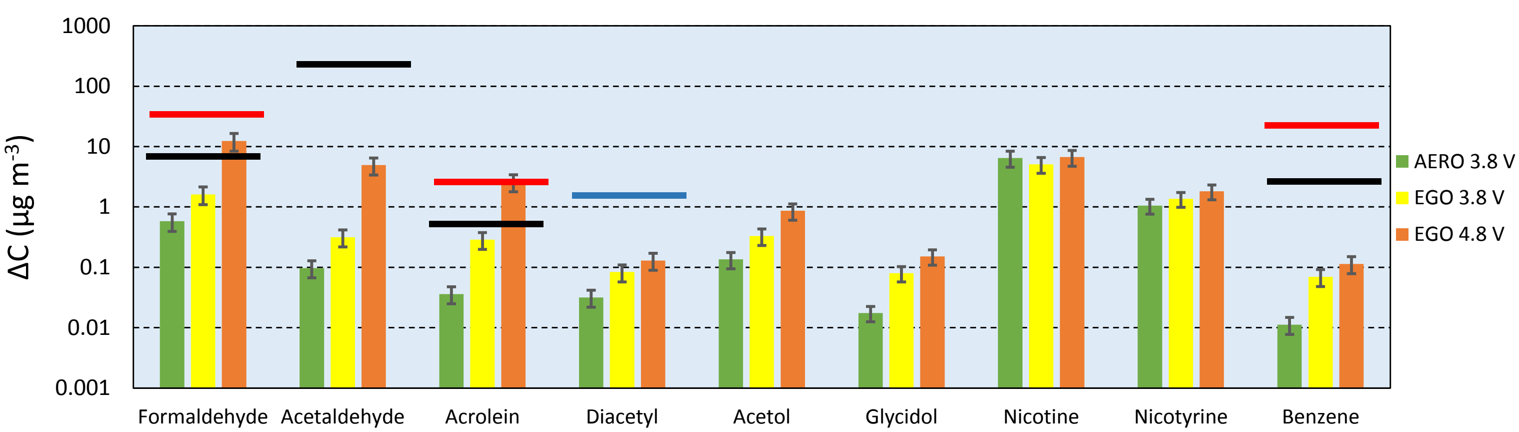
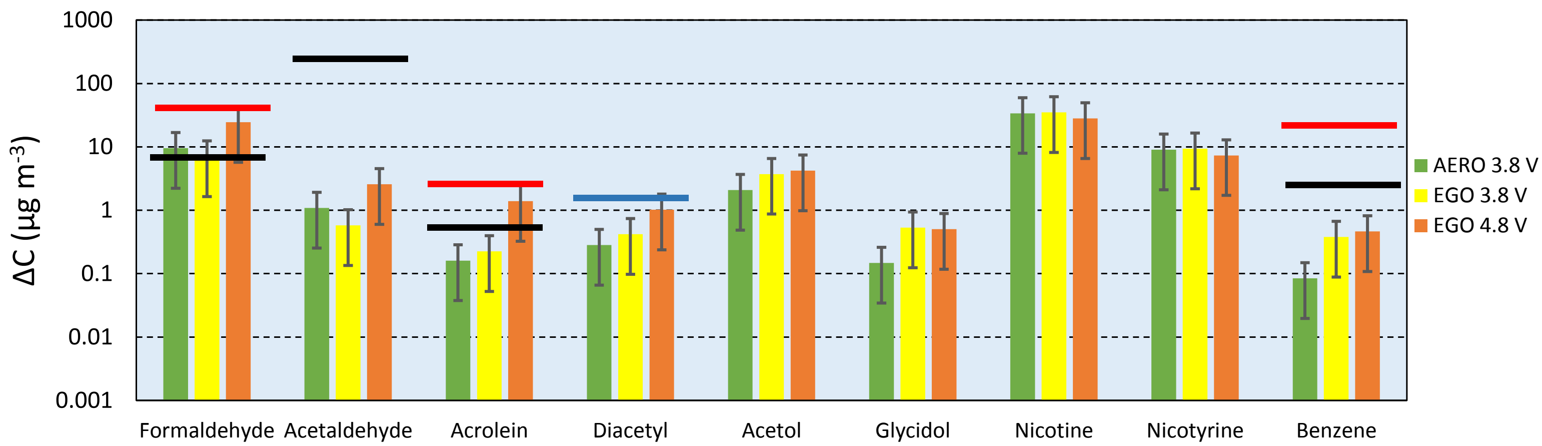


***Figure S4**. Change in average indoor air VOC concentration in vaping bars. Black and red lines represent California OEHHA Reference Exposure Levels for 8-h and acute 1-h exposures, respectively, for formaldehyde, acetaldehyde, acrolein and benzene. The blue line represents the NIOSH recommended 40-h workweek exposure level for diacetyl. Three different device/voltage combinations using the CT e-liquid were used to determine emission rates corresponding to: (A) frequent short vaping sessions (25 sessions of 10 puffs each), and (B) infrequent long vaping sessions (5 sessions of 50 puffs each).*

(A)



(B)

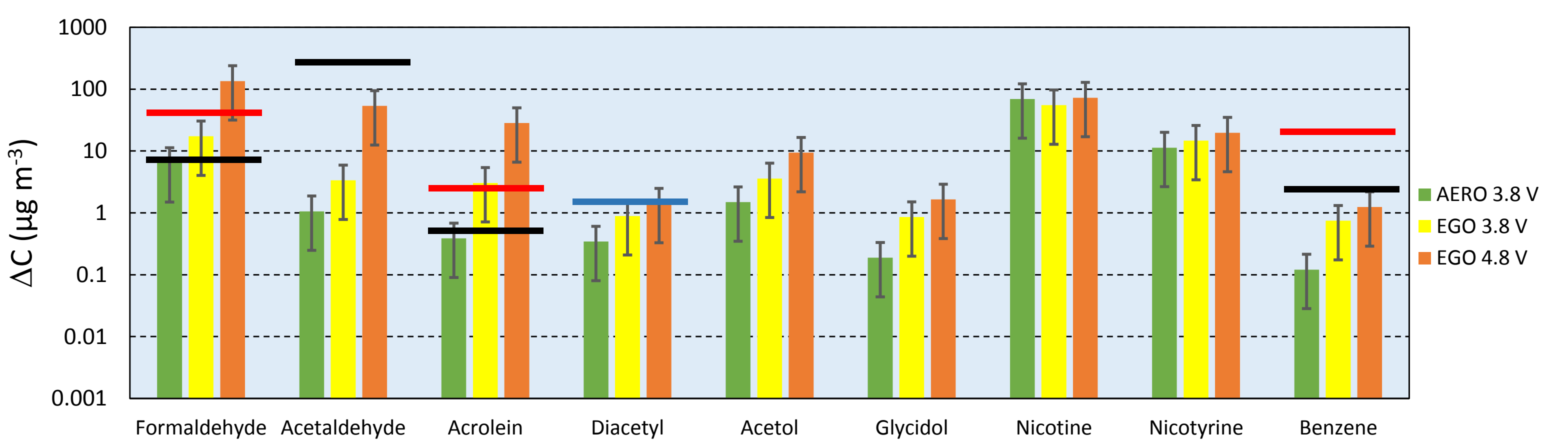


Table S4. *Physical characteristics (space volume, air exchange rates), occupancy and average number of lit cigarettes during a sampling period of at least 30 minutes for 17 bars studied by Waring and Siegel in 2007.[4] This data set was used in our evaluation of the impact of these parameters on indoor levels due to vaping, assuming that the vaping and smoking prevalences were the same. For each lit cigarette listed in the Waring and Siegel study, we computed 10 e-cigarette puffs. Reproduced with permission from Nature Publishing Group. Copyright 2007.*

Bar #	Volume (m^3)	Number of occupants	Average number of lit cigarettes	Air exchange rate (h^{-1})
1	284	23	5.0	1.3
2	1164	73	10.8	1.0
3	377	44	7.3	1.9
4	379	38	5.3	4.8
5	467	72	7.0	5.4
6	1167	89	9.4	1.2
7	826	69	9.2	1.7
8	419	20	4.0	0.9
9	351	204	8.8	NA
10	532	90	7.2	NA
11	816	99	3.3	NA
12	626	230	9.7	3.9
13	521	190	9.7	6.5
14	1995	187	10.0	0.6
15	677	186	13.0	1.7
16	886	79	7.3	1.6
17	2508	105	12.0	0.9

NA: not available

Figure S5: *Estimated DALYs for selected modeled scenarios. The boxes show the median and 95th percentile range of predicted health damage. (A) toxicant-specific impact estimated for the residential scenario in which the vaper consumes CT e-liquid using the EGO device at 3.8 V; (B) aggregated damage for six scenarios of home and bar exposures using three device/voltage combinations. In all cases, emission rates correspond to frequent and short vaping sessions (25 sessions of 10 puffs each). The figure includes the estimated damage due to secondhand and thirdhand smoke (SHS/THS) from combustion cigarettes calculated in our previous study. The DALYs are presented for full smoke and for the VOCs alone (excluding $PM_{2.5}$).*

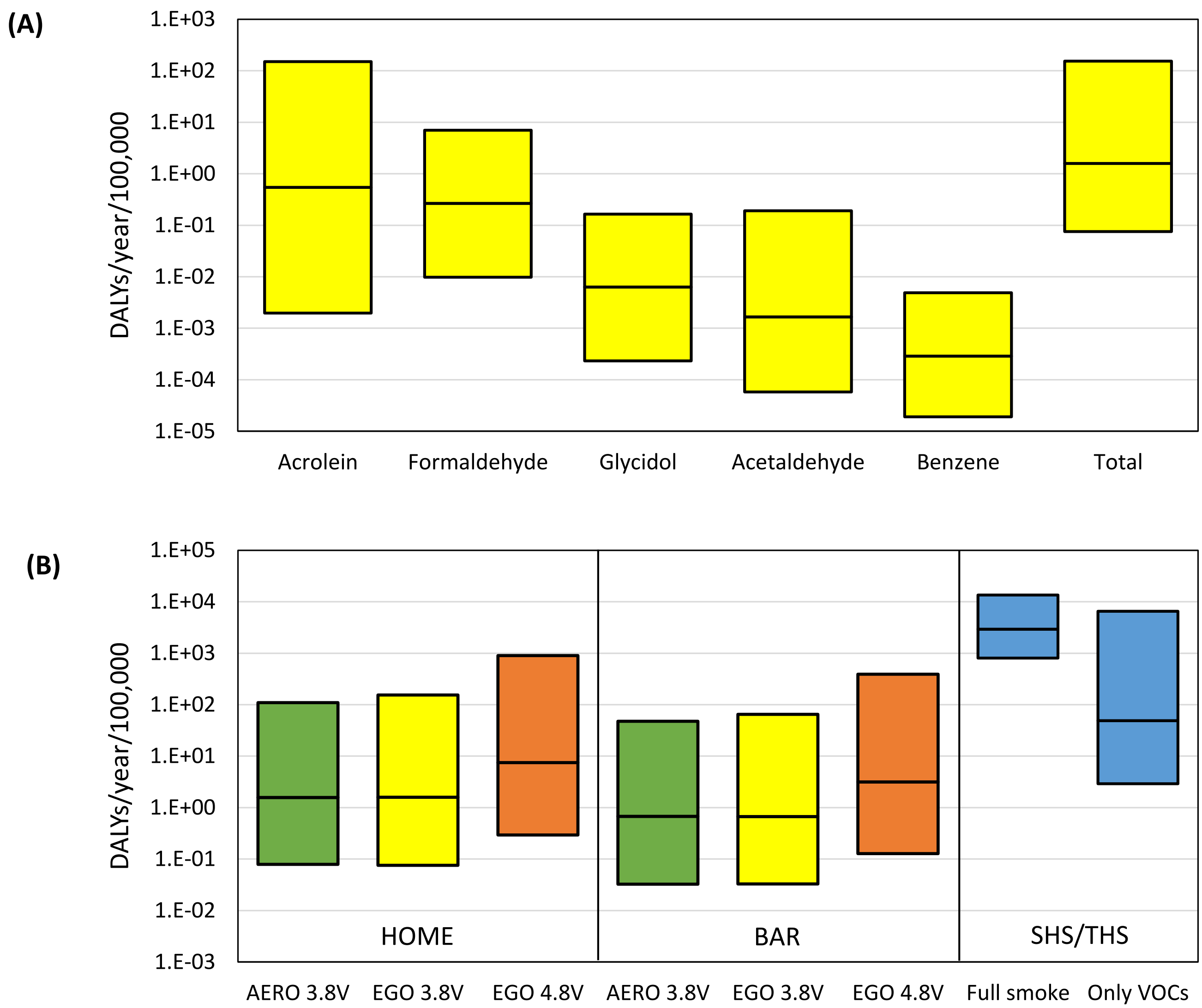
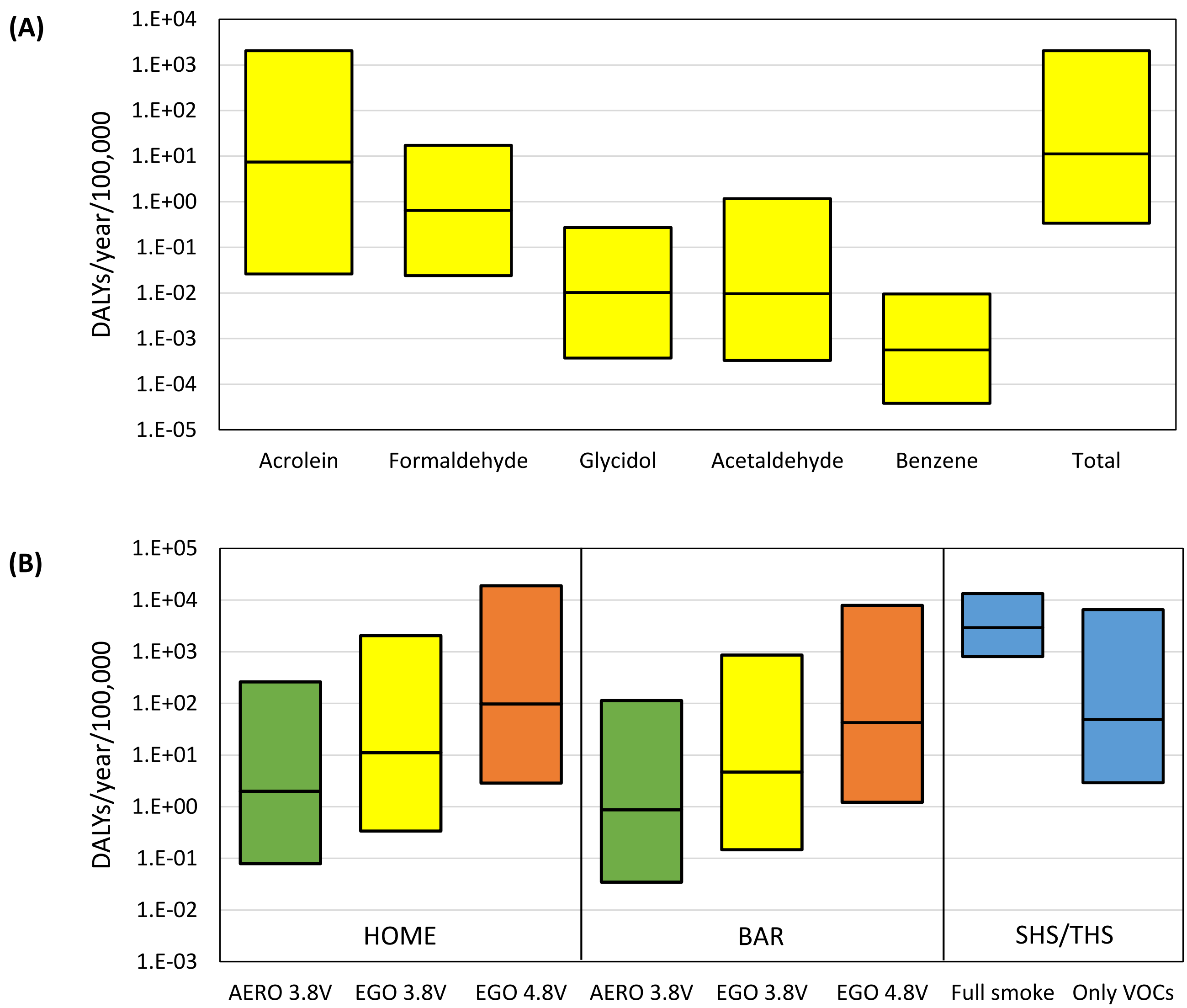


Figure S6: *Estimated DALYs for selected modeled scenarios. The boxes show the median and 95th percentile range of predicted health damage. (A) toxicant-specific impact estimated for the residential scenario in which the vaper consumes CT e-liquid using the EGO device at 3.8 V; (B) aggregated damage for six scenarios of home and bar exposures using three device/voltage combinations. In all cases, emission rates correspond to infrequent and long vaping sessions (5 sessions of 50 puffs each). The figure includes the estimated damage due to secondhand and thirdhand smoke (SHS/THS) from combustion cigarettes calculated in our previous study. The DALYs are presented for full smoke and for the VOCs alone (excluding $PM_{2.5}$).*



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