

Simultaneous Analysis of 22 Volatile Organic Compounds in Cigarette Smoke Using Gas Sampling Bags for High-Throughput SPME

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Table S-1. Regimen and cigarette design influence on vapor phase concentrations from 1R5F and 3R4F University of Kentucky reference cigarettes smoked under both ISO and Intense regimen conditions. Theoretical values were calculated with Equations 1 and 2.

Analyte	1R5F I/ISO	3R4F I/ISO	ISO 1R5F/3R4F	Intense 1R5F/3R4F
Furan	6.0	2.4	0.283	0.714
2,5-Dimethylfuran	6.2	2.7	0.184	0.420
Acetaldehyde	6.6	2.8	0.319	0.743
Vinyl Acetate	6.6	2.7	0.320	0.795
Benzene	6.7	2.7	0.308	0.767
1,3-Butadiene	7.0	2.5	0.329	0.911
Vinyl Chloride	7.3	2.6	0.262	0.732
Nitromethane	7.7	2.8	0.336	0.910
Methylethylketone	8.6	3.0	0.271	0.766
Butanal	9.1	3.1	0.292	0.848
2,3-Butanedione	10.1	3.9	0.289	0.754
Toluene	10.7	3.3	0.226	0.726
Methylvinylketone	10.8	3.5	0.251	0.784
2-Pentanone	11.1	3.5	0.212	0.677
3-Pentanone	11.7	3.6	0.205	0.670
<i>m/p</i> -Xylene	13.0	4.6	0.226	0.632
Acrylonitrile	14.2	3.6	0.251	0.983
<i>o</i> -Xylene	14.8	5.4	0.226	0.625
Ethylbenzene	16.4	4.9	0.214	0.723
Crotonaldehyde	18.5	4.4	0.176	0.744
3-Ethyltoluene	18.9	6.8	0.228	0.634
Styrene	24.7	7.5	0.232	0.766
Theoretical Ratios	5.3	2.8	0.31	0.60

Calculating Research Cigarette and Regimen Ratios

Equations 1 and 2 use smoke volume and dilution variables for each reference cigarette and smoking regimen. Using median puff numbers for these reference cigarettes to calculate smoke volumes, 1R5F smoke volume will increase from 210 mL (6 puffs of 35 mL) for ISO to 335.5 mL (6.1 puffs of 55 mL) for Intense and 3R4F smoke volume will increase from 283.5 mL (8.1 puffs of 35 mL) for ISO to 555.5 mL (10.1 puffs of 55 mL) for Intense. Thus, under Intense conditions, we estimate a 60% smoke volume increase for 1R5F and 96% volume increase for 3R4F, relative to ISO smoke volumes.

Although the 1R5F total smoke volume is less affected by increase in puff volume than the 3R4F, it is much more affected by filter tip ventilation blocking. Filter tip ventilation dilution factors are calculated based on reported filter tip ventilations, with 1R5F 70% ventilated¹ for a dilution factor of 0.30 and 3R4F 29% ventilated² for a dilution factor of 0.71.

Equation 1 shows that Intense conditions are expected to produce deliveries 5.3 times greater than ISO deliveries for 1R5F and 2.8 times greater for 3R4F. Using Equation 2, the relative concentrations for the two reference cigarettes, 1R5F/3R4F, are expected to be 0.31 under ISO conditions and 0.60 under Intense conditions. The actual ratios calculated from the QC means are given in Table S-1.

Equation 1. Smoking Regimen ratio Intense-to-ISO for 1R5F and 3R4F reference cigarettes

$$\frac{\text{Intense Volume}}{\text{ISO Volume} \times \text{Dilution Factor}}$$

$$1R5F \frac{\text{Intense}}{\text{ISO}} = \frac{335.5 \text{ mL}}{210 \text{ mL} \times 0.30} = 5.3$$

$$3R4F \frac{\text{Intense}}{\text{ISO}} = \frac{555.5 \text{ mL}}{283.5 \text{ mL} \times 0.71} = 2.8$$

Equation 2. Reference cigarette ratio 1R5F-to-3R4F for Intense and ISO regimens

$$\frac{1R5F \text{ Volume} \times 1R5F \text{ Dilution Factor}}{3R4F \text{ Volume} \times 3R4F \text{ Dilution Factor}}$$

$$ISO \frac{1R5F}{3R4F} = \frac{210 \text{ mL} \times 0.30}{283.5 \text{ Volume} \times 0.71} = 0.31$$

$$Intense \frac{1R5F}{3R4F} = \frac{335.5 \text{ mL} \times 1}{555.5 \text{ Volume} \times 1} = 0.60$$

ABBREVIATIONS

I, Intense Regimen (Canadian Intense or Health Canada Method); ISO, International Organization for Standardization
3402:1999 Regimen (Cambridge Filter or FTC Method)

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- (1) Haussmann, H. ; Patskan, G.; Rustemeier, K. *Philip Morris*. 2002, <http://legacy.library.ucsf.edu/tid/ids49c00>.
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