Statistical Analysis for Comparison of the Results Obtained by Capillary Columns and Packed Columns in the Determination of Water Yield in Smoke Condensates Analyzed in Cigarettes for the 24th Asia Collaborative Study *

by

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SUMMARY

Recently, capillary columns have been widely used in the methodology for the determination of water yields in smoke condensate, even though ISO 10362-1:1999, “*Cigarettes - Determination of water in smoke condensates – Part 1: Gas chromatographic method*” specifies a packed gas chromatographic column. As a result of a systematic review in 2015, ISO/TC126 decided to revise the standard to include the use of capillary columns.

The goal of this study was to confirm the comparability of water yields obtained from capillary column methodology to those yields from packed columns by the statistical analysis of yield data from the 24th Asia Collaborative Study which included 86 datasets submitted by 64 laboratories. After the exclusion of outliers by Cochran’s and Grubbs’ tests, the datasets were classified by GC column type and then mean water yields, and their repeatability and reproducibility were calculated for each type of column. No significant differences were observed in water yields between capillary and packed columns. Repeatability and reproducibility of water yields using capillary column were comparable to those using packed columns as described in ISO 10362-1:1999. From these results, it was confirmed that the capillary columns are an appropriate alternative to

packed columns for the gas chromatographic procedure described in ISO 10362-1:1999. [Beitr. Tabakforsch. Int. 29 (2020) 97–118]

ZUSAMMENFASSUNG

Zur gaschromatographischen Wasserbestimmung im Rauchkondensat von Zigaretten werden immer häufiger Kapillarsäulen verwendet, obwohl in der ISO Norm 10362-1:1999 “*Zigaretten – Wasserbestimmung in Rauchkondensaten – Teil 1: Gaschromatographisches Verfahren*” eine gepackte Trennsäule vorgeschrieben ist. 2015 beschloss ISO/TC 126 auf Basis einer systematischen Überprüfung der einschlägigen Literatur die Verwendung von Kapillarsäulen zur Quantifizierung des Wassers im Rauchkondensat zuzulassen und den Standard den realen Gegebenheiten in den Prüflabors anzupassen.

Ziel dieser Studie war es, die Vergleichbarkeit der gaschromatographisch bestimmten Wasserwerte des Hauptstromrauch-Kondensats von Zigaretten, die mittels gepackter Trennsäulen bzw. Kapillaren erhalten wurden, mithilfe statistischer Verfahren zu bestätigen. Dazu dienten 86 Datensätze aus 64 Laboratorien, die im Rahmen der 24. Asia Collaborative Study erhalten wurden. Nach Ausreißer-

Bereinigung über Cochran und Grubbs Tests wurden die Datensätze nach den verwendeten Typen der gaschromatographischen Trennkolonnen klassifiziert und die Mittelwerte für den Wassergehalt, deren Wiederholbarkeit und Reproduzierbarkeit für jeden Typ der eingesetzten Trennkolonnen berechnet.

Für die gemessenen quantitativen Wasserwerte zeigten sich keine signifikanten Unterschiede bei Verwendung der Kapillaren oder der gepackten Säulen. Auch die Wiederholbarkeit und Reproduzierbarkeit der mit den Kapillaren erhaltenen Wasserwerte entsprachen den in ISO 10362-1:1999 für gepackte Trennsäulen vorgegebenen. Die von uns erhaltenen Ergebnisse bestätigen, dass Kapillaren eine geeignete Alternative für die gaschromatographischen Wasserbestimmung nach ISO 10362-1:1999 darstellen. [Beitr. Tabakforsch. Int. 29 (2020) 97–118]

RESUME

Récemment, les colonnes capillaires ont été abondamment utilisées afin de doser méthodiquement les teneurs en eau dans le condensat de fumée même si la norme ISO 10362-1:1999 "*Cigarettes - Dosage de l'eau dans les condensats de fumée - Partie 1: Méthode par chromatographie en phase gazeuse*" mentionne spécifiquement les colonnes à remplissage pour toute chromatographie gazeuse. A la suite d'un réexamen systématique réalisé en 2015, le comité technique ISO/TC126 décida de revoir la norme afin d'inclure l'utilisation de colonnes capillaires. L'objectif de la présente étude était de confirmer la comparabilité des teneurs en eau relevées par la méthode recourant aux colonnes capillaires à celles mesurées dans les colonnes à remplissage par le biais d'une analyse statistique des données de rendement recensées par la 24^e étude collaborative asiatique qui inclut 86 jeux de données soumis par 64 laboratoires. Après l'exclusion des valeurs aberrantes à travers des tests de Cochran et de Grubbs, les jeux de données furent classés par type de colonne utilisé pour la chromatographie en phase gazeuse et ensuite par teneurs en eau médianes. Ensuite, la répétabilité et la reproductibilité furent calculées pour chaque type de colonne.

Des différences significatives des teneurs en eau ne furent pas observées entre les colonnes capillaires et à remplissage. La répétabilité et la reproductibilité des teneurs en eau mesurées grâce aux colonnes capillaires furent comparables à celles observées sur les colonnes à remplissage prescrites dans la norme ISO 10362-1:1999. A la lumière de ces résultats, il fut confirmé que les colonnes capillaires constituaient une option alternative appropriée aux colonnes à remplissage dans le cadre de la chromatographie en phase gazeuse évoquée dans la norme ISO 10362-1:1999. [Beitr. Tabakforsch. Int. 29 (2020) 97–118]

INTRODUCTION

The international standard 10362-1:1999 "*Cigarette-Determination of water in smoke condensate - Part 1: Gas chromatographic method*" (1) specifies only packed columns in the methodology for water yield analysis even though recently the use of capillary columns for both water and

nicotine (2) has become relatively more popular across global laboratories.

Indeed, capillary columns were used in the recently updated CORESTA Recommended Method No 57, "*Determination of water in tobacco and tobacco products by gas chromatographic analysis*" (3).

Based on this situation, ISO/TC 126 decided in 2015 to create a Working Group 17 (WG 17) to revise ISO10362-1:1999 to include capillary columns as one of the methodology options, starting with discussion and a systematic review. At the first ISO/TC 126/WG 17 meeting, the necessity for a comparison of water yields using either packed or capillary columns in the methodology, was identified.

Yield data were gathered and analysed from several collaborative studies e.g., of 24th Asia Collaborative Study 2015 (ACS, the meeting was held in Bali in 2016), of the European Collaborative Study 2016 (EUCS, organized by the Committee on Tobacco and Tobacco Smoke of the German Institute for Standardization (DIN)) and of the CORESTA CM8 collaborative study 2017 (4). Water yield comparability was presented and confirmed in all collaborative studies at the WG17 meeting held in November 2017. The results from the monitor cigarette (CM8) from the CORESTA collaborative study were published by CRUMPLER *et al.* (4), but only one brand for test samples was used.

On the other hand, ACS 2015 and EUCS 2016 used five different brands for test samples. Although the results of EUCS didn't contain datasets obtained with the combination of packed columns and linear smoking machines, the results of ACS (5) contained datasets obtained with all combinations of GC columns and smoking machines. Consequently, WG17 decided to use the results of ACS for the revision of the international standard.

This paper has been written to provide a comprehensive statistical comparison in terms of water yield differences between packed and capillary columns obtained from the 24th Asia Collaborative Study (2015) covering cigarettes across a typical range of "tar" yields.

EXPERIMENTAL

Asia Collaborative Study – Participants

64 laboratories participated in the 24th Asia Collaborative Study (ACS) held in 2015. All participating laboratories are listed in Table A of Appendix A. The laboratories marked with an asterisk provided more than one dataset which were obtained by using various combinations of linear and rotary smoking machines.

In this study, 86 datasets were submitted with their water yields analysed. They consisted of 46 datasets measured by capillary column, 39 datasets measured by packed column, and 1 dataset without mention which column was used.

Protocol

Participants were requested to follow the protocol "ACS" to analyse five test samples, including CORESTA Monitor CM8 (6) as listed in Table 1, and to report on parameters as listed in Tables 2 and 3.

Table 1. List of samples.

Code	Sample name	Supplier	Origin	NFDPM level (mg/cig)	Butt length (mm)
A	Mevius One Box	JT	Japan	1	35
B	Marlboro Clear 3 Box	PMI	Lithuania	3	35
C	Kent 6 KS Box	RJR	USA	6	35
D	Mevius Box	JT	Japan	10	35
E	CORESTA Monitor (CM8)	COR	Germany	14.1*	33

Suppliers: JT: Japan Tobacco Inc., PMI: Philip Morris International, RJR: R J Reynolds, COR: CORESTA
CM8 was provided by Cerulean in this year.

* NFDPM was quoted from 'CORESTA Approved Monitor No.8 (CM8) use of condition, June 2015' (6).

Table 2. List of parameters to be reported.

	Outline
Test period	September 1 st to November 30 th , 2015
Data set / sample	One data set consists of 6 test results obtained from 6 runs. One test result was defined as the average yield obtained from 20 cigarettes in a single run.
Test parameters	TPM, water, nicotine, NFDPM, CO, puffs
Original data sets	86 data sets from 64 laboratories for each sample

Table 3. Dataset per sample.

Test parameter	Smoking machine	Number of runs	Reported data / sample
TPM (mg/cig)	Linear 20 port	6 runs 5 cig/port x 4 ports/run	6 test results, mean and standard deviation
Water (mg/cig)			
Nicotine (mg/cig)			
NFDPM (mg/cig)	Linear 16 port	4 ports/run	
CO (mg/cig)	Linear 10 port		
Puff count (puffs/cig)	Rotary	6 runs (20 cig/run)	

As shown in Table 1, the four sample brands covered the range in NFDPM from 1 to 10 mg/cig, NFDPM of CM8 was reported to be 14.1 mg/cig (6). CORESTA Monitor CM8 was provided by Cerulean or Borgwaldt KC year by year in turn and Cerulean provided it in that particular year. One dataset consists of six test results obtained from six runs, as shown in Table 2. One test result was defined as the average yield obtained from 20 cigarettes in a single run. For linear smoking machines, four ports per brand were used within each run, and five cigarettes were smoked per port. Rotary smoking machine always used 20 cigarettes per run.

Raw data

Raw datasets are listed in APPENDIX B with the type of smoking machine and GC column, water yields for each run, mean and standard deviation (SD) for five test samples.

Statistical analysis – Exclusion of outliers

Numerical outlier technique: Cochran's and Grubbs' tests were applied in accordance with ISO 5725-2:1994 (7) to exclude outlying datasets prior to the determination of repeatability and reproducibility. Cochran's test was applied to identify an outlier with statistically deviant standard deviation. Grubbs' test was applied to identify an outlier in a univariate dataset that follows an approximately normal distribution.

After Cochran's test, Grubbs' test was applied to the mean values of the remaining datasets according to chapter 7.3.4.3 in ISO 5725-2 (7). Grubbs' test consists of two types of tests. One is to determine whether the largest or smallest observation is the outlier, this is called the single Grubbs' test (chapter 7.3.4.1 in ISO 5725-2). The second test is to determine whether the two largest observations or two smallest observations are the outliers, it is called the double Grubbs' test (chapter 7.3.4.2 in ISO 5725-2).

In the first step, the datasets were sorted in descending order for mean value. The Grubbs' statistics G_p was calculated using the maximum mean value x_p , ground mean and standard deviation s . Where the Grubbs' statistics was higher than 1% of critical value (8), the maximum value was considered as outlier. The same process was applied for the dataset with the minimum mean value. When outliers are determined by single Grubbs' test, the Grubbs' test is completed. If there is no outlier in single Grubbs' test, double Grubbs' test for the two smallest or two largest observations should be applied.

Repeatability and reproducibility estimation

Water yield repeatability (r) and reproducibility (R) were calculated for all types of gas chromatographic columns and each type of GC column separately, with all types of smoking machines according to ISO 5725-2:1994 (7), by using the data that remained after the removal of outliers.

RESULTS

Statistical analysis

1. Mean and standard deviation

Mean and standard deviation for each dataset were calculated and are listed in Table 4.

The labcode was randomly assigned and is in no way related to the participation numbers of the laboratories, which were given in numerical order of data submission.

2. Exclusion of outliers

85 datasets, shown in Table 4, were sorted in descending order of their standard deviation. The test statistic C was calculated and compared with 1% of critical value. Cochran's critical values are given in ISO 5725-2 (7) only up to 40 numbers of data sets.

As the numbers of datasets exceeded 40 in this study, Cochran's critical value at corresponding numbers of datasets were calculated by use of the approximation in (9) which

Table 4. Mean and standard deviation (SD) of water yields for each data set (unit: mg/cig).

No.	Smoking machine ^a	GC column ^b	Lab. code	Sample A		Sample B		Sample C		Sample D		Sample E	
				Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD
1	R	C	01R	0.07	0.031	0.14	0.037	0.96	0.103	1.69	0.086	1.90	0.109
2	R	C	02R	0.09	0.061	0.30	0.084	1.01	0.154	1.93	0.207	2.23	0.172
3	L	P	03AL	0.08	0.066	0.17	0.053	0.45	0.046	1.03	0.053	1.21	0.052
4	R	P	03BR	0.07	0.052	0.15	0.031	0.55	0.111	1.22	0.167	1.34	0.182
5	L	P	04L	0.15	0.024	0.33	0.046	0.69	0.065	1.34	0.078	1.56	0.121
6	L	P	05L	0.10	0.029	0.29	0.042	0.68	0.057	1.54	0.076	1.72	0.092
7	L	C	06AL	0.09	0.030	0.38	0.176	0.61	0.121	1.38	0.228	1.62	0.393
8	L	C	06BL	0.20	0.104	0.35	0.237	0.55	0.180	1.00	0.216	1.50	0.481
9	R	C	07AR	0.12	0.035	0.43	0.056	0.96	0.048	1.90	0.097	2.16	0.132
10	R	C	07BR	0.10	0.036	0.35	0.039	0.92	0.036	1.83	0.116	2.17	0.033
11	L	C	07CL	0.07	0.022	0.19	0.042	0.58	0.017	1.23	0.151	1.43	0.050
12	R	C	08R	0.09	0.041	0.27	0.042	0.87	0.056	1.69	0.089	1.97	0.115
13	R	C	09R	0.08	0.080	0.23	0.041	0.80	0.118	1.55	0.107	1.90	0.090
14	R	C	10R	0.04	0.023	0.26	0.021	0.86	0.051	2.02	0.049	2.14	0.080
15	L	C	11L	0.06	0.043	0.21	0.043	0.49	0.131	1.21	0.130	1.32	0.074
16	R	P	12R	0.08	0.023	0.31	0.068	1.05	0.085	1.72	0.033	2.19	0.126
17	R	C	13AR	0.13	0.037	0.29	0.038	0.93	0.012	1.45	0.115	1.52	0.115
18	R	C	13BR	0.13	0.017	0.34	0.079	0.88	0.053	1.54	0.095	1.68	0.170
19	R	P	14R	0.17	0.017	0.37	0.071	0.86	0.088	1.67	0.179	1.90	0.096
20	R	C	15AR	0.14	0.053	0.32	0.042	0.97	0.055	1.69	0.037	1.92	0.066
21	L	C	15BL	0.13	0.085	0.17	0.100	0.51	0.113	1.13	0.138	1.52	0.215
22	R	P	16R	0.08	0.059	0.27	0.105	0.74	0.134	1.54	0.113	1.70	0.148
23	R	P	17AR	0.09	0.015	0.27	0.031	0.77	0.103	1.52	0.145	1.82	0.112
24	L	P	17BL	0.10	0.022	0.21	0.034	0.53	0.072	1.15	0.141	1.31	0.076
25	R	C	18AR	0.10	0.004	0.35	0.034	0.88	0.078	1.63	0.096	1.78	0.145
26	L	C	18BL	0.09	0.019	0.30	0.056	0.66	0.158	1.45	0.184	1.39	0.203
27	L	C	19AL	0.06	0.017	0.25	0.013	0.62	0.044	1.47	0.078	1.63	0.089
28	R	C	19BR	0.13	0.038	0.28	0.039	0.90	0.061	1.69	0.073	2.03	0.066
29	L	C	19CL	0.08	0.014	0.27	0.018	0.67	0.024	1.47	0.085	1.73	0.112
30	R	C	19DR	0.08	0.061	0.25	0.054	0.82	0.078	1.47	0.083	1.82	0.033
31	L	P	19EL	0.06	0.013	0.22	0.010	0.55	0.033	1.36	0.029	1.44	0.040
32	L	P	20L	0.06	0.014	0.27	0.039	0.63	0.073	1.45	0.058	1.62	0.054
33	L	C	21L	0.13	0.004	0.26	0.012	0.77	0.012	1.45	0.010	1.84	0.039
34	R	C	22R	0.11	0.083	0.29	0.061	0.87	0.156	1.80	0.197	2.06	0.101
35	R	C	23R	0.00	0.005	0.24	0.076	0.80	0.125	1.46	0.072	1.80	0.052
36	R	C	24AR	0.11	0.005	0.23	0.017	0.73	0.014	1.43	0.119	1.79	0.088
37	L	C	24BL	0.12	0.008	0.33	0.009	0.64	0.016	1.38	0.128	1.66	0.050
38	R	P	25R	0.10	0.014	0.37	0.043	1.03	0.116	1.94	0.170	2.20	0.213
39	R	C	26AR	0.14	0.051	0.31	0.066	0.91	0.045	1.92	0.227	2.13	0.137
40	R	C	26BR	0.14	0.052	0.38	0.044	1.07	0.063	2.03	0.130	2.33	0.077
41	L	C	27L	0.09	0.105	0.19	0.082	0.57	0.088	1.21	0.177	1.35	0.108
42	L	P	28L	0.21	0.078	0.33	0.103	0.70	0.119	1.55	0.154	1.87	0.167
43	L	P	29L	-	-	0.27	0.104	0.70	0.073	1.41	0.262	1.60	0.212
44	R	P	30R	0.09	0.022	0.35	0.064	1.03	0.077	2.03	0.121	2.10	0.105
45	L	P	31L	0.08	0.053	0.40	0.345	0.55	0.213	1.33	0.202	1.53	0.236
46	R	C	32AR	0.06	0.031	0.20	0.093	0.81	0.102	1.61	0.083	1.88	0.075
47	R	C	32BR	0.07	0.041	0.29	0.106	0.88	0.138	1.73	0.120	1.95	0.161
48	R	C	33R	0.05	0.011	0.24	0.041	0.70	0.085	1.36	0.155	1.58	0.110
49	R	P	34R	0.16	0.072	0.39	0.084	1.21	0.134	2.26	0.244	2.57	0.321
50	L	P	35L	0.11	0.092	0.62	0.371	0.84	0.234	1.75	0.261	2.21	0.219
51	R	C	36AR	0.17	0.015	0.52	0.030	0.89	0.056	1.37	0.053	2.30	0.060
52	R	C	36BR	0.19	0.034	0.52	0.025	0.94	0.036	1.46	0.069	2.43	0.051
53	R	C	37AR	0.08	0.084	0.20	0.098	0.70	0.183	1.53	0.231	1.78	0.341
54	L	C	37BL	0.11	0.087	0.42	0.181	0.85	0.171	1.31	0.178	1.70	0.152
55	R	P	38R	0.14	0.071	0.28	0.024	0.86	0.060	1.73	0.100	1.88	0.073
56	R	P	39R	0.13	0.048	0.35	0.069	1.03	0.150	1.91	0.203	2.01	0.518
57	R	P	40R	0.14	0.084	0.37	0.076	1.30	0.329	2.44	0.287	2.70	0.219
58	R	C	41R	0.11	0.031	0.25	0.010	0.83	0.100	1.42	0.117	1.78	0.106

Table 4. Continued.

No.	Smoking machine	GC column	Lab. code	Sample A		Sample B		Sample C		Sample D		Sample E	
				Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD
59	L	C	42L	0.10	0.017	0.26	0.044	0.57	0.052	1.19	0.040	1.52	0.104
60	L	P	43AL	0.21	0.057	0.44	0.112	0.75	0.032	1.36	0.072	1.63	0.136
61	L	P	43BL	0.20	0.014	0.47	0.178	0.73	0.015	1.35	0.064	1.58	0.069
62	L	C	44AL	0.11	0.105	0.27	0.186	0.55	0.150	1.29	0.151	1.66	0.129
63	L	C	44BL	0.07	0.108	0.22	0.035	0.61	0.138	1.35	0.186	1.58	0.156
64	R	P	45R	0.06	0.026	0.23	0.032	0.70	0.074	1.58	0.168	1.71	0.073
65	L	P	46L	0.03	0.054	0.14	0.108	0.50	0.087	1.03	0.126	1.01	0.079
66	L	P	47L	0.19	0.072	0.42	0.125	0.78	0.099	1.55	0.172	1.70	0.259
67	L	C	48L	0.10	0.004	0.30	0.010	0.77	0.018	1.30	0.037	1.78	0.028
68	R	P	49R	0.21	0.071	0.33	0.117	1.05	0.104	1.85	0.108	1.94	0.129
69	R	P	50AR	0.07	0.054	0.23	0.040	0.77	0.034	1.63	0.128	1.83	0.113
70	R	P	50BR	0.04	0.031	0.19	0.039	0.75	0.084	1.65	0.083	1.85	0.047
71	L	P	50CL	0.09	0.045	0.25	0.081	0.56	0.074	1.38	0.098	1.46	0.127
72	R	C	51R	0.11	0.023	0.40	0.053	0.98	0.121	1.95	0.122	2.19	0.160
73	R	C	52R	0.00	0.000	0.05	0.062	0.64	0.123	1.79	0.167	2.18	0.192
74	L	P	53L	0.06	0.015	0.26	0.025	0.75	0.010	1.60	0.070	1.69	0.047
75	R	C	54R	0.09	0.021	0.25	0.026	0.81	0.091	1.50	0.090	1.85	0.064
76	R	UN	55R	0.44	0.150	0.41	0.139	0.94	0.120	1.25	0.192	1.97	0.195
77	L	P	56L	1.43	0.368	1.84	0.713	2.47	0.936	3.82	1.050	4.33	1.388
78	R	P	57R	0.13	0.023	0.35	0.053	0.97	0.045	1.99	0.104	2.26	0.088
79	L	P	58L	0.07	0.028	0.23	0.091	0.52	0.051	1.22	0.112	1.50	0.113
80	L	P	59L	0.72	0.607	1.00	0.660	1.24	0.637	1.79	0.493	3.27	0.758
81	R	P	60AR	0.07	0.015	0.30	0.039	0.85	0.099	1.58	0.085	2.17	0.127
82	L	P	60BL	0.07	0.021	0.27	0.046	0.66	0.079	1.61	0.114	2.41	0.243
83	R	P	61R	0.13	0.008	0.30	0.024	0.71	0.016	1.01	0.016	1.90	0.012
84	R	C	62R	0.04	0.043	0.31	0.134	1.04	0.162	2.26	0.288	2.35	0.326
85	L	C	63L	0.18	0.008	0.34	0.015	0.73	0.035	1.24	0.015	1.69	0.041
86	R	P	64R	0.04	0.015	0.22	0.073	0.59	0.102	1.41	0.162	1.43	0.170

^a Smoking machine R: rotary smoking machine, L: linear smoking machine

^b GC column C: capillary column, P: packed column, UN: unknown

Table 5. Results of outlier tests.

Sample	Cochran's test	Grubbs' test	Remaining data sets
A	59 L, 56 L, 55 R	N/A	82
B	56 L, 59 L, 35 L	N/A	82
C	56 L, 59 L, 40 R	N/A	82
D	56 L, 59 L	N/A	83
E	56 L, 59 L, 39 R	N/A	82

N/A: Not applicable

extends the Cochran's test beyond 40 data sets.

When the test statistics was higher than the critical value, the dataset was considered an outlier. After the exclusion of an outlier dataset, the test statistic C for the next dataset with a higher standard deviation was calculated and compared to the critical value. Prior to the analysis the maximum number of outlier tests was restricted to four to avoid an excessive exclusion of dataset. The results of Cochran's test are listed in Table 5. Applying Cochran's test, two or three datasets were excluded as outliers. Grubbs' test was applied for the mean values of the remaining datasets. There was no outlier in Grubbs' test. The excluded datasets determined by Cochran's test and Grubbs' test are listed in Table 5.

Table 6. Number of datasets classified by GC column type and smoking machine type.

Sample code	Total datasets	Column type	Total by GC column	Linear smoking	Rotary smoking
A	82	Capillary	46	17	29
		Packed	36	17	19
B	82	Capillary	46	17	29
		Packed	36	17	19
C	82	Capillary	46	17	29
		Packed	36	18	18
D	83	Capillary	46	17	29
		Packed	37	18	19
E	82	Capillary	46	17	29
		Packed	36	18	18

Two or three datasets from a total of 85 datasets were excluded from further statistical evaluation. The number of datasets classified by GC column type and smoking machine type is listed in Table 6.

3. Comparison of capillary column with packed column

Datasets were classified by GC column type into capillary data and packed column data. Box plots of each column type for each test sample are shown in Figures 1 to 5.

Figure 1. Box plots of water yield for sample A.
 ◇ indicate mean values

Figure 2. Box plots of water yield for sample B.

Figure 3. Box plots of water yield for sample C.

Figure 4. Box plots of water yield for sample D.

Figure 5. Box plots of water yield for sample E.

The diamond-shaped symbols indicate the mean values. The interquartile range (IQR) of capillary columns for sample A was narrower than the IQR of packed columns. IQR of capillary columns for samples B, C, D and E were almost identical to those of the packed columns. The *t*-test of Welch was applied to confirm the statistical difference in water yield determination by packed columns and capillary columns. The results of the *t*-test are listed in Table 7.

No significant difference between packed columns and capillary columns in water yield determination was observed in all test samples.

4. Comparison of water yields by smoking machine type and GC column type

Datasets were classified into four groups by the combination of GC column type and smoking machine type. Box plots for each test sample are shown in Figures 6 to 10.

Figure 6. Box plots of water yield for sample A.

Figure 7. Box plots of water yield for sample B.

Figure 8. Box plots of water yield for sample C.

Figure 9. Box plots of water yield for sample D.

Figure 10. Box plots of water yield for sample E.

Table 7. Results of *t*-test in water yields between capillary columns and packed columns.

Sample code	"Tar" (mg/cig)	Capillary (mg/cig)		Packed (mg/cig)		<i>t</i> -test ^a
		Mean	SD	Mean	SD	
A	1	0.097	0.043	0.104	0.052	ns
B	3	0.287	0.089	0.290	0.074	ns
C	6	0.785	0.155	0.753	0.188	ns
D	10	1.534	0.272	1.558	0.321	ns
E	14.1	1.836	0.287	1.791	0.376	ns

^a *t*-test ns: not significant

L/Cap means a combination of linear smoking machine and capillary column. L/Packed means a combination of linear smoking machine and packed column. R/Cap means a combination of rotary smoking machine and capillary column. R/Packed means a combination of rotary smoking machine and capillary column.

IQR and median of the four groups for samples A and B were almost identical. But IQR and median of rotary and linear smoking machines seemed to be different for samples C, D and E. The results of the *t*-test are listed in Tables 8 and 9. A statistically significant difference in water yields was not observed between capillary columns and packed columns within the same type of smoking machine. On the other hand, statistically significant differences in water yields were observed for samples C, D and E between rotary smoking machines and linear smoking machines within the same type of GC column.

5. Repeatability and reproducibility estimation

The estimated values, which were calculated for all types of GC columns, capillary columns and packed columns are listed in Table 10. In comparison with repeatability and reproducibility defined in ISO 10362-1:1999, the estimated repeatability and reproducibility tends to be smaller than in ISO 10362-1:1999.

DISCUSSION

Comparison of capillary column with packed column

CRUMPLER *et al.* (4) also reported that there was no significant difference in water yield of CM8 between packed columns and capillary columns.

In our study, we could show that no significant difference was observed for water yields in cigarette smoke condensate between capillary and packed columns, not only from CM8 but also from other test samples, covering the majority of "tar" value products that are sold in the market.

Comparison of water yields by smoking machine type and GC column type

There was no significant difference in water yields between linear type smoking machines and rotary type smoking machines for samples A and B, which had the lowest water yields. On the other hand, the water yields for samples C, D and E by rotary type smoking machines were higher than those by linear type smoking machine.

The differences in water yields between rotary and linear smoking machines were already observed in the CORESTA Harmonization Study in 1991 (10) and in the CORESTA Collaborative Study conducted by CORESTA CO Sub-Committee (11). Although the differences in CO yields and NFDPM were improved and the differences in water yields became smaller through the improvement of air flow around cigarettes, higher water yields were still observed in the results obtained with rotary smoking machines under the ISO smoking regime (4, 12). Nevertheless, such a difference is no real influence in case of evaluation of the data from each smoking machine type. Comparisons between the two types of columns were carried out with a wider range of "tar" yields for each smoking machine type. This evaluation did not show significant difference between the data from packed columns and capillary columns.

Furthermore it was confirmed that there was no significant difference in the lower range of water yields between packed columns and capillary columns, with or without distinction of smoking machine type.

Table 8. Results of *t*-test in water yields between capillary and packed column within same type of smoking machine (unit: mg/cig).

Sample code	Linear					Rotary				
	Capillary		Packed		<i>t</i> -test ^a	Capillary		Packed		<i>t</i> -test ^a
	Mean	SD	Mean	SD		Mean	SD	Mean	SD	
A	0.106	0.041	0.102	0.058	ns	0.092	0.044	0.101	0.047	ns
B	0.273	0.065	0.286	0.082	ns	0.29	0.101	0.296	0.068	ns
C	0.632	0.100	0.645	0.113	ns	0.874	0.103	0.861	0.188	ns
D	1.287	0.137	1.391	0.193	ns	1.676	0.229	1.718	0.338	ns
E	1.576	0.159	1.614	0.324	ns	1.988	0.23	1.969	0.346	ns

^a *t*-test ns: not significant

Table 9. Results of *t*-test in water yields between linear and rotary smoking machine within same type of GC column (unit: mg/cig).

Sample code	Capillary					Packed				
	Linear		Rotary		<i>t</i> -test ^a	Linear		Rotary		<i>t</i> -test ^a
	Mean	SD	Mean	SD		Mean	SD	Mean	SD	
A	0.106	0.041	0.092	0.044	ns	0.102	0.058	0.101	0.047	ns
B	0.273	0.065	0.290	0.101	ns	0.286	0.082	0.296	0.068	ns
C	0.632	0.100	0.874	0.103	**	0.645	0.113	0.861	0.188	**
D	1.287	0.137	1.676	0.229	**	1.391	0.193	1.718	0.338	**
E	1.576	0.159	1.988	0.230	**	1.614	0.324	1.969	0.346	**

^a *t*-test ns: not significant, ** 1% significant

Table 10. Estimated r and R for all water data, capillary columns and packed columns (unit: mg/cig).

Sample code	All data			Capillary columns			Packed columns		
	Mean	r	R	Mean	r	R	Mean	r	R
A	0.101	0.129	0.176	0.097	0.131	0.169	0.104	0.13	0.187
B	0.286	0.225	0.307	0.284	0.209	0.312	0.29	0.243	0.302
C	0.771	0.267	0.534	0.785	0.281	0.505	0.753	0.246	0.572
D	1.525	0.365	0.818	1.518	0.349	0.773	1.534	0.379	0.883
E	1.816	0.424	0.999	1.836	0.432	0.895	1.791	0.414	1.121

Table 11. Repeatability and reproducibility in ISO 10362-1:1999.

Mean value m_w (mg/cig)	Repeatability limit r (mg/cig)	Reproducibility limit R (mg/cig)
0.083	0.154	0.241
0.153	0.228	0.353
0.338	0.272	0.381
0.962	0.407	0.734
1.595	0.561	0.935
3.187	0.908	1.680

Comparison of estimated repeatability and reproducibility with the past results

The comparison of repeatability and reproducibility estimated by using all datasets as well as datasets classified by GC column type were made via an F -ratio test with a Bonferroni adjustment for multiple comparisons. No significant differences between capillary and packed columns were observed when comparing repeatability and reproducibility among the samples.

Estimated r and R listed in Table 10 were compared to those of ISO 10362-1:1999 (1) listed in Table 11 by use of 95% of upper limit of prediction bands (ULP) and lower limit of prediction bands (LLP). The ULP and LLP were determined by a linear regression analysis of mean, repeatability and reproducibility defined in ISO 10362-1:1999 (1).

The repeatability estimated by using all datasets as well as datasets classified by GC column type were plotted with those of ISO 10362-1:1999 and 95% of upper and lower limits for prediction bands (Figure 11).

The estimated repeatability for samples A and B were within the upper and lower limits for prediction bands. All of the estimated repeatability for samples C, D and E were smaller than 95% of lower limit for prediction band. This means that the estimated repeatability might be similar or smaller than the values in ISO 10362-1:1999.

The reproducibility estimated by using all datasets as well as datasets classified by GC column types were plotted with those of ISO 10362-1:1999 and 95% of upper and lower limits for prediction bands (Figure 12).

The estimated reproducibility of packed columns was almost within the 95% upper and lower limit of prediction bands. On the other hand, the estimated reproducibility of capillary columns was smaller than 95% of lower limit of prediction band. This means that the estimated reproducibility of capillary columns is better than the reproducibility in ISO10362-1: 1999.

The estimated r and R by capillary column, packed column and all types of GC column are within 95% of upper limit for prediction band.

The estimated r and R for all data, capillary column and packed column are confirmed to be comparable to those of ISO 10362-1:1999, and these values can cover a wider range of water yields by ISO Smoking Regime.

The comparative results of water yields and estimated r and R strongly suggests that capillary columns are an appropriate alternative column for the gas chromatographic procedure of ISO 10362-1.

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Figure 11. Comparison of estimated repeatability (r) for all, capillary and packed columns with those of ISO 10362-1 and upper and lower limits for prediction bands.
95% LLP: 95% of lower limit for prediction bands
95% ULP: 95% of upper limit for prediction bands

Figure 12. Comparison of estimated reproducibility (R) for all, capillary and packed columns with those of ISO 10362-1 and upper and lower limits for prediction bands.
95% LLP: 95% of lower limit for prediction bands
95% ULP: 95% of upper limit for prediction bands

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APPENDIX A. Table A. List of Participating Laboratories

No.	Name of participating laboratories	Country
1	Papierfabrik Wattens GmbH & Co KG	Austria
2	British American Tobacco Bangladesh	Bangladesh
3	Philip Morris Brazil Industria & Comercio Ltda	Brazil
4*	RBH Inc.	Canada
5	Beijing Tobacco Monopoly Bureau	China
6	China National Tobacco Corporation Shandong Branch	China
7	China National Tobacco Corporation Sichuan Branch	China
8*	China National Tobacco Quality Supervision & Test Centre	China
9	China Tobacco Co. Shannxi Provincial Co.	China
10	Guangdong Tobacco Quality Supervision and Test Station	China
11	Guizhou Province Tobacco Quality Supervision & Test Station	China
12	Henan Tobacco Quality Supervision & Test Station	China
13	Hubei Tobacco Quality Supervision and Test Station	China
14	Inner Mongolia Tob. Monopoly Quality Supervision and Test Center	China
15	Ji Lin Tobacco Quality Supervision & Inspection Station	China
16	Shanghai Tobacco Group Co., Ltd	China
17	Yunnan Comtestor co., LTD	China
18	Yunnan Tobacco Quality Supervision & Test Station	China
19	Borgwaldt KC GmbH	Germany
20*	JT International Germany GmbH	Germany
21	Reemtsma Cigarettenfabriken GmbH	Germany
22	Hong Kong Government Laboratory	Hong Kong
23*	Godfrey Phillips India Ltd.	India
24*	ITC Ltd.	India
25	VST Industries Ltd.	India
26*	PT. Bentoel Prima	Indonesia
27*	PT. Djarum	Indonesia
28*	PT. Gudang Garam Tbk.	Indonesia
29	PT. Gelora Djaja	Indonesia
30*	PT. HM Sampoerna. Tbk	Indonesia
31	PT. Nojorono Tob. Intl.	Indonesia
32	PT. Sentosa Abadi Purwosari	Indonesia
33*	PT Sumatra Tobacco Trading Company	Indonesia
34	UPT PSMB-Lembaga Tembakau Jember	Indonesia
35*	Japan Tobacco Inc.	Japan
36	TIOJ Testing Laboratory	Japan
37	Royal Scientific Society	Jordan
38	BAT Korea	Korea
39	Korea Conformity Laboratories (KCL)	Korea
40	KT&G	Korea
41	Ministry of Food and Drug Safety	Korea
42*	Philip Morris Korea	Korea
43	Tobacco Smoke Analysis Center	Korea
44	Public Health Laboratory	Macao
45	BAT AsPac Service Centre	Malaysia
46	National Public Health Laboratory	Malaysia
47*	Philip Morris Mexico Productos Y Servicios	Mexico
48	Surya Nepal Pvt. Ltd.	Nepal
49	Pakistan Tobacco Company	Pakistan
50*	Mighty Corporation	Philippines
51	PMFTC Inc.	Philippines
52	British American Tobacco Singapore	Singapore
53	Philip Morris International	Switzerland
54	Food & Drug Administration, Ministry of Health & Welfare	Taiwan
55*	Taiwan Cigarette and Liquor Cop.	Taiwan
56	Taiwan Tobacco and Liquor Corporation -1	Taiwan
57	Taiwan Tobacco and Liquor Corporation -2	Taiwan
58	Thailand Tobacco Monopoly	Thailand
59*	Essentra Scientific Services	U.K.
60	Altria Client Services	U.S.A.
61	Enthalpy Analytical, Inc.	U.S.A.
62	R.J. Reynolds Tobacco Co.	U.S.A.
63	National Laboratory & Research Center	UAE
64	Compañia Industrial de Tabacos Montepaz S.A.	Uruguay

Note: Laboratories marked with * provided more than one data set obtained by using various combinations of linear and rotary smoking machines.

APPENDIX B. Raw Data

A unique alpha-numeric code was assigned to each data set received from a laboratory reflecting the type of smoking machine used and the specific data set submitted.

The numerals (01–64) in the code denote the laboratory, alphabet characters A, B, C, D and E represent the specific data set and the alphabet characters L or R refer to the linear or rotary smoking machine used by that laboratory.

Table B1. Raw data of water yields for sample A (unit: mg/cig)

Table B2. Raw data of water yields for sample B (unit: mg/cig)

Table B3. Raw data of water yields for sample C (unit: mg/cig)

Table B4. Raw data of water yields for sample D (unit: mg/cig)

Table B5. Raw data of water yields for sample E (unit: mg/cig)

Table B1. Raw data of water yields for sample A (unit: mg/cig).

No.	Smoking machine	GC column type	Lab. Code	No. of run						Mean	SD
				1	2	3	4	5	6		
1	R	Capillary	01R	0.02	0.04	0.08	0.10	0.06	0.09	0.07	0.031
2	R	Capillary	02R	0.15	0.17	0.02	0.04	0.12	0.06	0.09	0.061
3	L	Packed	03AL	0.04	0.15	0.17	0.03	0.02	0.05	0.08	0.066
4	R	Packed	03BR	0.13	0.05	0.13	0.01	0.03	0.05	0.07	0.052
5	L	Packed	04L	0.17	0.11	0.17	0.17	0.14	0.16	0.15	0.024
6	L	Packed	05L	0.07	0.08	0.09	0.11	0.11	0.15	0.10	0.029
7	L	Capillary	06AL	0.12	0.08	0.10	0.04	0.12	0.08	0.09	0.030
8	L	Capillary	06BL	0.33	0.22	0.06	0.29	0.12	0.15	0.20	0.104
9	R	Capillary	07AR	0.19	0.08	0.11	0.11	0.13	0.11	0.12	0.035
10	R	Capillary	07BR	0.14	0.13	0.05	0.10	0.08	0.07	0.10	0.036
11	L	Capillary	07CL	0.06	0.08	0.08	0.03	0.09	0.08	0.07	0.022
12	R	Capillary	08R	0.16	0.08	0.06	0.12	0.06	0.06	0.09	0.041
13	R	Capillary	09R	0.19	0.01	0.10	0.01	0.16	0.02	0.08	0.080
14	R	Capillary	10R	0.00	0.03	0.06	0.06	0.06	0.02	0.04	0.023
15	L	Capillary	11L	0.10	0.02	0.11	0.08	0.02	0.02	0.06	0.043
16	R	Packed	12R	0.07	0.05	0.08	0.09	0.10	0.12	0.08	0.023
17	R	Capillary	13AR	0.10	0.12	0.10	0.13	0.12	0.20	0.13	0.037
18	R	Capillary	13BR	0.14	0.14	0.11	0.11	0.12	0.15	0.13	0.017
19	R	Packed	14R	0.16	0.17	0.16	0.19	0.18	0.14	0.17	0.017
20	R	Capillary	15AR	0.20	0.22	0.13	0.10	0.11	0.10	0.14	0.053
21	L	Capillary	15BL	0.11	0.09	0.09	0.02	0.19	0.26	0.13	0.085
22	R	Packed	16R	0.03	0.05	0.13	0.07	0.02	0.17	0.08	0.059
23	R	Packed	17AR	0.08	0.10	0.08	0.09	0.09	0.12	0.09	0.015
24	L	Packed	17BL	0.13	0.12	0.09	0.09	0.07	0.11	0.10	0.022
25	R	Capillary	18AR	0.09	0.10	0.10	0.10	0.09	0.10	0.10	0.004
26	L	Capillary	18BL	0.09	0.08	0.11	0.06	0.07	0.10	0.09	0.019
27	L	Capillary	19AL	0.03	0.07	0.06	0.05	0.06	0.08	0.06	0.017
28	R	Capillary	19BR	0.13	0.18	0.12	0.09	0.17	0.09	0.13	0.038
29	L	Capillary	19CL	0.09	0.09	0.06	0.06	0.08	0.07	0.08	0.014
30	R	Capillary	19DR	0.07	0.10	0.17	0.11	0.01	0.01	0.08	0.061
31	L	Packed	19EL	0.07	0.07	0.04	0.07	0.05	0.06	0.06	0.013
32	L	Packed	20L	0.09	0.06	0.06	0.06	0.06	0.05	0.06	0.014
33	L	Capillary	21L	0.13	0.12	0.13	0.13	0.13	0.13	0.13	0.004
34	R	Capillary	22R	0.04	0.10	0.05	0.09	0.11	0.27	0.11	0.083
35	R	Capillary	23R	0.01	0.01	0.00	0.00	0.01	0.00	0.00	0.005
36	R	Capillary	24AR	0.10	0.11	0.11	0.10	0.11	0.10	0.11	0.005
37	L	Capillary	24BL	0.12	0.12	0.11	0.13	0.12	0.11	0.12	0.008
38	R	Packed	25R	0.09	0.08	0.11	0.10	0.10	0.12	0.10	0.014
39	R	Capillary	26AR	0.18	0.15	0.09	0.09	0.09	0.21	0.14	0.051
40	R	Capillary	26BR	0.18	0.14	0.09	0.06	0.20	0.15	0.14	0.052
41	L	Capillary	27L	0.28	0.12	0.03	0.00	0.01	0.08	0.09	0.105
42	L	Packed	28L	0.09	0.19	0.17	0.31	0.25	0.26	0.21	0.078
43	L	Packed	29L	n.s. ^a	n.s.	n.s.	n.s.	n.s.	n.s.	n.s.	n.s.
44	R	Packed	30R	0.12	0.08	0.10	0.11	0.08	0.06	0.09	0.022
45	L	Packed	31L	0.03	0.11	0.08	0.13	0.00	0.12	0.08	0.053
46	R	Capillary	32AR	0.08	0.02	0.09	0.09	0.03	0.07	0.06	0.031
47	R	Capillary	32BR	0.01	0.05	0.08	0.13	0.06	0.10	0.07	0.041
48	R	Capillary	33R	0.05	0.07	0.05	0.03	0.05	0.06	0.05	0.011
49	R	Packed	34R	0.27	0.10	0.12	0.23	0.17	0.09	0.16	0.072
50	L	Packed	35L	0.06	0.10	0.15	0.27	0.00	0.09	0.11	0.092
51	R	Capillary	36AR	0.20	0.18	0.16	0.17	0.17	0.16	0.17	0.015
52	R	Capillary	36BR	0.18	0.17	0.24	0.17	0.16	0.23	0.19	0.034
53	R	Capillary	37AR	0.00	0.04	0.21	0.05	0.01	0.14	0.08	0.084
54	L	Capillary	37BL	0.01	0.16	0.13	0.13	0.22	0.00	0.11	0.087
55	R	Packed	38R	0.07	0.07	0.09	0.25	0.17	0.17	0.14	0.071
56	R	Packed	39R	0.22	0.06	0.13	0.12	0.14	0.12	0.13	0.048

Table B1. Continued.

No.	Smoking machine	GC column type	Lab. Code	No. of run						Mean	SD
				1	2	3	4	5	6		
57	R	Packed	40R	0.04	0.04	0.20	0.20	0.23	0.13	0.14	0.084
58	R	Capillary	41R	0.16	0.12	0.10	0.13	0.07	0.09	0.11	0.031
59	L	Capillary	42L	0.12	0.09	0.08	0.10	0.09	0.12	0.10	0.017
60	L	Packed	43AL	0.20	0.17	0.18	0.18	0.18	0.32	0.21	0.057
61	L	Packed	43BL	0.19	0.18	0.18	0.21	0.20	0.21	0.20	0.014
62	L	Capillary	44AL	0.13	0.20	0.14	0.14	0.14	-0.10	0.11	0.105
63	L	Capillary	44BL	-0.04	-0.03	0.05	0.03	0.19	0.21	0.07	0.108
64	R	Packed	45R	0.08	0.04	0.05	0.09	0.06	0.02	0.06	0.026
65	L	Packed	46L	0.00	0.13	0.00	0.00	0.00	0.06	0.03	0.054
66	L	Packed	47L	0.30	0.18	0.10	0.23	0.20	0.13	0.19	0.072
67	L	Capillary	48L	0.09	0.10	0.10	0.10	0.10	0.10	0.10	0.004
68	R	Packed	49R	0.24	0.28	0.09	0.28	0.19	0.19	0.21	0.071
69	R	Packed	50AR	0.01	0.07	0.10	0.15	0.07	0.01	0.07	0.054
70	R	Packed	50BR	0.03	0.05	0.05	0.00	0.08	0.00	0.04	0.031
71	L	Packed	50CL	0.06	0.04	0.10	0.13	0.14	0.04	0.09	0.045
72	R	Capillary	51R	0.12	0.10	0.13	0.13	0.08	0.08	0.11	0.023
73	R	Capillary	52R	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.000
74	L	Packed	53L	0.08	0.06	0.05	0.05	0.07	0.04	0.06	0.015
75	R	Capillary	54R	0.11	0.10	0.07	0.10	0.06	0.11	0.09	0.021
76	R	unknown	55R	0.56	0.38	0.19	0.38	0.56	0.56	0.44	0.150
77	L	Packed	56L	0.88	1.58	1.50	1.99	1.34	1.27	1.43	0.368
78	R	Packed	57R	0.13	0.14	0.13	0.13	0.10	0.17	0.13	0.023
79	L	Packed	58L	0.04	0.05	0.08	0.11	0.08	0.04	0.07	0.028
80	L	Packed	59L	0.23	0.57	1.82	0.35	1.00	0.33	0.72	0.607
81	R	Packed	60AR	0.08	0.09	0.06	0.07	0.05	0.06	0.07	0.015
82	L	Packed	60BL	0.05	0.07	0.07	0.11	0.06	0.06	0.07	0.021
83	R	Packed	61R	0.13	0.13	0.14	0.13	0.12	0.14	0.13	0.008
84	R	Capillary	62R	0.01	0.12	0.02	0.00	0.05	0.04	0.04	0.043
85	L	Capillary	63L	0.19	0.17	0.18	0.19	0.18	0.19	0.18	0.008
86	R	Packed	64R	0.04	0.02	0.06	0.02	0.04	0.03	0.04	0.015

^a n.s. = no submission

Table B2. Raw data of water yields for sample B (unit: mg/cig).

No.	Smoking machine	GC column type	Lab. code	No. of run						Mean	SD
				1	2	3	4	5	6		
1	R	Capillary	01R	0.08	0.11	0.14	0.14	0.19	0.15	0.14	0.037
2	R	Capillary	02R	0.30	0.37	0.20	0.22	0.30	0.42	0.30	0.084
3	L	Packed	03AL	0.15	0.24	0.23	0.18	0.12	0.12	0.17	0.053
4	R	Packed	03BR	0.16	0.18	0.13	0.18	0.11	0.13	0.15	0.031
5	L	Packed	04L	0.33	0.25	0.35	0.33	0.31	0.39	0.33	0.046
6	L	Packed	05L	0.27	0.26	0.25	0.26	0.34	0.34	0.29	0.042
7	L	Capillary	06AL	0.27	0.44	0.29	0.36	0.23	0.71	0.38	0.176
8	L	Capillary	06BL	0.50	0.19	0.14	0.75	0.30	0.19	0.35	0.237
9	R	Capillary	07AR	0.49	0.47	0.39	0.36	0.48	0.39	0.43	0.056
10	R	Capillary	07BR	0.37	0.36	0.31	0.30	0.35	0.41	0.35	0.039
11	L	Capillary	07CL	0.21	0.13	0.25	0.21	0.20	0.16	0.19	0.042
12	R	Capillary	08R	0.32	0.30	0.26	0.20	0.26	0.25	0.27	0.042
13	R	Capillary	09R	0.28	0.24	0.20	0.16	0.24	0.24	0.23	0.041
14	R	Capillary	10R	0.28	0.25	0.25	0.29	0.27	0.24	0.26	0.021
15	L	Capillary	11L	0.17	0.20	0.25	0.27	0.17	0.18	0.21	0.043
16	R	Packed	12R	0.30	0.32	0.36	0.42	0.23	0.27	0.31	0.068
17	R	Capillary	13AR	0.28	0.28	0.32	0.23	0.33	0.32	0.29	0.038
18	R	Capillary	13BR	0.50	0.32	0.29	0.30	0.32	0.31	0.34	0.079
19	R	Packed	14R	0.24	0.35	0.44	0.38	0.42	0.40	0.37	0.071
20	R	Capillary	15AR	0.35	0.35	0.28	0.34	0.33	0.25	0.32	0.042
21	L	Capillary	15BL	0.27	0.19	0.30	0.14	0.07	0.06	0.17	0.100
22	R	Packed	16R	0.13	0.34	0.30	0.25	0.19	0.42	0.27	0.105
23	R	Packed	17AR	0.24	0.26	0.23	0.30	0.30	0.29	0.27	0.031
24	L	Packed	17BL	0.23	0.25	0.25	0.19	0.19	0.17	0.21	0.034
25	R	Capillary	18AR	0.29	0.38	0.36	0.37	0.35	0.34	0.35	0.034
26	L	Capillary	18BL	0.21	0.28	0.31	0.32	0.38	0.31	0.30	0.056
27	L	Capillary	19AL	0.23	0.26	0.25	0.24	0.26	0.26	0.25	0.013
28	R	Capillary	19BR	0.29	0.27	0.25	0.34	0.26	0.23	0.28	0.039
29	L	Capillary	19CL	0.28	0.28	0.26	0.24	0.28	0.25	0.27	0.018
30	R	Capillary	19DR	0.26	0.27	0.26	0.33	0.22	0.17	0.25	0.054
31	L	Packed	19EL	0.23	0.23	0.22	0.21	0.21	0.23	0.22	0.010
32	L	Packed	20L	0.31	0.30	0.22	0.24	0.31	0.26	0.27	0.039
33	L	Capillary	21L	0.27	0.25	0.26	0.26	0.27	0.24	0.26	0.012
34	R	Capillary	22R	0.21	0.25	0.29	0.30	0.38	0.34	0.29	0.061
35	R	Capillary	23R	0.30	0.26	0.12	0.28	0.31	0.17	0.24	0.076
36	R	Capillary	24AR	0.21	0.22	0.23	0.26	0.24	0.23	0.23	0.017
37	L	Capillary	24BL	0.32	0.32	0.34	0.33	0.33	0.34	0.33	0.009
38	R	Packed	25R	0.35	0.34	0.43	0.41	0.38	0.32	0.37	0.043
39	R	Capillary	26AR	0.33	0.44	0.31	0.27	0.25	0.29	0.31	0.066
40	R	Capillary	26BR	0.40	0.39	0.36	0.30	0.44	0.38	0.38	0.044
41	L	Capillary	27L	0.32	0.23	0.18	0.07	0.19	0.17	0.19	0.082
42	L	Packed	28L	0.19	0.38	0.22	0.40	0.37	0.44	0.33	0.103
43	L	Packed	29L	0.17	0.28	0.41	0.33	0.13	0.30	0.27	0.104
44	R	Packed	30R	0.42	0.42	0.30	0.27	0.36	0.31	0.35	0.064
45	L	Packed	31L	0.14	0.13	0.77	0.65	0.00	0.71	0.40	0.345
46	R	Capillary	32AR	0.21	0.22	0.16	0.20	0.06	0.35	0.20	0.093
47	R	Capillary	32BR	0.22	0.18	0.25	0.27	0.33	0.48	0.29	0.106
48	R	Capillary	33R	0.21	0.28	0.25	0.21	0.30	0.21	0.24	0.041
49	R	Packed	34R	0.54	0.39	0.35	0.39	0.40	0.28	0.39	0.084
50	L	Packed	35L	0.92	0.26	1.08	0.84	0.35	0.25	0.62	0.371
51	R	Capillary	36AR	0.56	0.52	0.48	0.55	0.53	0.50	0.52	0.030
52	R	Capillary	36BR	0.48	0.53	0.51	0.50	0.55	0.53	0.52	0.025
53	R	Capillary	37AR	0.17	0.33	0.04	0.19	0.18	0.27	0.20	0.098
54	L	Capillary	37BL	0.12	0.32	0.64	0.49	0.41	0.52	0.42	0.181
55	R	Packed	38R	0.27	0.25	0.32	0.28	0.26	0.29	0.28	0.024
56	R	Packed	39R	0.46	0.26	0.37	0.31	0.36	0.32	0.35	0.069

Table B2. Continued.

No.	Smoking machine	GC column type	Lab. code	No. of run						Mean	SD
				1	2	3	4	5	6		
57	R	Packed	40R	0.30	0.32	0.40	0.37	0.51	0.34	0.37	0.076
58	R	Capillary	41R	0.26	0.24	0.25	0.25	0.24	0.24	0.25	0.010
59	L	Capillary	42L	0.24	0.20	0.32	0.23	0.28	0.29	0.26	0.044
60	L	Packed	43AL	0.65	0.40	0.35	0.38	0.37	0.47	0.44	0.112
61	L	Packed	43BL	0.83	0.40	0.36	0.42	0.40	0.41	0.47	0.178
62	L	Capillary	44AL	0.28	0.08	0.42	0.40	0.44	0.01	0.27	0.186
63	L	Capillary	44BL	0.21	0.16	0.24	0.22	0.26	0.24	0.22	0.035
64	R	Packed	45R	0.27	0.26	0.23	0.20	0.23	0.19	0.23	0.032
65	L	Packed	46L	0.00	0.05	0.14	0.24	0.28	0.11	0.14	0.108
66	L	Packed	47L	0.55	0.55	0.25	0.45	0.30	0.40	0.42	0.125
67	L	Capillary	48L	0.31	0.29	0.30	0.28	0.30	0.29	0.30	0.010
68	R	Packed	49R	0.54	0.31	0.19	0.31	0.28	0.36	0.33	0.117
69	R	Packed	50AR	0.24	0.21	0.28	0.28	0.20	0.19	0.23	0.040
70	R	Packed	50BR	0.17	0.16	0.18	0.19	0.27	0.19	0.19	0.039
71	L	Packed	50CL	0.22	0.24	0.23	0.32	0.37	0.14	0.25	0.081
72	R	Capillary	51R	0.44	0.42	0.41	0.35	0.31	0.44	0.40	0.053
73	R	Capillary	52R	0.01	0.05	0.00	0.06	0.17	0.02	0.05	0.062
74	L	Packed	53L	0.25	0.29	0.24	0.25	0.30	0.25	0.26	0.025
75	R	Capillary	54R	0.26	0.25	0.29	0.22	0.25	0.22	0.25	0.026
76	R	unknown	55R	0.56	0.56	0.38	0.38	0.19	0.38	0.41	0.139
77	L	Packed	56L	1.23	0.92	2.19	2.43	1.56	2.72	1.84	0.713
78	R	Packed	57R	0.35	0.45	0.34	0.33	0.32	0.30	0.35	0.053
79	L	Packed	58L	0.21	0.39	0.13	0.25	0.23	0.16	0.23	0.091
80	L	Packed	59L	0.25	1.20	1.15	0.41	2.09	0.87	1.00	0.660
81	R	Packed	60AR	0.33	0.30	0.28	0.26	0.25	0.35	0.30	0.039
82	L	Packed	60BL	0.32	0.24	0.20	0.28	0.24	0.31	0.27	0.046
83	R	Packed	61R	0.30	0.29	0.30	0.28	0.34	0.27	0.30	0.024
84	R	Capillary	62R	0.30	0.12	0.26	0.25	0.46	0.47	0.31	0.134
85	L	Capillary	63L	0.35	0.34	0.31	0.35	0.33	0.34	0.34	0.015
86	R	Packed	64R	0.16	0.12	0.21	0.29	0.31	0.23	0.22	0.073

Table B3. Raw data of water yields for sample C (unit: mg/cig).

No.	Smoking machine	GC column type	Lab. code	No. of run						Mean	SD
				1	2	3	4	5	6		
1	R	Capillary	01R	0.87	0.83	1.09	1.00	0.90	1.04	0.96	0.103
2	R	Capillary	02R	1.25	1.06	0.81	0.92	1.09	0.95	1.01	0.154
3	L	Packed	03AL	0.46	0.49	0.50	0.45	0.41	0.38	0.45	0.046
4	R	Packed	03BR	0.50	0.68	0.49	0.68	0.50	0.42	0.55	0.111
5	L	Packed	04L	0.72	0.62	0.66	0.63	0.74	0.78	0.69	0.065
6	L	Packed	05L	0.60	0.69	0.68	0.63	0.76	0.71	0.68	0.057
7	L	Capillary	06AL	0.63	0.64	0.67	0.48	0.45	0.77	0.61	0.121
8	L	Capillary	06BL	0.60	0.38	0.41	0.43	0.84	0.66	0.55	0.180
9	R	Capillary	07AR	1.00	0.98	1.01	0.93	0.90	0.92	0.96	0.048
10	R	Capillary	07BR	0.97	0.96	0.87	0.91	0.91	0.91	0.92	0.036
11	L	Capillary	07CL	0.58	0.60	0.58	0.57	0.55	0.59	0.58	0.017
12	R	Capillary	08R	0.94	0.88	0.90	0.80	0.80	0.87	0.87	0.056
13	R	Capillary	09R	0.88	0.73	0.79	0.61	0.95	0.81	0.80	0.118
14	R	Capillary	10R	0.92	0.88	0.80	0.91	0.86	0.81	0.86	0.051
15	L	Capillary	11L	0.39	0.53	0.57	0.27	0.56	0.61	0.49	0.131
16	R	Packed	12R	1.12	0.91	1.10	1.04	1.01	1.14	1.05	0.085
17	R	Capillary	13AR	0.93	0.94	0.94	0.94	0.91	0.93	0.93	0.012
18	R	Capillary	13BR	0.82	0.81	0.91	0.92	0.92	0.92	0.88	0.053
19	R	Packed	14R	0.87	0.81	0.77	0.97	0.79	0.96	0.86	0.088
20	R	Capillary	15AR	1.01	0.93	1.01	0.88	0.99	1.01	0.97	0.055
21	L	Capillary	15BL	0.60	0.46	0.69	0.40	0.45	0.44	0.51	0.113
22	R	Packed	16R	0.58	0.69	0.66	0.79	0.72	0.97	0.74	0.134
23	R	Packed	17AR	0.70	0.76	0.96	0.71	0.78	0.68	0.77	0.103
24	L	Packed	17BL	0.62	0.57	0.55	0.47	0.52	0.42	0.53	0.072
25	R	Capillary	18AR	0.75	0.90	0.89	0.88	1.00	0.88	0.88	0.078
26	L	Capillary	18BL	0.66	0.65	0.90	0.67	0.65	0.40	0.66	0.158
27	L	Capillary	19AL	0.56	0.58	0.64	0.64	0.68	0.61	0.62	0.044
28	R	Capillary	19BR	0.98	0.81	0.93	0.91	0.90	0.84	0.90	0.061
29	L	Capillary	19CL	0.66	0.67	0.64	0.70	0.66	0.70	0.67	0.024
30	R	Capillary	19DR	0.81	0.82	0.96	0.83	0.74	0.76	0.82	0.078
31	L	Packed	19EL	0.56	0.52	0.56	0.51	0.53	0.60	0.55	0.033
32	L	Packed	20L	0.71	0.63	0.59	0.73	0.55	0.58	0.63	0.073
33	L	Capillary	21L	0.78	0.76	0.77	0.79	0.78	0.76	0.77	0.012
34	R	Capillary	22R	0.71	0.77	0.78	0.84	1.03	1.09	0.87	0.156
35	R	Capillary	23R	0.90	0.90	0.61	0.68	0.81	0.89	0.80	0.125
36	R	Capillary	24AR	0.75	0.73	0.72	0.72	0.72	0.71	0.73	0.014
37	L	Capillary	24BL	0.64	0.61	0.64	0.66	0.64	0.63	0.64	0.016
38	R	Packed	25R	1.20	1.12	0.87	1.04	0.96	0.99	1.03	0.116
39	R	Capillary	26AR	0.89	0.91	0.99	0.86	0.91	0.88	0.91	0.045
40	R	Capillary	26BR	1.08	1.02	1.13	0.97	1.10	1.13	1.07	0.063
41	L	Capillary	27L	0.64	0.60	0.69	0.52	0.47	0.49	0.57	0.088
42	L	Packed	28L	0.51	0.70	0.85	0.79	0.64	0.72	0.70	0.119
43	L	Packed	29L	0.67	0.63	0.72	0.83	0.71	0.64	0.70	0.073
44	R	Packed	30R	1.12	1.11	1.01	0.95	1.02	0.94	1.03	0.077
45	L	Packed	31L	0.71	0.52	0.67	0.14	0.60	0.67	0.55	0.213
46	R	Capillary	32AR	0.72	0.80	0.77	0.94	0.71	0.93	0.81	0.102
47	R	Capillary	32BR	1.02	1.00	0.84	0.95	0.76	0.68	0.88	0.138
48	R	Capillary	33R	0.72	0.81	0.76	0.71	0.60	0.61	0.70	0.085
49	R	Packed	34R	1.38	1.29	1.33	1.08	1.13	1.07	1.21	0.134
50	L	Packed	35L	0.89	0.76	1.17	1.04	0.61	0.59	0.84	0.234
51	R	Capillary	36AR	0.97	0.86	0.94	0.91	0.82	0.86	0.89	0.056
52	R	Capillary	36BR	0.95	0.93	0.98	0.93	0.97	0.88	0.94	0.036
53	R	Capillary	37AR	0.82	0.62	0.60	0.48	0.67	1.00	0.70	0.183
54	L	Capillary	37BL	0.66	0.83	1.05	0.68	0.84	1.05	0.85	0.171
55	R	Packed	38R	0.88	0.79	0.96	0.81	0.83	0.89	0.86	0.060
56	R	Packed	39R	1.10	0.85	1.28	0.98	1.02	0.94	1.03	0.150

Table B3. Continued.

No.	Smoking machine	GC column type	Lab. code	No. of run						Mean	SD
				1	2	3	4	5	6		
57	R	Packed	40R	1.09	0.93	1.23	1.19	1.84	1.53	1.30	0.329
58	R	Capillary	41R	0.92	0.95	0.73	0.73	0.88	0.75	0.83	0.100
59	L	Capillary	42L	0.60	0.56	0.50	0.60	0.53	0.64	0.57	0.052
60	L	Packed	43AL	0.79	0.75	0.74	0.74	0.70	0.78	0.75	0.032
61	L	Packed	43BL	0.70	0.72	0.73	0.74	0.74	0.73	0.73	0.015
62	L	Capillary	44AL	0.60	0.31	0.70	0.67	0.43	0.58	0.55	0.150
63	L	Capillary	44BL	0.49	0.68	0.46	0.61	0.84	0.58	0.61	0.138
64	R	Packed	45R	0.69	0.68	0.85	0.67	0.64	0.69	0.70	0.074
65	L	Packed	46L	0.46	0.43	0.44	0.66	0.46	0.52	0.50	0.087
66	L	Packed	47L	0.88	0.90	0.83	0.68	0.68	0.73	0.78	0.099
67	L	Capillary	48L	0.77	0.79	0.78	0.78	0.74	0.76	0.77	0.018
68	R	Packed	49R	1.10	0.85	1.14	1.10	1.05	1.08	1.05	0.104
69	R	Packed	50AR	0.78	0.79	0.81	0.78	0.77	0.71	0.77	0.034
70	R	Packed	50BR	0.78	0.64	0.82	0.65	0.81	0.81	0.75	0.084
71	L	Packed	50CL	0.61	0.54	0.61	0.62	0.43	0.52	0.56	0.074
72	R	Capillary	51R	0.92	0.99	0.79	0.97	1.11	1.11	0.98	0.121
73	R	Capillary	52R	0.68	0.51	0.48	0.68	0.67	0.81	0.64	0.123
74	L	Packed	53L	0.73	0.75	0.76	0.75	0.75	0.74	0.75	0.010
75	R	Capillary	54R	0.92	0.68	0.81	0.80	0.73	0.89	0.81	0.091
76	R	unknown	55R	0.75	0.94	0.94	1.13	0.94	0.94	0.94	0.120
77	L	Packed	56L	1.40	1.45	2.24	2.81	3.22	3.68	2.47	0.936
78	R	Packed	57R	0.92	0.98	0.99	0.91	1.00	1.02	0.97	0.045
79	L	Packed	58L	0.53	0.57	0.50	0.58	0.48	0.45	0.52	0.051
80	L	Packed	59L	0.62	1.55	0.88	1.34	0.75	2.32	1.24	0.637
81	R	Packed	60AR	0.86	1.02	0.90	0.75	0.81	0.77	0.85	0.099
82	L	Packed	60BL	0.66	0.55	0.72	0.65	0.60	0.77	0.66	0.079
83	R	Packed	61R	0.72	0.73	0.70	0.70	0.69	0.69	0.71	0.016
84	R	Capillary	62R	0.87	0.82	1.13	1.08	1.24	1.10	1.04	0.162
85	L	Capillary	63L	0.74	0.75	0.70	0.79	0.70	0.71	0.73	0.035
86	R	Packed	64R	0.43	0.63	0.50	0.61	0.69	0.67	0.59	0.102

Table B4. Raw data of water yields for sample D (unit: mg/cig).

No.	Smoking machine	GC column type	Lab. code	No. of run						Mean	SD
				1	2	3	4	5	6		
1	R	Capillary	01R	1.58	1.59	1.79	1.73	1.75	1.70	1.69	0.086
2	R	Capillary	02R	2.16	2.03	1.76	1.66	2.02	-	1.93	0.207
3	L	Packed	03AL	1.01	1.00	1.08	1.05	1.09	0.95	1.03	0.053
4	R	Packed	03BR	1.20	1.48	1.06	1.36	1.18	1.07	1.22	0.167
5	L	Packed	04L	1.31	1.33	1.24	1.42	1.31	1.45	1.34	0.078
6	L	Packed	05L	1.51	1.48	1.47	1.54	1.68	1.55	1.54	0.076
7	L	Capillary	06AL	1.28	1.25	1.49	1.80	1.22	1.24	1.38	0.228
8	L	Capillary	06BL	1.19	1.07	0.73	0.89	1.28	0.83	1.00	0.216
9	R	Capillary	07AR	2.00	1.84	2.05	1.86	1.80	1.88	1.90	0.097
10	R	Capillary	07BR	1.95	2.00	1.71	1.77	1.80	1.75	1.83	0.116
11	L	Capillary	07CL	1.25	1.19	1.44	1.32	1.15	1.00	1.23	0.151
12	R	Capillary	08R	1.70	1.69	1.75	1.79	1.67	1.53	1.69	0.089
13	R	Capillary	09R	1.62	1.46	1.61	1.47	1.69	1.43	1.55	0.107
14	R	Capillary	10R	2.01	2.11	2.01	1.97	2.04	2.02	2.02	0.049
15	L	Capillary	11L	1.09	1.14	1.08	1.38	1.19	1.35	1.21	0.130
16	R	Packed	12R	1.71	1.75	1.71	1.76	1.74	1.67	1.72	0.033
17	R	Capillary	13AR	1.55	1.50	1.36	1.28	1.58	1.45	1.45	0.115
18	R	Capillary	13BR	1.62	1.42	1.55	1.46	1.67	1.51	1.54	0.095
19	R	Packed	14R	1.81	1.74	1.39	1.80	1.49	1.77	1.67	0.179
20	R	Capillary	15AR	1.74	1.67	1.64	1.70	1.67	1.72	1.69	0.037
21	L	Capillary	15BL	1.12	1.05	1.29	1.00	1.31	1.01	1.13	0.138
22	R	Packed	16R	1.45	1.44	1.53	1.70	1.45	1.65	1.54	0.113
23	R	Packed	17AR	1.58	1.54	1.71	1.33	1.60	1.37	1.52	0.145
24	L	Packed	17BL	1.25	1.18	1.25	1.22	1.14	0.88	1.15	0.141
25	R	Capillary	18AR	1.52	1.64	1.51	1.68	1.66	1.76	1.63	0.096
26	L	Capillary	18BL	1.57	1.17	1.65	1.46	1.54	1.28	1.45	0.184
27	L	Capillary	19AL	1.38	1.36	1.51	1.56	1.50	1.48	1.47	0.078
28	R	Capillary	19BR	1.73	1.62	1.79	1.71	1.69	1.59	1.69	0.073
29	L	Capillary	19CL	1.53	1.54	1.38	1.36	1.44	1.55	1.47	0.085
30	R	Capillary	19DR	1.54	1.40	1.56	1.48	1.48	1.34	1.47	0.083
31	L	Packed	19EL	1.38	1.36	1.39	1.34	1.39	1.32	1.36	0.029
32	L	Packed	20L	1.38	1.39	1.49	1.50	1.41	1.50	1.45	0.058
33	L	Capillary	21L	1.47	1.45	1.46	1.45	1.45	1.44	1.45	0.010
34	R	Capillary	22R	1.52	1.65	1.82	1.82	1.94	2.07	1.80	0.197
35	R	Capillary	23R	1.49	1.50	1.34	1.41	1.50	1.52	1.46	0.072
36	R	Capillary	24AR	1.51	1.42	1.20	1.53	1.46	1.46	1.43	0.119
37	L	Capillary	24BL	1.56	1.34	1.24	1.27	1.34	1.50	1.38	0.128
38	R	Packed	25R	2.16	2.03	2.02	1.96	1.80	1.69	1.94	0.170
39	R	Capillary	26AR	2.00	1.60	2.15	2.16	1.72	1.90	1.92	0.227
40	R	Capillary	26BR	2.12	1.84	2.19	1.95	2.10	1.98	2.03	0.130
41	L	Capillary	27L	1.32	1.36	1.37	1.08	1.17	0.93	1.21	0.177
42	L	Packed	28L	1.33	1.57	1.65	1.76	1.58	1.43	1.55	0.154
43	L	Packed	29L	1.06	1.23	1.39	1.78	1.37	1.63	1.41	0.262
44	R	Packed	30R	2.21	2.04	1.98	1.84	2.07	2.03	2.03	0.121
45	L	Packed	31L	1.56	1.08	1.31	1.55	1.13	1.34	1.33	0.202
46	R	Capillary	32AR	1.70	1.62	1.69	1.60	1.52	1.51	1.61	0.083
47	R	Capillary	32BR	1.94	1.80	1.59	1.72	1.68	1.68	1.73	0.120
48	R	Capillary	33R	1.25	1.50	1.55	1.41	1.15	1.29	1.36	0.155
49	R	Packed	34R	2.61	2.50	2.17	2.15	2.16	1.97	2.26	0.244
50	L	Packed	35L	1.90	1.85	2.03	1.82	1.57	1.31	1.75	0.261
51	R	Capillary	36AR	1.39	1.33	1.36	1.31	1.46	1.36	1.37	0.053
52	R	Capillary	36BR	1.45	1.36	1.41	1.51	1.55	1.48	1.46	0.069
53	R	Capillary	37AR	1.70	1.59	1.55	1.13	1.46	1.79	1.53	0.231
54	L	Capillary	37BL	1.11	1.29	1.36	1.31	1.17	1.62	1.31	0.178
55	R	Packed	38R	1.65	1.63	1.73	1.91	1.73	1.74	1.73	0.100
56	R	Packed	39R	1.88	1.67	2.16	2.10	1.96	1.70	1.91	0.203

Table B4. Continued.

No.	Smoking machine	GC column type	Lab. code	No. of run						Mean	SD
				1	2	3	4	5	6		
57	R	Packed	40R	2.13	2.15	2.44	2.37	2.84	2.70	2.44	0.287
58	R	Capillary	41R	1.64	1.40	1.36	1.29	1.41	1.43	1.42	0.117
59	L	Capillary	42L	1.14	1.14	1.20	1.21	1.20	1.24	1.19	0.040
60	L	Packed	43AL	1.45	1.25	1.36	1.34	1.34	1.43	1.36	0.072
61	L	Packed	43BL	1.40	1.28	1.36	1.28	1.44	1.35	1.35	0.064
62	L	Capillary	44AL	1.27	1.14	1.50	1.43	1.25	1.13	1.29	0.151
63	L	Capillary	44BL	1.50	1.57	1.29	1.21	1.09	1.46	1.35	0.186
64	R	Packed	45R	1.84	1.41	1.74	1.49	1.49	1.52	1.58	0.168
65	L	Packed	46L	1.01	0.87	1.05	0.94	1.24	1.06	1.03	0.126
66	L	Packed	47L	1.63	1.50	1.75	1.30	1.70	1.43	1.55	0.172
67	L	Capillary	48L	1.27	1.33	1.32	1.30	1.33	1.24	1.30	0.037
68	R	Packed	49R	1.94	1.84	1.95	1.76	1.93	1.69	1.85	0.108
69	R	Packed	50AR	1.70	1.70	1.66	1.77	1.52	1.43	1.63	0.128
70	R	Packed	50BR	1.60	1.54	1.72	1.76	1.69	1.61	1.65	0.083
71	L	Packed	50CL	1.40	1.32	1.40	1.27	1.55	1.33	1.38	0.098
72	R	Capillary	51R	1.98	2.02	1.85	2.08	1.99	1.75	1.95	0.122
73	R	Capillary	52R	1.66	1.72	1.71	1.76	1.75	2.12	1.79	0.167
74	L	Packed	53L	1.59	1.61	1.66	1.63	1.46	1.62	1.60	0.070
75	R	Capillary	54R	1.44	1.53	1.55	1.35	1.60	1.53	1.50	0.090
76	R	unknown	55R	1.31	1.50	1.31	1.13	0.94	1.31	1.25	0.192
77	L	Packed	56L	2.43	2.72	3.91	5.00	4.11	4.76	3.82	1.050
78	R	Packed	57R	2.00	2.13	1.99	2.06	1.83	1.93	1.99	0.104
79	L	Packed	58L	1.19	1.32	1.04	1.33	1.28	1.16	1.22	0.112
80	L	Packed	59L	1.22	1.99	2.13	2.47	1.64	1.29	1.79	0.493
81	R	Packed	60AR	1.45	1.64	1.55	1.53	1.69	1.60	1.58	0.085
82	L	Packed	60BL	1.69	1.74	1.68	1.49	1.46	1.62	1.61	0.114
83	R	Packed	61R	1.00	1.02	1.00	0.99	1.03	0.99	1.01	0.016
84	R	Capillary	62R	1.92	1.98	2.54	2.19	2.30	2.63	2.26	0.288
85	L	Capillary	63L	1.23	1.23	1.26	1.22	1.24	1.25	1.24	0.015
86	R	Packed	64R	1.27	1.65	1.26	1.30	1.42	1.55	1.41	0.162

Table B5. Raw data of water yields for sample E (unit: mg/cig).

No.	Smoking machine	GC column type	Lab. code	No. of run						Mean	SD
				1	2	3	4	5	6		
1	R	Capillary	01R	1.96	2.06	1.93	1.79	1.78	1.85	1.90	0.109
2	R	Capillary	02R	2.40	2.19	2.10	2.09	2.48	2.09	2.23	0.172
3	L	Packed	03AL	1.20	1.22	1.21	1.30	1.16	1.16	1.21	0.052
4	R	Packed	03BR	1.15	1.47	1.32	1.58	1.44	1.12	1.34	0.182
5	L	Packed	04L	1.47	1.60	1.53	1.65	1.40	1.73	1.56	0.121
6	L	Packed	05L	1.58	1.64	1.74	1.81	1.81	1.71	1.72	0.092
7	L	Capillary	06AL	1.41	1.63	1.56	2.20	1.04	1.85	1.62	0.393
8	L	Capillary	06BL	1.14	0.74	1.97	1.87	1.46	1.80	1.50	0.481
9	R	Capillary	07AR	2.27	2.29	1.92	2.19	2.18	2.14	2.16	0.132
10	R	Capillary	07BR	2.16	2.16	2.18	2.20	2.12	2.21	2.17	0.033
11	L	Capillary	07CL	1.48	1.46	1.43	1.41	1.45	1.34	1.43	0.050
12	R	Capillary	08R	2.03	2.11	2.04	1.94	1.78	1.93	1.97	0.115
13	R	Capillary	09R	1.99	1.97	1.91	1.84	1.93	1.75	1.90	0.090
14	R	Capillary	10R	2.20	2.19	2.23	2.13	2.07	2.02	2.14	0.080
15	L	Capillary	11L	1.32	1.28	1.36	1.26	1.24	1.44	1.32	0.074
16	R	Packed	12R	2.08	2.32	2.37	2.10	2.09	2.15	2.19	0.126
17	R	Capillary	13AR	1.69	1.53	1.48	1.42	1.60	1.38	1.52	0.115
18	R	Capillary	13BR	1.80	1.65	1.69	1.36	1.81	1.78	1.68	0.170
19	R	Packed	14R	2.04	1.76	1.90	1.90	1.84	1.96	1.90	0.096
20	R	Capillary	15AR	1.98	1.97	1.83	1.88	1.97	1.86	1.92	0.066
21	L	Capillary	15BL	1.41	1.85	1.73	1.46	1.33	1.36	1.52	0.215
22	R	Packed	16R	1.58	1.73	1.51	1.88	1.64	1.85	1.70	0.148
23	R	Packed	17AR	1.76	1.84	1.87	1.63	1.96	1.85	1.82	0.112
24	L	Packed	17BL	1.20	1.41	1.31	1.36	1.33	1.25	1.31	0.076
25	R	Capillary	18AR	1.72	1.68	1.71	1.64	1.96	1.97	1.78	0.145
26	L	Capillary	18BL	1.32	1.77	1.30	1.17	1.41	1.37	1.39	0.203
27	L	Capillary	19AL	1.48	1.60	1.59	1.71	1.71	1.67	1.63	0.089
28	R	Capillary	19BR	1.92	2.05	2.08	2.01	2.11	2.04	2.03	0.066
29	L	Capillary	19CL	1.76	1.59	1.76	1.61	1.88	1.80	1.73	0.112
30	R	Capillary	19DR	1.83	1.82	1.85	1.76	1.83	1.83	1.82	0.033
31	L	Packed	19EL	1.49	1.49	1.45	1.40	1.41	1.42	1.44	0.040
32	L	Packed	20L	1.60	1.67	1.67	1.66	1.57	1.55	1.62	0.054
33	L	Capillary	21L	1.76	1.85	1.86	1.86	1.85	1.85	1.84	0.039
34	R	Capillary	22R	2.07	1.89	2.10	2.02	2.18	2.12	2.06	0.101
35	R	Capillary	23R	1.88	1.83	1.80	1.74	1.74	1.78	1.80	0.052
36	R	Capillary	24AR	1.66	1.89	1.84	1.79	1.70	1.83	1.79	0.088
37	L	Capillary	24BL	1.64	1.67	1.74	1.63	1.59	1.66	1.66	0.050
38	R	Packed	25R	2.13	2.44	2.37	2.34	1.91	2.03	2.20	0.213
39	R	Capillary	26AR	2.12	1.96	2.24	2.33	2.03	2.07	2.13	0.137
40	R	Capillary	26BR	2.28	2.29	2.32	2.34	2.48	2.28	2.33	0.077
41	L	Capillary	27L	1.46	1.48	1.30	1.22	1.37	1.25	1.35	0.108
42	L	Packed	28L	1.67	2.15	1.95	1.84	1.86	1.75	1.87	0.167
43	L	Packed	29L	1.22	1.62	1.64	1.68	1.59	1.87	1.60	0.212
44	R	Packed	30R	2.17	2.16	2.13	1.94	2.21	2.01	2.10	0.105
45	L	Packed	31L	1.33	1.72	1.88	1.30	1.38	1.59	1.53	0.236
46	R	Capillary	32AR	1.99	1.81	1.80	1.94	1.92	1.84	1.88	0.075
47	R	Capillary	32BR	2.11	1.94	2.16	1.86	1.91	1.72	1.95	0.161
48	R	Capillary	33R	1.71	1.69	1.56	1.55	1.55	1.41	1.58	0.110
49	R	Packed	34R	2.97	2.83	2.55	2.62	2.07	2.36	2.57	0.321
50	L	Packed	35L	2.20	2.31	2.50	1.98	2.35	1.94	2.21	0.219
51	R	Capillary	36AR	2.25	2.22	2.38	2.29	2.35	2.28	2.30	0.060
52	R	Capillary	36BR	2.44	2.49	2.40	2.45	2.47	2.35	2.43	0.051
53	R	Capillary	37AR	1.96	1.50	1.56	1.39	2.12	2.18	1.78	0.341
54	L	Capillary	37BL	1.53	1.77	1.84	1.55	1.64	1.89	1.70	0.152
55	R	Packed	38R	1.78	1.84	1.94	1.85	1.96	1.94	1.88	0.073
56	R	Packed	39R	2.06	1.96	2.32	2.18	2.50	1.02	2.01	0.518

Table B5. Continued.

No.	Smoking machine	GC column type	Lab. code	No. of run						Mean	SD
				1	2	3	4	5	6		
57	R	Packed	40R	2.47	2.52	2.75	2.54	2.98	2.92	2.70	0.219
58	R	Capillary	41R	1.90	1.82	1.79	1.58	1.80	1.80	1.78	0.106
59	L	Capillary	42L	1.44	1.43	1.68	1.55	1.60	1.44	1.52	0.104
60	L	Packed	43AL	1.86	1.55	1.46	1.62	1.60	1.69	1.63	0.136
61	L	Packed	43BL	1.55	1.61	1.46	1.59	1.65	1.63	1.58	0.069
62	L	Capillary	44AL	1.60	1.66	1.56	1.58	1.91	1.64	1.66	0.129
63	L	Capillary	44BL	1.71	1.43	1.49	1.45	1.82	1.60	1.58	0.156
64	R	Packed	45R	1.74	1.68	1.80	1.75	1.69	1.59	1.71	0.073
65	L	Packed	46L	0.89	0.97	1.05	0.96	1.05	1.11	1.01	0.079
66	L	Packed	47L	1.85	1.88	1.53	2.05	1.50	1.40	1.70	0.259
67	L	Capillary	48L	1.80	1.78	1.77	1.77	1.73	1.81	1.78	0.028
68	R	Packed	49R	1.90	1.95	1.91	1.79	2.18	1.91	1.94	0.129
69	R	Packed	50AR	1.77	1.77	2.02	1.91	1.79	1.72	1.83	0.113
70	R	Packed	50BR	1.82	1.89	1.91	1.82	1.87	1.79	1.85	0.047
71	L	Packed	50CL	1.39	1.52	1.45	1.68	1.42	1.31	1.46	0.127
72	R	Capillary	51R	1.94	2.44	2.21	2.16	2.22	2.15	2.19	0.160
73	R	Capillary	52R	2.15	1.93	2.11	2.24	2.13	2.51	2.18	0.192
74	L	Packed	53L	1.71	1.73	1.63	1.74	1.64	1.67	1.69	0.047
75	R	Capillary	54R	1.92	1.74	1.87	1.88	1.86	1.80	1.85	0.064
76	R	unknown	55R	2.06	2.25	2.06	1.69	1.88	1.88	1.97	0.195
77	L	Packed	56L	2.14	4.08	6.49	4.21	4.49	4.59	4.33	1.388
78	R	Packed	57R	2.28	2.19	2.39	2.24	2.32	2.15	2.26	0.088
79	L	Packed	58L	1.45	1.40	1.37	1.54	1.68	1.53	1.50	0.113
80	L	Packed	59L	2.29	3.61	3.99	2.46	4.06	3.23	3.27	0.758
81	R	Packed	60AR	2.21	2.05	2.21	1.98	2.28	2.29	2.17	0.127
82	L	Packed	60BL	2.18	2.19	2.68	2.74	2.32	2.35	2.41	0.243
83	R	Packed	61R	1.90	1.91	1.89	1.88	1.91	1.90	1.90	0.012
84	R	Capillary	62R	2.09	1.99	2.73	2.75	2.18	2.34	2.35	0.326
85	L	Capillary	63L	1.75	1.66	1.65	1.73	1.67	1.67	1.69	0.041
86	R	Packed	64R	1.56	1.34	1.32	1.23	1.42	1.69	1.43	0.170