Model Development and Validation of Personal Exposure to Volatile Organic Compound Concentrations

Supplemental Material

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SAMPLING METHODOLOGY

The VOC sampled were n-hexane, benzene, toluene, ethylbenzene, o-xylene, m-xylene, p-xylene, styrene, 1,3,5-trimethylbenzene, 1,2,4-trimethylbenzene, p-isopropyltoluene, pyridine, 3-ethenylpyridine, 1,3-butadiene and naphthalene.

Two methods were used for sampling the main group of VOC compounds and 1,3-butadiene (BUT) separately. VOC and 1,3-butadiene were collected in sorbent tubes packed with a dual adsorbent bed separated and plugged with unsilanised glass wool and fitted with appropriate ferrules and Swagelok caps as described in detail by (Kim et al. 1999). The sorbent material were Tenax GR and Carbotrap to collect VOC compounds and Carbopack B and Carbosieve SIII to collect 1,3-butadiene. The tubes were conditioned with helium for one hour at 275°C and 360°C for VOC and 1,3-butadiene respectively prior to the first usage or after the analysis of highly polluted samples. All collected samples were kept in refrigerated conditions after sampling and prior to analysis.

Personal Exposure Sampling

Each subject was sampled for a group of VOC and 1,3-butadiene (separately) for a total of five consecutive 24-hour periods using one personal sampler pump (SKC model PCXR8), connected to two different sorbent tubes. The active-sampling setup was enclosed in a small portable aluminium briefcase and additional power was supplied via camcorder batteries connected to the pumps. The flowrates used were 40 mL min^{-1} for VOC and 30 mL min^{-1} for 1,3-butadiene and 3 L min^{-1} for PAH.

Researchers met the subjects daily early in the morning to collect the sampler corresponding to the previous 24-hours, to supply a new 24-h sampler ready for the new day and to check that all the questionnaires were correctly completed.

Collection of the personal exposure, home and workplace samples was spread over two years from May 2005 to May 2007. Personal exposure samples were collected mainly in weekdays, but 3% of the data was collected on weekend days.

Subject Related Microenvironment Sampling

During the period when personal exposure was being measured there was a simultaneous programme of measurement of subject-related microenvironments such as subject specific workplaces (40 cases) and

home environments (77 cases) for one day. As most of the volunteers were office workers, most of the workplaces were offices (85%). Other workplaces that were sampled were a health centre (7.5%), a nursery/playschool (2.5%), a laboratory (2.5%) and a garden centre (2.5%).

Home and workplace sampling was performed with a bespoke stationary microenvironment sampler box, which contained one A.C. powered pump (Model VC0101, Nitto Kohki Co Ltd) connected to the sorbent tubes, and a programmable controller (Siemens LOGO! 24RC) that allowed the sampler to collect two consecutive samples over specified time periods.

The main VOC group were monitored at 80 mL min^{-1} during 2 consecutive 12-h periods for home microenvironment (day and nighttime) and at 120 mL min^{-1} during 8-h periods for workplace concentrations. 1,3-Butadiene was sampled concurrently with the other VOCs for the same sampling periods at 60 mL min^{-1} for home microenvironment and at 90 mL min^{-1} for workplace samples.

Other Microenvironment Sampling

In addition to the collection of subject related microenvironments, a seasonal programme of measurement of other microenvironments that members of the public visit during their daily activities was carried out. These other microenvironment measurements, were non-subject specific, independent from the subject's sampling programme and included street microenvironments (i.e. trafficked roadside locations, background streets, pedestrian streets and parks, 150 cases), transport microenvironments (i.e. cars, trains, bus, tube, coach stations, train stations and car parks, 122 cases), indoor microenvironments (i.e. pubs, restaurants, libraries, museums, supermarket, hair dresser and department store, 39 cases) and other home environments (i.e. kitchen, garden, garages and spare bedrooms, 83 cases). Summer samples were collected during May-August 2006 and May 2007. The same microenvironments were sampled in the winter campaign from November 2006 to February 2007. The sampler was supervised by a researcher at all times during the sampling interval. Meteorological data and description of each microenvironment sampling event were recorded.

A D.C. powered stationary microenvironment sampler box was designed and was intended to be used in microenvironments where no power supply was available for sampling during restricted time periods (2 hours). VOC and 1,3-butadiene were monitored at 360 and 240 mL min^{-1} during 2-h periods.

Street and transport microenvironments were sampled for 2-hours twice per day at rush hour (07:00-09:00) and during the afternoon (13:00-15:00). Indoor samples and parks samples were collected once during daytime hours for two hours, preferably 13:00-15:00, although some pub samples were collected during the evening time (18:00-20:00).

ANALYTICAL METHODOLOGY

1,3-butadiene was sampled and analysed separately from the other VOC due to its high volatility. The VOC and 1,3-butadiene methods were based on techniques previously developed and validated in our laboratory (Kim et al. 1999; Kim et al. 2001) and briefly comprise the thermal desorption of the compounds from the sampling tube in a thermal desorption unit (AEROTrap Auto-Sampler TEKMAR 6016), cryogenic preconcentration in a cryotrap (AEROTrap Desorber TEKMAR 6000) and subsequent analysis by Gas Chromatography (Agilent Technologies 6890 N Network GC System) and a Mass Spectrometry (Agilent Technologies 5973 Network Mass Selective Detector). The detector was set to quantify the analytes in single ion monitoring (SIM) mode. Further details of the analytical method are described in the Supporting Information.

VOC compounds were separated using a Varian CP7723 CP Wax 52CB column (50-m length x 0.25-mm ID x 0.20 µm film thickness), whilst two columns were used to analyse BUT. The first 20% of the samples were analysed using a capillary column Varian CP7552 CP-PoraPLOT Q (52.5m x 0.32mm i.d. x 10 µm film thickness), and the remaining samples were quantified using a Varian CP7352 CP-PoraBOND Q (50.0m x 0.32mm i.d. x 5 µm film thickness).

Calibration of the VOC and 1,3-butadiene analytical methods was performed as described by Kim and coworkers. The certified standards were purchased from LGC Promochem, Greyhound Chemservice, UltraScientific and Restek Corporation.

QA-QC in the VOC and BUT analytical methods included (a) instrument performance check and tuning prior to initial calibration, (b) initial five or six-point calibration curve, (c) analysis of laboratory blank at the beginning of a batch, (d) standard check at the beginning and end of each batch, (e) re-conditioning of highly exposed tubes and (f) random analysis of duplicate standards.

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List of abbreviations used in Tables S2, S3 and S4.

ABBREVIATION	DEFINITION
HEX	n-Hexane
BENZ	Benzene
TOL	Toluene
ETBZ	Ethylbenzene
P-XYL	p-Xylene
M-XYL	m-Xylene
PYR	Pyrene
O-XYL	o-Xylene
135-TMB	1,3,5-trimethylbenzene
STY	Styrene
P-ISO	p-isopropyltoluene
124-TMB	1,2,4-trimethylbenzene
3-EP	3-ethenylpyridine
NAPH	Naphthalene
1,3-BUT	1,3-butadiene
-99	Missing data – no data reported on the time-activity data questionnaires
-	No strata applicable for particular microenvironment.
Bham	Birmingham subjects
FL	First Line house
NFL	Non First Line house
IG	House with Integral Garage
NIG	House without Integral Garage
ETS	Microenvironment with Environmental Tobacco Smoke
NETS	Microenvironment without Environmental Tobacco Smoke

Supplemental Material, Table 1. Subject characteristics description

Characteristic	Percentage of cases MATCH Project
Gender	
Female	57
Male	43
Age	
18-25	18
26-35	31
36-45	15
46-55	13
56-65	17
66+	6
Occupation category	
Administration/office worker	48
Cleaning	1
Education	6
Food/Hospitality	7
Health	7
Housewife	4
Manufacturing	1
Police	1
Research and development	7
Retired	7
Student	10
Unemployed	1
Time spent per microenvironment	
Indoors at home	62
Indoors at work	16
Other indoors	12
Outdoors	4
In transit	6
Time spent traveling to workplace	
Not applicable	17
Less than 5 minutes	47
Less than 30 minutes	32
More than 30 minutes	4
ETS exposure	
ETS exposed at least 1 day	43
ETS exposed at home	12
Not ETS exposed at home	88
ETS exposed at work	8
Not ETS exposed at work	92
Activities relevant to VOC and PAH concentrations	
Cleaning	61
Aerosol/Perfume use	55
Solvent use	8
Candle burning	13
Photocopier/Printer	41
Lighted fire in fireplace	11
Other fossil fuel use	4
Refueling car	23
DIY-Hobbies	12
Cooking characteristics	
Natural gas	47
Electricity	53
Use of cooker hood	36
No use of cooker hood	64
Geographical location	
London	11
West Midlands	79
Wales	10
Home location	
Urban	38
Suburban	42
Rural	20
Other	
Living in houses with attached garages	16
Living in trafficked roadsides	44

Supplemental Material, Table 2. Characterisation of VOC (µg m-3) personal exposure concentrations in the full dataset (including extreme cases) (N=500), the training dataset (N=370) and the validation dataset (N=120)

	ALL DATASET						TRAINING DATASET						VALIDATION DATASET					
Statistics	Max/Min		Arithmetic		Geometric		Max/Min		Arithmetic		Geometric		Max/Min		Arithmetic		Geometric	
	Min	Max	Mean	SD	Mean	SD	Min	Max	Mean	SD	Mean	SD	Min	Max	Mean	SD	Mean	SD
n-Hexane	0.06	109.6	3.6	8.26	1.67	3.04	0.06	29.25	2.61	3.61	1.59	2.60	0.16	31.93	3.45	5.80	1.44	3.50
Benzene	0.15	30.2	2.2	2.48	1.64	2.01	0.16	8.97	1.76	1.31	1.43	1.87	0.62	13.26	2.06	1.88	1.65	1.82
Toluene	0.06	407.3	19.68	34.26	11.53	2.65	0.14	134.1	16.62	17.32	10.90	2.57	1.48	97.13	13.43	14.73	9.30	2.33
Ethylbenzene	0.06	181.9	3.2	10.62	1.48	2.72	0.06	32.69	2.05	3.27	1.29	2.40	0.16	14.77	2.23	2.95	1.39	2.49
p-Xylene	n.d.	213.8	3.08	11.85	1.26	3.05	n.d.	40.77	1.90	3.31	1.13	2.55	0.13	16.10	1.83	2.59	1.12	2.51
m-Xylene	0.01	575.4	7.72	30.49	3.23	3.01	0.01	89.22	4.77	8.21	2.79	2.72	0.30	34.64	4.93	6.15	3.04	2.59
m+p-Xylene	0.01	789	10.8	42.3	4.49	6.06	0.01	130	6.67	11.5	3.92	5.26	0.43	50.7	6.76	8.73	4.15	5.10
Pyridine	n.d.	6.92	0.25	0.36	0.15	2.56	n.d.	3.71	0.25	0.41	0.16	2.34	0.02	1.05	0.25	0.25	0.15	2.88
o-Xylene	0.04	173.7	3.59	11.22	1.61	2.83	0.05	49.81	2.44	4.49	1.43	2.55	0.15	17.29	2.35	3.33	1.41	2.54
1,3,5-Trimethylbenzene	0.01	40.74	0.96	2.7	0.44	2.8	0.01	40.46	0.85	2.67	0.41	2.68	0.05	5.24	0.57	0.84	0.35	2.45
Styrene	0.08	61.66	1.31	4.58	0.63	2.38	0.07	45.02	1.04	3.23	0.59	2.20	0.15	22.77	1.35	3.29	0.66	2.65
p-Isopropyltoluene	n.d.	12.88	1.07	0.94	0.8	2.28	0.04	7.98	1.11	0.99	0.82	2.22	n.d.	3.00	0.91	0.65	0.71	2.14
1,2,4-Trimethylbenzene	0.03	102.3	3.5	8.63	1.57	2.94	0.02	99.97	2.95	7.58	1.42	2.87	0.06	26.05	2.29	4.22	1.27	2.64
3-Ethenylpyridine	n.d.	6.92	0.29	0.59	0.1	3.94	0.01	6.32	0.30	0.69	0.09	3.84	n.d.	2.04	0.31	0.47	0.10	4.74
Naphthalene	0.02	14.21	0.74	1.06	0.53	2.03	0.02	12.59	0.71	1.17	0.51	2.02	0.06	3.87	0.60	0.67	0.45	1.98
1,3-Butadiene	n.d.	6.31	0.4	0.71	0.14	5.23	n.d.	5.48	0.33	0.53	0.14	3.83	0.01	5.95	0.47	0.97	0.17	3.95

Supplemental Material, Table 3. Microenvironment concentrations used in Model 4, in µg/m^3

Location	HEX	BENZ	TOL	ETBZ	P-XYL	M-XYL	PYR	O-XYL	135-TMB	STY	P-ISO	124-TMB	3-EP	NAPH	1,3-BUT
Art Gallery/Museum	0,42	0,84	2,29	0,44	0,32	0,85	0,09	0,45	0,35	0,32	0,20	1,17	0,04	0,37	0,02
Bus	0,91	1,89	6,92	1,50	1,47	3,82	0,05	2,00	0,44	0,36	0,19	1,60	0,09	0,52	0,45
Bus In London	1,65	3,97	14,70	2,23	2,38	5,89	0,06	2,96	0,88	0,93	0,30	2,75	0,08	0,82	0,19
Bus Stop	0,91	2,19	5,84	1,01	1,00	2,50	0,04	1,37	0,33	0,23	0,02	1,10	0,04	0,29	0,22
Car Park	1,91	3,79	13,66	2,03	2,16	5,42	0,04	2,61	0,55	0,44	0,12	2,10	0,04	0,47	0,60
Car/Taxi	1,91	3,79	13,66	2,03	2,16	5,42	0,04	2,61	0,55	0,44	0,12	2,10	0,04	0,47	0,60
City Centre	1,91	3,79	13,66	2,03	2,16	5,42	0,04	2,61	0,55	0,44	0,12	2,10	0,04	0,47	0,60
Friends/Relatives House	2,81	1,98	17,98	1,72	1,68	4,09	0,17	1,99	0,60	0,86	1,03	2,27	0,13	0,79	0,25
Garden Centre/Nursery/Home Greenhouse/Craft Centre	0,21	0,58	0,82	0,20	0,14	0,32	0,04	0,18	0,05	0,09	0,10	0,55	0,11	0,09	0,02
Garden/Courtyard/Balcony/Beer Garden	0,40	0,99	2,67	0,78	0,51	0,91	0,05	0,61	0,13	0,12	0,02	0,45	0,07	0,14	0,14
GP Surgery/Health Centre /Hospital/ Hospice/ Dentist/ /Chiropodist/Opticians	0,61	0,75	4,24	0,61	0,54	1,21	0,14	0,71	0,58	0,66	0,52	2,09	0,05	0,50	0,16
Hairdressers/Tanning or Beauty or Nail Salon	0,22	0,42	1,75	1,10	1,10	2,67	0,07	1,12	0,12	0,16	0,17	0,45	0,03	0,24	-
Home	2,81	1,98	17,98	1,72	1,68	4,09	0,17	1,99	0,60	0,86	1,03	2,27	0,13	0,79	0,25
Home - Bathroom	2,81	1,98	17,98	1,72	1,68	4,09	0,17	1,99	0,60	0,86	1,03	2,27	0,13	0,79	0,25
Home - Bedroom/Spare Room/Upstairs	2,81	1,98	17,98	1,72	1,68	4,09	0,17	1,99	0,60	0,86	1,03	2,27	0,13	0,79	0,25
Home - Kitchen/Breakfast Room	0,72	1,09	5,14	0,48	0,44	1,16	0,57	0,53	0,24	0,68	0,99	0,87	0,66	0,37	1,13
Home - Living Room/Lounge/Sitting Room/Dining Room/Downstairs	2,81	1,98	17,98	1,72	1,68	4,09	0,17	1,99	0,60	0,86	1,03	2,27	0,13	0,79	0,25
Home - Other	2,81	1,98	17,98	1,72	1,68	4,09	0,17	1,99	0,60	0,86	1,03	2,27	0,13	0,79	0,25
Laboratory	54,46	1,26	3,22	22,28	6,88	51,52	0,02	6,91	0,16	0,77	0,01	0,58	0,00	0,19	0,02
Library	1,27	1,33	4,95	1,06	0,93	2,37	0,05	1,18	0,23	0,54	0,21	0,84	0,05	0,75	0,56
Other Indoors	0,42	0,84	2,29	0,44	0,32	0,85	0,09	0,45	0,35	0,32	0,20	1,17	0,04	0,37	0,02
Other Outdoors	0,69	1,35	4,11	0,71	0,70	1,69	0,03	0,88	0,22	0,13	0,02	0,73	0,02	0,17	0,07
Park/Resevoir/Lake/Canal/Woodland/Forest/Ski Park/Cemetry	0,21	0,58	0,82	0,20	0,14	0,32	0,04	0,18	0,05	0,09	0,10	0,55	0,11	0,09	0,02
Pub/Bar/Social Club	1,41	4,94	14,42	2,32	1,75	6,07	3,78	2,11	0,47	1,48	0,88	1,85	4,95	0,56	5,20
Restaurant/Cafe/Tea Room	0,94	1,33	4,27	0,89	0,65	1,78	0,58	0,96	0,33	0,34	1,26	1,26	0,82	0,23	0,96
Shopping Centre	0,41	0,74	14,69	0,95	1,17	3,00	0,07	1,79	0,12	0,29	0,17	0,50	0,07	0,33	-
Shops	0,41	0,74	14,69	0,95	1,17	3,00	0,07	1,79	0,12	0,29	0,17	0,50	0,07	0,33	-
Street	0,69	1,35	4,11	0,71	0,70	1,69	0,03	0,88	0,22	0,13	0,02	0,73	0,02	0,17	0,07
Supermarket/Retail Park	0,32	0,93	2,70	0,53	0,38	1,01	0,11	0,53	0,44	0,44	0,25	1,36	0,05	0,46	-
Train in London	0,43	1,19	4,97	0,58	0,52	1,61	0,06	0,69	0,14	0,31	0,28	0,74	0,06	0,54	0,17
Train	0,22	1,44	6,94	0,99	1,03	2,51	0,07	1,26	0,43	0,47	0,34	1,39	0,13	1,01	0,09
Train/Tube Station	0,66	1,35	3,39	0,69	0,61	1,79	0,05	0,96	0,24	0,24	0,04	0,98	0,06	0,28	0,15
Tube	1,70	2,20	11,73	1,59	1,61	3,96	0,10	1,96	0,67	2,60	0,34	2,26	0,10	2,23	0,21
Work - Kitchen/Common Room/Staff Room /Cafeteria /Canteen	1,05	1,16	4,32	1,23	1,21	3,23	0,11	1,49	0,26	0,54	0,46	1,33	0,07	0,37	0,08
Work - Office At Different Site/Conference Centre	1,05	1,16	4,32	1,23	1,21	3,23	0,11	1,49	0,26	0,54	0,46	1,33	0,07	0,37	0,08
Work/Educational Institute - Office	1,05	1,16	4,32	1,23	1,21	3,23	0,11	1,49	0,26	0,54	0,46	1,33	0,07	0,37	0,08

Supplemental Material, Table 4. Microenvironment concentrations used in Model 5 and Model 6 – Part 1, in µg/m^3

Location	Strata	HEX	BENZ	TOL	ETBZ	P-XYL	M-XYL	PYR	O-XYL	135-TMB	STY	P-ISO	124-TMB	3-EP	NAPH	1,3-BUT
Art Gallery/Museum	summer	0.63	0.67	1.45	0.27	0.20	0.53	0.05	0.29	0.18	0.09	0.09	0.78	0.02	0.18	0.01
	winter	0.22	1.01	3.12	0.61	0.44	1.17	0.13	0.61	0.52	0.55	0.31	1.56	0.06	0.56	0.02
Bus	summer	0.95	1.21	5.42	1.48	1.43	3.77	0.04	2.13	0.43	0.34	0.17	1.65	0.06	0.37	0.07
	winter	0.87	2.57	8.42	1.51	1.52	3.87	0.06	1.86	0.46	0.37	0.22	1.55	0.12	0.68	1.02
Bus London	summer	1.94	5.43	21.54	3.16	3.44	8.60	0.06	4.28	1.26	1.30	0.44	3.95	0.11	1.13	0.29
Bus Stop	summer	0.82	1.55	4.40	0.79	0.72	1.92	0.05	1.10	0.22	0.18	0.04	0.80	0.03	0.21	0.08
	winter	0.99	2.83	7.28	1.24	1.27	3.08	0.03	1.65	0.44	0.29	0.00	1.41	0.05	0.37	0.35
Car Park	summer	1.24	2.00	6.28	0.99	0.93	2.54	0.04	1.39	0.34	0.31	0.06	1.44	0.05	0.41	0.05
	winter	2.58	5.58	21.04	3.07	3.39	8.30	0.03	3.82	0.76	0.57	0.18	2.75	0.04	0.53	1.15
Car/Taxi	summer	1.24	2.00	6.28	0.99	0.93	2.54	0.04	1.39	0.34	0.31	0.06	1.44	0.05	0.41	0.05
	winter	2.58	5.58	21.04	3.07	3.39	8.30	0.03	3.82	0.76	0.57	0.18	2.75	0.04	0.53	1.15
City Centre	summer	0.26	0.34	1.19	0.20	0.16	0.41	0.01	0.22	0.04	0.02	0.00	0.18	0.00	0.04	0.03
	winter	0.25	0.79	1.34	0.27	0.25	0.61	0.02	0.31	0.08	0.06	0.00	0.27	0.01	0.08	0.06
Garden Centre/Nursery/Home Greenhouse/Craft Centre	summer	0.28	0.52	0.64	0.18	0.11	0.24	0.05	0.15	0.05	0.08	0.28	1.55	0.19	0.08	0.00
	winter	0.00	0.80	0.93	0.22	0.18	0.45	0.02	0.21	0.04	0.10	0.00	0.14	0.01	0.10	0.04
GP Surgery/Health Centre/Hospital/Hospice/Dentist /Chiropodist/Opticians	-	0.61	0.75	4.24	0.61	0.54	1.21	0.14	0.71	0.58	0.66	0.52	2.09	0.05	0.50	0.16
Gym/Leisure Centre/Swimming Baths	summer	0.43	0.62	4.99	0.72	0.76	1.93	0.06	1.04	0.14	0.19	0.16	0.59	0.05	0.37	0.01
	winter	0.37	1.25	3.56	0.74	0.64	1.60	0.08	0.81	0.38	0.63	0.17	1.16	0.06	0.41	0.02
Hairdressers/Tanning or Beauty or Nail Salon		0.22	0.42	1.75	1.10	1.10	2.67	0.07	1.12	0.12	0.16	0.17	0.45	0.03	0.24	-
Laboratory	Health centre	54.46	1.26	3.22	22.28	6.88	51.52	0.02	6.91	0.16	0.77	0.01	0.58	0.00	0.19	0.02
	University	-	4.20	8.30	0.70	0.60	1.90	-	0.80	0.10	0.20	0.20	0.50	-	0.10	0.20
Library	summer	0.41	0.60	1.98	0.71	0.71	1.80	0.06	0.99	0.14	0.20	0.20	0.57	0.05	0.60	-
	winter	0.53	1.49	4.00	0.88	0.84	2.02	0.04	1.01	0.24	0.71	0.04	0.76	0.05	0.25	-
Other Indoors	summer	0.43	0.62	4.99	0.72	0.76	1.93	0.06	1.04	0.14	0.19	0.16	0.59	0.05	0.37	0.01
	winter	0.37	1.25	3.56	0.74	0.64	1.60	0.08	0.81	0.38	0.63	0.17	1.16	0.06	0.41	0.02
Park/Resevoir/Lake/Canal/Woodland/Forest/Ski Park/Cemetry	summer	0.28	0.52	0.64	0.18	0.11	0.24	0.05	0.15	0.05	0.08	0.28	1.55	0.19	0.08	0.00
	winter	0.00	0.80	0.93	0.22	0.18	0.45	0.02	0.21	0.04	0.10	0.00	0.14	0.01	0.10	0.04
Shopping Centre	-	0.41	0.74	14.69	0.95	1.17	3.00	0.07	1.79	0.12	0.29	0.17	0.50	0.07	0.33	-
Shops	-	0.41	0.74	14.69	0.95	1.17	3.00	0.07	1.79	0.12	0.29	0.17	0.50	0.07	0.33	-
Supermarket/Retail Park	summer	0.41	0.74	14.69	0.95	1.17	3.00	0.07	1.79	0.12	0.29	0.17	0.50	0.07	0.33	-
	winter	0.28	1.55	9.09	1.16	1.31	3.15	0.08	1.62	0.57	0.64	0.60	1.85	0.18	1.43	0.07
Train	summer	0.42	0.73	2.93	0.53	0.44	1.32	0.07	0.64	0.14	0.29	0.24	0.58	0.05	0.37	0.19
	winter	0.62	2.36	7.88	1.02	1.13	3.77	0.05	1.38	0.24	0.43	0.28	1.24	0.06	0.85	0.38
Train/Tube Station	summer	0.62	1.10	2.50	0.59	0.47	1.48	0.05	0.82	0.16	0.29	0.02	0.75	0.05	0.22	0.05
	winter	0.61	1.34	2.09	0.42	0.40	1.04	0.06	0.53	0.23	0.18	0.01	0.74	0.08	0.24	0.29
Tube	-	1.62	2.65	12.81	1.67	1.73	4.18	0.11	2.13	0.74	3.06	0.49	2.49	0.13	2.41	0.25

Supplemental Material, Table 5. Microenvironment concentrations used in Model 5 and Model 6 – Part 2, in µg/m^3

Location	Strata 1	Strata 2	HEX	BENZ	TOL	ETBZ	P-XYL	M-XYL	PYR	O-XYL	135-TMB	STY	P-ISO	124-TMB	3-EP	NAPH	1,3-BUT
Friends/Relatives House	Urban	FL-ETS	1.4	1.2	22.2	1.0	1.0	2.5	0.67	1.2	0.4	0.7	1.0	1.1	1.31	0.7	0.2
	Urban	NFL-NETS	1.8	1.2	8.0	1.7	1.7	5.0	0.2	3.4	2.0	1.7	2.0	0.7	0.3	0.6	0.3
	Suburban	FL-ETS	1.0	1.9	7.1	0.9	0.7	1.6	0.67	0.9	0.7	0.7	0.9	0.8	1.31	0.5	0.2
	Suburban	FL-NETS	1.0	1.9	7.1	0.9	0.7	1.6	0.2	0.9	0.7	0.7	0.9	0.8	0.1	0.5	0.2
	Suburban	NFL-ETS	1.9	1.3	6.7	1.0	1.0	2.1	0.67	1.2	0.4	0.7	0.9	0.7	1.31	0.5	0.2
	Suburban	NFL-NETS	1.9	1.3	6.7	1.0	1.0	2.1	0.1	1.2	0.4	0.7	0.9	0.7	0.1	0.5	0.2
	Suburban	-99-ETS	1.9	1.3	6.7	1.0	1.0	2.1	0.67	1.2	0.4	0.7	0.9	0.7	1.31	0.5	0.2
	Suburban	-99/-NETS	1.9	1.3	6.7	1.0	1.0	2.1	0.1	1.2	0.4	0.7	0.9	0.7	0.1	0.5	0.2
	-99	FL-NETS	1.0	1.9	7.1	0.9	0.7	1.6	0.2	0.9	0.7	0.7	0.9	0.8	0.1	0.5	0.2
	-99	-99	1.0	1.9	7.1	0.9	0.7	1.6	0.2	0.9	0.7	0.7	0.9	0.8	0.1	0.5	0.2
	Rural	FL-NETS	0.9	1.2	5.7	0.6	0.6	1.3	0.1	0.7	0.2	0.3	0.6	0.7	0.0	0.8	0.1
	Rural	NFL-NETS	1.6	1.9	8.7	1.6	1.2	2.1	0.1	1.4	0.5	0.6	0.8	1.0	0.1	0.5	0.3
	Rural	NFL-ETS	1.6	1.9	8.7	1.6	1.2	2.1	0.67	1.4	0.5	0.6	0.8	1.0	1.31	0.5	0.3
Garden/Courtyard/Balcony/ /Beer Garden	garden	summer	0.32	0.86	1.80	0.34	0.29	0.69	0.02	0.34	0.07	0.10	0.00	0.24	0.01	0.25	0.00
		winter	0.29	1.77	3.51	0.84	0.80	2.12	0.05	0.89	0.20	0.24	0.11	0.64	0.01	0.32	0.16
	London Street BS	summer-daytime	1.71	1.73	7.11	1.08	1.02	2.45	0.05	1.20	0.34	0.31	0.05	1.11	0.07	0.26	0.06
	pedestrian	summer	0.34	0.72	1.69	0.30	0.21	0.56	0.04	0.32	0.10	0.08	0.01	0.47	0.03	0.12	0.01
		winter	0.37	1.62	4.95	2.95	1.46	1.22	0.05	1.57	0.20	0.14	0.00	0.63	0.06	0.19	0.68
	suburban-BS	winter	0.41	1.26	3.26	0.61	0.60	1.45	0.02	0.71	0.17	0.10	0.01	0.54	0.02	0.16	0.02
HOME All	Urban	FL-ETS	0.55	1.07	4.29	0.80	0.58	1.56	0.74	0.74	0.17	0.80	0.29	0.70	1.16	0.41	
	Urban	FL-NETS	1.4	1.5	17.1	1.1	1.0	2.7	0.1	1.3	0.6	0.7	1.1	2.2	0.1	0.7	0.3
	Urban	NFL-ETS	2.8	1.6	11.6	2.2	1.8	5.7	0.3	4.4	1.9	1.8	1.3	0.8	0.4	0.6	0.2
	Urban	NFL-NETS	1.5	1.0	6.7	0.7	0.6	1.6	0.1	0.8	0.2	0.5	1.1	0.6	0.0	0.3	0.3
	Suburban	FL-ETS-IG	1.0	1.9	7.1	0.9	0.7	1.6	0.67	0.9	0.7	0.7	0.9	0.8	1.31	0.5	0.2
	Suburban	FL-ETS	0.56	1.52	67.10	0.87	0.74	1.83	0.92	0.86	0.31	0.69	1.54	1.04	1.46	0.61	1.32
	Suburban	FL-IG	3.3	2.0	16.7	1.5	1.6	3.8	0.1	1.8	0.9	0.7	1.2	2.5	0.1	0.9	0.4
	Suburban	FL-NETS-NIG	1.1	1.6	4.3	1.4	1.1	1.4	0.2	2.2	0.7	0.8	1.2	1.1	0.1	0.7	0.3
	Suburban	NFL-ETS-IG	3.47	3.11	24.17	3.15	3.16	7.68	0.42	2.88	0.87	0.75	1.16	4.67	0.70	0.31	0.72
	Suburban	NFL-ETS	3.04	2.11	6.61	0.91	0.66	2.05	0.19	1.76	0.99	0.74	0.77	2.08	0.46	0.30	0.75
	Suburban	NFL-IG	1.5	1.1	7.3	0.9	0.8	2.1	0.1	1.1	0.6	0.4	0.7	1.8	0.1	0.6	0.1
	Suburban	NFL-NETS-NIG	1.6	1.2	4.6	1.0	0.9	1.7	0.1	0.9	0.3	0.6	0.9	0.8	0.1	0.5	0.3
	Rural	FL-IG	6.9	6.4	46.9	5.8	7.2	16.4	0.1	7.5	1.9	0.8	1.3	9.3	0.0	0.7	0.2
	Rural	FL-NETS-NIG	0.6	1.2	4.6	0.6	0.5	1.3	0.1	0.7	0.2	0.3	0.5	0.7	0.0	0.7	0.1
	Rural	NFL-IG	1.3	1.8	16.3	2.0	2.1	3.1	0.1	2.5	0.9	0.8	1.2	4.1	0.0	0.7	0.2
	Rural	NFL-NETS-NIG	1.5	2.8	7.5	1.7	1.3	1.0	0.1	1.7	0.5	0.6	0.7	1.0	0.0	0.9	0.1
Other Outdoors	Urban	Summer	0.26	0.34	1.19	0.20	0.16	0.41	0.01	0.22	0.04	0.02	0.00	0.18	0.00	0.04	0.03
	Urban	Winter	0.25	0.79	1.34	0.27	0.25	0.61	0.02	0.31	0.08	0.06	0.00	0.27	0.01	0.08	0.06
	Suburnan	Winter	0.41	1.26	3.26	0.61	0.60	1.45	0.02	0.71	0.17	0.10	0.01	0.54	0.02	0.16	0.02
	Rural	Summer	0.09	0.45	0.25	0.07	0.05	0.05	0.03	0.04	0.00	0.05	0.00	0.01	0.03	0.05	0.02
		Winter	0.33	0.88	0.51	0.05	0.04	0.09	0.01	0.05	0.01	0.06	0.00	0.04	0.00	0.06	0.03
Pub/Bar/Social Club	urban	ETS	0.81	1.90	8.28	1.36	1.28	3.58	1.50	1.86	0.30	0.66	0.90	1.38	2.69	0.33	2.55
	urban	NFL-NETS-summer	0.43	0.56	1.77	0.47	0.35	0.97	0.01	0.31	0.05	0.18	0.05	0.15	0.02	0.12	1.66
	urban	NFL-NETS-winter	0.61	0.76	1.86	0.30	0.24	0.62	0.36	0.30	0.04	0.14	1.70	0.31	0.06	0.16	0.55
	non urban	ETS-summer	0.81	2.22	8.09	1.12	0.85	2.33	1.53	1.11	0.21	0.75	0.55	0.93	3.22	0.35	14.48
	non urban	NFL-NETS-summer	0.52	0.92	2.80	0.58	0.41	1.06	0.41	0.73	0.09	0.24	0.59	0.44	0.72	0.17	0.43
	non urban	ETS-winter	3.15	11.75	38.17	6.98	5.00	19.24	9.08	6.08	1.31	3.47	1.64	5.06	10.26	1.21	6.62
	non urban	NFL-NETS-winter	0.98	5.03	10.67	1.30	1.02	3.34	4.08	1.09	0.31	1.49	0.80	1.10	5.02	0.49	2.18
Restaurant/Cafe/Tea Room	urban	ETS-summer	0.81	1.90	8.28	1.36	1.28	3.58	1.50	1.86	0.30	0.66	0.90	1.38	2.69	0.33	2.55
	urban	ETS-winter	1.94	4.30	10.41	1.49	1.33	3.90	2.83	1.51	0.43	1.16	0.83	1.50	4.52	0.48	0.81
	urban	NFL-NETS-summer	0.43	0.56	1.77	0.47	0.35	0.97	0.01	0.31	0.05	0.18	0.05	0.15	0.02	0.12	1.66
	urban	NFL-NETS-winter	0.61	0.76	1.86	0.30	0.24	0.62	0.36	0.30	0.04	0.14	1.70	0.31	0.06	0.16	0.55
	urban	FL-NETS-summer	1.01	1.45	4.77	0.71	0.52	1.48	0.66	0.69	0.20	0.41	2.30	0.90	1.19	0.23	1.11
	urban	FL-NETS-winter	0.99	3.01	7.80	1.22	1.16	3.32	1.63	1.54	1.68	0.76	2.13	5.75	2.28	0.40	1.95
	non urban	ETS-summer	0.81	2.22	8.09	1.12	0.85	2.33	1.53	1.11	0.21	0.75	0.55	0.93	3.22	0.35	14.48
	non urban	NFL-NETS-summer	0.52	0.92	2.80	0.58	0.41	1.06	0.41	0.73	0.09	0.24	0.59	0.44	0.72	0.17	0.43
	non urban	ETS-winter	3.15	11.75	38.17	6.98	5.00	19.24	9.08	6.08	1.31	3.47	1.64	5.06	10.26	1.21	6.62
	non urban	NFL-NETS-winter	0.98	5.03	10.67	1.30	1.02	3.34	4.08	1.09	0.31	1.49	0.80	1.10	5.02	0.49	2.18
	non urban	FL-NETS-winter	2.12	1.69	4.21	0.67	0.59	1.55	0.65	0.77	0.20	0.33	1.90	0.62	1.01	0.41	0.83
	non urban	FL-NETS-summer	0.90	0.55	6.42	2.22	1.18	3.20	0.10	2.03	0.27	0.17	0.47	1.39	0.05	0.16	0.15
Street	London	FL	1.29	1.27	4.31	0.78	0.77	1.78	0.08	0.92	0.28	0.18	0.08	0.84	0.08	0.19	0.03
	Rest locations	NFL=BS-daytime	1.71	1.73	7.11	1.08	1.02	2.45	0.05	1.20	0.34	0.31	0.05	1.11	0.07	0.26	0.06
		FL-Summer	1.09	1.38	4.78	0.83	0.75	2.00	0.05	1.10	0.24	0.17	0.04	0.89	0.07	0.17	0.16
		FL-winter	1.12	2.63	7.04	1.32	1.31	3.29	0.03	1.56	0.38	0.25	0.01	1.20	0.02	0.29	0.52
		NFL-urban-Summer	0.26	0.34	1.19	0.20	0.16	0.41	0.01	0.22	0.04	0.02	0.00	0.18	0.00	0.04	0.03
		NFL-Urban-Winter	0.25	0.79	1.34	0.27	0.25	0.61	0.02	0.31	0.08	0.06	0.00	0.27	0.01	0.08	0.06
		NFL-Suburban-Summer	0.69	0.76	2.25	0.35	0.25	0.68	0.03	0.41	0.06	0.06	0.00	0.27	0.01	0.08	
		NFL-suburban-Winter	0.41	1.26	3.26	0.61	0.60	1.45	0.02	0.71	0.17	0.10	0.01	0.54	0.02	0.16	0.02
		urban-pedestrian	0.37	1.62	4.95	2.95	1.46	1.22	0.05	1.57	0.20	0.14	0.00	0.63	0.06	0.19	0.68
Work - Kitchen/Common Room/Staff Room/Cafeteria/Canteen	London	FL	1.27	0.96	4.67	1.35	1.27	3.31	0.14	1.55	0.31	0.37	0.39	1.20	0.18	0.31	0.04
Work - Office at Different Site/Conference Centre		NFL	0.60	0.70	2.69	0.76	0.86	2.33	0.13	1.09	0.16	0.25	0.57	3.79	0.10	0.30	0.02
Work/Educational Institute - Office	Wales	NFL	0.34	2.01	2.78	0.39	0.39	0.93	0.06	0.46	0.16	0.29	0.41	0.58	0.04	0.41	0.08
	Bham -urban	FL	1.17	1.50	7.29	1.35	1.23	3.31	0.06	1.51	0.40	0.69	0.53	1.55	0.04	0.37	0.19
		NFL	1.15	1.34	6.55	2.26	1.79	5.17	0.18	1.94	0.32	1.15	0.56	1.24	0.08	0.41	0.14
	Bham-suburban	FL	1.17	1.50	7.29	1.35	1.23	3.31	0.06	1.51	0.40	0.69	0.53	1.55	0.04	0.37	0.19
		NFL	1.36	0.82	3.14	1.17	1.35	3.47	0.09	1.80	0.24	0.43	0.39	0.82	0.05	0.38	0.06

Supplemental Material, Table 6. Sensitivity analysis of model evolution measured as correlation coefficient (R^2) and standard error of the estimate (in µg m^{-3}) in the VOC logged training dataset

	Model 1		Model 2		Model 3		Model 4		Model 5		Model 6		Model 7	
Number of Samples	**(N=77)**		**(N=40)**		**(N=37)**		**(N=375)**		**(N=375)**		**(N=375)**		**(N=375)**	
Statistic	**R^2**	**SE**	**R^2**	**SE**	**R^2**	**SE**	**R^2**	**SE**	**R^2**	**SE**	**R^2**	**SE**	**R^2**	**SE**
Hexane	0.331[(a)]	1.95	0.243[(a)]	2.24	0.200[(a)]	0.11	0.401[(a)]	0.24	0.025	0.22	0.289[(a)]	0.19	0.127[(a)]	0.16
Benzene	0.675[(a)]	1.38	0.236[(a)]	1.66	0.653[(a)]	0.11	0.392[(a)]	0.17	0.120[(a)]	0.18	0.354[(a)]	0.14	0.130[(a)]	0.08
Toluene	0.666[(a)]	1.62	0.288[(a)]	2.04	0.594[(a,b)]	0.14	0.496[(a)]	0.26	0.114[(a)]	0.26	0.288[(a)]	0.20	0.005	0.06
Ethylbenzene	0.436[(a)]	1.78	0.137	2.00	0.482[(a)]	0.12	0.457[(a)]	0.20	0.078[(a)]	0.21	0.450[(a)]	0.18	NVE	NVE
p-Xylene	0.497[(a)]	1.78	0.239[(a)]	2.04	0.520[(a,b)]	0.15	0.470[(a)]	0.00	0.096[(a)]	0.23	0.461[(a)]	0.19	0.018	0.09
m-Xylene	0.474[(a)]	1.82	0.268[(a)]	2.04	0.509[(a)]	0.13	0.422[(a)]	0.23	0.115[(a)]	0.22	0.412[(a)]	0.20	NVE	NVE
Pyridine	0.250[(a)]	1.78	0.003	1.95	0.254[(a)]	0.17	0.427[(a)]	0.24	0.263[(a)]	0.27	0.283[(a)]	0.23	0.221[(a)]	0.24
o-Xylene	0.502[(a)]	1.74	0.184[(a)]	2.00	0.530[(a,b)]	0.15	0.468[(a)]	0.21	0.127[(a)]	0.22	0.462[(a)]	0.19	0.017	0.1
1,3,5-Trimethylbenzene	0.693[(a)]	1.70	0.124	2.34	0.735[(a)]	0.16	0.601[(a)]	0.21	0.161[(a)]	0.24	0.302[(a)]	0.38	0.030[(a)]	0.17
Styrene	0.359[(a)]	1.86	0.084	1.74	0.375[(a)]	0.09	0.464[(a)]	0.19	0.105[(a)]	0.21	0.317[(a)]	0.18	0.001	0.14
p-Isopropyltoluene	0.518[(a)]	1.62	0.061	1.70	0.497[(a)]	0.10	0.439[(a)]	0.19	0.048[(a)]	0.15	0.253[(a)]	0.15	NVE	NVE
1,2,4-Trimethylbenzene	0.731[(a)]	1.70	0.159	2.34	0.778[(a)]	0.15	0.599[(a)]	0.22	0.196[(a)]	0.25	0.386[(a)]	0.30	0.116[(a)]	0.17
3-Ethenylpyridine	0.260[(a)]	2.24	0.000	2.40	0.239	0.34	0.506[(a)]	0.34	0.387[(a)]	0.36	0.322[(a)]	0.35	0.330[(a)]	0.39
Naphthalene	0.478[(a)]	1.58	0.215[(a)]	1.70	0.291[(a)]	0.07	0.511[(a)]	0.18	0.092[(a)]	0.17	0.282[(a)]	0.19	0.008	0.14
1,3-Butadiene	0.266[(a)]	2.14	0.015	2.04	0.533[(a)]	0.27	0.132[(a)]	0.42	0.036[(a)]	0.33	0.288[(a)]	0.26	0.122[(a)]	0.21

(a) Represent significant correlation values at 0.01 level.
(b) The workplace concentration coefficient γ is significant at the 0.01 level.
NVE : No Variable Entered in the Stepwise regression.

Supplemental Material, Table 7. Sensitivity analysis of model evolution measured as correlation coefficient (R^2), adjusted correlation coefficient (R^2_{adj}) and standard error of the estimate (in µg m^{-3}) in the VOC training dataset obtained from three different combinations of training data selected randomly.

		Model 1			Model 2			Model 3			Model 4			Model 5			Model 6			Model 7		
Number of Samples		**(N=77)**			**(N=40)**			**(N=37)**			**(N=375)**			**(N=375)**			**(N=375)**			**(N=375)**		
Statistic		**R^2**	**R^2_{adj}**	**SE**	**R2**	**R2adj**	**SE**	**R2**	**R2adj**	**SE**	**R^2**	**R^2_{adj}**	**SE**	**R2**	**R2adj**	**SE**	**R2**	**R2adj**	**SE**	**R2**	**R2adj**	**SE**
Hexane	AM	0.139	0.123	1.344	0.157	0.122	0.979	0.190	0.153	1.189	0.370	0.036	2.917	0.016	0.023	1.438	0.404	0.402	1.778	0.119	0.117	1.25
	STD	0.047	0.046	0.036	0.061	0.060	0.215	0.130	0.134	0.194	0.003	0.004	0.164	0.006	0.007	0.435	0.029	0.029	0.039	0.003	0.003	0.01
Benzene	AM	0.761	0.756	0.706	0.109	0.072	0.486	0.820	0.812	0.653	0.313	0.235	0.985	0.121	0.040	0.835	0.448	0.446	0.647	0.121	0.118	0.37
	STD	0.009	0.009	0.020	0.041	0.044	0.083	0.013	0.014	0.048	0.003	0.003	0.028	0.007	0.009	0.205	0.040	0.040	0.005	0.000	0.000	0.00
Toluene	AM	0.473	0.464	5.761	0.157	0.147	4.154	0.476	0.475	5.410	0.463	0.211	13.50	0.091	0.203	7.676	0.527	0.526	8.317	0.032	0.029	2.38
	STD	0.301	0.306	3.882	0.135	0.098	3.268	0.405	0.384	3.459	0.053	0.070	0.566	0.009	0.057	3.018	0.031	0.032	0.173	0.001	0.001	0.01
Ethylbenzene	AM	0.075	0.062	0.343	0.270	0.257	1.112	0.290	0.257	0.975	0.423	0.073	1.351	0.037	0.002	0.753	0.756	0.756	1.411	0.007	0.004	3.76
	STD	0.070	0.039	0.177	0.167	0.168	0.085	0.149	0.158	0.128	0.008	0.010	0.048	0.001	0.001	0.265	0.044	0.045	0.072	0.002	0.002	0.01
p-Xylene	AM	0.477	0.467	1.140	0.119	0.094	0.354	0.296	0.264	1.132	0.487	0.116	1.324	0.096	0.061	0.854	0.759	0.758	1.206	NVE	NVE	NVE
	STD	0.060	0.061	0.079	0.086	0.068	0.255	0.077	0.083	0.089	0.009	0.011	0.032	0.014	0.018	0.320	0.080	0.080	0.161			
m-Xylene	AM	0.467	0.457	2.773	0.099	0.062	1.034	0.269	0.236	2.541	0.467	0.105	3.392	0.069	0.031	2.091	0.750	0.749	3.160	0.005	0.003	0.92
	STD	0.035	0.035	0.118	0.036	0.035	0.467	0.120	0.128	0.259	0.007	0.010	0.110	0.005	0.007	0.720	0.067	0.068	0.257	0.002	0.001	0.00
Pyridine	AM	0.360	0.348	0.115	0.001	0.042	0.004	0.367	0.336	0.067	0.157	0.064	0.473	0.136	0.050	0.270	0.661	0.660	0.155	0.226	0.224	0.17
	STD	0.221	0.227	0.008	0.002	0.003	0.000	0.160	0.170	0.012	0.011	0.015	0.056	0.021	0.027	0.070	0.062	0.062	0.005	0.013	0.013	0.00
o-Xylene	AM	0.475	0.465	1.441	0.096	0.081	0.591	0.235	0.210	1.248	0.492	0.119	1.466	0.096	0.036	1.047	0.788	0.787	1.756	0.006	0.003	0.54
	STD	0.046	0.046	0.080	0.080	0.045	0.079	0.022	0.041	0.055	0.016	0.020	0.026	0.010	0.013	0.415	0.042	0.042	0.120	0.002	0.002	0.00
1,3,5-Trimethylbenzene	AM	0.507	0.498	0.906	0.006	0.036	0.112	0.447	0.422	0.536	0.460	0.276	0.434	0.140	0.077	0.303	0.781	0.780	0.938	0.020	0.017	0.59
	STD	0.040	0.040	0.093	0.002	0.006	0.069	0.089	0.091	0.184	0.052	0.070	0.025	0.006	0.008	0.038	0.024	0.024	0.182	0.006	0.006	0.00
Styrene	AM	0.329	0.329	0.779	0.006	0.035	0.074	0.074	0.037	0.353	0.578	0.072	0.726	0.208	0.064	0.426	0.844	0.843	1.386	0.019	0.016	0.35
	STD	0.534	0.533	0.576	0.007	0.005	0.067	0.060	0.058	0.376	0.010	0.014	0.040	0.016	0.021	0.303	0.009	0.009	0.045	0.001	0.001	0.00
p-Isopropyltoluene	AM	0.262	0.248	0.356	0.049	0.029	0.108	0.343	0.313	0.250	0.337	0.112	0.476	0.042	0.009	0.234	0.458	0.456	0.465	NVE	NVE	NVE
	STD	0.090	0.090	0.013	0.040	0.027	0.007	0.174	0.183	0.025	0.010	0.013	0.008	0.003	0.003	0.037	0.021	0.022	0.011			
1,2,4-Trimethylbenzene	AM	0.537	0.528	2.898	0.005	0.036	0.244	0.492	0.470	1.982	0.502	0.305	1.662	0.217	0.048	1.111	0.809	0.809	2.364	0.031	0.028	1.83
	STD	0.023	0.022	0.192	0.007	0.005	0.128	0.080	0.081	0.592	0.044	0.064	0.080	0.013	0.018	0.239	0.036	0.036	0.061	0.001	0.001	0.00
3-Ethenylpyridine	AM	0.510	0.501	0.253	0.021	0.019	0.036	0.450	0.425	0.203	0.242	0.114	0.560	0.185	0.107	0.317	0.688	0.687	0.266	0.291	0.289	0.32
	STD	0.224	0.230	0.012	0.015	0.016	0.007	0.066	0.071	0.021	0.017	0.023	0.065	0.022	0.030	0.094	0.060	0.060	0.006	0.005	0.005	0.00
Naphthalene	AM	0.403	0.392	0.144	0.297	0.280	0.136	0.388	0.422	0.225	0.447	0.304	0.861	0.117	0.110	0.302	0.513	0.511	0.640	0.030	0.027	0.23
	STD	0.144	0.145	0.110	0.240	0.229	0.019	0.314	0.220	0.179	0.014	0.019	0.043	0.053	0.071	0.237	0.002	0.002	0.026	0.002	0.002	0.00
1,3-Butadiene	AM	0.128	0.109	0.049	0.023	0.022	0.187	0.556	0.522	0.122	0.092	0.026	0.507	0.046	0.001	0.402	0.197	0.195	0.293	0.009	0.007	0.16
	STD	0.037	0.036	0.013	0.008	0.014	0.237	0.067	0.095	0.002	0.008	0.011	0.026	0.001	0.001	0.012	0.038	0.038	0.011	0.005	0.004	0.00

Supplemental Material, Table 8. Detailed list of add-on variables (A_m and F_n), un-standardised variable coefficients (βm and γn), standardised variable coefficient (Beta), t-statistic and its significance and partial correlations of the variables entered in the development of Model 6 as defined in Equation 6. Concentrations are measured in µg m^{-3}, time variables are measured in minutes and Inverse of time variables in $minutes^{-1}$

Model	Variables	Un-standardised coefficients (β_m, γ_n)		Standardised coefficient	t-statistic	Sig.	Correlations			% cases report add-on	Reference supporting variable
		β_m or γ_n	Std. Error	Beta			Zero-order	Partial	Semi-partial		
n-Hexane	(Constant)	1.687	0.170		9.920	0.000					
(R^2=0.385)	DICHOTOMOUS VARIABLES A_m										
	Volunteer has paints stored in the garage	6.675	0.556	0.520	11.995	0.000	0.514	0.552	0.519	7	(Edwards et al. 2005; Zuraimi et al. 2006)
	Volunteer visited hospital	3.830	0.921	0.181	4.160	0.000	0.188	0.224	0.180	3	
	Additional heating sources at home	4.134	1.661	0.108	2.489	0.013	0.093	0.136	0.108	3	
	Volunteer works in a factory	0.093	1.659	0.002	0.056	0.956	-0.022	0.003	0.002	1	(Edwards et al. 2005)
	Volunteer works with solvents in the lab	7.221	1.289	0.243	5.601	0.000	0.215	0.295	0.242	9	(Edwards et al. 2005)
	TIME VARIABLES F_n										
	Time exposed to constant ETS	0.008	0.003	0.129	2.967	0.003	0.163	0.161	0.128	6	
Benzene	(Constant)	0.609	0.196		3.108	0.002					
(R^2=0.469)	DICHOTOMOUS VARIABLES A_m										
	Benzene Modelled	0.140	0.082	0.096	1.696	0.091	0.316	0.093	0.068	100	
	Volunteer has paints stored in the garage	1.905	0.210	0.405	9.082	0.000	0.464	0.447	0.364	7	
	Car kept in the garage	1.049	0.215	0.219	4.889	0.000	0.382	0.260	0.196	7	(Batterman et al. 2006)
	Urban subject	0.380	0.133	0.140	2.854	0.005	-0.094	0.155	0.114	38	(Edwards et al. 2005)
	Volunteer visited hospital	1.320	0.316	0.170	4.171	0.000	0.183	0.223	0.167	3	
	Commute by electric or diesel train	0.350	0.179	0.083	1.962	0.051	0.023	0.107	0.079	10	(Edwards et al. 2005)
	Additional heating sources at home	2.087	0.668	0.148	3.122	0.002	0.175	0.169	0.125	3	
	Gas used as main heating	0.455	0.123	0.172	3.714	0.000	0.032	0.200	0.149	60	
	TIME VARIABLES F_n										
	Time exposed to constant or frequent ETS	0.003	0.001	0.279	5.994	0.000	0.285	0.313	0.240	15	(Heavner et al. 1995)
	Time commuting in a car	0.005	0.001	0.153	3.597	0.000	0.243	0.194	0.144	11	
Toluene	(Constant)	5.584	1.203		4.643	0.000					
(R^2=0.513)	DICHOTOMOUS VARIABLES A_m										
	Toluene Modelled	0.394	0.095	0.172	4.159	0.000	0.245	0.224	0.160	100	
	Open plan kitchen + living room	7.335	1.715	0.178	4.276	0.000	0.084	0.230	0.165	21	
	Incense burning	2.499	3.484	0.029	0.717	0.474	0.028	0.040	0.028	4	
	Volunteer has paints stored in the garage	12.534	2.690	0.199	4.659	0.000	0.208	0.249	0.180	7	(Ilgen et al. 2001)
	Car kept in the garage	8.820	2.714	0.138	3.250	0.001	0.141	0.177	0.125	7	(Jia et al. 2008; Song et al. 2007)
	London subject	7.940	2.102	0.151	3.777	0.000	0.054	0.204	0.146	11	(Jia et al. 2008; Song et al. 2007)
	Volunteer visited hospital	25.329	4.022	0.247	6.298	0.000	0.247	0.328	0.243	3	(Song et al. 2007)
	Drawing or painting with colours	23.955	5.766	0.167	4.154	0.000	0.271	0.224	0.160	1	(Song et al. 2007)
	Volunteer works in a factory	9.808	7.171	0.053	1.368	0.172	0.011	0.075	0.053	1	(Song et al. 2007)
	Additional Gas heating appliances	5.753	3.567	0.064	1.613	0.108	0.041	0.089	0.062	13	
	Wrapping Christmas presents and cards	41.584	7.264	0.225	5.725	0.000	0.218	0.301	0.221	1	(Jia et al. 2008)
	TIME VARIABLES F_n										
	Time doing manicure, gardening or glues	0.321	0.026	0.480	12.144	0.000	0.474	0.557	0.468	2	(Ilgen et al. 2001)
Ethylbenzene	(Constant)	0.981	0.198		4.944	0.000					
(R^2=0.813)	DICHOTOMOUS VARIABLES A_m										
	Ethylbenzene Modelled	0.156	0.156	0.032	0.995	0.320	0.117	0.055	0.024	100	
	Volunteer has paints stored in the garage	1.668	0.309	0.142	5.393	0.000	0.183	0.284	0.128	7	(Ilgen et al. 2001)
	Car kept in the garage	1.807	0.321	0.152	5.637	0.000	0.159	0.296	0.134	7	(Song et al. 2007)
	Volunteer visited hospital	2.113	0.463	0.109	4.559	0.000	0.088	0.243	0.108	3	(Song et al. 2007)
	Carpet been fumigated	19.158	0.836	0.546	22.929	0.000	0.525	0.783	0.545	1	(Yang et al. 2002)
	New carpet fitted at home	0.202	0.200	0.025	1.006	0.315	-0.015	0.055	0.024	1	
	Additional heating sources at home	3.113	1.057	0.089	2.945	0.003	0.082	0.160	0.070	3	(Song et al. 2007)
	Volunteer works in a factory	3.881	0.836	0.111	4.645	0.000	0.085	0.247	0.110	1	(Song et al. 2007)
	TIME VARIABLES F_n										
	Time painting or in presence of painters	0.074	0.003	0.675	28.345	0.000	0.662	0.841	0.674	3	(Ilgen et al. 2001; Song et al. 2007)

Supplemental Material, Table 8 Cont.

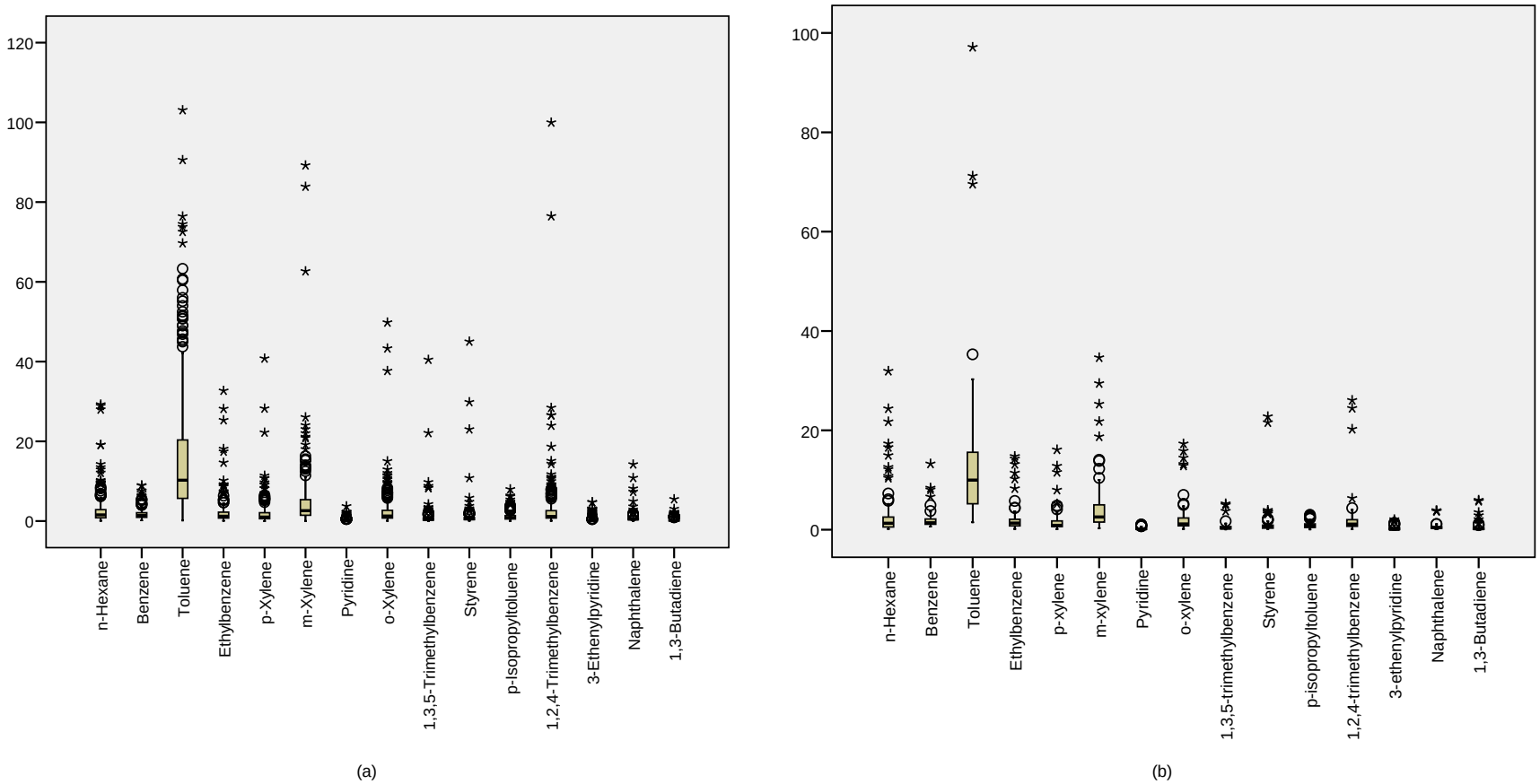
Model	Variables	Un-standardised coefficients (β_m, γ_n) β_m or γ_n	Std. Error	Standardised coefficient Beta	t-statistic	Sig.	Correlations Zero-order	Partial	Semi-partial	% cases report add-on	Reference supporting variable
p-Xylene	(Constant)	0.620	0.184		3.374	0.001					
(R^2=0.819)	DICHOTOMOUS VARIABLES A_m										
	p-Xylene Modelled	0.423	0.150	0.095	2.814	0.005	0.180	0.152	0.066	100	
	Storage of lawn mower in garage	1.760	0.337	0.131	5.222	0.000	0.200	0.275	0.122	7	(Song et al. 2007)
	Car kept in the garage	2.157	0.321	0.179	6.717	0.000	0.205	0.345	0.157	7	(Song et al. 2007)
	Volunteer visited hospital	2.028	0.460	0.103	4.409	0.000	0.091	0.235	0.103	3	(Song et al. 2007)
	Carpet been fumigated	5.857	0.828	0.165	7.072	0.000	0.141	0.361	0.165	1	(Yang et al. 2002)
	Additional heating sources at home	2.510	1.157	0.071	2.169	0.031	0.113	0.118	0.051	3	(Song et al. 2007)
	Volunteer works in a factory	5.552	0.828	0.157	6.707	0.000	0.134	0.345	0.156	1	(Song et al. 2007)
	Time painting or in presence of painters	0.092	0.003	0.828	35.487	0.000	0.818	0.889	0.828	3	(Ilgen et al. 2001; Song et al. 2007)
m-Xylene	(Constant)	1.491	0.327		4.560	0.000					
(R^2=0.833)	DICHOTOMOUS VARIABLES A_m										
	m-Xylene Modelled	0.514	0.097	0.121	5.321	0.000	0.175	0.280	0.119	100	
	Car kept in the garage	6.533	0.680	0.219	9.606	0.000	0.191	0.465	0.215	7	(Song et al. 2007)
	Volunteer visited hospital	4.570	1.090	0.094	4.192	0.000	0.076	0.224	0.094	3	(Song et al. 2007)
	Carpet been fumigated	14.123	1.967	0.161	7.178	0.000	0.138	0.366	0.161	1	(Yang et al. 2002)
	Volunteer works in a factory	14.725	1.968	0.168	7.483	0.000	0.144	0.379	0.167	1	(Song et al. 2007)
	TIME VARIABLES F_n										
	Time painting or in presence of painters	0.348	0.012	1.268	28.262	0.000	0.799	0.840	0.632	3	(Ilgen et al. 2001; Song et al. 2007)
	Time in presence of painters	-0.168	0.014	-0.531	-11.84	0.000	0.558	-0.544	-0.265	1	(Ilgen et al. 2001; Song et al. 2007)
Pyridine	(Constant)	0.165	0.015		10.735	0.000					
(R^2=0.699)	DICHOTOMOUS VARIABLES A_m										
	Pyridine Modelled	-0.221	0.041	-0.291	-5.441	0.000	0.336	-0.285	-0.161	100	
	ETS	0.059	0.034	0.065	1.739	0.083	0.420	0.095	0.051	30	(Heavner et al. 1995)
	TIME VARIABLES F_n										
	Time in presence of ETS	0.001	0.000	0.208	3.268	0.001	0.730	0.176	0.097	30	(Heavner et al. 1995)
	Time exposed to constant ETS	0.004	0.000	0.528	12.391	0.000	0.682	0.561	0.366	6	(Heavner et al. 1995)
	Time in presence of frequent ETS	0.002	0.000	0.537	8.921	0.000	0.496	0.439	0.264	11	(Heavner et al. 1995)
o-Xylene	(Constant)	0.381	0.191		1.995	0.047					
(R^2=0.832)	DICHOTOMOUS VARIABLES A_m										
	o-Xylene Modelled	0.671	0.106	0.132	6.350	0.000	0.206	0.328	0.128	100	
	Car kept in the garage	2.664	0.339	0.163	7.865	0.000	0.140	0.395	0.159	7	(Song et al. 2007)
	Volunteer visited hospital	2.177	0.538	0.082	4.049	0.000	0.070	0.216	0.082	3	(Song et al. 2007)
	Carpet been fumigated	7.501	0.972	0.156	7.721	0.000	0.130	0.389	0.156	1	(Yang et al. 2002)
	Volunteer works in a factory	12.118	0.971	0.252	12.477	0.000	0.228	0.564	0.252	1	(Song et al. 2007)
	TIME VARIABLES F_n										
	Time painting or in presence of painters	0.208	0.006	1.384	34.089	0.000	0.776	0.881	0.687	3	(Ilgen et al. 2001)
	Time in presence of painters	-0.120	0.007	-0.695	-17.13	0.000	0.493	-0.684	-0.345	1	(Ilgen et al. 2001)
1,3,5-Trimethylbenzene	(Constant)	-0.148	0.110		-1.342	0.180					
	DICHOTOMOUS VARIABLES A_m										
(R^2=0.788)	1,3,5-Trimethylbenzene Modelled	0.689	0.198	0.079	3.481	0.001	0.271	0.187	0.075	100	
	Car kept in the garage	1.023	0.229	0.105	4.459	0.000	0.114	0.237	0.096	7	(Jia et al. 2008)
	Garage connected to the kitchen	1.132	0.265	0.100	4.272	0.000	0.111	0.227	0.092	5	(Jia et al. 2008)
	Use of gas cooker	0.244	0.031	0.187	7.804	0.000	0.504	0.392	0.168	44	
	Volunteer works in a factory	0.966	0.618	0.034	1.562	0.119	0.012	0.085	0.034	1	(Watson et al. 2001)
	TIME VARIABLES F_n										
	Time in painting	0.143	0.004	0.802	34.265	0.000	0.879	0.882	0.739	3	(Lai et al. 2004)
Styrene	(Constant)	0.209	0.171		1.224	0.222					
(R^2=0.868)	DICHOTOMOUS VARIABLES A_m										
	Styrene Modelled	0.796	0.248	0.064	3.208	0.001	0.035	0.172	0.064	100	
	Wood burning in a fireplace	2.503	0.489	0.102	5.117	0.000	0.094	0.268	0.102	2	(Austin et al. 2001)
	Carpet been fumigated	31.987	0.688	0.926	46.475	0.000	0.922	0.930	0.925	1	(Zuraimi et al. 2006)

Supplemental Material, Table 8 Cont.

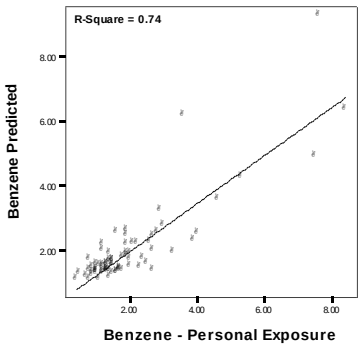
Model	Variables	Un-standardised coefficients (β_m, γ_n) β_m or γ_n	Std. Error	Standardised coefficient Beta	t-statistic	Sig.	Correlations Zero-order	Partial	Semi-partial	% cases report add-on	Reference supporting variable
p-isopropyltoluene (R^2=0.484)	(Constant)	0.329	0.152		2.166	0.031					
	DICHOTOMOUS VARIABLES A_m										
	p-Isopropyltoluene Modelled	0.534	0.181	0.123	2.945	0.003	0.136	0.160	0.116	100	
	Incense burning	0.485	0.203	0.097	2.390	0.017	0.143	0.130	0.094	2	
	Redecoration	0.257	0.086	0.129	3.001	0.003	0.146	0.163	0.118	44	
	Subject works as a chiropodist	3.756	0.428	0.353	8.769	0.000	0.340	0.434	0.346	1	
	Drawing or painting with colours	1.305	0.338	0.158	3.865	0.000	0.154	0.208	0.153	1	(Scorecard 2006)
	Additional Gas heating appliances	0.642	0.215	0.124	2.981	0.003	0.092	0.162	0.118	13	
	Not use of cooker hood	0.288	0.213	0.055	1.350	0.178	0.024	0.074	0.053	3	
	TIME VARIABLES F_n										
	Inverse Time since antimould use	3.923	0.613	0.255	6.401	0.000	0.230	0.332	0.253	1	
	Time in the gym	0.004	0.001	0.125	3.087	0.002	0.135	0.167	0.122	9	
	Time in painting	0.030	0.003	0.449	11.242	0.000	0.451	0.526	0.444	3	(Scorecard 2006)
1,2,4-Trimethylbenzene (R^2=0.862)	(Constant)	-0.138	0.280		-0.494	0.621					
	DICHOTOMOUS VARIABLES A_m										
	1,2,4-Trimethylbenzene Modelled	0.716	0.154	0.100	4.639	0.000	0.115	0.246	0.094	100	
	Car kept in the garage	4.164	0.625	0.151	6.665	0.000	0.191	0.343	0.135	7	(Jia et al. 2008)
	Garage connected to the kitchen	4.337	0.709	0.135	6.113	0.000	0.177	0.317	0.124	5	(Jia et al. 2008)
	Use of gas cooker	0.642	0.081	0.173	7.879	0.000	0.465	0.396	0.159	44	
	Volunteer works in a factory	3.902	1.645	0.048	2.372	0.018	0.025	0.129	0.048	1	(Watson et al. 2001)
	TIME VARIABLES F_n										
	Time in painting	0.416	0.011	0.822	37.466	0.000	0.873	0.899	0.758	3	(Lai et al. 2004)
3-Ethenylpyridine (R^2=0.750)	(Constant)	0.109	0.022		4.912	0.000					
	DICHOTOMOUS VARIABLES A_m										
	3-Ethenylpyridine Modelled	-0.337	0.052	-0.318	-6.472	0.000	0.370	-0.333	-0.172	100	
	ETS	0.178	0.051	0.116	3.482	0.001	0.468	0.187	0.092	30	(Heavner et al. 1995)
	TIME VARIABLES F_n										
	Time in presence of ETS	0.001	0.000	0.227	3.970	0.000	0.761	0.212	0.105	30	(Heavner et al. 1995)
	Time exposed to constant ETS	0.003	0.000	0.215	5.204	0.000	0.711	0.273	0.138	6	(Heavner et al. 1995)
	Time exposed to constant or frequent ETS	0.004	0.000	0.647	9.808	0.000	0.777	0.472	0.260	15	(Heavner et al. 1995)
Naphthalene (R^2=0.418)	(Constant)	0.381	0.082		4.659	0.000					
	DICHOTOMOUS VARIABLES A_m										
	Incense burning	0.994	0.248	0.168	4.006	0.000	0.146	0.214	0.167	2	
	Photocopier, fax or printer in the house	0.306	0.135	0.097	2.272	0.024	0.205	0.123	0.095	18	(Zuraimi et al. 2006)
	Gas used as main heating	0.273	0.102	0.115	2.671	0.008	0.045	0.145	0.111	59	
	Packing or unpacking clothes	1.188	0.906	0.055	1.311	0.191	0.040	0.072	0.055	1	(Edwards et al. 2005)
	TIME VARIABLES F_n										
	Inverse time carpet was replaced in kitchen	0.921	0.693	0.058	1.329	0.185	0.068	0.073	0.055	7	
	Inverse time carpet was replaced in livingroom	0.164	0.333	0.021	0.493	0.622	0.001	0.027	0.021	7	
	Inverse time packing or unpacking clothes	20.078	1.435	0.600	13.991	0.000	0.603	0.608	0.584	1	(Edwards et al. 2005)
1,3-Butadiene (R^2=0.487)	(Constant)	0.115	0.036		3.232	0.001					
	DICHOTOMOUS VARIABLES A_m										
	Solvent use	0.112	0.135	0.034	0.834	0.405	0.117	0.046	0.033	4	
	Subject visited a petrol station	0.178	0.106	0.068	1.678	0.094	0.107	0.092	0.066	4	
	Commute by bus	0.108	0.070	0.062	1.538	0.125	0.094	0.084	0.060	13	(Curren et al. 2006)
	Garage connected to the kitchen	0.401	0.091	0.176	4.403	0.000	0.145	0.235	0.173	5	
	Additional Gas heating appliances	0.666	0.112	0.238	5.969	0.000	0.198	0.312	0.234	13	
	TIME VARIABLES F_n										
	Time travelling	0.001	0.000	0.059	1.458	0.146	0.042	0.080	0.057	12	(Curren et al. 2006)
	Time in presence of ETS	0.001	0.000	0.149	1.969	0.050	0.389	0.108	0.077	30	(Heavner et al. 1995; Kim et al. 2001)
	Time exposed to constant or frequent ETS	0.001	0.000	0.236	3.150	0.002	0.375	0.171	0.124	15	(Heavner et al. 1995; Kim et al. 2001)
	Time wrapping Christmas presents and cards	0.015	0.001	0.431	10.685	0.000	0.448	0.506	0.419	1	
	Inverse Time since antimould use	2.001	0.338	0.241	5.925	0.000	0.247	0.310	0.232	1	

Supplemental Material, Table 9. Detailed list of dichotomous variables (D_l), un-standardised variable coefficients (δ_l), standardised variable coefficient (Beta), t-statistic and its significance and partial correlations of the variables entered in the development of Model 7 as defined in Equation 7. Concentrations are measured in µg m^{-3}

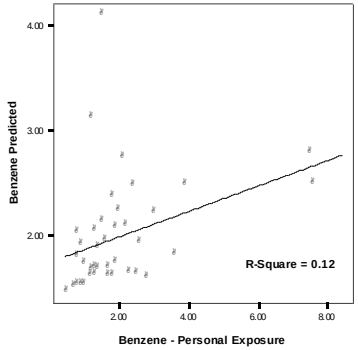
Model	Variables	Unstandardized coefficients		Standardized coefficient	t-statistic	Sig.	Correlations		
		δ_l	Std. Error	Beta			Zero-order	Partial	Semipartial
n-Hexane	(Constant)	1.91	0.21		9.01	0.00			
	IG	3.25	0.50	0.34	6.56	0.00	0.33	0.34	0.34
	ETS_home	1.45	0.60	0.12	2.40	0.02	0.12	0.13	0.12
Benzene	(Constant)	1.47	0.09		17.10	0.00			
	IG	0.87	0.18	0.25	4.73	0.00	0.24	0.25	0.25
	ETS	0.50	0.15	0.17	3.34	0.00	0.17	0.18	0.17
Toluene	(Constant)	14.30	1.28		11.18	0.00			
	FL	4.90	1.86	0.14	2.63	0.01	0.14	0.14	0.14
Ethylbenzene	(Constant)	2.41	0.24		9.97	0.00			
	FL	-0.77	0.35	-0.12	-2.17	0.03	-0.12	-0.12	-0.12
p-Xylene	NVE								
m-Xylene	(Constant)	5.65	0.61		9.32	0.00			
	FL	-1.87	0.88	-0.11	-2.12	0.03	-0.11	-0.11	-0.11
Pyridine	(Constant)	0.13	0.02		5.61	0.00			
	ETS	0.32	0.05	0.35	6.69	0.00	0.42	0.34	0.32
	ETS_home	0.28	0.07	0.21	4.04	0.00	0.33	0.22	0.20
o-Xylene	(Constant)	2.96	0.33		8.93	0.00			
	FL	-1.10	0.48	-0.12	-2.28	0.02	-0.12	-0.12	-0.12
1,3,5-Trimethylbenzene	(Constant)	0.67	0.15		4.50	0.00			
	ETS_home	1.78	0.47	0.20	3.81	0.00	0.20	0.20	0.20
Styrene	(Constant)	0.76	0.22		3.46	0.00			
	urban	0.74	0.36	0.11	2.06	0.04	0.11	0.11	0.11
p-isopropyltoluene	NVE								
1,2,4-Trimethylbenzene	(Constant)	2.08	0.46		4.53	0.00			
	ETS_home	4.63	1.34	0.18	3.45	0.00	0.18	0.18	0.18
	IG	2.46	1.08	0.12	2.27	0.02	0.12	0.12	0.12
3-Ethenylpyridine	(Constant)	0.07	0.04		1.86	0.06			
	ETS	0.58	0.08	0.38	7.57	0.00	0.47	0.38	0.35
	ETS_home	0.58	0.11	0.25	5.08	0.00	0.39	0.27	0.24
Naphthalene	(Constant)	0.78	0.08		9.30	0.00			
	ETS_home	0.65	0.21	0.17	3.16	0.00	0.16	0.17	0.17
	suburban	-0.31	0.13	-0.13	-2.47	0.01	-0.12	-0.13	-0.13
1,3-Butadiene	(Constant)	0.28	0.04		7.27	0.00			
	ETS	0.34	0.06	0.29	5.57	0.00	0.28	0.29	0.29
	urban	-0.14	0.06	-0.13	-2.56	0.01	-0.12	-0.14	-0.13



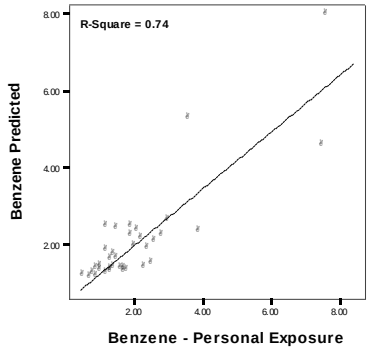
Supplemental Material, Figure 1. Boxplot distribution of personal exposure concentrations (μg/m^3) contained in the (a) training dataset and (b) validation dataset. Y-axis represents personal exposure concentrations (μg/m^3)



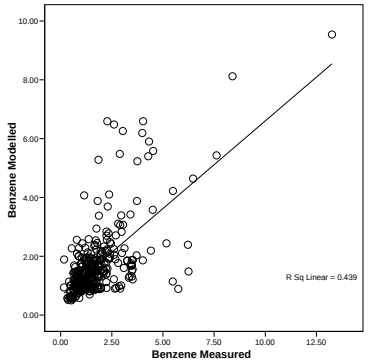
(a) Model 1



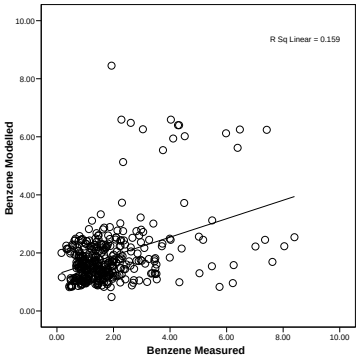
(b) Model 2



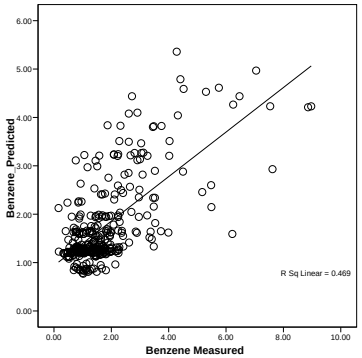
(c) Model 3



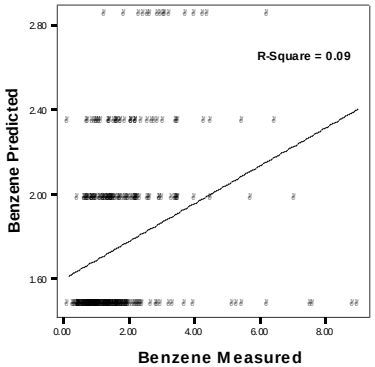
(d) Model 4



(e) Model 5



(f) Model 6



(g) Model 7

Supplemental Material, Figure 2. Benzene concentrations (in µg m^{-3}) predicted vs. concentration measured in training dataset used in (a) Model 1, (b) Model 2, (c) Model 3, (d) Model 4, (e) Model 5, (f) Model 6 and (g) Model 7