Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supporting Information

Behavior of carbon monoxide, nitrogen oxides, and ozone in vehicle cabin with a passenger

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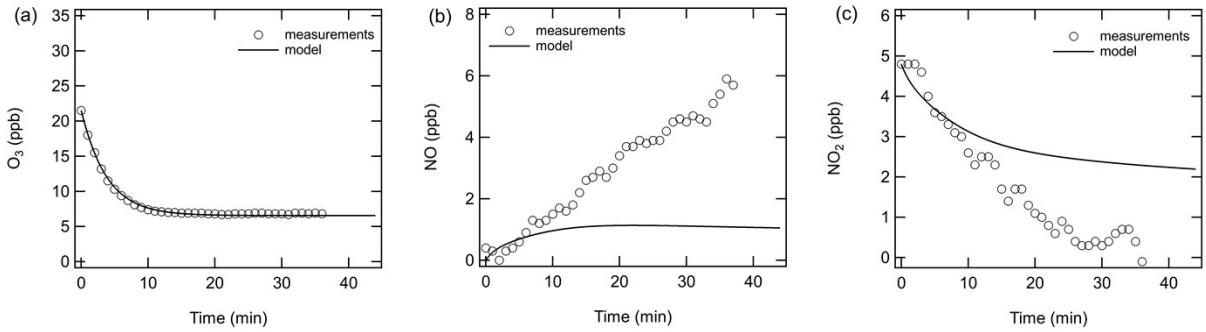

Figure S1: Concentrations of (a) O_3, (b) NO and (c) NO_2 predicted by the model at midnight when an ozone production rate of 8.1×10^8 molecule cm^{-3} s^{-1} was included in the model in order to match ozone concentrations. All other parameters were kept consistent with those found in Table S1.

Table S1: Gas-phase reactions and deposition rates to vehicle surfaces included in the kinetic model.

Reaction	**Rate (cm^6 s^{-2}, cm^3 s^{-1} or s^{-1})**	**Comment or reference**
$O_3 + h\nu \rightarrow O + O_2$	0 (midnight), ≤ 2.3×10^{-8} (midday and sunset)	2.3×10^{-8} s^{-1} was measured indoors in direct sunlight in Table S5 of a different study [26] (values are likely to be lower as the inside of the car will not be in direct sunlight). Model results are insensitive at all values ≤ 2.3×10^{-8} s^{-1}.
$O + O_2 (+ M) \rightarrow O_3 (+ M)$	1.4×10^{-14}	IUPAC recommended value
$NO + O_3 \rightarrow NO_2 + O_2$	1.9×10^{-14}	IUPAC recommended value
$NO_2 + h\nu \rightarrow NO + O$	0 (midnight), ≤ 1.4×10^{-4} (midday and sunset)	1.4×10^{-3} s^{-1} was measured indoors in direct sunlight in Table S10 of a different study [26] (values are likely to be lower as the inside of the car will not be in direct sunlight. The transmission through car windows may also be different. Therefore, the value

		was divided by at least a factor of 10). NO_2 decay rates are insensitive at all values ≤ 1.4×10^{-4} s^{-1}.
$O_3 + NO_2 \rightarrow NO_3 + O_2$	3.5×10^{-17}	IUPAC recommended value
$NO_2 + NO_3 (+ M) \rightarrow N_2O_5 (+ M)$	3.5×10^{-12}	IUPAC recommended value
$N_2O_5 (+ M) \rightarrow NO_2 + NO_3 (+ M)$	6.9×10^{-2}	IUPAC recommended value
$N_2O_5 + H_2O \rightarrow 2HNO_3$ (on surfaces)	Varied	So far not sensitive in the model
O_3 + 6-MHO → Products	4.3×10^{-16}	EPIWIN
O_3 + Geranyl acetone → Products	8.6×10^{-16}	EPIWIN
O_3 + Isoprene → Products	1.3×10^{-17}	EPIWIN
O_3 reaction with gas-phase VOCs or deposition to car surfaces	3.0×10^{-3} (first order loss rate from the gas-phase).	It is known that ozone will react with indoor surfaces
NO_2 deposition to car surfaces with a certain yield of NO	1.5×10^{-3} (first order loss rate from the gas-phase). NO yield was set to 0.4 - 1 as this gave the best fit to the data	There are papers that suggest that one of the products of NO_2 deposition to surfaces is NO (e.g. [22])

$CO + OH \rightarrow CO_2 + H$	2.1×10^{-13}	IUPAC recommended value
$H + O_2 \rightarrow HO_2$	1.0×10^{-12}	IUPAC recommended value
$HO_2 + NO \rightarrow NO_2 + OH$	8.5×10^{-12}	IUPAC recommended value
$OH + NO_2 \rightarrow HNO_3$	3.0×10^{-11}	IUPAC recommended value
$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	1.6×10^{-12}	IUPAC recommended value
$H_2O_2 + h\nu \rightarrow OH + OH$	0 (midnight), $\leq 1.4 \times 10^{-7}$ (midday and sunset)	1.4×10^{-7} s^{-1} was measured indoors in direct sunlight in Table S5 of a different study [26] (values are likely to be lower as the inside of the car will not be in direct sunlight). Model results are insensitive at all values $\leq 1.4 \times 10^{-7}$ s^{-1}.
$H_2O_2 + OH \rightarrow HO_2 + H_2O$	1.7×10^{-12}	IUPAC recommended value