Supporting Information for "The London Hybrid Exposure Model (LHEM): Improving human exposure estimates to NO_2 and $PM_{2.5}$ in an urban setting"

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Appendix A. Deriving weighting factors for the London Travel Demand Survey (LTDS) (Provided by David Wilby, Statistical Analyst, TfL)

The objective of the weighting process is to derive expansion factors, which weight the LTDS dataset to the Greater London population (see Section 2.1). The weighting process currently considers the Greater London sample of households, with the top 1% removed to avoid the influence of outliers. In total 6 weights were derived and added to the final dataset used in the LHEM model:

Household weighting factors: First a weight was created for each household representing both the survey's sampling rate and response rate. The next step was to adjust the expansion factors to give an even distribution of households across the days of the week and then a weight was created to represent estimates of the household structure by London borough. The household structure was taken from GLA midyear estimates, (https://www.london.gov.uk/sites/default/files/update-04-2015-2014rnd-trend-proj-methodology.pdf) and all weights were provided by TfL as part of the survey output.

Person weighting factors: Building on the capped and rescaled household weights, the person sample was aggregated by gender and age, and weighted to match population estimates of gender and age by borough. Analysis was also undertaken to check that the weighted data reflects the population size and composition in each borough. Both household and person weights were finally adjusted to account for the effect of school terms.

Appendix B. Illustrative video of the LTDS data & exposure results

http://www.londonair.org.uk/Research/lhem_pm25_animation/

Appendix C. Output from the CMAQ-urban model for Great Britain

Figure S1 provides a picture of the output, from the CMAQ-urban model, of annual average NO_2 across Great Britain. The CMAQ model was run hourly for 2011, at 10km x 10km grid resolution, with the ADMS roads model providing hourly air pollution predictions at 20m x 20m within urban areas and close to major roads between urban areas. Whilst only NO_2 is provided the model also predicts PM components in three size bins which are combined to give estimates of $PM_{2.5}$ and PM_{10} mass, as well as NO_X and Ozone. Finally, the hourly model output has been summarised as an average hour of the day for each 20m grid location, encompassing both the long term nature of the exposure estimates made with LHEM, whilst recognising the need to account for the time of travel during the day.

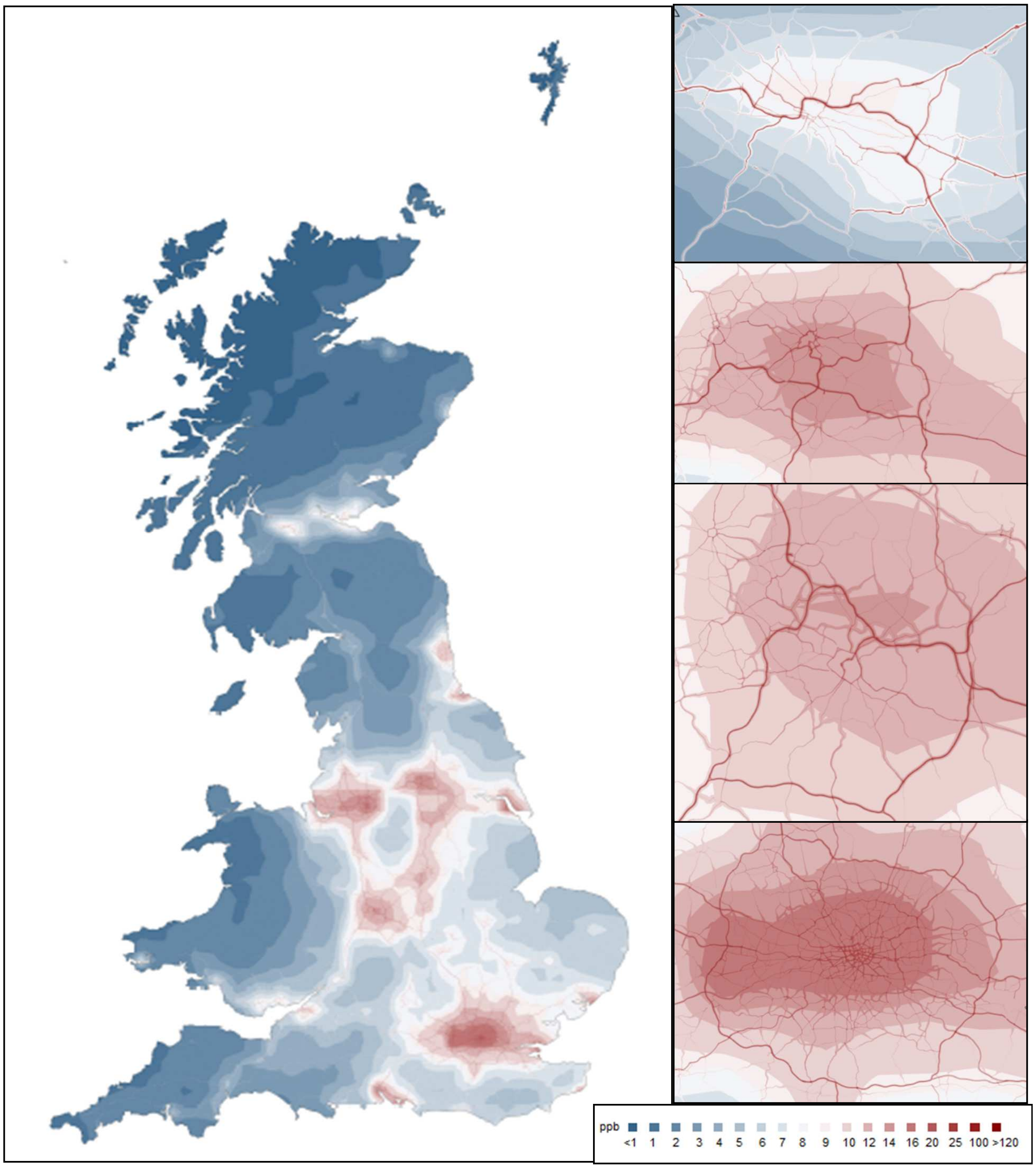

Figure S1. Example NO_2 air pollution predictions from the CMAQ-urban model. Within urban areas and along major roads the CMAQ-urban model predictions are at 20 x 20m grid resolution. In rural areas the grid resolution is 10 x 10 km.

Appendix C1. CMAQ-Urban air quality model evaluation

The source of outdoor air quality concentrations in the LHEM is the CMAQ-Urban model, described elsewhere by Beevers et al.[1] and providing average hour of the day outdoor air pollution concentrations throughout Great Britain, the latter being required since individuals often travel beyond London. Here, CMAQ-Urban 2011 annual average NO_2 and $PM_{2.5}$ have been evaluated using the protocols described in Derwent et al.[2] against up to 89 monitoring stations across Great Britain (see Table S1). In addition, since human exposure has been estimated by hour of the day, we have also included diurnal profiles for three different measurements site types: roadside, (including kerbside) for sites within 5m of a road, urban background (including suburban) for sites within urban areas but beyond the influence of individual local sources, and rural sites, for those outside urban areas (see Figure S2).

Table S1. Model evaluation statistics for CMAQ-urban predictions of outdoor NO_2 and $PM_{2.5}$ concentrations in the UK

Species	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
NO_2	89	1.00	0.5	3.7	0.03	0.18	4.9	0.90
$PM_{2.5}$	66	1.00	-1.4	2.2	-0.10	0.15	2.6	0.77

The CMAQ-urban model is able to predict NO_2 concentrations well across the UK and with an r value of 0.9, is able to explain 81% of the measured variability. There is a small normalised mean bias (NMB) of 3%, although as seen in Figure S2, the model tends to over predict the diurnal variation of average NO_2, especially at roadside sites and over predicts rural concentrations throughout the day.

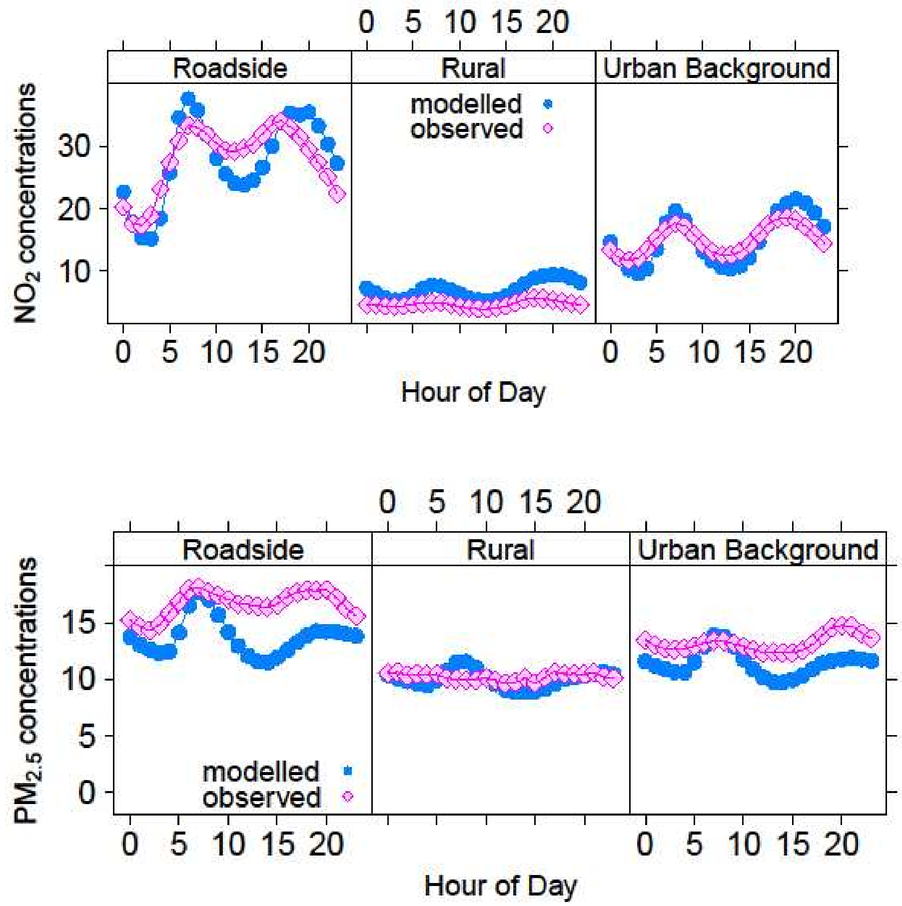

Figure S2. Modelled vs Observed hour of day average NO_2 (ppb) and $PM_{2.5}$ ($\mu g\ m^{-3}$) outdoor concentrations at UK monitoring sites.

Annual average $PM_{2.5}$ concentrations are also reasonably well predicted with the r values of 0.77 and an NMB value of -0.1 (see Table S1) and whilst rural diurnal $PM_{2.5}$ concentrations are also reasonably well predicted, the model shows a greater diurnal variation in concentrations than shown by the measurements. This is particularly the case for roadside sites where, despite predicting the early morning peak concentration well, the afternoon and evening periods are under-predicted meaning that the exposure impacts of road transport modes, walking and cycling will be under-predicted for $PM_{2.5}$.

Appendix D. Indoor/Outdoor ratios

There are important differences between the postcode-averaged $PM_{2.5}$ I/O ratios (Figure 1), which fall within a range of 0.35 to 0.86, and those for NO_2 (Figure S3), which fall between the range 0.11 to 0.59. The differences are mainly due to the assumptions regarding pollutant behaviour. $PM_{2.5}$ was modelled with a deposition rate of 0.19 h^{-1} and with a penetration factor of 0.8 when windows were closed and 1.0 when they were open[3], the latter representing a small fraction of all hours when internal temperatures exceeded a specified threshold. In contrast NO_2 was modelled with a deposition rate of 0.87h^{-1} and a penetration factor of 1.0 at all times[4]. The lack of penetration factor and higher deposition rate for NO_2 results in a lower range of estimated I/O ratios than that predicted for $PM_{2.5}$.

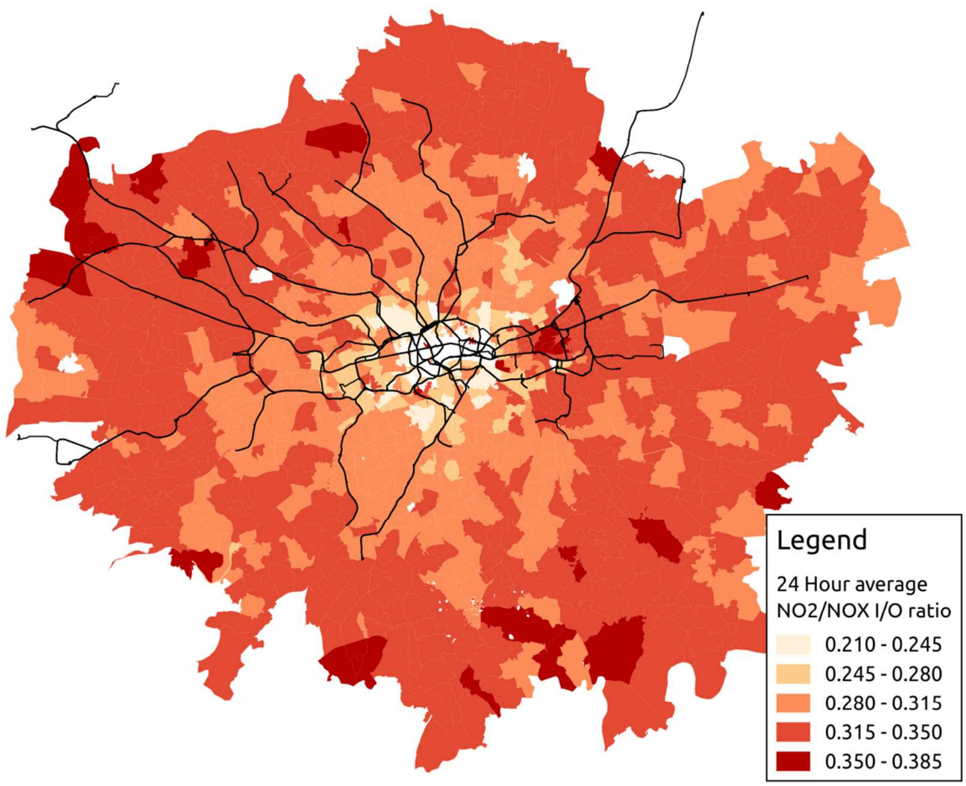

Figure S3. 24 hour average indoor to outdoor ratios (I/O) for NO_2 concentrations at each postcode in London

Appendix E. In-vehicle model assumptions and sensitivity tests

Equation 1 within the main manuscript describes a mass balance equation commonly used[5–7] to derive pollutant concentrations in enclosed environments. The mass balance equation is solved analytically. The general solution is given below (Equation 2) where $b = \lambda_{win} \cdot C_{out} + Q/V$, $a = \lambda_{win} + n\lambda_{HVAC} + V_g(A^*/V)$ and the subscript 0 denotes the initial conditions.

$$C_{in} = \left(C_{in_0} - \frac{b_0}{a_0}\right) \cdot \exp(-a \cdot t) + \frac{b}{a} \qquad (1)$$

Values for the characteristics (volumes, surfaces, numbers of people) of each vehicle type (bus, car, train etc.) are used in the in-vehicle exposure module of the LHEM (Table S2). The velocities with which pollutants are deposited on vehicles' surfaces are adopted from the values used in INDAIR model[8] that is 1.8 10^{-4} ms^{-1} for $PM_{2.5}$ and 1.2 10^{-4} ms^{-1} for NO_2 in the base case calculations and 8.6 10^{-4} ms^{-1} for $PM_{2.5}$ and 2.4 10^{-4} ms^{-1} for NO_2 in the sensitivity test run number 4.

The air exchange rates for cars/taxis are taken from published studies[9,10] and assume semi-opened windows, with the air-conditioning off, resulting in values of 2.8 h^{-1} while stationary and 30.3 h^{-1} during the journey. The air exchange rates used for buses and coaches between stops was taken as 1.25 h^{-1}, and at stops was 24 h^{-1}. These are similar to other in-vehicle studies [6]. In the case of train trips, an average air exchange rate of 5.2 h^{-1} was assumed through the mechanical ventilation system[11] between stops, and 10 h^{-1} at stops (to reflect door opening). For simplicity, the number of people between two stops and active passengers at each stop is assumed constant throughout a journey (Table S2).

The re-suspension rates per person for $PM_{2.5}$ has been adopted from current literature[12], and for people walking indoors was assumed to be 0.71 and 1200 µg $ac.no^{-1}$ h^{-1} whilst moving and at stops.

Table S2. LHEM vehicle characteristics.

Transport mode	Area (m^2)/ Volume (m^3) (per car/coach)	Number of passengers/ active people (per car/coach)	Number of passengers/ active people for sensitivity test 3 (per car/coach)
Car/van/taxi	0.7/2.5	-	-
Coach/school bus	30/66	50/0	50/0
Dial a ride	7.7/15.5	30/0	30/0
Public bus	57/105	50/10	87/20
Train	62/224	40/10	40/20
DLR	74/260	70/30	140/60
Tram	17/60	30/10	30/10

Appendix F. LHEM exposure relationships

It is important to understand whether the journeys undertaken in the LTDS survey are part of people's daily routine or are unusual, for example, going on holiday, and whether this effects the pollutant correlation discussed in Section 3.3. To do this the LHEM exposure scatter plots in Figure 4 of the main manuscript have been split by whether individuals took 'fewer' (pink), 'more' (cyan) or a their 'usual' (purple) number of journeys in a day (Figure S4), with the 'missing' (green) category included, where there was no response to this question. For the times that this question was answered, all show similar relationships to that of the right panel of Figure 4 in the main manuscript.

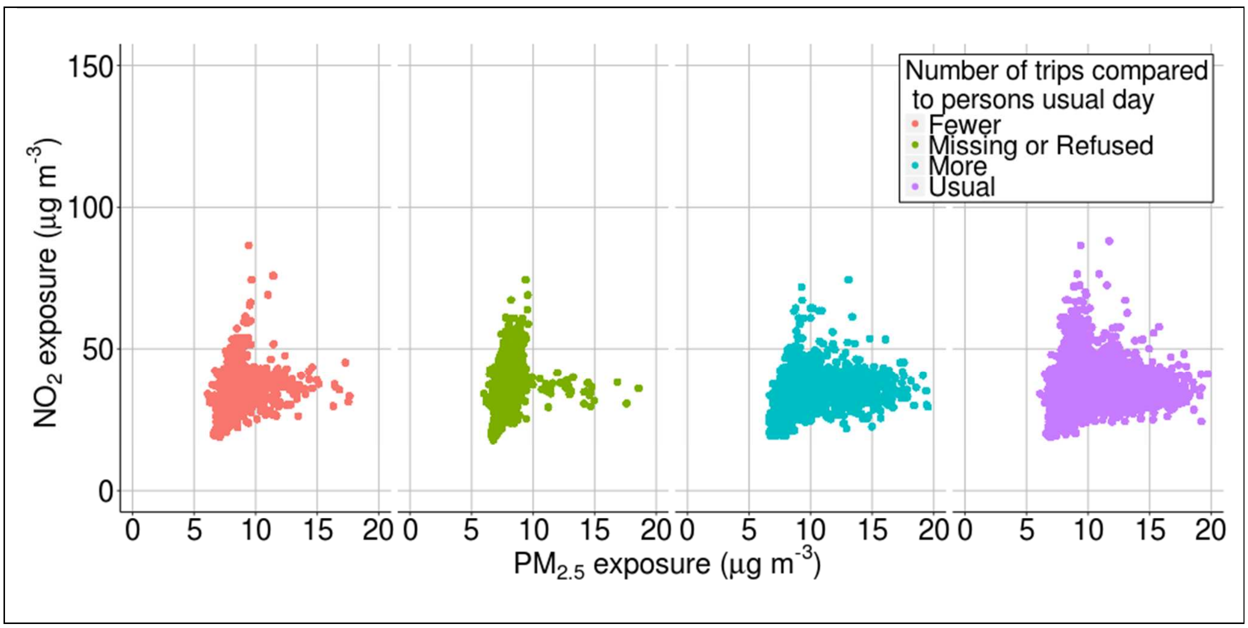

Figure S4. The relationship between the daily mean $PM_{2.5}$ vs. NO_2 exposure estimated using the LHEM model, split by normal number of trips

Appendix G. Microenvironments

Mean concentrations (and range) for each microenvironment output from CMAQ-Urban, the I/O ratios, and the in-vehicle model.

Table S3. Concentrations within microenvironments

Microenvironment	$PM_{2.5}$ (µg m^{-3}) (mean, range)	NO_2 (µg m^{-3}) (mean, range)
Walk	13.7 (6.4 – 40.5)	44.8 (2.9 – 372.1)
Cycle	15.1 (9.2 – 38.3)	55.3 (12.6 – 298)
Motorcycle	16.9 (9.1 – 43.0)	75.0 (11.4 – 348)
Driving	14.6 (6.0 – 53.7)	57.2 (1.8 - 404)
Bus	14.5 (5.0 – 44.0)	58.2 (7.8 - 364)
Underground & DLR	91.5 (5.3-94.0)	57.6 (9.3 – 261)
Train	13.5 (5.6 – 33.4)	40.4 (2.6 – 252.7)
Indoor	7.9 (3.1 – 26.0)	10.9 (0.5 – 75.4)
Outdoor	13.6 (5.9 – 54.0)	35.7 (2.0 – 406.0)

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