Supplementary File 1 –
KCLurban model description, evaluation and outputs

Model summary

The KCLurban model used a kernel modelling technique, based upon the ADMS[1,2], to describe the initial dispersion from each emissions source. The contribution from each source has been summed onto a fixed 20m x 20m grid across London assuming that one can calculate the contribution of any source to total air pollution concentrations by applying each kernel and adjusting for the source strength. The kernels were produced using an emissions source of unity, either 1 g s^{-1} (point and jet sources), 1 g m^{-3} s^{-1} (volume sources) or a 1 g km^{-1} s^{-1} (road sources) and hourly meteorological measurements from the UK Meteorological Office site at Heathrow. Data from the Heathrow site is recorded at a height of 10 metres and includes measurements of temperature, wind speed, wind direction, precipitation, relative humidity and cloud cover. The KCLurban model used emissions from the London Atmospheric Emissions Inventory (LAEI)[3] and for road traffic emissions using King's well established emissions modelling methods, combined with emissions factors from the UK specific roadside measurements of Carslaw[4] and for non-exhaust emissions, based upon the work of Harrison[5].

Treatment of sources in KCLurban

To predict air quality concentrations in London the KCLurban model sums together three source categories. First, for rural sources outside the model domain, use was made of rural NO_X, PM_{10}, $PM_{2.5}$ and monthly OX (NO_2 + O_3), measurements taken from a combination of Harwell, Rochester Stoke and Maidstone monitoring sites, part of the UK AURN network (http://uk-air.defra.gov.uk/data/). Second, within the model domain, but greater than 500m from a receptor location, London sources were represented as shallow volumes of 1x1 km horizontal dimension and 2m vertically for road traffic, and 50m vertically for other sources. Because emissions from biomass burning are not well represented in the London emissions inventory an additional 1.05 µg m^{-3} of PM was also included, based upon the work of Fuller[4]. Third, for those sources within 500m of a receptor location, a detailed treatment of road/rail/aircraft and gas combustion sources was used.

Sources within the KCLurban model include: road transport (exhaust and non-exhaust), large regulated industrial processes, small regulated industrial processes, large boiler plant, gas heating (domestic and industrial-commercial), oil combustion sources (domestic and commercial), coal combustion sources (domestic and commercial), agricultural and natural sources, rail, ships, airports and others (sewage plant etc). In modelling the emissions from large industrial processes use was made of emissions data and stack conditions (height, temperature, volume flow rate) for each source.

Representing road sources

Within 500m of a road, where strong concentration gradients exist, a highly detailed treatment of road sources is required. In KCLurban we modelled road emissions as a series of road links 10 m long and based on geographically accurate Ordnance Survey road map data. To reflect the important separation of two or more lanes of traffic, on large roads/motorways, each side of the road was modelled separately. Six road categories (and associated kernels) were used in London, including open roads (motorway), typical roads (average urban roads surrounded by low rise buildings) and 4 types of street canyon (classified by their orientation: north-south, east-west, southwest-northeast and southeast-northwest). The "typical roads" had a road width of 20m and a building height of 10m and "street canyons" had a width of 30m and a building height of 25m. The "street canyon" width and height details were manually sampled from the 3D building model in London http://www.casa.ucl.ac.uk/news/newsStory.asp?ID=80. There are approximately 2.25 million 10m road sources in the KCLurban model.

Representing railway sources

Railway sources were treated in much the same way as for roads, i.e. by using the rail network emissions broken into 10m sections. Whilst trains in London are predominantly electric, the line running west from Paddington station and the line running north from St Pancras station includes many diesel trains and represents a significant source of NO_X and PM emissions. For diesel trains, the emissions release height was taken to be 5m and the NO_2/NO_X exhaust ratio was assumed to be similar to large HGVs at 13%.

Representing gas combustion sources

Gas combustion is a very important source of NO_X in London[3], and in the KCLurban model a detailed representation of the height of release, spatial distribution of gas sources and temporal change in emissions throughout the year has been included. Through analysis of the 3D model of buildings in London (http://www.casa.ucl.ac.uk/news/newsStory.asp?ID=80) the height of release from gas sources was varied from 1m (domestic housing), through 30m for small commercial premises to 75m for large commercial office buildings. Gas heating sources were represented spatially by points located at 50m intervals throughout the minor road network and set back from the road by 20m, assuming that the majority of buildings follow the road network. Model kernels representing the varied release conditions from these sources were then applied to domestic and commercial gas emissions summarised in 1 x 1km grids across London. Finally, a detailed treatment of the emissions variation by hour of the day and month of the year was included in the model and was based upon UK gas use statistics (http://www.decc.gov.uk/en/content/cms/statistics/energy_stats/source/gas/gas.aspx).

Representing Heathrow airport

At Heathrow airport, emissions from aircraft during approach, landing, taxi out, taxi in, hold, take off, initial climb and climb out were represented using the same method as for roads, i.e. as individual sources 10m apart. Auxiliary Power Unit (APU) emissions and engine testing on the airport were

represented as stationary point sources. Other sources such as heating plant, public and staff car parks, car rental, taxis queues and fire training ground emissions were represented horizontally as volume sources of 1 x 1 km, 50m high, and for airside vehicles 2m high.

Takeoff is the aircraft mode that provides one of the largest contributions to ground-level NO_X and PM concentrations. During takeoff each accelerating aircraft engine was represented by horizontal stationary jet sources at 10 m intervals along the runway, from the start of the ground-roll to where the aircraft leaves the ground. The effect of accelerating aircraft was included to reflect the maximum emission close to the start of the ground-roll, thereby reproducing the steep emission gradient along the runway.

Of importance in estimating ground level concentrations from Jet plumes is their rapid change in temperature and velocity over short distances, as well as the effect of aircraft speed. By comparing modelled and measured data close to Heathrow airport we showed that buoyant jet plumes could be accurately modelled by varying the jet release temperature assumptions. The hourly variation of aircraft emissions was reproduced using aircraft movements made available by the UK Civil Aviation Authority. Jet velocities were varied for the different aircraft operational settings of take off, approach and taxiing and were assumed to be 85 %, 30 % and 7 % of full thrust, respectively. Finally, account was taken of the rapidly reducing effect of aircraft emissions to ground level concentrations at different aircraft heights. The aircraft NO_2/NO_X emissions ratio was assumed to be 11%.

Predicting NO_2 and O_3 concentrations

The method for converting NO_X to NO_2 used the well established relationships of Carslaw et al[6] and was based upon an analysis of measurements at both background and roadside sites, included the influence of NO_2 emitted directly from the vehicle exhaust. O_3 concentrations were predicted through methods described in Clapp and Jenkins[7], combined with knowledge of monthly OX entering London, and taken from the Harwell monitoring site, the model's predictions of NO_2 and at roadside the magnitude of primary NO_2 emitted from vehicle exhausts.

KCLurban model evaluation

The KCLurban model is well established for use in public health research[8] and has been submitted to the UK Model Inter-comparison Exercise, run by King's on behalf of DEFRA (http://uk-air.defra.gov.uk/library/reports?report_id=777). To understand the annual performance of the KCLurban model predictions, an evaluation process has been undertaken against fixed site measurements from the London Air Quality Network (LAQN) and Defra's Automatic Urban and Rural Network (AURN) covering all the years from 2003 to 2010. This has been based upon our extensive experience of model evaluation, including King's participation in both phases of the UK Model Inter-comparison Exercise, run by King's on behalf of DEFRA (http://uk-air.defra.gov.uk/library/reports?report_id=777).

For NO_x and NO_2, modelled data has been evaluated against measurement data from monitoring sites with an annual data capture rate of > 75 %. This has resulted in a minimum of 62 site comparisons in 2003 and a maximum of 100 comparisons in 2008 (Table 2, Figure 5 and Figure 6). For both pollutants, a strong linear relationship is observed between the variables and high correlation coefficients were found for both NO_x (varying between 0.79 in 2009 and 0.92 in 2008) and NO_2 (varying between 0.85 in 2009 and 0.93 in 2008). Additionally, for both pollutants the normalised mean gross error (NMGE) is relatively low and for NO_X has a maximum of 23% in 2010 and for NO_2 has a maximum of 16% in 2007. The KCLurban model exhibits little overall bias for NO_2 predictions, with the normalised mean bias (NMB) varying between – 8.5 % in 2003 and 6.8 % in 2007, although a small but consistent under prediction of NO_x concentrations is observed: NMB varies between –4.9 % in 2004 and -15.4 % in 2003.

Modelled PM_{10} concentrations have been evaluated against measurements from a minimum of 49 monitoring sites in 2003 and a maximum of 76 sites in 2008, all of which have a data capture rate of > 75 % (Table 2, Figure 7). The correlation coefficient, r, for PM_{10} concentrations indicates a reasonably strong agreement, varying between 0.65 in 2007 and 0.85 in 2005. Overall NMGE in the modelled concentrations is low varying between 7.9 % in 2003 and 13.5 % in 2007, and broadly comparable to that observed for NO_2. The KCLurban model exhibits little bias in predicting PM_{10} concentrations with NMB varying between -0.87 % in 2003 and 6.8 % in 2006.

There are significantly fewer measurements of $PM_{2.5}$ than for other pollutants within London. As a result $PM_{2.5}$ concentrations have been evaluated against measurements from a minimum of only 4 monitoring sites in 2003 and a maximum of 21 sites in 2009, all of which have a data capture rate of > 75 % (Table 2, Figure 8). It is prudent therefore not to over interpret the results for some years. The NMGE varies between 11 % in 2008 and 42 % in 2003 (n=4)), NMB varies between 0.19 % in 2008 and 42.1 % in 2003 (n=4) and the correlation coefficient, r varies between 0.26 in 2010 and 1 in 2004 (n=5) is also not as consistently strong as for NO_X, NO_2 and PM_{10}. It is also important to note that a transition between TEOM based measurements to TEOM-FDMS machine has occurred in a piecemeal way during the period between 2003 and 2010. Whilst the FDMS instruments do not suffer nitrate loss, they are more complex to run and once again add a level of uncertainty to the observations which does not exist for PM_{10}, NO_X, NO_2 or O_3.

There are fewer measurements of O_3, with a minimum of 24 monitoring sites in 2003 and a maximum of 37 sites in 2007, all of which have a data capture rate of > 75 % (Table 2, Figure 9). The NMGE varies between 9.2 % in 2007 and 22.1 % in 2010, the NMB varies between -11.5 % in 2003 and 21.7 % in 2010 and the value of r between measured and modelled concentrations varies between 0.79 in 2005 and 0.89 in 2009 and is broadly comparable to that observed for NO_X.

Table 2. Values of the spearman correlation coefficient (r), root mean square error (RMSE), normalised mean gross error (NMGE) and normalised mean bias (NMB) for observed vs. modelled annual average concentrations for each of the years between 2003 and 2010

Year	Pollutant	Number of monitoring sites (n)	Normalised mean bias (NMB)	Normalised mean gross error (NMGE)	Root mean square error (RMSE)	Spearman correlation coefficient (r)
2003	NOx	62	−0.154	0.21	18	0.88
2004	NOx	70	−0.049	0.19	17	0.91
2005	NOx	84	−0.108	0.2	21	0.88
2006	NOx	85	−0.136	0.21	21	0.86
2007	NOx	90	−0.069	0.2	18	0.88
2008	NOx	100	−0.120	0.2	18	0.92
2009	NOx	96	−0.091	0.23	22	0.79
2010	NOx	87	−0.132	0.23	22	0.86
2003	NO_2	62	−0.085	0.13	4.7	0.9
2004	NO_2	70	0.018	0.12	5.2	0.92
2005	NO_2	84	−0.015	0.13	6.1	0.91
2006	NO_2	85	−0.049	0.13	6.1	0.91
2007	NO_2	90	0.068	0.16	6	0.9
2008	NO_2	100	−0.011	0.13	5.1	0.93
2009	NO_2	96	0.031	0.15	5.5	0.85
2010	NO_2	87	−0.014	0.14	5.8	0.89
2003	PM_{10}	49	−0.0087	0.079	4	0.71
2004	PM_{10}	59	0.0604	0.124	4.6	0.76
2005	PM_{10}	62	0.0391	0.095	3.5	0.85
2006	PM_{10}	73	0.0068	0.111	5.2	0.73
2007	PM_{10}	70	0.0441	0.135	5.8	0.65
2008	PM_{10}	76	−0.0067	0.104	4.1	0.78
2009	PM_{10}	74	0.0418	0.117	3.7	0.78
2010	PM_{10}	68	0.0415	0.13	4.2	0.71
2003	$PM_{2.5}$	4	0.4207	0.42	6.9	0.97
2004	$PM_{2.5}$	5	0.3474	0.35	5.2	1
2005	$PM_{2.5}$	9	0.2143	0.26	3.9	0.67
2006	$PM_{2.5}$	9	0.1533	0.18	2.8	0.84
2007	$PM_{2.5}$	14	0.0431	0.12	2.1	0.82
2008	$PM_{2.5}$	15	0.0019	0.11	2	0.74
2009	$PM_{2.5}$	21	0.104	0.15	2.8	0.59
2010	$PM_{2.5}$	20	0.0157	0.15	2.8	0.26
2003	O_3	24	−0.115	0.124	2.7	0.87
2004	O_3	25	−0.033	0.095	2	0.82
2005	O_3	29	−0.019	0.095	2	0.79
2006	O_3	29	−0.047	0.095	2.2	0.81
2007	O_3	37	0.053	0.092	1.9	0.87
2008	O_3	36	0.086	0.103	2.3	0.87
2009	O_3	34	0.138	0.148	2.8	0.89

2010	O_3	32	0.217	0.221	4	0.85

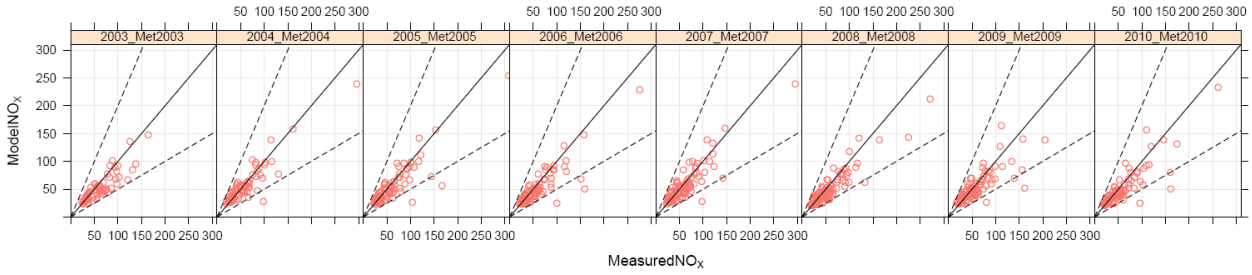

Figure 5 Scatter plots of annual average modelled vs. measured NO_X concentrations (µg m^{-3}) for 2003 to 2010

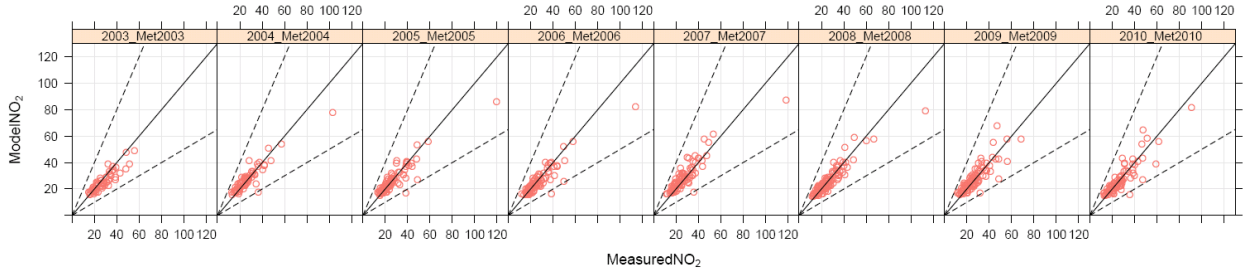

Figure 6 Scatter plots of annual average modelled vs. measured NO_2 concentrations (µg m^{-3}) for 2003 to 2010

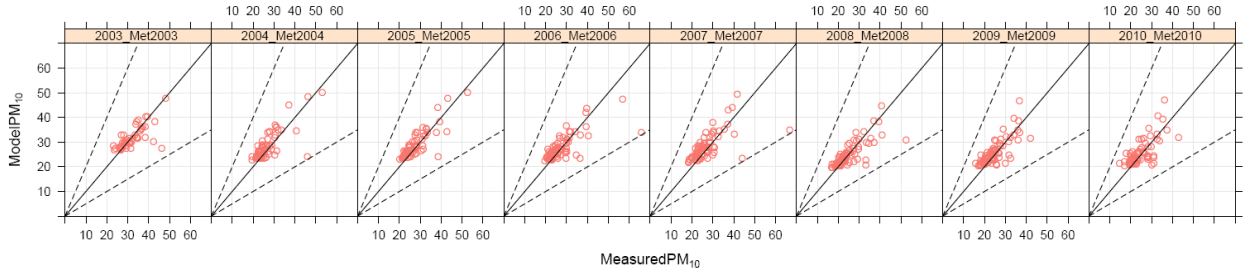

Figure 7 Scatter plots of annual average modelled vs. measured PM_{10} concentrations (µg m^{-3}) for 2003 to 2010

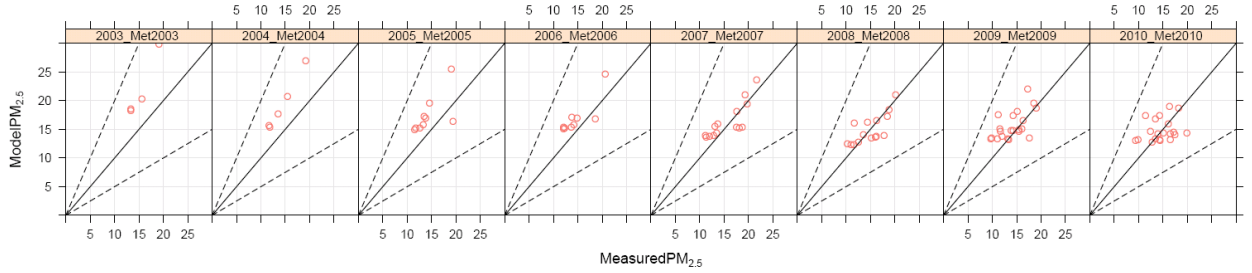

Figure 8 Scatter plots of annual average modelled vs. measured $PM_{2.5}$ concentrations (µg m^{-3}) for 2003 to 2010

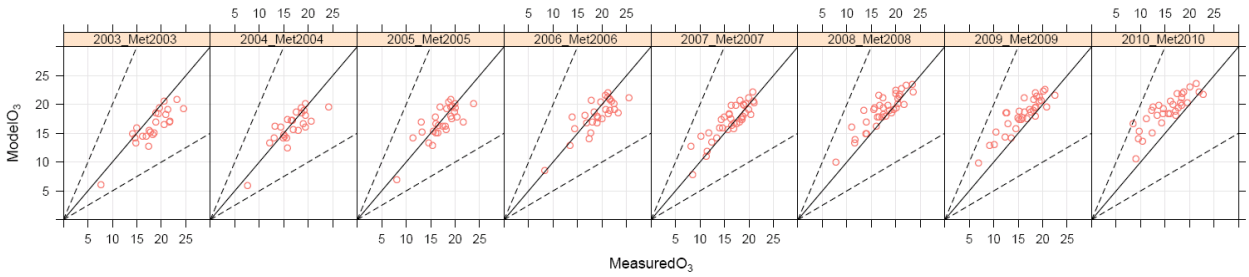

Figure 9 Scatter plots of annual average modelled vs. measured O_3 concentrations (µg m^{-3}) for 2003 to 2010

KCLurban's example model results

This section provides graphical examples of the outputs produced by the KCLurban model. Figure 10 illustrates mapped concentrations of NO_2 for the London area up to and including the M25 in the year 2008. The map highlights the importance of road traffic as a source of air pollution. London's major roads are plainly visible and in the majority of cases, the highest concentrations are predicted at, or immediately adjacent to, these major roads. Central London is also highlighted as a problem area. The concentrations in central London are amongst the highest in London and reflect the high density of emission sources. Heathrow airport to the west of the city is also clearly visible, as is the Paddington railway line (running due west from central London).

The KCLurban model outputs have subsequently been manipulated to produce concentrations at postcode level. Figure 11 shows postcode address centroid annual mean NO_2 concentrations, in the year 2008, interpolated from 20m grid model predictions using a bi-linear interpolation technique.

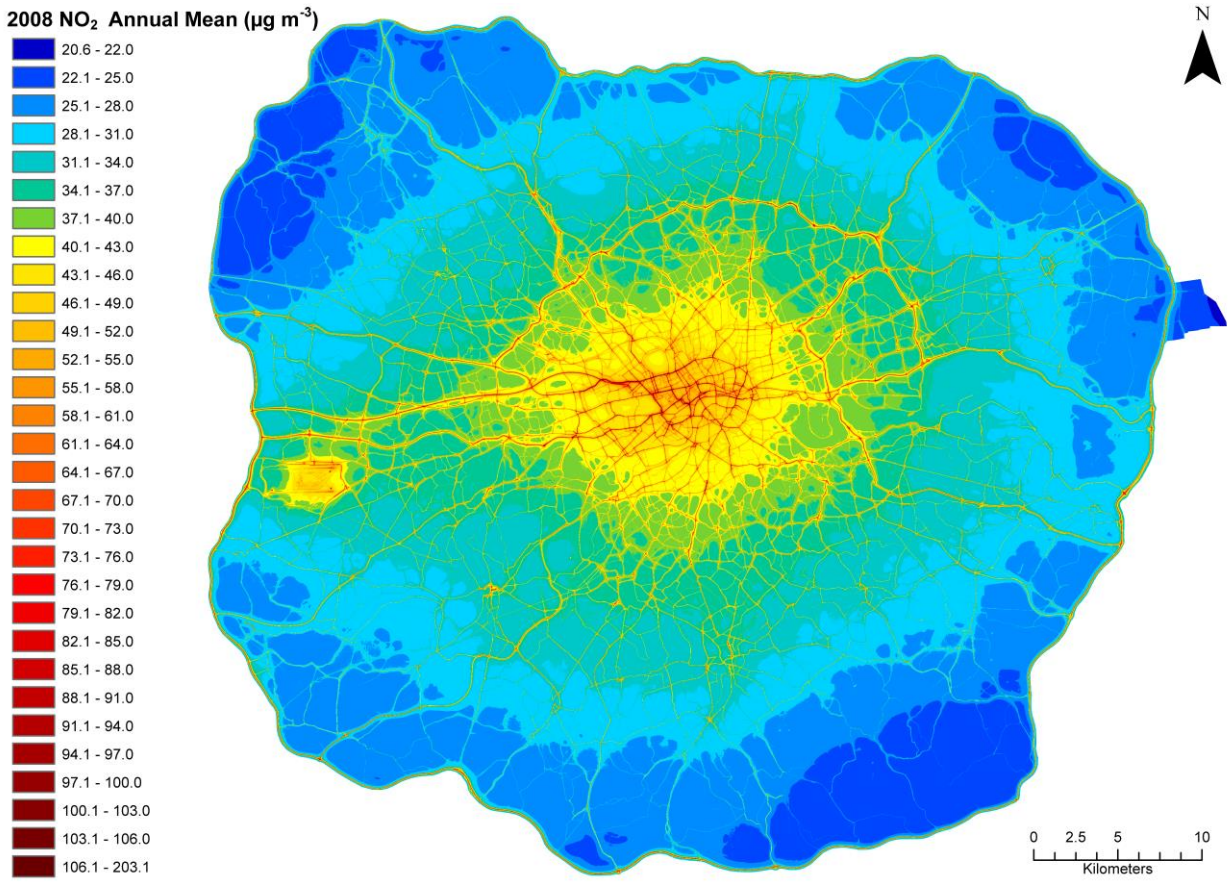

Figure 10 Annual mean NO_2 concentrations in 2008

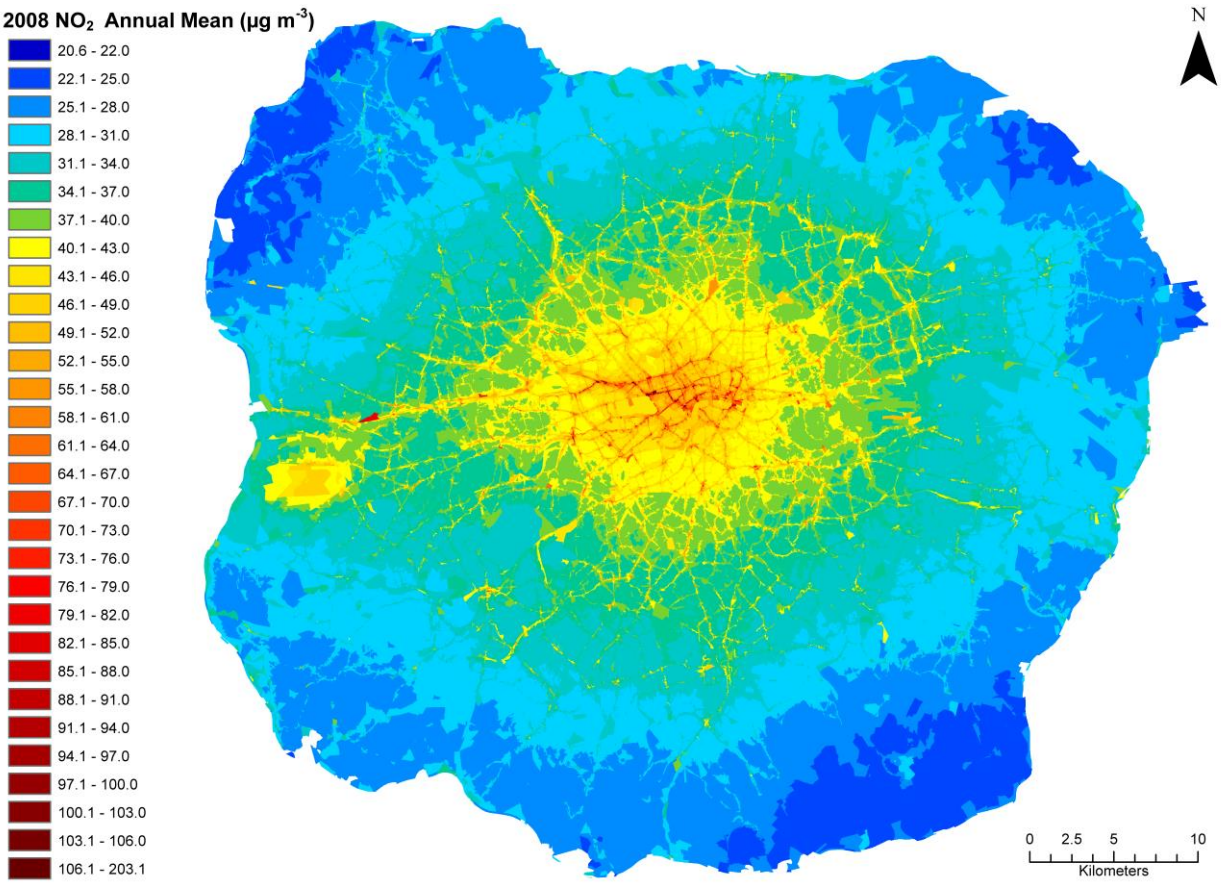

Figure 11 Annual mean NO_2 concentrations in 2008 at postcode address centroids

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