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Defra urban model evaluation analysis – Phase 1

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Executive summary

This report provides a summary of the evaluation of models used for the assessment of urban air quality. Specifically, this report considers the prediction of annual mean concentrations of NO_x, NO₂, O₃, PM₁₀ and PM_{2.5} for a large sample of measurements sites in London. In addition, the evaluation of hourly predictions is considered for a subset of models and receptor locations. The report focuses on a range of quantitative metrics commonly used for model evaluation together with a series of graphical comparisons that aim to reveal some of the characteristics of each model. While the comparisons are not exhaustive, they are presented in such a way as to easily allow further analysis by each modelling group. The principal aim of this report is to provide information to the *Air Quality Modelling Review Steering Group* to assist their deliberations concerning the future use of air quality models by Defra.

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Contents

1	Introduction	6
1.1	Document history	6
1.2	Background	6
1.3	Methods used	6
2	Data preparation	7
3	Analysis examples	8
3.1	Annual mean NO _x and NO ₂ concentrations	8
3.1.1	Relative Directive Error, <i>RDE</i>	17
3.2	Annual mean O ₃	19
3.3	Annual mean PM ₁₀	21
3.3.1	Relative Directive Error, <i>RDE</i>	25
3.4	Annual mean PM _{2.5}	26
4	Hourly analysis	30
4.1	Data preparation	30
4.2	Evaluation metrics	34
4.3	Scatter plots	39
4.4	Temporal variations	46
4.5	Conditional quantiles	49
A	Model performance evaluation statistics	56
A	Urban modelling receptor information	58

List of Figures

1	Scatter plot of measured versus predicted annual mean NO_x concentrations.	10
2	Graphical summary of FAC for each model by site type for NO_x	11
3	Graphical summary of mean bias for each model by site type for NO_x	11
4	Graphical summary of RMSE for each model by site type for NO_x	12
5	Graphical summary of the correlation coefficient, r , for each model by site type for NO_x	12
6	Scatter plot of measured versus predicted annual mean NO_2 concentrations.	14
7	Graphical summary of the FAC2 for each model by site type for NO_2	15
8	Graphical summary of the mean bias for each model by site type for NO_2	15
9	Graphical summary of the RMSE for each model by site type for NO_2	16
10	Graphical summary of the correlation coefficient, r , for each model by site type for NO_2	16
11	The RDE for annual mean NO_2 concentrations by group.	18
12	Measured vs. modelled annual mean O_3 concentrations for each model.	20
13	Measured vs. modelled annual mean PM_{10} concentrations for each model.	22
14	Graphical summary of FAC for each model by site type for PM_{10}	23
15	Graphical summary of mean bias for each model by site type for PM_{10}	23
16	Graphical summary of RMSE for each model by site type for PM_{10}	24
17	Graphical summary of the correlation coefficient, r , for each model by site type for PM_{10}	24
18	The RDE for annual mean PM_{10} concentrations by group.	25
19	Measured vs. modelled annual mean $\text{PM}_{2.5}$ concentrations for each model.	27
20	Graphical summary of FAC for each model by site type for $\text{PM}_{2.5}$	28
21	Graphical summary of mean bias for each model by site type for $\text{PM}_{2.5}$	28
22	Graphical summary of RMSE for each model by site type for $\text{PM}_{2.5}$	29
23	Graphical summary of the correlation coefficient, r , for each model by site type for $\text{PM}_{2.5}$	29
24	Scatter plot of measured vs. modelled NO_x concentrations using the CERC model.	39
25	Scatter plot of measured vs. modelled NO_x concentrations using the CERC queue model.	40
26	Scatter plot of measured vs. modelled NO_x concentrations using the KCL model.	41
27	Scatter plot of measured vs. modelled NO_2 concentrations using the CERC model.	42
28	Scatter plot of measured vs. modelled NO_2 concentrations using the KCL model.	43
29	Scatter plot of measured vs. modelled O_3 concentrations using the CERC model.	44
30	Scatter plot of measured vs. modelled O_3 concentrations using the KCL model.	45
31	Temporal variations in NO_x at the Shaftesbury Avenue site using the CERC model.	46
32	Temporal variations in NO_x at the Shaftesbury Avenue site using the KCL-CMAQ model.	47
33	Temporal variations in NO_x at the Greenwich Eltham site using the CERC model.	47
34	Temporal variations in NO_x at the Greenwich Eltham site using the KCL-CMAQ model.	48
35	Example of the use of conditional quantiles applied to the ADMS Urban model at London Bloomsbury for hourly NO_x concentrations. The blue line shows the results for a perfect model. In this case the observations cover a range from 0 to $700 \mu\text{g m}^{-3}$. The red line shows the median value of the predictions. The maximum predicted value is close to $700 \mu\text{g m}^{-3}$, which shows the range of predictions from the model is similar to that of the observations. The shading shows the predicted quantile intervals i.e. the 25/75th and the 10/90th. A perfect model would lie on the blue line and have a very narrow spread. There is still some spread because even for a perfect model a specific quantile interval will contain a range of values. However, for the number of bins used in this plot the spread will be very narrow. Finally, the histogram shows the counts of predicted values.	50

36	Conditional quantile plot for hourly NO_x concentrations across all sites.	51
37	Conditional quantile plot for hourly NO_2 concentrations across all sites.	52
38	Conditional quantile plot for hourly NO_2 concentrations across all sites.	53
39	Conditional quantile plot for hourly PM_{10} concentrations across all sites.	53
40	Conditional quantile plot for hourly $\text{PM}_{2.5}$ concentrations across all sites.	54

List of Tables

1	Summary model evaluation statistics for annual mean NO _x	9
2	Summary model evaluation statistics for annual mean NO ₂	13
3	Summary of the Maximum Relative Directive Error for annual mean NO ₂ by group (%).	17
4	Summary model evaluation statistics for annual mean O ₃	19
5	Summary model evaluation statistics for annual mean PM ₁₀	21
6	Summary of the Maximum Relative Directive Error for annual mean PM ₁₀ by group (%).	25
7	Summary model evaluation statistics for annual mean PM _{2.5}	26
8	Summary model evaluation statistics for hourly mean NO _x	35
9	Summary model evaluation statistics for hourly mean NO ₂	36
10	Summary model evaluation statistics for hourly mean O ₃	37
11	Summary model evaluation statistics for hourly mean PM ₁₀	38
12	Site/receptor details relevant to the urban modelling groups.	59
12	Site/receptor details relevant to the urban modelling groups.	60

1 Introduction

1.1 Document history

This document has had the following updates.

12th January 2011 Changed model name “BRUTO” to “BRUTAL”.

8th February 2011 Fixed scatter plots to ensure same scaling.

Added total number of data points ‘n’ to the summary statistics; useful to gauge whether sample sizes are large enough to draw meaningful inferences from.

Changed names used in hourly modelling to make it clearer what is modelled/measured.

Confirmed CERC-queue results were used correctly.

23rd February 2011 Added new section on conditional quantiles — [subsection 4.5](#).

24th February 2011 Added analysis on how well model performance compares with Directive requirements ([subsubsection 3.1.1](#) and [subsubsection 3.3.1](#))

15th April 2011 Changed name of models run by CERC, plus other mostly minor edits.

1.2 Background

This document will summarise the evaluation of air pollution models as part of Defra’s model evaluation exercise. Model evaluation can be a complex and time consuming task. The results presented in this report are focused on providing some input to the Defra Model Evaluation exercise. The performance statistics used here have mostly been guided by [Derwent et al. \(2010\)](#). [Dennis et al. \(2010\)](#) provide useful and more general framework for model evaluation. They distinguish between several types of evaluation:

Operational evaluation in which model predictions are compared with data in an overall sense using a variety of statistical measures;

Diagnostic Evaluation in which the relative interplay of chemical and physical processes captured by the model are analysed to assess if the overall operation of the model is correct;

Dynamic Evaluation in which the ability of the modelling system to capture observed changes in emissions or meteorology is analysed; and,

Probabilistic Evaluation in which various statistical techniques are used to capture joint uncertainty in model predictions and observations.

On this basis, the evaluation carried out here forms a small part of *operational evaluation* and to a lesser extent *diagnostic evaluation*. By the same token, considerably more in-depth analysis would be possible and perhaps desirable but that is currently beyond the scope of the Defra work.

1.3 Methods used

This document blends text with code in that the whole document must be ‘run’ to produce it. Each time a version of this documentation is produced, all the code is run at the same time to generate all the various outputs e.g. plots and tables. This process is described in [Leisch \(2002\)](#). There are several reasons for adopting this approach:

- It provides a good way of presenting and distilling a large amount of information; hopefully an advantage to the modelling steering group.

- Every plot, table or statistic is entirely reproducible by anyone. An up to date version of R and R package called **openair** is all that is required. The commands shown can be pasted into R and all the workings are shown in a logical sequence.
- The approach makes it much easier to deal with revised results from models. For example, if modelling groups discover a problem with their results, a new set of results can be analysed very quickly and all the plots, tables etc. updated accordingly. Account can be taken of such changes at the last minute.
- It is clear that this document can only show a limited amount of information given the number of modelling groups, receptor points and the wide range of analyses that could potentially be undertaken. However, by showing the commands used to carry out the analysis, the modelling groups can choose to undertake further more detailed analysis should they wish to.
- Finally, this approach is fully transparent. All the code and methods used in the analysis are open to scrutiny by anyone.

All the code used in this document is based on R and use is also made of existing functions in **openair** to help with the evaluation. Several new functions have also been written related to model performance statistics.

Where possible we have tried to use files and file names as directly supplied by the modelling groups, as this ought to make it easier for each group to understand exactly the data used in the evaluation. In some cases minor editing of these files was necessary e.g. to change column names. Where more major manipulation was necessary, this is shown in the document.

This document was produced using R version 2.13.0 and **openair** version 0.4-16.

2 Data preparation

Modelling includes NO_x , NO_2 , O_3 , PM_{10} $\text{PM}_{2.5}$. All predictions should be in $\mu\text{g m}^{-3}$ for annual means (for NO_x the results should be in $\mu\text{g m}^{-3}$ as NO_2). For the particle metrics it is assumed that gravimetric-equivalent predictions will be made. All the analyses in this report relate to 2008 i.e. emissions inventory and ambient measurements.

Details of the receptors etc can be found in [Appendix A](#). Note that for PM_{10} and $\text{PM}_{2.5}$ the measured concentrations are expressed gravimetrically using the Volatile Correction Model.

Note that once all the model results are available they will be compiled into a consistent data set and imported in a straightforward way. It is expected that all the data would be imported using a couple of lines of code.

First it is necessary to load **openair** and some additional functions to help with the evaluation, including ensuring that the times are displayed in GMT:

```
library(openair)
source("~/Projects/modelEvaluation/modStats.R")
## make sure all times are displayed in GMT
Sys.setenv(TZ = "GMT")
## set file paths
setwd("~/Projects/modelEvaluation/urban")
```

Next we import the measured data from a pre-prepared file.

```
urban.meas <- read.csv("urban_template_complete.csv", header = TRUE)
```

KCL have provided two sets of results. The first set uses their urban model for London using fixed assumptions about background concentrations external to London i.e. the *ERG Toolkit*. The second set uses the CMAQ model, which explicitly models all UK and European sources and thus does not rely on assumed background concentrations. The latter model results only include NO_x , NO_2 and O_3 . The ERG Toolkit is referred to as 'KCLurban' and the CMAQ-based modelling as 'KCLurbanCMAQ'.

Import the KCL data and merge with measurements:

```
KCLurban <- read.csv("urbanTemplate_KCL_final_Year2008.csv", header = TRUE)
KCLurban <- merge(KCLurban, urban.meas, by = c("id", "site.code", "easting", "northing", "site.type"))
## add model group name
KCLurban$group <- "KCLurban"
```

The KCL-CMAQ results:

```
KCLurbanCMAQ <- read.csv("urbanTemplate_KCLCMAQ_final_Year2008.csv", header = TRUE)
KCLurbanCMAQ <- merge(KCLurbanCMAQ, urban.meas, by = c("id", "site.code", "easting", "northing",
                                                    "site.type"))
## add model group name
KCLurbanCMAQ$group <- "KCLurbanCMAQ"
```

And the BRUTAL results:

```
BRUTAL <- read.csv("urbanTemplateV1.3_UKIAMBRUTAL_Data4MIP_01Dec10.csv", header = TRUE)
BRUTAL <- merge(BRUTAL, urban.meas, by = c("id", "site.code", "easting", "northing", "site.type"))
BRUTAL$group <- "BRUTAL"
```

The AEA pollution climate mapping (PCM) results:

```
PCM <- read.csv("pcm_urbanTemplateV1.3.csv", header = TRUE, na.strings = "N/A")
PCM <- merge(PCM, urban.meas, by = c("id", "site.code", "easting", "northing", "site.type"))
PCM$group <- "PCM"
```

The CERC results are imported as follows. Note that CERC produced two sets: the first where all hours of the year were modelled and the second where only hours where there were valid monitored values were available.

Note that there are some difficulties comparing the hourly models (CERC and KCL) with annual models. The annual models essentially assume that data capture rates are 100% because they cannot take account of partial years. Conversely, the hourly models can predict concentrations consistent with the measurements e.g. they could take account of missing hours in the wintertime. It is not possible therefore to ensure complete consistency in the comparisons. However, by choosing a relatively high data capture rate of 75% these issues are mitigated somewhat. The hourly models would however be expected to provide more representative predictions that allow a consistent comparison with the measurements.

```
ADMSUrban <- read.csv("urbanTemplateV13CERC(valid monitoring hours only).csv", header = TRUE)
ADMSUrban <- merge(ADMSUrban, urban.meas, by = c("id", "site.code", "easting", "northing", "site.type"))
ADMSUrban$group <- "ADMSUrban"
```

CERC (17 December 2010) have provided an additional set of results that aims to treat vehicle queuing. We refer to these results as ADMSUrban.queue.

```
ADMSUrban.queue <- read.csv("urbanTemplateV13(valid monitoring hours only)16Dec.csv", header = TRUE,
                           na.strings = c("x", "n/a"))
ADMSUrban.queue <- merge(ADMSUrban.queue, urban.meas, by = c("id", "site.code", "easting", "northing",
                                                            "site.type"))
ADMSUrban.queue$group <- "ADMSUrban.queue"
```

Now we can combine all the model results:

```
all.results <- rbind.fill(KCLurban, BRUTAL, PCM, ADMSUrban, KCLurbanCMAQ, ADMSUrban.queue)
```

3 Analysis examples

3.1 Annual mean NO_x and NO₂ concentrations

First we will extract the NO_x and NO₂ data and apply a data capture threshold.

Not every group predicted at every receptor, which could therefore introduce an inconsistency into the analysis. The code below therefore extracts receptors where all groups made a prediction.

```
nox.results <- subset(all.results, nox.count > 0.75 * 8784)
## extract only those results where all groups made a prediction
## sites where this is true
fullSites <- with(nox.results, tapply(N0x, site.code, function(x) length(na.omit(x))))
fullSites <- fullSites[fullSites == length(unique(nox.results$group))]
nox.results <- subset(nox.results, site.code %in% names(fullSites))
```

Model evaluation statistics can be estimated using the `modStats` function. Note that these statistics will be defined and explained later. These numerical summaries can easily be added to e.g. to provide means, 95th percentile values etc. In using the function below, it is supplied with the data (`nox.results`), the analysis type (statistics by site i.e. `type = "site"`), the modelled results column is called `"NOx"` and the observations column in this case is `"nox.meas"`.

```
noxStats <- modStats(nox.results, type = c("site.type", "group"), obs = "nox.meas", mod = "NOx")
```

Table 1: Summary model evaluation statistics for annual mean NO_x .

site.type	group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
kerbside	ADMSUrban	7	0.71	-73.70	80.76	-0.32	0.35	113.55	0.77
kerbside	ADMSUrban.queue	7	0.86	-53.63	60.69	-0.23	0.26	82.04	0.89
kerbside	BRUTAL	7	0.43	-129.15	129.96	-0.56	0.57	184.49	0.21
kerbside	KCLurban	7	0.86	-60.23	79.39	-0.26	0.35	106.88	0.75
kerbside	KCLurbanCMAQ	7	0.57	-57.86	72.36	-0.25	0.32	79.85	0.95
kerbside	PCM	7	0.86	-74.53	81.72	-0.32	0.36	119.02	0.77
roadside	ADMSUrban	30	1.00	-22.78	23.64	-0.17	0.18	27.94	0.94
roadside	ADMSUrban.queue	30	1.00	-14.29	18.89	-0.11	0.14	21.77	0.93
roadside	BRUTAL	30	1.00	-35.26	38.33	-0.27	0.29	46.10	0.79
roadside	KCLurban	30	0.93	-14.35	28.00	-0.11	0.21	41.47	0.61
roadside	KCLurbanCMAQ	30	0.87	-31.89	46.58	-0.24	0.35	59.96	0.63
roadside	PCM	30	0.97	16.20	41.68	0.12	0.32	50.06	0.42
suburban	ADMSUrban	11	1.00	-4.51	8.23	-0.09	0.16	9.20	0.45
suburban	ADMSUrban.queue	11	1.00	-4.51	8.23	-0.09	0.16	9.20	0.45
suburban	BRUTAL	11	1.00	-7.48	8.73	-0.15	0.17	9.87	0.62
suburban	KCLurban	11	1.00	-4.26	7.09	-0.08	0.14	8.18	0.52
suburban	KCLurbanCMAQ	11	1.00	-15.37	15.37	-0.30	0.30	17.23	0.36
suburban	PCM	11	1.00	-6.14	7.56	-0.12	0.15	9.17	0.59
urban background	ADMSUrban	29	1.00	5.62	14.64	0.08	0.21	18.14	0.79
urban background	ADMSUrban.queue	29	1.00	5.62	14.64	0.08	0.21	18.14	0.79
urban background	BRUTAL	29	0.93	-2.71	18.15	-0.04	0.25	25.35	0.33
urban background	KCLurban	29	1.00	1.43	10.66	0.02	0.15	13.70	0.80
urban background	KCLurbanCMAQ	29	0.97	-11.02	17.21	-0.15	0.24	22.91	0.66
urban background	PCM	29	0.97	-4.67	12.13	-0.07	0.17	17.73	0.65

```
scatterPlot(nox.results, x = "nox.meas", y = "NOx", type = "group", mod.line = TRUE,
            pch = 16, smooth = FALSE, group = "site.type", xlim = c(0, 550), ylim = c(0, 550))
```

```
scatterPlot(noxStats, x = "group", y = "FAC2", type = "site.type", key = FALSE, pch = 16, cex = 1.5)
```

```
scatterPlot(noxStats, x = "group", y = "MB", type = "site.type", key = FALSE, pch = 16, cex = 1.5)
```

```
scatterPlot(noxStats, x = "group", y = "RMSE", type = "site.type", key = FALSE, pch = 16, cex = 1.5,
            ref.y = 0)
```

```
scatterPlot(noxStats, x = "group", y = "r", type = "site.type", key = FALSE, pch = 16, cex = 1.5)
```

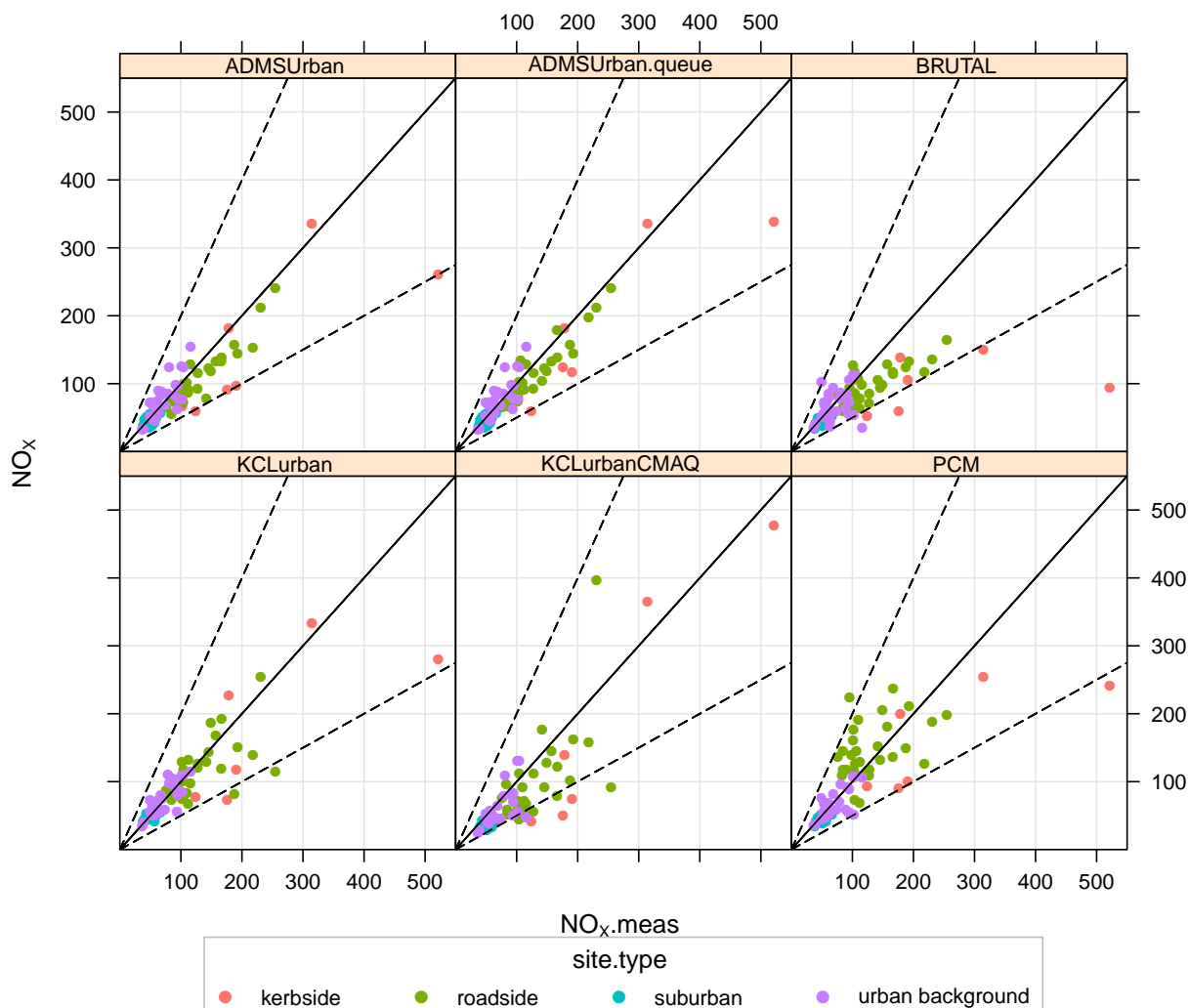


Figure 1: Scatter plot of measured versus predicted annual mean NO_x concentrations.

```
modStats(nox.results, type = c("site.type", "group"), obs = "no2.meas", mod = "NO2")
```

```
scatterPlot(nox.results, x = "no2.meas", y = "NO2", type = "group", mod.line = TRUE,
  pch = 16, smooth = FALSE, group = "site.type", xlim = c(0, 250), ylim = c(0, 250))
```

```
no2Stats <- modStats(nox.results, type = c("site.type", "group"), obs = "no2.meas", mod = "NO2")
```

```
scatterPlot(no2Stats, x = "group", y = "FAC2", type = "site.type", key = FALSE, pch = 16, cex = 1.5)
```

```
scatterPlot(no2Stats, x = "group", y = "MB", type = "site.type", key = FALSE, pch = 16, cex = 1.5,
  ref.y = 0)
```

```
scatterPlot(no2Stats, x = "group", y = "RMSE", type = "site.type", key = FALSE, pch = 16, cex = 1.5)
```

```
scatterPlot(no2Stats, x = "group", y = "r", type = "site.type", key = FALSE, pch = 16, cex = 1.5)
```

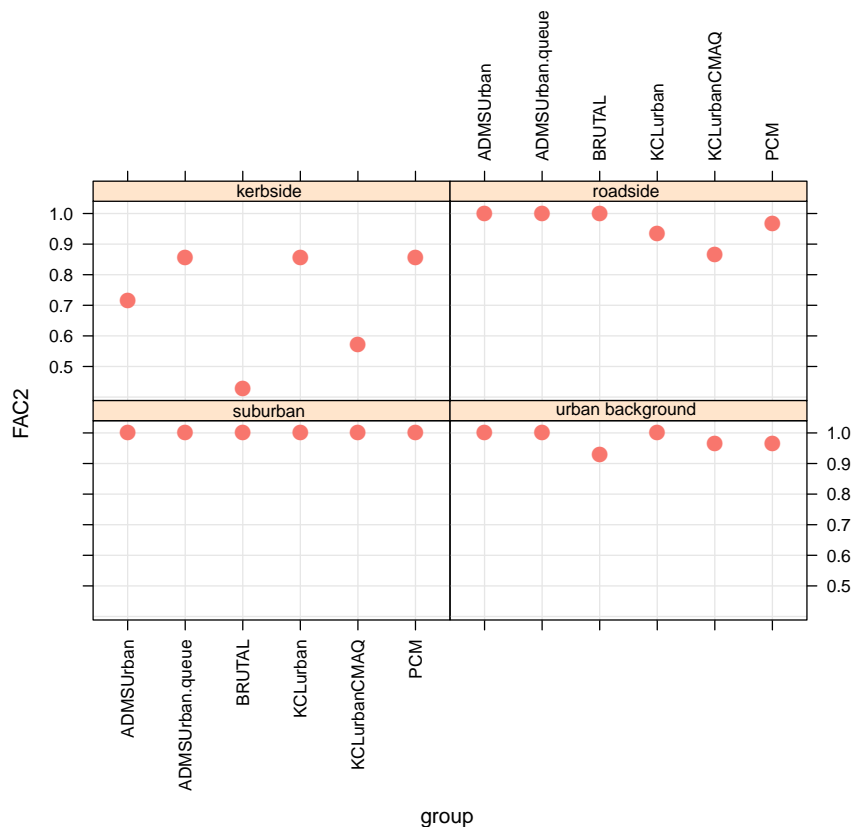


Figure 2: Graphical summary of FAC for each model by site type for NO_x.

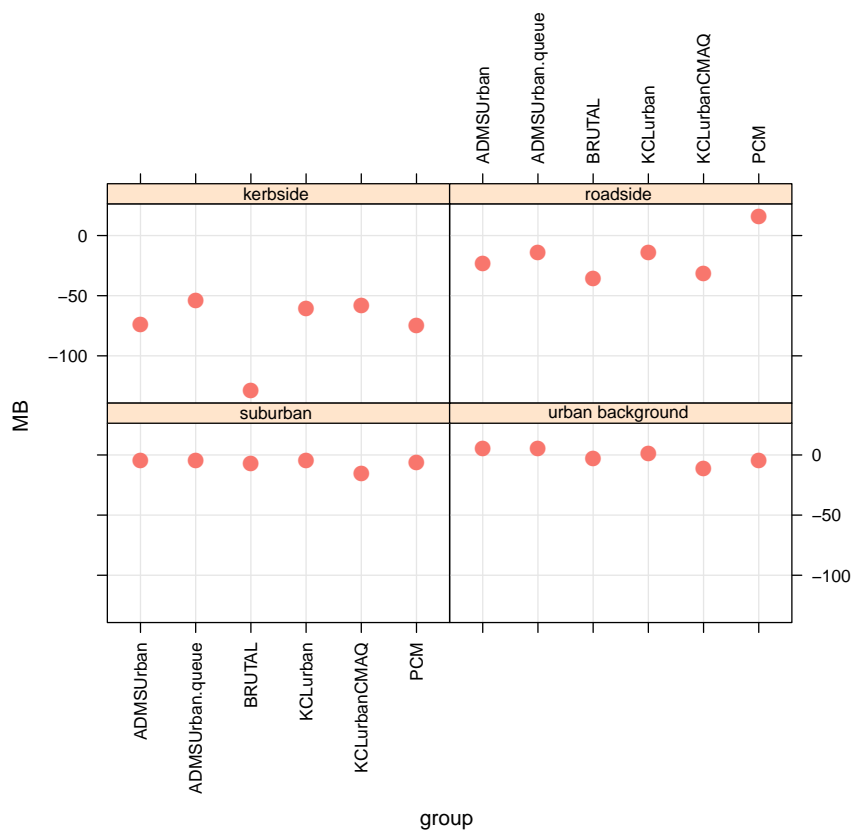


Figure 3: Graphical summary of mean bias for each model by site type for NO_x.

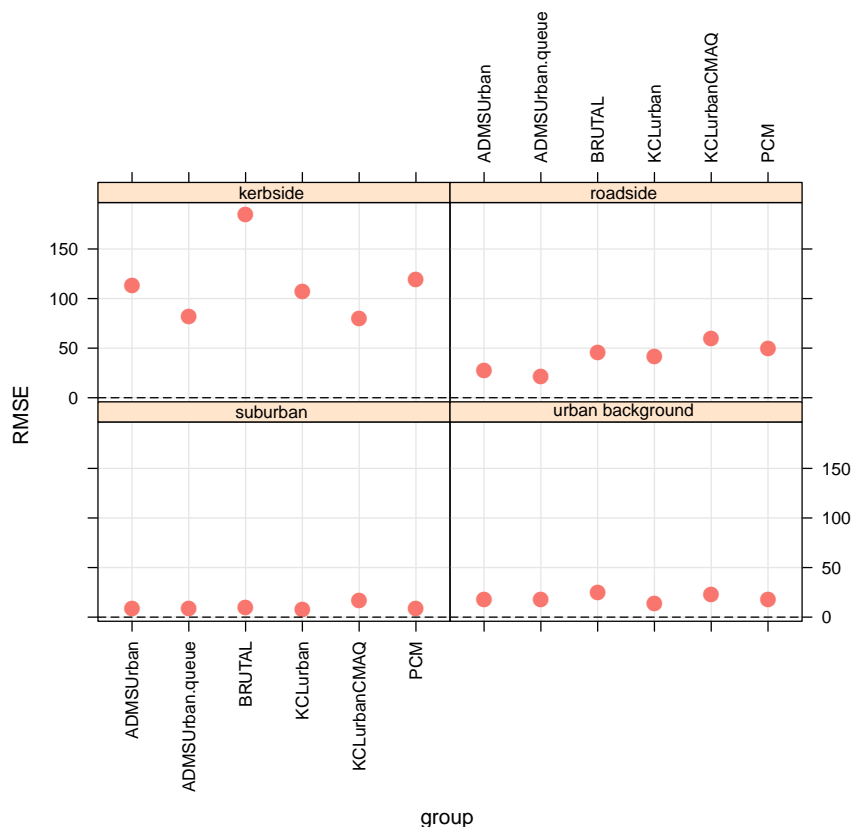


Figure 4: Graphical summary of RMSE for each model by site type for NO_x.

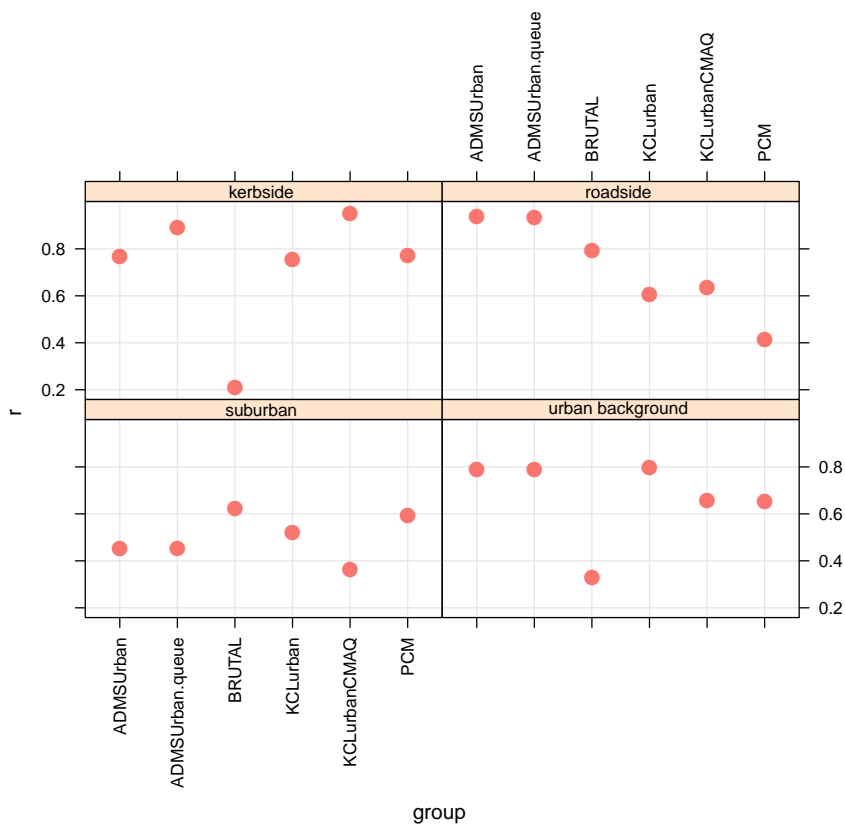


Figure 5: Graphical summary of the correlation coefficient, r , for each model by site type for NO_x.

Table 2: Summary model evaluation statistics for annual mean NO₂.

site.type	group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
kerbside	ADMSUrban	7	0.86	-29.00	30.48	-0.31	0.32	47.54	0.73
kerbside	ADMSUrban.queue	7	1.00	-22.59	24.07	-0.24	0.26	37.53	0.86
kerbside	BRUTAL	7	0.71	-39.61	42.24	-0.42	0.45	67.09	0.15
kerbside	KCLurban	7	0.86	-25.84	28.77	-0.27	0.31	45.59	0.75
kerbside	KCLurbanCMAQ	7	0.86	-21.94	24.26	-0.23	0.26	29.39	0.93
kerbside	PCM	7	1.00	-25.53	27.26	-0.27	0.29	43.15	0.81
roadside	ADMSUrban	30	1.00	-6.12	7.70	-0.11	0.14	9.94	0.86
roadside	ADMSUrban.queue	30	1.00	-3.42	6.00	-0.06	0.11	7.75	0.89
roadside	BRUTAL	30	1.00	-3.02	9.30	-0.05	0.16	11.67	0.69
roadside	KCLurban	30	1.00	-2.19	8.44	-0.04	0.15	11.12	0.72
roadside	KCLurbanCMAQ	30	1.00	-4.22	10.32	-0.07	0.18	14.22	0.76
roadside	PCM	30	1.00	7.93	16.02	0.14	0.28	19.69	0.38
suburban	ADMSUrban	11	1.00	-1.26	3.34	-0.04	0.11	3.89	0.39
suburban	ADMSUrban.queue	11	1.00	-1.26	3.34	-0.04	0.11	3.89	0.39
suburban	BRUTAL	11	1.00	-2.15	4.07	-0.07	0.13	4.29	0.40
suburban	KCLurban	11	1.00	0.10	2.65	0.00	0.09	3.23	0.38
suburban	KCLurbanCMAQ	11	1.00	-2.02	3.82	-0.07	0.12	4.41	0.27
suburban	PCM	11	1.00	-3.00	3.97	-0.10	0.13	4.85	0.33
urban background	ADMSUrban	29	1.00	0.77	4.42	0.02	0.11	5.47	0.85
urban background	ADMSUrban.queue	29	1.00	0.77	4.42	0.02	0.11	5.47	0.85
urban background	BRUTAL	29	0.97	-3.13	7.12	-0.08	0.17	9.76	0.56
urban background	KCLurban	29	1.00	0.42	3.67	0.01	0.09	4.97	0.87
urban background	KCLurbanCMAQ	29	1.00	-0.20	4.34	-0.00	0.11	6.15	0.84
urban background	PCM	29	1.00	-3.34	4.82	-0.08	0.12	7.23	0.77

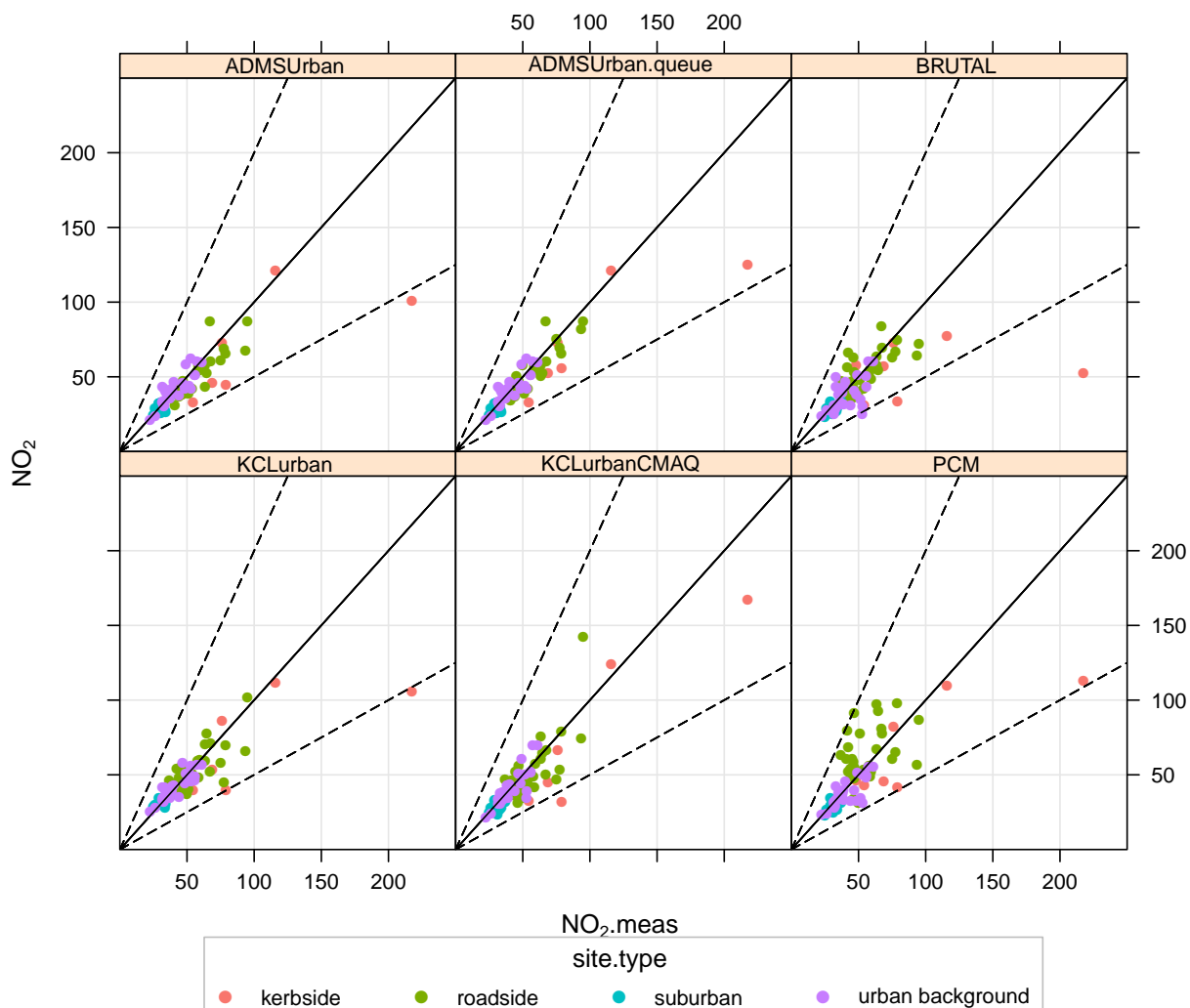


Figure 6: Scatter plot of measured versus predicted annual mean NO_2 concentrations.

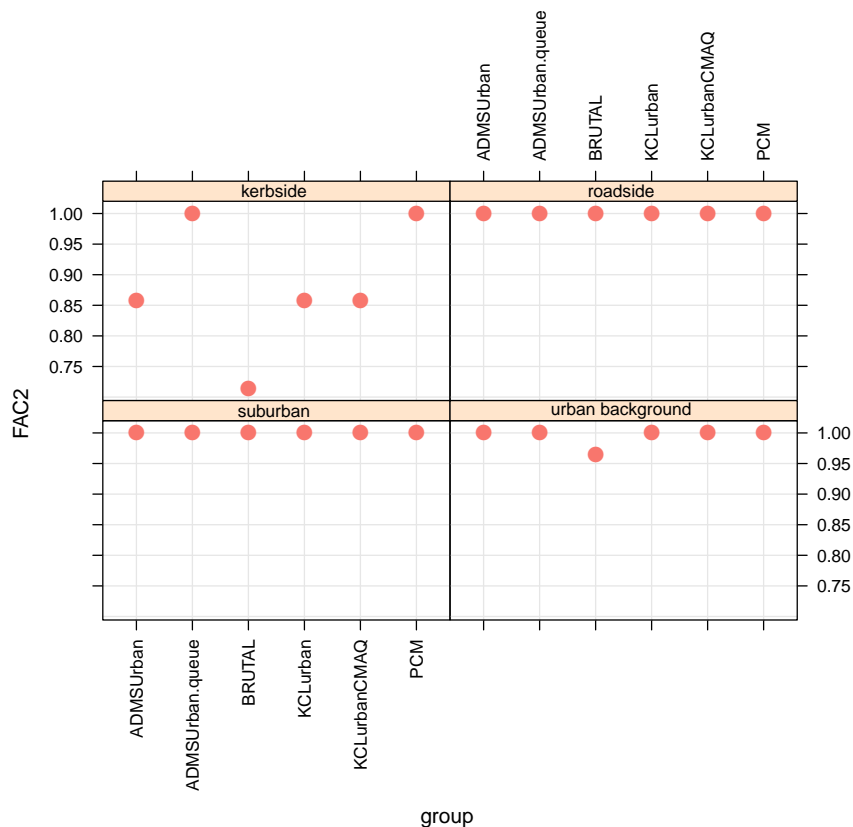


Figure 7: Graphical summary of the FAC2 for each model by site type for NO₂.

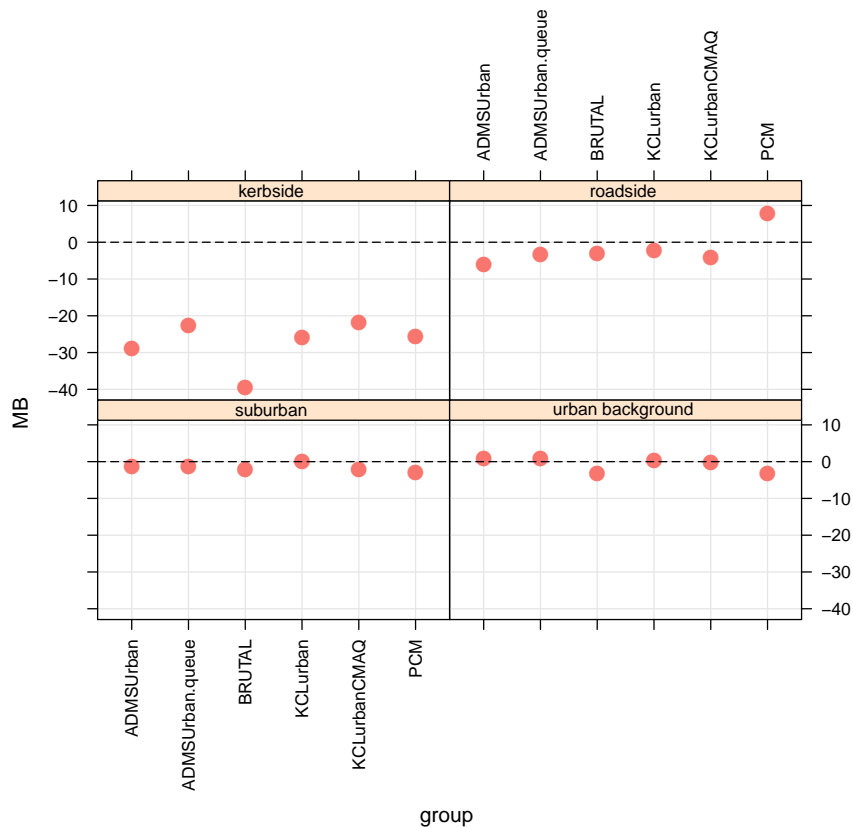


Figure 8: Graphical summary of the mean bias for each model by site type for NO₂.

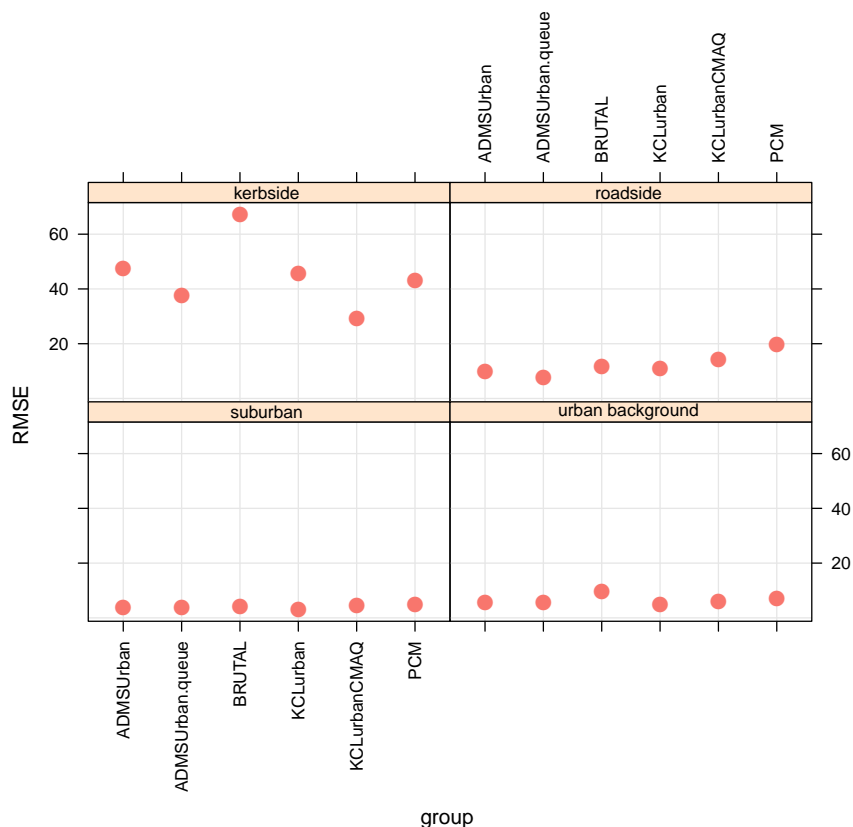


Figure 9: Graphical summary of the RMSE for each model by site type for NO₂.

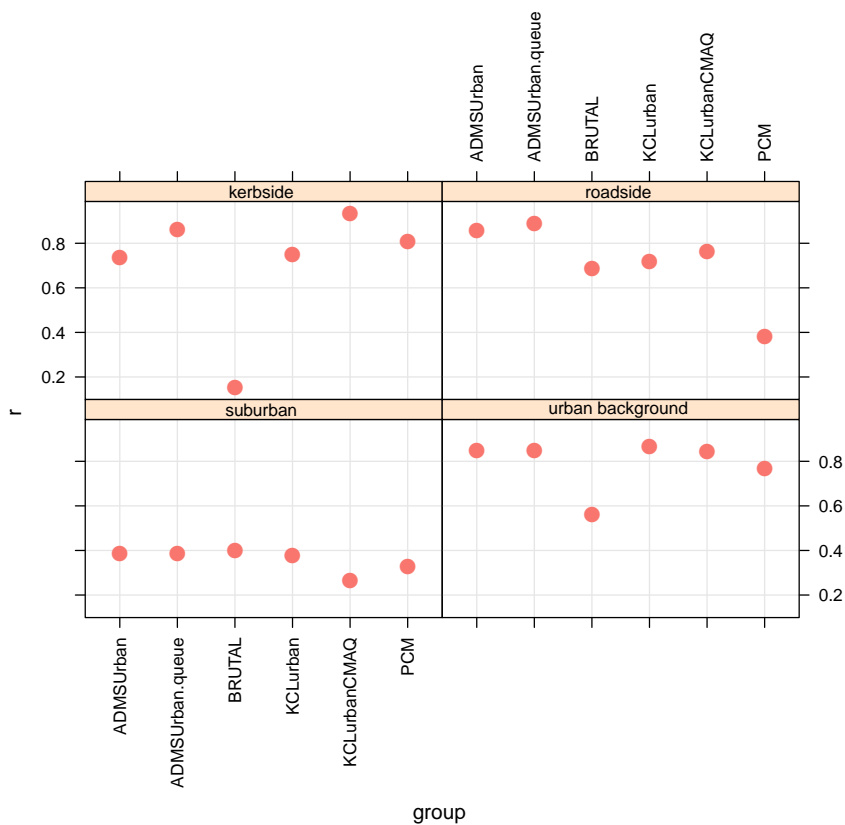


Figure 10: Graphical summary of the correlation coefficient, r , for each model by site type for NO₂.

3.1.1 Relative Directive Error, RDE

We have also considered how the predictive performance of the models compare with the Directive requirements. It seems that the Directive requirements for model performance are ambiguous.¹ The FAIRMODE report attempts to provide some clarification in this respect by defining *Relative Directive Error (RDE)*:

$$RDE = \frac{|O_{LV} - M_{LV}|}{LV} \quad (1)$$

where O_{LV} is the closest observed concentration to the limit value concentration (LV) and M_{LV} is the correspondingly ranked modelled concentration. The RDE is expressed as a percentage. The maximum of this value found at 90% of the available stations is then the *Maximum Relative Directive Error (MRDE)*.

For the PM₁₀ daily LV the daily means are ranked and closest observed concentration to 50 µg m⁻³ recorded. The corresponding ranked modelled value is then calculated. These two values are then input into [Equation 1](#).

For annual means [Equation 1](#) is used directly without any ranking. This slightly bizarre procedure allows models to be judged against Directive requirements. The PM₁₀ procedure will be applied in [subsection 3.3](#).

The RDE for NO₂ is calculated as follows:

```
nox.results$RDE.NO2 <- 100 * abs((nox.results$no2.meas - nox.results$NO2)) / 40
```

The RDE results for NO₂ are plotted in [Figure 11](#). The RDE is then interpreted as the 90th percentile value i.e. there is some allowance for outliers. However, the FAIRMODE report is rather tentative about the interpretation of 90% suggesting it should not be taken literally e.g. no allowance for outliers if there are fewer than 10 sites in a conurbation. However, there are easily sufficient sites in London for this statistic to be calculated in a direct way.

```
scatterPlot(nox.results, x = "group", y = "RDE.NO2")
```

The 90th percentile values are shown in [Table 3](#). The Directive specifies that the models should have a value < 30% at an overall comparison across the territory of a member state. This inter-comparison exercise only focuses on London as subset of the UK so is therefore not suitable for the application of the RDE statistic. The RDE will in effect penalise conurbations with higher concentrations of NO₂ such as London, because there are a lot of sites with annual means >40 µg m⁻³. The value will always be higher in areas such as London where concentrations are high, and lower in areas where the limit value is not exceeded. Furthermore, the absolute error in annual mean predictions tends to increase with increasing concentration and [Equation 1](#) will tend to penalise these sites because the denominator is fixed at 40 µg m⁻³. These results therefore show the model performance for a subset of data and as such is not comparable with the scenario at which the FAIRMODE guidance is aimed. Unsurprisingly then, none of the models are within 30% — although the CERC and KCLurban models are close to this value.

```
RDE.NO2 <- with(nox.results, tapply(RDE.NO2, group, function (x) quantile(x, prob = 0.9, na.rm = T)))
```

Table 3: Summary of the Maximum Relative Directive Error for annual mean NO₂ by group (%).

ADMSUrban	ADMSUrban.queue	BRUTAL	KCLurban	KCLurbanCMAQ	PCM
33.76	30.53	56.51	33.78	46.27	66.05

¹Guidance on the use of models for the European Air Quality Directive A working document of the Forum for Air Quality Modelling in Europe, FAIRMODE ETC/ACC report Version 6.1.

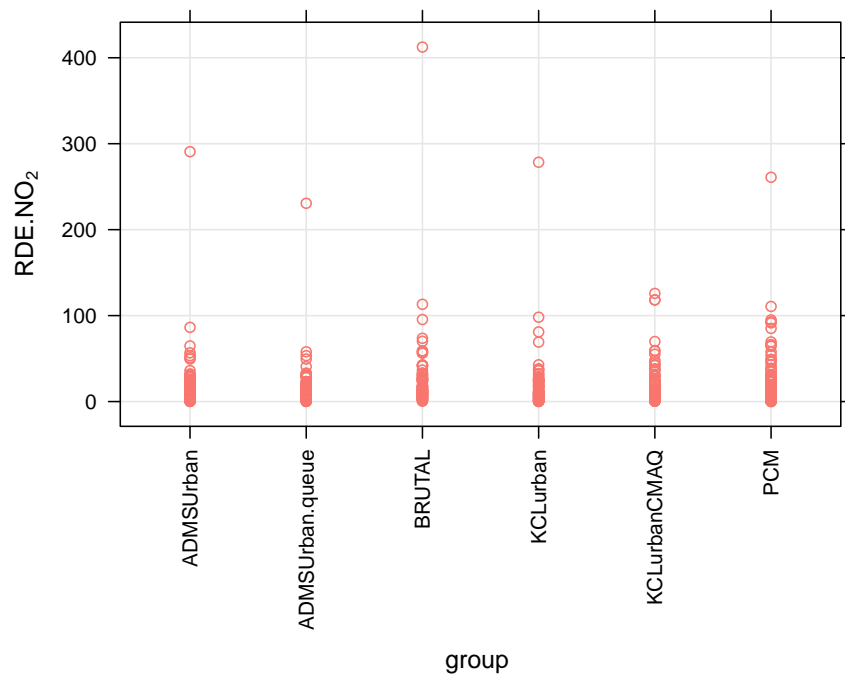


Figure 11: The RDE for annual mean NO₂ concentrations by group.

3.2 Annual mean O₃

Ozone data measurements with a data capture of >75% are first extracted and the BRUTAL/PCM model results omitted.

```
o3.results <- subset(all.results, o3.count > 0.75 * 8784 & group != BRUTAL & group != PCM)
```

And the model evaluation statistics are:

```
o3Stats <- modStats(o3.results, type = c("site.type", "group"), obs = "o3.meas", mod = "O3")
```

Table 4: Summary model evaluation statistics for annual mean O₃.

site.type	group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
airport	ADMSUrban	1	1.00	0.28	0.28	0.01	0.01	0.28	
airport	ADMSUrban.queue	1	1.00	0.28	0.28	0.01	0.01	0.28	
airport	KCLurban	1	1.00	3.99	3.99	0.11	0.11	3.99	
airport	KCLurbanCMAQ	0							
kerbside	ADMSUrban	1	1.00	2.43	2.43	0.16	0.16	2.43	
kerbside	ADMSUrban.queue	1	1.00	2.43	2.43	0.16	0.16	2.43	
kerbside	KCLurban	1	1.00	2.82	2.82	0.18	0.18	2.82	
kerbside	KCLurbanCMAQ	1	1.00	3.69	3.69	0.24	0.24	3.69	
roadside	ADMSUrban	9	1.00	4.81	4.81	0.16	0.16	5.81	0.85
roadside	ADMSUrban.queue	9	1.00	4.80	4.80	0.16	0.16	5.81	0.85
roadside	KCLurban	11	1.00	2.27	3.63	0.07	0.12	4.83	0.74
roadside	KCLurbanCMAQ	11	1.00	8.04	9.57	0.26	0.31	10.28	0.60
suburban	ADMSUrban	8	1.00	-0.08	1.65	-0.00	0.04	2.10	0.92
suburban	ADMSUrban.queue	8	1.00	-0.08	1.65	-0.00	0.04	2.10	0.92
suburban	KCLurban	9	1.00	1.85	3.15	0.05	0.08	3.50	0.74
suburban	KCLurbanCMAQ	7	1.00	10.30	10.30	0.25	0.25	10.76	0.41
urban background	ADMSUrban	14	1.00	0.32	2.90	0.01	0.08	3.84	0.65
urban background	ADMSUrban.queue	14	1.00	0.32	2.90	0.01	0.08	3.84	0.65
urban background	KCLurban	15	1.00	2.93	3.79	0.08	0.11	4.97	0.63
urban background	KCLurbanCMAQ	14	1.00	8.42	8.63	0.24	0.24	9.95	0.58

```
scatterPlot(o3.results, x = "o3.meas", y = "O3", type = "group", mod.line = TRUE,
            pch = 16, smooth = FALSE, group = "site.type", cex = 1.5,
            xlim = c(0, 60), ylim = c(0, 60))
```

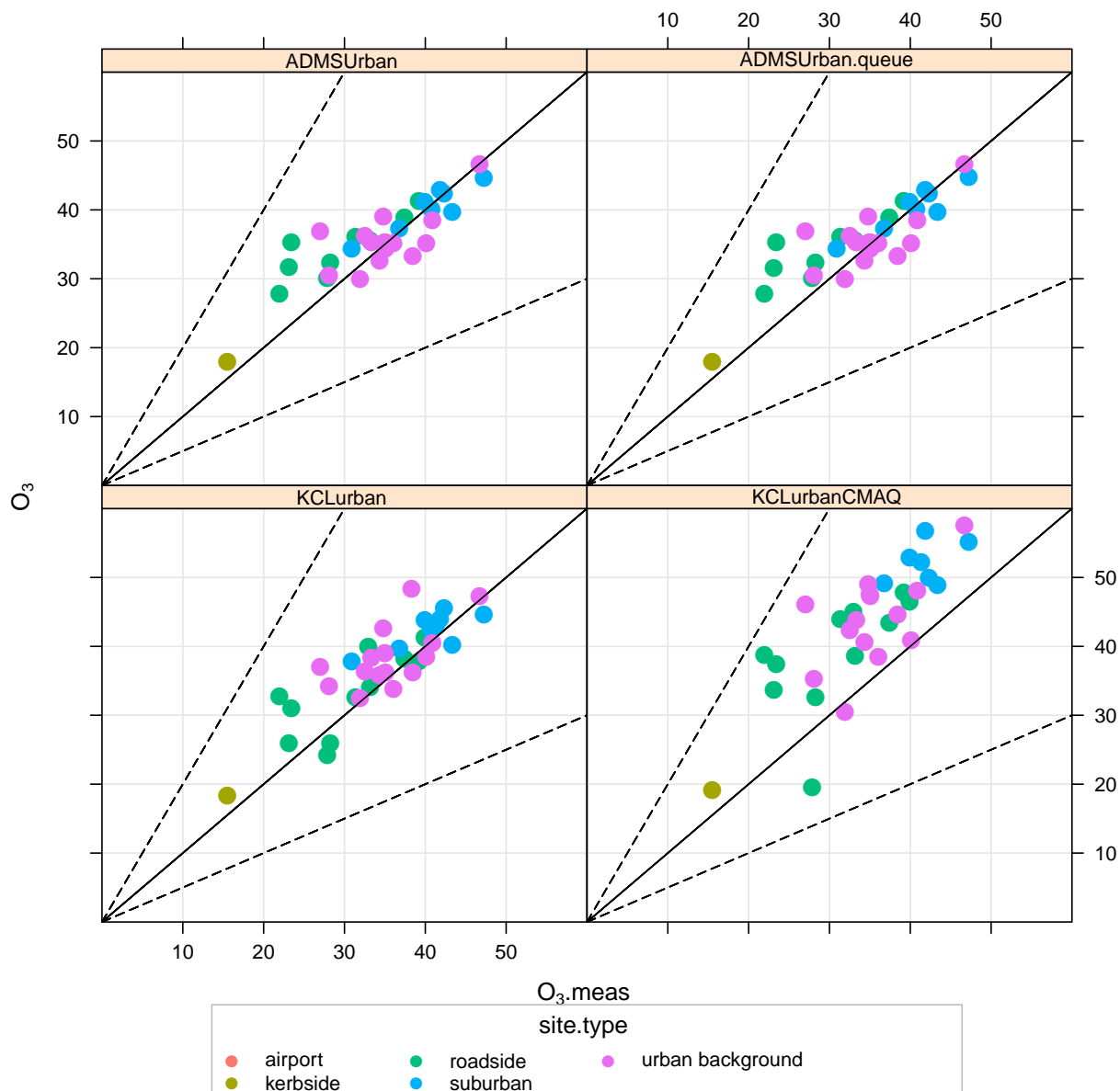


Figure 12: Measured vs. modelled annual mean O_3 concentrations for each model.

3.3 Annual mean PM₁₀

```
pm10.results <- subset(all.results, pm10.count > 0.75 * 8784 & group != "KCLurbanCMAQ")
## extract only those results where all groups made a prediction
## sites where this is true
fullSites <- with(pm10.results, tapply(PM10, site.code, function(x) length(na.omit(x))))
fullSites <- fullSites[fullSites == length(unique(pm10.results$group))]
pm10.results <- subset(pm10.results, site.code %in% names(fullSites))
```

And the model evaluation statistics are:

```
pm10Stats <- modStats(pm10.results, type = c("site.type", "group"), obs = "pm10.meas", mod = "PM10")
```

Table 5: Summary model evaluation statistics for annual mean PM₁₀.

site.type	group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
kerbside	ADMSUrban	6	1.00	-4.80	4.80	-0.15	0.15	6.04	0.76
kerbside	ADMSUrban.queue	6	1.00	-3.81	3.81	-0.12	0.12	5.08	0.81
kerbside	BRUTAL	6	1.00	-4.73	5.30	-0.15	0.17	6.63	0.57
kerbside	KCLurban	6	1.00	-7.14	7.14	-0.23	0.23	8.31	0.67
kerbside	PCM	6	1.00	-4.22	4.47	-0.13	0.14	5.33	0.84
roadside	ADMSUrban	17	1.00	-1.24	2.06	-0.05	0.08	3.11	0.66
roadside	ADMSUrban.queue	17	1.00	-0.63	1.91	-0.02	0.07	2.92	0.66
roadside	BRUTAL	17	1.00	-0.69	2.87	-0.03	0.11	3.84	0.35
roadside	KCLurban	17	1.00	-4.57	4.57	-0.18	0.18	5.53	0.57
roadside	PCM	17	1.00	-0.02	2.55	-0.00	0.10	3.18	0.57
suburban	ADMSUrban	8	1.00	1.81	1.81	0.09	0.09	2.08	0.39
suburban	ADMSUrban.queue	8	1.00	1.81	1.81	0.09	0.09	2.08	0.39
suburban	BRUTAL	8	1.00	1.05	1.63	0.05	0.08	1.97	0.08
suburban	KCLurban	8	1.00	-1.69	1.72	-0.09	0.09	2.03	0.05
suburban	PCM	8	1.00	0.52	1.20	0.03	0.06	1.39	0.27
urban background	ADMSUrban	19	1.00	1.00	1.50	0.05	0.07	1.84	0.63
urban background	ADMSUrban.queue	19	1.00	1.00	1.50	0.05	0.07	1.84	0.63
urban background	BRUTAL	19	1.00	1.43	1.86	0.07	0.09	2.11	0.72
urban background	KCLurban	19	1.00	-2.50	2.52	-0.12	0.12	2.93	0.72
urban background	PCM	19	1.00	0.21	1.21	0.01	0.06	1.45	0.70

```
scatterPlot(pm10.results, x = "pm10.meas", y = "PM10", type = "group", mod.line = TRUE,
            pch = 16, smooth = FALSE, group = "site.type", xlim = c(0, 40), ylim = c(0, 40))
```

```
scatterPlot(pm10Stats, x = "group", y = "FAC2", type = "site.type", key = FALSE, pch = 16, cex = 1.5)
```

```
scatterPlot(pm10Stats, x = "group", y = "MB", type = "site.type", key = FALSE, pch = 16, cex = 1.5,
            ref.y = 0)
```

```
scatterPlot(pm10Stats, x = "group", y = "RMSE", type = "site.type", key = FALSE, pch = 16, cex = 1.5)
```

```
scatterPlot(pm10Stats, x = "group", y = "r", type = "site.type", key = FALSE, pch = 16, cex = 1.5)
```

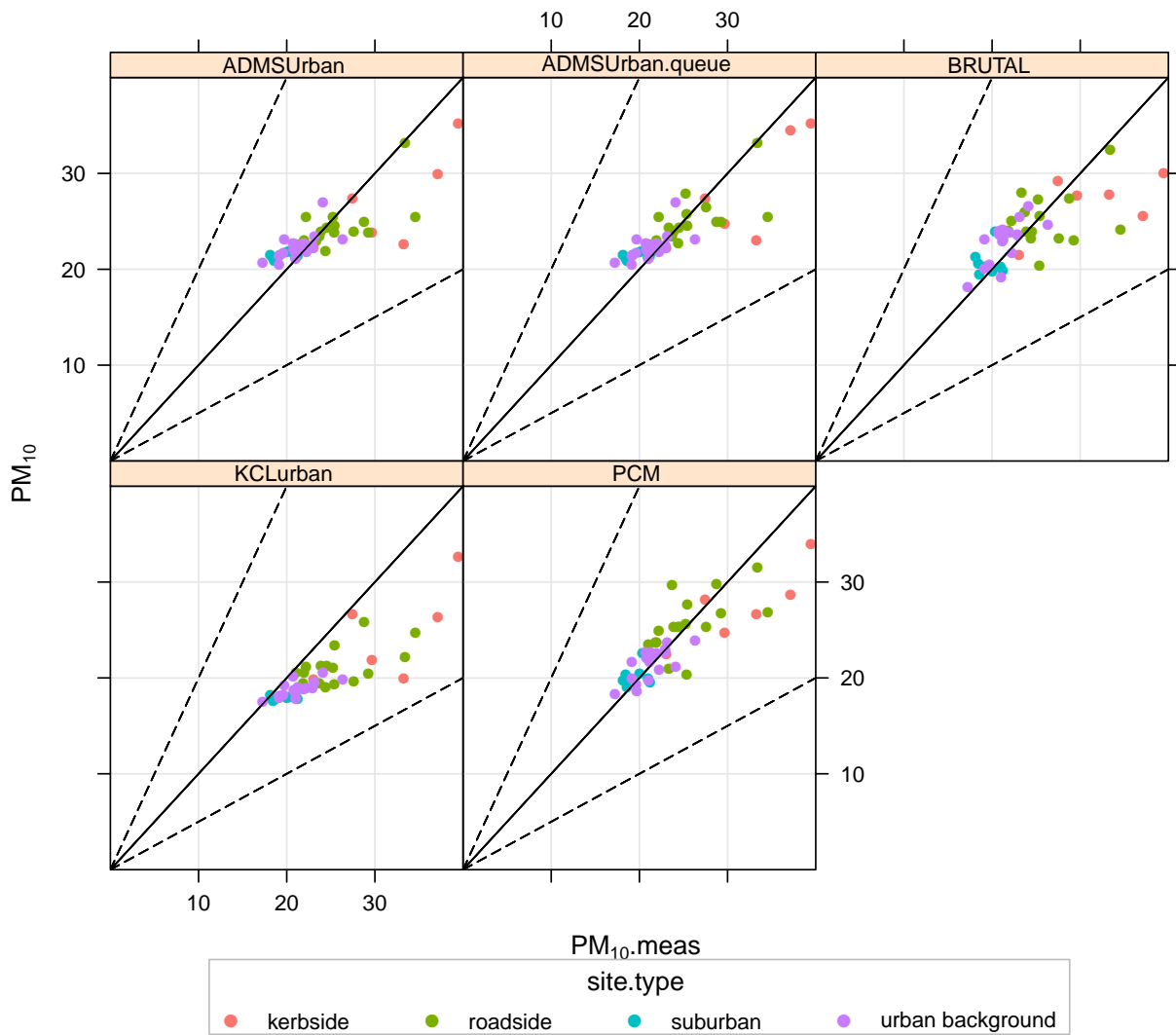


Figure 13: Measured vs. modelled annual mean PM_{10} concentrations for each model.

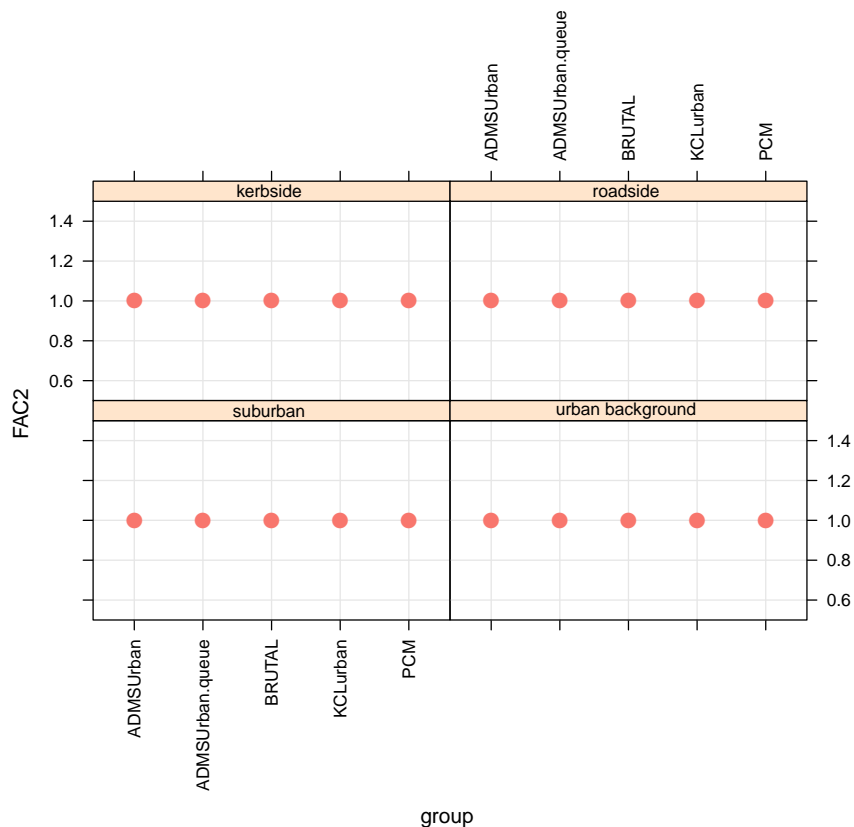


Figure 14: Graphical summary of FAC for each model by site type for PM₁₀.

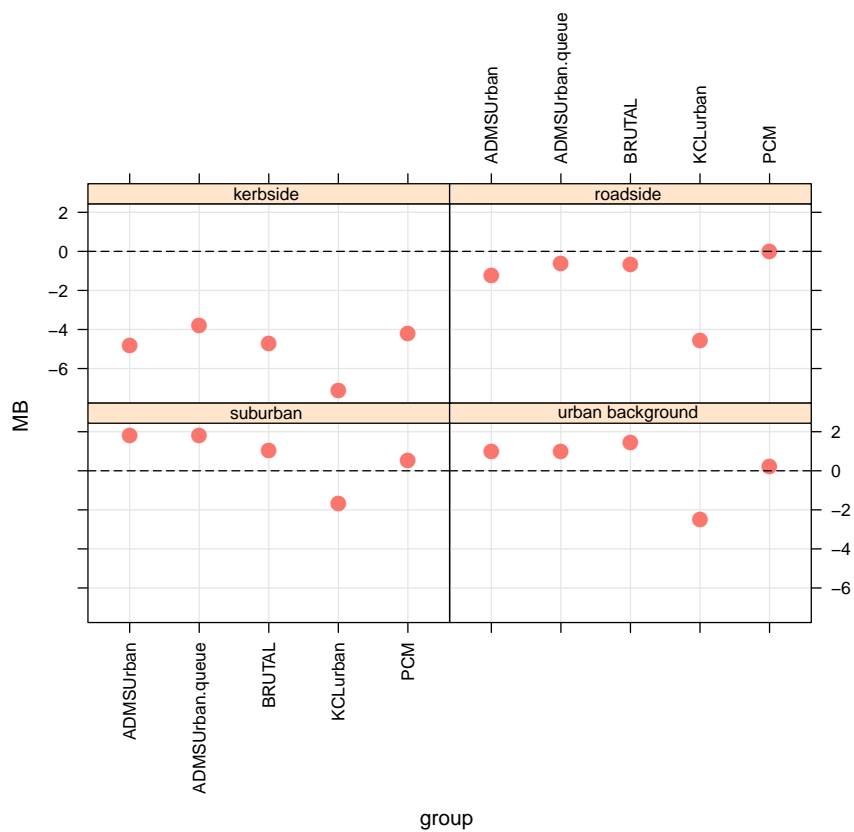


Figure 15: Graphical summary of mean bias for each model by site type for PM₁₀.

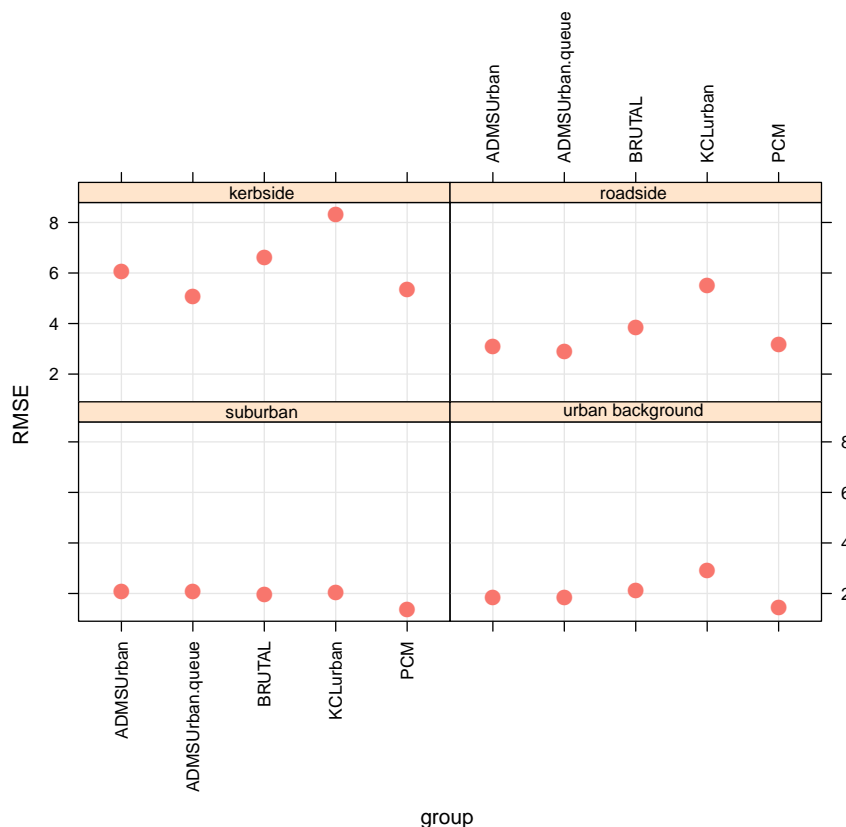


Figure 16: Graphical summary of RMSE for each model by site type for PM_{10} .

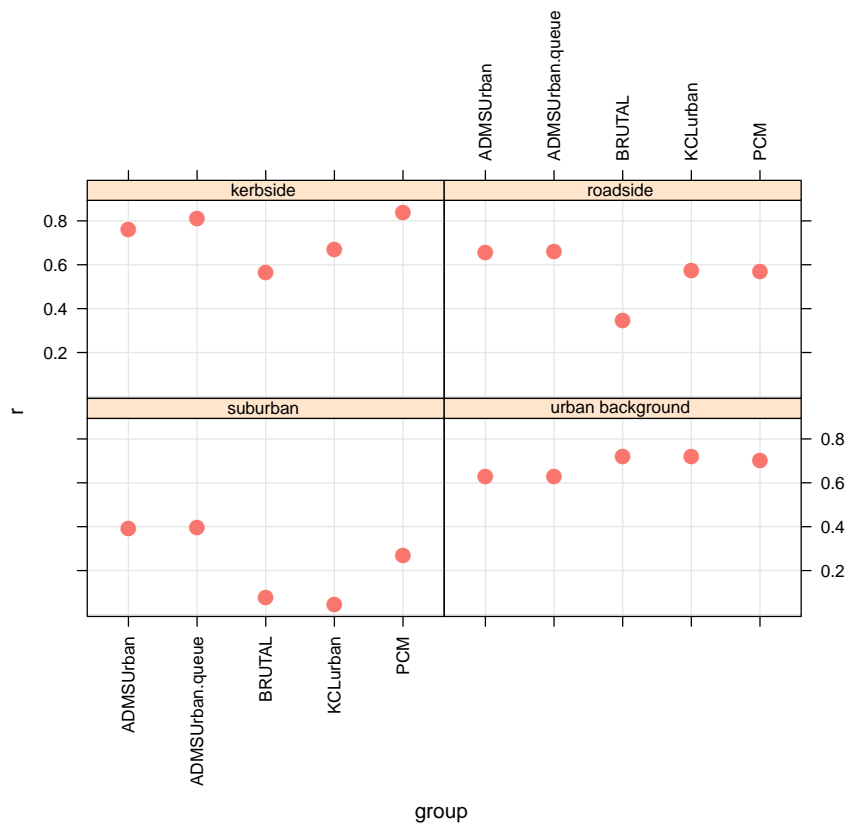


Figure 17: Graphical summary of the correlation coefficient, r , for each model by site type for PM_{10} .

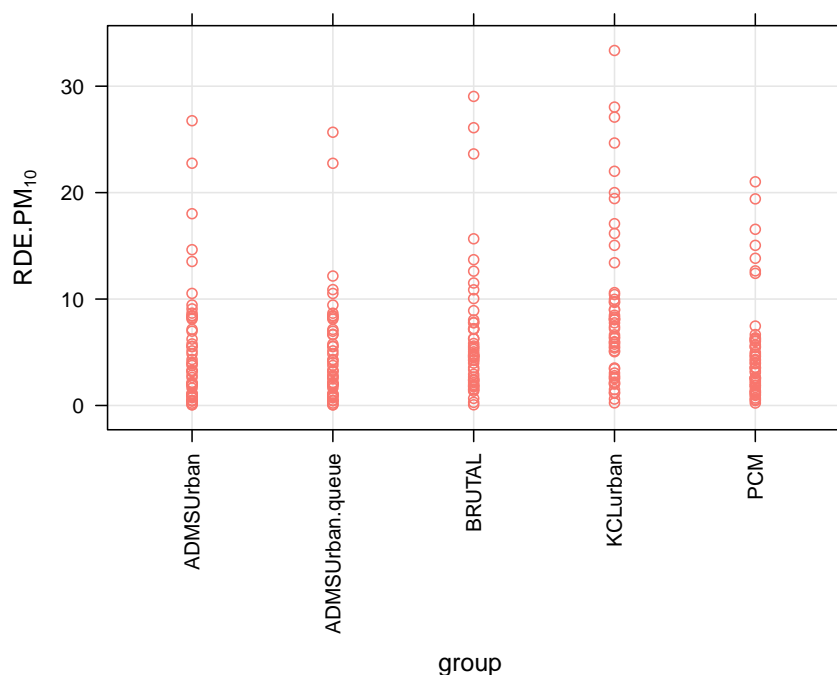


Figure 18: The RDE for annual mean PM_{10} concentrations by group.

3.3.1 Relative Directive Error, *RDE*

```
pm10.results$RDE.PM10 <- 100 * abs((pm10.results$pm10.meas - pm10.results$PM10)) / 40
```

The RDE results for PM_{10} are plotted in Figure 18. The RDE is calculated in the same way as for NO_2 shown in subsection 3.1.1. It should be noted, as in the case of NO_2 , that the RDE would be applied to national scale data and not London in isolation. These results therefore show the model performance for a subset of data and as such is not comparable with Directive requirements.

```
scatterPlot(pm10.results, x = "group", y = "RDE.PM10")
```

The 90th percentile values are shown in Table 6. The Directive specifies that the models should have a value $< 50\%$, which all models meet comfortably. The reason why the models meet the uncertainty requirement for PM_{10} so easily compared with NO_2 is because the PM_{10} concentrations are much lower than NO_2 .

```
RDE.PM10 <- with(pm10.results, tapply(RDE.PM10, group, function (x) quantile(x, prob = 0.9, na.rm = T)))
```

Table 6: Summary of the Maximum Relative Directive Error for annual mean PM_{10} by group (%).

ADMSUrban	ADMSUrban.queue	BRUTAL	KCLurban	PCM
10.83	9.55	12.73	20.20	12.77

3.4 Annual mean PM_{2.5}

```
pm25.results <- subset(all.results, pm25.count > 0.75 * 8784 & group != "KCLurbanCMAQ" & group != "BRUTAL")
## extract only those results where all groups made a prediction
## sites where this is true
fullSites <- with(pm25.results, tapply(PM2.5, site.code, function(x) length(na.omit(x))))
fullSites <- fullSites[fullSites == length(unique(pm25.results$group))]
pm25.results <- subset(pm25.results, site.code %in% names(fullSites))
```

And the model evaluation statistics are:

```
pm25Stats <- modStats(pm25.results, type = c("site.type", "group"), obs = "pm25.meas", mod = "PM2.5")
```

Table 7: Summary model evaluation statistics for annual mean PM_{2.5}.

site.type	group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
kerbside	ADMSUrban	1	1.00	2.86	2.86	0.14	0.14	2.86	
kerbside	ADMSUrban.queue	1	1.00	2.86	2.86	0.14	0.14	2.86	
kerbside	KCLurban	1	1.00	1.81	1.81	0.09	0.09	1.81	
kerbside	PCM	1	1.00	0.95	0.95	0.05	0.05	0.95	
roadside	ADMSUrban	9	1.00	-1.88	2.74	-0.13	0.18	3.37	0.21
roadside	ADMSUrban.queue	9	1.00	-1.59	2.90	-0.11	0.19	3.43	0.06
roadside	KCLurban	9	1.00	-1.16	1.79	-0.08	0.12	2.16	0.68
roadside	PCM	9	1.00	3.00	3.16	0.20	0.21	3.49	0.70
suburban	ADMSUrban	1	1.00	-0.62	0.62	-0.06	0.06	0.62	
suburban	ADMSUrban.queue	1	1.00	-0.61	0.61	-0.06	0.06	0.61	
suburban	KCLurban	1	1.00	0.22	0.22	0.02	0.02	0.22	
suburban	PCM	1	1.00	2.83	2.83	0.26	0.26	2.83	
urban background	ADMSUrban	2	1.00	-2.07	2.07	-0.14	0.14	2.59	-1.00
urban background	ADMSUrban.queue	2	1.00	-2.07	2.07	-0.14	0.14	2.59	-1.00
urban background	KCLurban	2	1.00	-1.85	1.85	-0.13	0.13	2.18	-1.00
urban background	PCM	2	1.00	1.94	1.94	0.14	0.14	2.54	-1.00

Save all the statistics for external processing if necessary.

```
save(noxStats, no2Stats, o3Stats, pm10Stats, pm25Stats, file = "urbanStats.RData")
```

```
scatterPlot(pm25.results, x = "pm25.meas", y = "PM2.5", type = "group", mod.line = TRUE,
            pch = 16, smooth = FALSE, group = "site.type",
            cex = 1.5, xlim = c(0, 21), ylim = c(0, 21))
```

```
scatterPlot(pm25Stats, x = "group", y = "FAC2", type = "site.type", key = FALSE, pch = 16, cex = 1.5)
```

```
scatterPlot(pm25Stats, x = "group", y = "MB", type = "site.type", key = FALSE, pch = 16, cex = 1.5,
            ref.y = 0)
```

```
scatterPlot(pm25Stats, x = "group", y = "RMSE", type = "site.type", key = FALSE, pch = 16, cex = 1.5)
```

```
scatterPlot(pm25Stats, x = "group", y = "r", type = "site.type", key = FALSE, pch = 16, cex = 1.5)
```

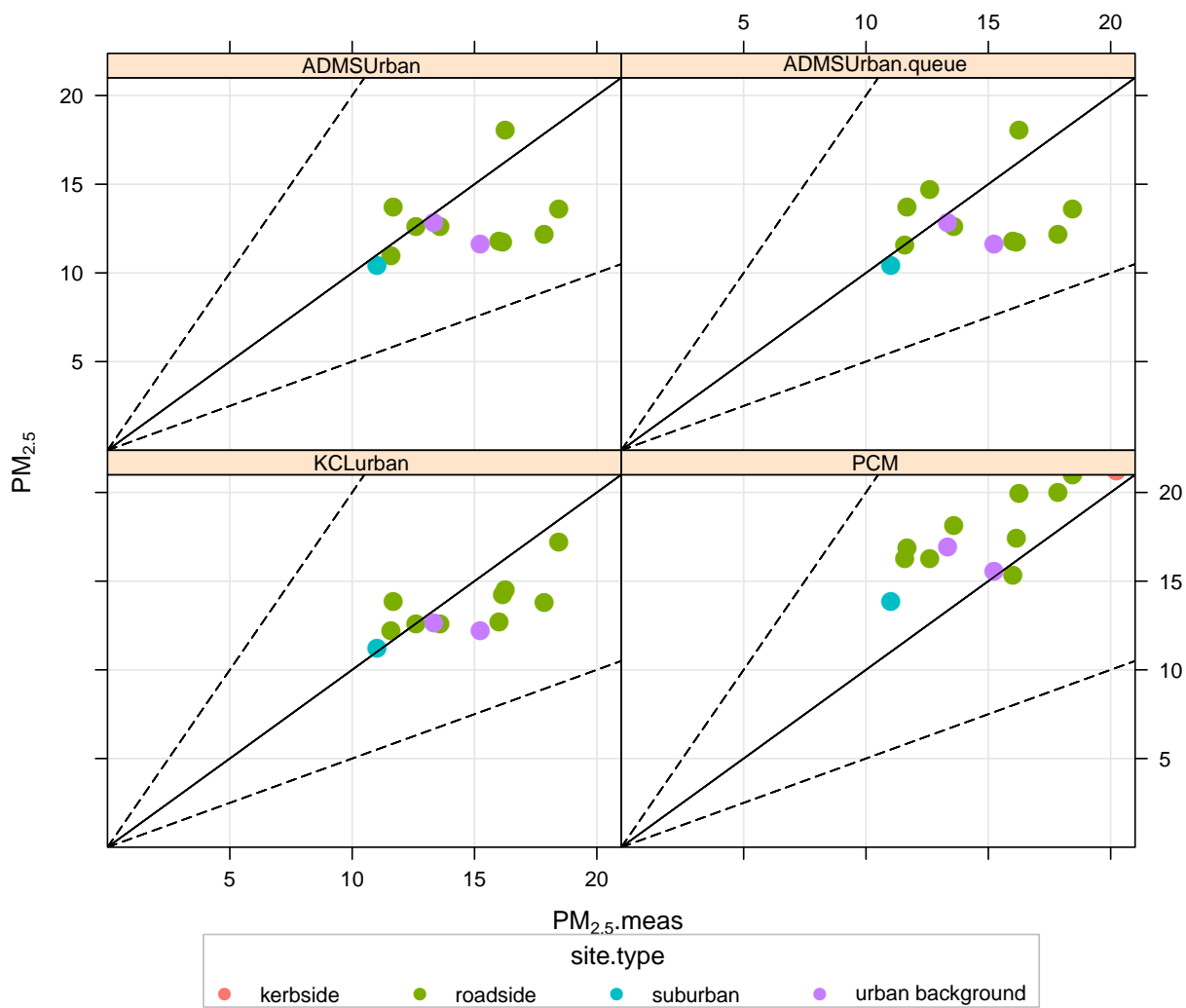


Figure 19: Measured vs. modelled annual mean $PM_{2.5}$ concentrations for each model.

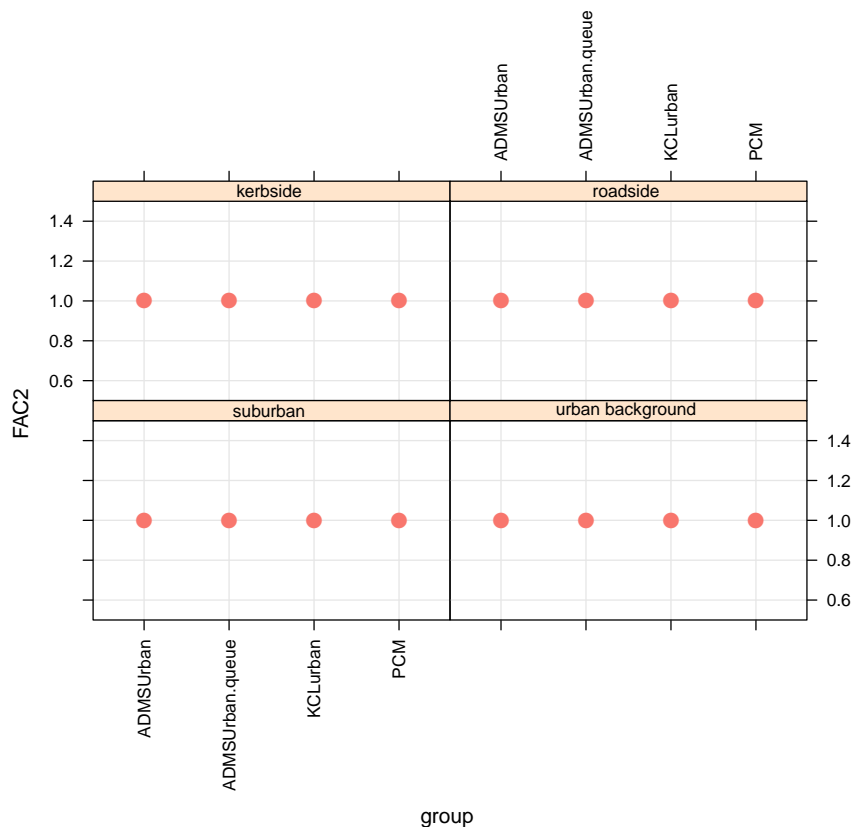


Figure 20: Graphical summary of FAC for each model by site type for $PM_{2.5}$.

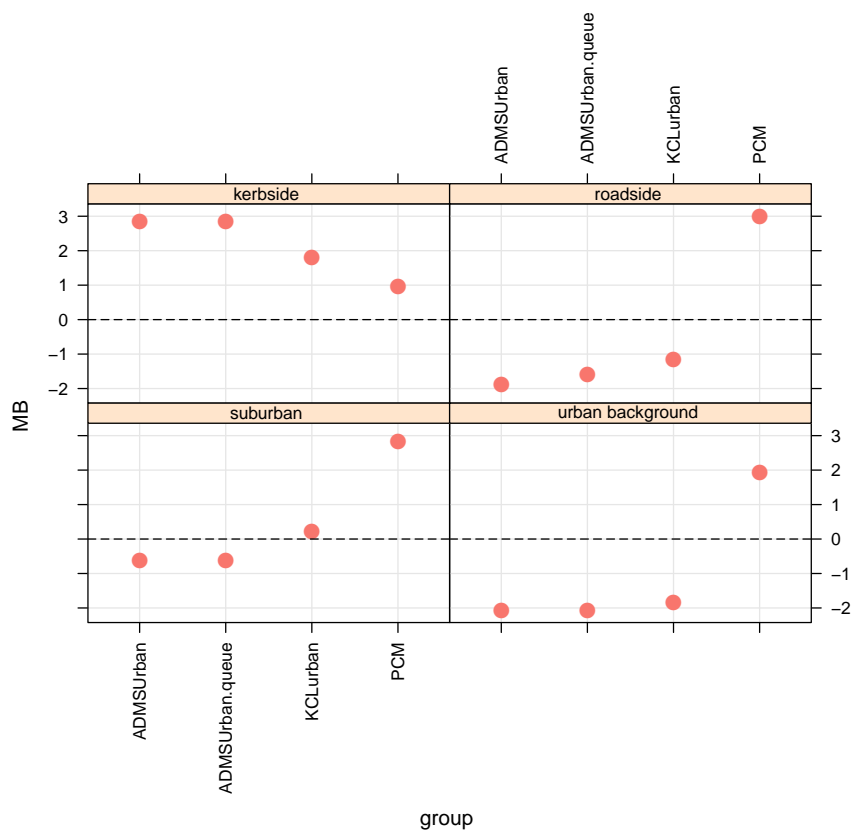


Figure 21: Graphical summary of mean bias for each model by site type for $PM_{2.5}$.

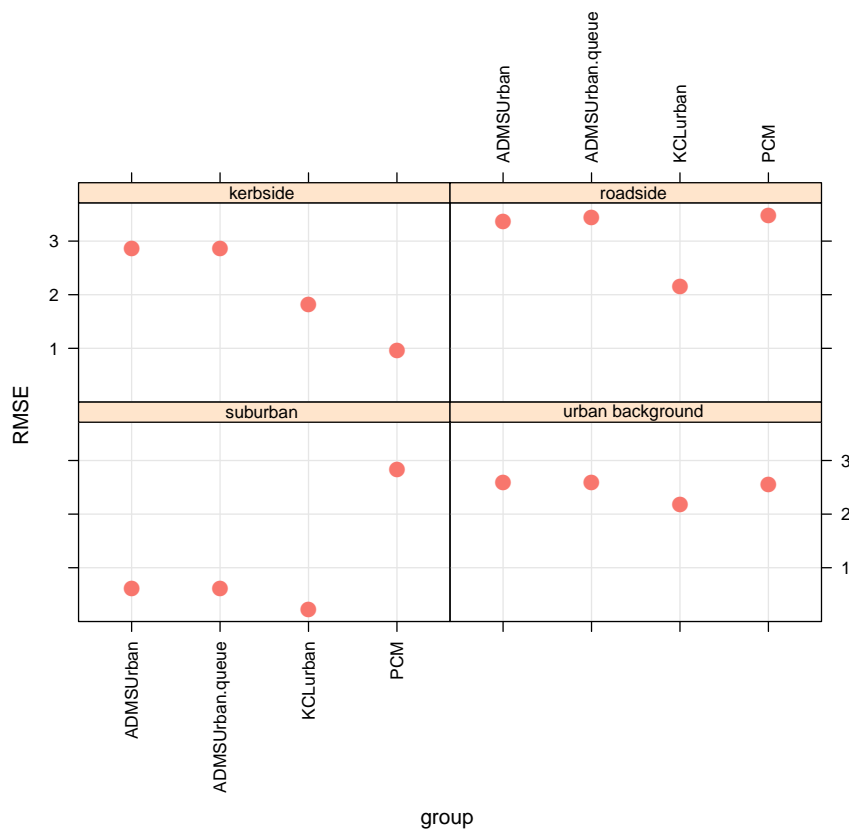


Figure 22: Graphical summary of RMSE for each model by site type for $PM_{2.5}$.

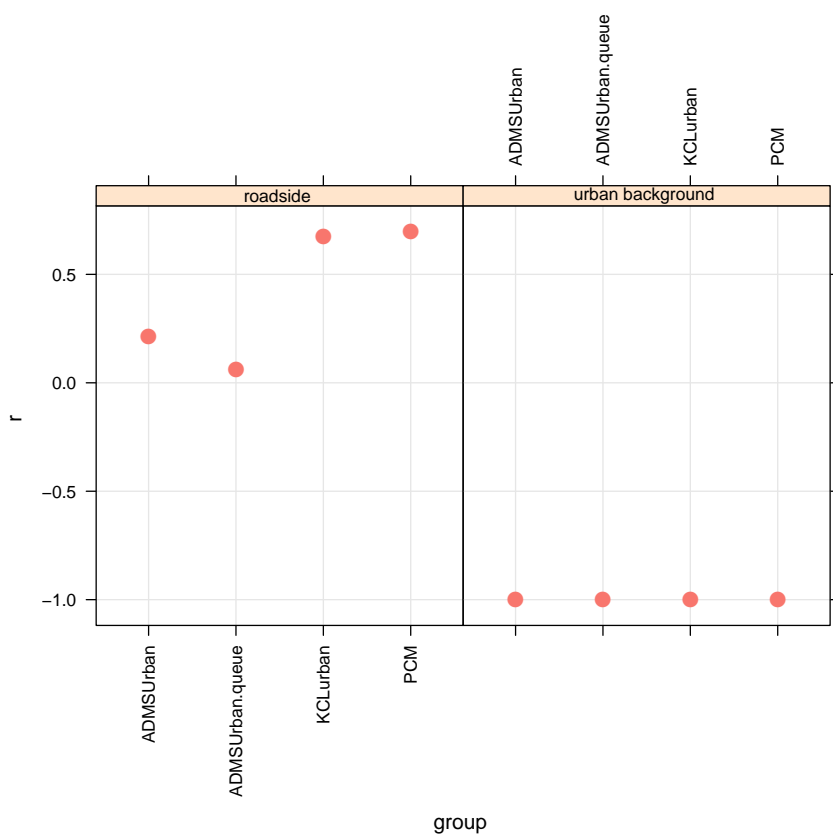


Figure 23: Graphical summary of the correlation coefficient, r , for each model by site type for $PM_{2.5}$.

4 Hourly analysis

4.1 Data preparation

This sections considers the hourly predictions from the KCL and CERC models. Neither BRUTAL nor the PCM models provide hourly outputs.

The KCL data are imported as follows.

```
## note different data order here
KCL.hourly <- import("KCLRoadsideNOxO3Hourly.csv")
```

```
      date1      date2      month      day      hour site.code site.name site.type
"POSIXct" "POSIXt" "integer" "integer" "integer" "factor" "factor" "factor"
      NOx      NO2      O3
"numeric" "numeric" "numeric"
```

```
KCL.hourly$group <- "KCLurbanCMAQ"
```

The CERC data are in several files and need some pre-processing. Missing data are shown as **-999**.

```
## data are sites by column; need to stack and combine
nox <- import("HourlyNOxCERC.csv", na.strings = "-999")
```

```

date1    date2    BL0    BX1    CD3    CR4    EA1    EA2
"POSIXct" "POSIXt" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
  EN1    GR4    HG1    KC1    LB4    LW2    TD0    TH1
"numeric" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
  TH2
"numeric"
```

```
## stack data
nox <- melt(nox, id.vars = "date")
names(nox) <- c("date", "site.code", "NOx")
## NO2
no2 <- import("HourlyNO2CERC.csv", na.strings = "-999")
```

```

date1    date2    BL0    BX1    CD3    CR4    EA1    EA2
"POSIXct" "POSIXt" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
  EN1    GR4    HG1    KC1    LB4    LW2    TD0    TH1
"numeric" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
  TH2
"numeric"
```

```
## stack data
no2 <- melt(no2, id.vars = "date")
names(no2) <- c("date", "site.code", "NO2")
## O3
o3 <- import("HourlyO3CERC.csv", na.strings = "-999")
```

```

date1    date2    BL0    BX1    EA1    EA2    GR4    KC1
"POSIXct" "POSIXt" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
  TD0    TH1
"numeric" "numeric"
```

```
## stack data
o3 <- melt(o3, id.vars = "date")
names(o3) <- c("date", "site.code", "O3")
## PM10
pm10 <- import("HourlyPM10CERC.csv", na.strings = "-999")
```

```

date1    date2    BL0    BX1    CD3    CR4    EA2    GR4
"POSIXct" "POSIXt" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
  HG1    KC1    LB4    LW2    TH1
"numeric" "numeric" "numeric" "numeric" "numeric"
```

```
## stack data
pm10 <- melt(pm10, id.vars = "date")
names(pm10) <- c("date", "site.code", "PM10")
## PM2.5
pm25 <- import("HourlyPM25CERC.csv", na.strings = "-999")
```

```

date1    date2    BL0    BX1    EA2    GR4    KC1    TD0
"POSIXct" "POSIXt" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
```

```
## stack data
pm25 <- melt(pm25, id.vars = "date")
names(pm25) <- c("date", "site.code", "PM2.5")
```

Now the data can be combined:


```
ADMSUrban.hourly <- rbind.fill(nox, no2, o3, pm10, pm25)
ADMSUrban.hourly$group <- "ADMSUrban"
```

Note also that CERC produced an alternative set of predictions that aimed to take better account of vehicle queuing. These data are imported as follows.

```
## data are sites by column; need to stack and combine
nox <- import("HourlyNOx(16Dec).csv", na.strings = "-999")
```

```

date1    date2    BL0    BX1    CD3    CR4    EA1    EA2
"POSIXct" "POSIXt" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
  EN1    GR4    HG1    KC1    LB4    LW2    TD0    TH1
"numeric" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
  TH2
"numeric"
```

```
## stack data
nox <- melt(nox, id.vars = "date")
names(nox) <- c("date", "site.code", "NOx")
## NO2
no2 <- import("HourlyNO2(16Dec).csv", na.strings = "-999")
```

```

date1    date2    BL0    BX1    CD3    CR4    EA1    EA2
"POSIXct" "POSIXt" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
  EN1    GR4    HG1    KC1    LB4    LW2    TD0    TH1
"numeric" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
  TH2
"numeric"
```

```
## stack data
no2 <- melt(no2, id.vars = "date")
names(no2) <- c("date", "site.code", "NO2")
## O3
o3 <- import("HourlyO3(16Dec).csv", na.strings = "-999")
```

```

date1    date2    BL0    BX1    EA1    EA2    GR4    KC1
"POSIXct" "POSIXt" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
  TD0    TH1
"numeric" "numeric"
```

```
## stack data
o3 <- melt(o3, id.vars = "date")
names(o3) <- c("date", "site.code", "O3")
## PM10
pm10 <- import("HourlyPM10(16Dec).csv", na.strings = "-999")
```

```

date1    date2    BL0    BX1    CD3    CR4    EA2    GR4
"POSIXct" "POSIXt" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
  HG1    KC1    LB4    LW2    TH1
"numeric" "numeric" "numeric" "numeric" "numeric"
```

```
## stack data
pm10 <- melt(pm10, id.vars = "date")
names(pm10) <- c("date", "site.code", "PM10")
## PM2.5
pm25 <- import("HourlyPM25(16Dec).csv", na.strings = "-999")
```

```

date1    date2    BL0    BX1    EA2    GR4    KC1    TD0
"POSIXct" "POSIXt" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
```

```
## stack data
pm25 <- melt(pm25, id.vars = "date")
names(pm25) <- c("date", "site.code", "PM2.5")
## combine and name
ADMSUrban.hourly.queue <- rbind.fill(nox, no2, o3, pm10, pm25)
ADMSUrban.hourly.queue$group <- "ADMSUrbanQueue"
```

The CERC and the KCL data can now be combined:

```
urban.hourly <- rbind.fill(ADMSUrban.hourly, KCL.hourly, ADMSUrban.hourly.queue)
```

These results need to be combined with measurements. These can be downloaded using the `importKCL` function as shown below. However, for the sake of speed, these data are imported from a pre-prepared file.

```
## to imprt using importKCL
urban.meas <- importKCL(site = c("BL0", "BX1", "CD3", "CR4", "EA1", "EA2", "EN1", "GR4", "HG1", "KC1", "LB4",
                                "LW2", "TD0", "TH1", "TH2"), year = 2008)
```

And to import pre-prepared values:

```
## this loads a data frame called urban.meas
load("urbanMeas.RData")
## rename some fields
urban.meas <- rename(urban.meas, c(nox = "nox.meas", no2 = "no2.meas", o3 = "o3.meas",
                                   pm10 = "pm10.meas", pm25 = "pm25.meas", code = "site.code"))
```

Finally, all these data can be combined, ready for processing.

```
urban.hourly <- merge(urban.hourly, urban.meas, by = c("date", "site.code"), all = TRUE)
## rename to make axes clearer
urban.hourly <- rename(urban.hourly, c(NOx = "nox.mod", NO2 = "no2.mod", O3 = "o3.mod",
                                       PM10 = "pm10.mod", PM2.5 = "pm25.mod"))
```

4.2 Evaluation metrics

First we consider the evaluation statistics by group and by site.

```
NOx.stats <- modStats(urban.hourly, type = c("group", "site"), obs = "nox.meas", mod = "nox.mod")
```

```
NO2.stats <- modStats(urban.hourly, type = c("group", "site"), obs = "no2.meas", mod = "no2.mod")
```

```
O3.stats <- modStats(urban.hourly, type = c("group", "site"), obs = "no2.meas", mod = "o3.mod")
```

```
PM10.stats <- modStats(urban.hourly, type = c("group", "site"), obs = "pm10.meas", mod = "pm10.mod")
```

Table 8: Summary model evaluation statistics for hourly mean NO_x.

group	site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
ADMSurban	Camden - Bloomsbury	8316	0.84	4.50	39.29	0.05	0.43	62.75	0.65
ADMSurban	Bexley - Slade Green	8175	0.75	-12.41	27.17	-0.23	0.50	54.58	0.60
ADMSurban	Camden - Shaftesbury Avenue	8250	0.74	-17.24	71.57	-0.10	0.43	101.05	0.55
ADMSurban	Croydon - George Street	8192	0.83	30.18	42.99	0.32	0.45	72.06	0.75
ADMSurban	Ealing - Ealing Town Hall	8291	0.75	18.67	36.99	0.29	0.58	64.18	0.67
ADMSurban	Ealing - Acton Town Hall	7307	0.80	-7.61	51.44	-0.06	0.42	81.90	0.66
ADMSurban	Enfield 1 - Bushhill Park	6782	0.77	-11.13	21.49	-0.24	0.46	44.13	0.60
ADMSurban	Greenwich - Eltham	8020	0.73	7.77	21.35	0.20	0.55	43.97	0.67
ADMSurban	Haringey - Haringey Town Hall	8326	0.83	-8.08	29.93	-0.11	0.41	59.06	0.68
ADMSurban	Kensington and Chelsea - North Ken	7592	0.63	24.12	34.55	0.50	0.71	55.59	0.64
ADMSurban	Lambeth - Brixton Road	7413	0.51	-259.34	275.59	-0.50	0.53	358.24	0.63
ADMSurban	Lewisham - New Cross	7914	0.70	-27.36	66.40	-0.19	0.45	99.31	0.64
ADMSurban	Richmond - National Physical Laboratory	8131	0.77	1.56	19.42	0.04	0.54	41.44	0.65
ADMSurban	Tower Hamlets - Poplar	8317	0.79	15.37	27.87	0.28	0.51	49.54	0.68
ADMSurban	Tower Hamlets - Mile End Road	8182	0.60	-60.36	69.61	-0.43	0.50	99.40	0.62
ADMSurban		0							
ADMSurbanQueue	Camden - Bloomsbury	8316	0.84	4.50	39.29	0.05	0.43	62.75	0.65
ADMSurbanQueue	Bexley - Slade Green	8175	0.75	-12.41	27.17	-0.23	0.50	54.58	0.60
ADMSurbanQueue	Camden - Shaftesbury Avenue	8250	0.74	-17.24	71.57	-0.10	0.43	101.05	0.55
ADMSurbanQueue	Croydon - George Street	8192	0.83	30.18	42.99	0.32	0.45	72.06	0.75
ADMSurbanQueue	Ealing - Ealing Town Hall	8291	0.75	18.67	36.99	0.29	0.58	64.18	0.67
ADMSurbanQueue	Ealing - Acton Town Hall	7307	0.80	-7.61	51.44	-0.06	0.42	81.90	0.66
ADMSurbanQueue	Enfield 1 - Bushhill Park	6782	0.77	-11.13	21.49	-0.24	0.46	44.13	0.60
ADMSurbanQueue	Greenwich - Eltham	8020	0.73	7.77	21.35	0.20	0.55	43.97	0.67
ADMSurbanQueue	Haringey - Haringey Town Hall	8326	0.83	-8.08	29.93	-0.11	0.41	59.06	0.68
ADMSurbanQueue	Kensington and Chelsea - North Ken	7592	0.63	24.12	34.55	0.50	0.71	55.59	0.64
ADMSurbanQueue	Lambeth - Brixton Road	7413	0.62	-181.51	237.07	-0.35	0.46	313.80	0.60
ADMSurbanQueue	Lewisham - New Cross	7914	0.70	-27.36	66.40	-0.19	0.45	99.31	0.64
ADMSurbanQueue	Richmond - National Physical Laboratory	8131	0.77	1.56	19.42	0.04	0.54	41.44	0.65
ADMSurbanQueue	Tower Hamlets - Poplar	8317	0.79	15.37	27.87	0.28	0.51	49.54	0.68
ADMSurbanQueue	Tower Hamlets - Mile End Road	8182	0.63	-35.59	68.99	-0.26	0.50	97.86	0.53
ADMSurbanQueue		0							
KCLurbanCMAQ	Camden - Bloomsbury	8175	0.78	-10.85	40.45	-0.12	0.43	62.79	0.60
KCLurbanCMAQ	Bexley - Slade Green	8027	0.70	-17.26	29.94	-0.31	0.54	59.47	0.56
KCLurbanCMAQ	Camden - Shaftesbury Avenue	8101	0.78	26.70	82.19	0.16	0.48	125.35	0.57
KCLurbanCMAQ	Croydon - George Street	8048	0.60	-40.86	48.03	-0.44	0.51	76.40	0.51
KCLurbanCMAQ	Ealing - Ealing Town Hall	8150	0.75	-19.63	32.32	-0.30	0.49	68.69	0.57
KCLurbanCMAQ	Ealing - Acton Town Hall	7454	0.70	-14.69	64.35	-0.11	0.50	104.40	0.53
KCLurbanCMAQ	Enfield 1 - Bushhill Park	6512	0.66	-13.09	25.20	-0.28	0.54	50.17	0.52
KCLurbanCMAQ	Greenwich - Eltham	7943	0.72	-6.23	21.39	-0.15	0.53	46.37	0.53
KCLurbanCMAQ	Haringey - Haringey Town Hall	8182	0.75	0.73	37.13	0.01	0.49	69.97	0.60
KCLurbanCMAQ	Kensington and Chelsea - North Ken	7365	0.72	1.18	26.04	0.02	0.54	47.46	0.49
KCLurbanCMAQ	Lambeth - Brixton Road	7234	0.75	-34.76	225.78	-0.07	0.43	325.74	0.61
KCLurbanCMAQ	Lewisham - New Cross	7789	0.64	-17.98	72.17	-0.12	0.49	105.95	0.60
KCLurbanCMAQ	Richmond - National Physical Laboratory	7992	0.73	-8.08	20.70	-0.22	0.56	46.55	0.49
KCLurbanCMAQ	Tower Hamlets - Poplar	8182	0.75	2.12	28.50	0.04	0.51	51.36	0.54
KCLurbanCMAQ	Tower Hamlets - Mile End Road	8036	0.72	38.20	77.52	0.28	0.56	113.70	0.58
KCLurbanCMAQ		0							

Table 9: Summary model evaluation statistics for hourly mean NO₂.

group	site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
ADMSurban	Camden - Bloomsbury	8316	0.91	-4.04	15.76	-0.07	0.29	21.05	0.66
ADMSurban	Bexley - Slade Green	8175	0.80	-5.52	12.53	-0.17	0.38	18.03	0.68
ADMSurban	Camden - Shaftesbury Avenue	8250	0.82	-12.86	27.02	-0.16	0.34	34.63	0.49
ADMSurban	Croydon - George Street	8192	0.93	4.83	15.50	0.10	0.31	23.87	0.74
ADMSurban	Ealing - Ealing Town Hall	8268	0.89	3.52	12.79	0.09	0.33	18.14	0.73
ADMSurban	Ealing - Acton Town Hall	7301	0.90	-3.74	18.21	-0.06	0.31	26.07	0.68
ADMSurban	Enfield 1 - Bushhill Park	6782	0.82	-4.84	11.06	-0.16	0.36	15.61	0.68
ADMSurban	Greenwich - Eltham	8019	0.80	3.61	10.57	0.14	0.41	16.45	0.71
ADMSurban	Haringey - Haringey Town Hall	8326	0.88	1.63	12.13	0.04	0.33	16.79	0.70
ADMSurban	Kensington and Chelsea - North Ken	7592	0.80	9.07	14.38	0.28	0.44	19.91	0.71
ADMSurban	Lambeth - Brixton Road	7412	0.48	-115.95	119.19	-0.53	0.55	151.02	0.53
ADMSurban	Lewisham - New Cross	7914	0.77	-11.65	25.05	-0.18	0.39	33.81	0.62
ADMSurban	Richmond - National Physical Laboratory	8131	0.79	0.60	10.11	0.02	0.42	16.24	0.72
ADMSurban	Tower Hamlets - Poplar	8317	0.91	3.42	11.85	0.09	0.32	16.94	0.73
ADMSurban	Tower Hamlets - Mile End Road	8182	0.76	-19.81	23.83	-0.31	0.38	30.77	0.61
ADMSurban		0							
ADMSurbanQueue	Camden - Bloomsbury	8316	0.91	-4.04	15.76	-0.07	0.29	21.05	0.66
ADMSurbanQueue	Bexley - Slade Green	8175	0.80	-5.52	12.53	-0.17	0.38	18.03	0.68
ADMSurbanQueue	Camden - Shaftesbury Avenue	8250	0.82	-12.86	27.02	-0.16	0.34	34.63	0.49
ADMSurbanQueue	Croydon - George Street	8192	0.93	4.83	15.50	0.10	0.31	23.87	0.74
ADMSurbanQueue	Ealing - Ealing Town Hall	8268	0.89	3.52	12.79	0.09	0.33	18.14	0.73
ADMSurbanQueue	Ealing - Acton Town Hall	7301	0.90	-3.74	18.21	-0.06	0.31	26.07	0.68
ADMSurbanQueue	Enfield 1 - Bushhill Park	6782	0.82	-4.84	11.06	-0.16	0.36	15.61	0.68
ADMSurbanQueue	Greenwich - Eltham	8019	0.80	3.61	10.57	0.14	0.41	16.45	0.71
ADMSurbanQueue	Haringey - Haringey Town Hall	8326	0.88	1.63	12.13	0.04	0.33	16.79	0.70
ADMSurbanQueue	Kensington and Chelsea - North Ken	7592	0.80	9.07	14.38	0.28	0.44	19.91	0.71
ADMSurbanQueue	Lambeth - Brixton Road	7412	0.61	-91.93	102.88	-0.42	0.47	133.35	0.53
ADMSurbanQueue	Lewisham - New Cross	7914	0.77	-11.65	25.05	-0.18	0.39	33.81	0.62
ADMSurbanQueue	Richmond - National Physical Laboratory	8131	0.79	0.60	10.11	0.02	0.42	16.24	0.72
ADMSurbanQueue	Tower Hamlets - Poplar	8317	0.91	3.42	11.85	0.09	0.32	16.94	0.73
ADMSurbanQueue	Tower Hamlets - Mile End Road	8182	0.79	-12.66	22.90	-0.20	0.36	30.19	0.55
ADMSurbanQueue		0							
KCLurbanCMAQ	Camden - Bloomsbury	8175	0.90	-2.83	16.52	-0.05	0.30	21.85	0.60
KCLurbanCMAQ	Bexley - Slade Green	8027	0.80	-1.93	12.83	-0.06	0.39	17.67	0.63
KCLurbanCMAQ	Camden - Shaftesbury Avenue	8101	0.93	0.69	24.18	0.01	0.30	31.97	0.48
KCLurbanCMAQ	Croydon - George Street	8048	0.76	-14.14	18.95	-0.28	0.38	25.10	0.62
KCLurbanCMAQ	Ealing - Ealing Town Hall	8127	0.85	-3.75	13.03	-0.10	0.34	18.27	0.67
KCLurbanCMAQ	Ealing - Acton Town Hall	7448	0.84	-1.16	22.15	-0.02	0.37	31.25	0.56
KCLurbanCMAQ	Enfield 1 - Bushhill Park	6512	0.73	-2.87	12.94	-0.10	0.43	17.49	0.59
KCLurbanCMAQ	Greenwich - Eltham	7942	0.77	2.03	11.12	0.08	0.43	15.90	0.65
KCLurbanCMAQ	Haringey - Haringey Town Hall	8182	0.79	10.60	16.68	0.29	0.46	21.97	0.67
KCLurbanCMAQ	Kensington and Chelsea - North Ken	7365	0.79	3.93	13.75	0.12	0.42	18.84	0.61
KCLurbanCMAQ	Lambeth - Brixton Road	7233	0.78	-48.26	85.50	-0.22	0.39	113.90	0.55
KCLurbanCMAQ	Lewisham - New Cross	7789	0.77	1.01	25.78	0.02	0.41	35.07	0.55
KCLurbanCMAQ	Richmond - National Physical Laboratory	7992	0.74	0.03	11.32	0.00	0.47	17.17	0.62
KCLurbanCMAQ	Tower Hamlets - Poplar	8182	0.86	5.27	13.83	0.14	0.37	18.34	0.64
KCLurbanCMAQ	Tower Hamlets - Mile End Road	8036	0.88	13.35	22.07	0.21	0.35	28.31	0.67
KCLurbanCMAQ		0							

Table 10: Summary model evaluation statistics for hourly mean O₃.

group	site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
ADMSurban	Camden - Bloomsbury	8246	0.66	2.10	11.02	0.07	0.39	14.75	0.78
ADMSurban	Bexley - Slade Green	8097	0.76	-0.45	11.69	-0.01	0.27	16.21	0.82
ADMSurban	Camden - Shaftesbury Avenue	0							
ADMSurban	Croydon - George Street	0							
ADMSurban	Ealing - Ealing Town Hall	8277	0.70	-1.34	11.06	-0.04	0.31	15.49	0.80
ADMSurban	Ealing - Acton Town Hall	8046	0.57	10.80	14.10	0.46	0.60	18.20	0.77
ADMSurban	Enfield 1 - Bushhill Park	0							
ADMSurban	Greenwich - Eltham	8086	0.76	0.74	10.73	0.02	0.27	14.85	0.83
ADMSurban	Haringey - Haringey Town Hall	0							
ADMSurban	Kensington and Chelsea - North Ken	8281	0.69	-5.69	12.07	-0.15	0.31	17.38	0.80
ADMSurban	Lambeth - Brixton Road	0							
ADMSurban	Lewisham - New Cross	0							
ADMSurban	Richmond - National Physical Laboratory	8247	0.79	-3.14	11.66	-0.07	0.24	16.60	0.82
ADMSurban	Tower Hamlets - Poplar	8306	0.69	-5.90	12.46	-0.14	0.31	17.48	0.81
ADMSurban	Tower Hamlets - Mile End Road	0							
ADMSurban		0							
ADMSurbanQueue	Camden - Bloomsbury	8246	0.66	2.10	11.02	0.07	0.39	14.75	0.78
ADMSurbanQueue	Bexley - Slade Green	8097	0.76	-0.45	11.69	-0.01	0.27	16.21	0.82
ADMSurbanQueue	Camden - Shaftesbury Avenue	0							
ADMSurbanQueue	Croydon - George Street	0							
ADMSurbanQueue	Ealing - Ealing Town Hall	8277	0.70	-1.34	11.06	-0.04	0.31	15.49	0.80
ADMSurbanQueue	Ealing - Acton Town Hall	8046	0.57	10.80	14.10	0.46	0.60	18.20	0.77
ADMSurbanQueue	Enfield 1 - Bushhill Park	0							
ADMSurbanQueue	Greenwich - Eltham	8086	0.76	0.74	10.73	0.02	0.27	14.85	0.83
ADMSurbanQueue	Haringey - Haringey Town Hall	0							
ADMSurbanQueue	Kensington and Chelsea - North Ken	8281	0.69	-5.69	12.07	-0.15	0.31	17.38	0.80
ADMSurbanQueue	Lambeth - Brixton Road	0							
ADMSurbanQueue	Lewisham - New Cross	0							
ADMSurbanQueue	Richmond - National Physical Laboratory	8247	0.79	-3.14	11.66	-0.07	0.24	16.60	0.82
ADMSurbanQueue	Tower Hamlets - Poplar	8306	0.69	-5.90	12.46	-0.14	0.31	17.48	0.81
ADMSurbanQueue	Tower Hamlets - Mile End Road	0							
ADMSurbanQueue		0							
KCLurbanCMAQ	Camden - Bloomsbury	8104	0.58	7.14	16.17	0.25	0.57	20.84	0.58
KCLurbanCMAQ	Bexley - Slade Green	7947	0.67	6.95	19.36	0.16	0.45	24.90	0.55
KCLurbanCMAQ	Camden - Shaftesbury Avenue	0							
KCLurbanCMAQ	Croydon - George Street	0							
KCLurbanCMAQ	Ealing - Ealing Town Hall	8129	0.63	12.04	19.03	0.34	0.54	24.03	0.61
KCLurbanCMAQ	Ealing - Acton Town Hall	7813	0.51	14.63	18.20	0.62	0.77	22.30	0.62
KCLurbanCMAQ	Enfield 1 - Bushhill Park	0							
KCLurbanCMAQ	Greenwich - Eltham	7941	0.67	12.38	20.69	0.31	0.52	25.95	0.53
KCLurbanCMAQ	Haringey - Haringey Town Hall	0							
KCLurbanCMAQ	Kensington and Chelsea - North Ken	8140	0.64	6.05	18.39	0.16	0.48	23.89	0.58
KCLurbanCMAQ	Lambeth - Brixton Road	0							
KCLurbanCMAQ	Lewisham - New Cross	0							
KCLurbanCMAQ	Richmond - National Physical Laboratory	8106	0.74	7.57	19.11	0.16	0.40	24.69	0.56
KCLurbanCMAQ	Tower Hamlets - Poplar	8171	0.64	0.58	18.18	0.01	0.45	23.81	0.55
KCLurbanCMAQ	Tower Hamlets - Mile End Road	0							
KCLurbanCMAQ		0							

Table 11: Summary model evaluation statistics for hourly mean PM₁₀.

group	site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
ADMSurban	Camden - Bloomsbury	6734	0.90	0.76	7.21	0.03	0.32	10.63	0.68
ADMSurban	Bexley - Slade Green	8099	0.83	3.11	7.15	0.17	0.39	10.21	0.65
ADMSurban	Camden - Shaftesbury Avenue	8291	0.86	-4.06	10.00	-0.14	0.34	15.09	0.53
ADMSurban	Croydon - George Street	8296	0.88	2.69	7.41	0.12	0.33	10.74	0.67
ADMSurban	Ealing - Ealing Town Hall	0							
ADMSurban	Ealing - Acton Town Hall	8300	0.91	0.33	7.38	0.01	0.31	11.17	0.69
ADMSurban	Enfield 1 - Bushhill Park	0							
ADMSurban	Greenwich - Eltham	7848	0.89	0.56	6.96	0.03	0.33	10.70	0.63
ADMSurban	Haringey - Haringey Town Hall	5436	0.87	2.69	7.60	0.13	0.36	10.98	0.66
ADMSurban	Kensington and Chelsea - North Ken	8213	0.88	1.68	6.92	0.08	0.33	10.25	0.68
ADMSurban	Lambeth - Brixton Road	6345	0.90	-6.75	11.75	-0.18	0.32	22.90	0.43
ADMSurban	Lewisham - New Cross	7879	0.90	-0.42	7.73	-0.02	0.31	11.52	0.66
ADMSurban	Richmond - National Physical Laboratory	0							
ADMSurban	Tower Hamlets - Poplar	8321	0.90	-0.00	7.06	-0.00	0.31	10.72	0.67
ADMSurban	Tower Hamlets - Mile End Road	0							
ADMSurban		0							
ADMSurbanQueue	Camden - Bloomsbury	6734	0.90	0.76	7.21	0.03	0.32	10.63	0.68
ADMSurbanQueue	Bexley - Slade Green	8099	0.83	3.11	7.15	0.17	0.39	10.21	0.65
ADMSurbanQueue	Camden - Shaftesbury Avenue	8291	0.86	-4.06	10.00	-0.14	0.34	15.09	0.53
ADMSurbanQueue	Croydon - George Street	8296	0.88	2.69	7.41	0.12	0.33	10.74	0.67
ADMSurbanQueue	Ealing - Ealing Town Hall	0							
ADMSurbanQueue	Ealing - Acton Town Hall	8300	0.91	0.33	7.38	0.01	0.31	11.17	0.69
ADMSurbanQueue	Enfield 1 - Bushhill Park	0							
ADMSurbanQueue	Greenwich - Eltham	7848	0.89	0.56	6.96	0.03	0.33	10.70	0.63
ADMSurbanQueue	Haringey - Haringey Town Hall	5436	0.87	2.69	7.60	0.13	0.36	10.98	0.66
ADMSurbanQueue	Kensington and Chelsea - North Ken	8213	0.88	1.68	6.92	0.08	0.33	10.25	0.68
ADMSurbanQueue	Lambeth - Brixton Road	6345	0.88	-2.22	13.03	-0.06	0.36	23.47	0.38
ADMSurbanQueue	Lewisham - New Cross	7879	0.90	-0.42	7.73	-0.02	0.31	11.52	0.66
ADMSurbanQueue	Richmond - National Physical Laboratory	0							
ADMSurbanQueue	Tower Hamlets - Poplar	8321	0.90	-0.00	7.06	-0.00	0.31	10.72	0.67
ADMSurbanQueue	Tower Hamlets - Mile End Road	0							
ADMSurbanQueue		0							
KCLurbanCMAQ	Camden - Bloomsbury	0							
KCLurbanCMAQ	Bexley - Slade Green	0							
KCLurbanCMAQ	Camden - Shaftesbury Avenue	0							
KCLurbanCMAQ	Croydon - George Street	0							
KCLurbanCMAQ	Ealing - Ealing Town Hall	0							
KCLurbanCMAQ	Ealing - Acton Town Hall	0							
KCLurbanCMAQ	Enfield 1 - Bushhill Park	0							
KCLurbanCMAQ	Greenwich - Eltham	0							
KCLurbanCMAQ	Haringey - Haringey Town Hall	0							
KCLurbanCMAQ	Kensington and Chelsea - North Ken	0							
KCLurbanCMAQ	Lambeth - Brixton Road	0							
KCLurbanCMAQ	Lewisham - New Cross	0							
KCLurbanCMAQ	Richmond - National Physical Laboratory	0							
KCLurbanCMAQ	Tower Hamlets - Poplar	0							
KCLurbanCMAQ	Tower Hamlets - Mile End Road	0							
KCLurbanCMAQ		0							

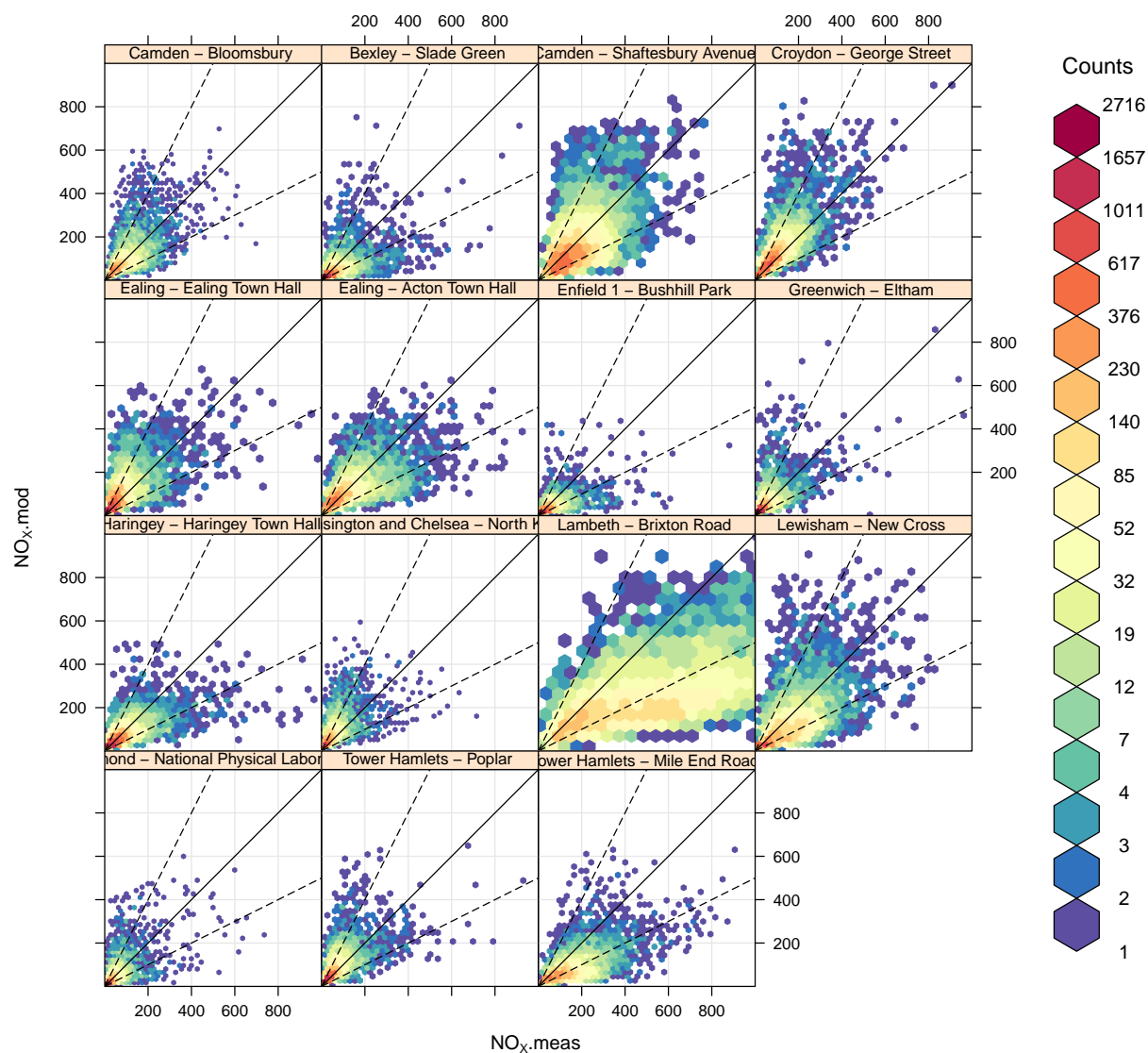


Figure 24: Scatter plot of measured vs. modelled NO_x concentrations using the CERC model.

4.3 Scatter plots

```
scatterPlot(subset(urban.hourly, group == "ADMSUrban"), x = "nox.meas", y = "nox.mod", mod.line = TRUE,
            type = "site", method = "hexbin", xlim = c(0, 1000), ylim = c(0, 1000))
```

```
scatterPlot(subset(urban.hourly, group == "ADMSUrbanQueue"), x = "nox.meas", y = "nox.mod", mod.line = TRUE,
            type = "site", method = "hexbin", xlim = c(0, 1000), ylim = c(0, 1000))
```

```
scatterPlot(subset(urban.hourly, group == "KCLUrbanCMAQ"), x = "nox.meas", y = "nox.mod", mod.line = TRUE,
            type = "site", method = "hexbin", xlim = c(0, 1000), ylim = c(0, 1000))
```

```
scatterPlot(subset(urban.hourly, group == "ADMSUrban"), x = "no2.meas", y = "no2.mod", mod.line = TRUE,
            type = "site", method = "hexbin", xlim = c(0, 600), ylim = c(0, 600))
```

```
scatterPlot(subset(urban.hourly, group == "KCLUrbanCMAQ"), x = "no2.meas", y = "no2.mod", mod.line = TRUE,
            type = "site", method = "hexbin", xlim = c(0, 600), ylim = c(0, 600))
```

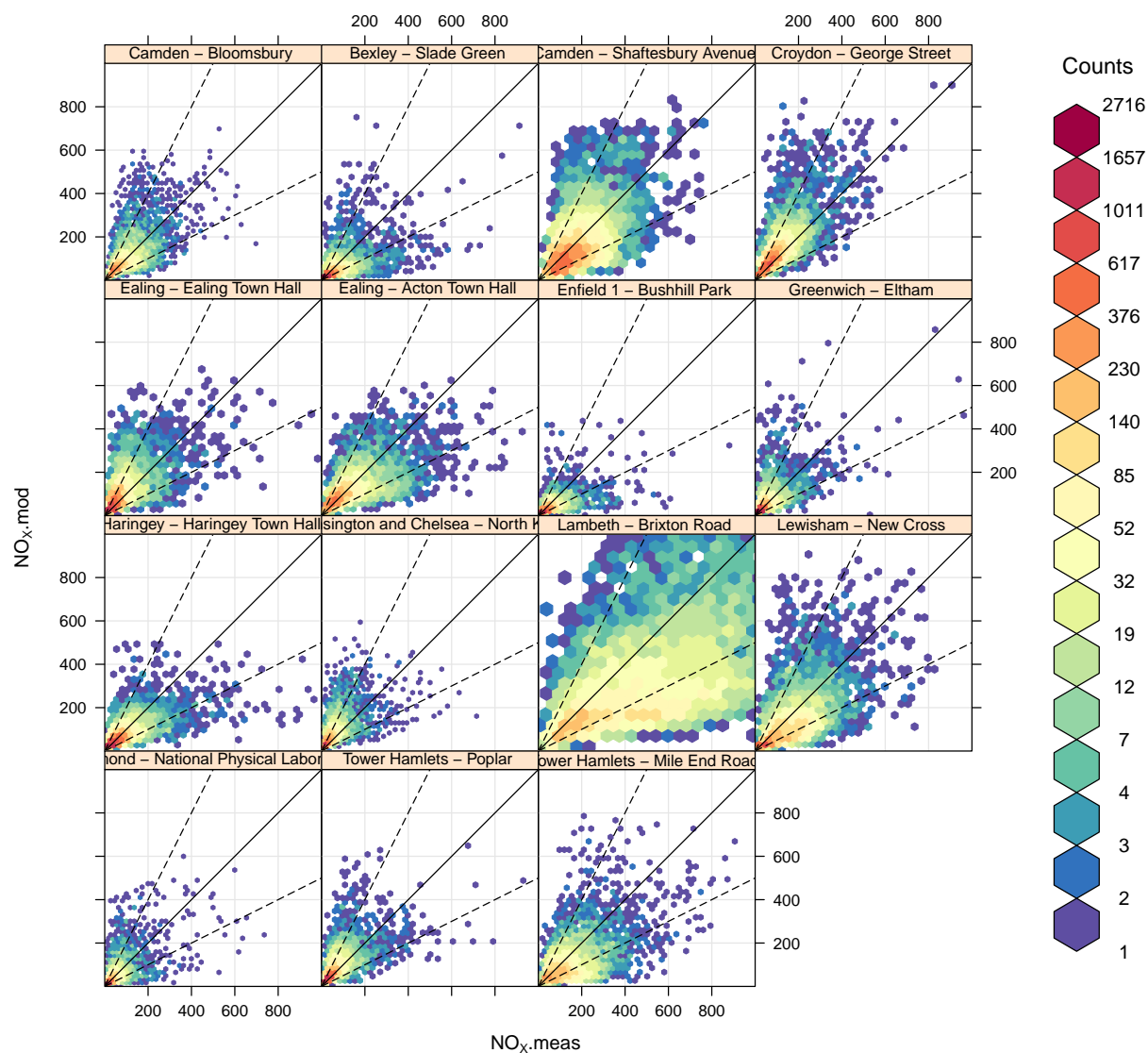



Figure 25: Scatter plot of measured vs. modelled NO_x concentrations using the CERC queue model.

```
scatterPlot(subset(urban.hourly, group == "ADMSurban"), x = "o3.meas", y = "o3.mod", mod.line = TRUE,
            type = "site", method = "hexbin", xlim = c(0, 180), ylim = c(0, 180))
```

```
scatterPlot(subset(urban.hourly, group == "KCLurbanCMAQ"), x = "o3.meas", y = "o3.mod", mod.line = TRUE,
            type = "site", method = "hexbin", xlim = c(0, 180), ylim = c(0, 180))
```

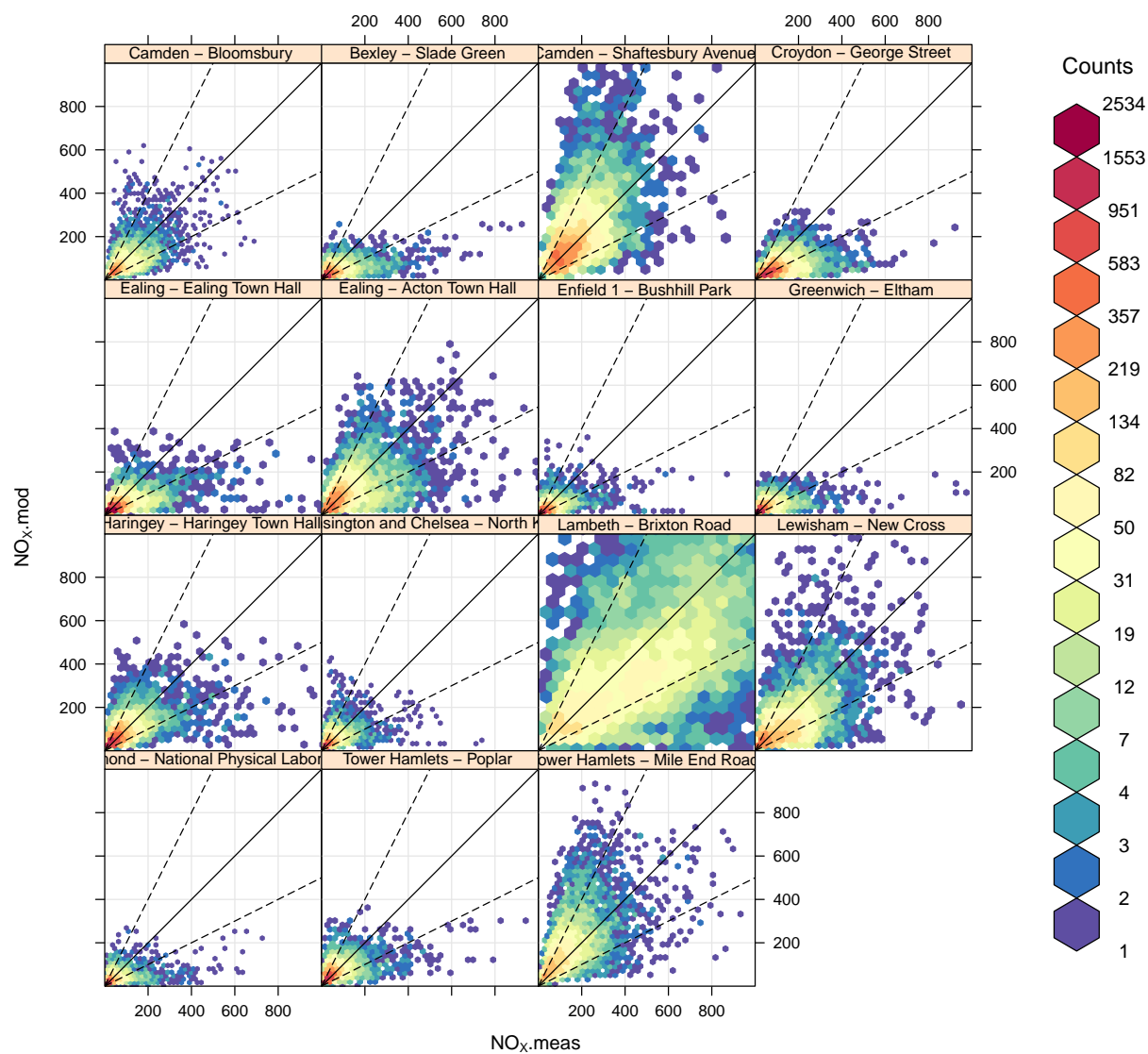


Figure 26: Scatter plot of measured vs. modelled NO_x concentrations using the KCL model.

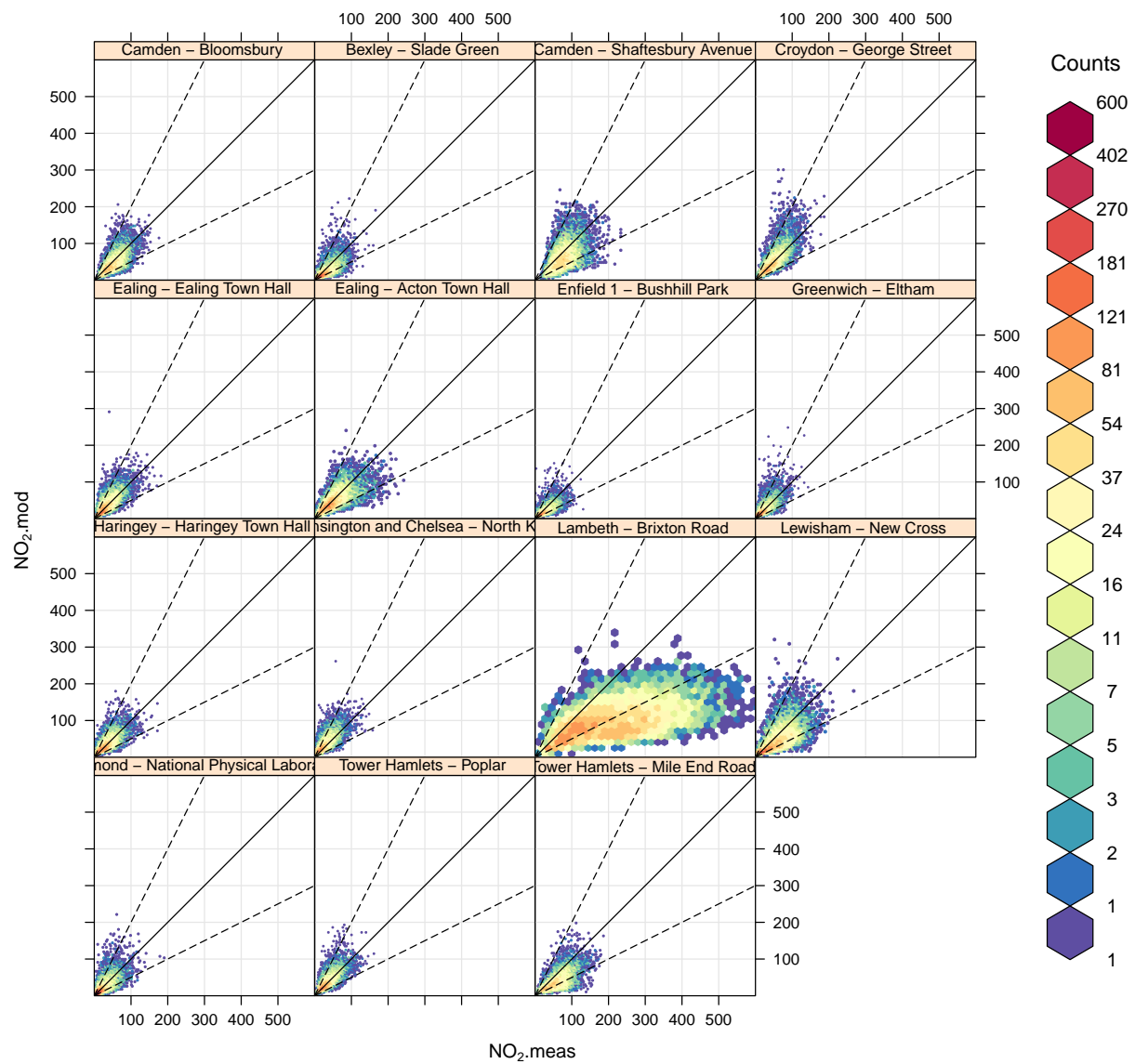


Figure 27: Scatter plot of measured vs. modelled NO₂ concentrations using the CERC model.

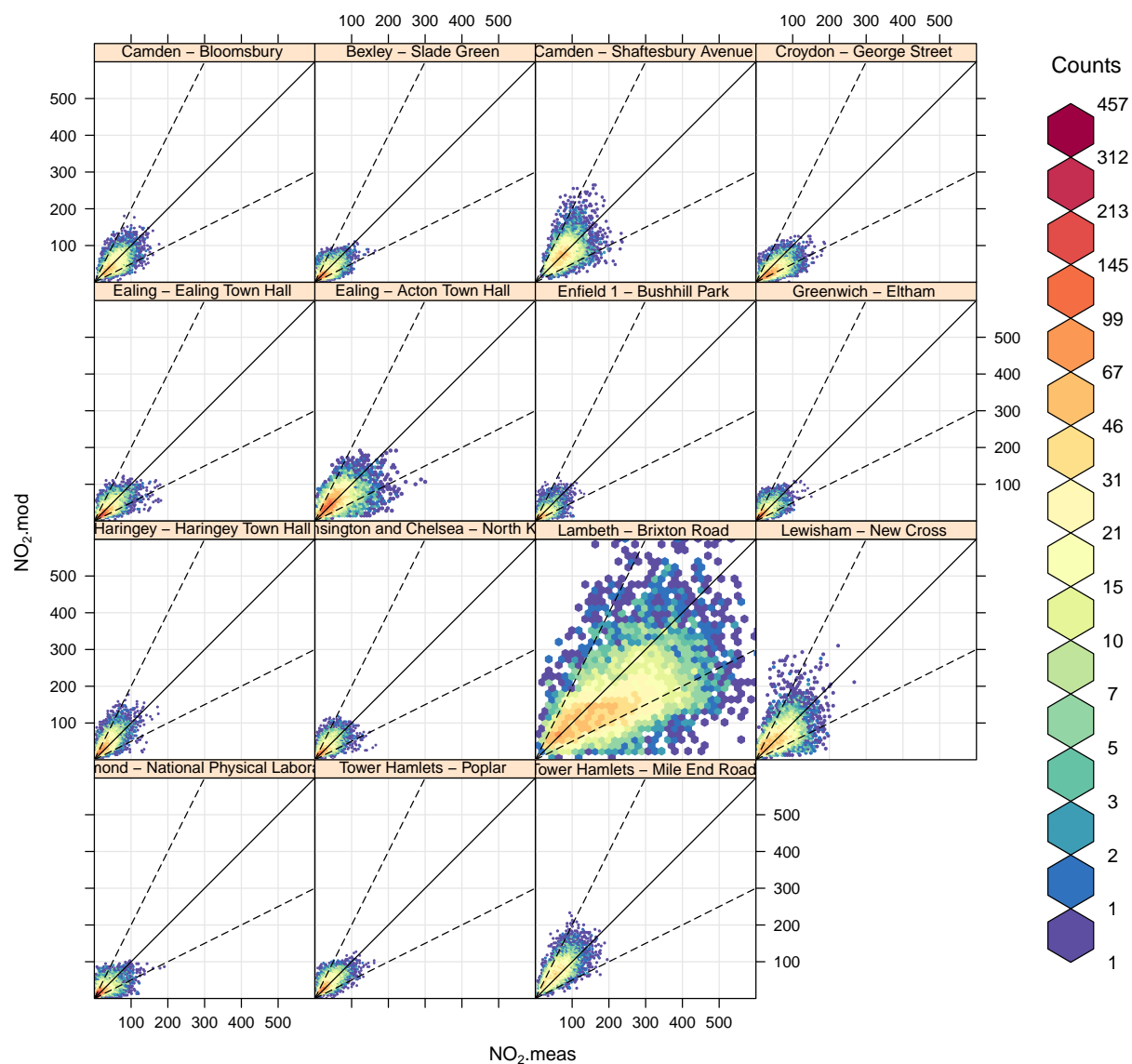


Figure 28: Scatter plot of measured vs. modelled NO_2 concentrations using the KCL model.

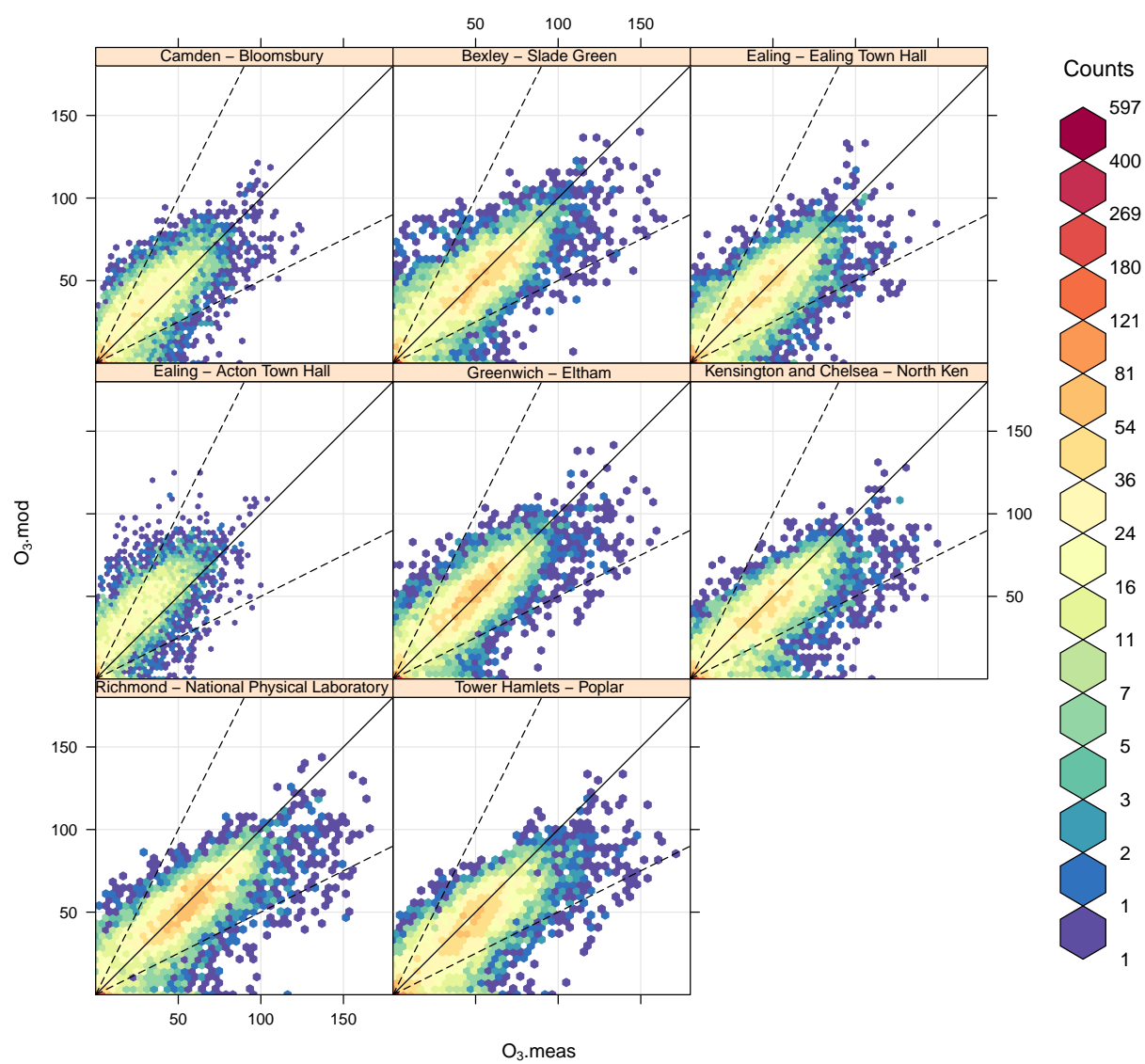


Figure 29: Scatter plot of measured vs. modelled O₃ concentrations using the CERC model.

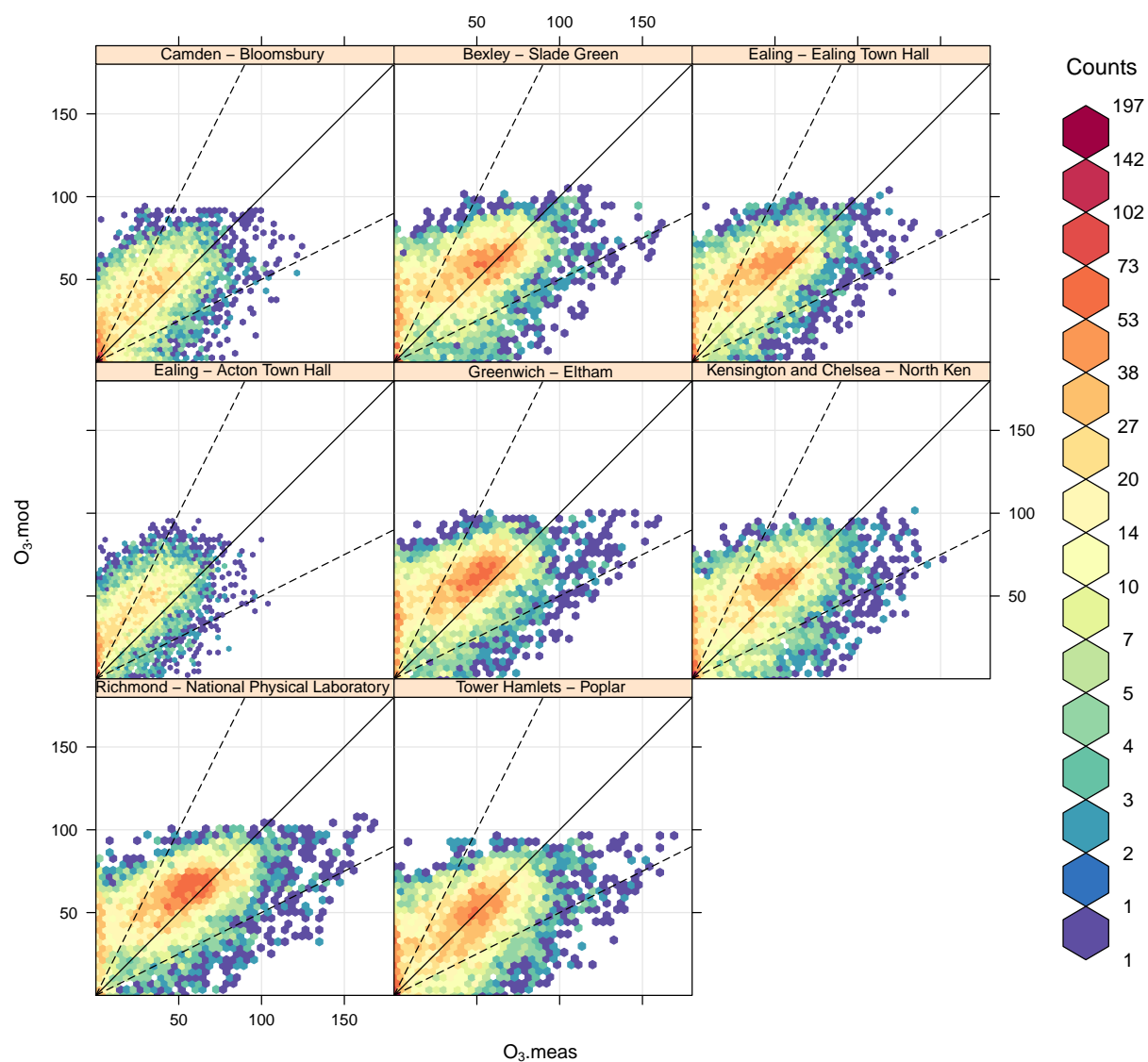


Figure 30: Scatter plot of measured vs. modelled O_3 concentrations using the KCL model.

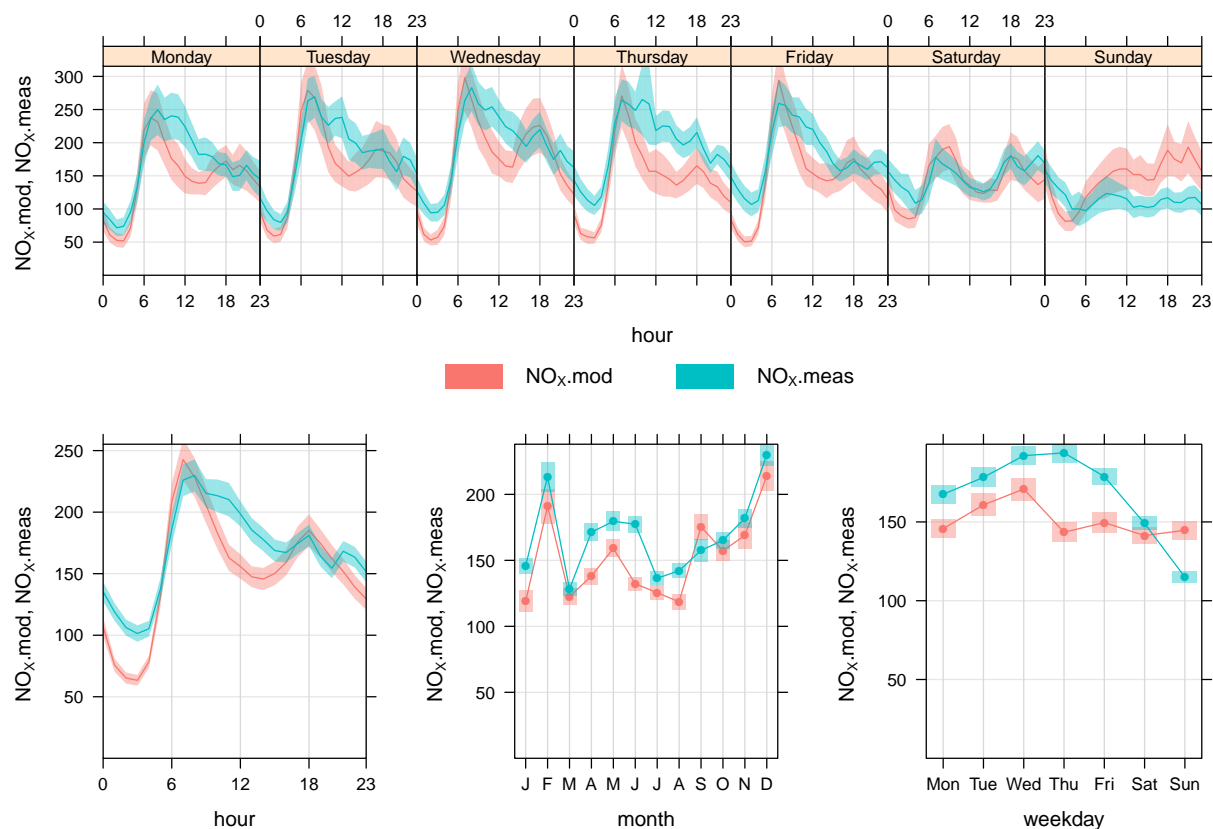


Figure 31: Temporal variations in NO_x at the Shaftesbury Avenue site using the CERC model.

4.4 Temporal variations

With so many sites to consider, only two have been chosen for plotting here: the Ealing Town Hall site (EA1, urban background) and the Camden Shaftesbury Avenue site (CD3, roadside).

```
timeVariation(subset(urban.hourly, site.code == "CD3" & group == "ADMSurban"),
  pollutant = c("nox.mod", "nox.meas"), ylim = c(0, NA))
```

```
timeVariation(subset(urban.hourly, site.code == "CD3" & group == "KCLurbanCMAQ"),
  pollutant = c("nox.mod", "nox.meas"), ylim = c(0, NA))
```

```
timeVariation(subset(urban.hourly, site.code == "GR4" & group == "ADMSurban"),
  pollutant = c("nox.mod", "nox.meas"), ylim = c(0, NA))
```

```
timeVariation(subset(urban.hourly, site.code == "GR4" & group == "KCLurbanCMAQ"),
  pollutant = c("nox.mod", "nox.meas"), ylim = c(0, NA))
```

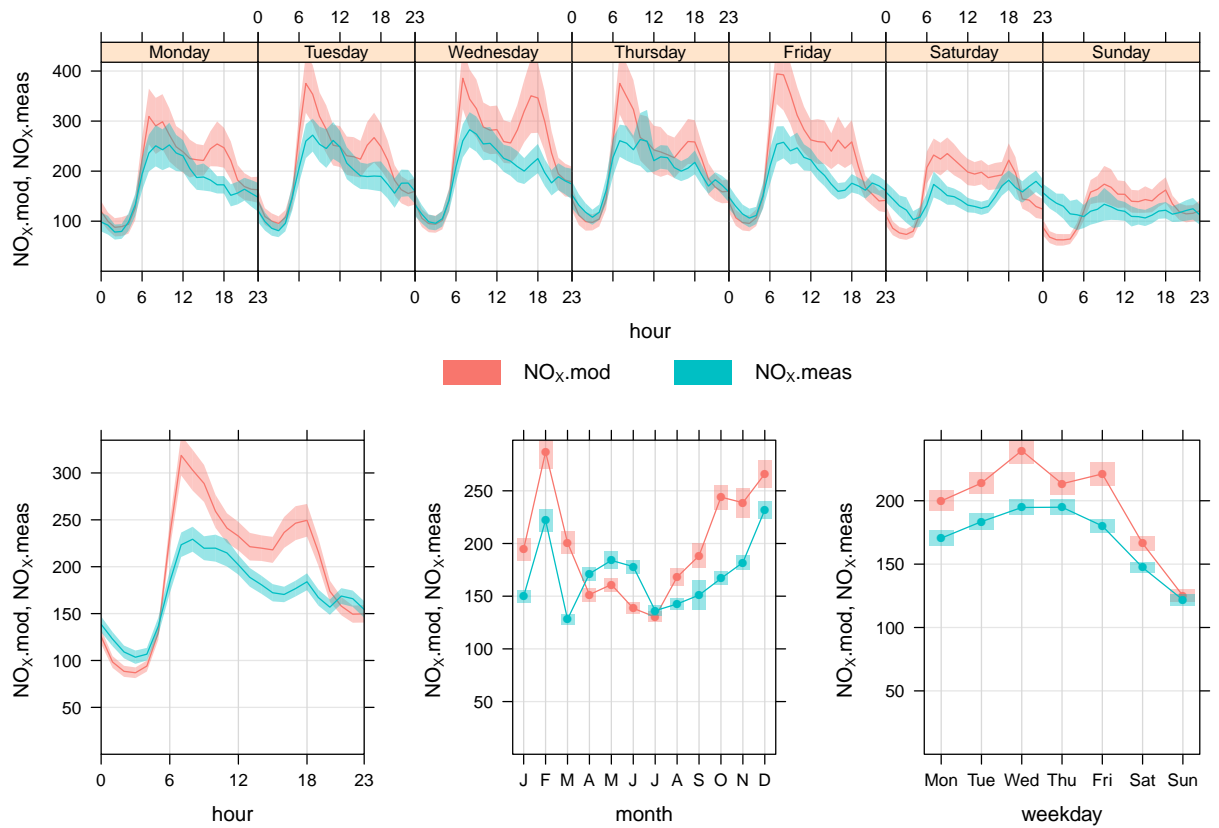


Figure 32: Temporal variations in NO_x at the Shaftesbury Avenue site using the KCL-CMAQ model.

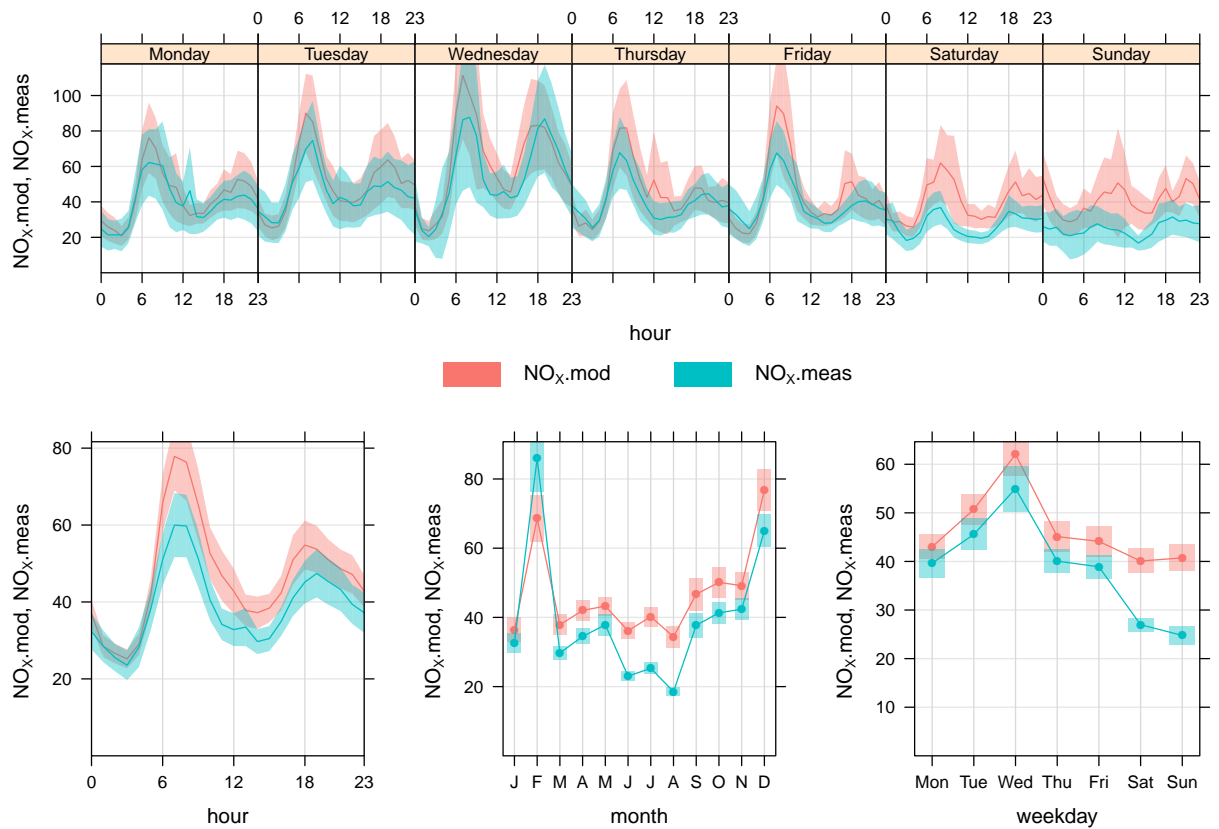


Figure 33: Temporal variations in NO_x at the Greenwich Eltham site using the CERC model.

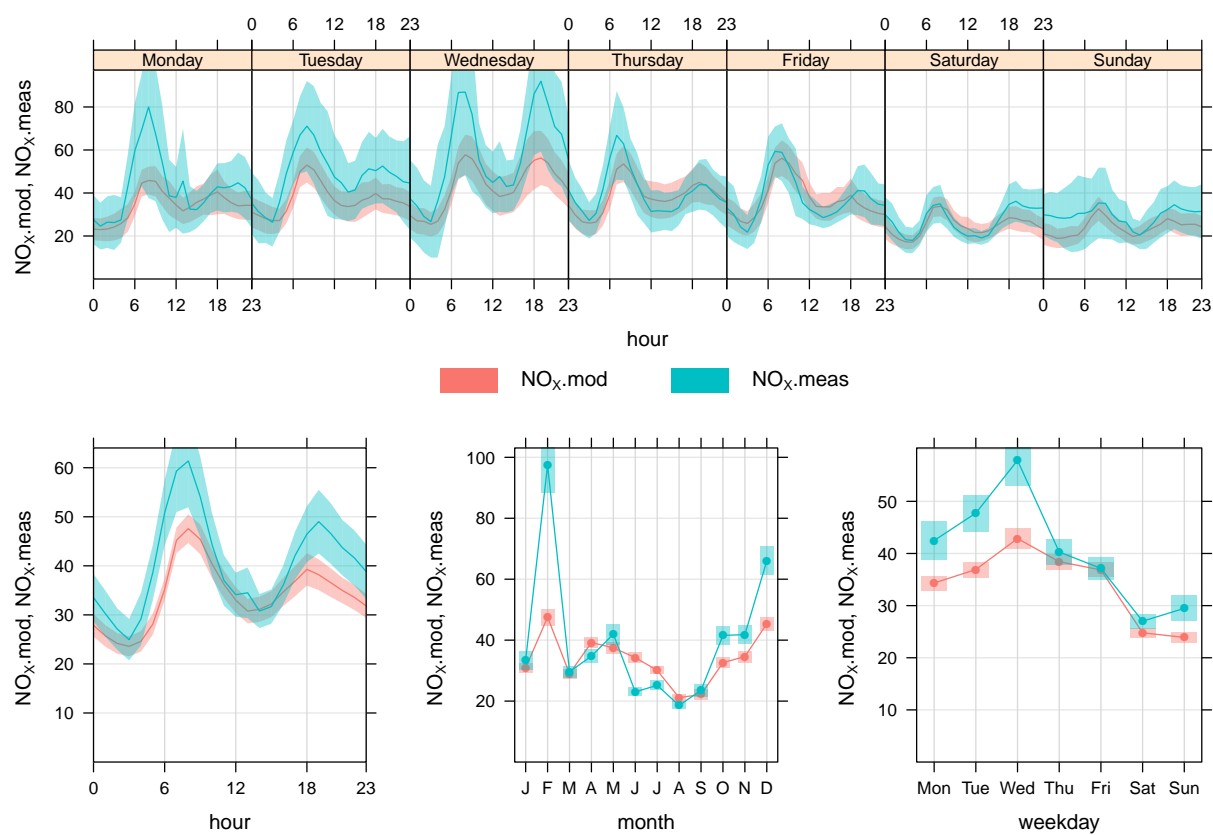


Figure 34: Temporal variations in NO_x at the Greenwich Eltham site using the KCL-CMAQ model.

4.5 Conditional quantiles

Conditional quantiles are a very useful way of considering model performance against observations for continuous measurements [Wilks \(2005\)](#). The conditional quantile plot splits the data into evenly spaced bins. For each predicted value bin e.g. from 0 to 10 $\mu\text{g m}^{-3}$ the *corresponding* values of the observations are identified and the median, 25/75th and 10/90 percentile (quantile) calculated for that bin. The data are plotted to show how these values vary across all bins. For a time series of observations and predictions that agree precisely the median value of the predictions will equal that for the observations for each bin.

The conditional quantile plot differs from the quantile-quantile plot (Q-Q plot) that is often used to compare observations and predictions. A Q-Q plot separately considers the distributions of observations and predictions, whereas the conditional quantile uses the corresponding observations for a particular interval in the predictions. Take as an example two time series, the first a series of real observations and the second a lagged time series of the same observations representing the predictions. These two time series will have identical (or very nearly identical) distributions (e.g. same median, minimum and maximum). A Q-Q plot would show a straight line showing perfect agreement, whereas the conditional quantile will not. This is because in any interval of the predictions the corresponding observations now have different values.

Plotting the data in this way shows how well predictions agree with observations and can help reveal many useful characteristics of how well model predictions agree with observations — across the full distribution of values. A single plot can therefore convey a considerable amount of information concerning model performance. The `conditionalQuantile` function in **openair** allows conditional quantiles to be considered in a flexible way e.g. by considering how they vary by season. We first demonstrate the usage with some sample data before applying it to the urban data.

First, the data are extracted and then plotted as shown in [Figure 35](#). In addition to the text in the caption, these results show that there is a tendency for the model to over estimate NO_x concentrations as the concentrations increase (as seen by the divergence of the red line from the blue line for increasingly high NO_x). The other point to note in [Figure 35](#) is that the percentile shading shows that the predictions become increasingly worse as the concentration of NO_x increases, as shown by their broadening.

A comprehensive analysis would consider each site separately for each pollutant. However, given the time available we only consider results across all receptors split by model used.

In the following plots ([Figure 36](#) to [Figure 40](#)) the following points can be made.

NO_x — [Figure 36](#) The ADMS Urban queue model does a better job of capturing higher concentrations than the base ADMS Urban model. There is a tendency for higher NO_x concentrations in the KCLurbanCMAQ model to be under estimated.

NO_2 — [Figure 37](#) Again the ADMS Urban queue model captures the higher concentrations better than the base model.

O_3 — [Figure 38](#) These results show that the ADMS Urban models do well in capturing O_3 concentrations across the full range of observed values. This is shown by how close the median line is to the blue (perfect model) line. The KCLurbanCMAQ are not as good as they have broader percentile distributions and the higher concentrations are not captured as well as the ADMS Urban models.

PM_{10} — [Figure 39](#) Hourly PM_{10} concentrations seem to be difficult to capture as these plots show that the higher concentrations are not predicted well and the percentile ranges are broad.

$\text{PM}_{2.5}$ — [Figure 40](#) The results for $\text{PM}_{2.5}$ are better than for PM_{10} , although again the higher concentrations are not as well predicted.

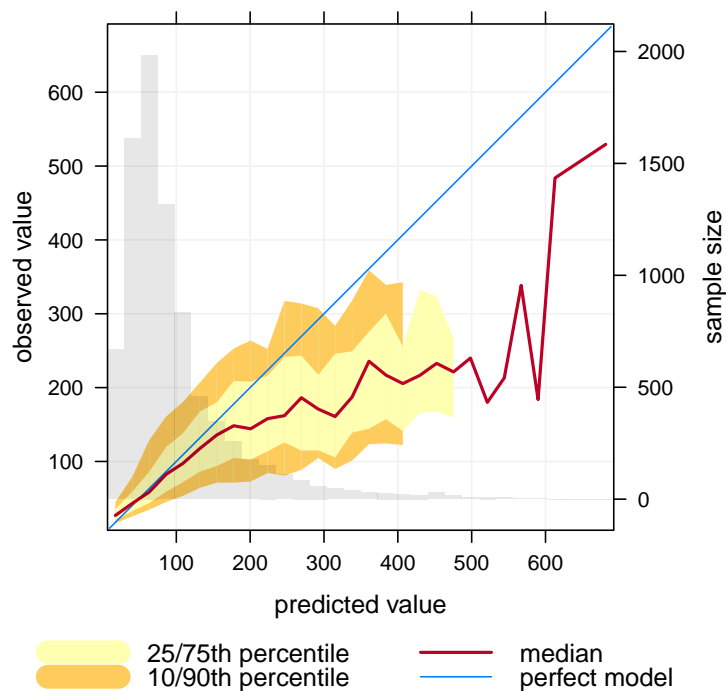


Figure 35: Example of the use of conditional quantiles applied to the ADMS Urban model at London Bloomsbury for hourly NO_x concentrations. The blue line shows the results for a perfect model. In this case the observations cover a range from 0 to $700 \mu\text{g m}^{-3}$. The red line shows the median value of the predictions. The maximum predicted value is close to $700 \mu\text{g m}^{-3}$, which shows the range of predictions from the model is similar to that of the observations. The shading shows the predicted quantile intervals i.e. the 25/75th and the 10/90th. A perfect model would lie on the blue line and have a very narrow spread. There is still some spread because even for a perfect model a specific quantile interval will contain a range of values. However, for the number of bins used in this plot the spread will be very narrow. Finally, the histogram shows the counts of predicted values.

Note that much more interpretation would be possible with other analysis e.g. by site, by day of the week and so on, that might help better understand the conditions under which model performance is poor.

```
conditionalQuantile(subset(urban.hourly, site.code == "BL0" & group == "ADMSurban"),
  obs = "nox.meas", mod = "nox.mod")
```

```
conditionalQuantile(urban.hourly, obs = "nox.meas", mod = "nox.mod", type = "group")
```

```
conditionalQuantile(urban.hourly, obs = "no2.meas", mod = "no2.mod", type = "group")
```

```
conditionalQuantile(urban.hourly, obs = "o3.meas", mod = "o3.mod", type = "group")
```

```
conditionalQuantile(urban.hourly, obs = "pm10.meas", mod = "pm10.mod", type = "group")
```

```
conditionalQuantile(urban.hourly, obs = "pm25.meas", mod = "pm25.mod", type = "group")
```

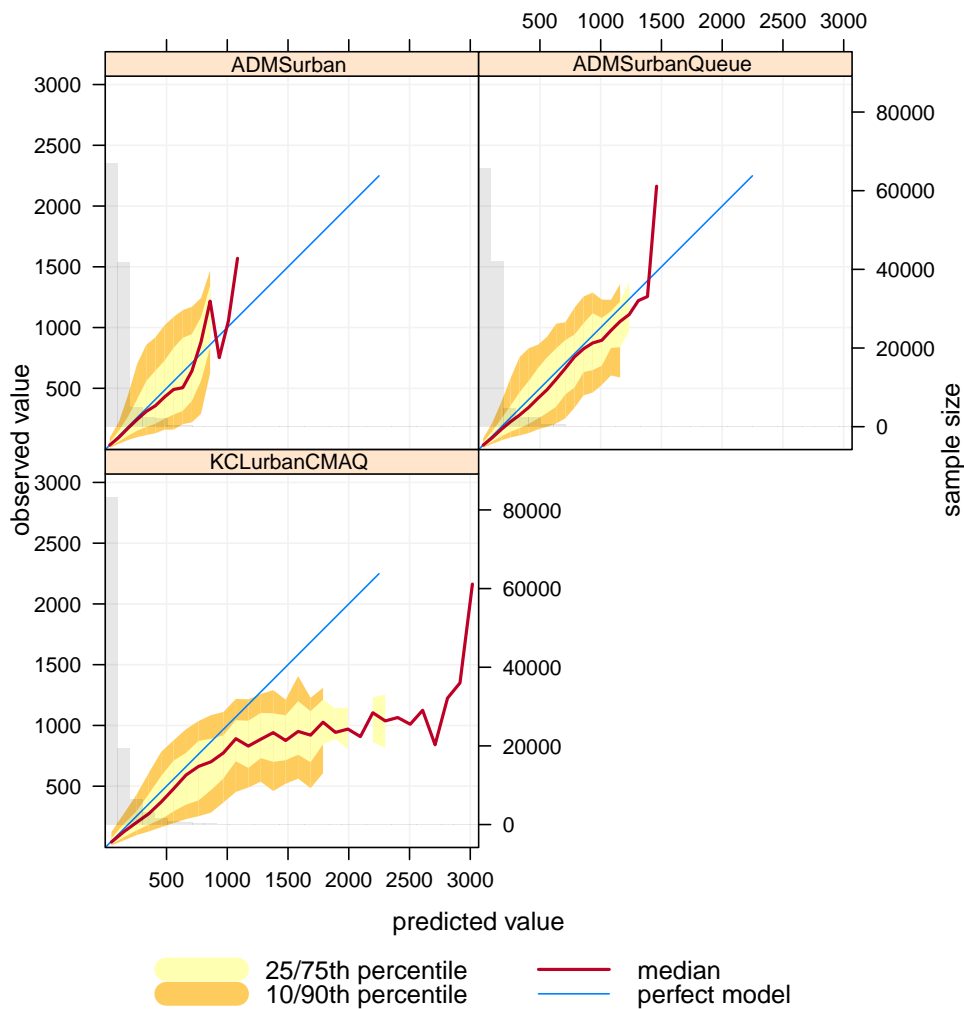


Figure 36: Conditional quantile plot for hourly NO_x concentrations across all sites.

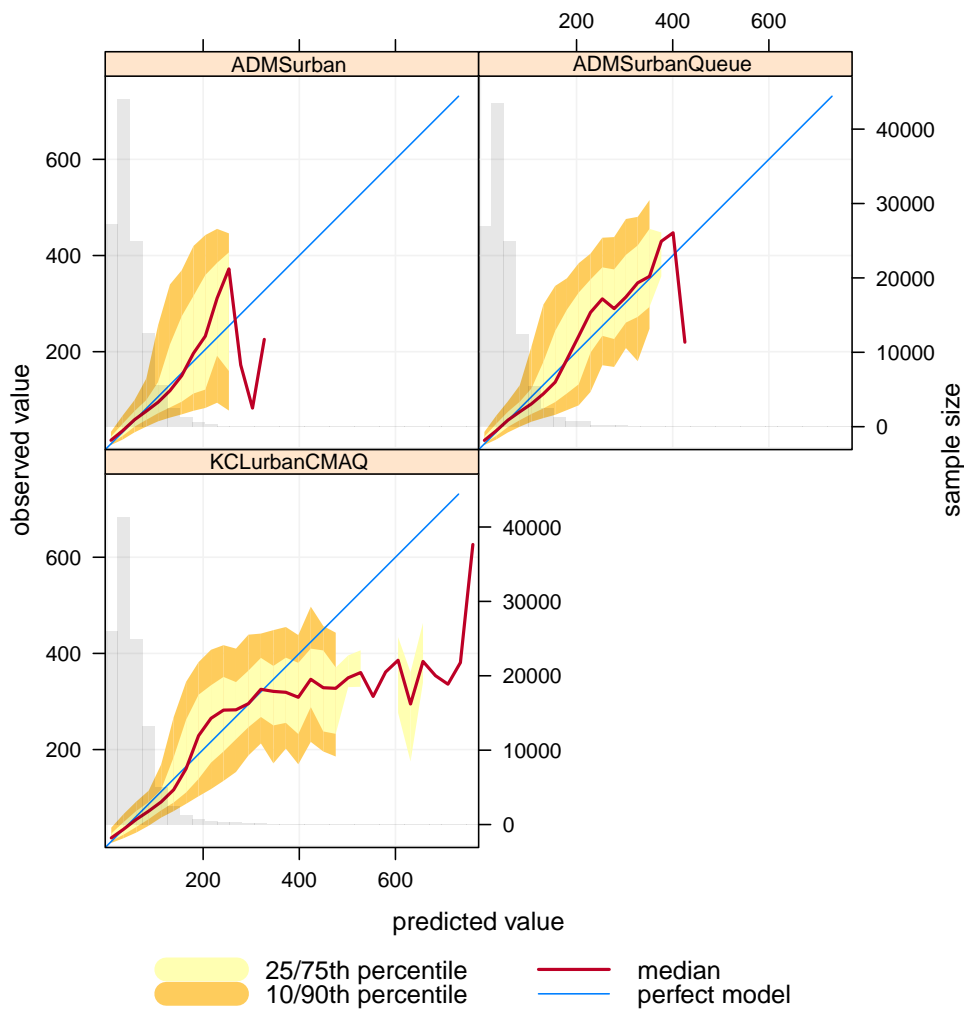


Figure 37: Conditional quantile plot for hourly NO₂ concentrations across all sites.

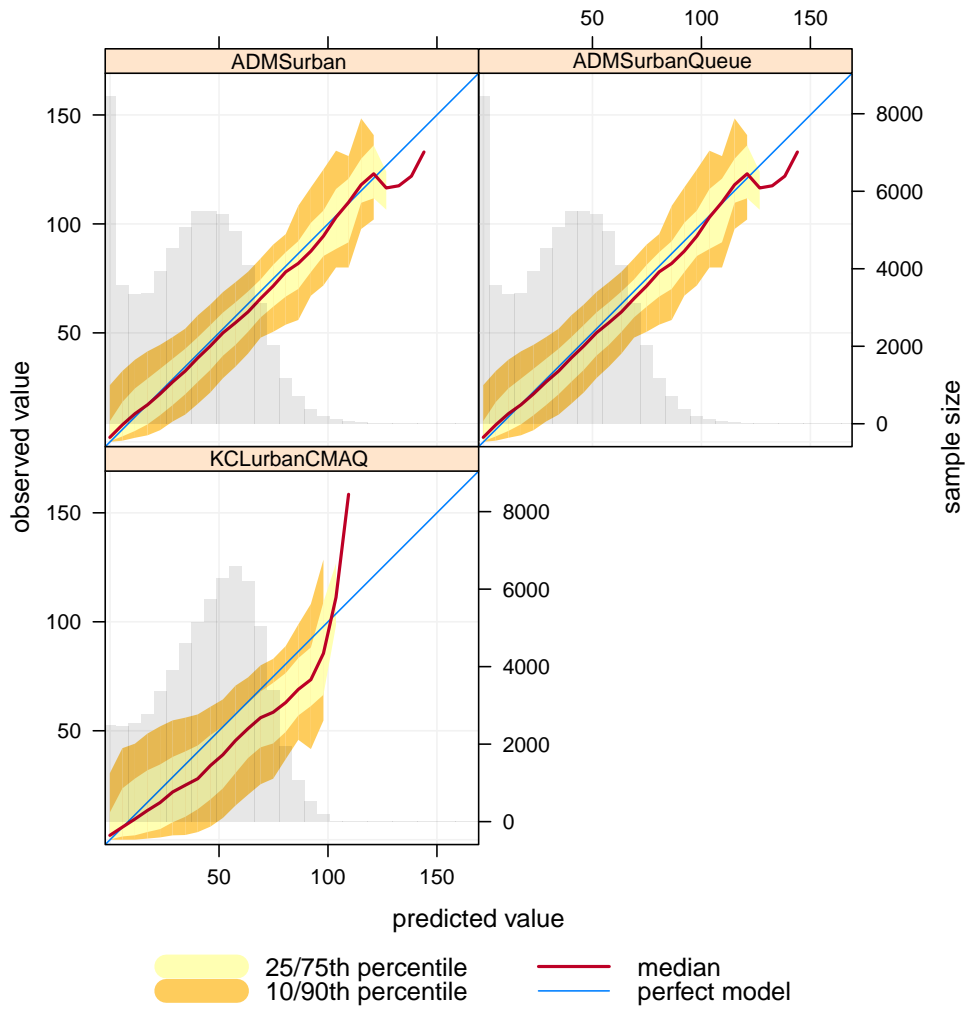


Figure 38: Conditional quantile plot for hourly NO_2 concentrations across all sites.

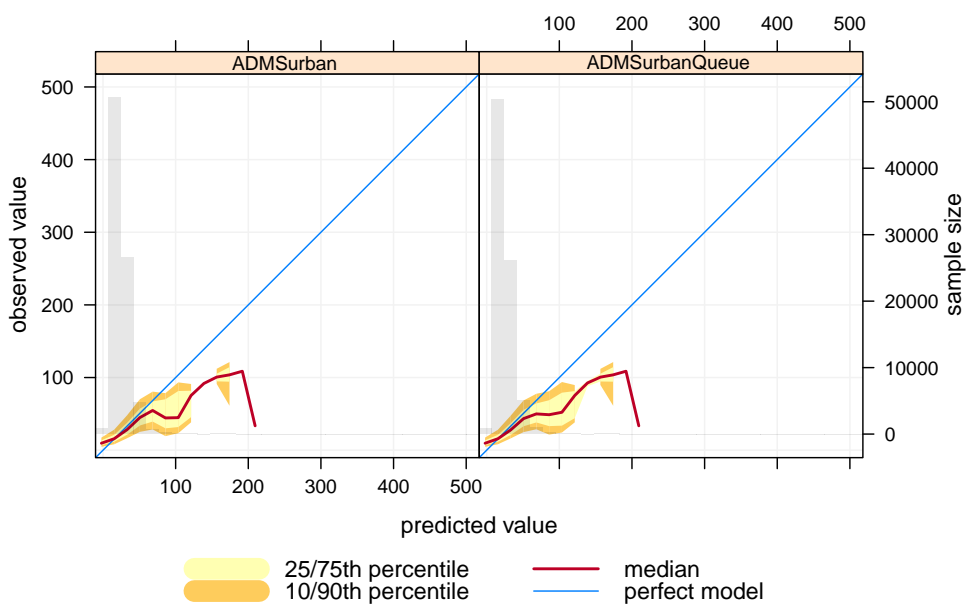


Figure 39: Conditional quantile plot for hourly PM_{10} concentrations across all sites.

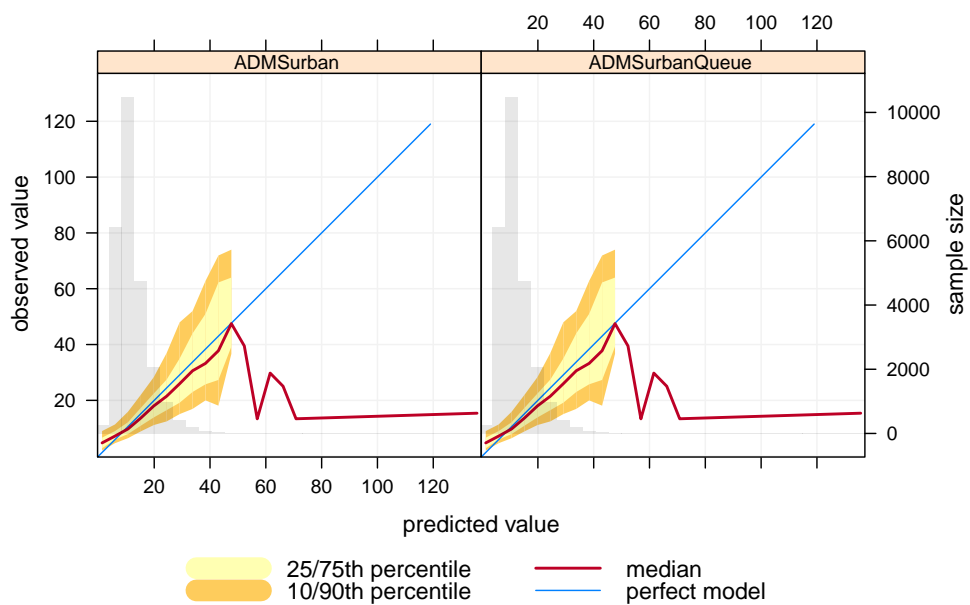


Figure 40: Conditional quantile plot for hourly $PM_{2.5}$ concentrations across all sites.

Acknowledgements

We appreciate the contributions made by the following organisations to the evaluation exercises: Imperial College London, University of Hertfordshire, AEA, Cambridge Environmental Research Consultants, The Joint Environment Programme (JEP), King's College London, University of York, Norwegian Meteorological Institute, CEH, University of Nottingham, The Met Office, RdScientific, the University of Edinburgh, Nicholson Environmental, The Environment Agency, NCAS and the University of Birmingham. We would like to thank the Met Office for providing the meteorological data used in this study and to the data providers including the AURN, the London Air Quality Network (LAQN) and the UK Eutrophying and Acidifying atmospheric Pollutants (UKEAP) network.

References

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A Model performance evaluation statistics

There are a very wide range of evaluation statistics that can be used to assess model performance. There is, however, no single statistic that encapsulates all aspects of interest. For this reason it is useful to consider several performance statistics and also to understand the sort of information or insight they might provide. The performance statistics used here have mostly been guided by [Derwent et al. \(2010\)](#).

In the following definitions, O_i represents the i th observed value and M_i represents the i th modelled value for a total of n observations.

Fraction of predictions within a factor of two, *FAC2*

The fraction of modelled values within a factor of two of the observed values are the fraction of model predictions that satisfy:

$$0.5 \leq \frac{M_i}{O_i} \leq 2.0 \quad (2)$$

Mean bias, *MB*

The mean bias provides a good indication of the mean over or under estimate of predictions. Mean bias in the same units as the quantities being considered.

$$MB = \frac{1}{n} \sum_{i=1}^N M_i - O_i \quad (3)$$

Mean Gross Error, *MGE*

The mean gross error provides a good indication of the mean error regardless of whether it is an over or under estimate. Mean gross error is in the same units as the quantities being considered.

$$MGE = \frac{1}{n} \sum_{i=1}^N |M_i - O_i| \quad (4)$$

Normalised mean bias, *NMB*

The normalised mean bias is useful for comparing pollutants that cover different concentration scales and the mean bias is normalised by dividing by the observed concentration.

$$NMB = \frac{\sum_{i=1}^n M_i - O_i}{\sum_{i=1}^n O_i} \quad (5)$$

Normalised mean gross error, *NMGE*

The normalised mean gross error further ignores whether a prediction is an over or under estimate.

$$NMGE = \frac{\sum_{i=1}^n |M_i - O_i|}{\sum_{i=1}^n O_i} \quad (6)$$

Root mean squared error, $RMSE$

The RMSE is a commonly used statistic that provides a good overall measure of how close modelled values are to predicted values.

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (M_i - O_i)^2}{n}} \quad (7)$$

Correlation coefficient, r

The (Pearson) correlation coefficient is a measure of the strength of the linear relationship between two variables. If there is perfect linear relationship with positive slope between the two variables, $r = 1$. If there is a perfect linear relationship with negative slope between the two variables $r = -1$. A correlation coefficient of 0 means that there is no linear relationship between the variables.

$$r = \frac{1}{(n-1)} \sum_{i=1}^n \left(\frac{M_i - \bar{M}}{\sigma_M} \right) \left(\frac{O_i - \bar{O}}{\sigma_O} \right) \quad (8)$$

A Urban modelling receptor information

Table 12: Site/receptor details relevant to the urban modelling groups.

site code	existing	northing	site name	site type	hourly?	PM10 technique	PM2.5 technique	NO _x & NO ₂	PM10	PM2.5	O ₃
1	BG1	551053	Barking and Dagenham - Rush Green	suburban		TEOM		x	x		
2	BG2	548043	Barking and Dagenham - Scrattons Farm	suburban		BAM		x	x		
3	BG3	543955	Barking and Dagenham - North Street	kerbside		TEOM	FDMS	x	x	x	
4	BL0	530123	Camden - Bloomsbury	urban background	x	TEOM		x	x		
5	BN1	526342	Barnet - Tally Ho Corner	kerbside		TEOM		x	x		
6	BN2	524370	Barnet - Finchley	urban background		TEOM		x	x		
7	BT1	519560	Brent - Kingsbury	suburban		TEOM	TEOM	x	x	x	
8	BT4	520866	Brent - Ilea	roadside		TEOM		x	x	x	
9	BT6	521619	Brent - John Kable Primary School	roadside		TEOM		x	x		
10	BT7	525173	Brent - St Marys Primary School	urban background		TEOM		x	x		
11	BX1	551860	Bexley - Slade Green	suburban	x	TEOM	TEOM	x	x	x	
12	BX2	549975	Bexley - Belvedere	suburban		TEOM		x	x		
13	BX7	552615	Bexley - Thames Road North	roadside		TEOM	TEOM	x	x	x	
14	BX8	552566	Bexley - Thames Road South	roadside		TEOM	TEOM	x	x	x	
15	BX7	540518	Bromley - Harwood Avenue	roadside		BAM		x	x		
16	CD1	526629	Camden - Swiss Cottage	kerbside		TEOM		x	x		
17	CD3	530057	Camden - Shaftesbury Avenue	roadside		TEOM		x	x		
18	CD4	530511	Camden - St Martins College (NOX 1)	urban background	x			x	x		
19	CD5	530511	Camden - St Martins College (NOX 2)	urban background				x	x		
20	CR2	531123	Croydon - Purley Way	roadside				x	x		
21	CR4	532583	Croydon - George Street	roadside	x	TEOM		x	x		
22	CR5	530626	Croydon - Norbury	kerbside				x	x		
23	CR6	531369	Croydon - Euston Road	suburban				x	x		
24	CRD2	526530	London Cromwell Rd2	roadside				x	x		
25	CT1	532235	City of London - Senator House	urban background				x	x		x
26	CT3	533480	City of London - Sir John Cass School	urban background		BAM		x	x		
27	CT6	532527	City of London - Walbrook Wharf	roadside				x	x		
28	CY1	533901	Crystal Palace - Crystal Palace Parade	roadside		TEOM		x	x		
29	EA1	517541	Ealing - Ealing Town Hall	urban background	x			x	x		
30	EA2	520304	Ealing - Acton Town Hall	roadside	x		TEOM	x	x		
31	EA6	518537	Ealing - Hanger Lane Gyratory	roadside				x	x		
32	EA7	511677	Ealing - Southall	urban background		TEOM		x	x		
33	EL1	511403	Elmbridge - Bell Farm Hersham	urban background		TEOM		x	x		
34	EL2	514024	Elmbridge - Esher High Street	roadside				x	x		
35	EN1	533900	Enfield - Bushhill Park	suburban	x	BAM		x	x		
36	EN3	535440	Enfield - Salisbury School	urban background		BAM		x	x		
37	EN4	535025	Enfield - Derby Road	roadside		TEOM		x	x		
38	EN5	529894	Enfield - Bowes Primary School	roadside		TEOM	TEOM	x	x		
39	GB6	544997	Greenwich and Bexley - Falconwood	roadside		TEOM	FDMS	x	x		
40	GNO	544084	Greenwich - A206 Burrage Grove	roadside		FDMS	FDMS	x	x		
41	GN2	540169	Greenwich - Millennium Village	urban background		FDMS	FDMS	x	x		
42	GN3	545560	Greenwich - Plumstead High Street	roadside		FDMS	FDMS	x	x		
43	GR4	543978	Greenwich - Eltham	suburban	x	TEOM	FDMS	x	x		
44	GR5	538960	Greenwich - Trafalgar Road	roadside		TEOM		x	x		
45	GR7	538141	Greenwich - Blackheath	roadside		TEOM		x	x		
46	GR8	540200	Greenwich - Woolwich Flyover	roadside		TEOM	TEOM	x	x		
47	GR9	541879	Greenwich - Westhorpe Avenue	roadside		TEOM	FDMS	x	x		
48	HF1	523420	Hammersmith and Fulham - Broadway	roadside				x	x		
49	HF2	523625	Hammersmith and Fulham - Brook Green	urban background		TEOM		x	x		
50	HG1	533891	Haringey - Haringey Town Hall	roadside	x	TEOM		x	x		
51	HG2	529894	Haringey - Priory Park	urban background		BAM		x	x		
52	H10	506945	Hillingdon - Sipson Road	suburban				x	x		
53	H11	510835	Hillingdon - South Ruislip	roadside		TEOM		x	x		
54	H12	506990	Hillingdon - Hillingdon Hospital	roadside		TEOM		x	x		
55	H13	509551	Hillingdon - Oxford Avenue	roadside		TEOM		x	x		
56	HK4	534830	Hackney - Clapton	urban background		TEOM	TEOM	x	x		
57	HK6	532947	Hackney - Old Street	roadside		TEOM	FDMS	x	x		
58	HR1	517877	Harrow - Stanmore	urban background		TEOM		x	x		
59	HR2	513504	Harrow - Pinner Road	roadside		TEOM		x	x		

Table 12: Site/receptor details relevant to the urban modelling groups.

site code	existing	northing	site name	site type	hourly?	PM _{2.5} technique	PM ₁₀ technique	NO _x & NO ₂	PM ₁₀	PM _{2.5}	O ₃
60	HRL	508299	London Harrington	airport				x			x
61	H52	510371	Hounslow - Grantford	suburban		TEOM		x	x		
62	H54	521083	Hounslow - Chiswick High Road	roadside		TEOM		x	x		x
63	H55	517423	Hounslow - Brentford	roadside		TEOM		x	x		
64	H56	513653	Hounslow - Heston Road	roadside		TEOM		x	x		
65	H57	509332	Hounslow - Hatton Cross	urban background		TEOM		x	x		
66	HV1	182516	Havering - Rainham	roadside				x	x		
67	HV3	551105	Havering - Romford	roadside		TEOM		x	x		
68	IS2	530698	Islington - Holloway Road	roadside		TEOM		x	x		
69	IS6	531325	Islington - Arsenal	roadside		TEOM		x	x		
70	KC1	524046	Kensington and Chelsea - North Ken	urban background	x		FDMS	x	x		x
71	KC2	179646	Kensington and Chelsea - Cromwell Road	roadside				x	x		
72	KC3	527551	Kensington and Chelsea - Knightsbridge	roadside				x	x		
73	KC4	180020	Kensington and Chelsea - Kings Road	roadside				x	x		
74	KC5	527264	Kensington and Chelsea - Earls Court Rd	kerbside				x	x		
75	LB1	525671	Kensington and Chelsea - Earsls Court Rd	roadside		BAM		x	x		
76	LB3	532137	Lambeth - Christchurch Road	urban background		BAM		x	x		
77	LB4	531070	Lambeth - Loughborough Junct	kerbside	x	BAM		x	x		
78	LB5	530317	Lambeth - Brixton Road	roadside		BAM		x	x		
79	LH0	508300	Hillingdon - Harrington	urban background		TEOM	FDMS	x	x		x
80	LH2	508393	Heathrow Airport	urban background		TEOM		x	x		x
81	LW1	537675	Lewisham - Catford	urban background				x	x		x
82	LW2	536241	Lewisham - New Cross	roadside	x	TEOM		x	x		x
83	MY1	528216	Westminster - Marylebone Road	kerbside		TEOM	TEOM	x	x		x
84	RB1	544377	Redbridge - Perth Terrace	urban background		BAM		x	x		x
85	RB3	544555	Redbridge - Fullwell Cross	kerbside		BAM	BAM	x	x		
86	RB4	540823	Redbridge - Gardner Close	roadside		BAM	BAM	x	x		
87	RB5	540017	Redbridge - South Woodford	roadside		BAM		x	x		
88	RI1	522498	Richmond - Castelnau	roadside		TEOM		x	x		
89	RI2	522989	Richmond - Barnes Wetlands	suburban		TEOM		x	x		
90	SK1	532240	Southwark - Larcom Street	urban background		TEOM		x	x		x
91	ST3	164513	Sutton - Carshalton	suburban				x	x		x
92	ST4	528925	Sutton - Wallington	kerbside				x	x		
93	ST6	522557	Sutton - Worcester Park	kerbside				x	x		
94	TD0	515600	Richmond - National Physical Laboratory	suburban	x		FDMS	x	x		x
95	TH1	537509	Tower Hamlets - Poplar	urban background	x	TEOM		x	x		x
96	TH2	535927	Tower Hamlets - Mile End Road	roadside	x			x	x		
97	TH3	535100	Tower Hamlets - Bethnal Green	urban background		TEOM	FDMS	x	x		x
98	TH4	538290	Tower Hamlets - Blackwall	roadside				x	x		x
99	TK1	560900	Thurrock - London Road (Grays)	urban background		TEOM		x	x		x
100	TK2	565738	Thurrock - Purfleet	roadside		BAM		x	x		
101	TK3	569356	Thurrock - Stanford-le-Hope	roadside		TEOM		x	x		
102	TK8	556698	Thurrock - London Road (Purfleet)	roadside		BAM		x	x		
103	WA2	525774	Wandsworth - Town Hall	urban background				x	x		x
104	WA6	527712	Wandsworth - Tooting	roadside		TEOM		x	x		
105	WLI1	538389	Waltham forest - Dawlish Road	urban background		TEOM		x	x		
106	WL4	191071	Waltham Forest - Crooked Billet	kerbside		TEOM		x	x		
107	WL5	537802	Waltham Forest - Leyton	urban background		TEOM		x	x		
108	WM0	529802	Westminster - Horseferry Road	urban background				x	x		x
109	WM4	529992	Westminster - Charing Cross Library	roadside				x	x		
110	CR3	532336	Croydon - Thornton Heath	suburban		TEOM		x	x		x
111	CT8	532829	City of London - Upper Thames Street	roadside		TEOM		x	x		
112	EI0	514323	Ealing - Greenford	urban background		TEOM		x	x		
113	FR1	485063	Rushmoor - Medway Drive	roadside		TEOM		x	x		
114	MV3	517033	Mole Valley - Donking	urban background		TEOM		x	x		
115	NM2	538661	Newham - Cam Road	roadside		TEOM		x	x		x
116	NM3	539889	Newham - Wren Close	urban background		TEOM		x	x		x
117	BX3	547323	Bexley - Thamesmead	suburban				x	x		
118	BX9	551860	Bexley - Slade Green FDMS	suburban			TEOM	x	x		
							FDMS				x