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Defra regional and transboundary 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 regional air quality. Specifically, this report considers the prediction of hourly mean ozone concentrations at receptors across the UK. 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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1 Introduction

1.1 Document history

This document has had the following updates.

13th January 2011 New figures that aim to show all sites and models by month and by day; both for the mean concentration of O_3 and the maximum value. See Figure 50 to Figure 53.

13th January 2011 Minor update of AQUM.GEMS results from the Met Office, due to Met Office post-processing issue.

18th January 2011 Added O_3 map from AEA via NetCDF file (page 63).

26th January 2011 Updated University of Hertfordshire results following use of erroneous shipping emissions. This update also includes the map.

3rd February 2011 Added new section on weekday-weekend response of O_3 for models and measurements (subsection 3.10) to help show how O_3 concentrations respond to changes in emissions.

4 February 2011 New EMEP4UK results which should have solved the hourly spikes — due to a switch in the preporcessor between WRF and EMEP.

7th February 2011 Added more analysis to subsection 3.8 on higher percentile concentrations of O_3. The main purpose was to examine how well the model capture higher concentrations of O_3 through considering the mean bias.

Also ensured that scatter plots in subsection 3.5 use the same x-y scaling.

Added subsection 3.9 on AOT40.

10th February 2011 Added an alternative AQUM model referred to as "AQUM.MACC". The previous AQUM model is now referred to as "AQUM.GEMS". [Met Office to provide text on the differences between the two.]

11th February 2011 Revised University of Herfordshire CMAQ.UH results processed for receptors and map.

16th February 2011 Added a new section on conditional quantiles to explore different aspects of model performance — subsection 3.2.

15th April 2011 Few minor changes to tables.

1.2 Background

This document summarises 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. The same is also true of any errors in the code itself. 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 on 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

A summary of the ozone sites is given in Table 1. Both OS easting/northings and latitude/longitude have been provided. Note that all analyses in this report relate to 2006.

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.

Table 1: Details of ozone monitoring sites to be used in the model intercomparison

	site.name	site.code	OS.easting	OS.northing	latitude	longitude
1	Aston Hill	AH	329902	290062	52 30 14N	03 02 03W
2	Bottesford	BOT	479768	337654	52 55 49N	00 48 53W
3	Bush Estate	BUSH	324626	663880	55 51 44N	03 12 22W
4	Eskdalemuir	ESK	323500	602800	55 18 55N	03 12 22W
5	Glazebury	GLAZ	368733	396034	53 27 36N	02 28 19W
6	High Muffles	HM	477535	493865	54 20 04N	00 48 33W
7	Harwell	HAR	446772	186020	51 34 16N	01 19 36W
8	Ladybower	LB	416575	389565	53 24 12N	01 45 07W
9	Lullington Heath	LH	553855	101740	50 47 37N	00 10 53E
10	Lough Navar	LN	206500	354500	54 26 22N	07 54 01W
11	Rochester	ROCH	583133	176220	51 27 22N	00 38 06E
12	Sibton	SIB	636295	271870	52 17 40N	01 27 49E
13	Strath Vaich	SV	234829	874785	57 44 04.04N	04 46 35.70W
14	Yarner Wood	YW	278605	78948	50 35 51N	03 42 59W
15	Wicken Fen	WFEN	556310	269210	52 17 55N	00 17 27E

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 path to data files
setwd("~/Projects/modelEvaluation/regional")
```

Next we import some pre-prepared data — hourly mean O_3 concentrations at 15 sites for 2006 and the pre-prepared model results data. Details are given in Appendix C about how the model data were prepared.

```
load("ozoneMeasurements.RData")
load("modelData.Rdata")
```

3 Analysis examples

3.1 Statistical metrics

Model evaluation statistics can be estimated using the `modStats` function. These statistics are described in Appendix B. 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 (`emep`), the analysis type (statistics by site i.e. `type = "site"`), the modelled results column is called `"mod"` and the observations column in this case is `"o3"`.

Note that the function `modStats` can be used to provide more detailed information that could help with model evaluation. For example, it might be useful to understand how model performance varies with site *and* season. In **openair** there are a very wide range of built in ways of partitioning (conditioning) the data including by year, day of the week, weekday/weekend, month, hour of the day, wind sector (if wind direction data is present) and by *any* other numerical variable if present e.g. wind speed. This is easily done by supplying another argument to `type`, as shown throughout this document.

```
modStats(emep, type = "site", mod = "mod", obs = "o3")
```

```
modStats(empUnified, type = "site", mod = "mod", obs = "o3")
```

Table 2: Summary model evaluation statistics for EMEP4UK.

site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
Aston.Hill	7840	0.93	-8.99	14.34	-0.12	0.20	19.81	0.70
Bottesford	8450	0.86	2.69	13.45	0.05	0.25	18.75	0.75
Bush.Estate	8325	0.93	5.52	12.11	0.09	0.21	16.33	0.70
Eskdalemuir	8389	0.89	9.55	14.57	0.16	0.25	19.43	0.71
Glazebury	6476	0.76	3.43	14.30	0.07	0.30	19.36	0.78
High.Muffles	7573	0.91	5.76	14.88	0.10	0.25	19.77	0.72
Harwell	7926	0.87	3.88	13.59	0.07	0.25	18.37	0.75
Ladybower	8041	0.80	13.91	19.12	0.28	0.38	23.53	0.67
Lullington.Heath	7599	0.88	-1.20	15.15	-0.02	0.24	21.97	0.68
Lough.Navar	8386	0.79	21.30	22.22	0.45	0.47	26.93	0.67
Rochester	8361	0.77	1.29	14.48	0.03	0.29	20.13	0.75
Sibton	7788	0.89	0.60	13.99	0.01	0.24	19.25	0.73
Strath.Vaich	7326	0.98	-6.64	11.79	-0.09	0.16	15.30	0.76
Yarner.Wood	8174	0.90	4.79	15.07	0.08	0.24	20.28	0.66
Wicken.Fen	7293	0.90	-7.64	17.03	-0.11	0.25	23.67	0.75

Table 3: Summary model evaluation statistics for EMEP Unified.

site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
Aston.Hill	8093	0.93	-3.19	13.64	-0.04	0.19	18.58	0.71
Bottesford	8658	0.82	8.71	16.30	0.17	0.31	21.99	0.71
Bush.Estate	8580	0.91	6.17	13.43	0.11	0.23	18.11	0.65
Eskdalemuir	8659	0.87	10.76	15.72	0.19	0.27	21.15	0.67
Glazebury	6476	0.73	14.34	19.39	0.30	0.41	25.73	0.72
High.Muffles	7844	0.86	9.23	18.45	0.16	0.32	24.13	0.60
Harwell	8196	0.84	9.44	16.05	0.17	0.30	21.61	0.73
Ladybower	8313	0.79	12.75	19.31	0.26	0.39	24.57	0.64
Lullington.Heath	7807	0.86	5.19	18.13	0.08	0.30	25.64	0.57
Lough.Navar	8658	0.79	21.21	22.25	0.45	0.47	27.10	0.66
Rochester	8633	0.77	9.25	16.99	0.19	0.35	22.77	0.71
Sibton	8060	0.83	1.29	17.68	0.02	0.31	24.55	0.53
Strath.Vaich	7326	0.98	-3.00	11.84	-0.04	0.16	15.33	0.70
Yarner.Wood	8446	0.89	7.40	16.74	0.12	0.27	22.31	0.63
Wicken.Fen	7565	0.88	-0.98	17.96	-0.01	0.27	23.61	0.72

```
modStats(NAME, type = "site", mod = "mod", obs = "o3")
```

```
modStats(AQUM.GEMS, type = "site", mod = "mod", obs = "o3")
```

```
modStats(AQUM.MACC, type = "site", mod = "mod", obs = "o3")
```

```
modStats(CMAQ.AEA, type = "site", mod = "mod", obs = "o3")
```

```
modStats(OSRM, type = "site", mod = "mod", obs = "o3")
```

```
modStats(CMAQ.UH, type = "site", mod = "mod", obs = "o3")
```

```
modStats(CMAQ.KCL, type = "site", mod = "mod", obs = "o3")
```

Table 4: Summary model evaluation statistics for the NAME model.

site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
Aston.Hill	8093	0.95	-10.63	17.11	-0.15	0.24	22.23	0.61
Bottesford	8659	0.83	5.07	16.59	0.10	0.32	21.97	0.66
Bush.Estate	8580	0.92	0.67	14.02	0.01	0.24	18.69	0.55
Eskdalemuir	8659	0.88	4.27	15.36	0.07	0.26	19.83	0.59
Glazebury	6476	0.74	5.87	17.73	0.12	0.37	23.24	0.68
High.Muffles	7844	0.90	2.85	15.30	0.05	0.26	20.25	0.68
Harwell	8196	0.85	2.34	16.31	0.04	0.30	21.41	0.63
Ladybower	8313	0.84	6.65	16.16	0.13	0.33	20.46	0.66
Lullington.Heath	7807	0.88	1.90	17.48	0.03	0.28	23.60	0.62
Lough.Navar	8658	0.81	14.22	18.61	0.30	0.39	24.49	0.49
Rochester	8633	0.77	-0.31	16.82	-0.01	0.34	21.63	0.68
Sibton	8060	0.87	6.82	17.51	0.12	0.31	23.00	0.64
Strath.Vaich	7326	0.98	-8.00	16.23	-0.11	0.22	20.53	0.52
Yarner.Wood	8446	0.90	1.41	18.19	0.02	0.29	23.56	0.50
Wicken.Fen	7565	0.88	-3.91	20.03	-0.06	0.30	26.25	0.65

Table 5: Summary model evaluation statistics for the AQUM.GEMS model.

site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
Aston.Hill	8093	0.82	-14.00	18.50	-0.19	0.26	24.58	0.72
Bottesford	8659	0.74	-4.14	18.07	-0.08	0.34	23.91	0.68
Bush.Estate	8580	0.82	-4.88	18.11	-0.08	0.31	24.00	0.47
Eskdalemuir	8659	0.83	0.19	18.01	0.00	0.31	23.75	0.54
Glazebury	6476	0.66	-1.47	19.61	-0.03	0.41	25.48	0.64
High.Muffles	7844	0.80	-6.55	18.38	-0.11	0.32	23.42	0.68
Harwell	8196	0.73	-9.03	18.30	-0.17	0.34	23.27	0.70
Ladybower	8313	0.76	1.62	19.65	0.03	0.40	24.17	0.59
Lullington.Heath	7807	0.82	-6.88	16.50	-0.11	0.27	21.61	0.77
Lough.Navar	8658	0.83	10.01	18.34	0.21	0.39	23.95	0.51
Rochester	8633	0.61	-11.28	20.40	-0.23	0.42	26.00	0.64
Sibton	8060	0.80	-4.03	17.38	-0.07	0.31	22.32	0.71
Strath.Vaich	7326	0.93	-11.64	19.35	-0.16	0.27	23.94	0.51
Yarner.Wood	8446	0.81	-3.82	20.45	-0.06	0.33	26.15	0.53
Wicken.Fen	7565	0.80	-10.09	20.64	-0.15	0.31	26.55	0.72

Table 6: Summary model evaluation statistics for the AQUM.MACC model.

site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
Aston.Hill	8091	0.94	8.75	17.56	0.12	0.24	21.03	0.75
Bottesford	8657	0.79	16.39	21.48	0.31	0.41	27.06	0.74
Bush.Estate	8578	0.86	17.74	23.19	0.31	0.40	27.82	0.56
Eskdalemuir	8657	0.82	23.36	25.69	0.40	0.44	31.09	0.64
Glazebury	6474	0.70	19.69	24.06	0.41	0.51	30.39	0.71
High.Muffles	7842	0.84	15.20	21.81	0.26	0.38	26.18	0.73
Harwell	8194	0.81	11.63	19.05	0.21	0.35	23.87	0.76
Ladybower	8311	0.69	23.79	28.25	0.48	0.57	33.11	0.63
Lullington.Heath	7805	0.87	12.61	19.20	0.21	0.31	23.62	0.78
Lough.Navar	8656	0.67	35.73	36.38	0.76	0.77	40.67	0.59
Rochester	8631	0.74	6.37	18.68	0.13	0.38	24.00	0.69
Sibton	8058	0.84	16.77	21.53	0.30	0.38	26.25	0.76
Strath.Vaich	7324	0.96	13.33	17.65	0.18	0.24	21.83	0.61
Yarner.Wood	8444	0.83	20.41	24.86	0.33	0.40	30.63	0.63
Wicken.Fen	7563	0.84	11.05	19.41	0.17	0.29	24.97	0.76

Table 7: Summary model evaluation statistics for the CMAQ AEA model.

site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
Aston.Hill	7658	0.95	0.81	13.71	0.01	0.19	19.38	0.60
Bottesford	8205	0.78	7.05	18.11	0.13	0.34	23.11	0.68
Bush.Estate	8108	0.89	11.57	17.47	0.20	0.30	21.94	0.51
Eskdalemuir	8185	0.85	15.69	18.32	0.27	0.31	23.43	0.68
Glazebury	6113	0.69	1.26	18.81	0.03	0.39	23.96	0.68
High.Muffles	7402	0.87	9.72	18.12	0.17	0.31	22.70	0.68
Harwell	7738	0.79	7.51	18.56	0.14	0.34	23.73	0.66
Ladybower	7851	0.76	16.16	22.36	0.32	0.45	27.10	0.58
Lullington.Heath	7390	0.85	7.54	19.99	0.12	0.32	25.96	0.54
Lough.Navar	8184	0.72	27.93	28.53	0.59	0.60	32.96	0.60
Rochester	8158	0.39	-26.46	29.13	-0.53	0.59	36.53	0.50
Sibton	7612	0.84	6.31	17.35	0.11	0.30	22.18	0.67
Strath.Vaich	6930	0.97	5.11	13.15	0.07	0.18	16.87	0.64
Yarner.Wood	7980	0.87	12.49	18.88	0.20	0.30	24.41	0.61
Wicken.Fen	7224	0.87	0.62	17.91	0.01	0.27	23.41	0.74
	0							

Table 8: Summary model evaluation statistics for the OSRM model.

site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
Aston.Hill	8087	0.81	-11.40	21.31	-0.16	0.30	29.72	0.46
Bottesford	8659	0.71	-1.70	21.07	-0.03	0.40	28.26	0.49
Bush.Estate	8573	0.80	-0.44	19.37	-0.01	0.33	25.44	0.45
Eskdalemuir	8652	0.78	3.52	20.54	0.06	0.35	27.06	0.44
Glazebury	6476	0.62	7.74	25.04	0.16	0.53	32.68	0.42
High.Muffles	7837	0.72	-0.51	24.36	-0.01	0.42	31.11	0.41
Harwell	8189	0.71	0.10	21.63	0.00	0.40	29.17	0.49
Ladybower	8306	0.69	3.67	23.37	0.07	0.47	29.25	0.42
Lullington.Heath	7807	0.73	-1.34	23.62	-0.02	0.38	31.22	0.52
Lough.Navar	8651	0.71	19.09	26.60	0.40	0.56	32.58	0.42
Rochester	8626	0.62	2.55	23.89	0.05	0.49	31.12	0.49
Sibton	8053	0.72	1.05	23.58	0.02	0.41	30.24	0.48
Strath.Vaich	7326	0.86	-11.99	21.17	-0.17	0.29	27.65	0.40
Yarner.Wood	8439	0.74	1.71	24.20	0.03	0.39	31.25	0.40
Wicken.Fen	7558	0.73	-6.89	26.33	-0.10	0.40	34.81	0.42

Table 9: Summary model evaluation statistics for the CMAQ University of Hertfordshire model.

site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
Aston.Hill	8093	0.78	-15.01	24.59	-0.21	0.34	32.09	0.32
Bottesford	8659	0.75	10.20	24.23	0.19	0.46	31.19	0.36
Bush.Estate	8580	0.82	11.62	24.17	0.20	0.42	29.67	0.13
Eskdalemuir	8659	0.78	11.36	25.13	0.20	0.43	31.49	0.16
Glazebury	6476	0.65	17.91	29.82	0.38	0.63	37.60	0.31
High.Muffles	7844	0.83	4.60	21.55	0.08	0.37	26.24	0.47
Harwell	8196	0.75	-3.05	21.46	-0.06	0.40	27.90	0.38
Ladybower	8313	0.72	13.67	25.56	0.28	0.52	30.80	0.35
Lullington.Heath	7807	0.79	-10.03	19.85	-0.16	0.32	27.22	0.55
Lough.Navar	8658	0.63	18.79	31.54	0.40	0.67	37.88	0.06
Rochester	8633	0.76	1.37	17.52	0.03	0.36	22.37	0.63
Sibton	8060	0.84	-1.91	17.36	-0.03	0.31	21.96	0.64
Strath.Vaich	7326	0.86	-2.85	23.67	-0.04	0.33	28.71	0.16
Yarner.Wood	8446	0.67	-15.44	26.66	-0.25	0.42	33.54	0.38
Wicken.Fen	7565	0.79	-4.98	24.20	-0.08	0.37	31.22	0.46

Table 10: Summary model evaluation statistics for the CMAQ King's College London model.

site	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
Aston.Hill	7974	0.94	-1.80	15.80	-0.02	0.22	22.44	0.40
Bottesford	8516	0.77	9.36	20.72	0.18	0.40	26.42	0.49
Bush.Estate	8442	0.88	7.78	16.74	0.13	0.29	21.70	0.33
Eskdalemuir	8516	0.81	17.33	21.84	0.30	0.38	28.31	0.35
Glazebury	6333	0.64	-2.48	21.60	-0.05	0.45	28.01	0.50
High.Muffles	7702	0.82	12.93	22.35	0.22	0.39	27.66	0.44
Harwell	8053	0.80	9.40	19.96	0.17	0.37	26.05	0.46
Ladybower	8170	0.71	18.87	25.67	0.38	0.52	30.71	0.32
Lullington.Heath	7688	0.83	6.74	20.83	0.11	0.34	27.26	0.43
Lough.Navar	8515	0.71	27.29	29.05	0.58	0.61	34.46	0.32
Rochester	8490	0.72	7.52	21.29	0.15	0.44	27.22	0.46
Sibton	7917	0.80	12.52	21.96	0.22	0.39	27.42	0.45
Strath.Vaich	7184	0.95	6.65	15.84	0.09	0.22	20.52	0.37
Yarner.Wood	8303	0.87	6.58	19.53	0.10	0.31	24.92	0.41
Wicken.Fen	7433	0.82	-0.80	22.45	-0.01	0.34	29.31	0.51

The example below shows how to calculate the model evaluation statistics by site *and* season.

```
modStats(emep, type = c("site", "season"), mod = "mod", obs = "o3")
```

Table 11: Summary model evaluation statistics by site and season for EMEP4UK.

site	season	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
Aston.Hill	spring (MAM)	1736	0.97	-8.54	15.68	-0.10	0.18	20.00	0.45
Aston.Hill	summer (JJA)	2174	0.96	-11.18	17.83	-0.14	0.23	25.67	0.67
Aston.Hill	autumn (SON)	2056	0.97	-4.61	10.28	-0.07	0.16	13.52	0.68
Aston.Hill	winter (DJF)	1874	0.84	-11.68	13.49	-0.18	0.21	17.47	0.84
Bottesford	spring (MAM)	2203	0.92	5.84	13.87	0.09	0.22	18.80	0.67
Bottesford	summer (JJA)	2194	0.86	2.19	18.72	0.04	0.31	25.21	0.72
Bottesford	autumn (SON)	2175	0.87	3.48	11.21	0.08	0.25	15.05	0.74
Bottesford	winter (DJF)	1878	0.78	-1.34	9.39	-0.03	0.21	12.77	0.85
Bush.Estate	spring (MAM)	2130	0.97	3.92	11.55	0.06	0.16	15.58	0.66
Bush.Estate	summer (JJA)	2156	0.94	8.30	14.04	0.15	0.25	19.10	0.58
Bush.Estate	autumn (SON)	2166	0.90	8.36	12.67	0.16	0.25	16.26	0.66
Bush.Estate	winter (DJF)	1873	0.91	0.83	9.86	0.01	0.18	13.55	0.75
Eskdalemuir	spring (MAM)	2203	0.93	8.76	13.51	0.12	0.19	18.61	0.66
Eskdalemuir	summer (JJA)	2161	0.88	9.95	17.27	0.17	0.30	22.48	0.65
Eskdalemuir	autumn (SON)	2180	0.85	11.99	15.30	0.23	0.30	20.18	0.60
Eskdalemuir	winter (DJF)	1845	0.88	7.15	11.79	0.13	0.22	15.13	0.79
Glazebury	spring (MAM)	2200	0.83	5.45	14.69	0.10	0.26	19.99	0.69
Glazebury	summer (JJA)	2161	0.78	1.41	16.48	0.03	0.32	21.72	0.79
Glazebury	autumn (SON)	736	0.74	7.79	14.51	0.21	0.39	18.78	0.69
Glazebury	winter (DJF)	1379	0.62	1.03	10.15	0.03	0.32	13.97	0.84
High.Muffles	spring (MAM)	1735	0.98	1.12	12.47	0.01	0.16	17.33	0.67
High.Muffles	summer (JJA)	1945	0.94	3.65	17.94	0.05	0.27	24.11	0.60
High.Muffles	autumn (SON)	2117	0.85	13.69	16.62	0.31	0.38	20.60	0.61
High.Muffles	winter (DJF)	1776	0.86	3.14	11.81	0.06	0.24	15.19	0.79
Harwell	spring (MAM)	1905	0.88	8.58	16.53	0.14	0.26	21.94	0.58
Harwell	summer (JJA)	2002	0.92	3.83	15.52	0.06	0.26	20.89	0.75
Harwell	autumn (SON)	2172	0.87	4.67	12.66	0.09	0.26	16.63	0.68
Harwell	winter (DJF)	1847	0.80	-1.85	9.58	-0.04	0.21	12.42	0.89
Ladybower	spring (MAM)	2165	0.96	5.59	12.98	0.08	0.19	17.52	0.59
Ladybower	summer (JJA)	2147	0.73	16.37	22.67	0.32	0.44	27.30	0.67
Ladybower	autumn (SON)	2008	0.68	22.48	24.84	0.60	0.66	28.43	0.41
Ladybower	winter (DJF)	1721	0.82	11.30	15.74	0.28	0.39	18.09	0.82
Lullington.Heath	spring (MAM)	1400	0.88	4.51	17.77	0.06	0.25	24.42	0.45
Lullington.Heath	summer (JJA)	2196	0.89	-6.36	19.49	-0.09	0.26	28.39	0.63
Lullington.Heath	autumn (SON)	2139	0.89	0.19	14.28	0.00	0.25	19.18	0.63
Lullington.Heath	winter (DJF)	1864	0.86	-1.00	9.06	-0.02	0.19	12.16	0.86
Lough.Navar	spring (MAM)	2168	0.84	21.17	21.77	0.35	0.36	28.27	0.49
Lough.Navar	summer (JJA)	2181	0.79	19.53	21.26	0.45	0.49	24.87	0.74
Lough.Navar	autumn (SON)	2159	0.78	24.56	24.77	0.58	0.59	28.79	0.51
Lough.Navar	winter (DJF)	1878	0.76	19.76	20.92	0.45	0.47	25.38	0.69
Rochester	spring (MAM)	2170	0.80	2.56	16.17	0.04	0.27	22.77	0.64
Rochester	summer (JJA)	2198	0.82	-2.18	16.61	-0.04	0.29	22.14	0.75
Rochester	autumn (SON)	2122	0.73	2.96	14.48	0.07	0.35	19.87	0.66
Rochester	winter (DJF)	1871	0.71	2.00	10.03	0.05	0.26	13.66	0.85
Sibton	spring (MAM)	2194	0.92	3.84	14.40	0.06	0.22	19.96	0.58
Sibton	summer (JJA)	2185	0.93	-2.17	16.45	-0.03	0.25	22.38	0.71
Sibton	autumn (SON)	1612	0.85	2.36	13.89	0.05	0.29	18.98	0.68
Sibton	winter (DJF)	1797	0.82	-1.54	10.57	-0.03	0.23	13.69	0.81
Strath.Vaich	spring (MAM)	2205	1.00	-10.19	13.01	-0.12	0.15	16.24	0.71
Strath.Vaich	summer (JJA)	2051	1.00	-5.70	12.14	-0.09	0.18	15.59	0.71
Strath.Vaich	autumn (SON)	1704	0.95	-7.09	12.74	-0.11	0.19	16.85	0.53
Strath.Vaich	winter (DJF)	1366	0.97	-1.77	8.12	-0.03	0.13	10.50	0.82
Yarner.Wood	spring (MAM)	2173	0.93	2.29	16.66	0.03	0.21	21.90	0.34
Yarner.Wood	summer (JJA)	2123	0.92	4.65	16.39	0.07	0.25	22.87	0.70
Yarner.Wood	autumn (SON)	2008	0.90	10.82	14.67	0.20	0.27	19.12	0.60
Yarner.Wood	winter (DJF)	1870	0.86	1.38	12.15	0.03	0.22	15.92	0.77
Wicken.Fen	spring (MAM)	2155	0.94	-8.91	18.29	-0.11	0.23	22.59	0.67
Wicken.Fen	summer (JJA)	2170	0.90	-13.45	22.61	-0.17	0.29	31.88	0.73
Wicken.Fen	autumn (SON)	1892	0.86	0.25	12.52	0.01	0.26	17.22	0.74
Wicken.Fen	winter (DJF)	1076	0.88	-7.29	11.16	-0.13	0.20	14.25	0.87

It is difficult to digest lots of numerical results when so many models and sites are involved. A much better way is to plot the key statistics by site and model. To do this, it is first necessary to combine all the model results:

```
all.results <- rbind.fill(emep, emepUnified, ptm, NAME, AQUM.GEMS, AQUM.MACC, CMAQ.AEA, OSRM,
                          CMAQ.UH, CMAQ.KCL)
## how many rows of data is this? Lots!
nrow(all.results)
```

```
[1] 1319460
```

Now it is possible to display the results in a much more digestible way. First it is necessary to calculate the evaluation statistics by model and site as shown in the following plots for some of the evaluations statistics. Note that the results for the PTM are not strictly comparable with the other models because they are only available for Harwell at 15:00 GMT each day.

```
allStats <- modStats(all.results, type = c("group", "site"), mod = "mod", obs = "o3")
```

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

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

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

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

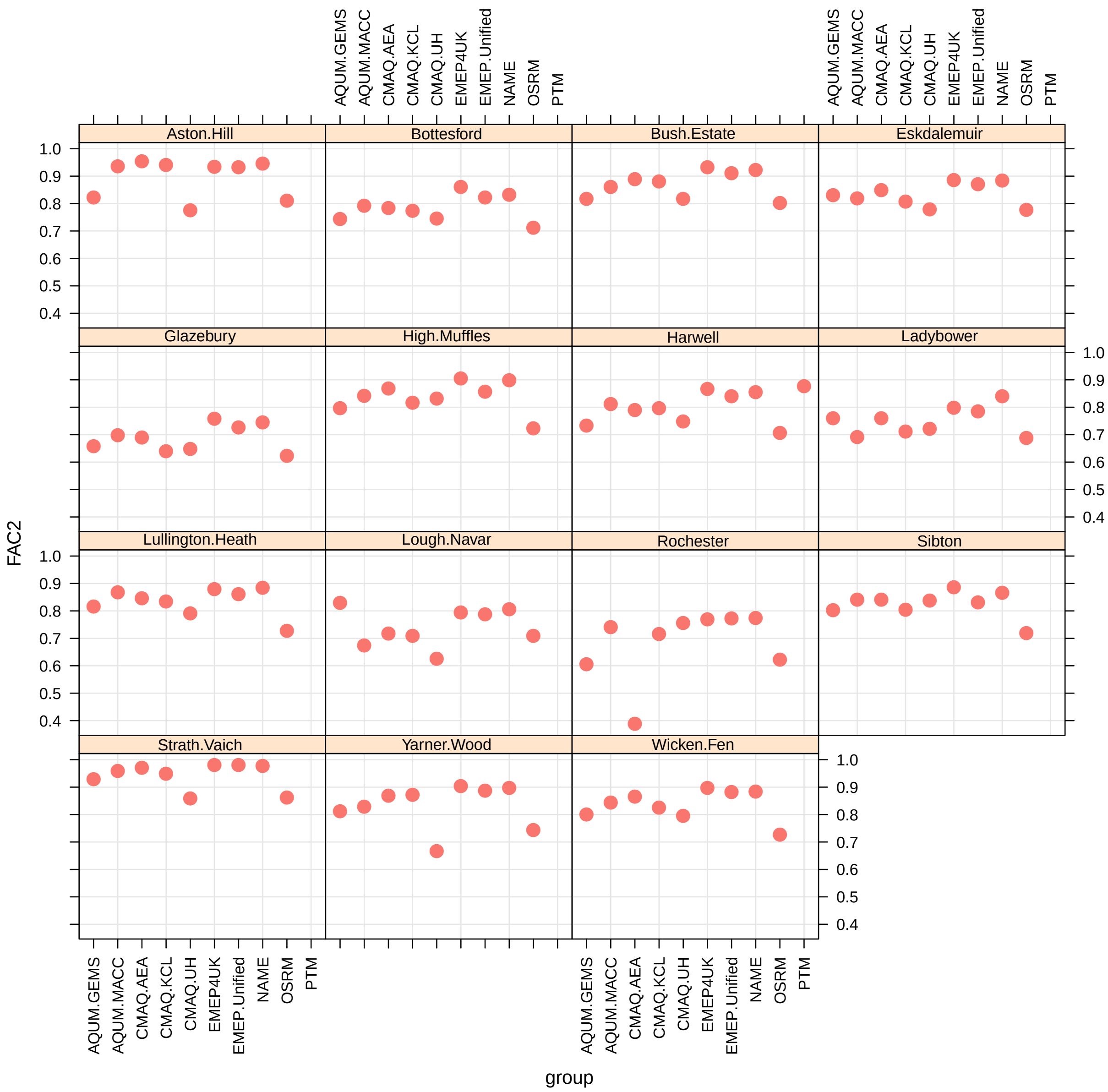

Figure 1: FAC2 by site and by model.

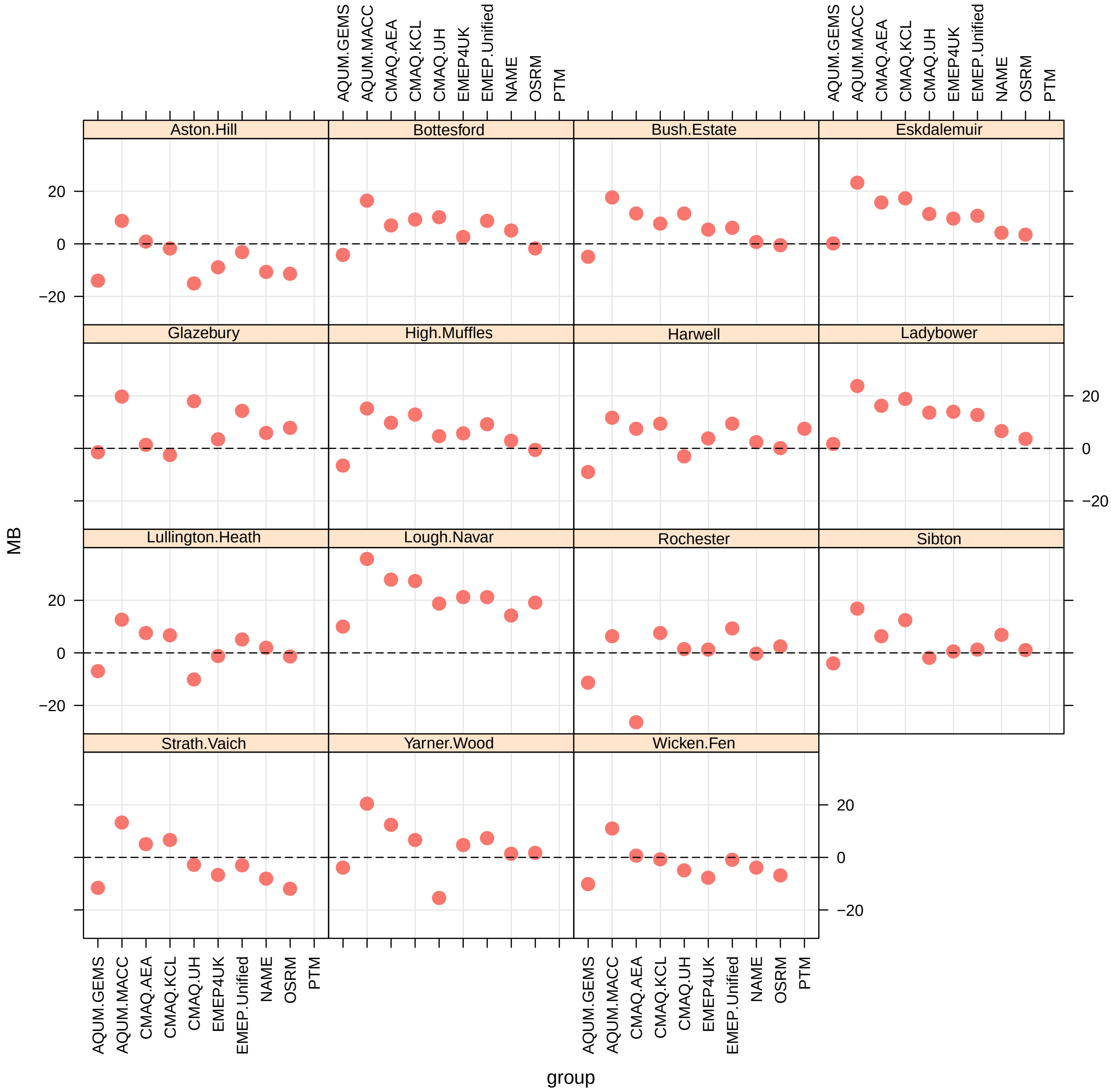

Figure 2: Mean bias by site and by model.

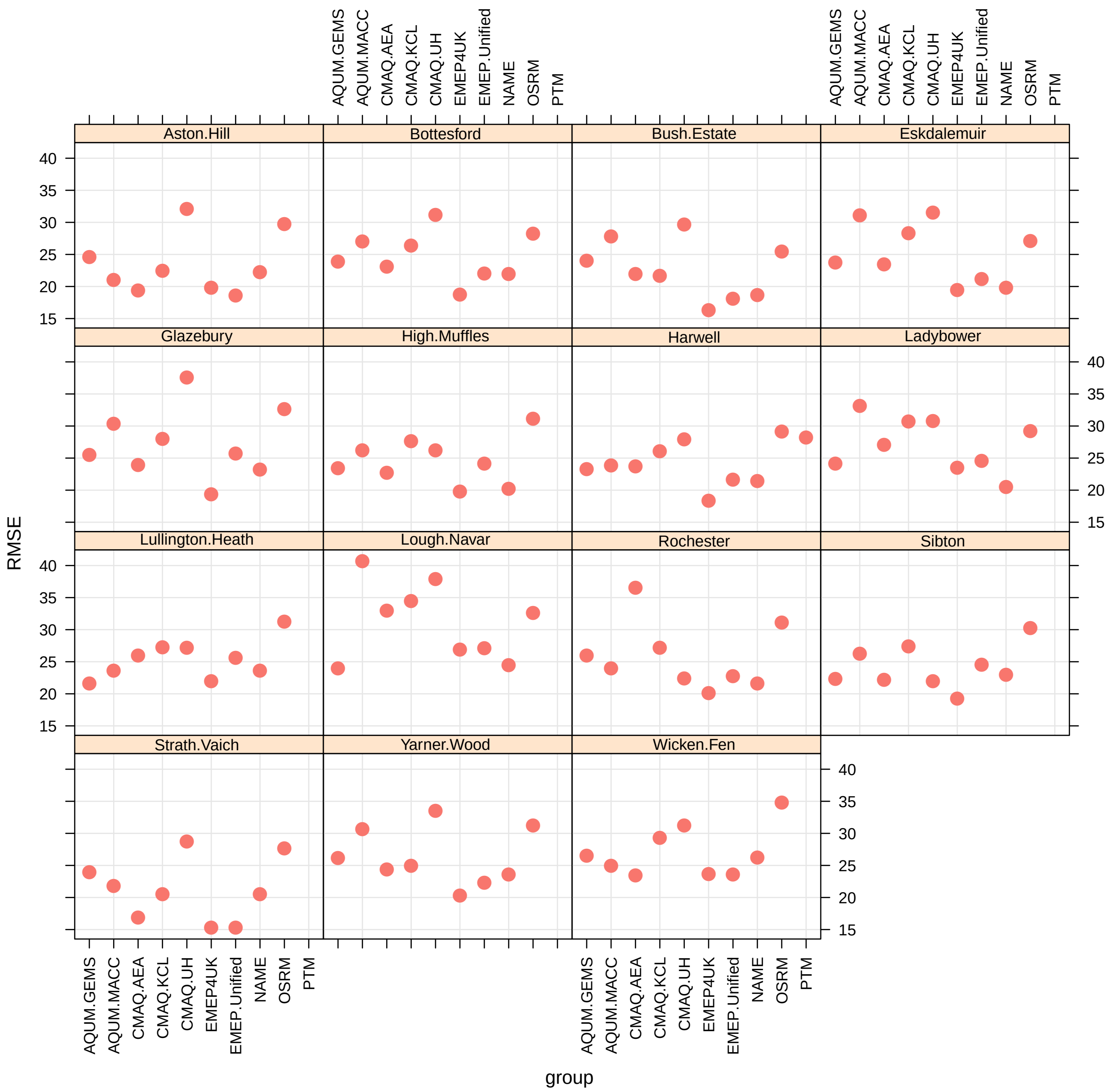

Figure 3: RMSE by site and model.

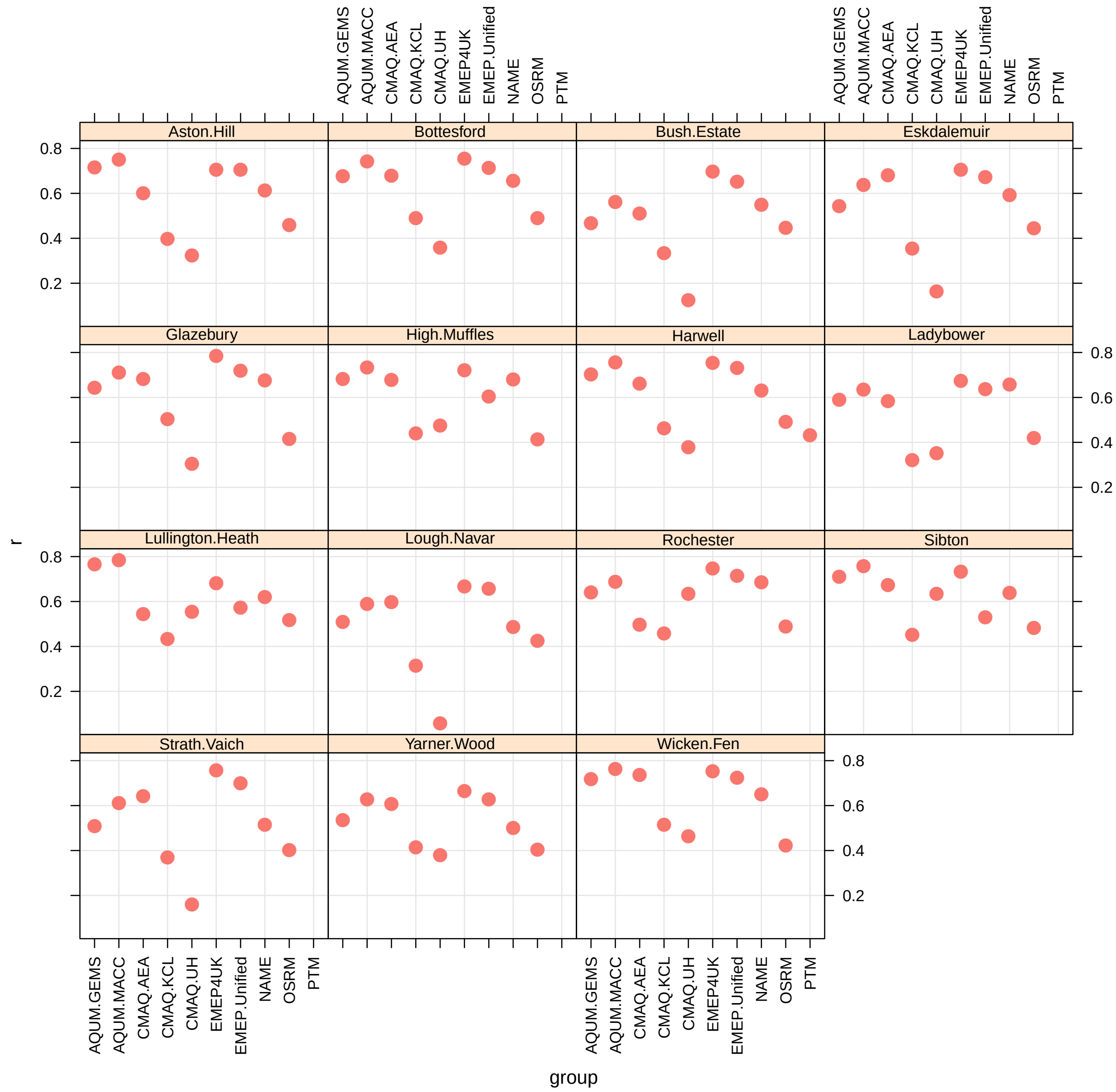

Figure 4: Correlation coefficient, r, by site and model.

3.2 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 μg 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 O_3 data.

The easiest way to understand conditional quantiles is to consider some real data. In this example we consider predictions from the NAME model at Lullington Heath as shown in Figure 5.

```
conditionalQuantile(subset(NAME, site == "Lullington.Heath"), mod = "mod", obs = "o3")
```

A 'good' model has the following characteristics in a conditional quantile plot:

- The predictions cover the full range of measured values. This would be shown by the red (median) prediction line covering the full width of the blue line (perfect predictions).
- Perfect predictions would show the overlap of the median line with the blue line i.e. the median line is straight and at an angle of 45 degrees. Departures from it demonstrate positive (median line below the perfect model line) or negative (median line above the perfect model line) bias in the predictions.
- The percentile bands should be narrow for good predictions.

On this basis the NAME predictions of O_3 at Lullington Heath (Figure 5) show the following characteristics. First, there is an absence of high concentration O_3 predictions because the median line reaches as far as 200 μg m^{-3}, where as the measurements extent to 250 μg m^{-3}. The lower percentile O_3 concentrations are captured well as shown by the overlap of the median line and the perfect model line for O_3 concentrations less than $\approx$70 μg m^{-3}. At concentrations above this level the NAME model tends to over estimate O_3 as shown by the departure of the median line from the perfect model line. There is also a tendency for O_3 predictions at higher levels to be worse because the percentile bands broaden for higher levels of O_3. A better indication of model performance can be gained when the models are compared with one another.

Lots of useful information can be gained into model performance by considering each model by season, using the command below, which plots data for Strath Vaich — shown in Figure 6. Some characteristics to note about Figure 6:

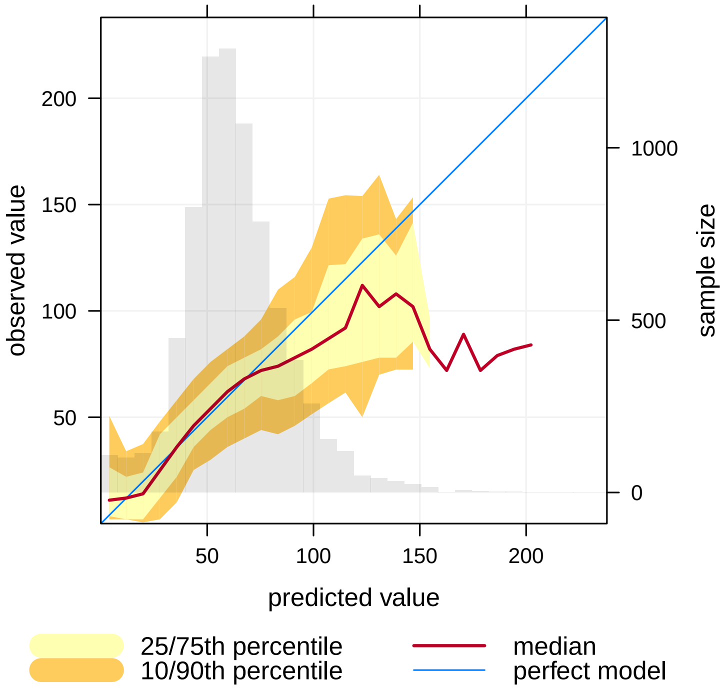

Figure 5: Example of the use of conditional quantiles applied to the NAME model at Lullington Heath for hourly O_3 concentrations. The blue line shows the results for a perfect model. In this case the observations cover a range from 0 to 250 $\mu g\ m^{-3}$. The red line shows the median value of the predictions. The maximum predicted value is 200 $\mu g\ m^{-3}$, somewhat less than the maximum observed value. 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.

- The EMEP models capture the wintertime O_3 concentrations well.
- There is more positive bias in the AQUM.MACC results compared with the AQUM.GEMS for all seasons except spring.
- The CMAQ.UH results and the OSRM results capture little of the variation across all seasons (shown by the almost horizontal median line).
- The CMAQ results in general do not have good coverage i.e. the median line is narrower than the blue "perfect" model line.

The results at a more polluted site (Lullington Heath) show different characteristics as shown in Figure 7. The EMEP models once again capture wintertime O_3 well. In terms of summertime O_3 the AQUM model(s) show best agreement with measurements.

```
conditionalQuantile(subset(all.results, site == "Strath.Vaich"), mod = "mod", obs = "o3",
                    type = c("season", "group"), key.columns = 4)
```

```
conditionalQuantile(subset(all.results, site == "Lullington.Heath"), mod = "mod", obs = "o3",
                    type = c("season", "group"), key.columns = 4)
```

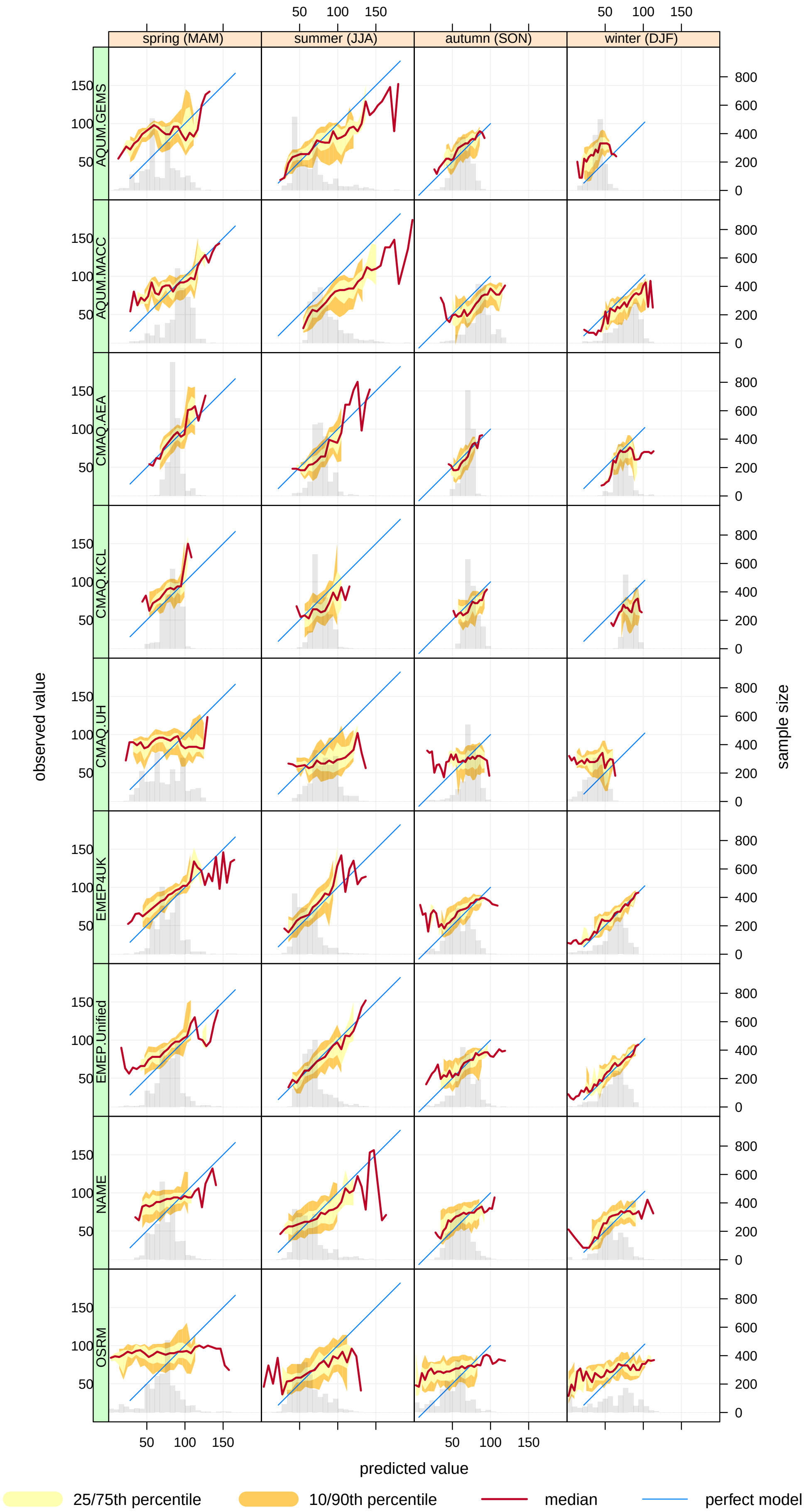

Figure 6: Conditional quantile plot by season and by model for Strath Vaich.

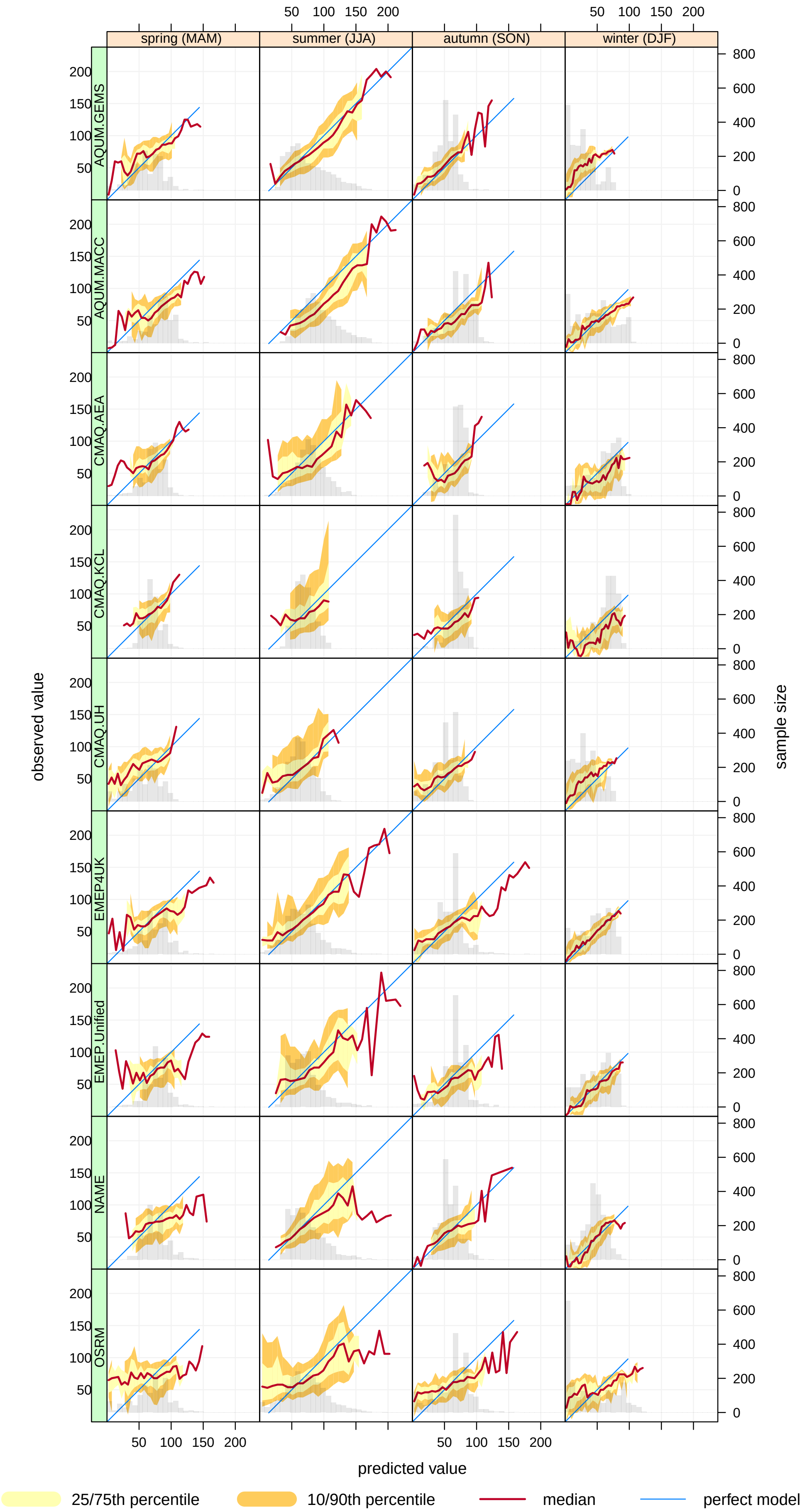

Figure 7: Conditional quantile plot by season and by model for Lullington Heath.

3.3 Comparisons at Harwell at 15:00 GMT

As noted above, the PTM model provides output at Harwell and the 15:00 each day. For a consistent comparison with other models it is necessary to select the same data from those model results. We can combine all the results, and select the appropriate site and time:

```
## select Harwell
harwell <- subset(all.results, site == "Harwell")
## select 15:00
harwell <- selectByDate(harwell, hour = 15)
```

Now it is possible to compare all the models on a similar basis. This time we choose to group by the modelling group and month.

```
all.stats <- modStats(harwell, type = c("group", "month"), mod = "mod", obs = "o3")
head(all.stats)
```

```
      group    month  n      FAC2          MB       MGE          NMB      NMGE     RMSE         r
5 AQUM.GEMS  January 30 0.1666667 -25.3266667 25.326667 -0.689473684 0.6894737 29.06779 0.7389934
4 AQUM.GEMS February 27 0.1851852 -35.1925926 35.192593 -0.633466667 0.6334667 38.85063 0.6948702
8 AQUM.GEMS    March 27 0.6666667 -30.5111111 31.607407 -0.422028689 0.4371926 34.61057 0.5400167
1 AQUM.GEMS    April 28 0.9285714 -19.1892857 21.910714 -0.248060942 0.2832410 26.10150 0.5856377
9 AQUM.GEMS      May 22 1.0000000  -0.5727273  9.927273 -0.006382979 0.1106383 13.53914 0.8496118
7 AQUM.GEMS     June 24 1.0000000  16.6833333 17.533333  0.189224953 0.1988658 22.53468 0.8889835
```

The data can be clearly summarised in an aggregate way:

```
modStats(harwell, type = "group", mod = "mod", obs = "o3")
```

```
          group   n      FAC2         MB      MGE         NMB      NMGE     RMSE         r
1     AQUM.GEMS 334 0.7784431 -13.173653 19.72156 -0.19262762 0.2883723 24.43033 0.8101726
2     AQUM.MACC 334 0.9011976   8.385629 16.67066  0.12261623 0.2437615 21.28679 0.8399143
3      CMAQ.AEA 329 0.8936170   9.724553 18.27325  0.14131528 0.2655433 24.47690 0.6928368
4      CMAQ.KCL 328 0.8810976   2.324207 18.53177  0.03410917 0.2719651 25.46200 0.5457169
5       CMAQ.UH 334 0.8113772 -11.161132 23.33358 -0.16320016 0.3411879 31.31166 0.4095081
6       EMEP4UK 323 0.9473684   7.318335 15.39576  0.10543364 0.2218033 21.02232 0.7563960
7   EMEP.Unified 334 0.9071856  10.036988 15.92092  0.14676272 0.2327986 21.84005 0.7829224
8          NAME 334 0.9101796  -1.789425 18.40721 -0.02616531 0.2691537 24.87846 0.6196814
9          OSRM 334 0.7814371  -9.152695 20.94946 -0.13383241 0.3063269 28.81127 0.6074468
10          PTM 334 0.8772455   7.392395 20.22216  0.10809299 0.2956921 28.24357 0.4311594
```

A scatter plot of these results is shown in Figure 8. This plot was generated by:

```
scatterPlot(harwell, x = "o3", y = "mod", mod.line = TRUE, type = "group", group = "month",
            smooth = FALSE)
```

It is perhaps more useful to plot some of the model performance statistics. Figure 9 shows the mean bias by model and Figure 10 shows the RMSE for each model.

```
scatterPlot(all.stats, x = "month", y = "MB", type = "group", key = FALSE, pch = 16,
            ref.y = 0)
```

```
scatterPlot(all.stats, x = "month", y = "RMSE", type = "group", key = FALSE, pch = 16)
```

The PTM does treat each percentile prediction as an independent model run and it is useful therefore to consider the predictions separately. Below we import the PTM data again and consider each of the percentile predictions.

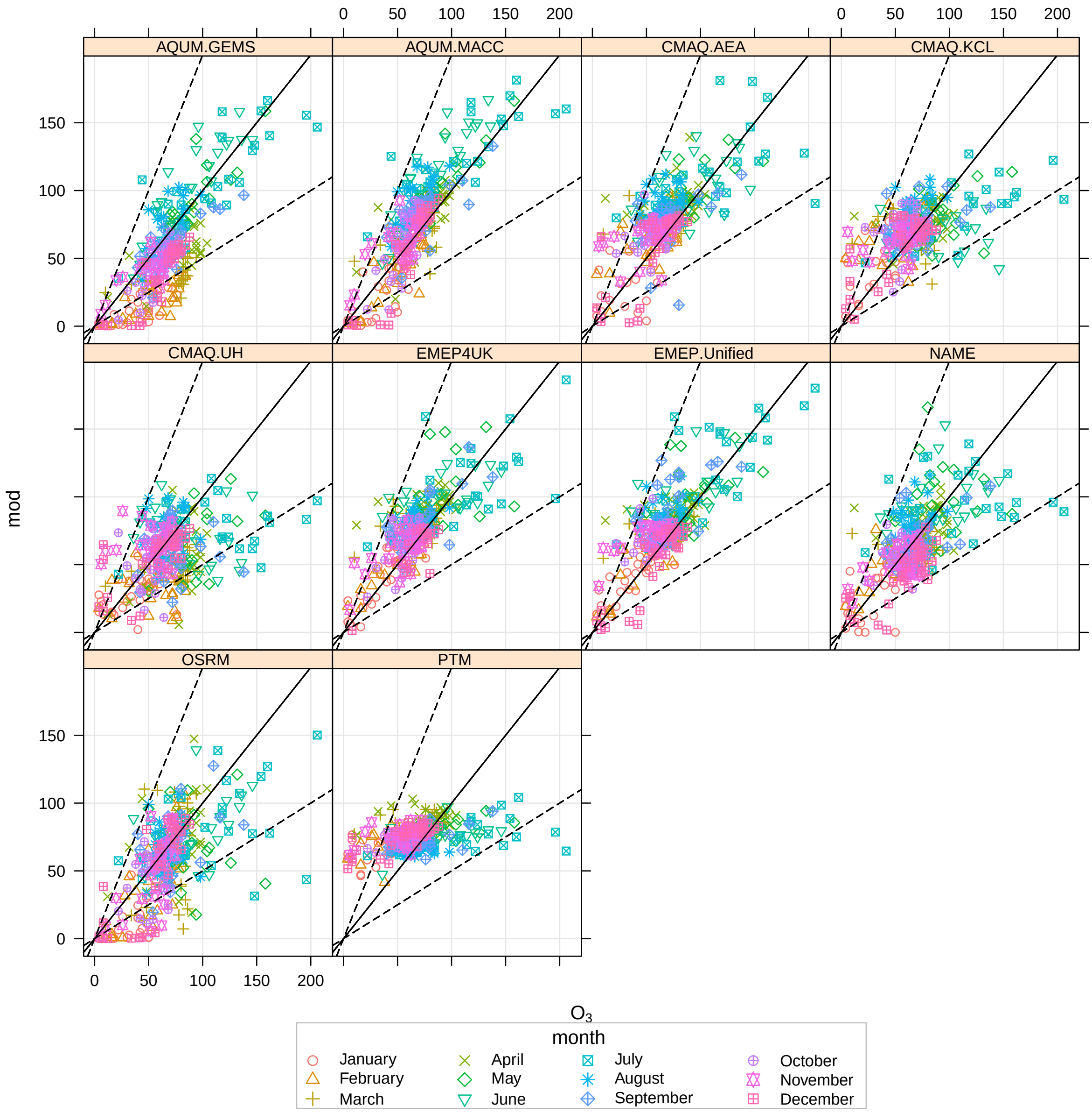

Figure 8: Plot of observed vs. modelled O_3 concentration at Harwell for hour 15:00.

```
## import the data
ptm.all <- import("ozoneTemplateV2 0_PTM.csv", data.at = 4, header.at = 3, date.name = "Date", time.name = "Date")
```

```
     date1       date2   X95..ile   X84..ile   X50..ile   X16..ile    X5..ile
"POSIXct"   "POSIXt" "numeric" "numeric" "numeric" "numeric" "numeric"
```

```
## change variable names
names(ptm.all)[2:6] <- c("P95", "P84", "P50", "P16", "P5")
## stack the data
ptm.all <- melt(ptm.all, measure.vars = 2:6)
names(ptm.all)[3] <- "mod"
## merge with measurements at Harwell but only by date
ptm.all <- merge(subset(ozone.meas, site == "Harwell"), ptm.all, by = "date", all = FALSE)
## only need hour = 15
ptm.all <- selectByDate(ptm.all, hour = 15)
```

Now it is possible to derive the statistics for these models:

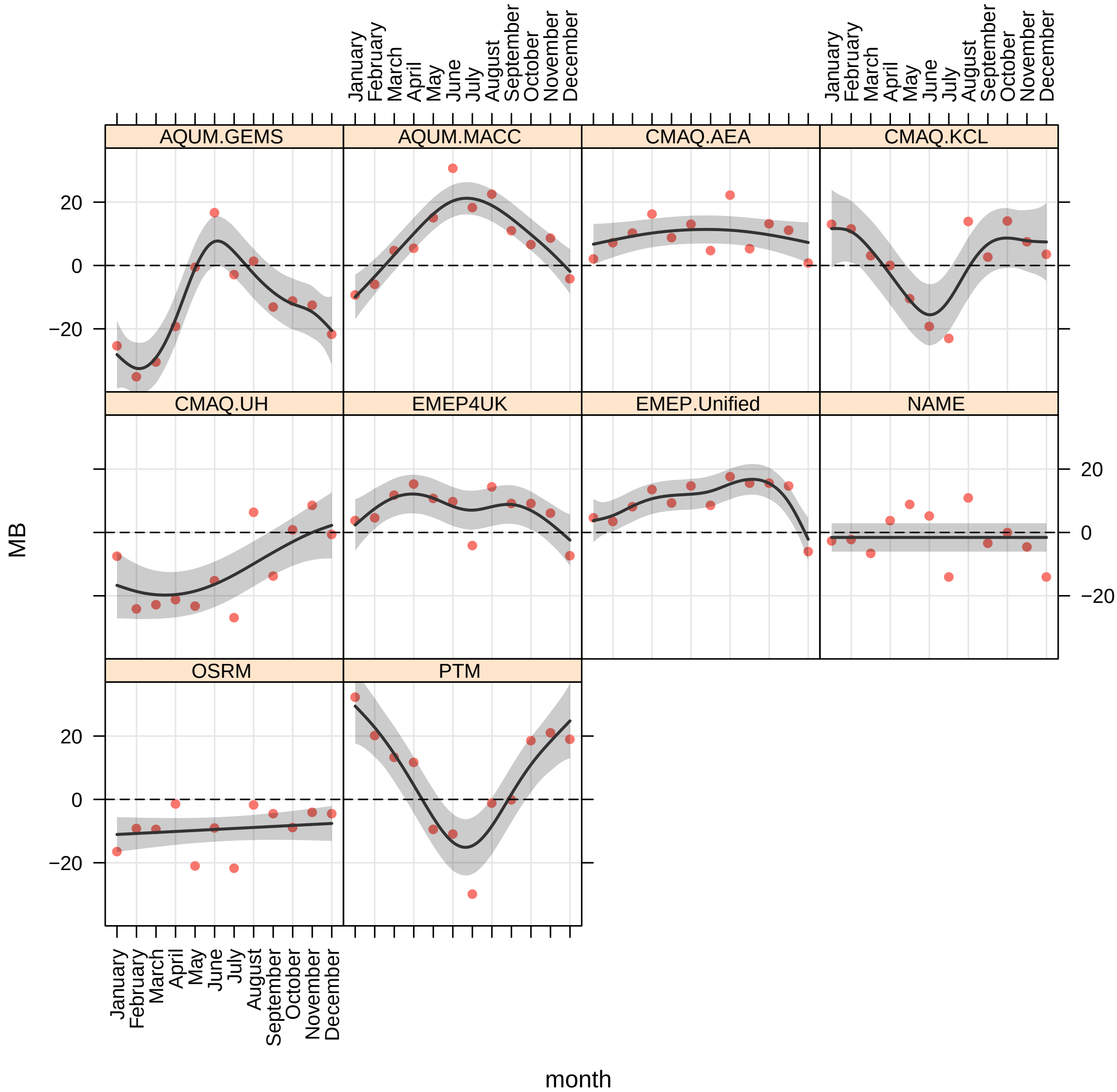

Figure 9: Plot of mean bias by model for Harwell at 15:00 GMT.

```
modStats(ptm.all, type = "variable", mod = "mod", obs = "o3")
```

```
  variable   n      FAC2         MB      MGE         NMB      NMGE     RMSE         r
5      P95 334 0.8233533  24.397485 28.19341  0.35674459 0.4122494 36.78251 0.4237818
4      P84 334 0.8622754  16.419251 23.40919  0.24008537 0.3422936 30.61505 0.5299844
3      P50 334 0.8772455   7.392395 20.22216  0.10809299 0.2956921 28.24357 0.4311594
1      P16 334 0.8712575  -2.842216 18.97647 -0.04155941 0.2774775 27.94162 0.3844891
2       P5 334 0.7874251 -14.501168 23.39572 -0.21203879 0.3420966 34.33598 0.2365358
```

A scatter plot of these results is shown in Figure 11.

```
scatterPlot(ptm.all, x = "o3", y = "mod", type = "variable", mod.line = TRUE, key = FALSE)
```

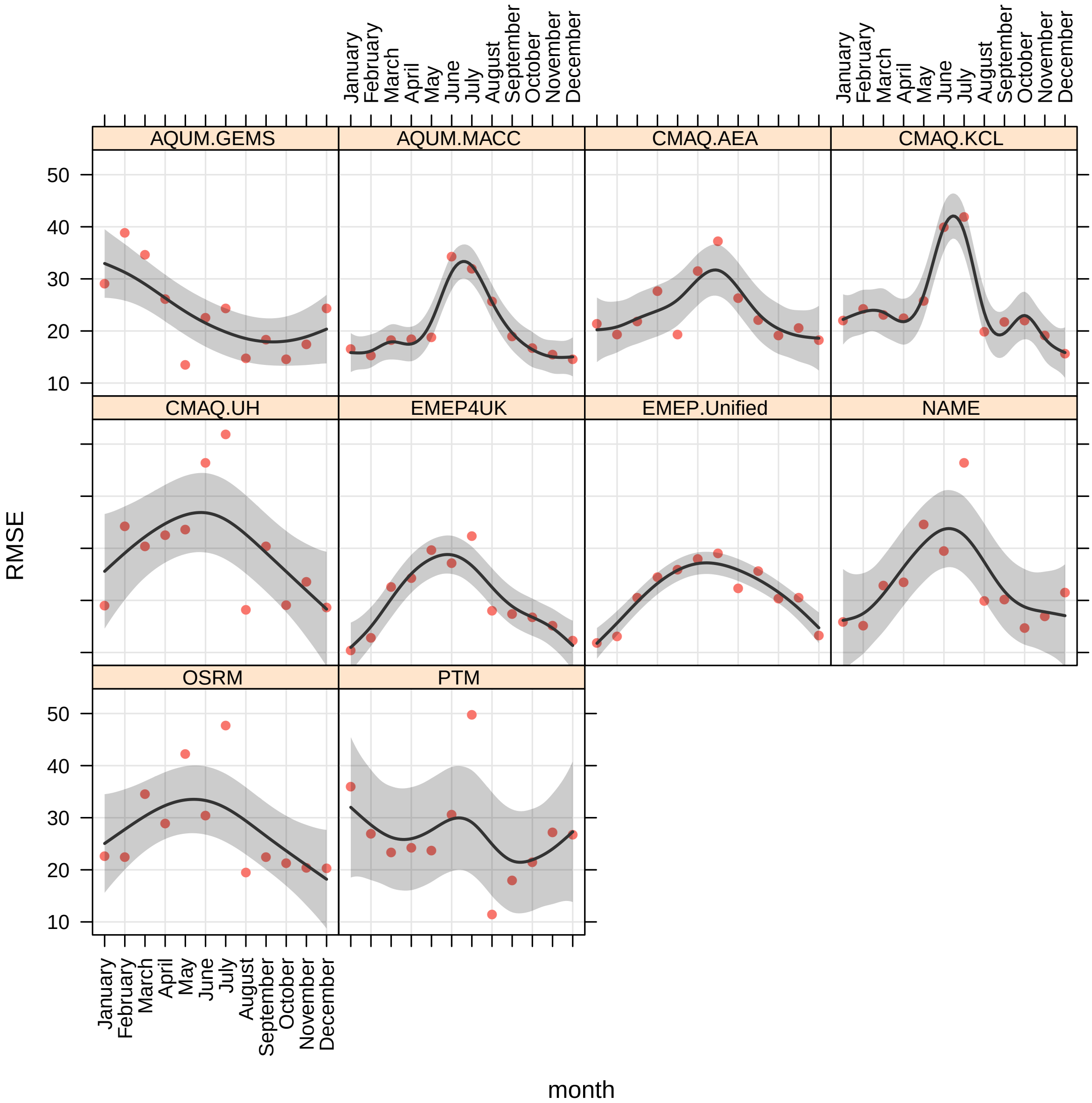

Figure 10: Plot of root mean square error (RMSE) by model for Harwell at 15:00 GMT.

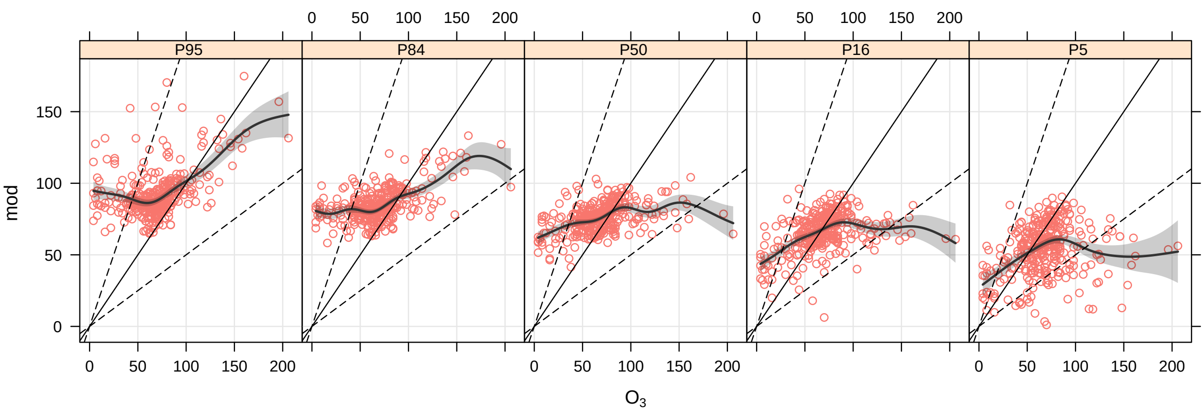

Figure 11: Scatter plot of of observed vs. modelled O_3 concentrations for different PTM models.

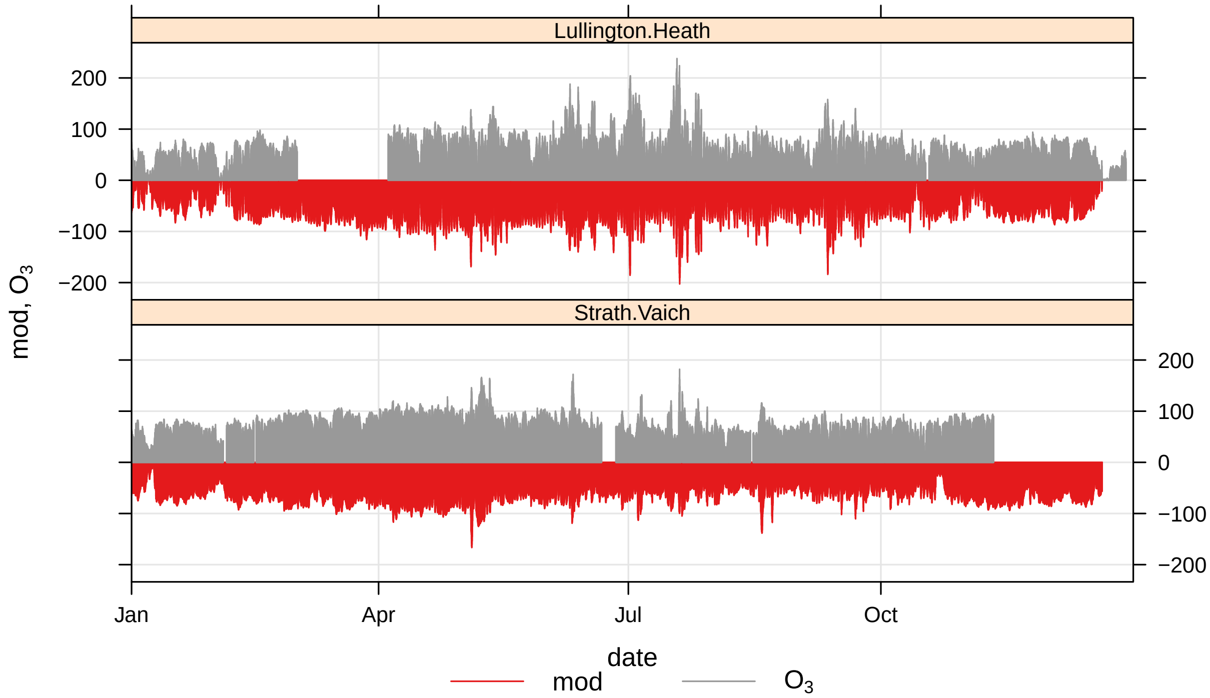

Figure 12: Time series of two sites using the EMEP4UK model.

3.4 Time series comparisons

We focus on only two sites in this section due to the amount of data to present: Lullington.Heath and Strath.Vaich. These two locations should provide an interesting contrast for comparison i.e. one site in the south-east of England influenced by regional-scale summertime episodes and one site in a remote area of Scotland more influenced by background or 'baseline' air masses. As before, other plots can easily be generated by each group.

```
emep.sub <- subset(emep, site %in% c("Lullington.Heath", "Strath.Vaich"))
timePlot(transform(emep.sub, mod = -1 * mod), pollutant = c("mod", "o3"), type = "site",
        layout = c(1, 2), plot.type = "h", lty = 1)
```

```
emepUnified.sub <- subset(emepUnified, site %in% c("Lullington.Heath", "Strath.Vaich"))
timePlot(transform(emepUnified.sub, mod = -1 * mod), pollutant = c("mod", "o3"), type = "site",
        layout = c(1, 2), plot.type = "h", lty = 1)
```

```
NAME.sub <- subset(NAME, site %in% c("Lullington.Heath", "Strath.Vaich"))
timePlot(transform(NAME.sub, mod = -1 * mod), pollutant = c("mod", "o3"), type = "site",
        layout = c(1, 2), plot.type = "h", lty = 1)
```

```
AQUM.GEMS.sub <- subset(AQUM.GEMS, site %in% c("Lullington.Heath", "Strath.Vaich"))
timePlot(transform(AQUM.GEMS.sub, mod = -1 * mod), pollutant = c("mod", "o3"), type = "site",
        layout = c(1, 2), plot.type = "h", lty = 1)
```

```
AQUM.MACC.sub <- subset(AQUM.MACC, site %in% c("Lullington.Heath", "Strath.Vaich"))
timePlot(transform(AQUM.MACC.sub, mod = -1 * mod), pollutant = c("mod", "o3"), type = "site",
        layout = c(1, 2), plot.type = "h", lty = 1)
```

```
CMAQ.AEA.sub <- subset(CMAQ.AEA, site %in% c("Lullington.Heath", "Strath.Vaich"))
timePlot(transform(CMAQ.AEA.sub, mod = -1 * mod), pollutant = c("mod", "o3"), type = "site",
        layout = c(1, 2), plot.type = "h", lty = 1)
```

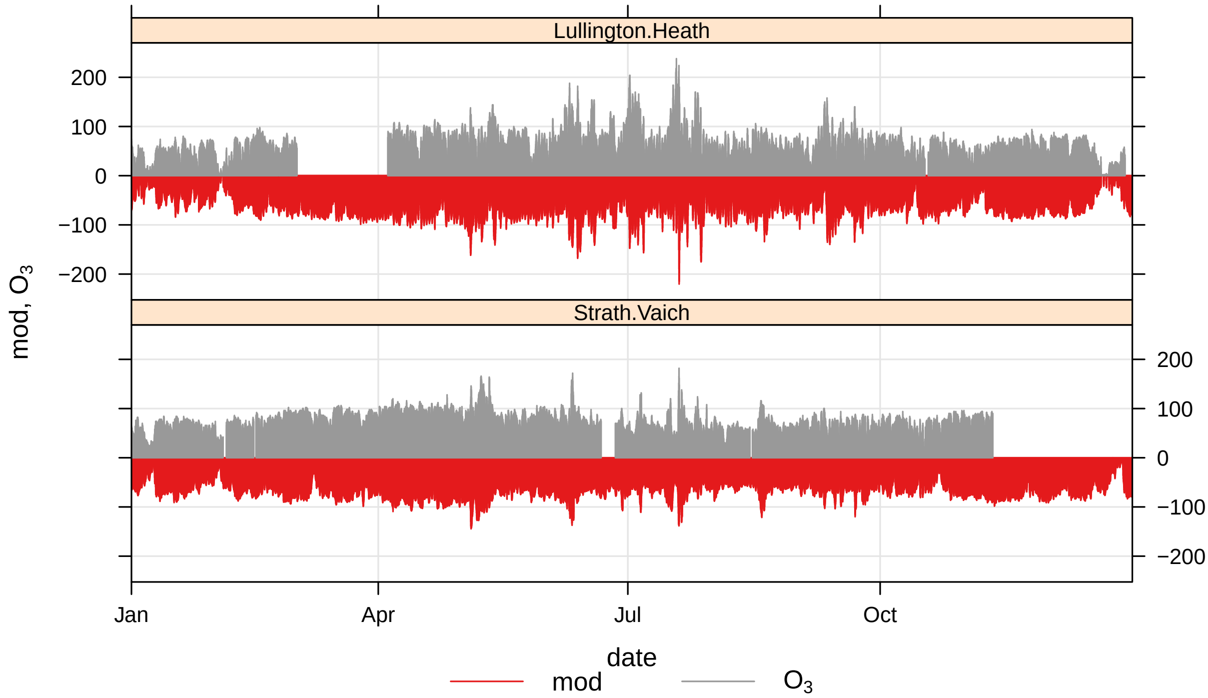

Figure 13: Time series of two sites using the EMEP Unified model.

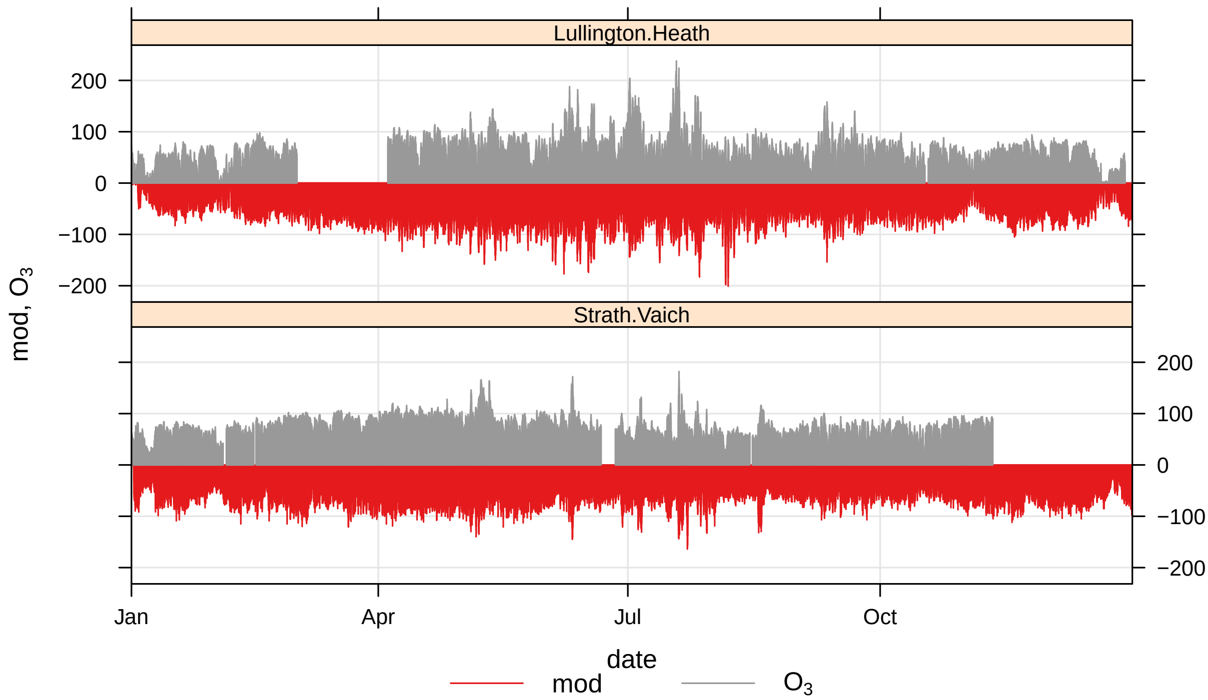

Figure 14: Time series of two sites using the NAME model.

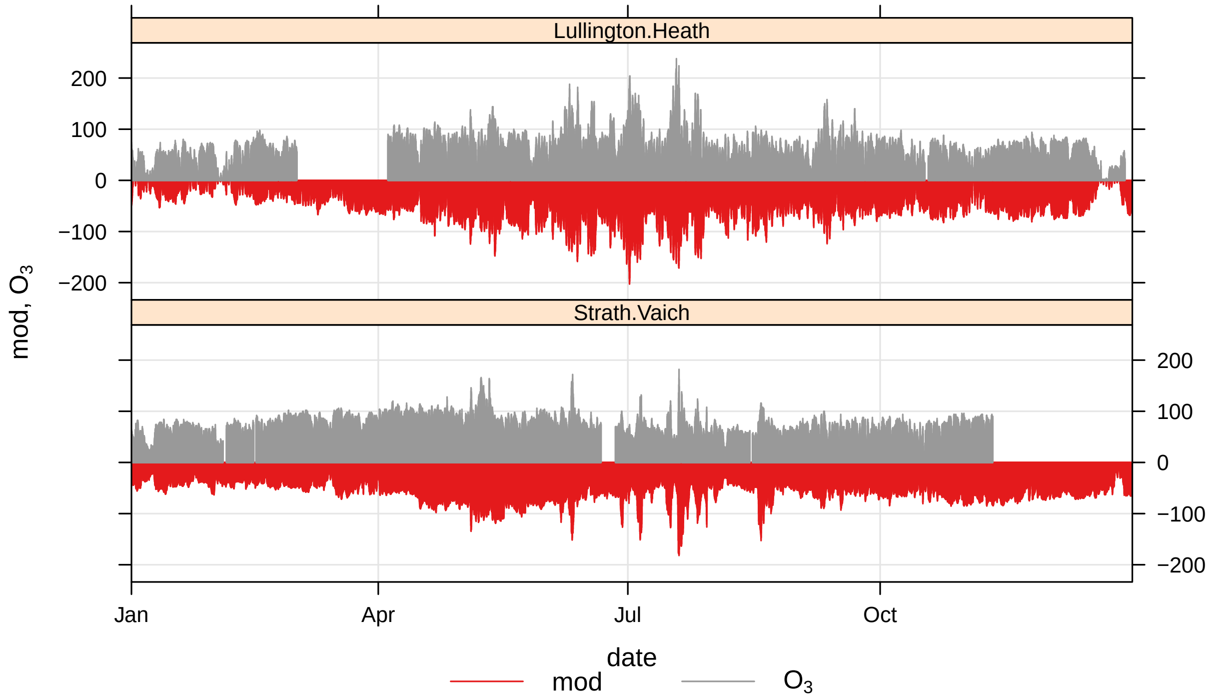

Figure 15: Time series of two sites using the AQUM.GEMS model.

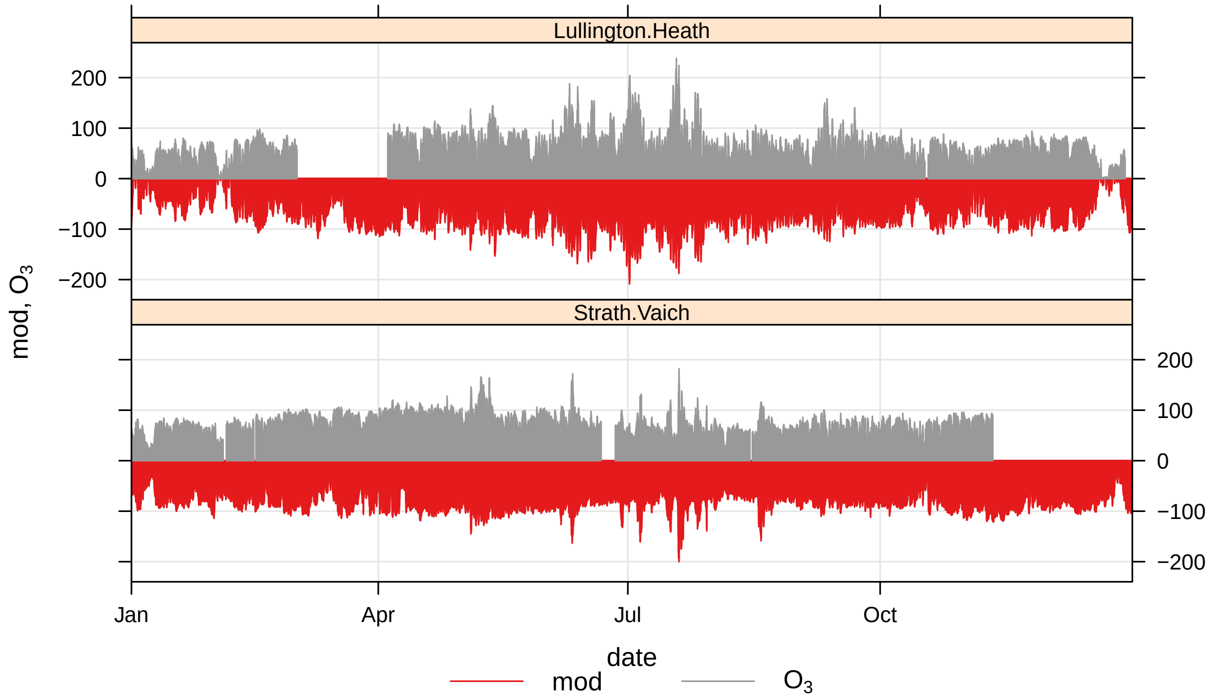

Figure 16: Time series of two sites using the AQUM.MACC model.

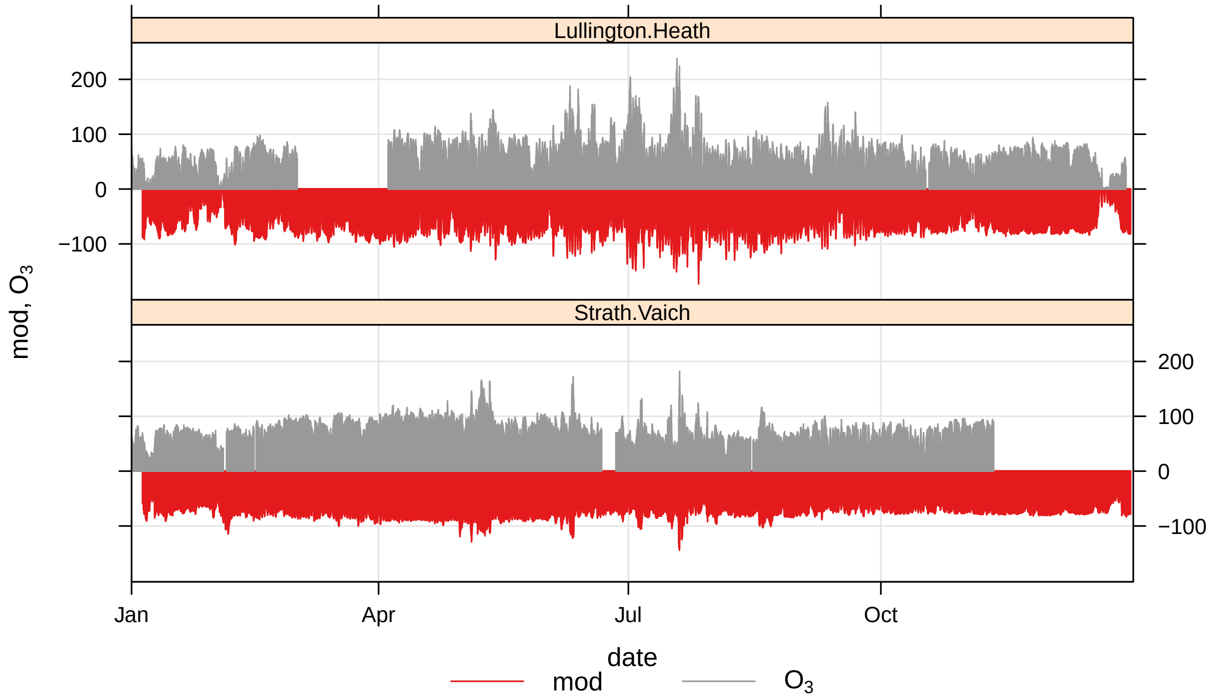

Figure 17: Time series of two sites using the CMAQ AEA model.

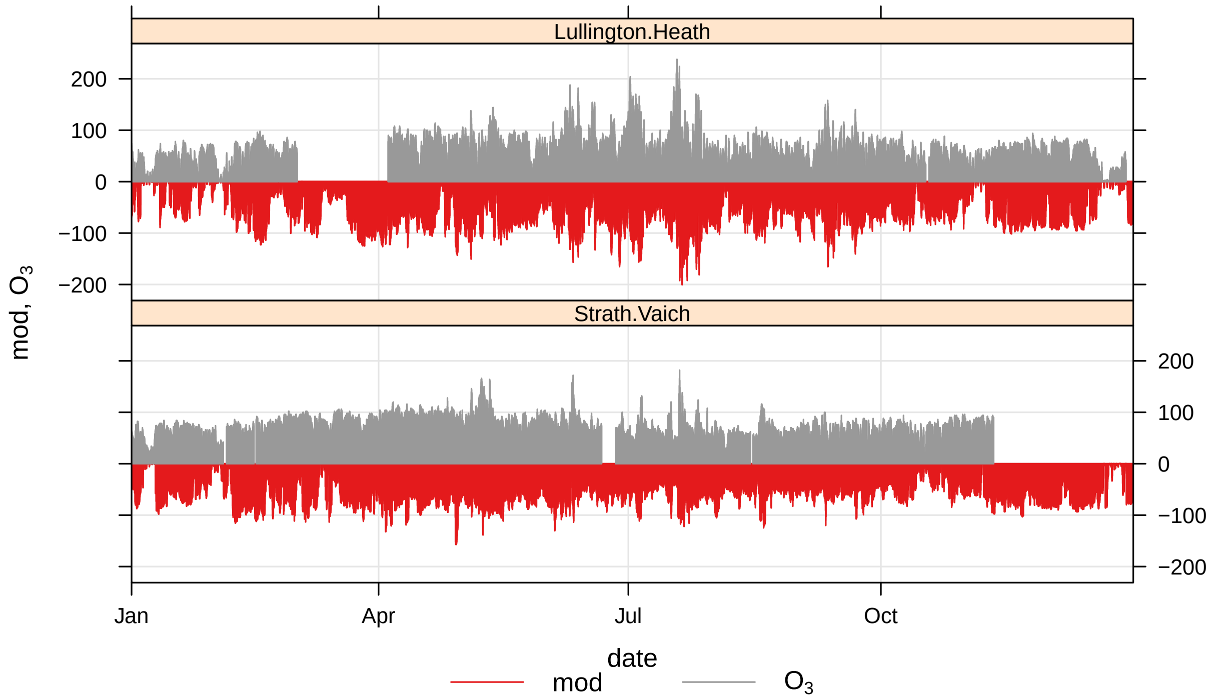

Figure 18: Time series of two sites using the OSRM model.

```
OSRM.sub <- subset(OSRM, site %in% c("Lullington.Heath", "Strath.Vaich"))
timePlot(transform(OSRM.sub, mod = -1 * mod), pollutant = c("mod", "o3"), type = "site",
         layout = c(1, 2), plot.type = "h", lty = 1)
```

```
CMAQ.UH.sub <- subset(CMAQ.UH, site %in% c("Lullington.Heath", "Strath.Vaich"))
timePlot(transform(CMAQ.UH.sub, mod = -1 * mod), pollutant = c("mod", "o3"), type = "site",
         layout = c(1, 2), plot.type = "h", lty = 1)
```

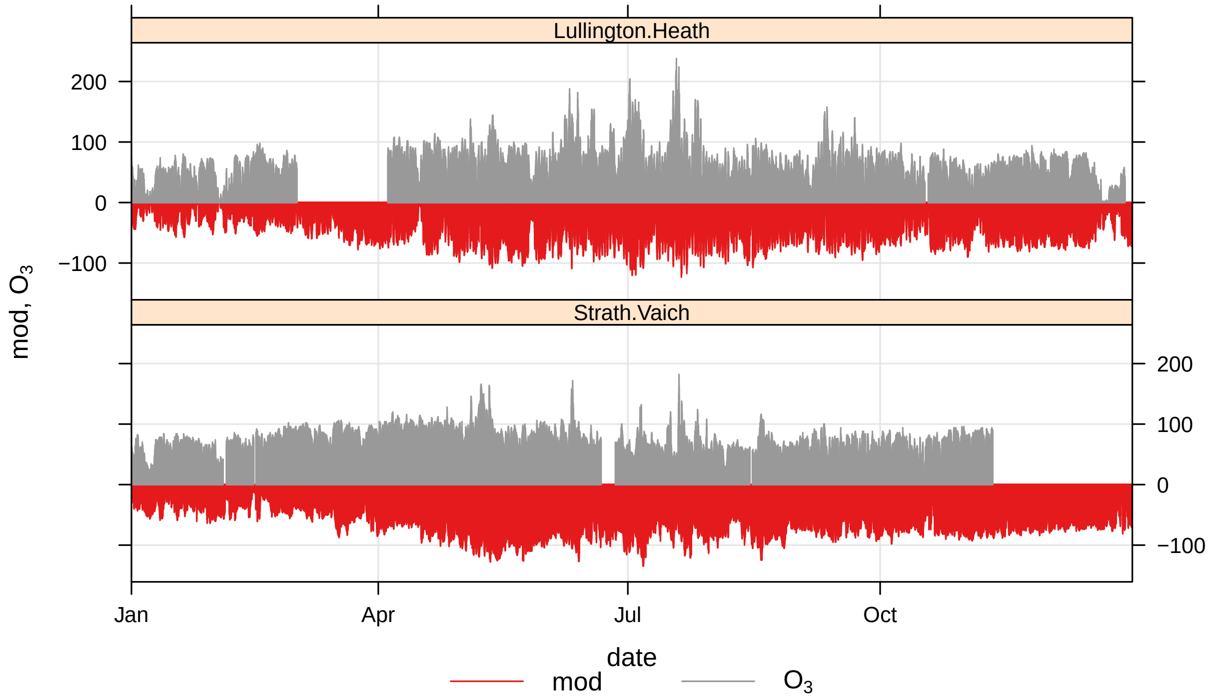

Figure 19: Time series of two sites using the CMAQ University of Hertfordshire model.

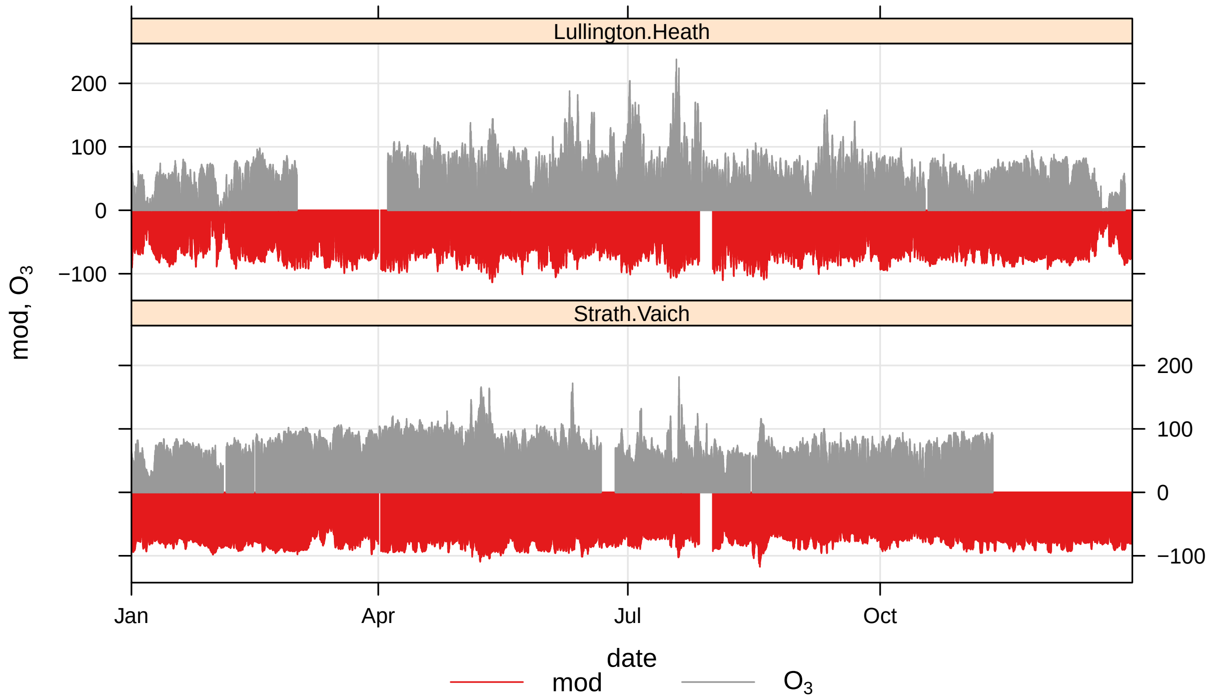

Figure 20: Time series of two sites using the CMAQ King's College London model.

```
CMAQ.KCL.sub <- subset(CMAQ.KCL, site %in% c("Lullington.Heath", "Strath.Vaich"))
timePlot(transform(CMAQ.KCL.sub, mod = -1 * mod), pollutant = c("mod", "o3"), type = "site",
         layout = c(1, 2), plot.type = "h", lty = 1)
```

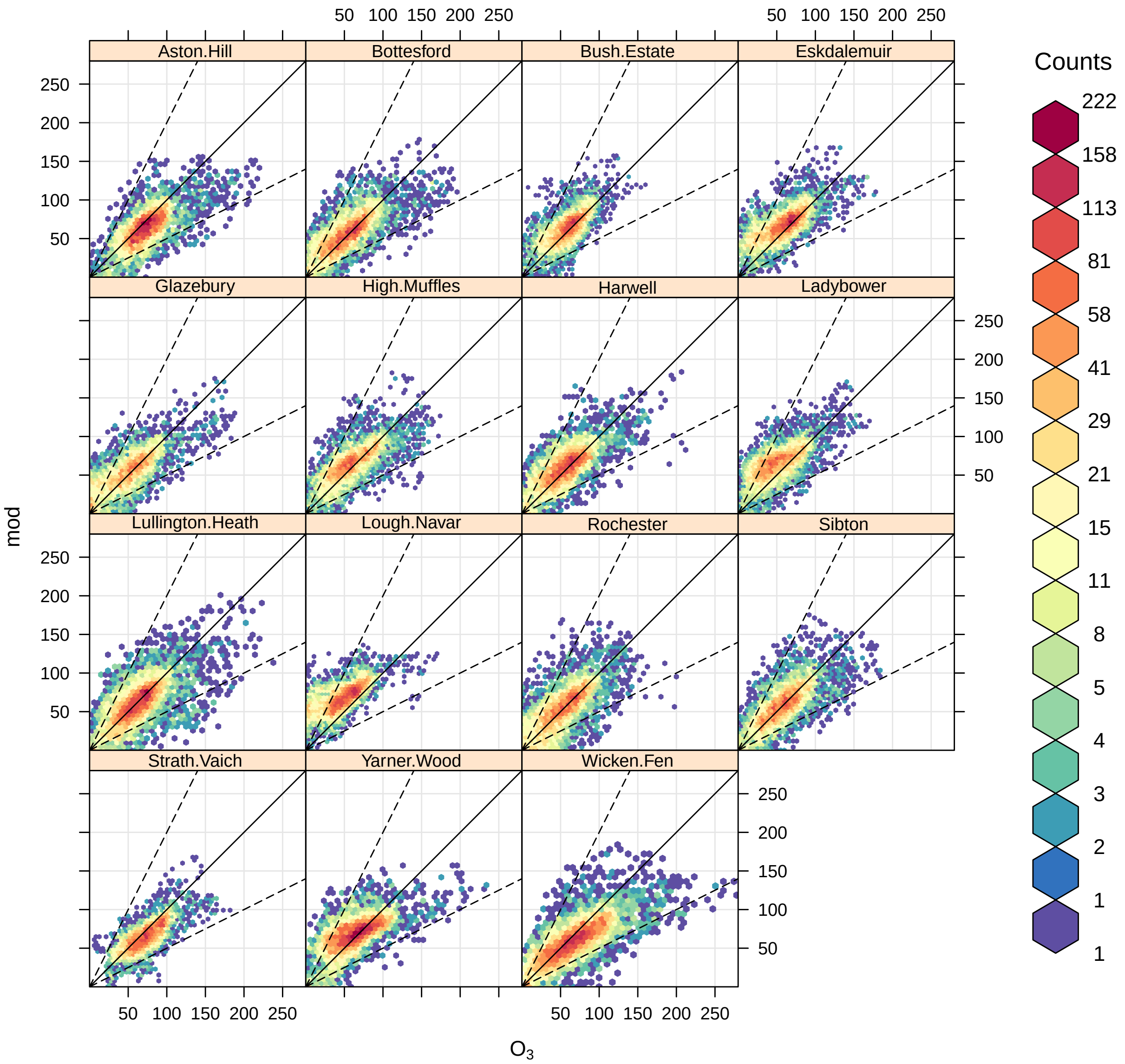

Figure 21: Scatter plot of observed hourly O_3 concentration vs. modelled for the EMEP4UK model. The dashed lines show the within factor of two (FAC2) region.

3.5 Scatter plots

Scatter plots are very useful to consider for model evaluation. With hourly data it can be very difficult to see how good a relationship is due to over-plotting. One way round this is to "bin" the data first, which we do here with hexagonal bins as shown in Figure 21. In this Figure it is much easier to see where the data lie and to get a feeling about bias etc. For example, consider the Aston Hill plot — it is apparent that the main bulk of the points lie below the 1:1 line and there is a negative bias (confirmed by considering Table 2).

```
scatterPlot(emep, x = "o3", y = "mod", type = "site", smooth = FALSE, mod.line = TRUE,
            method = "hexbin", xlim = c(0, 280), ylim = c(0, 280))
```

```
scatterPlot(NAME, x = "o3", y = "mod", type = "site", smooth = FALSE, mod.line = TRUE,
            method = "hexbin", xlim = c(0, 280), ylim = c(0, 280))
```

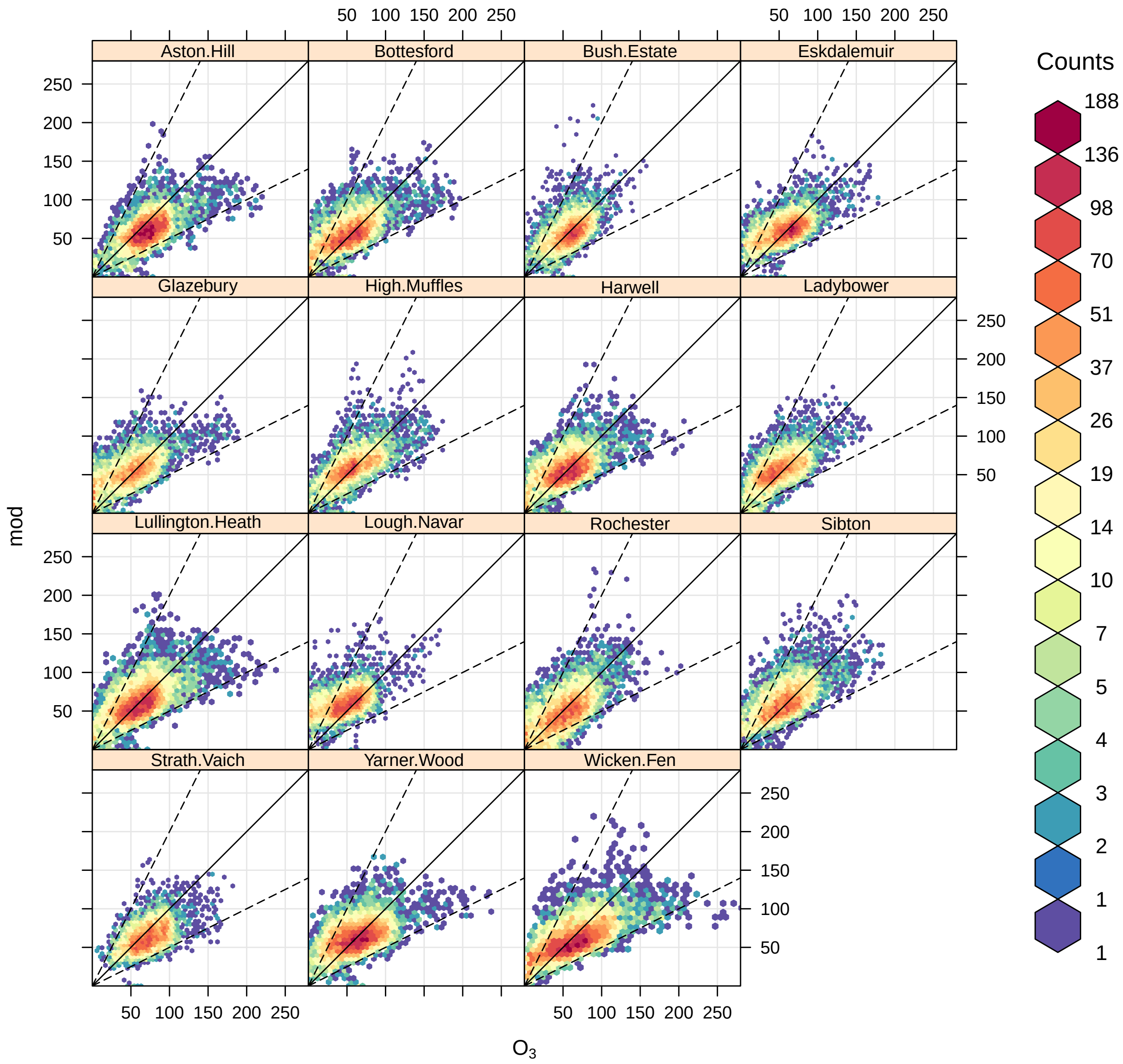

Figure 22: Scatter plot of observed hourly O_3 concentration vs. modelled for the NAME model. The dashed lines show the within factor of two (FAC2) region.

```
scatterPlot(emepUnified, x = "o3", y = "mod", type = "site", smooth = FALSE, mod.line = TRUE,
          method = "hexbin", xlim = c(0, 280), ylim = c(0, 280))
```

```
scatterPlot(AQUM.GEMS, x = "o3", y = "mod", type = "site", smooth = FALSE, mod.line = TRUE,
          method = "hexbin", xlim = c(0, 280), ylim = c(0, 280))
```

```
scatterPlot(AQUM.MACC, x = "o3", y = "mod", type = "site", smooth = FALSE, mod.line = TRUE,
          method = "hexbin", xlim = c(0, 280), ylim = c(0, 280))
```

```
scatterPlot(CMAQ.AEA, x = "o3", y = "mod", type = "site", smooth = FALSE, mod.line = TRUE,
          method = "hexbin", xlim = c(0, 280), ylim = c(0, 280))
```

```
scatterPlot(OSRM, x = "o3", y = "mod", type = "site", smooth = FALSE, mod.line = TRUE,
          method = "hexbin", xlim = c(0, 280), ylim = c(0, 280))
```

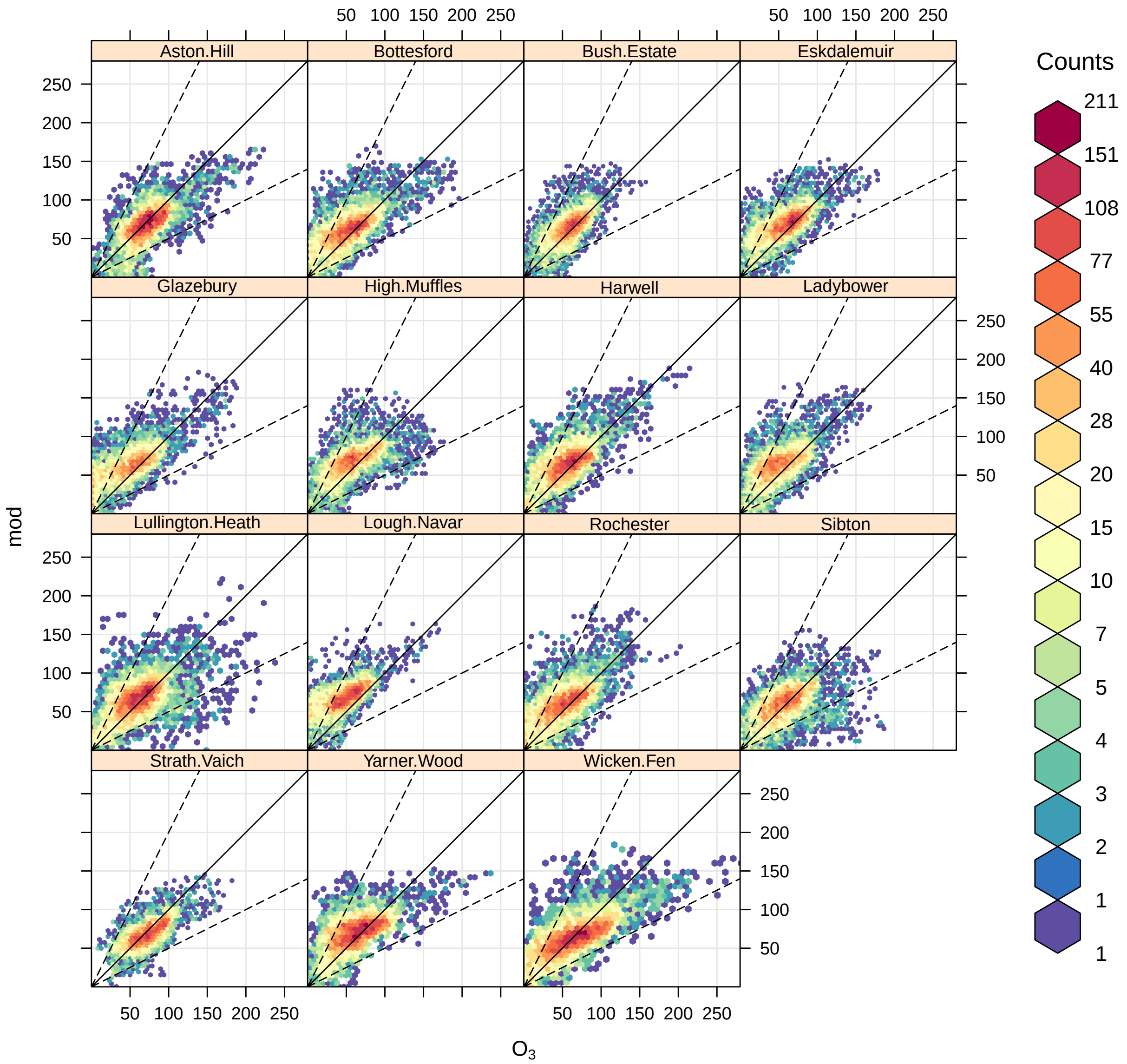

Figure 23: Scatter plot of observed hourly O_3 concentration vs. modelled for the EMEP Unified model. The dashed lines show the within factor of two (FAC2) region.

```
scatterPlot(CMAQ.UH, x = "o3", y = "mod", type = "site", smooth = FALSE, mod.line = TRUE,
          method = "hexbin", xlim = c(0, 280), ylim = c(0, 280))
```

```
scatterPlot(CMAQ.KCL, x = "o3", y = "mod", type = "site", smooth = FALSE, mod.line = TRUE,
          method = "hexbin", xlim = c(0, 280), ylim = c(0, 280))
```

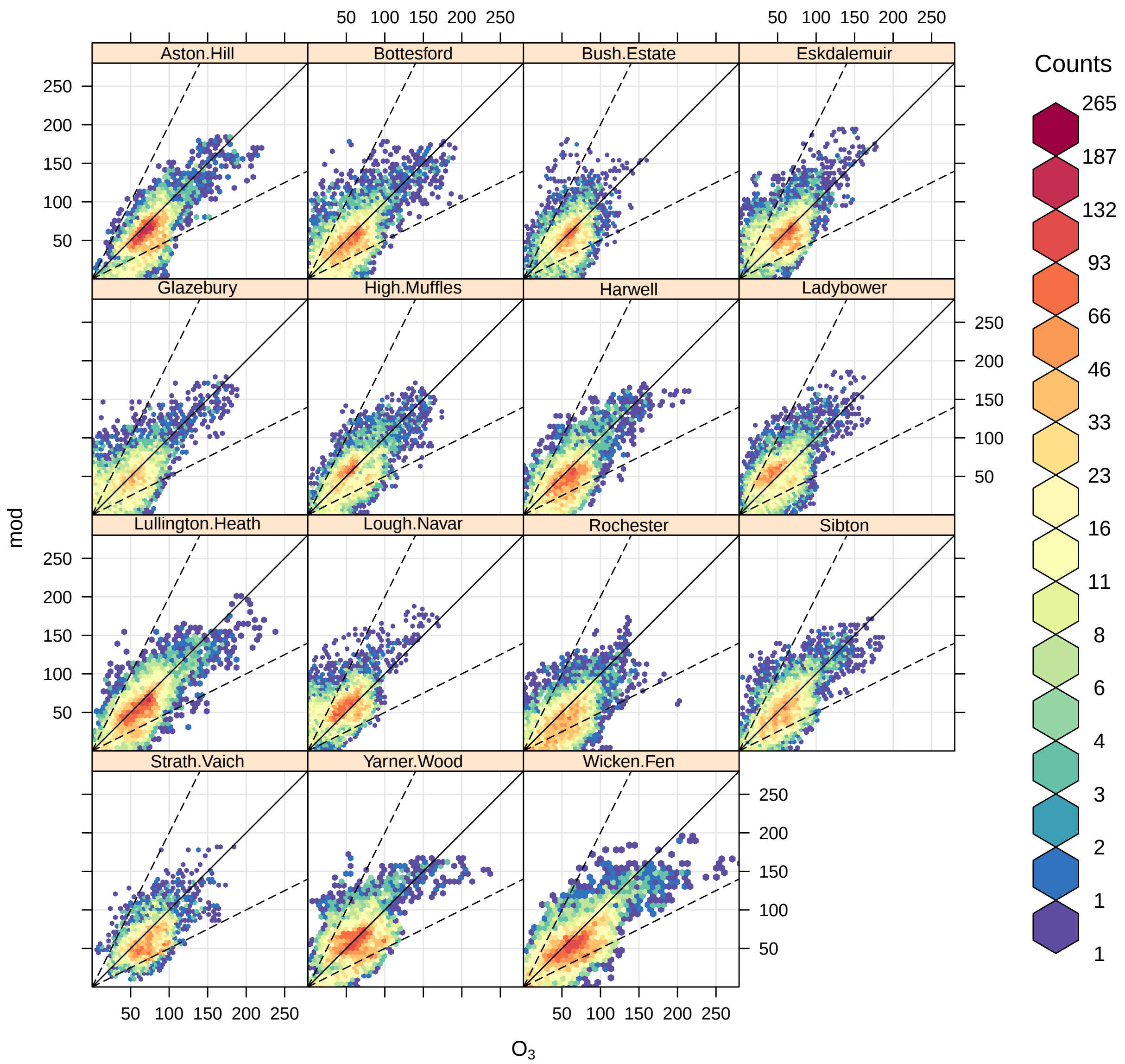

Figure 24: Scatter plot of observed hourly O_3 concentration vs. modelled for the AQUM.GEMS model. The dashed lines show the within factor of two (FAC2) region.

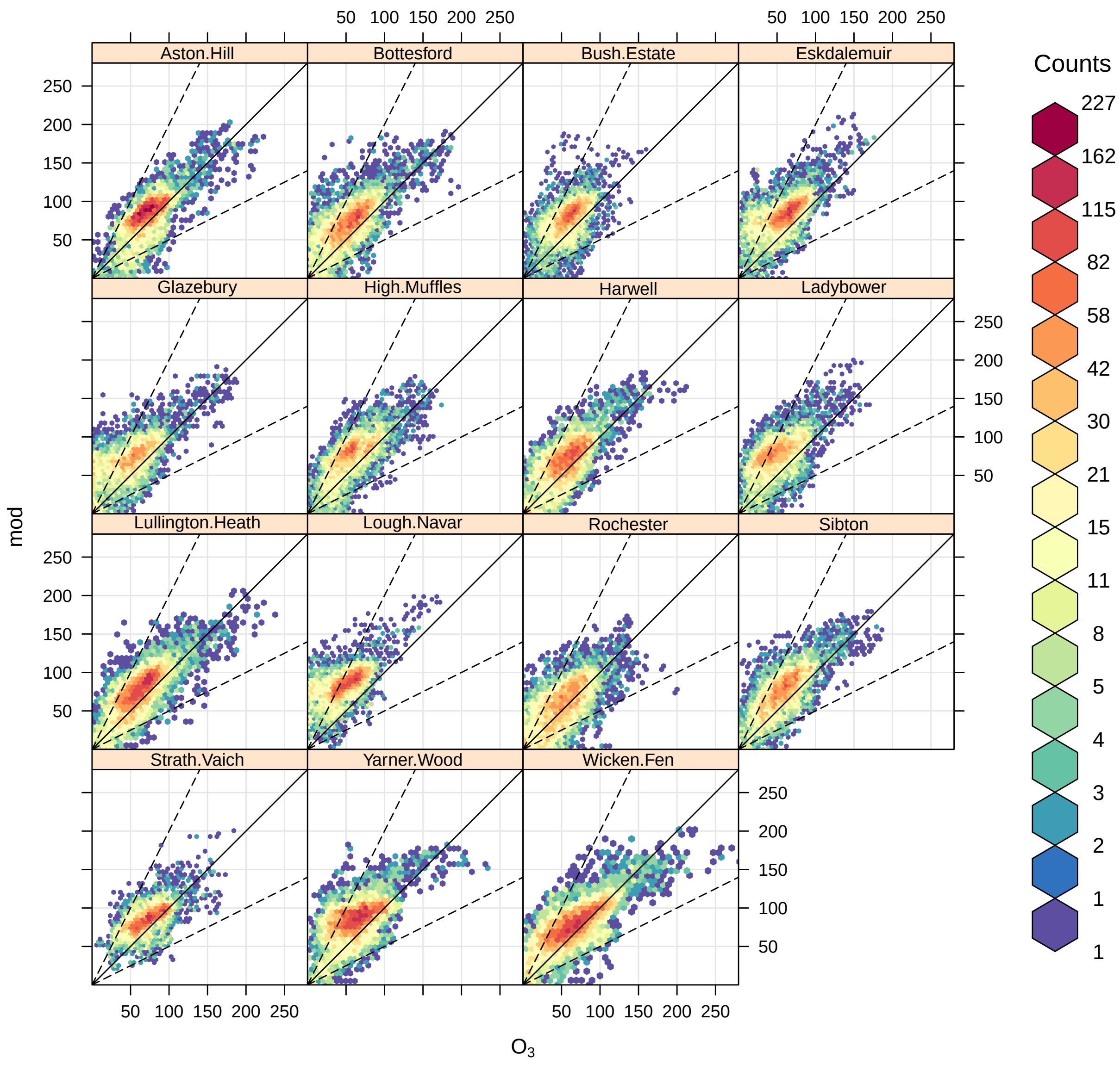

Figure 25: Scatter plot of observed hourly O_3 concentration vs. modelled for the AQUM.MACC model. The dashed lines show the within factor of two (FAC2) region.

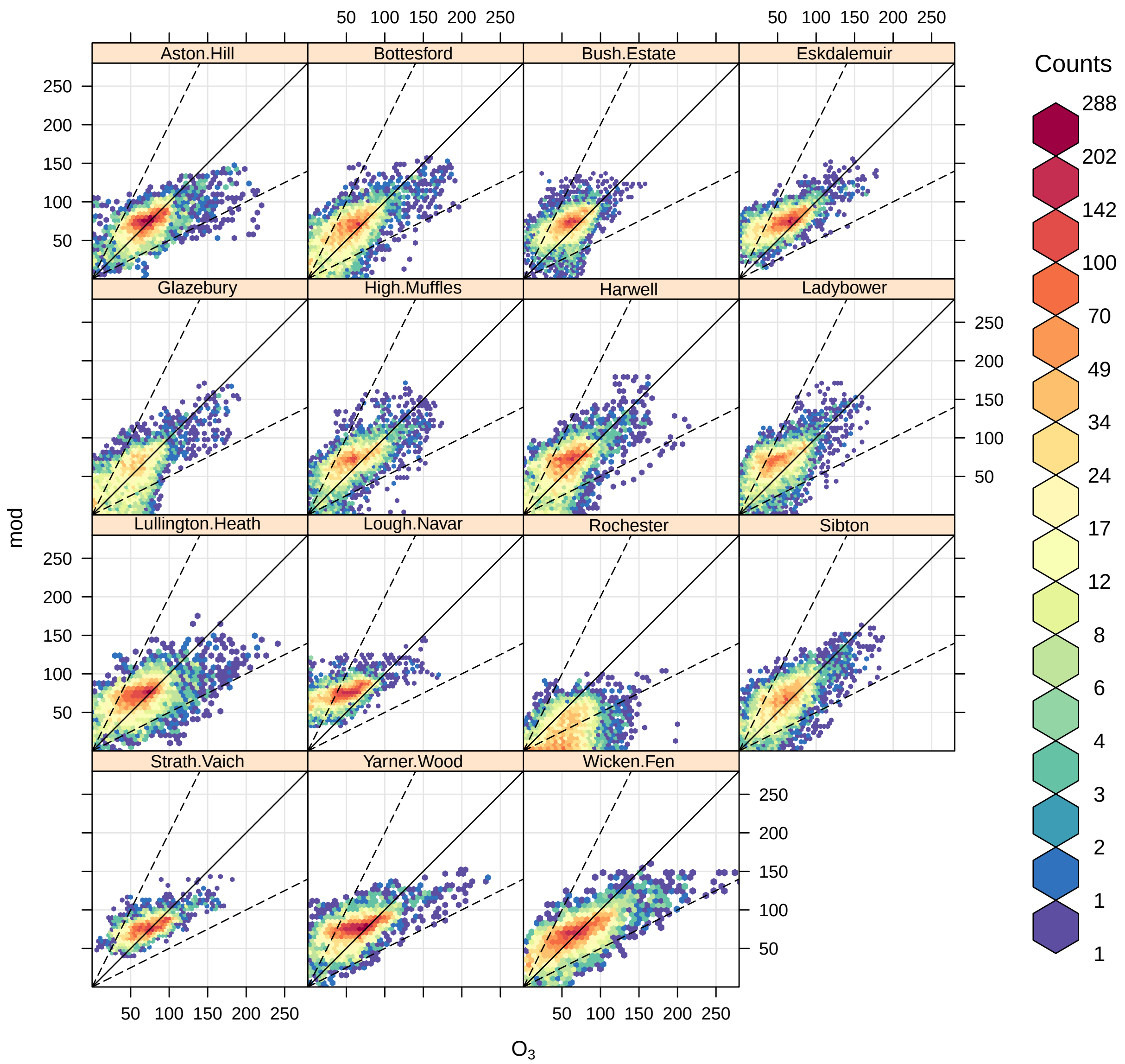

Figure 26: Scatter plot of observed hourly O_3 concentration vs. modelled for the AEA CMAQ model. The dashed lines show the within factor of two (FAC2) region.

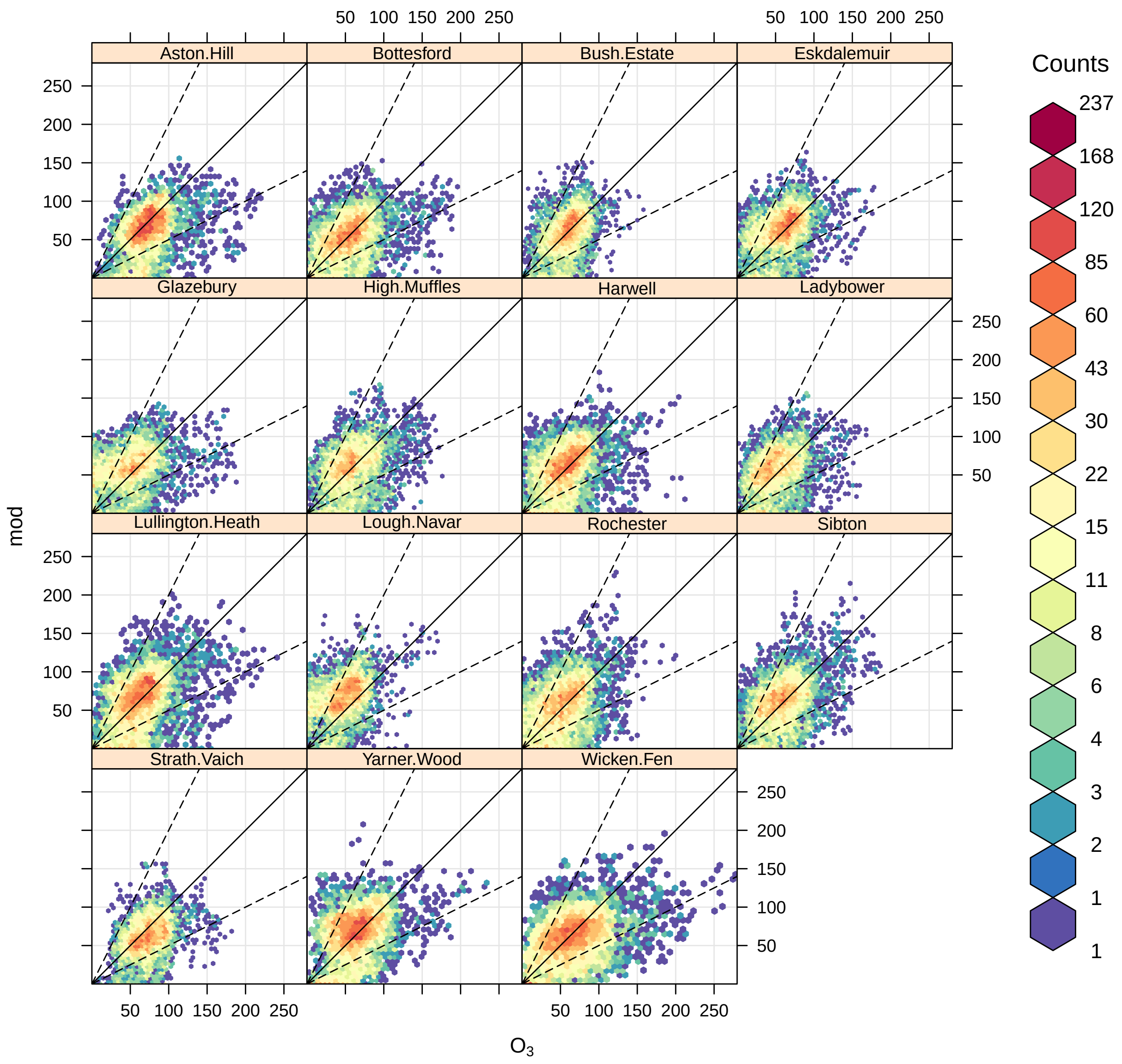

Figure 27: Scatter plot of observed hourly O_3 concentration vs. modelled for the OSRM model. The dashed lines show the within factor of two (FAC2) region.

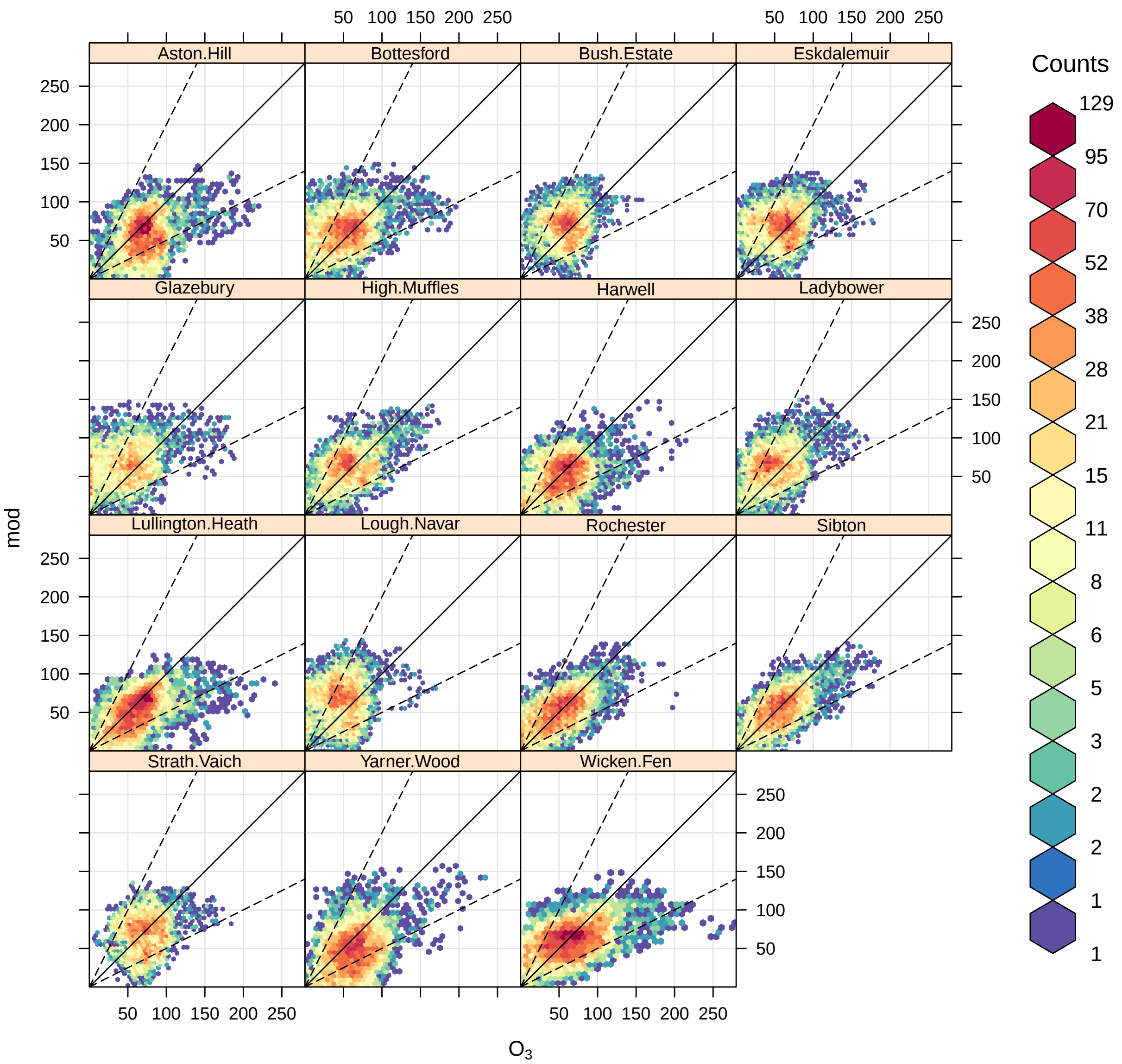

Figure 28: Scatter plot of observed hourly O_3 concentration vs. modelled for the CMAQ University of Hertfordshire model. The dashed lines show the within factor of two (FAC2) region.

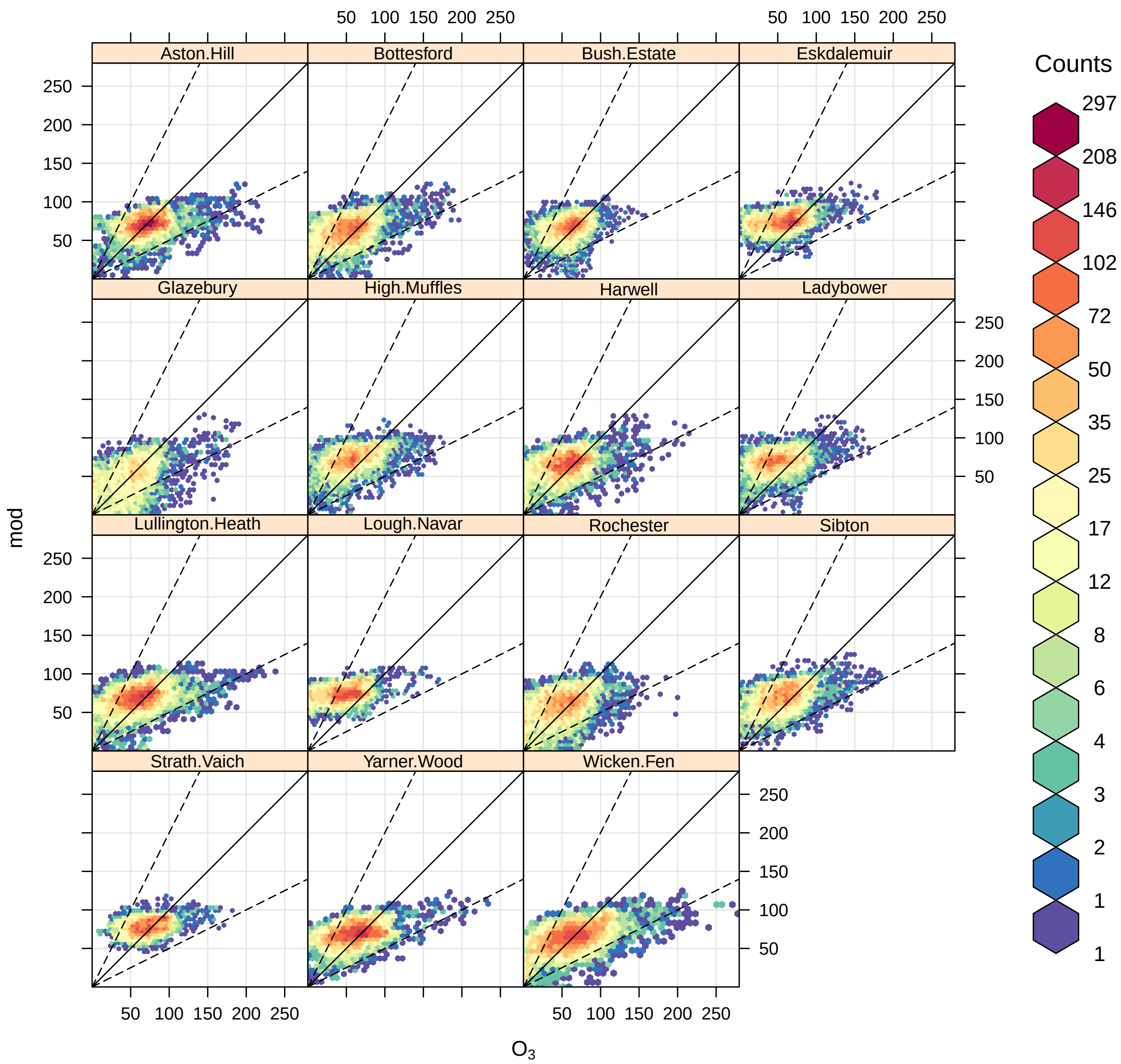

Figure 29: Scatter plot of observed hourly O_3 concentration vs. modelled for the CMAQ King's College London model. The dashed lines show the within factor of two (FAC2) region.

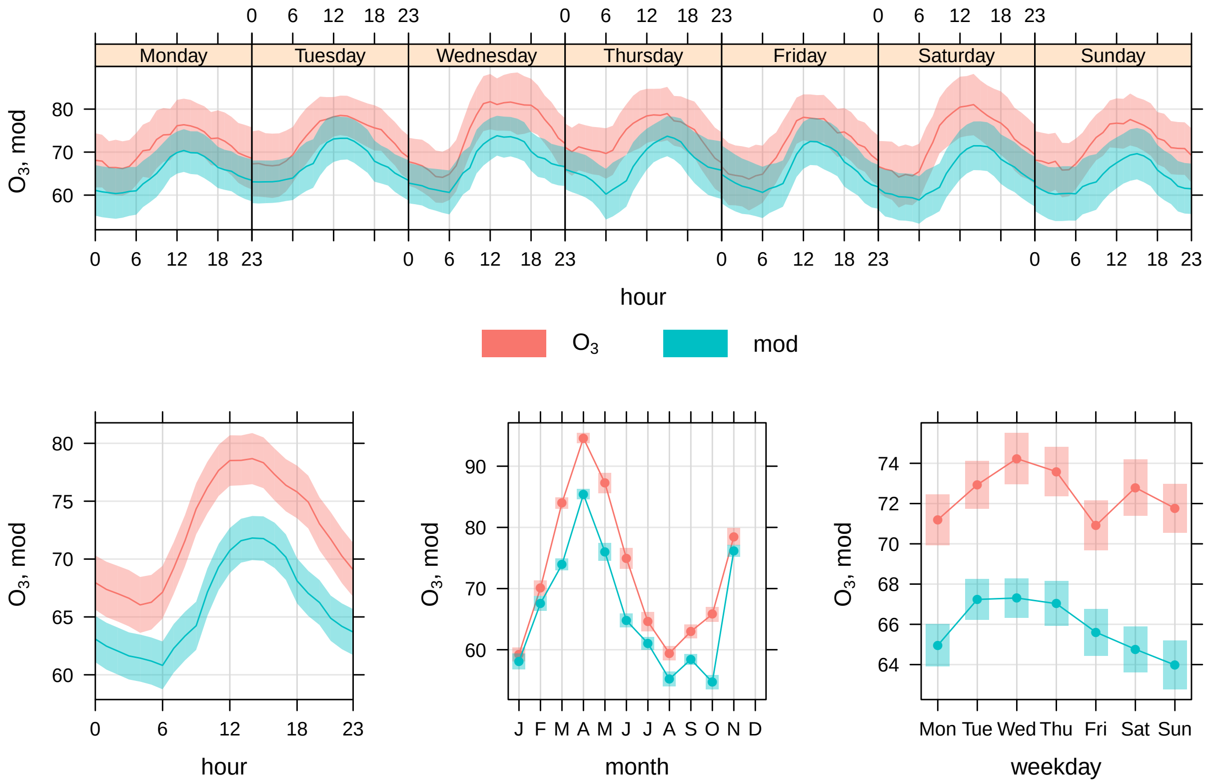

Figure 30: Temporal variation of modelled and observed hourly concentrations at Strath Vaich using the EMEP4UK model.

3.6 Temporal variations

It is also very useful to compare the temporal variations in modelled and observed concentrations. Here we compare two contrasting sites to consider the extent to which these characteristics are captured by the model.

Figure 30 shows how the model compares with measurements at Strath Vaich. The diurnal and seasonal variations are well-captured (maybe because of the large contribution from hemispheric O_3 that is fixed in the model?). However, the model does tend to produce lower estimates of O_3 concentrations. The results for Lullington Heath (Figure 31) are somewhat different and show that while the diurnal variation is captured quite well (apart from some slightly unusual dips), there is evidence that the magnitude of summer predictions is not well captured. This is also shown in Table 11 — one advantage of flexibly calculating the performance statistics (note the negative bias for Lullington Heath in summer).

```
timeVariation(subset(emep, site == "Strath.Vaich"), pollutant = c("o3", "mod"))
```

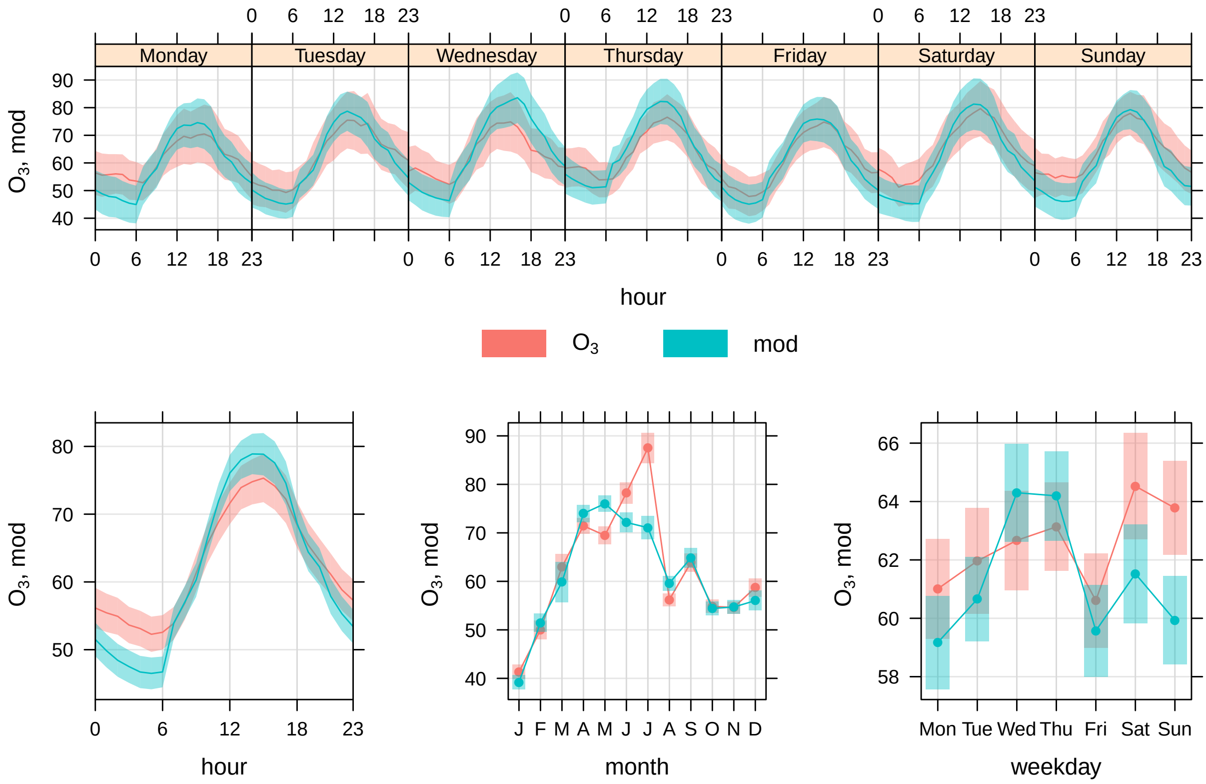

Figure 31: Temporal variation of modelled and observed hourly concentrations at Lullington Heath using the EMEP4UKmodel.

```
timeVariation(subset(emep, site == "Lullington.Heath"), pollutant = c("o3", "mod"))
```

```
timeVariation(subset(NAME, site == "Strath.Vaich"), pollutant = c("o3", "mod"))
```

```
timeVariation(subset(NAME, site == "Lullington.Heath"), pollutant = c("o3", "mod"))
```

```
timeVariation(subset(AQUM.GEMS, site == "Strath.Vaich"), pollutant = c("o3", "mod"))
```

```
timeVariation(subset(AQUM.GEMS, site == "Lullington.Heath"), pollutant = c("o3", "mod"))
```

```
timeVariation(subset(AQUM.MACC, site == "Strath.Vaich"), pollutant = c("o3", "mod"))
```

```
timeVariation(subset(AQUM.MACC, site == "Lullington.Heath"), pollutant = c("o3", "mod"))
```

```
timeVariation(subset(CMAQ.AEA, site == "Strath.Vaich"), pollutant = c("o3", "mod"))
```

```
timeVariation(subset(CMAQ.AEA, site == "Lullington.Heath"), pollutant = c("o3", "mod"))
```

```
timeVariation(subset(OSRM, site == "Strath.Vaich"), pollutant = c("o3", "mod"))
```

```
timeVariation(subset(OSRM, site == "Lullington.Heath"), pollutant = c("o3", "mod"))
```

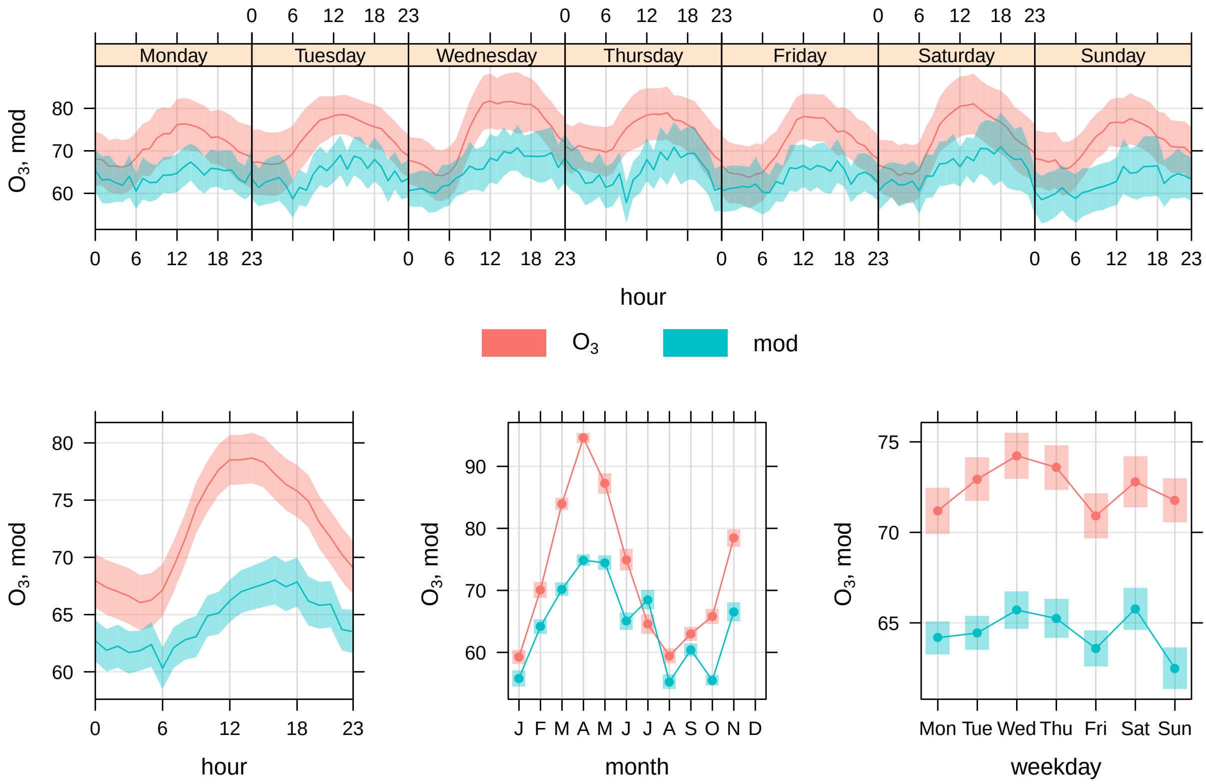

Figure 32: Temporal variation of modelled and observed hourly concentrations at Strath Vaich using the NAME model.

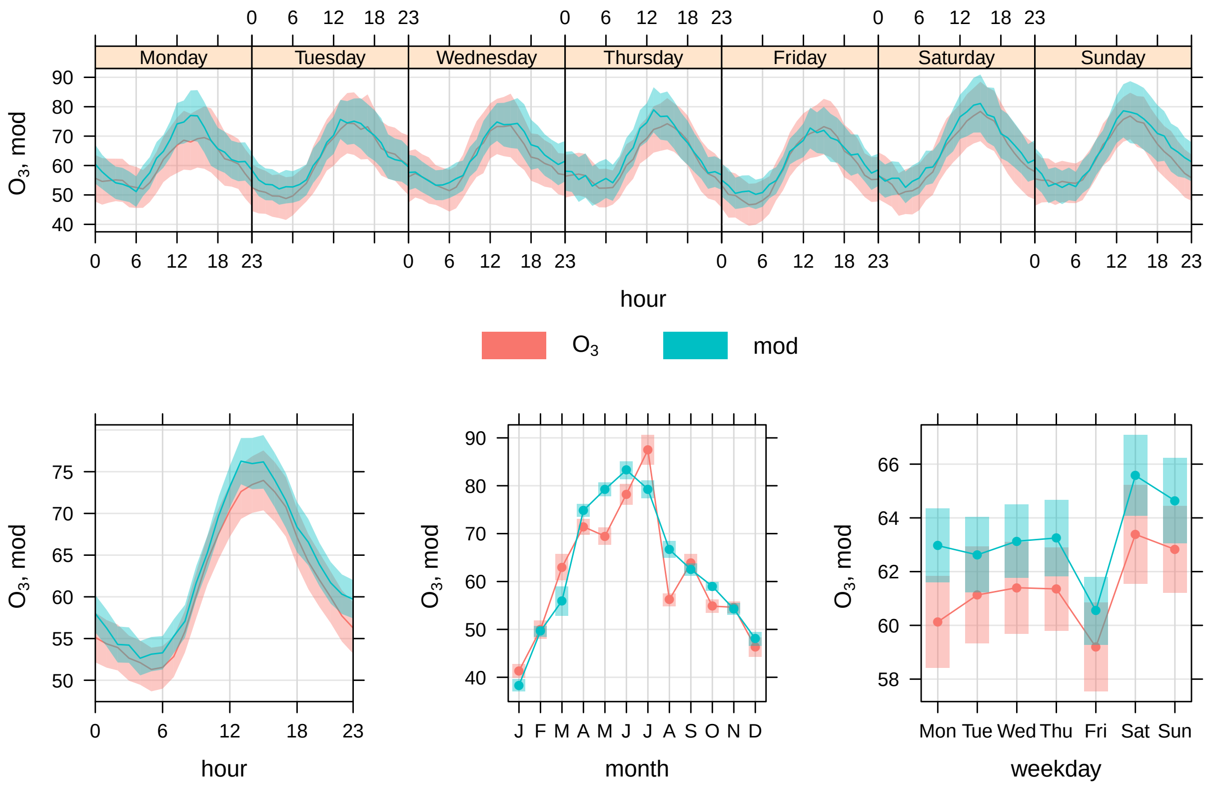

Figure 33: Temporal variation of modelled and observed hourly concentrations at Lullington Heath using the NAME model.

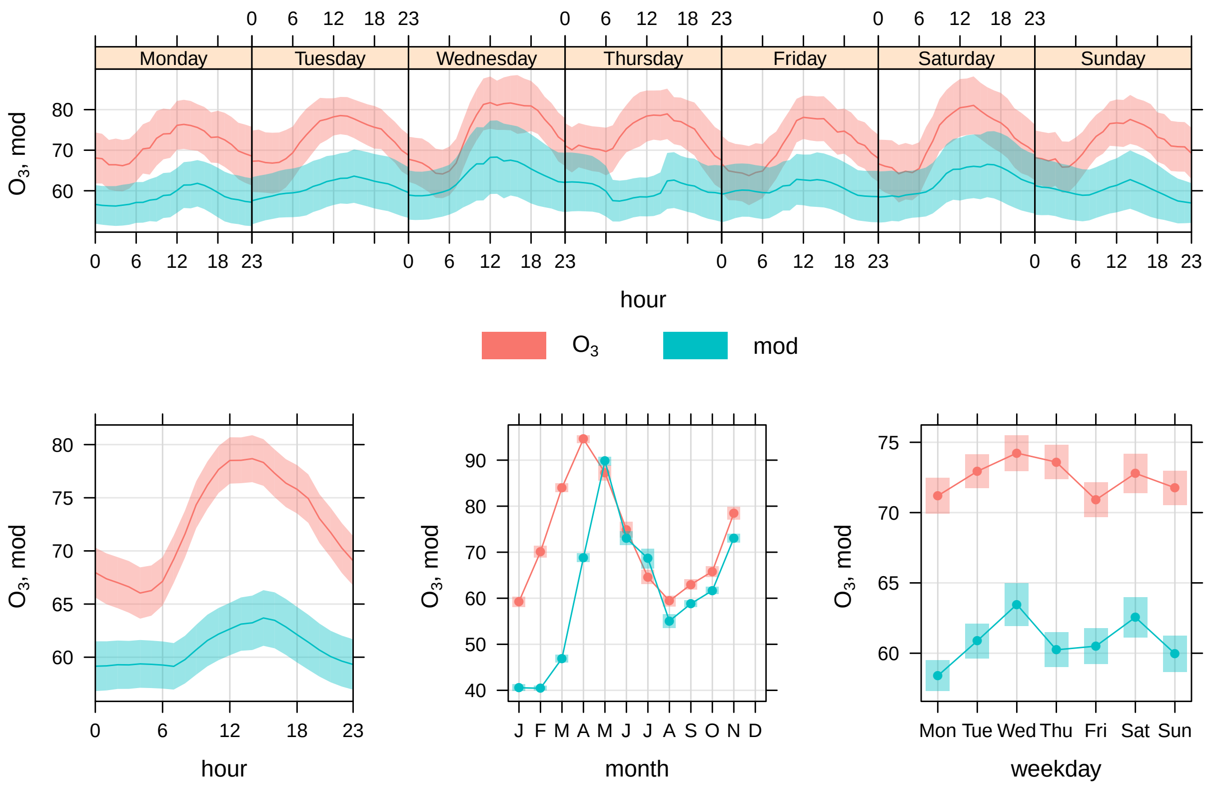

Figure 34: Temporal variation of modelled and observed hourly concentrations at Strath Vaich using the AQUM.GEMS model.

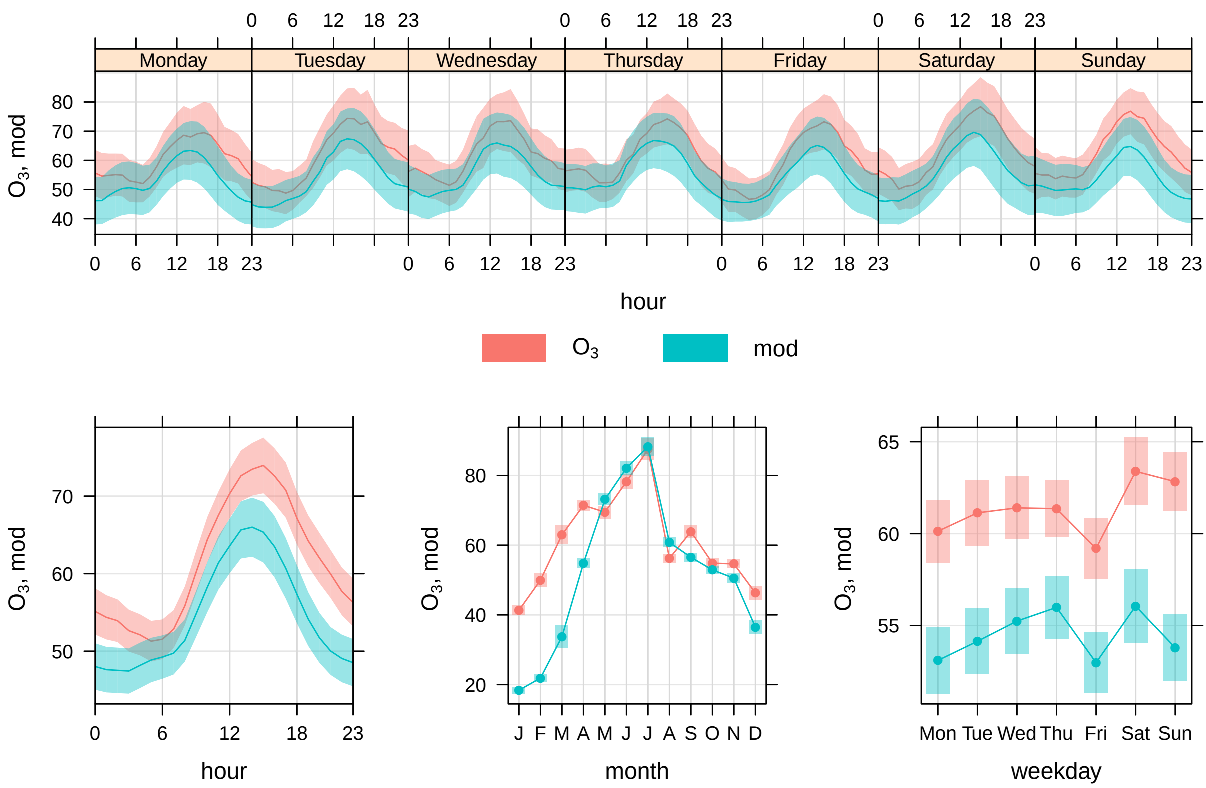

Figure 35: Temporal variation of modelled and observed hourly concentrations at Lullington Heath using the AQUM.GEMS model.

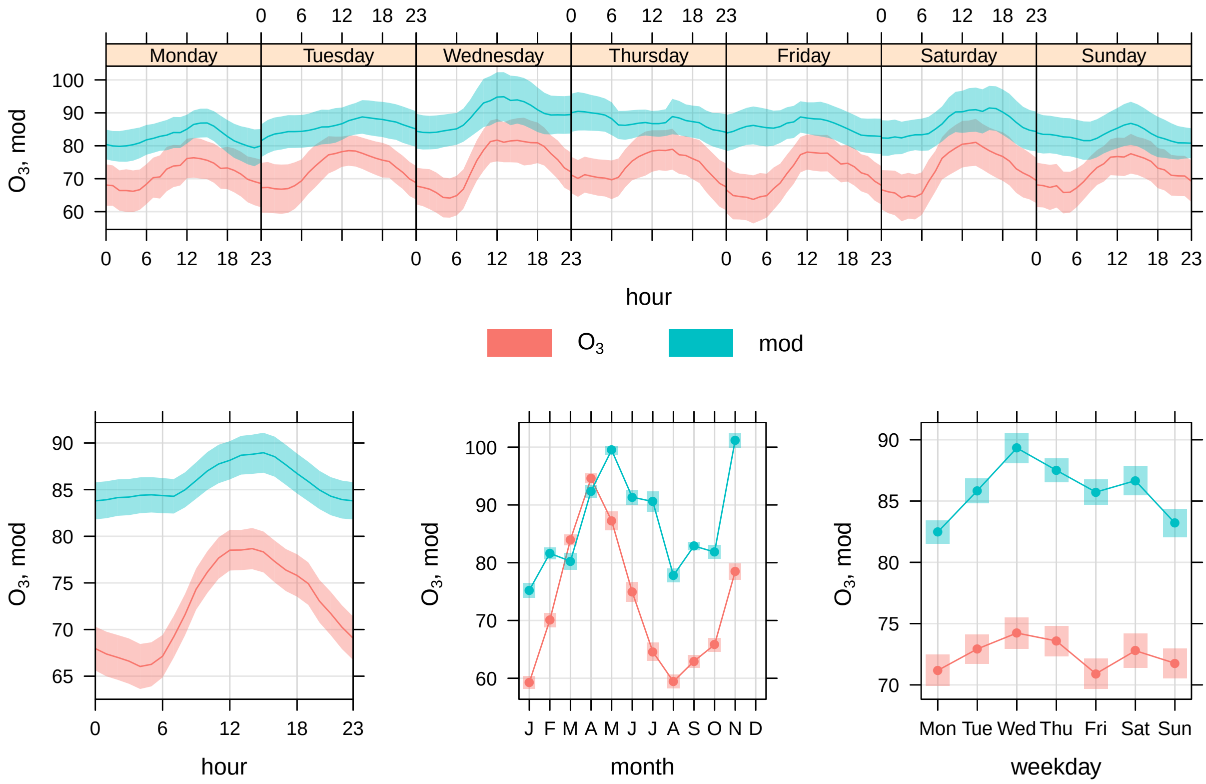

Figure 36: Temporal variation of modelled and observed hourly concentrations at Strath Vaich using the AQUM.MACC model.

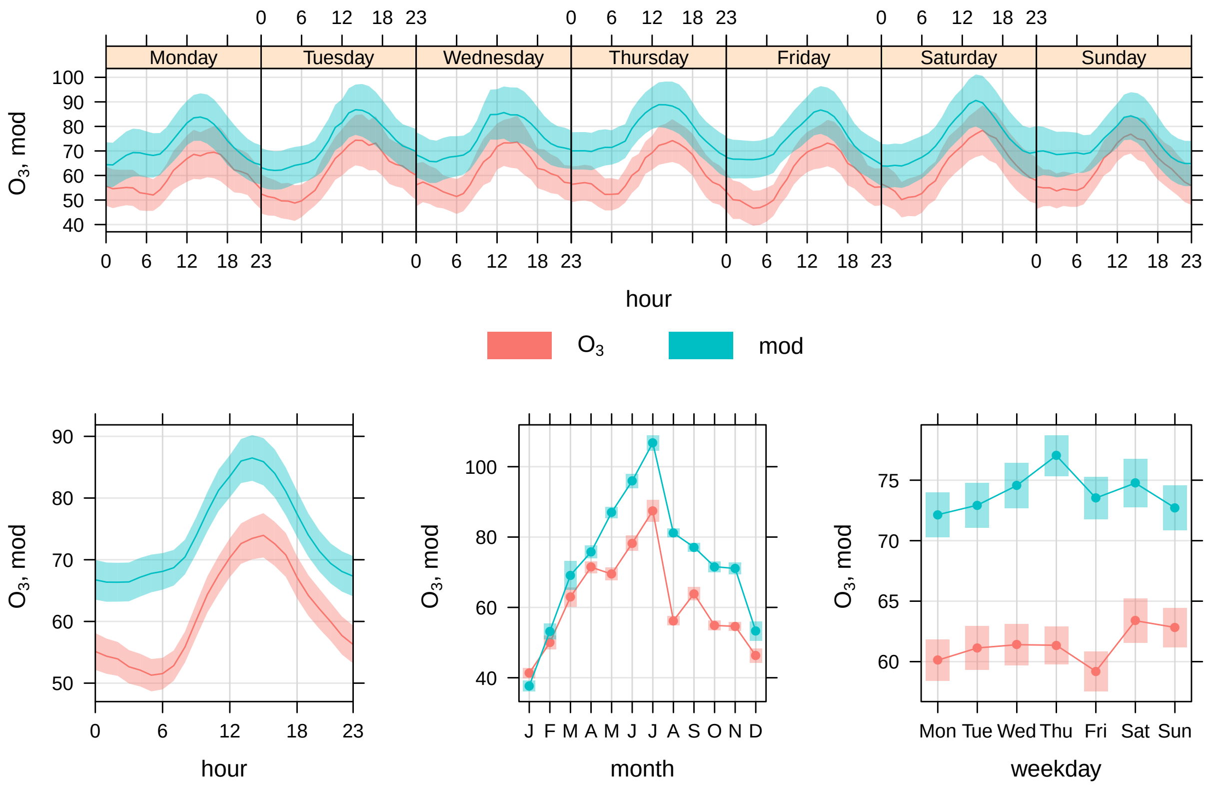

Figure 37: Temporal variation of modelled and observed hourly concentrations at Lullington Heath using the AQUM.MACC model.

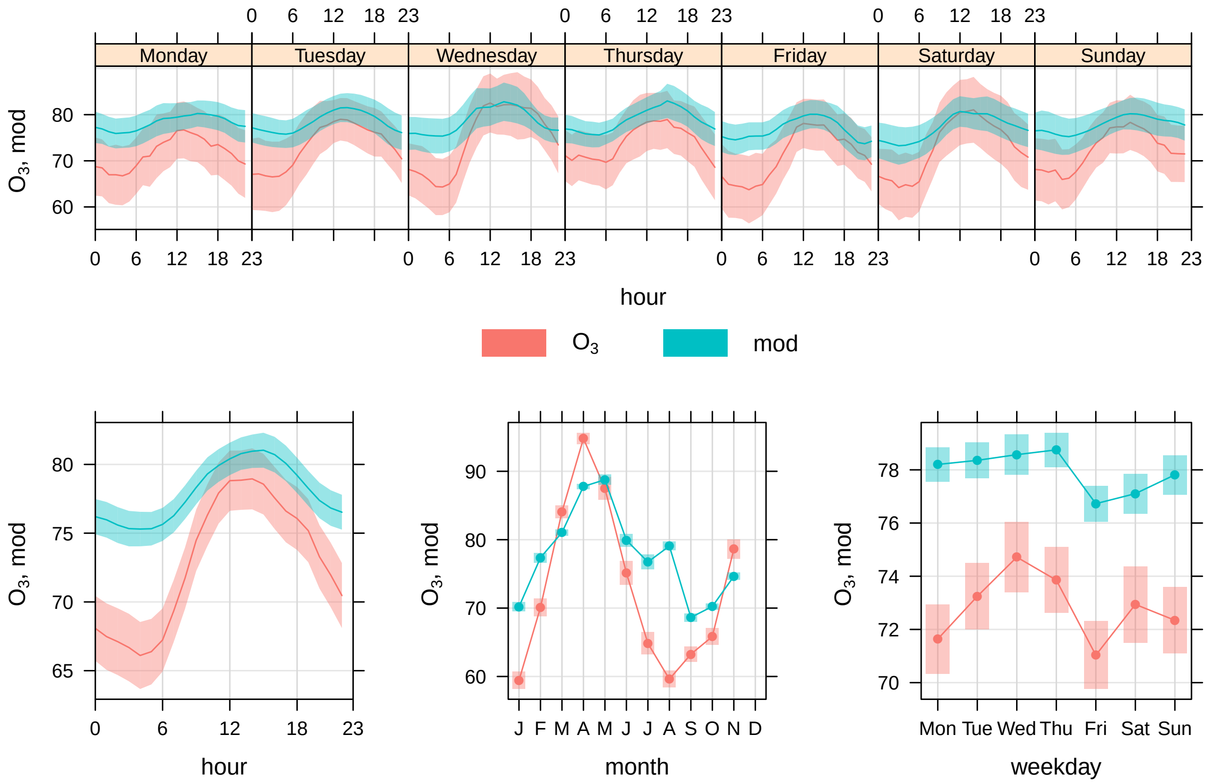

Figure 38: Temporal variation of modelled and observed hourly concentrations at Strath Vaich using the AEA CMAQ model.

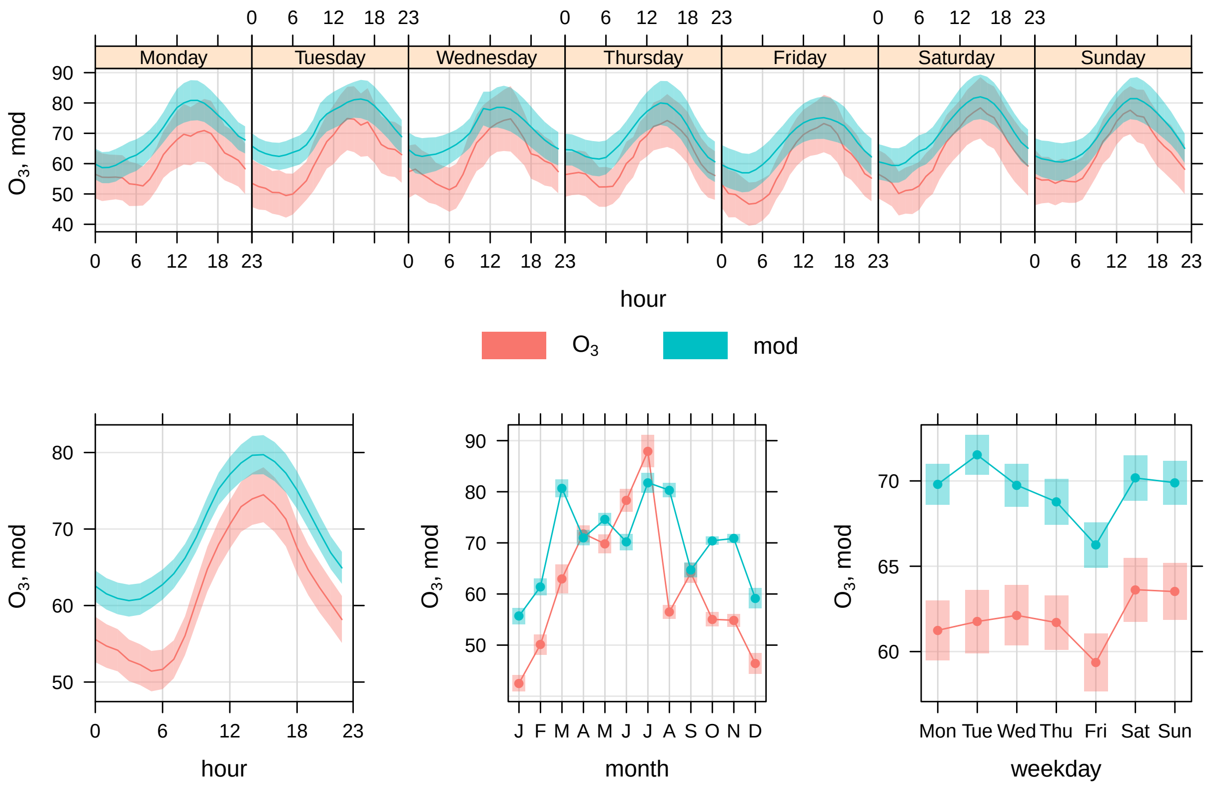

Figure 39: Temporal variation of modelled and observed hourly concentrations at Lullington Heath using the AEA CMAQ model.

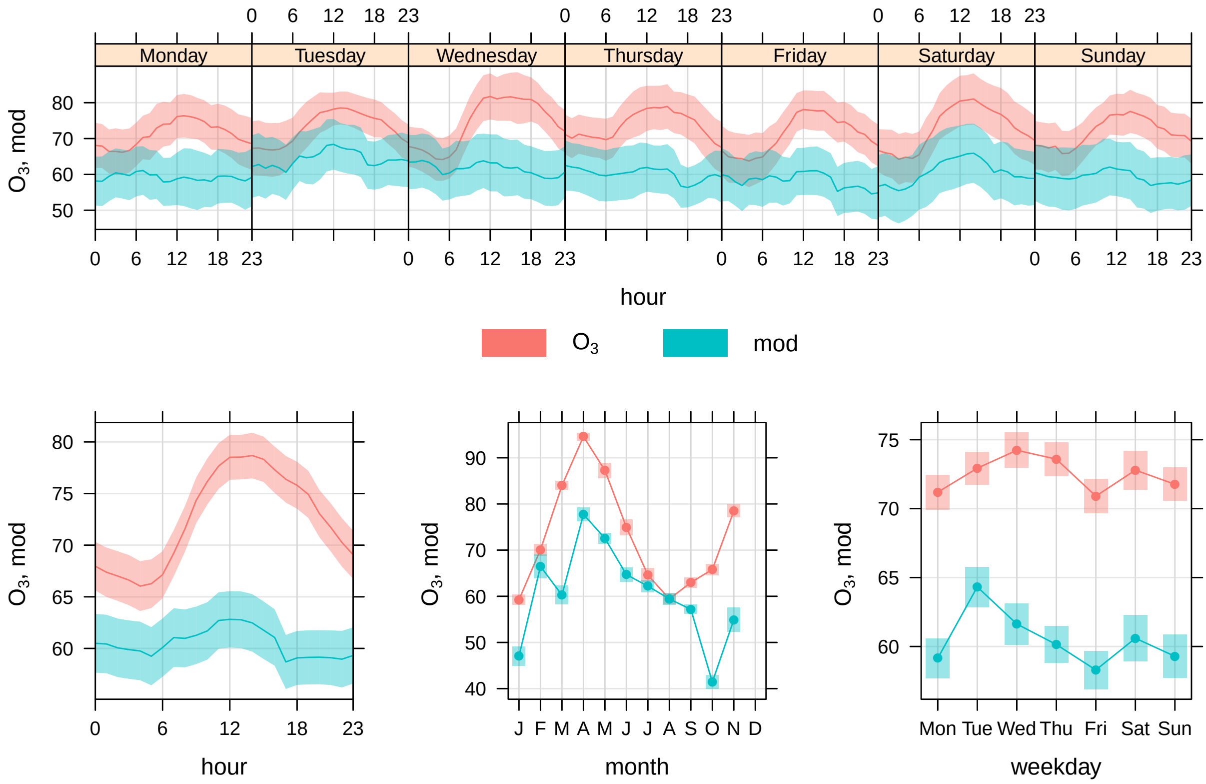

Figure 40: Temporal variation of modelled and observed hourly concentrations at Strath Vaich using the OSRM model.

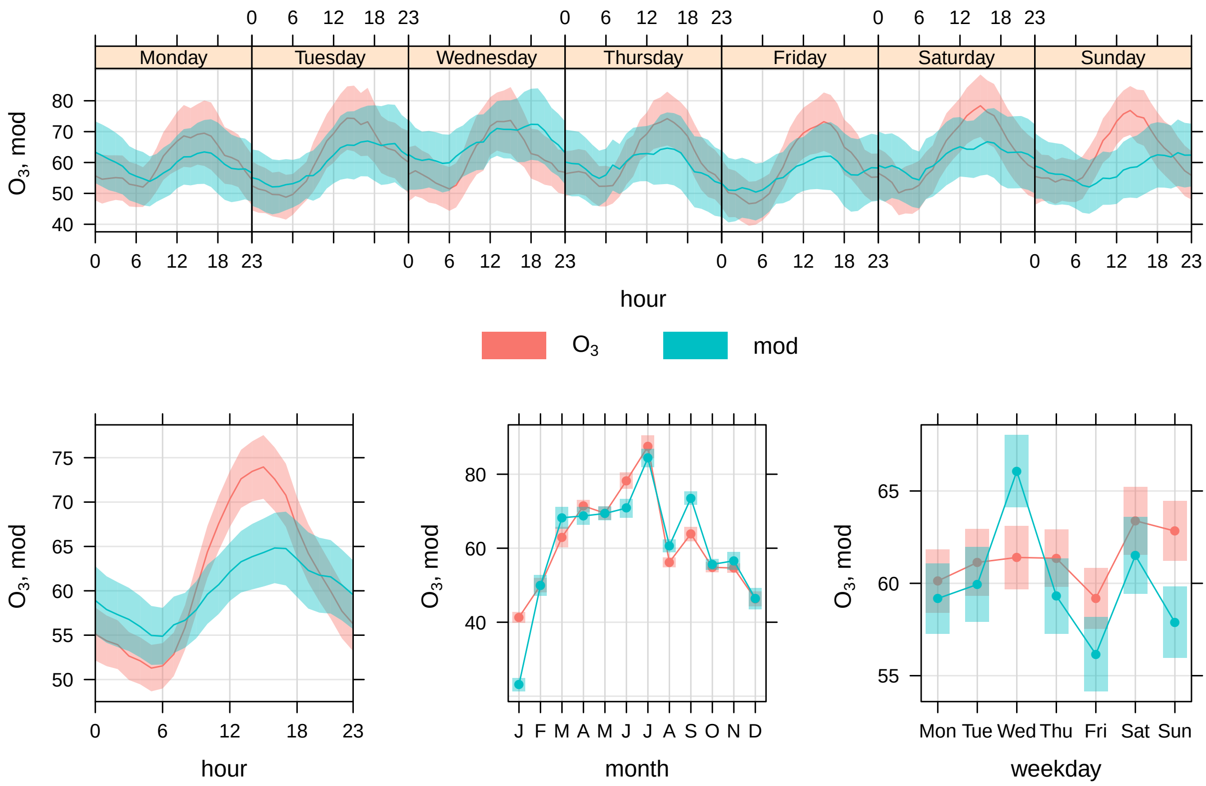

Figure 41: Temporal variation of modelled and observed hourly concentrations at Lullington Heath using the OSRM model.

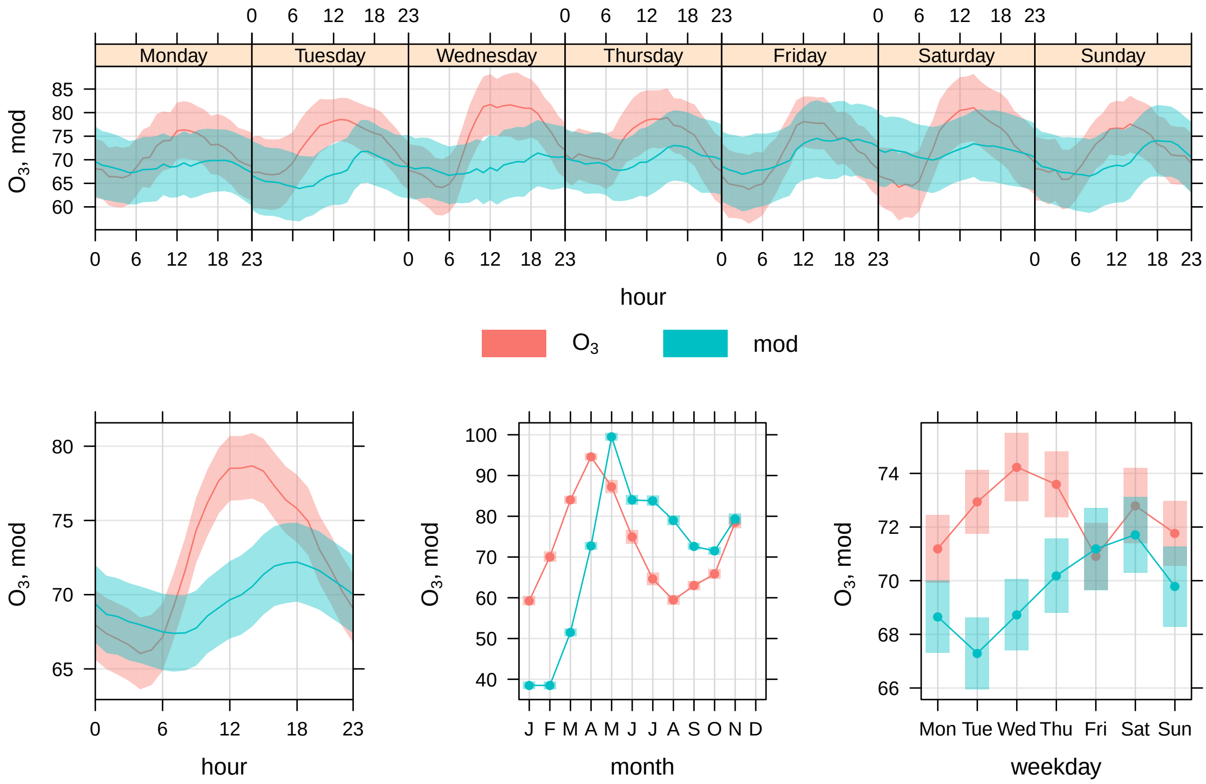

Figure 42: Temporal variation of modelled and observed hourly concentrations at Strath Vaich using the CMAQ University of Hertfordshire model.

```
timeVariation(subset(CMAQ.UH, site == "Strath.Vaich"), pollutant = c("o3", "mod"))
```

```
timeVariation(subset(CMAQ.UH, site == "Lullington.Heath"), pollutant = c("o3", "mod"))
```

```
timeVariation(subset(CMAQ.KCL, site == "Strath.Vaich"), pollutant = c("o3", "mod"))
```

```
timeVariation(subset(CMAQ.KCL, site == "Lullington.Heath"), pollutant = c("o3", "mod"))
```

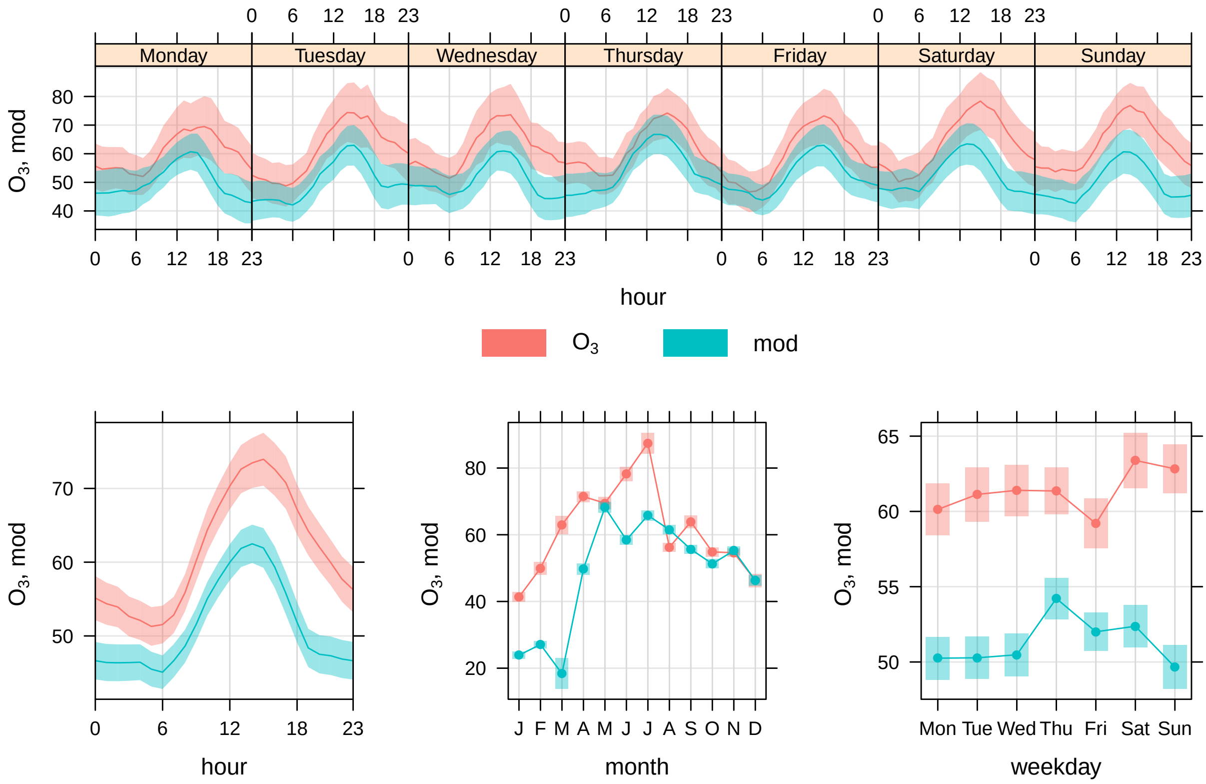

Figure 43: Temporal variation of modelled and observed hourly concentrations at Lullington Heath using the CMAQ University of Hertfordshire model.

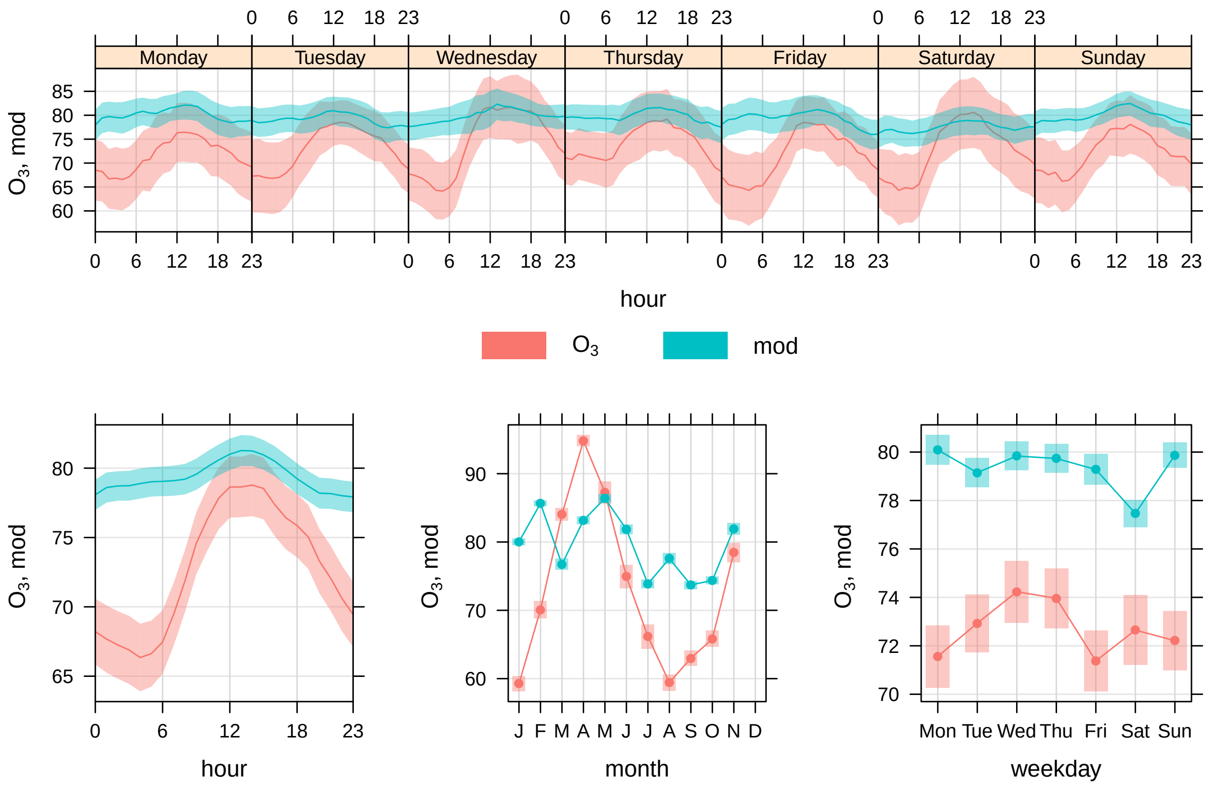

Figure 44: Temporal variation of modelled and observed hourly concentrations at Strath Vaich using the CMAQ King's College London model.

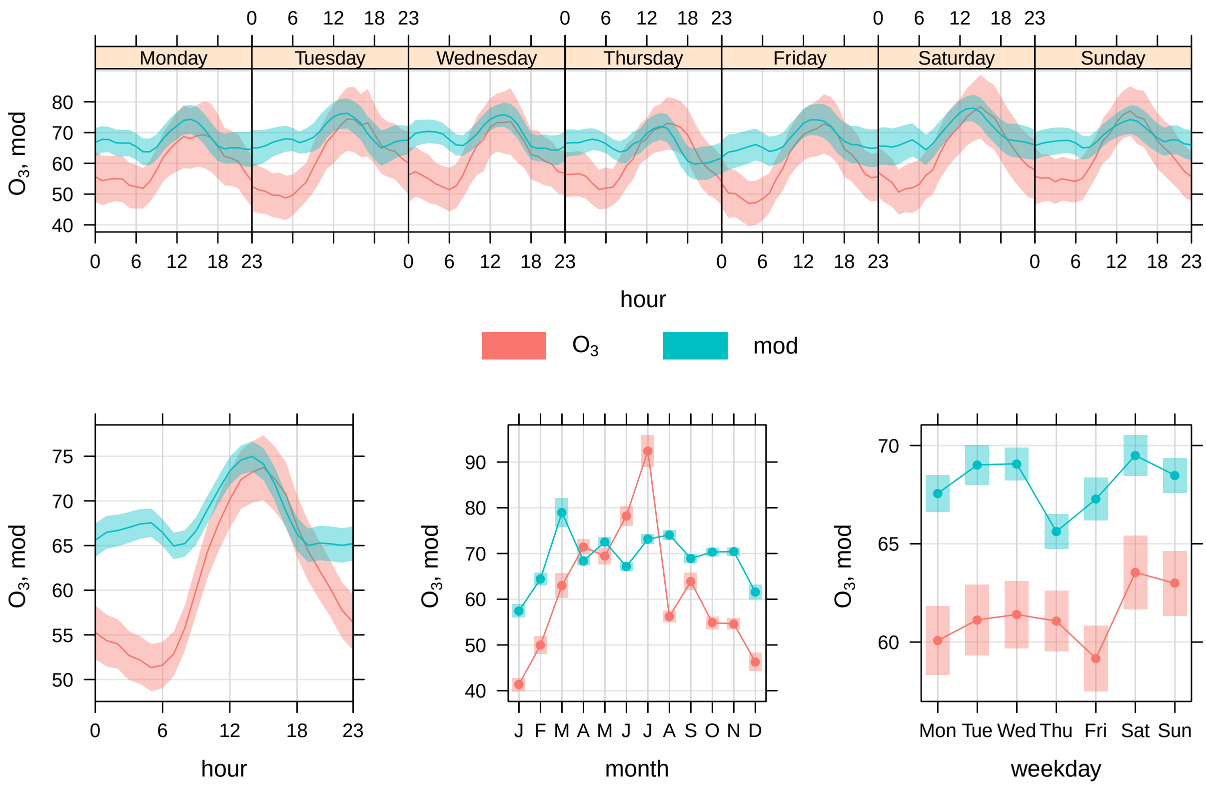

Figure 45: Temporal variation of modelled and observed hourly concentrations at Lullington Heath using the CMAQ King's College London model.

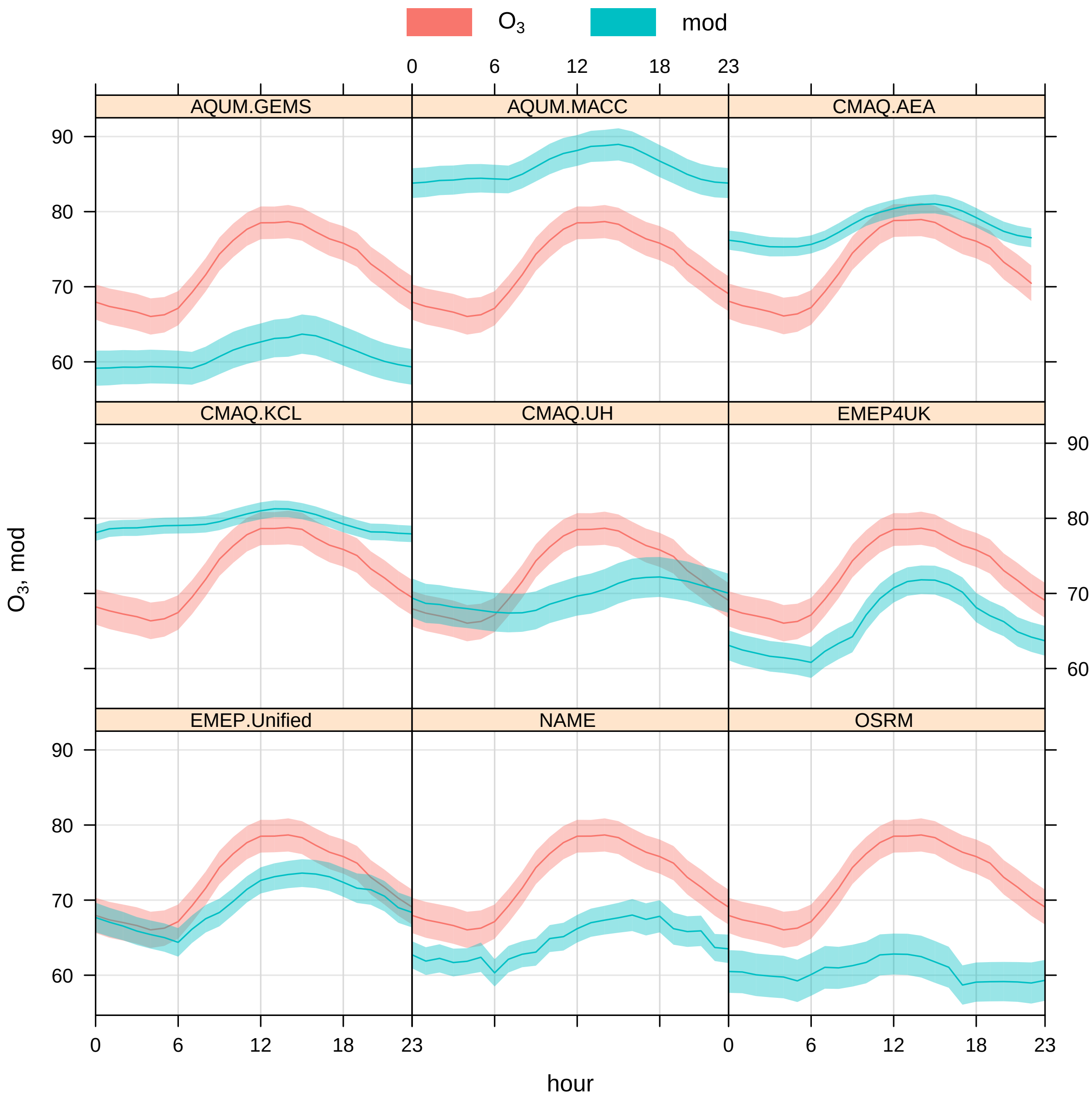

Figure 46: Diurnal variation of measured and predicted O_3 concentrations at Strath Vaich for all models.

It is perhaps better to compare specific temporal components of all the models together. This can be done as follows.

```
timeVar <- timeVariation(subset(all.results, site == "Strath.Vaich"),
                          pollutant = c("o3", "mod"), type = "group")
```

```
plot(timeVar, subset = "hour")
```

And for the monthly variations:

```
plot(timeVar, subset = "month")
```

```
timeVar <- timeVariation(subset(all.results, site == "Lullington.Heath"),
                          pollutant = c("o3", "mod"), type = "group")
```

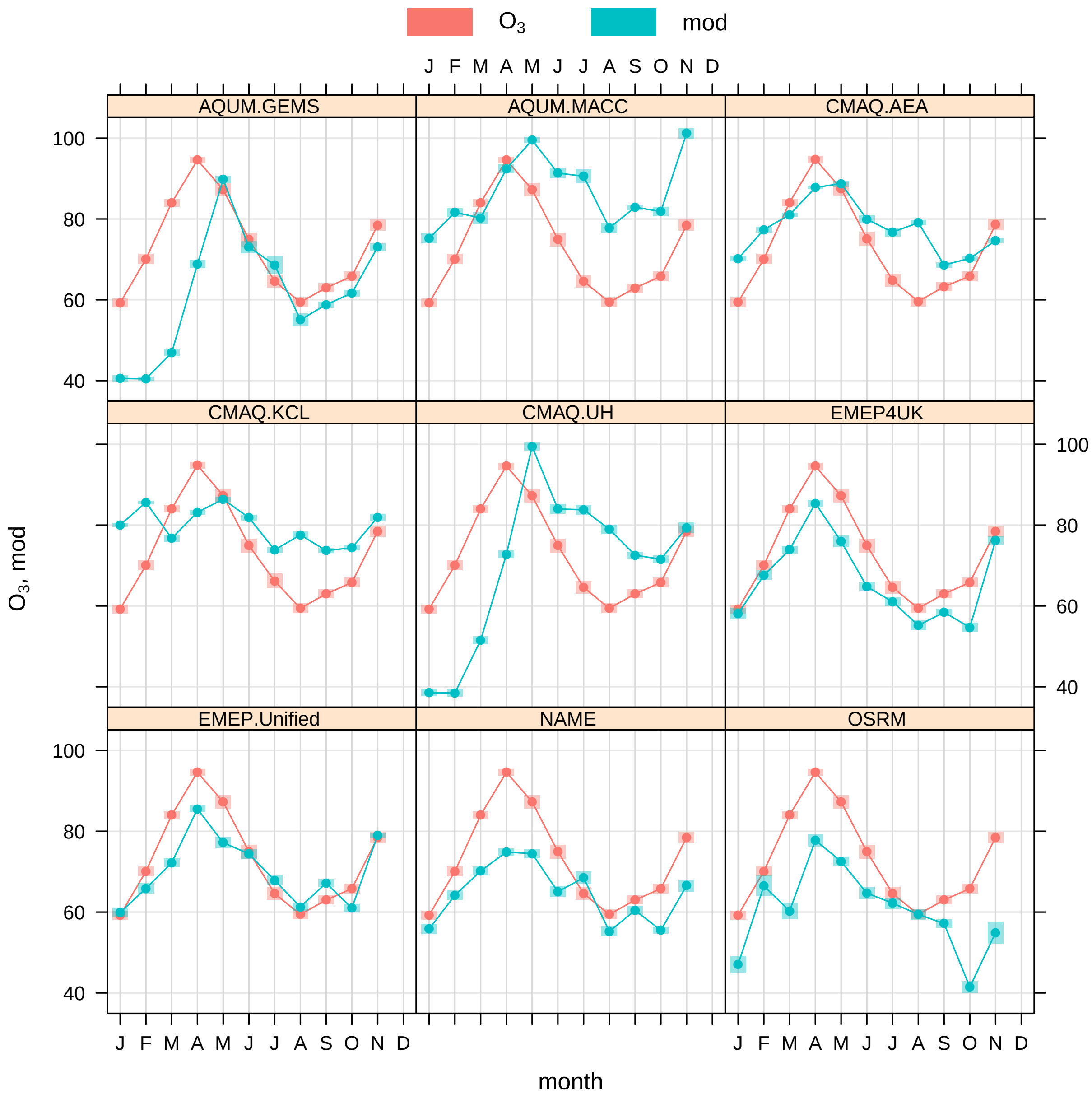

Figure 47: Monthly variation of measured and predicted O_3 concentrations at Strath Vaich for all models.

```
plot(timeVar, subset = "hour")
```

```
plot(timeVar, subset = "month")
```

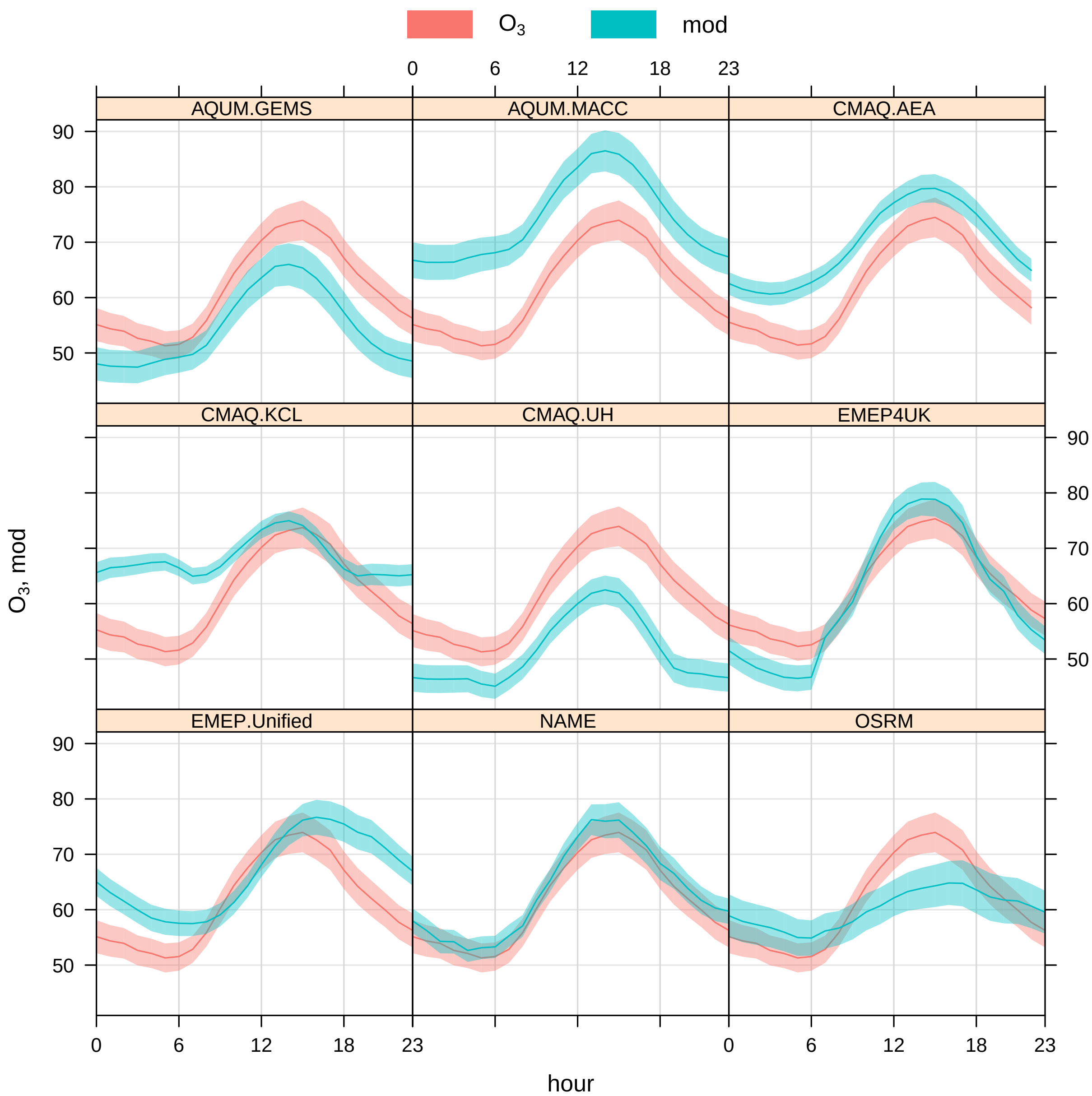

Figure 48: Diurnal variation of measured and predicted O_3 concentrations at Lullington Heath for all models.

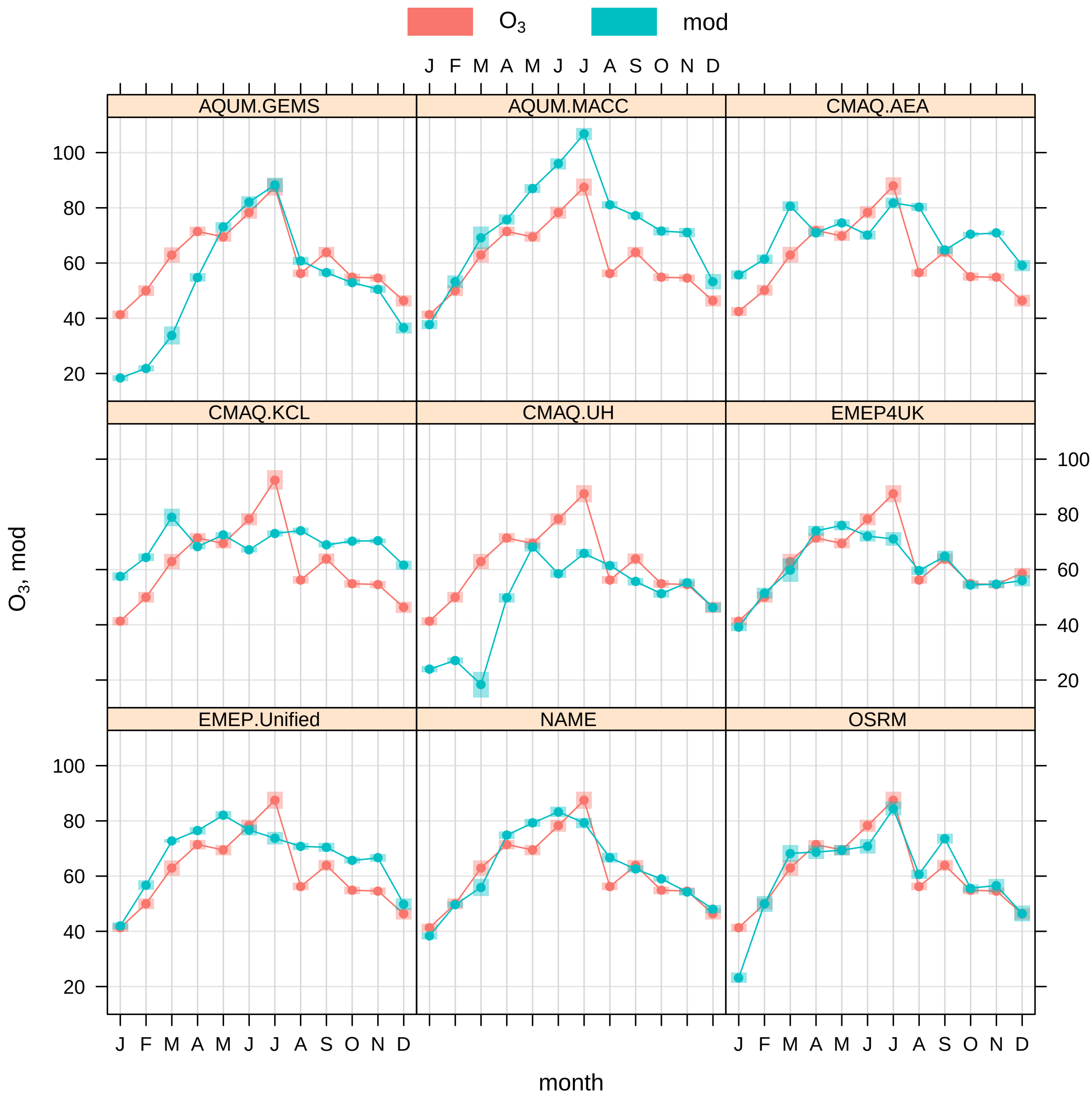

Figure 49: Monthly variation of measured and predicted O_3 concentrations at Lullington Heath for all models.

Another compact and useful way of viewing all the data together is to show the concentration of modelled O_3 by hour of the data, month of the year, site and by group. This may seem overly complex i.e. to show five variables in one plot — but it does help compare across all sites and all groups for two of the key temporal variations. In Figure 50 we force the scale to range from 0–120 $\mu g\ m^{-3}$ and will do the same with the measurements.

Similar plots have also been produced of the maximum O_3 concentration as shown in Figure 52 and Figure 53.

```
trendLevel(all.results, poll = "mod", type = c("site", "group"), limits = c(0, 120))
```

```
trendLevel(all.results, poll = "o3", type = "site", limits = c(0, 120), layout = c(15, 1))
```

```
trendLevel(all.results, poll = "mod", type = c("site", "group"), statistic = "max", limits = c(20, 230))
```

```
trendLevel(all.results, poll = "o3", type = "site", statistic = "max", layout = c(15, 1), limits = c(20, 230))
```

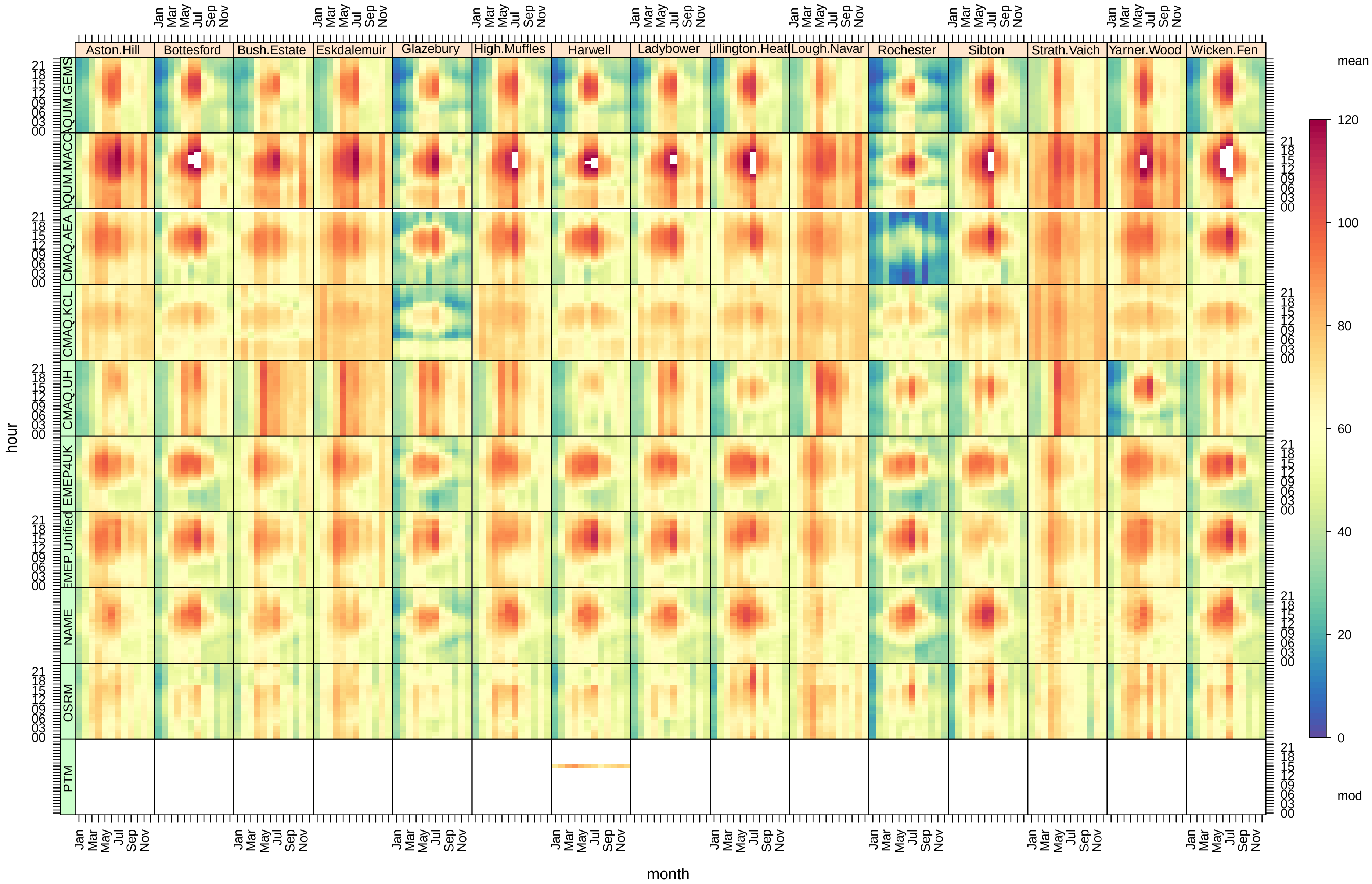

Figure 50: Mean modelled concentration of O_3 at all sites and for all groups, split by hour of the day and month of the year. This plot can be compared with the measurements shown in Figure 51

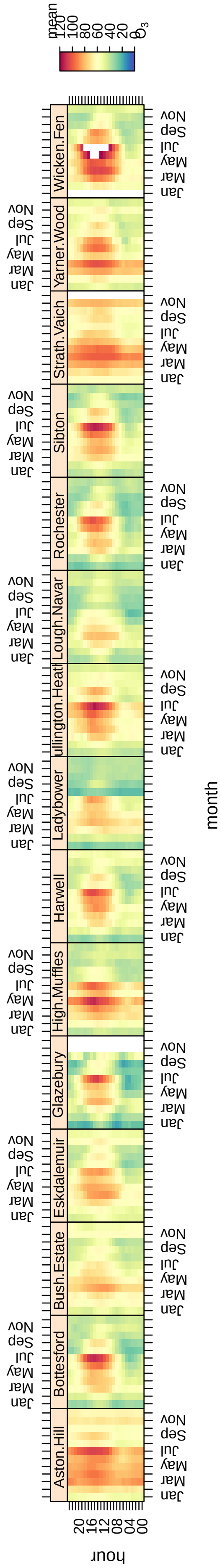

Figure 51: Mean measured concentration of O_3 at all sites, split by hour of the day and month of the year. This plot can be compared with the modelled values shown in Figure 50.

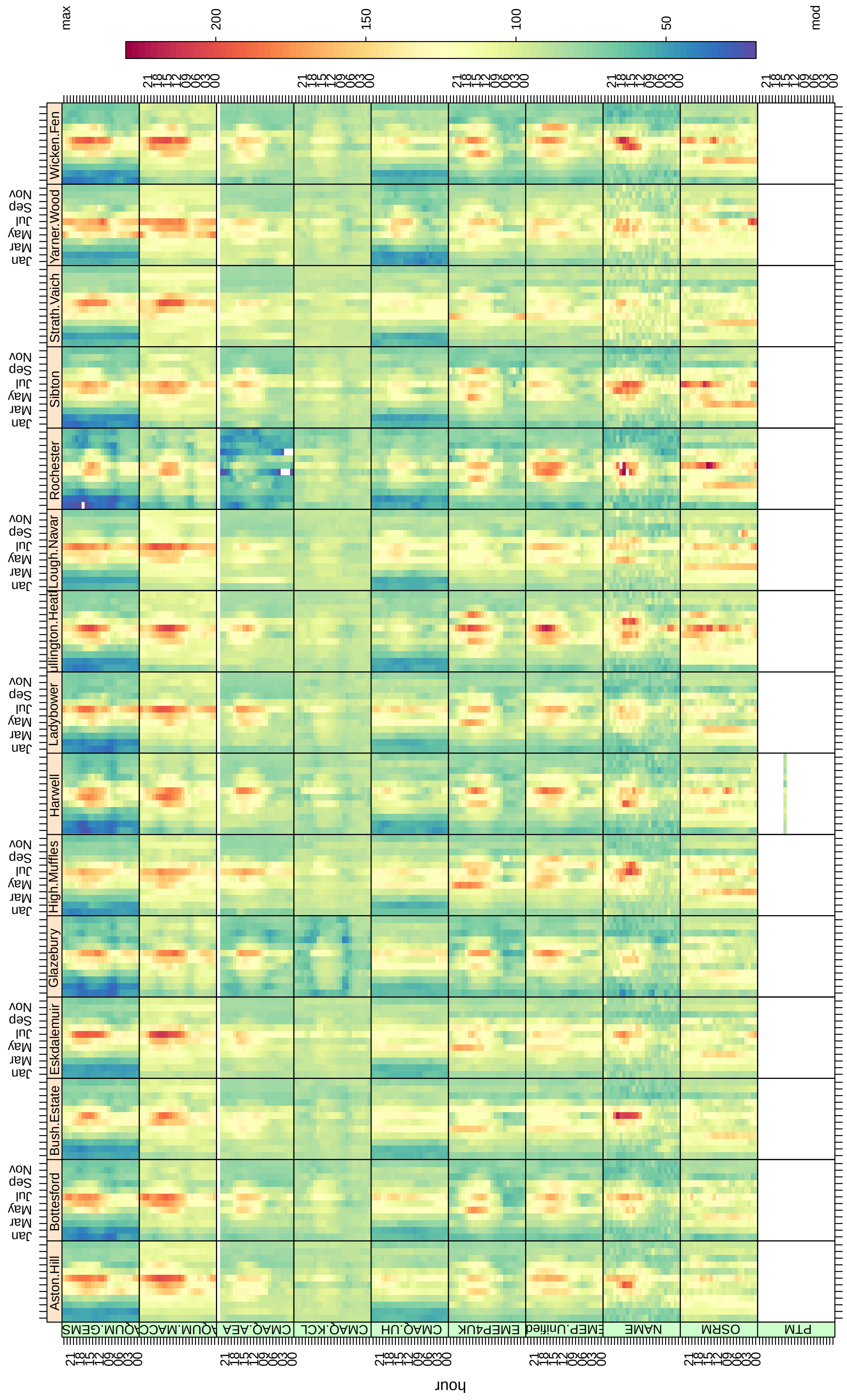

Figure 52: Maximum modelled concentration of O_3 at all sites and for all groups, split by hour of the day and month of the year. This plot can be compared with the measurements shown in Figure 53.

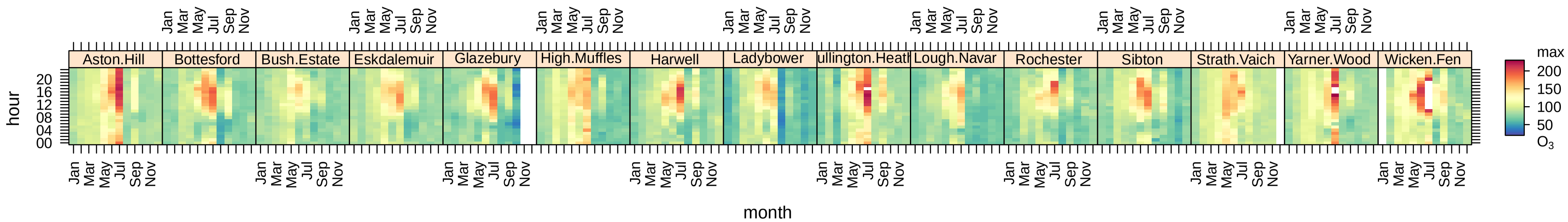

Figure 53: Mean measured concentration of O_3 at all sites, split by hour of the day and month of the year. This plot can be compared with the modelled values shown in Figure 52.

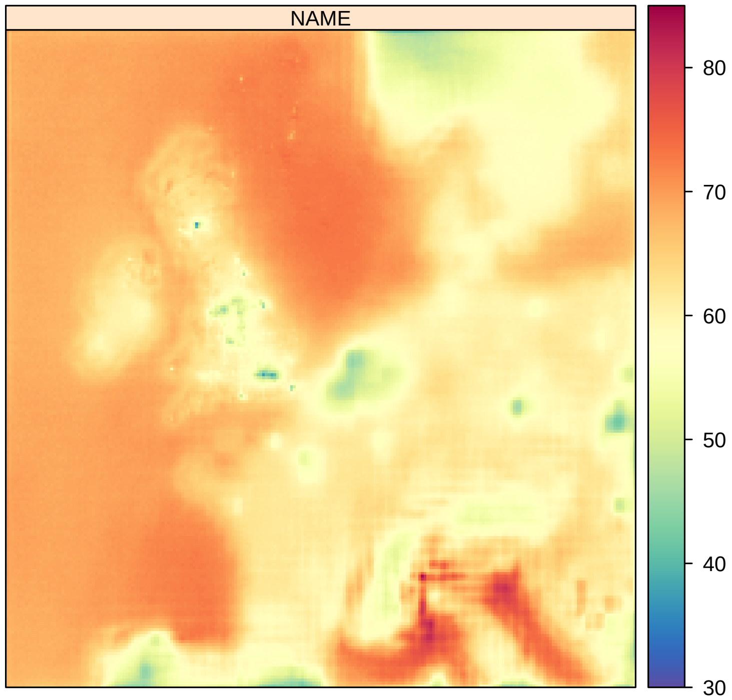

Figure 54: Map of predicted annual mean O_3 concentrations from the NAME model.

3.7 Maps

This section considers maps of annual mean surface concentrations of O_3 where available. The makeMap function has been written to produce consistent maps.

```
## import map data
mapNAME <- read.csv("metOfficeOzoneMap.csv", header = TRUE)
## convert units to ug
mapNAME$o3 <- 1000000 * mapNAME$o3
mapNAME$group <- "NAME"
makeMap(mapNAME, limits = c(30, 85))
```

The EMEP4UK map requires more work because the results are not on a regular grid but [some sort of map projection]. To plot the data in a consistent way to other models, the data are first interpolated onto a regular grid using bi-linear interpolation. The interpolation requires the R package "akima", which can be installed by typing this into R: install.packages("akima"). The function prepareGrid has been written to simplify this process. The series of steps below prepares the data for mapping and then produces the plot.

```
## import map data
mapEMEP <- read.csv("ozoneTemplateV3.0_EMEP4UK_rv3.7_final_SURFACEMAP.csv", header = TRUE)
## interpolate data to 200x200 grid
mapEMEP <- prepareGrid(mapEMEP, pollutant = "o3", group = "EMEP4UK")
## make map
makeMap(mapEMEP, limits = c(30, 85))
```

The data from AQUM.GEMS like EMEP4UK are not on a regular grid, and it is therefore necessary to carry out similar interpolation onto a regual grid for plotting in a consistent manner.

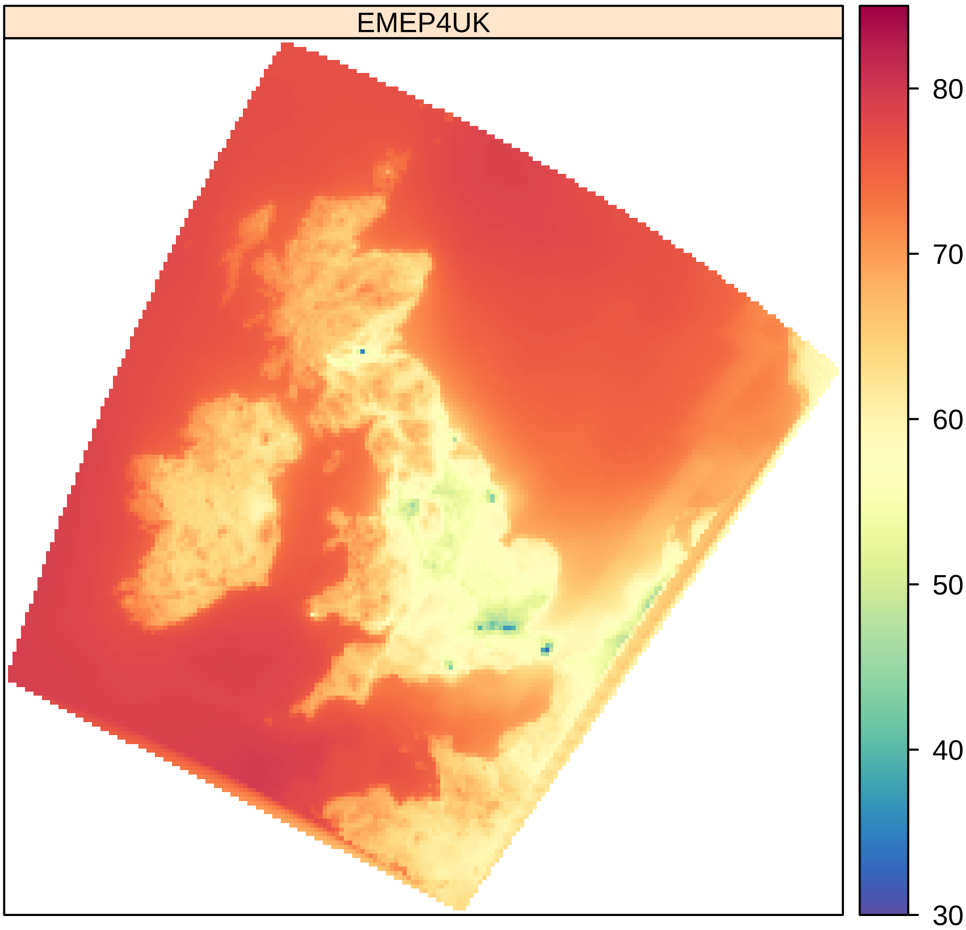

Figure 55: Map of predicted annual mean O_3 concentrations from the EMEP4UK model.

```
## read in data
mapAQUM.GEMS <- read.csv("2006_annual_mean_o3_AQUM.csv", header = TRUE)
## interpolate data to 200x200 grid
mapAQUM.GEMS <- prepareGrid(mapAQUM.GEMS, pollutant = "o3", group = "AQUM.GEMS")
## make map
makeMap(mapAQUM.GEMS, limits = c(30, 85))
```

```
## read in data
mapAQUM.MACC <- read.csv("2006_annual_mean_o3macc.csv", header = TRUE)
## interpolate data to 200x200 grid
mapAQUM.MACC <- prepareGrid(mapAQUM.MACC, pollutant = "o3", group = "AQUM.MACC")
## make map
makeMap(mapAQUM.MACC)
```

```
## mapCMAQ.UH <- read.csv("20101208_Ozone_UHmap.csv", header = TRUE)
## updated data provided 26 Jan 2011
## mapCMAQ.UH <- read.csv("~/Projects/modelEvaluation/regional/20110125_Ozone_UH_MAP.csv",
##                         header = TRUE)
## updated 11 Feb 2011
 mapCMAQ.UH <- read.csv("20110210_Ozone_UH_map.csv", header = TRUE)
## interpolate data to 200x200 grid
mapCMAQ.UH <- prepareGrid(mapCMAQ.UH, pollutant = "o3", group = "CMAQ.UH")
## make map
makeMap(mapCMAQ.UH)
```

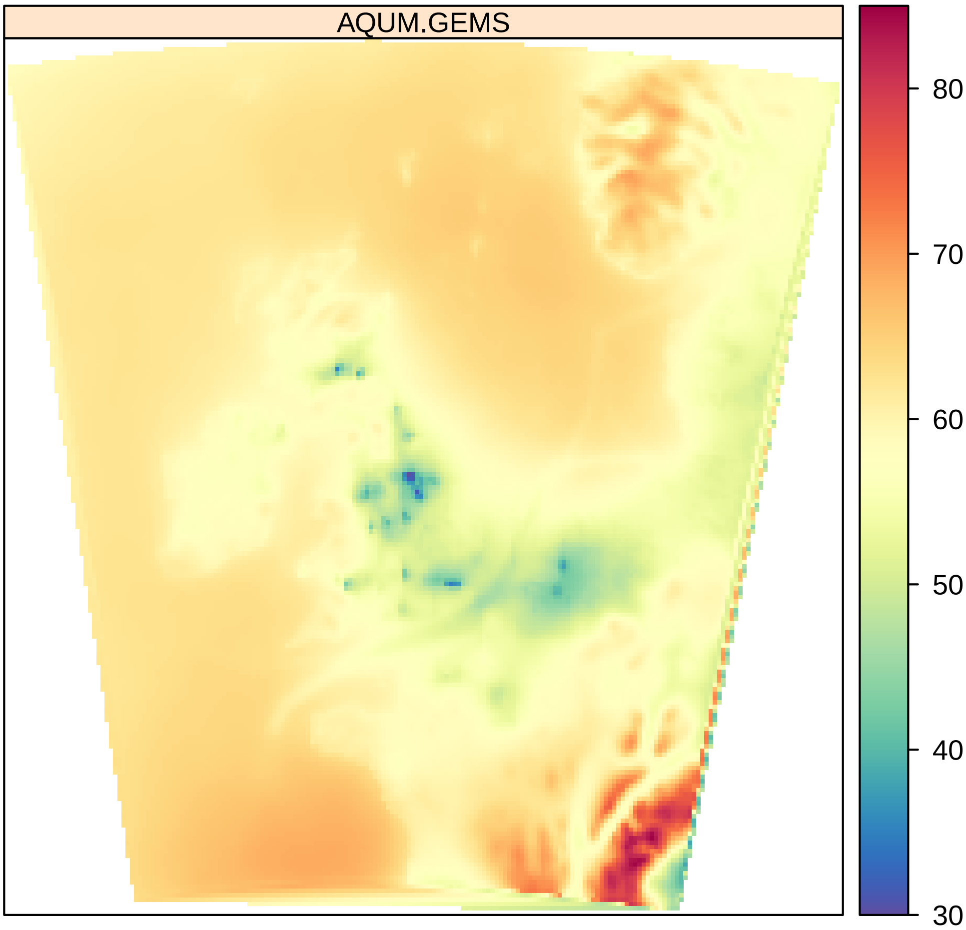

Figure 56: Map of predicted annual mean O_3 concentrations from the AQUM.GEMS model.

```
mapCMAQ.KCL <- read.csv("AnnualO3Average_ugm3_map_KCL_latlon_final.csv", header = TRUE)
## interpolate data to 200x200 grid
mapCMAQ.KCL <- prepareGrid(mapCMAQ.KCL, pollutant = "o3", group = "CMAQ.KCL")
## make map
makeMap(mapCMAQ.KCL)
```

```
mapOSRM <- read.csv("osrm_10km_10km_grid_annual_mean_2006.csv", header = TRUE)
makeMap(mapOSRM, lat = "northing", lon = "easting")
```

AEA supplied their data in two NetCDF files: one containing the O_3 predictions and the other information on the grid. These are imported and manipulated as follows (using the RNetCDF package).

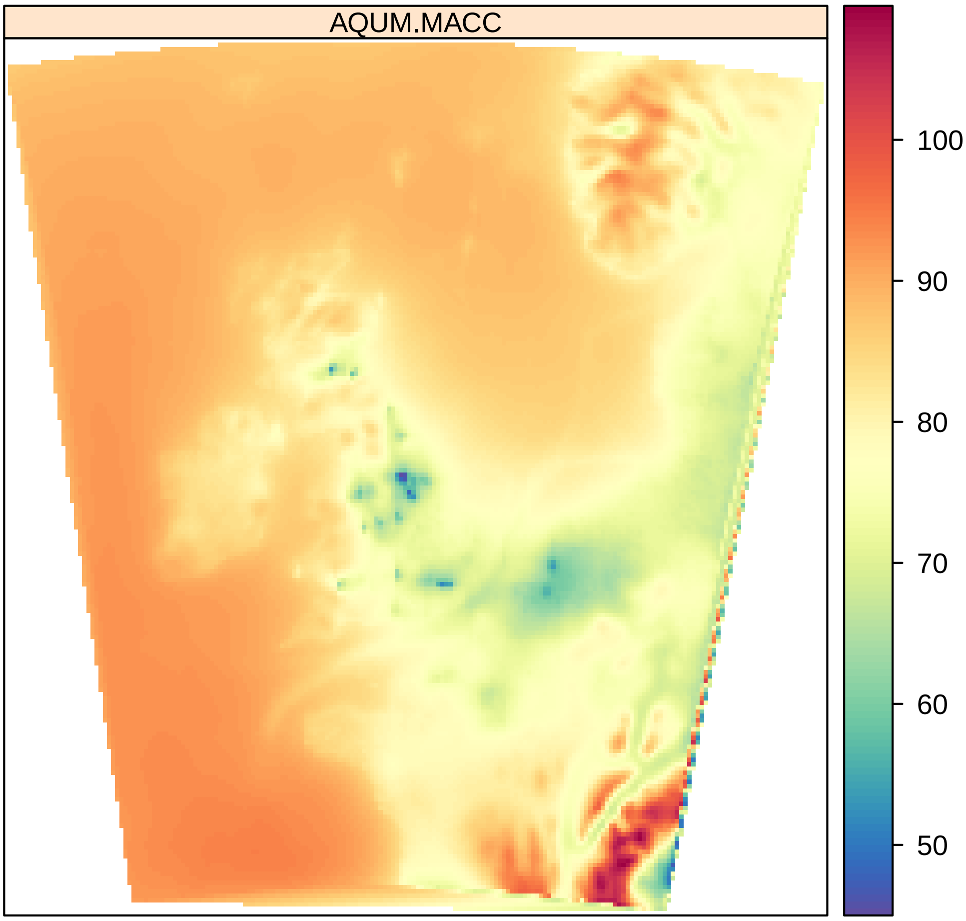

Figure 57: Map of predicted annual mean O_3 concentrations from the AQUM.MACC model.

```
## need to get in same 3-column format as the other models
library(RNetCDF)
o3AEAmap <- open.nc("AEA_ya03_2006.nc")
gridInfo <- open.nc("GRIDCRO2D_U1.nc")
o3Conc <- as.vector(var.get.nc(o3AEAmap, 1))  ## vecor of O3 concentrations
ndims <- (var.inq.nc(o3AEAmap, 1))$ndims
start <- rep(1, ndims)
count <- c(78, 98, 1, 1)
lat <- as.vector(var.get.nc(gridInfo, 1, start, count))
lon <- as.vector(var.get.nc(gridInfo, 2, start, count))
## make data frame for plotting
mapCMAQ.AEA <- data.frame(lat = lat, lon = lon, o3 = o3Conc)
mapCMAQ.AEA <- prepareGrid(mapCMAQ.AEA, pollutant = "o3", group = "CMAQ.AEA")
makeMap(mapCMAQ.AEA, pollutant = "o3")
```

The models predict O_3 over different spatial scales and map projections. It is useful to compare the predictions on the same basis and this is done below. We choose to plot over the spatial scale of the smallest geographic area i.e. the EMEP4UK results.

```
mapData <- rbind.fill(mapNAME, mapEMEP, mapAQUM.GEMS, mapAQUM.MACC, mapCMAQ.UH, mapCMAQ.KCL, mapCMAQ.AEA)
makeMap(mapData, xlim = range(mapEMEP$lon), ylim = range(mapEMEP$lat))
```

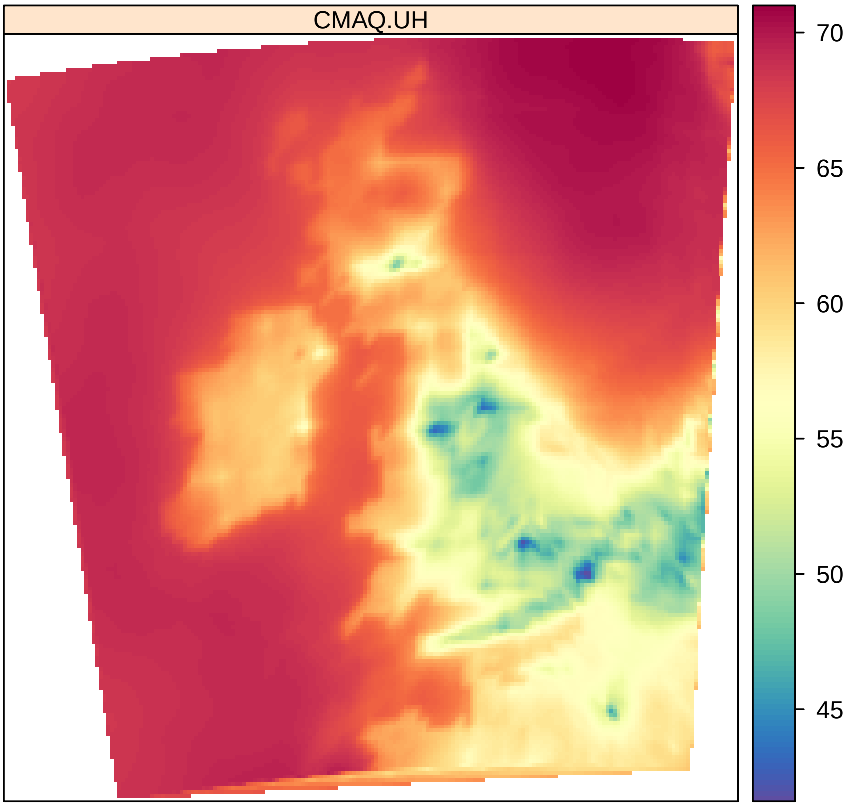

Figure 58: Map of predicted annual mean O_3 concentrations from the CMAQ University of Hertfordshire model.

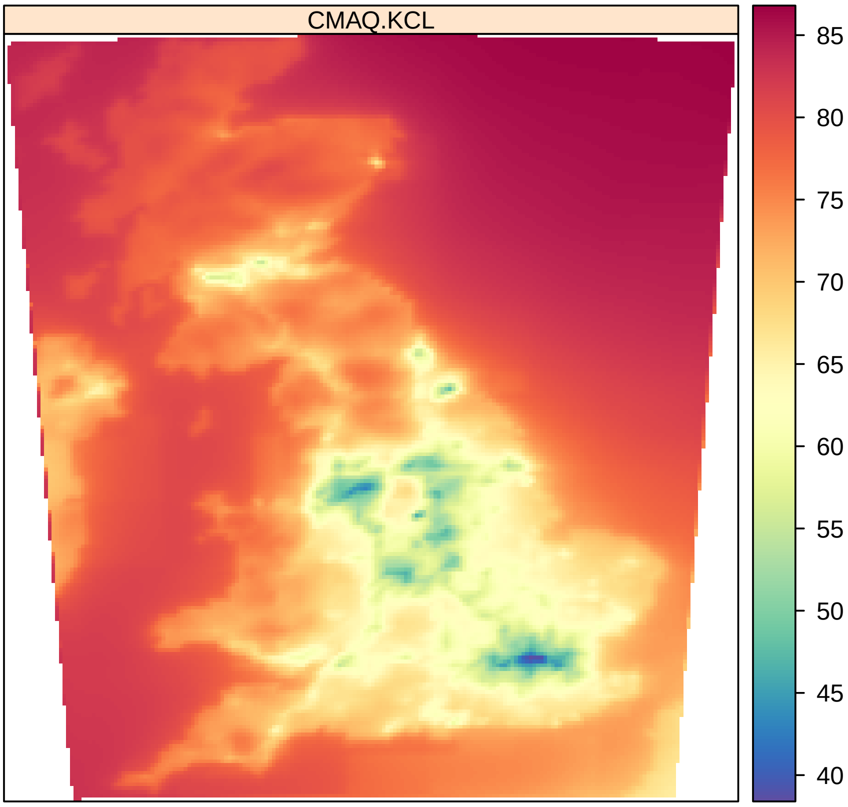

Figure 59: Map of predicted annual mean O_3 concentrations from the CMAQ King's College London model.

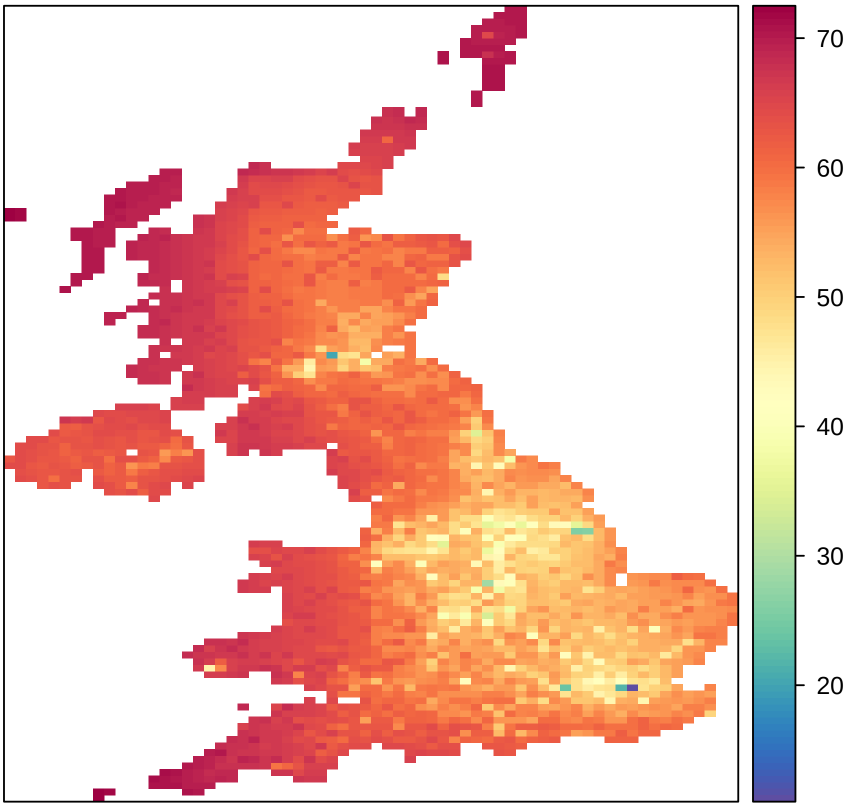

Figure 60: Map of predicted annual mean O_3 concentrations from the OSRM model.

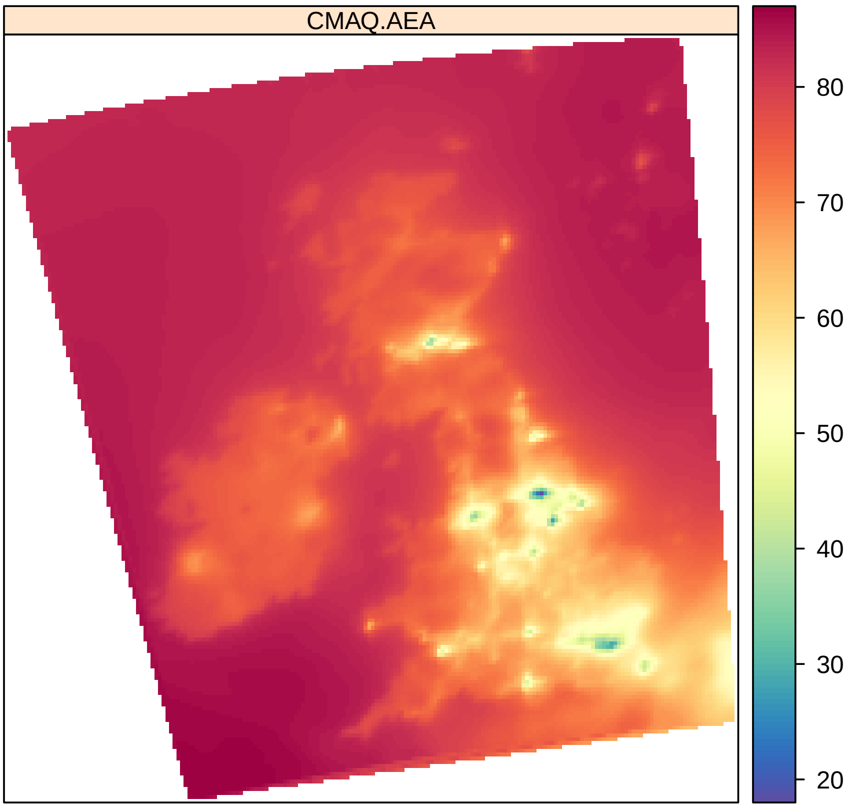

Figure 61: Map of predicted annual mean O_3 concentrations from the CMAQ AEA model.

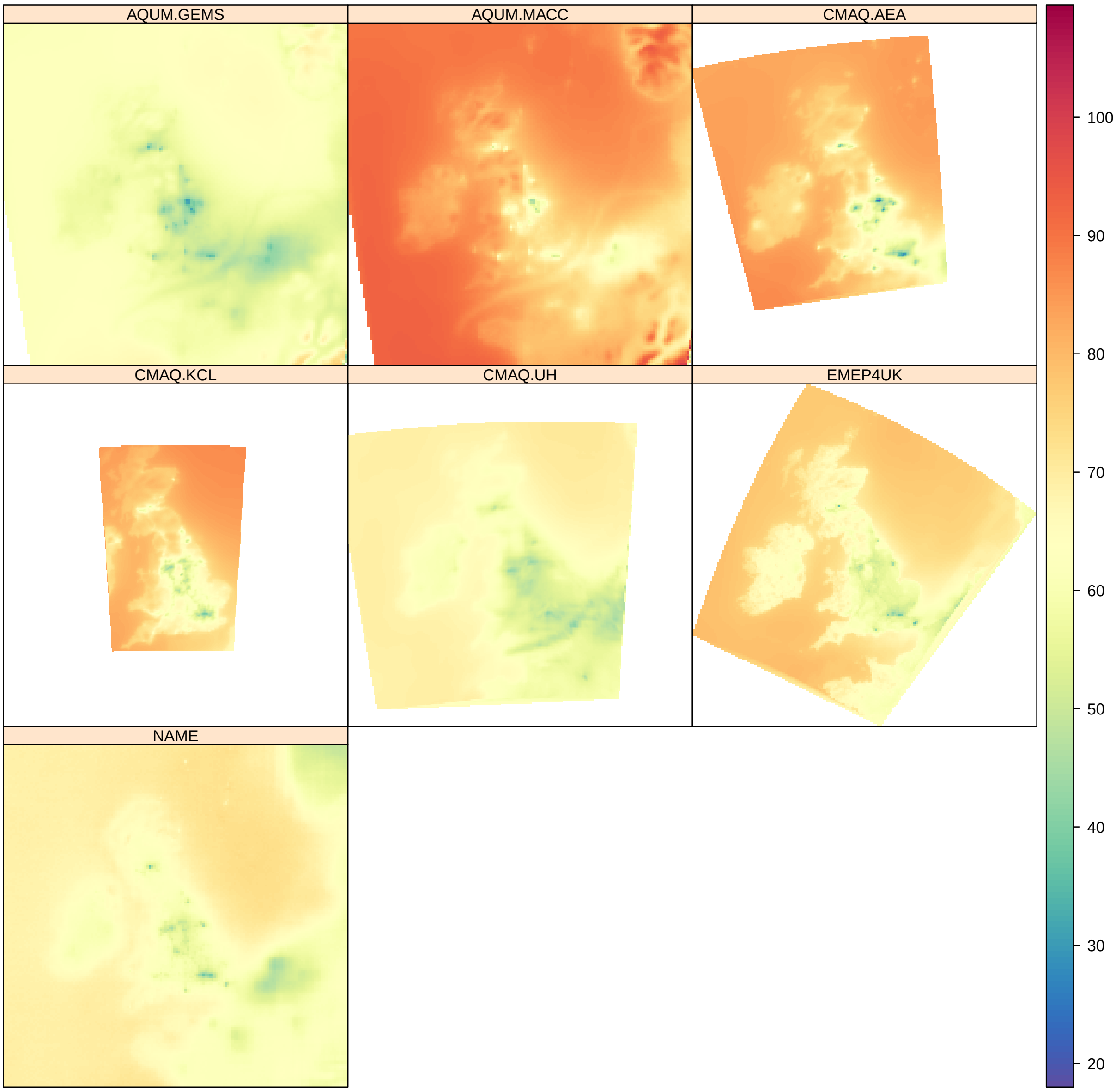

Figure 62: Surface annual mean O_3 concentrations predicted by each model over the same geographic area.

3.8 Rolling 8-hour means >100 µg m^{-3} and higher percentile O_3 concentrations

This section considers how well the models perform when calculating the number of hours where the rolling 8-hour mean O_3 concentration is >100 µg m^{-3} and the bias in predictions in general at higher concentrations of O_3. First we calculate the number of hours where the rolling mean 8-hour O_3 concentration is >100 µg m^{-3} using the `ozoneStats` function (a utility function written for this report). Note it is not possible to calculate these statistics for the PTM model.

```
o3.stats <- ozoneStats(subset(all.results, group != "PTM"))
```

A summary across all sites is given by:

```
modStats(o3.stats, type = "group", obs = "measured", mod = "modelled")
```

Table 12: Summary model evaluation statistics for the number of hours >100 µg m^{-3} rolling mean 8-hour O_3 concentration.

group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
AQUM.GEMS	15.00	0.73	96.20	148.07	0.29	0.45	176.29	0.71
AQUM.MACC	15.00	0.13	723.33	723.33	2.20	2.20	784.31	0.44
CMAQ.AEA	15.00	0.60	-72.67	137.73	-0.23	0.44	190.05	0.48
CMAQ.KCL	15.00	0.00	-287.87	287.87	-0.90	0.90	346.57	0.53
CMAQ.UH	15.00	0.33	31.93	311.67	0.10	0.95	362.14	-0.47
EMEP4UK	15.00	0.73	-75.47	155.60	-0.23	0.47	211.46	0.30
EMEP.Unified	15.00	0.67	22.07	172.20	0.07	0.52	192.38	0.39
NAME	15.00	0.73	-81.93	139.53	-0.25	0.42	198.19	0.49
OSRM	15.00	0.67	58.27	191.73	0.18	0.58	235.04	0.24

These results are probably more easily seen by plotting observed vs. modelled total hours.

```
scatterPlot(o3.stats, x = "measured", y = "modelled", type = "group", cex = 1.2,
            mod.line = TRUE, smooth = FALSE, group = "site")
```

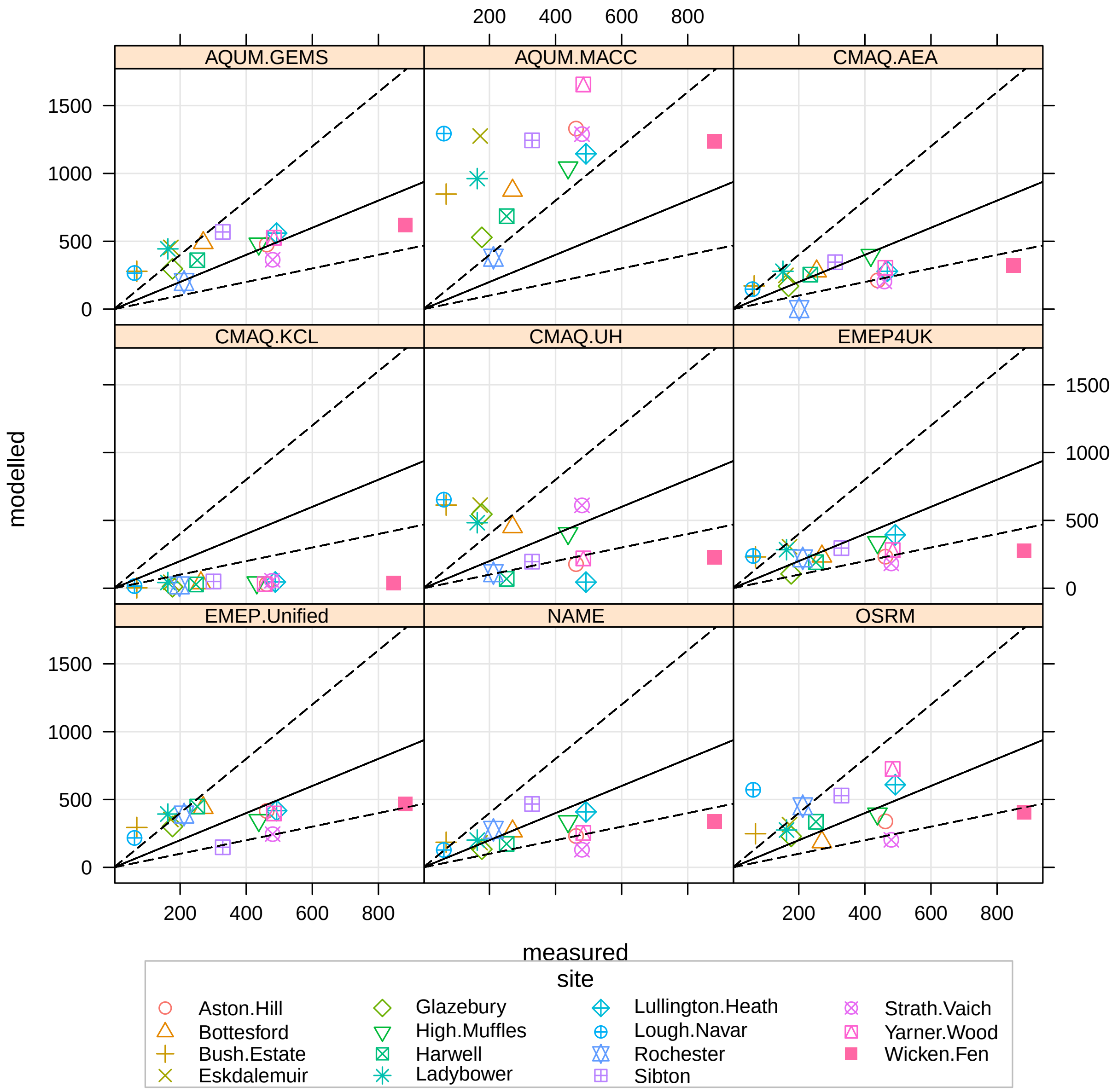

Figure 63: Measured vs. modelled number of hours where the rolling 8-hour mean O_3 concentration is >100 µg m^{-3}.

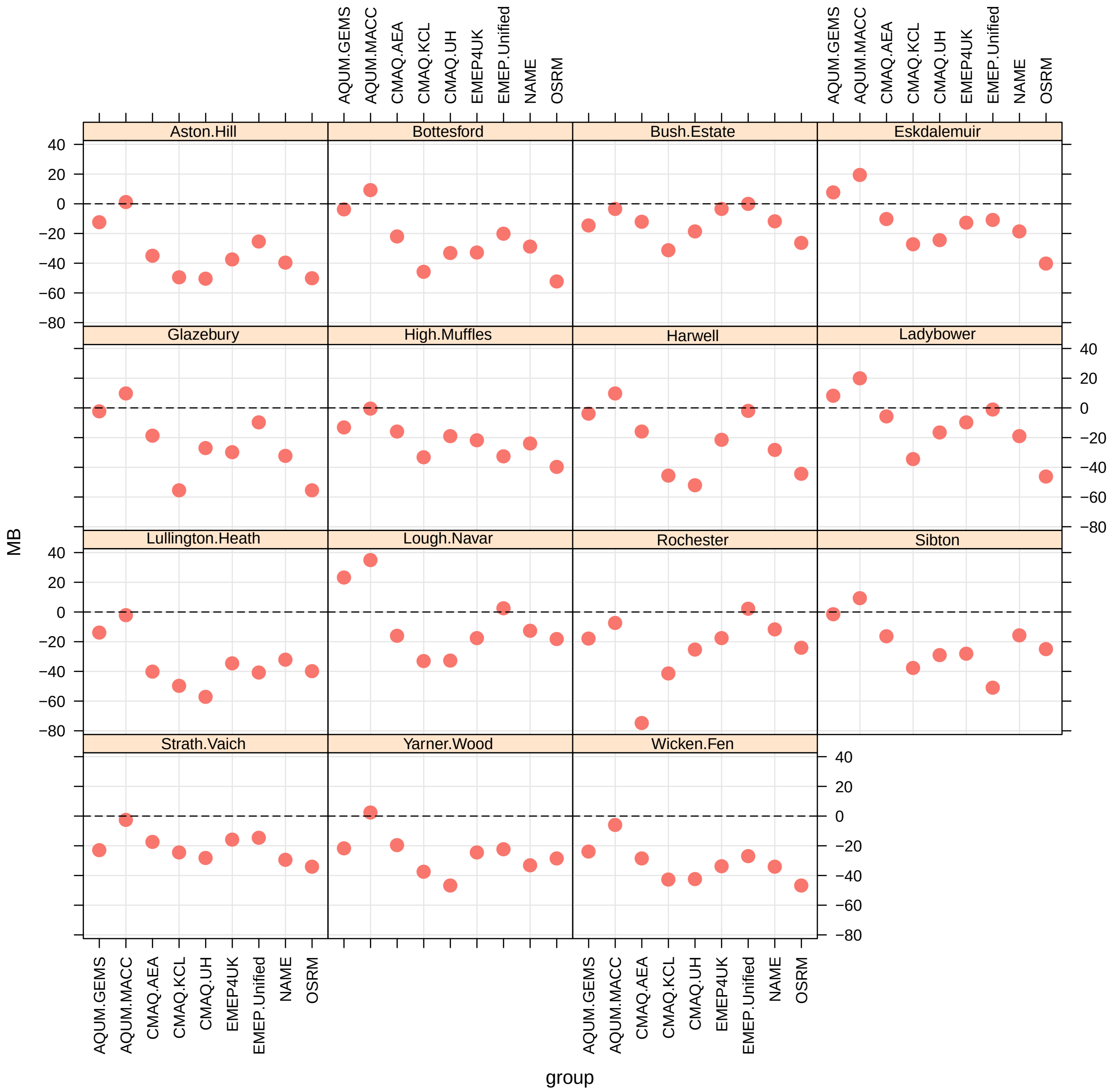

Figure 64: Mean bias of measured vs. modelled rolling 8-hour mean O_3 concentrations $gt100\ \mu g\ m^{-3}$. The dashed line is the zero-bias line.

It is also useful to know the extent to which the models show bias for the highest O_3 concentrations. There are various ways of considering this e.g. selecting whole days on which the maximum rolling 8-hour mean concentration exceeds 100 $\mu g\ m^{-3}$. We consider the simple case where measured rolling 8-hour mean concentrations exceed 100 $\mu g\ m^{-3}$ and compare the modelled results with those values. In general, as shown in Figure 64 most models tend to underestimate O_3 concentrations for these conditions. However, the AQUM.GEMS model tends to do rather better than other models in this respect.

```
epiStats <- modStats(subset(all.results, rollingO3Meas > 100), obs = "rollingO3Meas",
                     mod = "rollingO3Mod", type = c("group", "site"))
```

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

A more thorough investigating can easily be undertaken by considering different percentile concentrations of measured O_3 concentration, split by group and receptor location. The code below splits the measured O_3 concentrations into intervals determined by percentile levels of measured O_3 concentration. The percentile levels chosen were 50, 90, 95, 99 and 99.9 for hourly data. Note that these calculations base the percentiles on *all* measured O_3 concentrations. Therefore the analysis considers fixed ranges of O_3 concentration. The results are shown in Figure 65 and highlight that there is an increasing tendency for almost all models to under-predict O_3 concentrations as the O_3 concentration increases.

```
all.results$o3Interval <- cut(all.results$o3, breaks = quantile(all.results$o3,
                                             probs = c(0.5, 0.9, 0.95, 0.99, 0.999, 1), na.rm = TRUE))
## calculate model statsitics
percentileOzone <- modStats(all.results, obs = "o3", mod = "mod", type = c("site", "group", "o3Interval"))
```

```
scatterPlot(percentileOzone, x = "group", y = "MB", group = "o3Interval", type = "site", pch = 16,
           ref.y = 0, smooth = FALSE)
```

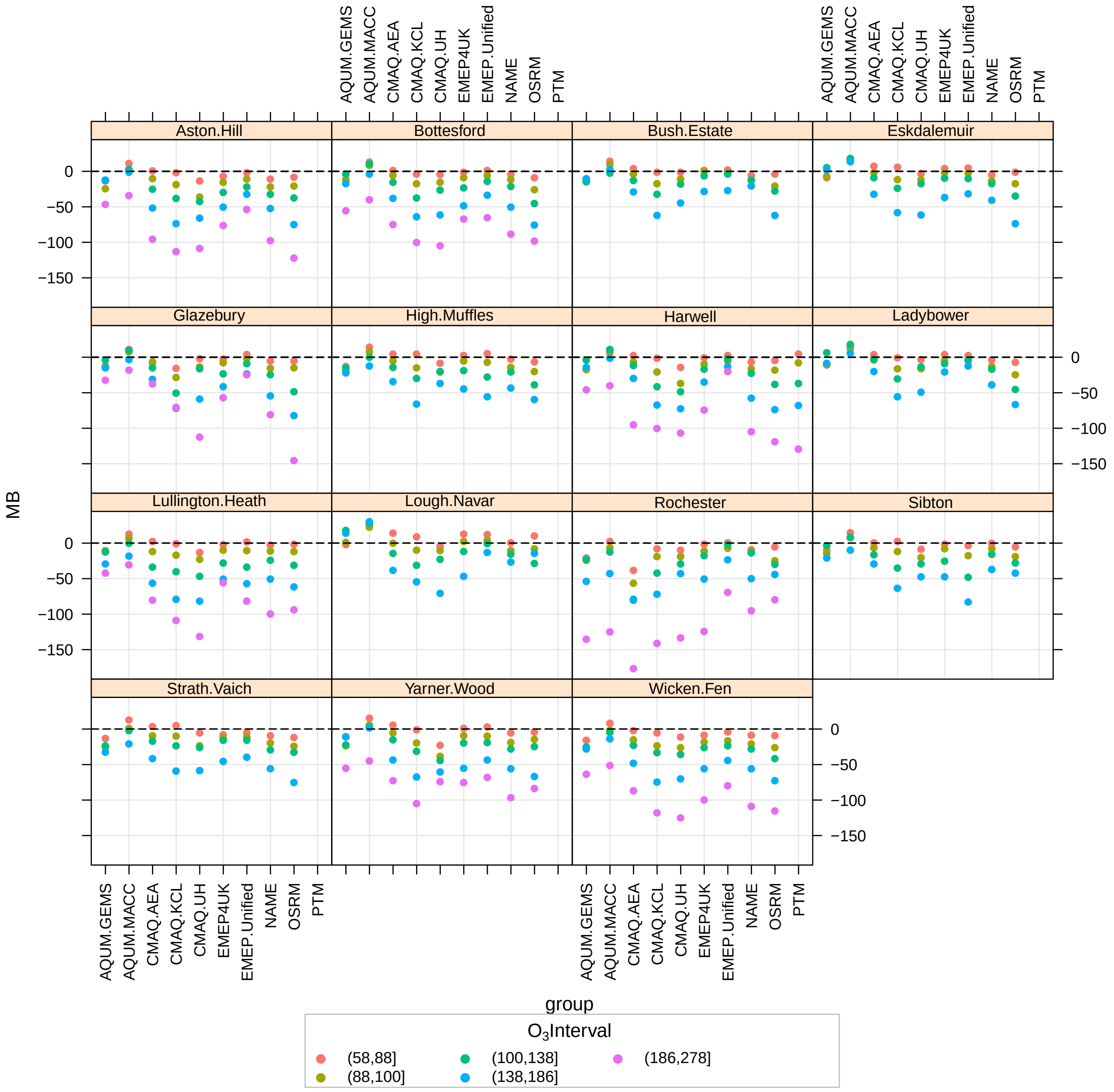

Figure 65: Mean bias in predicted O_3 concentration for different percentile levels of O_3 concentration split by model and receptor location. The dashed line is the zero-bias line.

3.9 Analysis of AOT40

This section briefly consider the analysis of the Accumulated dose of ozone Over a Threshold of 40 ppb (AOT40) — or in this case AOT80 because the units are in $\mu g\ m^{-3}$.

The calculation below subtracts 80 $\mu g\ m^{-3}$ from observed and modelled concentrations. Results less than 0 are set to zero. The results shown in Figure 66 and the table below.

```
all.results$AOT40Obs <- ifelse(all.results$o3 - 80 < 0 , 0, all.results$o3 - 80)
all.results$AOT40Mod <- ifelse(all.results$mod - 80 < 0 , 0, all.results$mod - 80)
## now sum these results for each site/model combination
AOT40 <- aggregate(subset(all.results, select = c(AOT40Obs, AOT40Mod)),
                   list(group = all.results$group, site = all.results$site), sum, na.rm = TRUE)
```

```
modStats(AOT40, obs = "AOT40Obs", mod = "AOT40Mod", type = "group")
```

```
         group  n      FAC2          MB       MGE         NMB      NMGE     RMSE          r
1    AQUM.GEMS 15 0.9333333    307.7333  8097.933  0.01242711 0.3270166 10065.08  0.7079632
2    AQUM.MACC 15 0.1333333  46394.5600 46394.560  1.87353855 1.8735385 49487.00  0.4660204
3     CMAQ.AEA 15 0.7333333  -1512.3427  9712.695 -0.06107251 0.3922250 12432.85  0.4340909
4     CMAQ.KCL 15 0.4000000 -11155.1627 13070.715 -0.45047582 0.5278310 17259.40  0.2956517
5      CMAQ.UH 15 0.4666667   -746.9671 16917.895 -0.03016456 0.6831906 20477.67 -0.4217398
6      EMEP4UK 15 0.7333333  -3627.3427  9356.223 -0.14648197 0.3778297 13172.50  0.3639761
7 EMEP.Unified 15 0.8666667   1406.2867  9913.060  0.05678968 0.4003163 11904.10  0.4984020
8         NAME 15 0.7333333  -5814.7133  8694.767 -0.23481394 0.3511183 12797.98  0.5523028
9         OSRM 15 0.8000000   4229.0107 12676.475  0.17077896 0.5119105 15407.22  0.1980435
10         PTM 15 0.0000000 -24707.6627 24707.663 -0.99776264 0.9977626 28202.27 -0.1188469
```

```
scatterPlot(AOT40, x = "AOT40Obs", y = "AOT40Mod", type = "group", group = "site", cex = 1.2,
           xlim = c(0, 80000), ylim = c(0, 80000))
```

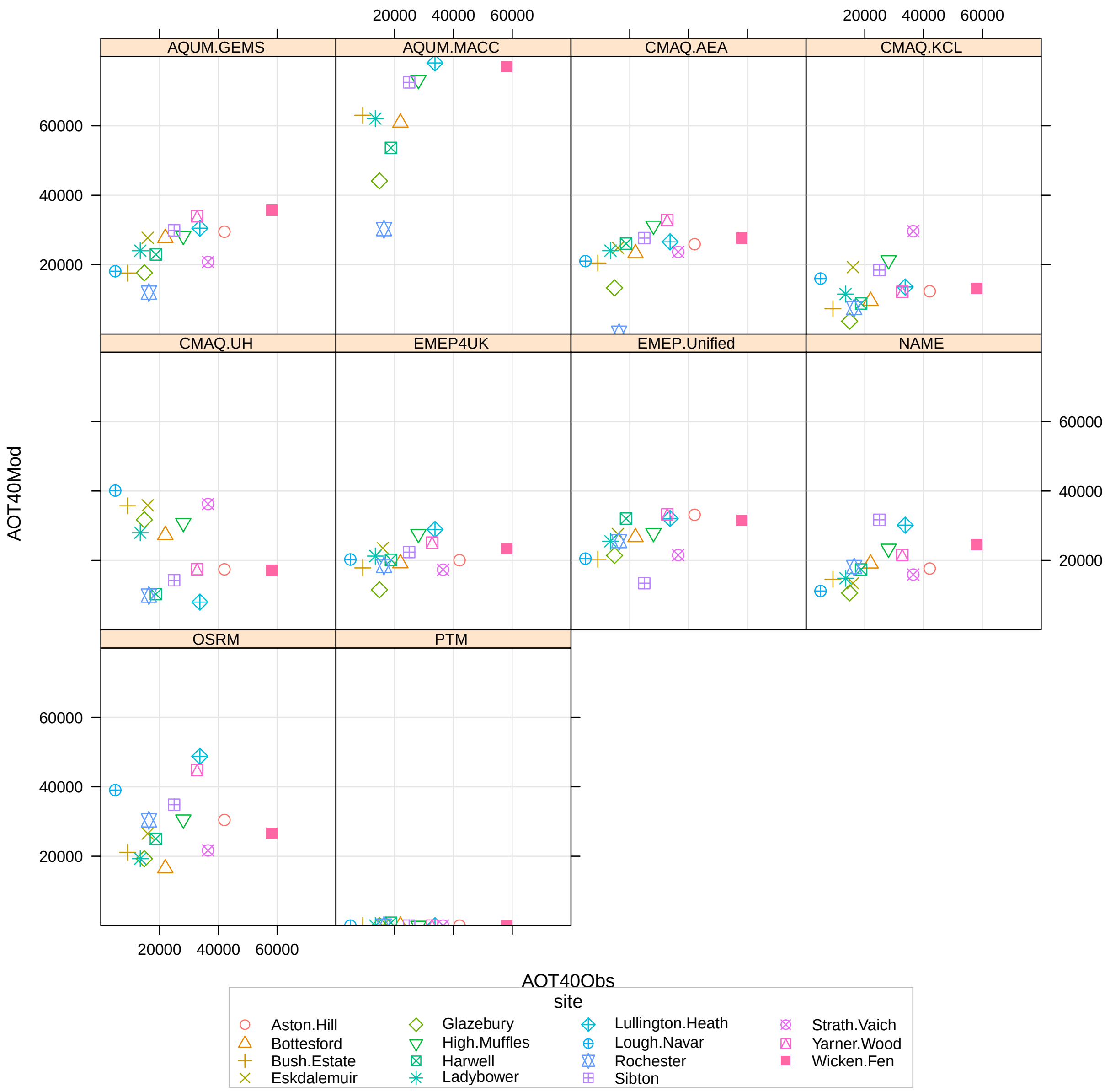

Figure 66: Comparison of modelled and measured AOT40 for each site/model combination.

3.10 Response of O_3 concentrations to changes in emissions:weekend-weekday analysis

Although it has been suggested that the models could usefully be tested to understand how O_3 predictions respond to emission changes by modelling a certain percentage reduction in NO_x and VOCs (e.g. 30% reduction) in phase two, it is possible to gain insight with the data we have now. One of the problems with testing lots of models to a change in emissions is that it is difficult to know which model(s) respond correctly because it is not known what "correct" is.

An alternative way of understanding these responses is to consider weekday-weekend changes. Emissions of VOCs and NO_x are lower during the weekends than weekdays and it is useful to use this difference to compare the models. Importantly, unlike a fixed emission reduction scenario, measured concentrations are also available with which to compare the models. Moreover, there are sufficient data over one year in order to show clear weekday-weekend differences. Care is still required in these comparisons because the models will be using slightly different assumptions concerning how emissions change by day of the week. However, in the absence of new model emission reduction scenarios, these weekday-weekend differences are very useful.

There are a few steps required to get the data into a format that makes it easy to analyse. The steps below should however be simpler than doing this from scratch, making use of **openair** functions and R. Note that in the weekday-weekend differences the mean of five weekdays is substracted from the mean of the two weekend days.

First it is necessary to label the data by weekday/weekend using the `cutData` function:

```
all.results <- cutData(all.results, "weekend")
head(all.results)
```

```
            date         site o3 rollingO3Meas    mod rollingO3Mod   group o3Interval AOT40Obs
25    2006-01-02   Aston.Hill 66         66.50 48.600     51.76250 EMEP4UK    (58,88]        0
8785  2006-01-02   Bottesford 36         38.50 28.300     29.68500 EMEP4UK       <NA>        0
17545 2006-01-02  Bush.Estate 36         45.50 38.240     34.96250 EMEP4UK       <NA>        0
26305 2006-01-02  Eskdalemuir  6         20.50 45.780     51.65500 EMEP4UK       <NA>        0
35065 2006-01-02    Glazebury  2         14.25 14.576     20.79175 EMEP4UK       <NA>        0
43825 2006-01-02 High.Muffles 28         45.75 56.240     60.36750 EMEP4UK       <NA>        0
      AOT40Mod weekend
25           0 weekday
8785         0 weekday
17545        0 weekday
26305        0 weekday
35065        0 weekday
43825        0 weekday
```

Now we need to aggregate the data by group, receptor and whether the day is a weekend or weekday:

```
delta <- ddply(all.results, .(site, group, weekend), numcolwise(mean), na.rm = TRUE)
head(delta)
```

```
        site     group weekend       o3 rollingO3Meas      mod rollingO3Mod AOT40Obs  AOT40Mod
1 Aston.Hill AQUM.GEMS weekday 72.07655      72.09178 57.72026     57.71811 5.362314  3.251474
2 Aston.Hill AQUM.GEMS weekend 71.57913      71.38040 57.58075     57.59017 4.787408  3.652341
3 Aston.Hill AQUM.MACC weekday 72.07655      72.09178 81.42171     81.37558 5.362314 10.550096
4 Aston.Hill AQUM.MACC weekend 71.57913      71.38040 80.26258     80.34823 4.787408 11.372778
5 Aston.Hill  CMAQ.AEA weekday 72.07655      72.09178 73.48143     73.26399 5.362314  3.053801
6 Aston.Hill  CMAQ.AEA weekend 71.57913      71.38040 72.35562     72.25355 4.787408  3.308599
```

To make it easy we need the responses in columns to allow the deltas to be calculated. This is done in a couple of steps:

```
delta <- melt(delta, id.vars = c("site", "group", "weekend"))
delta <- cast(delta, ... ~ weekend + variable)
## calculate weekday-weekend differences
delta <- transform(delta, deltaMeas = weekend_o3 - weekday_o3,
                   deltaMod = weekend_mod - weekday_mod)
head(delta)
```

```
       site     group weekday_o3 weekday_rollingO3Meas weekday_mod weekday_rollingO3Mod
1 Aston.Hill AQUM.GEMS   72.07655              72.09178    57.72026             57.71811
2 Aston.Hill AQUM.MACC   72.07655              72.09178    81.42171             81.37558
3 Aston.Hill  CMAQ.AEA   72.07655              72.09178    73.48143             73.26399
4 Aston.Hill  CMAQ.KCL   72.07655              72.09178    70.66321             70.70541
5 Aston.Hill   CMAQ.UH   72.07655              72.09178    56.41271             56.56033
6 Aston.Hill   EMEP4UK   72.07655              72.09178    64.44144             64.51226
  weekday_AOT40Obs weekday_AOT40Mod weekend_o3 weekend_rollingO3Meas weekend_mod
1         5.362314         3.251474   71.57913               71.3804    57.58075
2         5.362314        10.550096   71.57913               71.3804    80.26258
3         5.362314         3.053801   71.57913               71.3804    72.35562
4         5.362314         1.408753   71.57913               71.3804    69.77641
5         5.362314         1.888998   71.57913               71.3804    58.06071
6         5.362314         2.406854   71.57913               71.3804    63.42071
  weekend_rollingO3Mod weekend_AOT40Obs weekend_AOT40Mod  deltaMeas   deltaMod
1             57.59017         4.787408         3.652341 -0.4974211 -0.1395024
2             80.34823         4.787408        11.372778 -0.4974211 -1.1591263
3             72.25355         4.787408         3.308599 -0.4974211 -1.1258111
4             69.60418         4.787408         1.485539 -0.4974211 -0.8868051
5             57.69906         4.787408         2.238299 -0.4974211  1.6479996
6             63.26048         4.787408         2.258927 -0.4974211 -1.0207301
```

The model evaluation statistics by group are given by

```
modStats(delta, obs = "deltaMeas", mod = "deltaMod", type = "group")
```

```
          group  n       FAC2         MB      MGE        NMB      NMGE     RMSE         r
1     AQUM.GEMS 15 0.13333333 -1.7640000 2.041981 -0.6531316 0.7560557 2.437417 0.6921061
2     AQUM.MACC 15 0.13333333 -2.2505750 2.367001 -0.8332889 0.8763962 2.853676 0.6031785
3      CMAQ.AEA 15 0.00000000 -2.7897736 2.789774 -1.0329304 1.0329304 3.255686 0.6746077
4      CMAQ.KCL 15 0.20000000 -2.1586262 2.158626 -0.7992443 0.7992443 2.679603 0.7156421
5       CMAQ.UH 15 0.40000000 -0.7512296 1.966223 -0.2781473 0.7280060 2.386722 0.1577938
6       EMEP4UK 15 0.06666667 -2.5443607 2.605934 -0.9420648 0.9648627 3.111038 0.5899295
7  EMEP.Unified 15 0.33333333 -1.6264969 1.878649 -0.6022203 0.6955811 2.405655 0.5854334
8          NAME 15 0.53333333 -0.9684612 1.455372 -0.3585786 0.5388601 1.780568 0.7349152
9          OSRM 15 0.13333333 -2.3075868 2.428981 -0.8543979 0.8993449 2.837473 0.6704451
10          PTM  1 0.00000000 -3.8774853 3.877485 -1.0352004 1.0352004 3.877485        NA
```

which shows that most models do not replicate the weekday-weekend differences very well. Indeed only the NAME model has over half the differences within a factor of two. The principal characteristic however, is that all models tend to underestimate the increase in O_3 concentrations observed at weekends compared with weekdays.

NO_x measurements and predictions would help understand the extent to which this effect is caused by local emissions of NO; but these data are not currently available. Similarly it would be useful to explore whether the changes shown in Figure 67 are different in summer and winter months. This would help show for example the extent to which local NO_x emissions affect the results, which will be more prominent in winter. Another factor that could be important, but again is difficult to quantify, is the effect of grid size used in the models. A grid size too large to capture more local scale effects would tend to “compress” the predictions into a narrow band as is seen in Figure 67. Indeed, the issue of comparing point measurements with gridded predictions is well known and can be characterised. Regardless of the reason, these results show that most models do not capture the changes in O_3 concentrations between weekdays and weekends.

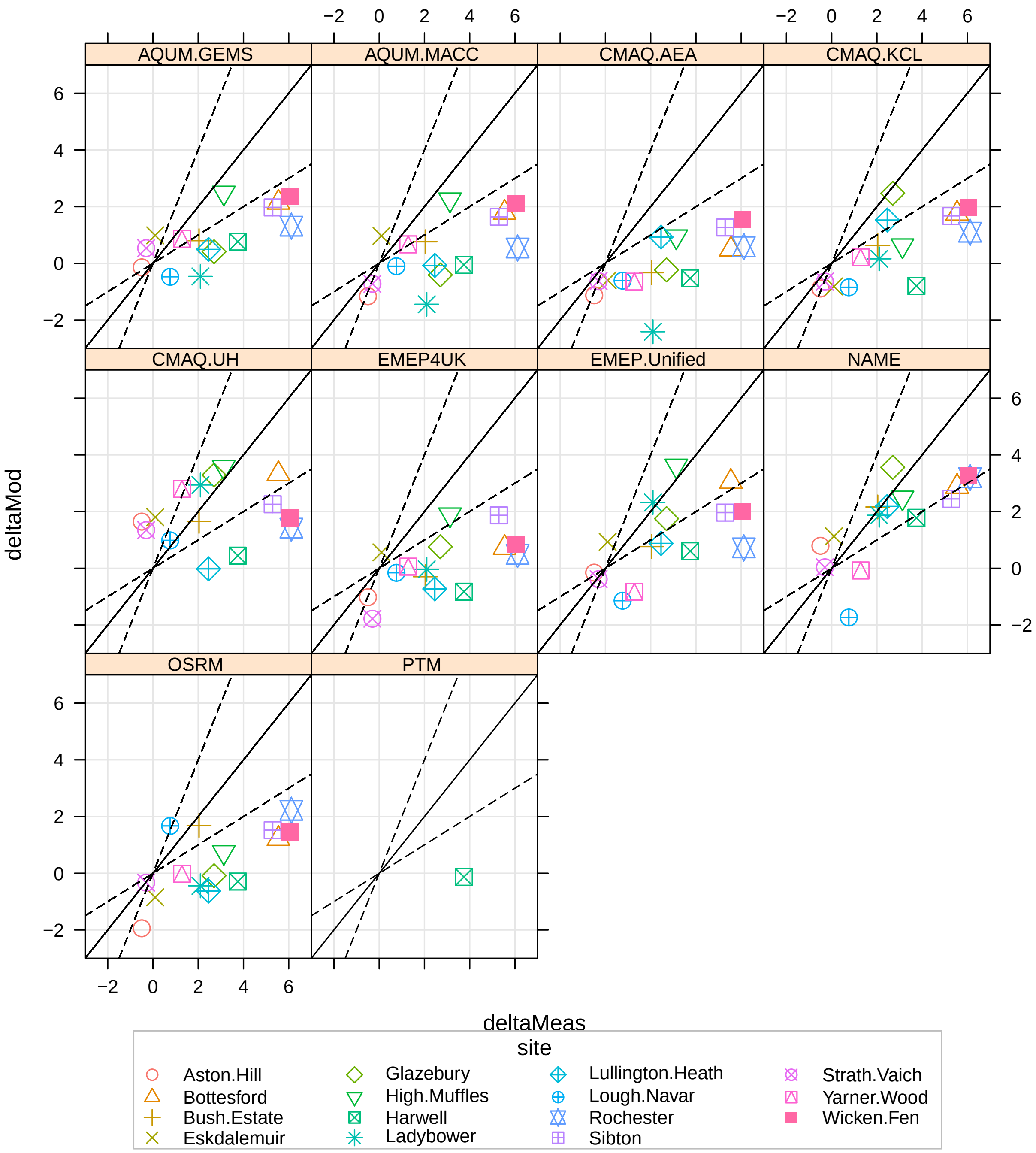

Figure 67: Weekend-weekday differences in measured and modelled O_3 concentrations at different receptors.

```
scatterPlot(delta, x = "deltaMeas", y = "deltaMod", type = c("group"), group = "site",
            xlim = c(-3, 7), ylim = c(-3, 7), mod.line = TRUE, cex = 1.5)
```

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A Example of using meteorological data

Most model evaluation studies focus on numeric metrics for compararing different models. While this type of evaluation is very useful, far more insight can be gained into model performance by analysing the data in other ways. This section shows a few examples of how combining predicted concentrations with meteorological data may help in understanding some of the *processes* that control O_3 concentrations. In essence these techniques make it much simpler to consider the dependence of O_3 concentrations on many other factors.

The Met Office have provided surface meteorological data for 10 surface sites across the UK.

To import the data:

```
## import a Met Office file for Lossiemouth
met <- read.csv("~/Projects/modelEvaluation/lossiemouthMet.csv", header = TRUE,
                na.strings = "n/a")
## make a date field
met$date <- ISOdatetime(year = met$year, month = met$month, day = met$day,
                        hour = met$hour, min = 0, sec = 0, tz = "GMT")
```

An example is provided of linking the met data from Lossiemouth with O_3 observations at Strath Vaich. First, a subset of the data are selected from the NAME model, which are then merged with the meteorological data.

```
strath <- subset(NAME, site == "Strath.Vaich")
## merge with the met data
strath <- merge(strath, met, by = "date", all = TRUE)
```

Now it is possible to obtain model performance statistics split by different levels of meteorological data. For example, how do these statistics vary by wind sector? The results below suggest less bias for southerly winds.

```
modStats(strath, type = "wd", mod = "mod", obs = "o3")
```

```
  wd    n      FAC2          MB      MGE         NMB      NMGE     RMSE         r
2  N  607 0.9868204  -9.9398682 15.58797 -0.13032443 0.2043783 19.56815 0.4982602
3 NE  426 0.9694836 -15.1018779 20.77606 -0.18532581 0.2549577 25.51199 0.3039773
1  E  941 0.9755579 -10.7911796 18.23369 -0.13890485 0.2347054 23.92092 0.5237564
6 SE  994 0.9849095  -1.9635815 14.66660 -0.03057427 0.2283687 18.85273 0.6222205
5  S  982 0.9887984  -0.9762729 13.02332 -0.01540427 0.2054904 16.61152 0.5117544
7 SW 1374 0.9687045  -6.5201994 15.84887 -0.09341572 0.2270688 19.82894 0.4847700
8  W 1419 0.9704017 -12.6173893 17.65037 -0.16319456 0.2282916 21.45229 0.4892936
4 NW  583 0.9897084 -10.7008576 15.84494 -0.13790009 0.2041910 19.57465 0.5198391
```

Or wind speed (more negative bias with increasing wind speed):

```
modStats(strath, type = "ws", mod = "mod", obs = "o3")
```

```
         ws    n      FAC2         MB      MGE         NMB      NMGE     RMSE          r
1   ws 0 to 5 1983 0.9662128  -1.810902 14.64741 -0.02977726 0.2408523 18.85434  0.4683541
3   ws 5 to 9 2034 0.9734513  -7.865492 16.54435 -0.11105843 0.2336014 21.21509  0.4368372
4  ws 9 to 13 1734 0.9861592 -10.537889 16.72209 -0.13497341 0.2141830 20.89497  0.4899580
2 ws 13 to 45 1570 0.9898089 -13.215796 17.27885 -0.15877078 0.2075832 21.26590  0.5084066
5        <NA>    5 1.0000000  -4.480000 15.36000 -0.06871166 0.2355828 17.84612 -0.9694559
```

Now it is possible to carry out lots of other analyses of these data. The example below aims to produce two bivariate polar plots.

A minimum number of points in any wind speed/direction bin is set to reduce the effect of single high values. Figure 68 confirms that the NAME model tends to under-predict O_3 concentrations at higher wind speeds, which may be indicative of how the model treats deposition processes.

```
polarPlot(strath, pollutant = c("o3", "mod"), min.bin = 2)
```

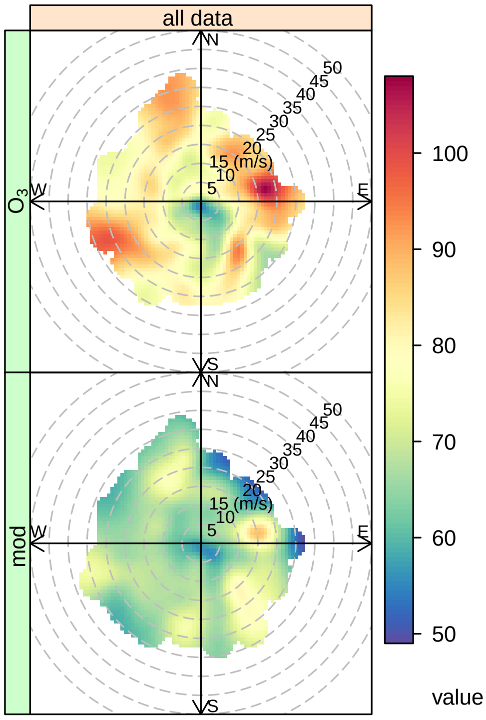

Figure 68: Example polar plot of modelled and observed O_3 concentrations at Strath Vaich using the NAME model.

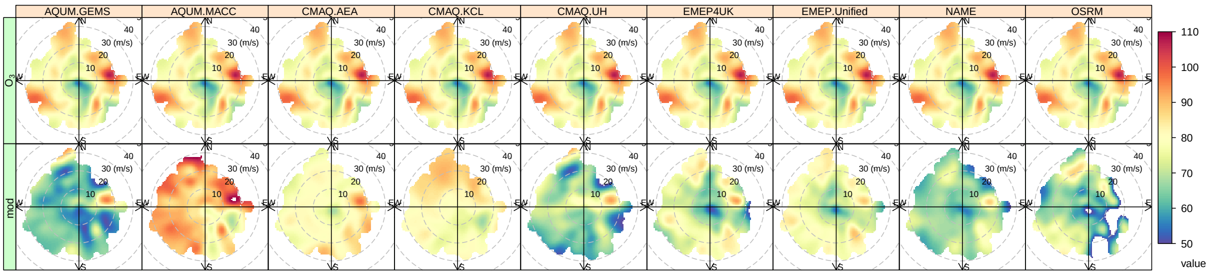

Figure 69: Example polar plot of modelled and observed O_3 concentrations at Strath Vaich for all models.

It is also possible with recent versions of **openair** to choose multiple pollutants and a single "type".

```
## use all results at Strath Vaich and merge with met data
strath <- merge(subset(all.results, site == "Strath.Vaich"), met, by = "date", all = TRUE)
## use limits to help show differences
polarPlot(subset(strath, group != "PTM"), poll=c("o3", "mod"), type = "group", min.bin = 2,
         upper = 35, limits = c(50, 110), ws.int = 10)
```

B 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 ith observed value and M_i represents the ith modelled value for a total of n observations.

Fraction of predictions within a factor or two, $FAC2$

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

$$0.5 \leq \frac{M_i}{O_i} \leq 2.0 \tag{1}$$

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.

$$MB = \frac{1}{n}\sum_{i=1}^{N} M_i - O_i \tag{2}$$

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.

$$MGE = \frac{1}{n}\sum_{i=1}^{N} |M_i - O_i| \tag{3}$$

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.

$$NMB = \frac{\sum\limits_{i=1}^{n} M_i - O_i}{\sum\limits_{i=1}^{n} O_i} \tag{4}$$

Normalised mean gross error, $NMGE$

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

$$NMGE = \frac{\sum\limits_{i=1}^{n} |M_i - O_i|}{\sum\limits_{i=1}^{n} O_i} \tag{5}$$

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.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(M_i - O_i)^2}{n}} \tag{6}$$

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.

$$r = \frac{1}{(n-1)} \sum_{i=1}^{n} \left(\frac{M_i - \overline{M}}{\sigma_M} \right) \left(\frac{O_i - \overline{O}}{\sigma_O} \right) \tag{7}$$

C Data import

This section deals with the importing of raw results files provided by each modelling group. This code may be useful if modellers wish to recreate the analyses with new data.

The EMEP4UK data are imported are some pre-processing is carried out to make future calculations easier. Note that the **openair** `rollingMean` function is used to calculate the rolling 8-hour mean, taking account of data capture rates >75%.

```
## emep4uk <- import("ozoneTemplateV3.0_EMEP4UK_rv3.7_final.csv")
## new EMEP data4 Feb 2011
emep4uk <- import("ozoneTemplateV2_0_EMEP4UKrv3.7_beta5_ugm3.csv")
```

```
          date1           date2      Aston.Hill      Bottesford     Bush.Estate
      "POSIXct"        "POSIXt"       "numeric"       "numeric"       "numeric"
     Eskdalemuir       Glazebury    High.Muffles         Harwell       Ladybower
      "numeric"       "numeric"       "numeric"       "numeric"       "numeric"
Lullington.Heath     Lough.Navar       Rochester          Sibton    Strath.Vaich
      "numeric"       "numeric"       "numeric"       "numeric"       "numeric"
      Yarner.Wood      Wicken.Fen
      "numeric"       "numeric"
```

```
emep4uk <- melt(emep4uk, id.vars = "date")
names(emep4uk) <- c("date", "site", "mod")
## calculate rolling 8-hour O3
emep4uk <- rollingMean(emep4uk, pollutant = "mod", new.name = "rollingO3Mod")
```

Then we merge these measured/modelled data sets together so that the analysis can proceed, adding a column 'group':

```
emep <- merge(ozone.meas, emep4uk, by = c("site", "date"), all = TRUE)
emep$group <- "EMEP4UK"
```

We also have results from the EMEP unified model, imported and prepared as follows:

```
empUnified <- import("ozoneTemplateV3.0_EMEP_rv3.7_beta9_final.csv")
```

```
          date1           date2      Aston.Hill      Bottesford     Bush.Estate
      "POSIXct"        "POSIXt"       "numeric"       "numeric"       "numeric"
     Eskdalemuir       Glazebury    High.Muffles         Harwell       Ladybower
      "numeric"       "numeric"       "numeric"       "numeric"       "numeric"
Lullington.Heath     Lough.Navar       Rochester          Sibton    Strath.Vaich
      "numeric"       "numeric"       "numeric"       "numeric"       "numeric"
      Yarner.Wood      Wicken.Fen
      "numeric"       "numeric"
```

```
emepUnified <- melt(emepUnified, id.vars = "date")
names(emepUnified) <- c("date", "site", "mod")
## calculate rolling 8-hour O3
emepUnified <- rollingMean(emepUnified, pollutant = "mod", new.name = "rollingO3Mod")
emepUnified <- merge(ozone.meas, emepUnified, by = c("site", "date"), all = TRUE)
emepUnified$group <- "EMEP.Unified"
```

The results from the PTM are in a somewhat different format. Predictions have only been made at Harwell and the PTM provides a distribution of results for one hour (15:00 GMT) each day. For the purposes of comparisons made here the median estimate from the PTM has been used.

The following code imports that data as provided and organises the data ready for analysis.

```
ptm <- import("ozoneTemplateV2 0_PTM.csv", data.at = 4, header.at = 3, date.name = "Date", time.name = "Date")
```

```
    date1      date2  X95..ile  X84..ile  X50..ile  X16..ile   X5..ile
"POSIXct"  "POSIXt" "numeric" "numeric" "numeric" "numeric" "numeric"
```

```
## only select the 50th percentile for now
ptm <- subset(ptm, select = c(date, X50..ile))
## change name to "mod"
names(ptm) <- c("date", "mod")
## add "site" field and assign Harwell (only receptor used in PTM)
ptm$site <- "Harwell"
## merge with ozone measurements
ptm <- merge(ozone.meas, ptm, by = c("site", "date"), all = TRUE)
## add model name
ptm$group <- "PTM"
```

The results for the NAME model are imported and prepared as follows:

```
NAME <- import("ozoneTemplateV3.0_MetOfficeNAME.csv")
```

```
          date1           date2      Aston.Hill      Bottesford     Bush.Estate
      "POSIXct"        "POSIXt"       "numeric"       "numeric"       "numeric"
     Eskdalemuir       Glazebury    High.Muffles         Harwell       Ladybower
      "numeric"       "numeric"       "numeric"       "numeric"       "numeric"
Lullington.Heath     Lough.Navar       Rochester          Sibton     Strath.Vaich
      "numeric"       "numeric"       "numeric"       "numeric"       "numeric"
     Yarner.Wood      Wicken.Fen
      "numeric"       "numeric"
```

```
## stack data
NAME <- melt(NAME, id.vars = "date")
names(NAME) <- c("date", "site", "mod")
## original units are in g/m3 - change to ug/m3
NAME$mod <- NAME$mod * 1000000
NAME <- rollingMean(NAME, pollutant = "mod", new.name = "rollingO3Mod")
## merge with observations
NAME <- merge(ozone.meas, NAME, by = c("site", "date"), all = TRUE)
## add model name
NAME$group <- "NAME"
```

The AQUM.GEMS results are imported and prerpared as follows:

```
## updated from file below on 13-01-2011
AQUM.GEMS <- import("sgkxs_03.csv")
```

```
          date1          date2     Aston.Hill     Bottesford    Bush.Estate
      "POSIXct"       "POSIXt"      "numeric"      "numeric"      "numeric"
     Eskdalemuir      Glazebury    High.Muffles        Harwell      Ladybower
      "numeric"      "numeric"      "numeric"      "numeric"      "numeric"
Lullington.Heath    Lough.Navar      Rochester         Sibton    Strath.Vaich
      "numeric"      "numeric"      "numeric"      "numeric"      "numeric"
     Yarner.Wood     Wicken.Fen
      "numeric"      "numeric"
```

```
## AQUM.GEMS <- import("2006_o3_AQUM.csv")
## stack data
AQUM.GEMS <- melt(AQUM.GEMS, id.vars = "date")
names(AQUM.GEMS) <- c("date", "site", "mod")
## calculate rolling 8-hour O3
AQUM.GEMS <- rollingMean(AQUM.GEMS, pollutant = "mod", new.name = "rollingO3Mod")
## merge with observations
AQUM.GEMS <- merge(ozone.meas, AQUM.GEMS, by = c("site", "date"), all = TRUE)
## add model name
AQUM.GEMS$group <- "AQUM.GEMS"
```

The AQUM.MACC results are imported and prerpared as follows:

```
AQUM.MACC <- import("2006_15sites_o3_macc.csv")
```

```
          date1          date2     Aston.Hill     Bottesford    Bush.Estate
      "POSIXct"       "POSIXt"      "numeric"      "numeric"      "numeric"
     Eskdalemuir      Glazebury    High.Muffles        Harwell      Ladybower
      "numeric"      "numeric"      "numeric"      "numeric"      "numeric"
Lullington.Heath    Lough.Navar      Rochester         Sibton    Strath.Vaich
      "numeric"      "numeric"      "numeric"      "numeric"      "numeric"
     Yarner.Wood     Wicken.Fen
      "numeric"      "numeric"
```

```
## stack data
AQUM.MACC <- melt(AQUM.MACC, id.vars = "date")
names(AQUM.MACC) <- c("date", "site", "mod")
## calculate rolling 8-hour O3
AQUM.MACC <- rollingMean(AQUM.MACC, pollutant = "mod", new.name = "rollingO3Mod")
## merge with observations
AQUM.MACC <- merge(ozone.meas, AQUM.MACC, by = c("site", "date"), all = TRUE)
## add model name
AQUM.MACC$group <- "AQUM.MACC"
```

The AEA CMAQ results are imported as follows:

```
CMAQ.AEA <- import("ozone_aea_cmaq_v1.csv")
```

```
          date1            date2       Aston.Hill      Bottesford     Bush.Estate
      "POSIXct"        "POSIXt"        "numeric"       "numeric"       "numeric"
    Eskdalemuir        Glazebury     High.Muffles         Harwell       Ladybower
      "numeric"        "numeric"       "numeric"       "numeric"       "numeric"
Lullington.Heath      Lough.Navar       Rochester          Sibton     Strath.Vaich
      "numeric"        "numeric"       "numeric"       "numeric"       "numeric"
     Yarner.Wood       Wicken.Fen
      "numeric"        "numeric"
```

```
## stack data
CMAQ.AEA <- melt(CMAQ.AEA, id.vars = "date")
names(CMAQ.AEA) <- c("date", "site", "mod")
## calculate rolling 8-hour O3
CMAQ.AEA <- rollingMean(CMAQ.AEA, pollutant = "mod", new.name = "rollingO3Mod")
## merge with observations
CMAQ.AEA <- merge(ozone.meas, CMAQ.AEA, by = c("site", "date"), all = TRUE)
## add model name
CMAQ.AEA$group <- "CMAQ.AEA"
```

The OSRM results are imported and processed as follows:

```
OSRM <- import("osrm_ozoneTemplateV3 0.csv")
```

```
          date1            date2       Aston.Hill      Bottesford     Bush.Estate
      "POSIXct"        "POSIXt"        "numeric"       "numeric"       "numeric"
    Eskdalemuir        Glazebury     High.Muffles         Harwell       Ladybower
      "numeric"        "numeric"       "numeric"       "numeric"       "numeric"
Lullington.Heath      Lough.Navar       Rochester          Sibton     Strath.Vaich
      "numeric"        "numeric"       "numeric"       "numeric"       "numeric"
     Yarner.Wood       Wicken.Fen
      "numeric"        "numeric"
```

```
## stack data
OSRM <- melt(OSRM, id.vars = "date")
names(OSRM) <- c("date", "site", "mod")
## calculate rolling 8-hour O3
OSRM <- rollingMean(OSRM, pollutant = "mod", new.name = "rollingO3Mod")
## merge with observations
OSRM <- merge(ozone.meas, OSRM, by = c("site", "date"), all = TRUE)
## add model name
OSRM$group <- "OSRM"
```

The University of Herfordshire CMAQ results:

```
## CMAQ.UH <- import("20101208_Ozone_UH.csv")
## revised results as of 26 Jan 2011
## CMAQ.UH <- import("20110126_Ozone_UH.csv")
CMAQ.UH <- import("20110210_Ozone_UH.csv")
```

```
          date1           date2      Aston.Hill     Bottesford    Bush.Estate
      "POSIXct"       "POSIXt"       "numeric"      "numeric"      "numeric"
    Eskdalemuir      Glazebury    High.Muffles        Harwell      Ladybower
      "numeric"      "numeric"       "numeric"      "numeric"      "numeric"
Lullington.Heath     Lough.Navar      Rochester         Sibton   Strath.Vaich
      "numeric"      "numeric"       "numeric"      "numeric"      "numeric"
     Yarner.Wood      Wicken.Fen
      "numeric"      "numeric"
```

```
## revised 11 Feb 2011
## stack data
CMAQ.UH <- melt(CMAQ.UH, id.vars = "date")
names(CMAQ.UH) <- c("date", "site", "mod")
## calculate rolling 8-hour O3
CMAQ.UH <- rollingMean(CMAQ.UH, pollutant = "mod", new.name = "rollingO3Mod")
## merge with observations
CMAQ.UH <- merge(ozone.meas, CMAQ.UH, by = c("site", "date"), all = TRUE)
## add model name
CMAQ.UH$group <- "CMAQ.UH"
```

King's College London CMAQ results:

```
CMAQ.KCL <- import("OzoneTemplateV3_KCL_9kmGrid_O3Modelling_final.csv")
```

```
          date1           date2      Aston.Hill     Bottesford    Bush.Estate
      "POSIXct"       "POSIXt"       "numeric"      "numeric"      "numeric"
    Eskdalemuir      Glazebury    High.Muffles        Harwell      Ladybower
      "numeric"      "numeric"       "numeric"      "numeric"      "numeric"
Lullington.Heath     Lough.Navar      Rochester         Sibton   Strath.Vaich
      "numeric"      "numeric"       "numeric"      "numeric"      "numeric"
     Yarner.Wood      Wicken.Fen
      "numeric"      "numeric"
```

```
## stack data
CMAQ.KCL <- melt(CMAQ.KCL, id.vars = "date")
names(CMAQ.KCL) <- c("date", "site", "mod")
## calculate rolling 8-hour O3
CMAQ.KCL <- rollingMean(CMAQ.KCL, pollutant = "mod", new.name = "rollingO3Mod")
## merge with observations
CMAQ.KCL <- merge(ozone.meas, CMAQ.KCL, by = c("site", "date"), all = TRUE)
## add model name
CMAQ.KCL$group <- "CMAQ.KCL"
```

The dat acan now be saved in an R *workspace*, which sores the data in a compressed format.

```
save(AQUM.GEMS, AQUM.MACC, CMAQ.AEA, CMAQ.KCL, CMAQ.UH, emep, emepUnified, NAME, OSRM, ptm,
    file = "modelData.Rdata")
```