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# Defra deposition model evaluation analysis – Phase 1

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## **Executive summary**

This report provides a summary of the evaluation of air quality models used for the assessment of deposition. The report considers a wide range of gaseous and wet deposition species. 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

**12th January 2011** Added CMAQ JEP maps.

**18th January 2011** Added transects for all species — extracted from maps for NAME, EMEP4UK, CMAQ-JEP and CMAP-University of Hertfordshire. Will need to come back to HARM results.

**26th January 2011** Wet deposition FRAME maps provided ([Figure 62](#), [Figure 70](#) and [Figure 78](#))

**2nd March 2011** Add FRAME lat/lon results for consistent mapping/transects with other models.

**15th April 2011** Comment about SO<sub>2</sub> concentrations and some minor modifications.

### 1.2 Background

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

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

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

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

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

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

### 1.3 Methods used

This document blends text with code in that the whole document must be 'run' to produce it. Each time a version of this documentation is produced, all the code is run at the same time to generate all the various outputs e.g. plots and tables. There are several reasons for adopting this approach:

- It provides a good way of presenting and distilling a large amount of information; hopefully an advantage to the modelling steering group.
- Every plot, table or statistic is entirely reproducible by anyone. An up to date version of R and R package called **openair** is all that is required. The commands shown can be pasted into R and all the workings are shown in a logical sequence.
- The approach makes it much easier to deal with revised results from models. For example, if modelling groups discover a problem with their results, a new set of results can be analysed very quickly and all the plots, tables etc. updated accordingly. Account can be taken of such changes at the last minute.

- It is clear that this document can only show a limited amount of information given the number of modelling groups, receptor points and the wide range of analyses that could potentially be undertaken. However, by showing the commands used to carry out the analysis, the modelling groups can choose to undertake further more detailed analysis should they wish to.
- Finally, this approach is fully transparent. All the code and methods used in the analysis are open to scrutiny by anyone.

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

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

The SO<sub>2</sub> concentration measurements were reviewed during the compilation of this report.<sup>1</sup> The principal issue relates to the accuracy of SO<sub>2</sub> measurements made by UV fluorescence instruments on the AURN at low ( $\approx 1$  ppb) concentration compared with Delta Denuders operated as part of the AGANet. In addition questions were raised around the treatment of data during rounding processes by different organisations which is being investigated further. The instruments used on the AURN fully meet the requirements of the Ambient Air Quality Directive (2008/50/EC) as they are the reference method EN 14212:2005 and provide data within the required data quality objectives, but at such low concentrations a degree of uncertainty is introduced which is not seen with the Delta Denuders. The Delta Denuders are not reference method. Readers should consider this when reviewing the performance of models compared with the SO<sub>2</sub> measurements as the variability between measurement data will introduce differences and uncertainty within the measured values. The issue will be considered in greater detail during Phase 2.

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

## 2 Data preparation

The details of the species to be predicted are shown in [Table 1](#). Unless stated otherwise the units used in all plots and tables are those shown in [Table 1](#).

Note that all analyses in this report relate to 2003.

**Table 1:** Details of deposition modelling.

species	note	units
SO <sub>2</sub>	from rural monitoring network	$\mu\text{g m}^{-3}$
NO <sub>2</sub>	from rural monitoring network	$\mu\text{g m}^{-3}$
ammonia	from rural monitoring network	$\mu\text{g m}^{-3}$
HNO <sub>3</sub>	DELTA sampler	$\text{mg m}^{-3}$
NH <sub>4</sub> <sup>+</sup>	DELTA sampler	$\text{mg m}^{-3}$
NO <sub>3</sub> <sup>-</sup>	DELTA sampler	$\text{mg m}^{-3}$
NO <sub>3</sub> <sup>-</sup>	DELTA sampler	$\text{mg m}^{-3}$
nss SO <sub>4</sub>	DELTA sampler	$\text{mg m}^{-3}$
nss sulphate	mean ion concentration in precipitation	micro.eq/l
nitrate	mean ion concentration in precipitation	micro.eq/l
ammonium	mean ion concentration in precipitation	micro.eq/l

The receptor-based results are straightforward to deal with across the different models. However, mapping the various outputs is more challenging because of the different map projections, spatial

<sup>1</sup>Professor Neil Cape (CEH) produced a document 'SO2\_comparisons.docx' which summarises these issues; sent by email on 2nd February 2011.

coverage and even units used by the different models. While it would be useful to plot all maps on the same basis, this has not been possible. However, the plots presented here should provide a good indication of the spatial prediction characteristics of the different models. Also note that because the models provide predictions at different spatial scales it may not be meaningful to attempt to plot spatial results on the same scale.

Not every group supplied transect information for the species of interest. We have therefore extracted the transects from the maps, which mostly had to be interpolated onto a regular grid of latitude and longitude. Because of the differences in spatial resolution between the models a vertical or horizontal transect was identified by finding the nearest point on the map grids to the latitude of longitude of interest. This provides a consistent, but not precise comparison between the models. The transects of interest were originally based on OS coordinates. However, because most models use latitude and longitude, these were converted. Again, because of various map projection differences, there is not a consistent OS line of northings that uniquely defines a line of consistent latitudes. These differences are small though. The vertical transect is therefore defined as being 4.05 W and 52.748–53.322 N. The horizontal transect is defined at 3.996–5.015 W and 55.065 N.

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")
## set working directory to make file paths easier
setwd("~/Projects/modelEvaluation/deposition")
## make sure all times are displayed in GMT
Sys.setenv(TZ = "GMT")
```

Next we import the results.

```
emep <- read.csv("depositionTemplateV1.0_EMEP4UK_rv3.7_final.csv", header = TRUE)
emep$group <- "EMEP4UK"
## also have EMEP Unified model results:
emepUnified <- read.csv("depositionTemplateV1.0_EMEP_rv3.7_beta9_final.csv", header = TRUE)
emepUnified$group <- "EMEP.Unified"
NAME <- read.csv("depositionTemplateV1.0_MetOfficeNAME.csv", header = TRUE)
NAME$group <- "NAME"
## HARM
HARM <- read.csv("depositionTemplateV1.0HARM2.csv", header = TRUE)
HARM$group <- "HARM"
## CMAQ JEP
CMAQ.JEP <- read.csv("depositionTemplateV1.0_JEP_CMAQv4.7_data.csv", header = TRUE)
CMAQ.JEP$group <- "CMAQ.JEP"
## FRAME
FRAME <- read.csv("depositionTemplateV1.0_FRAME_final.csv", header = TRUE)
FRAME$group <- "FRAME"
## CMAQ UH
CMAQ.UH <- read.csv("20101208_Deposition_UH.csv", header = TRUE)
CMAQ.UH$group <- "CMAQ.UH"
```

Now we can combine all the model results:

```
all.results <- rbind.fill(emep, emepUnified, NAME, HARM, CMAQ.JEP, FRAME, CMAQ.UH)
```

Some modellers have produced data that can be used for plotting surface concentration maps. These are imported below.

```

## import NAME air concentration data
mapNAME <- read.csv("NAME2003annual_airconcExtract.csv", header = TRUE)
## need to multiply by 10^6 to get ug/m3
mapNAME[, 3:9] <- mapNAME[, 3:9] * 1000000
mapNAME$group <- "NAME"
## import NAME wet deposition data
mapNAMEwet <- read.csv("NAME2003annual_wetdepExtractV2.csv", header = TRUE)
mapNAMEwet$group <- "NAME"
## FRAME air
mapFRAME <- read.csv("conc_MIP_run_10_8-02-0_2003unc.dat_latlon.csv", header = TRUE)
mapFRAME$group <- "FRAME"
## FRAME wet deposition data
mapFRAMEwet <- read.csv("prcon_MIP_run_10_8-02-0_2003unc.dat_latlon.csv", header = TRUE)
## CMAQ Uni Hertfordshire
mapUH <- read.csv("20101208_Deposition_map_UH.csv", header = TRUE)
mapUH$group <- "CMAQ.UH"

```

Maps for JEP data were in a matrix format, which were made into individual csv files. These are imported as follows.

```

## species in 12 csv files we want to import
species <- c("lat", "lon", "so2", "no2", "nh3", "hno3", "nh4", "no3", "nssSO4",
            "SO4precip", "NO3precip", "NH4precip")
## function to import data
importJEP <- function(species){
  theData <- read.csv(paste("JEP", species, ".csv", sep = ""),
                    header = FALSE)
  theData <- stack(theData)
  theData <- theData$value
  theData
}
## run the function
mapJEP <- lapply(species, importJEP)
## put data into columns
mapJEP <- do.call(cbind, mapJEP)
## make it a data frame
mapJEP <- as.data.frame(mapJEP)
names(mapJEP) <- species
mapJEP$group <- "CAMQ.JEP"

```

Finally, to help find the nearest point on a grid, the following function is defined:

```

nearest <- function(theData, lat = 55, lon = 0){
  if (!missing(lat)) {
    id <- which(abs(theData[, "lat"] - lat) == min(abs(theData[, "lat"] - lat)))
  } else {
    id <- which(abs(theData[, "lon"] - lon) == min(abs(theData[, "lon"] - lon)))
  }
  id
}

```

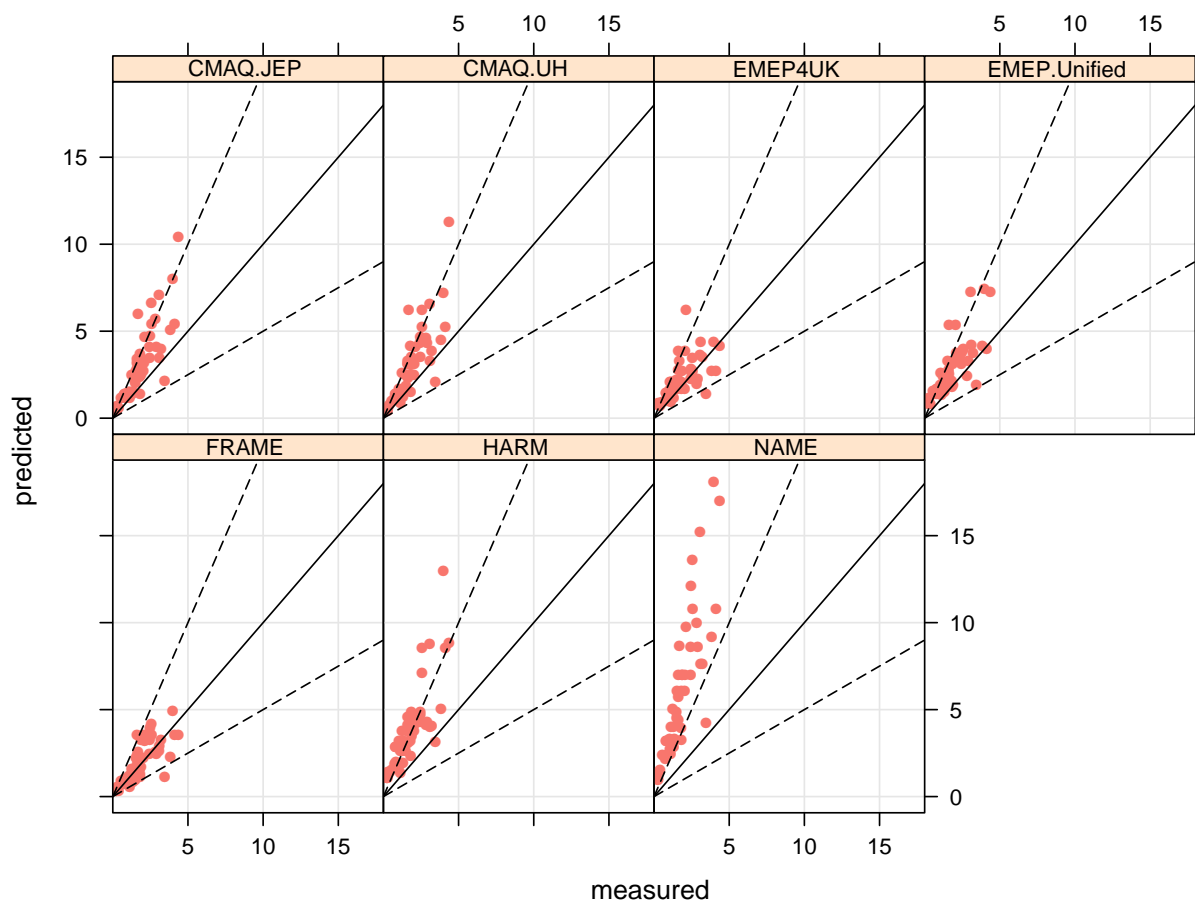
## 3 Analysis examples

### 3.1 Sulphur dioxide

First we will extract the SO<sub>2</sub> data.

```
so2.results <- subset(all.results, species == "SO2")
```

Model evaluation statistics can be estimated using the `modStats` function. These statistics are described in [Appendix A](#). 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 (`so2.results`),



**Figure 1:** Measured versus predicted annual mean  $\text{SO}_2$  concentrations ( $\mu\text{g m}^{-3}$ ).

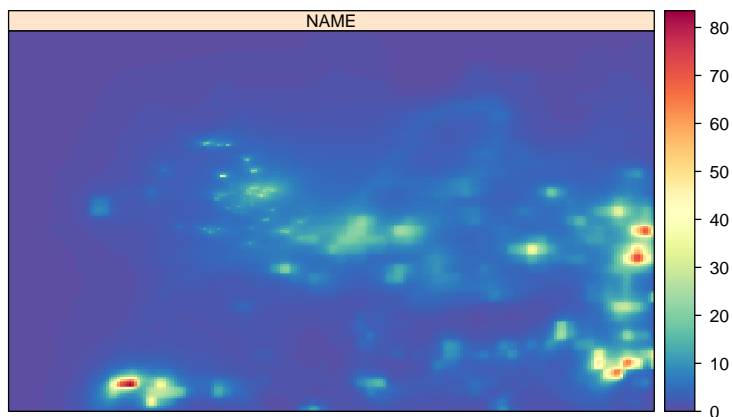
the analysis type (statistics by group i.e. `type = "group"`), the modelled results column is called `"predicted"` and the observations column in this case is `"measured"`.

```
S02stats <- modStats(so2.results, type = "group", mod = "predicted", obs = "measured")
```

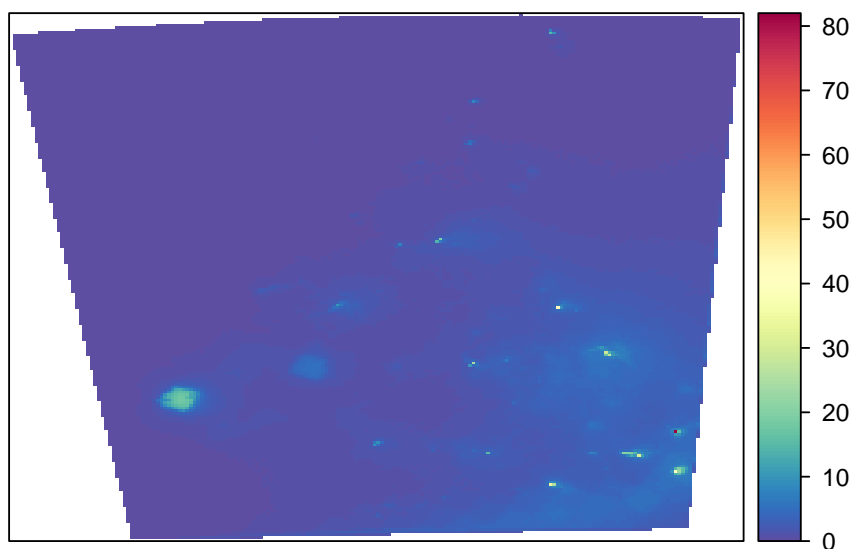
**Table 2:** Summary model evaluation statistics for annual mean  $\text{SO}_2$  concentrations.

group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
CMAQ.JEP	49.00	0.73	1.23	1.30	0.67	0.71	1.84	0.84
CMAQ.UH	49.00	0.84	1.18	1.26	0.64	0.68	1.81	0.82
EMEP4UK	49.00	0.86	0.41	0.71	0.22	0.39	1.00	0.66
EMEPUnified	49.00	0.73	0.98	1.06	0.53	0.58	1.42	0.77
FRAME	49.00	0.96	0.12	0.57	0.07	0.31	0.79	0.77
HARM	49.00	0.37	2.05	2.07	1.11	1.12	2.62	0.80
NAME	49.00	0.04	4.38	4.38	2.38	2.38	5.45	0.84

```
scatterPlot(so2.results, x = "measured", y = "predicted", type = "group", mod.line = TRUE,
            xlim = c(0, 18), smooth = FALSE, pch = 16, key = FALSE)
```



**Figure 2:** Annual mean SO<sub>2</sub> concentrations from the NAME model.



**Figure 3:** Annual mean SO<sub>2</sub> concentrations from the FRAME model.

```
makeMap(mapNAME, pollutant = "so2", aspect = "iso")
```

```
FRAMESO2 <- prepareGrid(mapFRAME, pollutant = "SO2")
makeMap(FRAMESO2, pollutant = "SO2", aspect = "iso")
```

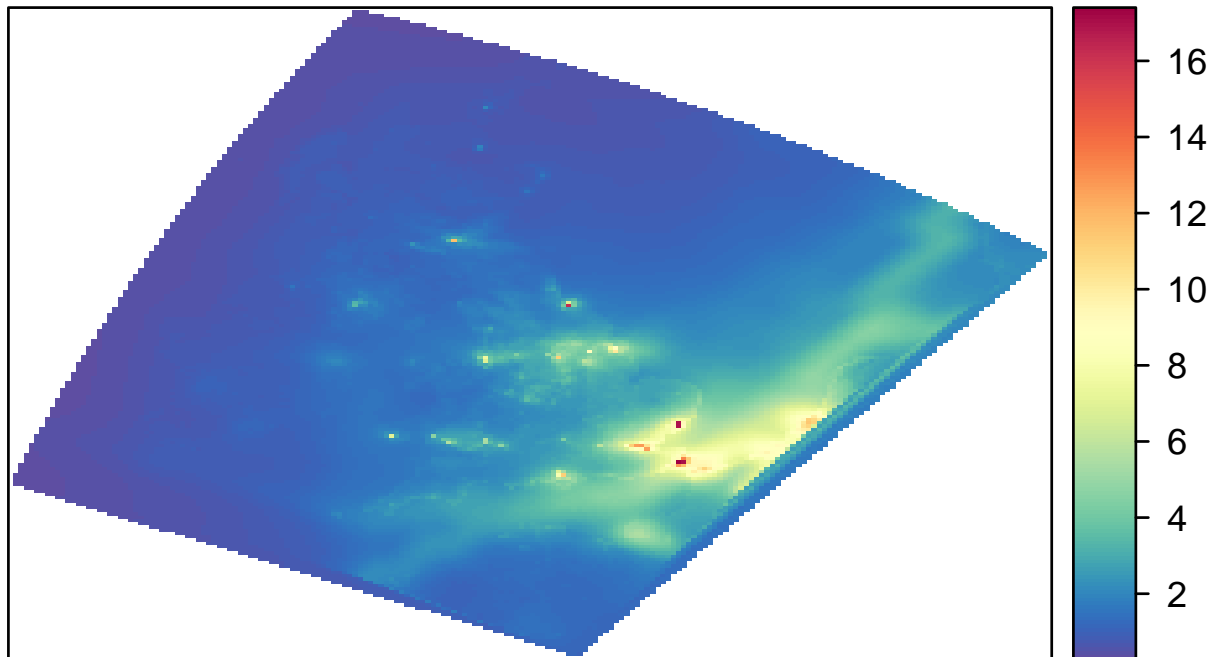
For the EMEP4UK data the results are in individual species files and the grid needs to be interpolated for plotting.

```
EMEPSO2 <- read.csv("depositionTemplateV1.0-EMEP4UK_rv3.7_final_SURFACE_MAP_SO2_ugm3.csv",
  header = TRUE, na.strings = "missing")
EMEPSO2 <- na.omit(EMEPSO2) ## remove missing data
EMEPSO2 <- prepareGrid(EMEPSO2, pollutant = "SO2.ugm3")
makeMap(EMEPSO2, pollu="SO2.ugm3", aspect = "iso")
```

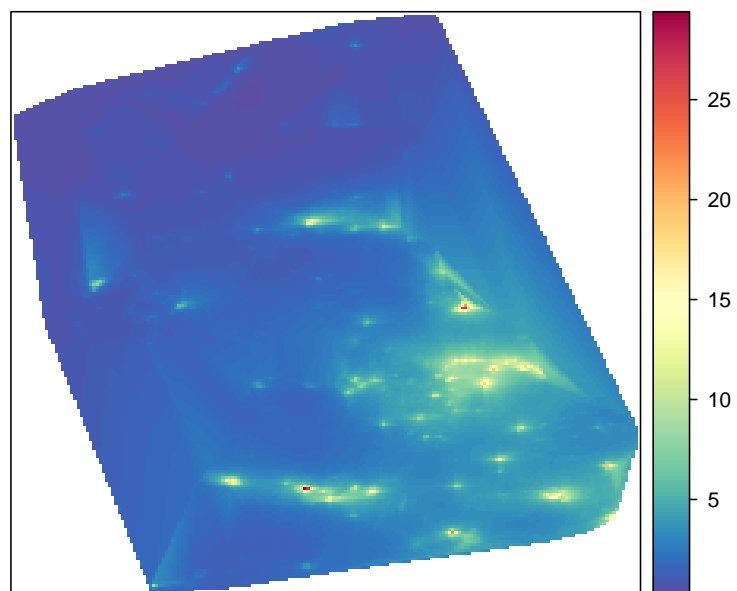
```
mapUHSO2 <- prepareGrid(mapUH, pollutant = "SO2")
makeMap(mapUHSO2, pollutant = "SO2", aspect = "iso")
```

```
mapJEPSO2 <- prepareGrid(mapJEP, pollutant = "so2")
makeMap(mapJEPSO2, pollutant = "so2", aspect = "iso")
```

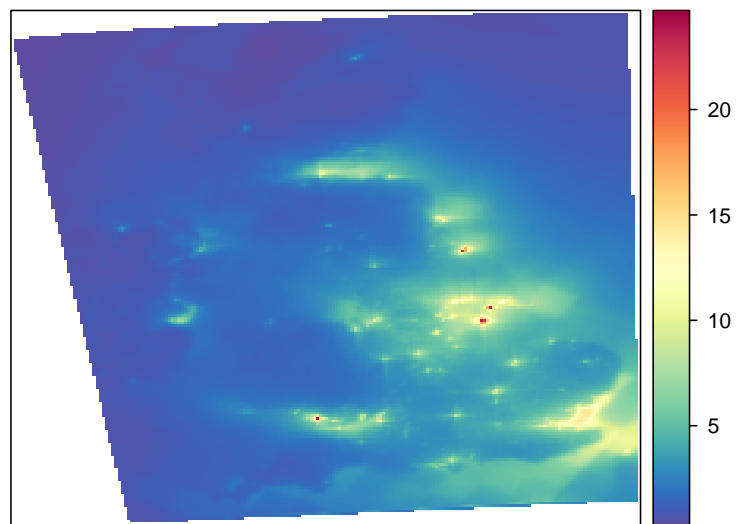




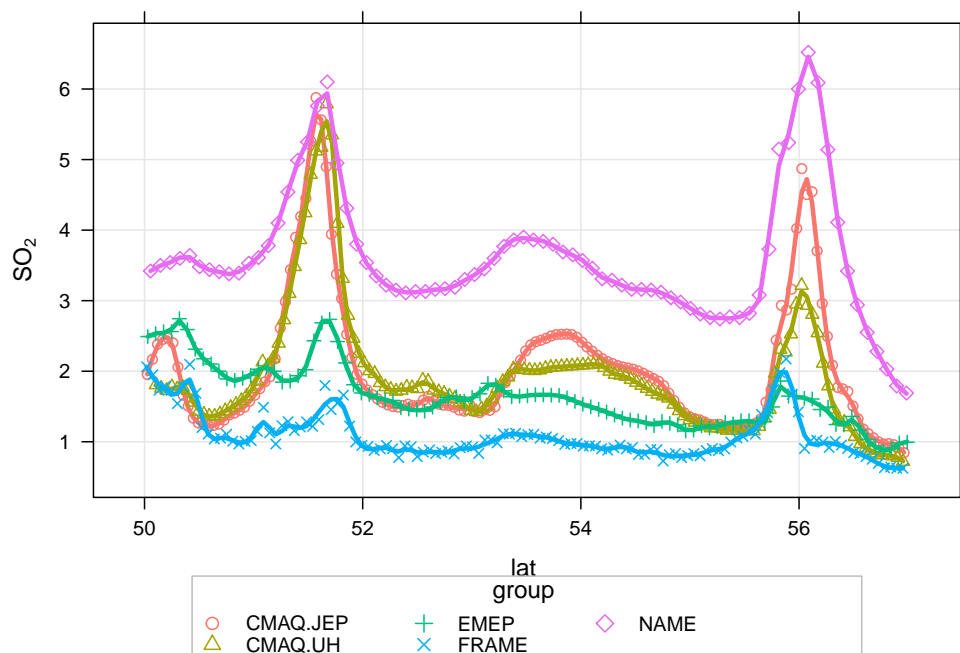
**Figure 4:** Annual mean SO<sub>2</sub> concentrations from the EMEP4UK model.



**Figure 5:** Annual mean SO<sub>2</sub> concentrations from the CMAQ University of Hertfordshire model.



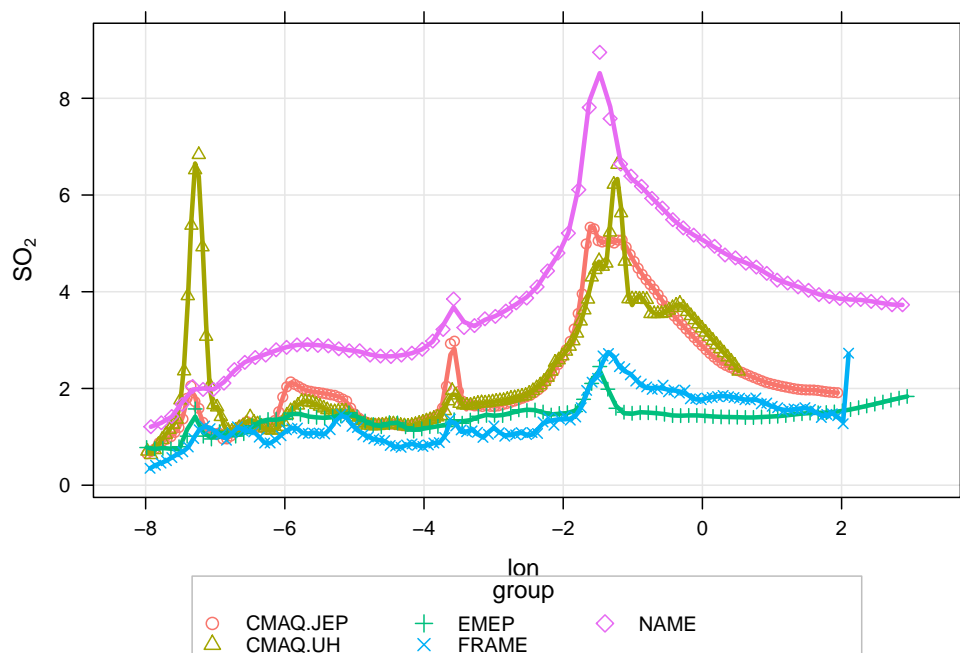
**Figure 6:** Annual mean SO<sub>2</sub> concentrations from the CMAQ JEP model.



**Figure 7:** Transect of SO<sub>2</sub> concentrations along  $-4.05$  longitude.

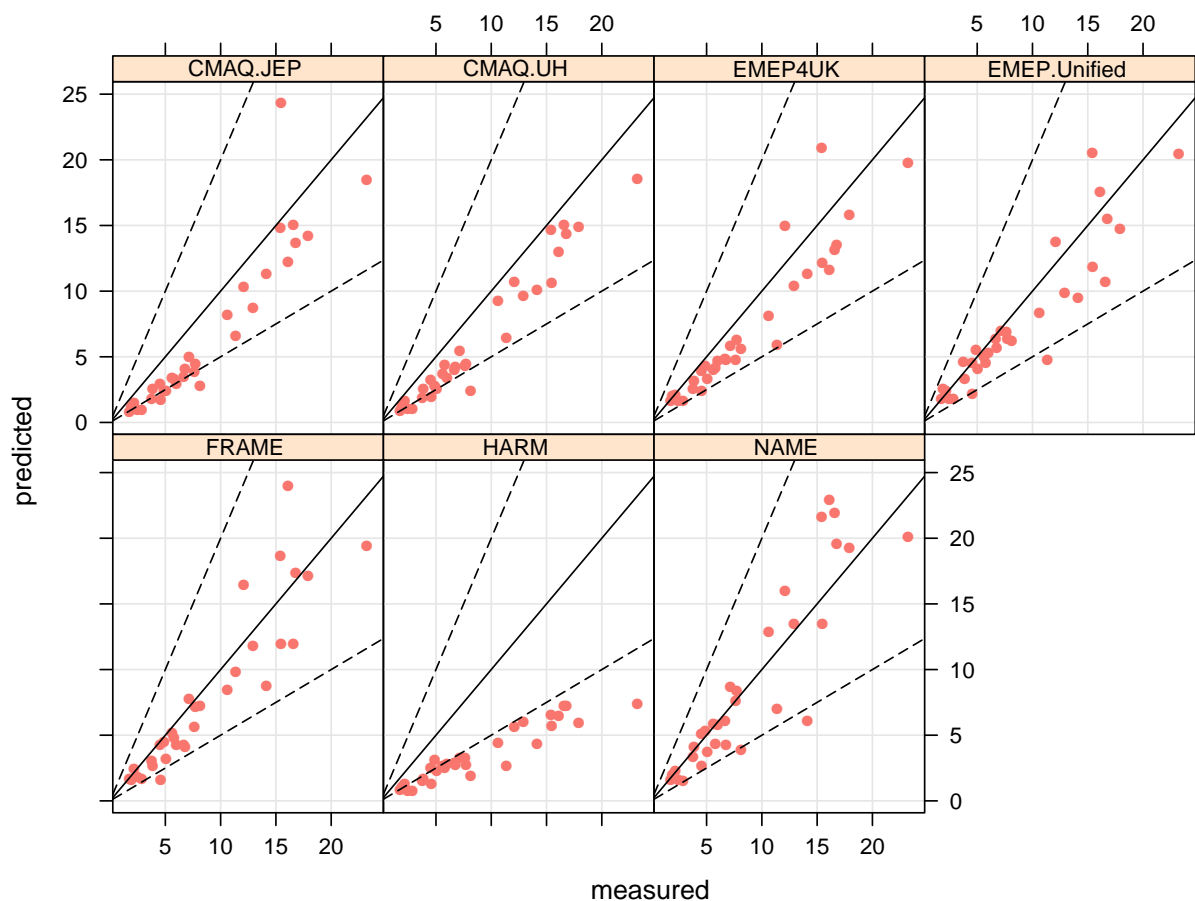
The transects require some work to extract from each of these maps.

```
## NAME
id <- nearest(mapNAME, lon = -4.05)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, so2))
names(transNAME)[3] <- "SO2"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPSO2, lon = -4.05)
transEMEP <- EMEPSO2[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, SO2.ugm3))
names(transEMEP)[3] <- "SO2"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMESO2, lon = -4.05)
transFRAME <- FRAMESO2[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, SO2))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHSO2, lon = -4.05)
transUH <- mapUHSO2[id , ]
transUH <- subset(transUH, select = c(lat, lon, SO2))
names(transUH)[3] <- "SO2"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPSO2, lon = -4.05)
transJEP <- mapJEPSO2[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, so2))
names(transJEP)[3] <- "SO2"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transSO2 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transSO2, lat > 50 & lat < 57), x = "lat", y = "SO2", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 8:** Transect of SO<sub>2</sub> concentrations along 55.065 latitude.

```
## NAME
id <- nearest(mapNAME, lat = 55.065)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, so2))
names(transNAME)[3] <- "SO2"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPSO2, lat = 55.065)
transEMEP <- EMEPSO2[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, SO2.ugm3))
names(transEMEP)[3] <- "SO2"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMESO2, lat = 55.065)
transFRAME <- FRAMESO2[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, SO2))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHSO2, lat = 55.065)
transUH <- mapUHSO2[id , ]
transUH <- subset(transUH, select = c(lat, lon, SO2))
names(transUH)[3] <- "SO2"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPSO2, lat = 55.065)
transJEP <- mapJEPSO2[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, so2))
names(transJEP)[3] <- "SO2"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transSO2 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transSO2, lon > -8 & lon < 3), x = "lon", y = "SO2", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 9:** Measured versus predicted annual mean  $\text{NO}_2$  concentrations ( $\mu\text{g m}^{-3}$ ).

### 3.2 Nitrogen dioxide

First we will extract the  $\text{NO}_2$  data.

```
no2.results <- subset(all.results, species == "NO2")
```

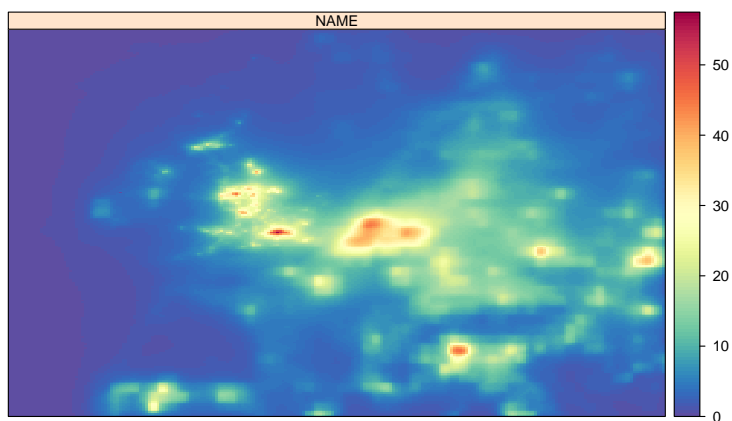
```
NO2stats <- modStats(no2.results, type = "group", mod = "predicted", obs = "measured")
```

**Table 3:** Summary model evaluation statistics for annual mean  $\text{NO}_2$  concentrations.

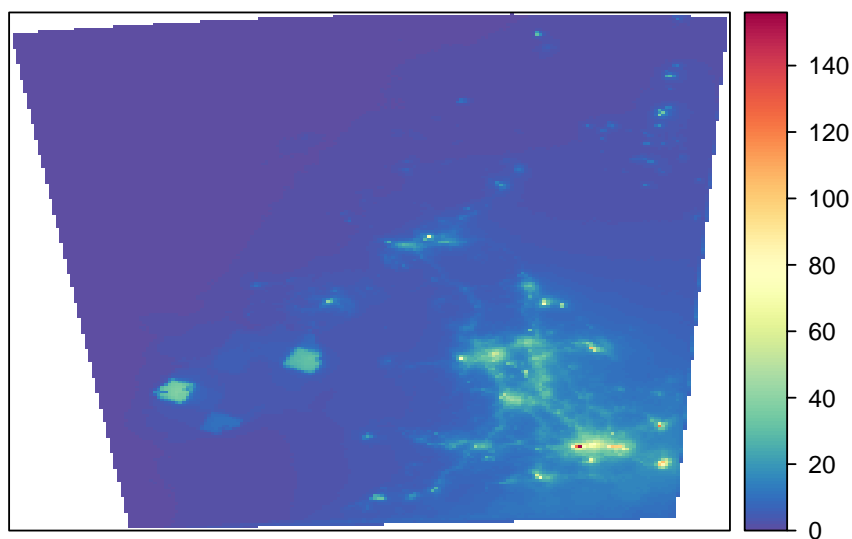
group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
CMAQ.JEP	32.00	0.72	-2.24	2.79	-0.25	0.32	3.23	0.92
CMAQ.UH	32.00	0.84	-2.41	2.41	-0.27	0.27	2.74	0.97
EMEP4UK	32.00	1.00	-1.58	2.11	-0.18	0.24	2.52	0.94
EMEPUnified	32.00	0.94	-1.13	1.80	-0.13	0.20	2.48	0.92
FRAME	32.00	0.97	-0.85	1.91	-0.10	0.22	2.60	0.92
HARM	32.00	0.12	-5.32	5.32	-0.60	0.60	6.47	0.94
NAME	32.00	0.94	0.02	2.05	0.00	0.23	2.95	0.91

```
scatterPlot(no2.results, x = "measured", y = "predicted", type = "group", mod.line = TRUE, smooth = FALSE,
            pch = 16, key = FALSE)
```

```
makeMap(mapNAME, pollutant = "no2", aspect = "iso")
```



**Figure 10:** Annual mean NO<sub>2</sub> concentrations from the NAME model.



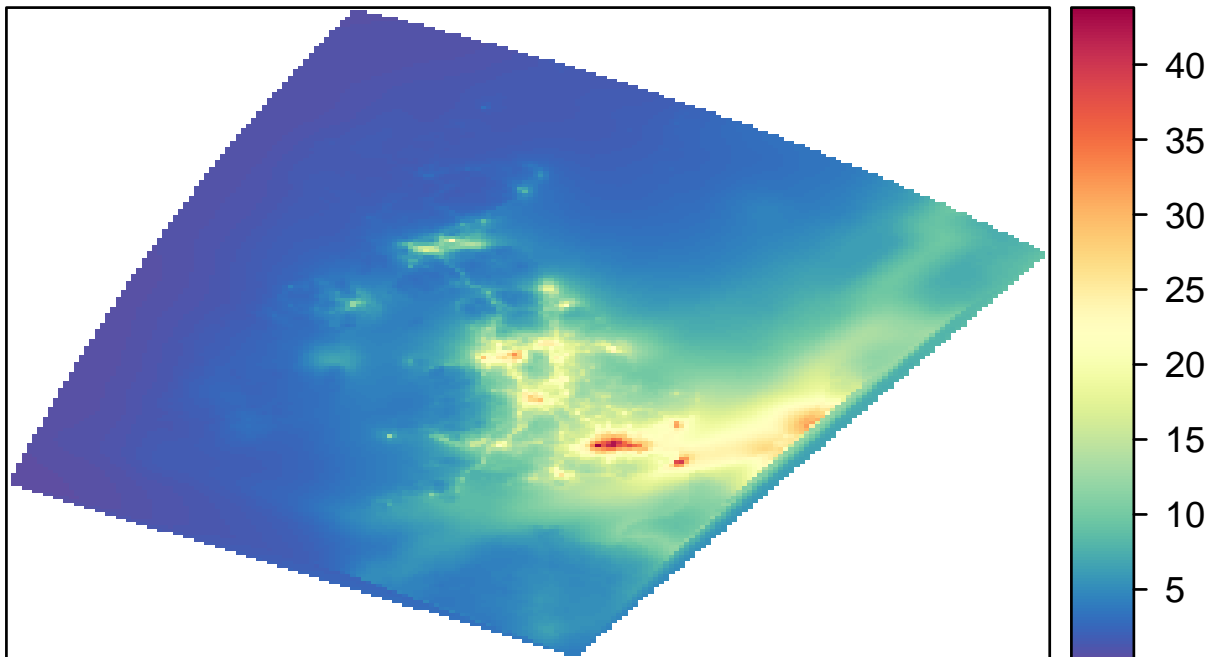
**Figure 11:** Annual mean NO<sub>2</sub> concentrations from the FRAME model.

```
FRAMENO2 <- prepareGrid(mapFRAME, pollutant = "NO2")
makeMap(FRAMENO2, pollutant = "NO2", aspect = "iso")
```

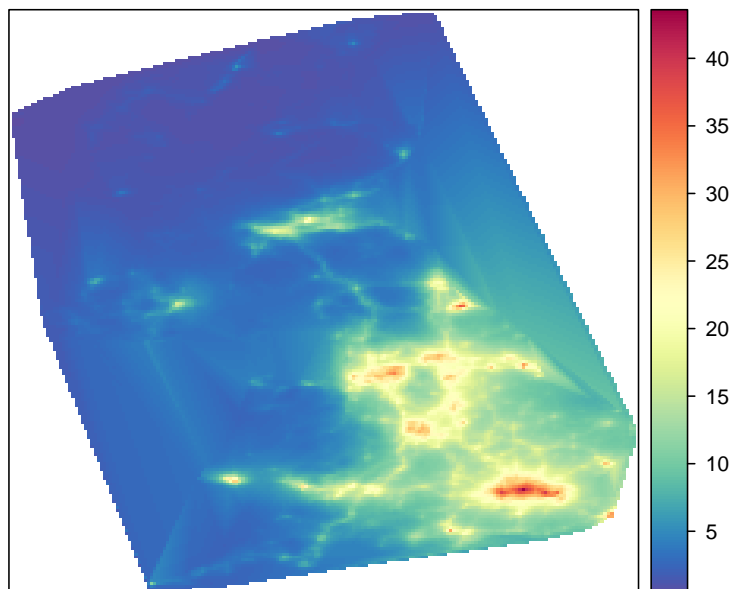
```
EMEPNO2 <- read.csv("depositionTemplateV1.0_EMEP4UK_rv3.7_final_SURFACE_MAP_NO2_ugm3.csv",
  header = TRUE, na.strings = "missing")
EMEPNO2 <- na.omit(EMEPNO2) ## remove missing data
EMEPNO2 <- prepareGrid(EMEPNO2, pollutant = "NO2.ugm3")
makeMap(EMEPNO2, pollu="NO2.ugm3", aspect = "iso")
```

```
mapUHN02 <- prepareGrid(mapUH, pollutant = "NO2")
makeMap(mapUHN02, pollutant = "NO2", aspect = "iso")
```

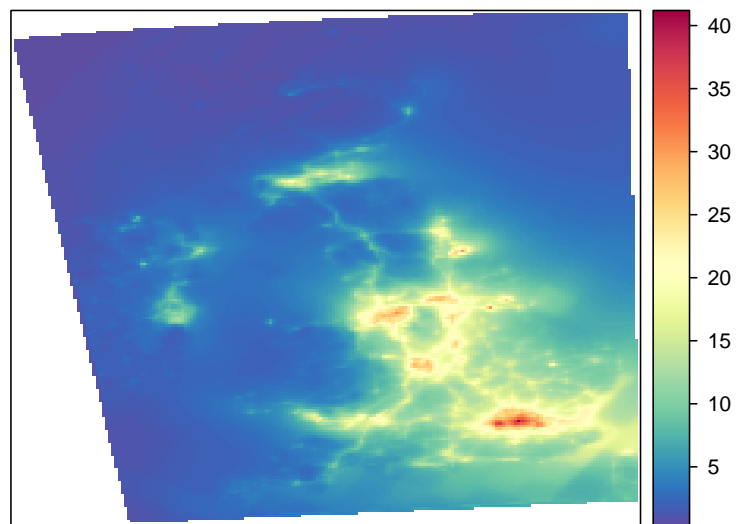
```
mapJEPNO2 <- prepareGrid(mapJEP, pollutant = "no2")
makeMap(mapJEPNO2, pollutant = "no2", aspect = "iso")
```



**Figure 12:** Annual mean NO<sub>2</sub> concentrations from the EMEP4UK model.

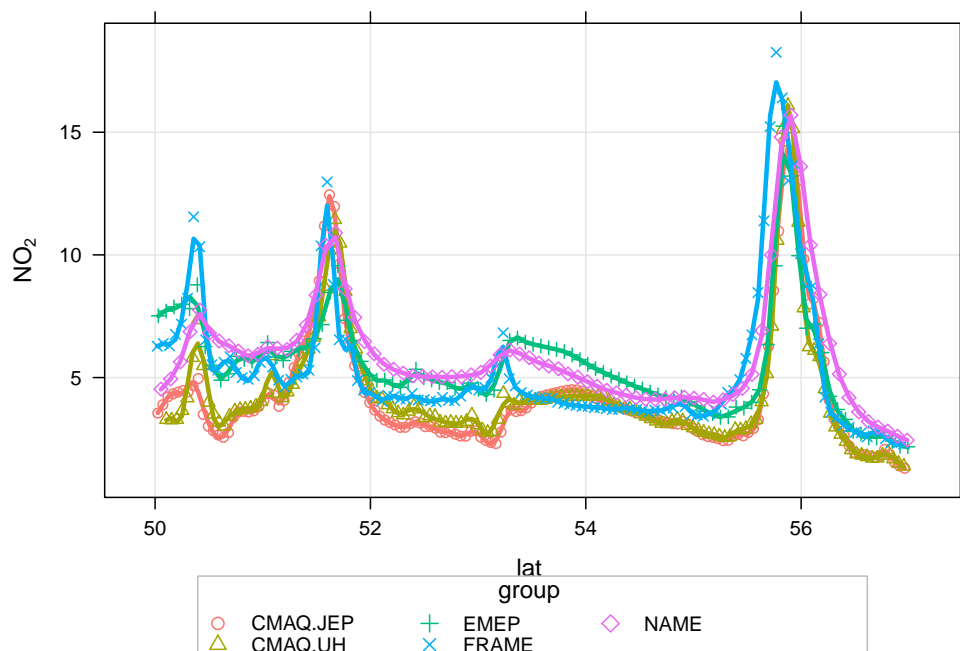


**Figure 13:** Annual mean NO<sub>2</sub> concentrations from the CMAQ University of Hertfordshire model.



**Figure 14:** Annual mean NO<sub>2</sub> concentrations from the CMAQ JEP model.

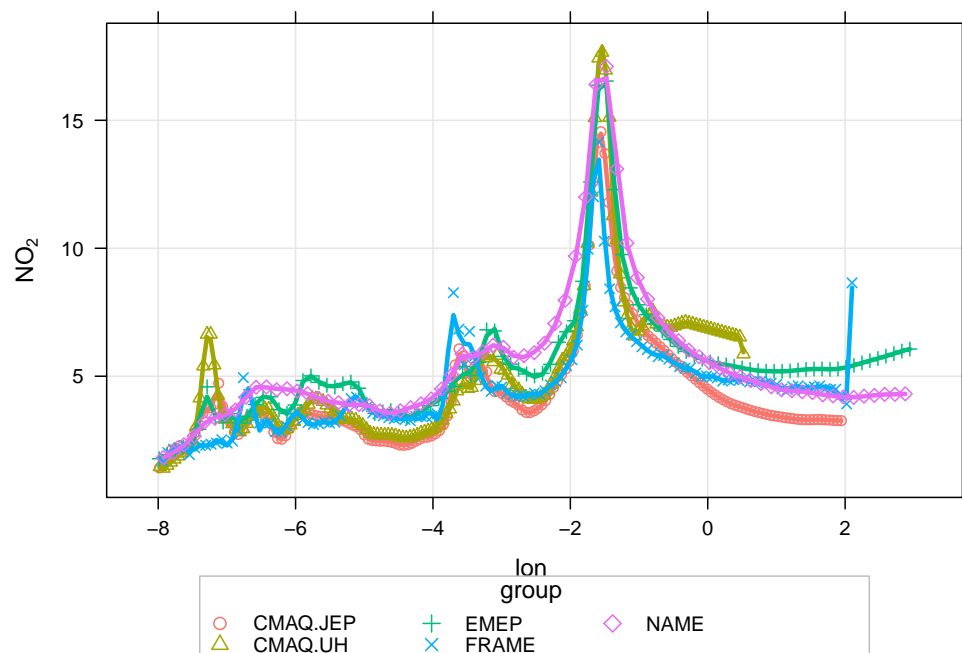




**Figure 15:** Transect of NO<sub>2</sub> concentrations along  $-4.05$  longitude.

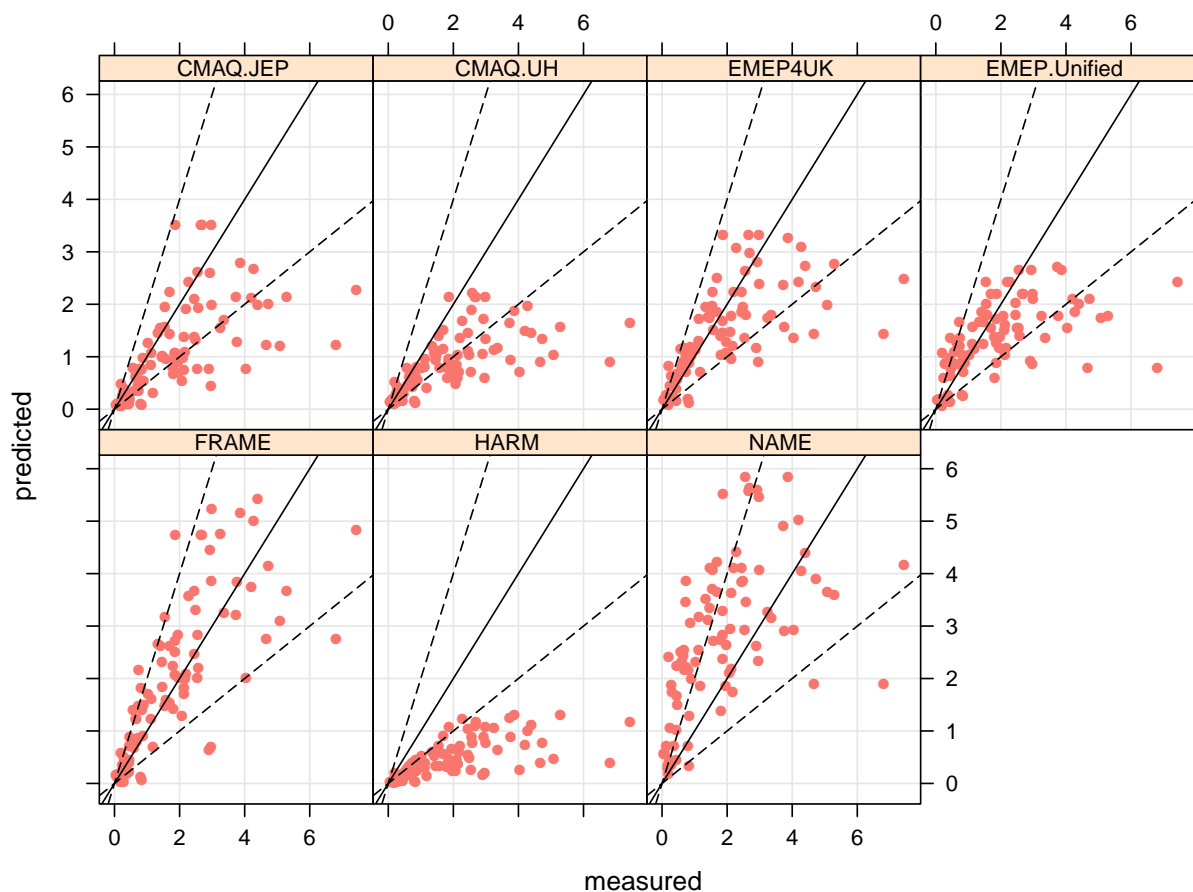
The transects require some work to extract from each of these maps.

```
## NAME
id <- nearest(mapNAME, lon = -4.05)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, no2))
names(transNAME)[3] <- "NO2"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPNO2, lon = -4.05)
transEMEP <- EMEPNO2[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, NO2.ugm3))
names(transEMEP)[3] <- "NO2"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMENO2, lon = -4.05)
transFRAME <- FRAMENO2[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, NO2))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHNO2, lon = -4.05)
transUH <- mapUHNO2[id , ]
transUH <- subset(transUH, select = c(lat, lon, NO2))
names(transUH)[3] <- "NO2"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPNO2, lon = -4.05)
transJEP <- mapJEPNO2[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, no2))
names(transJEP)[3] <- "NO2"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transNO2 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transNO2, lat > 50 & lat < 57), x = "lat", y = "NO2", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 16:** Transect of NO<sub>2</sub> concentrations along 55.065 latitude.

```
## NAME
id <- nearest(mapNAME, lat = 55.065)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, no2))
names(transNAME)[3] <- "NO2"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPNO2, lat = 55.065)
transEMEP <- EMEPNO2[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, NO2.ugm3))
names(transEMEP)[3] <- "NO2"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMENO2, lat = 55.065)
transFRAME <- FRAMENO2[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, NO2))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHN02, lat = 55.065)
transUH <- mapUHN02[id , ]
transUH <- subset(transUH, select = c(lat, lon, NO2))
names(transUH)[3] <- "NO2"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPNO2, lat = 55.065)
transJEP <- mapJEPNO2[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, no2))
names(transJEP)[3] <- "NO2"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transNO2 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transNO2, lon > -8 & lon < 3), x = "lon", y = "NO2", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 17:** Measured versus predicted annual mean ammonia concentrations ( $\mu\text{g m}^{-3}$ ).

### 3.3 Ammonia

First we will extract the ammonia data.

```
nh3.results <- subset(all.results, species == "NH3")
```

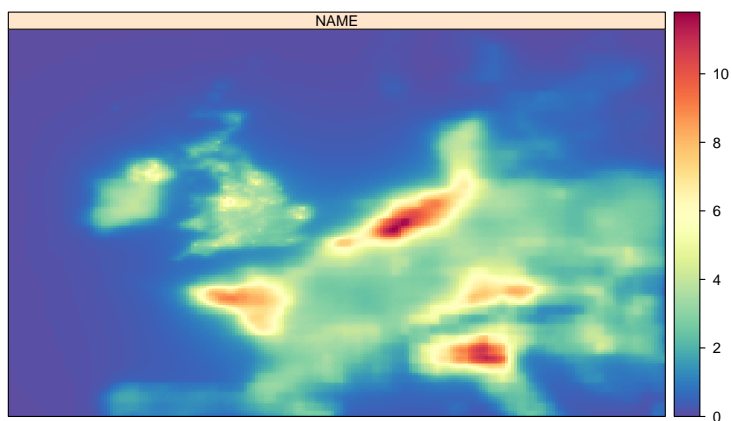
```
NH3stats <- modStats(nh3.results, type = "group", mod = "predicted", obs = "measured")
```

**Table 4:** Summary model evaluation statistics for annual mean ammonia concentrations.

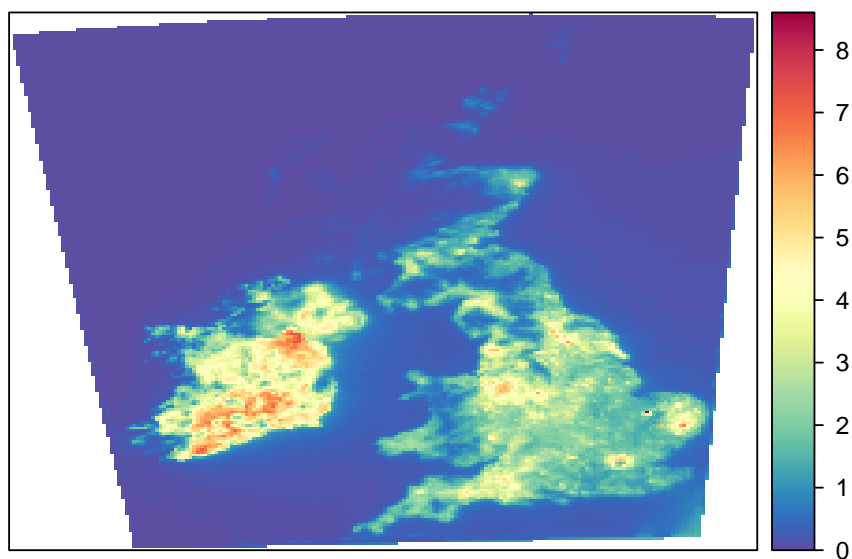
group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
CMAQ.JEP	87.00	0.62	-0.77	0.92	-0.40	0.48	1.45	0.61
CMAQ.UH	87.00	0.55	-1.02	1.05	-0.53	0.55	1.62	0.63
EMEP4UK	88.00	0.75	-0.47	0.78	-0.24	0.41	1.25	0.66
EMEPUnified	88.00	0.66	-0.57	0.87	-0.30	0.46	1.39	0.57
FRAME	88.00	0.78	0.14	0.75	0.07	0.39	1.08	0.75
HARM	88.00	0.10	-1.43	1.43	-0.75	0.75	1.95	0.66
NAME	88.00	0.53	0.89	1.34	0.47	0.70	1.67	0.56

```
scatterPlot(nh3.results, x = "measured", y = "predicted", type = "group", mod.line = TRUE,
            smooth = FALSE, pch = 16, key = FALSE)
```

```
makeMap(mapNAME, pollutant = "nh3", aspect = "iso")
```



**Figure 18:** Annual mean ammonia concentrations from the NAME model.



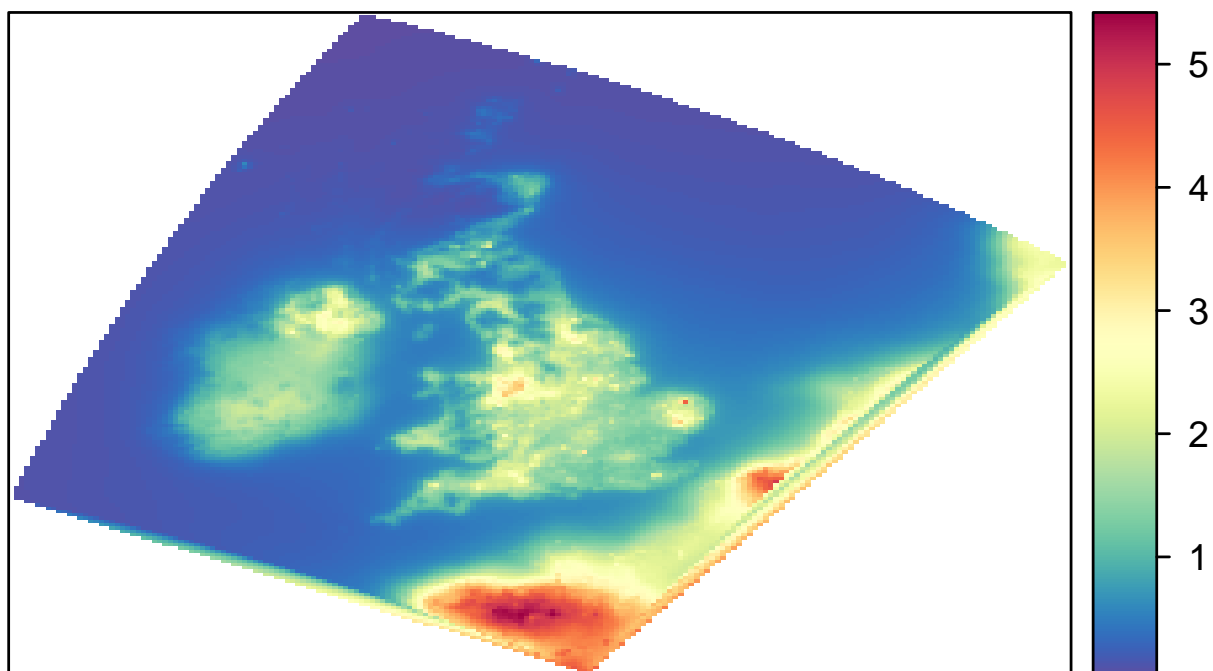
**Figure 19:** Annual mean ammonia concentrations from the FRAME model.

```
FRAMENH3 <- prepareGrid(mapFRAME, pollutant = "NH3")
makeMap(FRAMENH3, pollutant = "NH3", aspect = "iso")
```

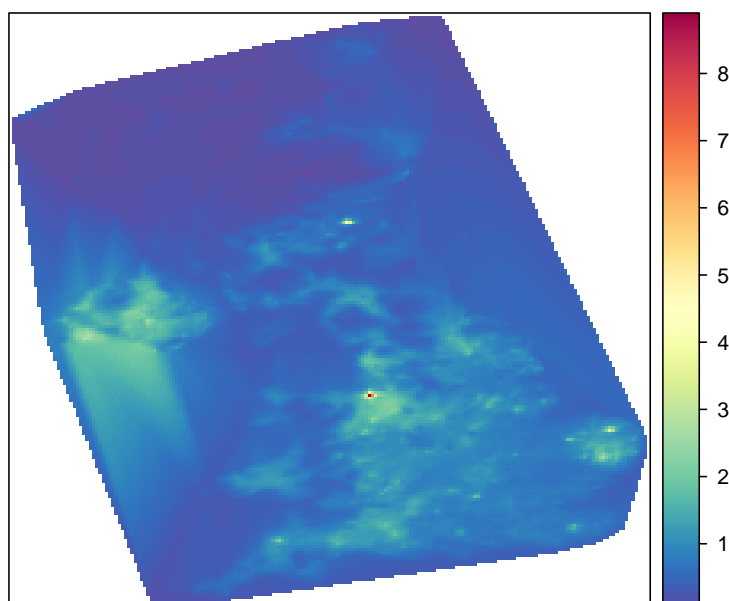
```
EMEPNH3 <- read.csv("depositionTemplateV1.0_EMEP4UK_rv3.7_final_SURFACE_MAP_NH3_ugm3.csv",
  header = TRUE, na.strings = "missing")
EMEPNH3 <- na.omit(EMEPNH3) ## remove missing data
EMEPNH3 <- prepareGrid(EMEPNH3, pollutant = "NH3.ugm3")
makeMap(EMEPNH3, pollu="NH3.ugm3", aspect = "iso")
```

```
mapUHNH3 <- prepareGrid(mapUH, pollutant = "NH3")
makeMap(mapUHNH3, pollutant = "NH3", aspect = "iso")
```

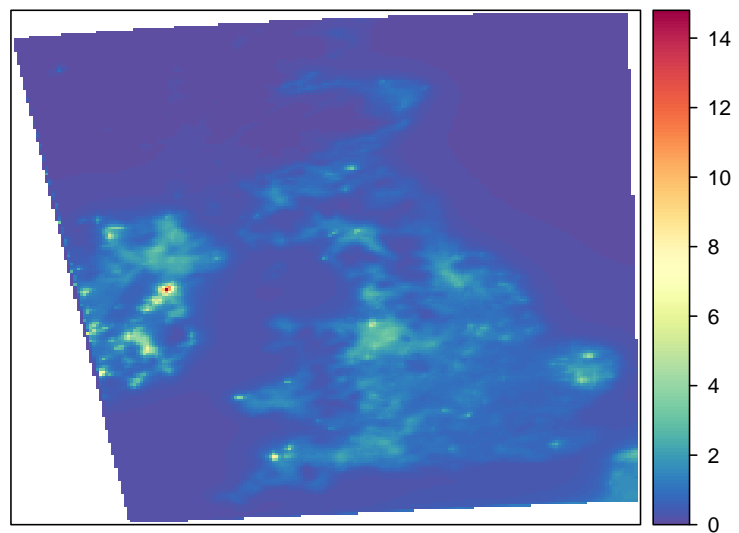
```
mapJEPNH3 <- prepareGrid(mapJEP, pollutant = "nh3")
makeMap(mapJEPNH3, pollutant = "nh3", aspect = "iso")
```



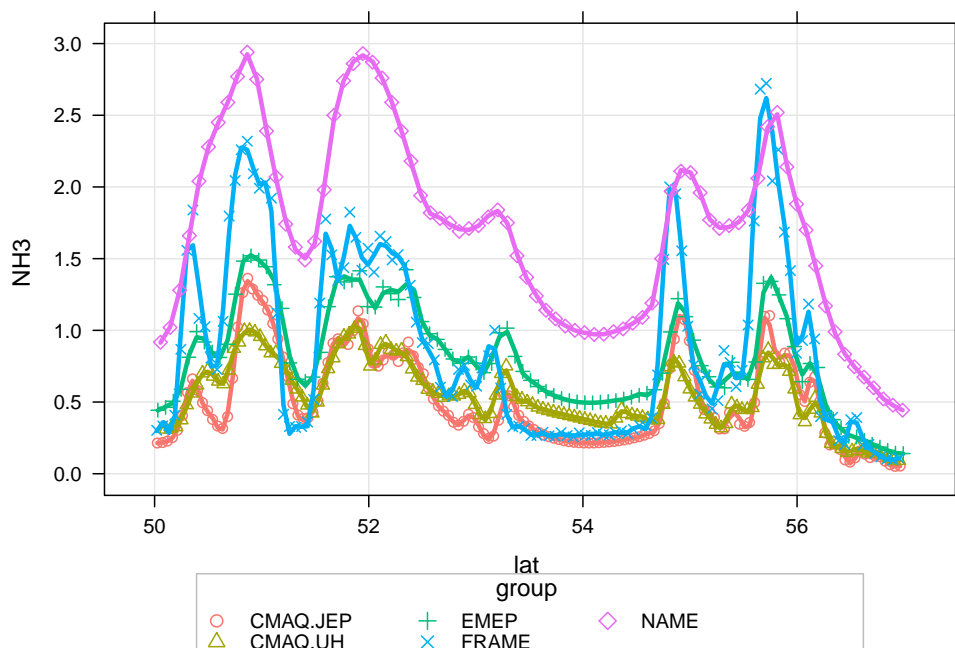
**Figure 20:** Annual mean ammonia concentrations from the EMEP4UK model.



**Figure 21:** Annual mean ammonia concentrations from the CMAQ University of Hertfordshire model.



**Figure 22:** Annual mean ammonia concentrations from the CMAQ JEP model.



**Figure 23:** Transect of ammonia concentrations along  $-4.05$  longitude.

The transects require some work to extract from each of these maps.

```
## NAME
id <- nearest(mapNAME, lon = -4.05)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, nh3))
names(transNAME)[3] <- "NH3"
transNAME$group <- "NAME"

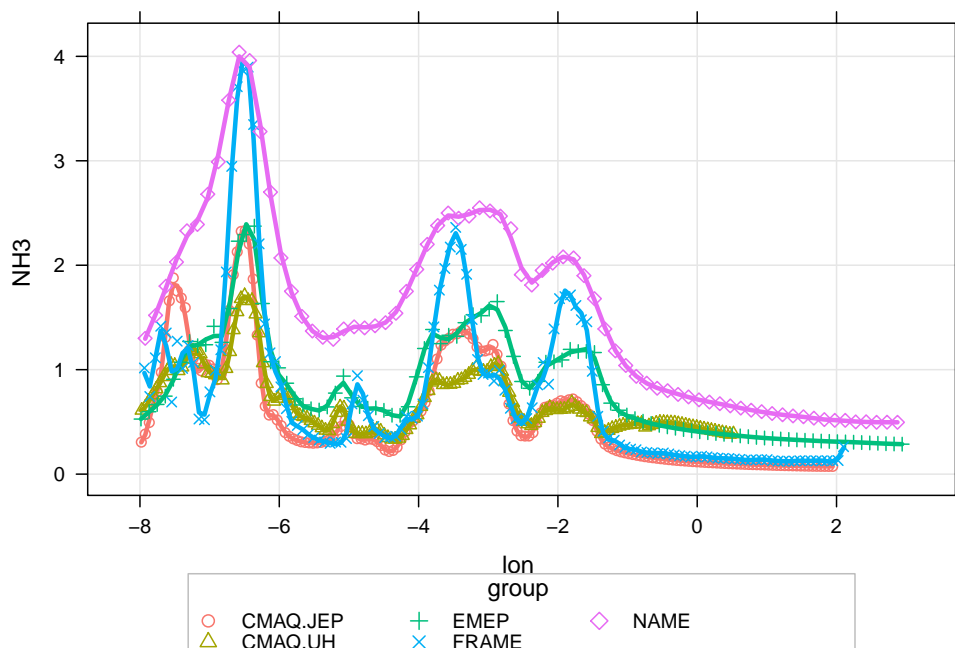
## EMEP
id <- nearest(EMEPNH3, lon = -4.05)
transEMEP <- EMEPNH3[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, NH3.ugm3))
names(transEMEP)[3] <- "NH3"
transEMEP$group <- "EMEP"

## FRAME
id <- nearest(FRAMENH3, lon = -4.05)
transFRAME <- FRAMENH3[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, NH3))
transFRAME$group <- "FRAME"

## CMAQ UH
id <- nearest(mapUHNH3, lon = -4.05)
transUH <- mapUHNH3[id , ]
transUH <- subset(transUH, select = c(lat, lon, NH3))
names(transUH)[3] <- "NH3"
transUH$group <- "CMAQ.UH"

## CMAQ JEP
id <- nearest(mapJEPNH3, lon = -4.05)
transJEP <- mapJEPNH3[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, nh3))
names(transJEP)[3] <- "NH3"
transJEP$group <- "CMAQ.JEP"

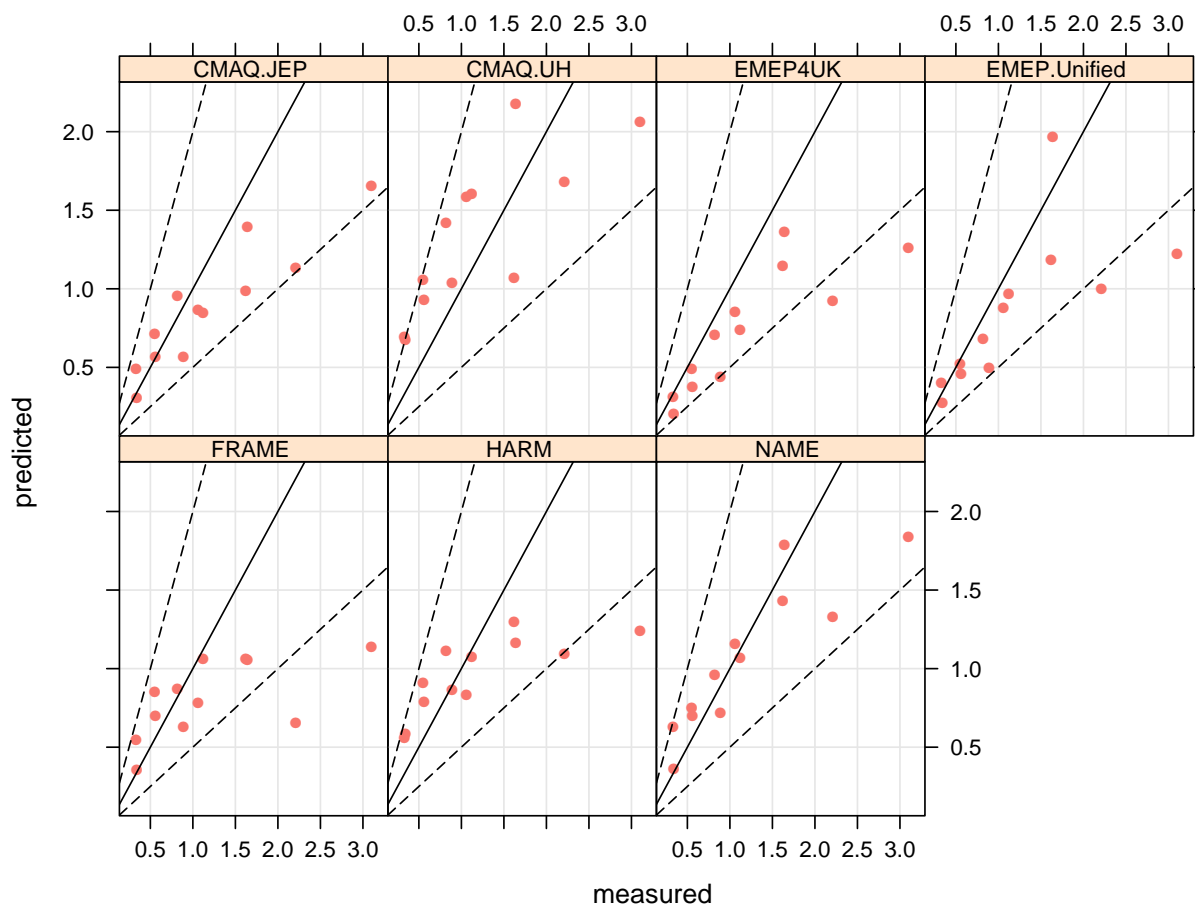
## now combine all the results
transNH3 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transNH3, lat > 50 & lat < 57), x = "lat", y = "NH3", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 24:** Transect of ammonia concentrations along 55.065 latitude.

```
## NAME
id <- nearest(mapNAME, lat = 55.065)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, nh3))
names(transNAME)[3] <- "NH3"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPNH3, lat = 55.065)
transEMEP <- EMEPNH3[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, NH3.ugm3))
names(transEMEP)[3] <- "NH3"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMENH3, lat = 55.065)
transFRAME <- FRAMENH3[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, NH3))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHNH3, lat = 55.065)
transUH <- mapUHNH3[id , ]
transUH <- subset(transUH, select = c(lat, lon, NH3))
names(transUH)[3] <- "NH3"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPNH3, lat = 55.065)
transJEP <- mapJEPNH3[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, nh3))
names(transJEP)[3] <- "NH3"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transNH3 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transNH3, lon > -8 & lon < 3), x = "lon", y = "NH3", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```





**Figure 25:** Measured versus predicted annual mean  $\text{HNO}_3$  concentrations ( $\mu\text{g m}^{-3}$ ).

### 3.4 Nitric acid

First we will extract the ammonia data.

```
hno3.results <- subset(all.results, species == "HNO3")
```

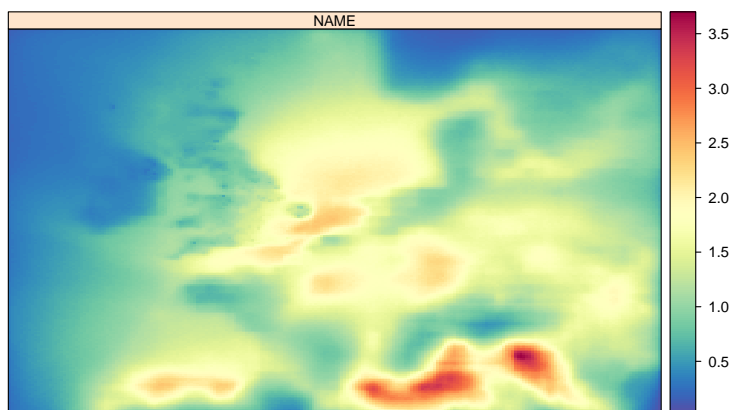
```
HNO3stats <- modStats(hno3.results, type = "group", mod = "predicted", obs = "measured")
```

**Table 5:** Summary model evaluation statistics for annual mean  $\text{HNO}_3$  concentrations.

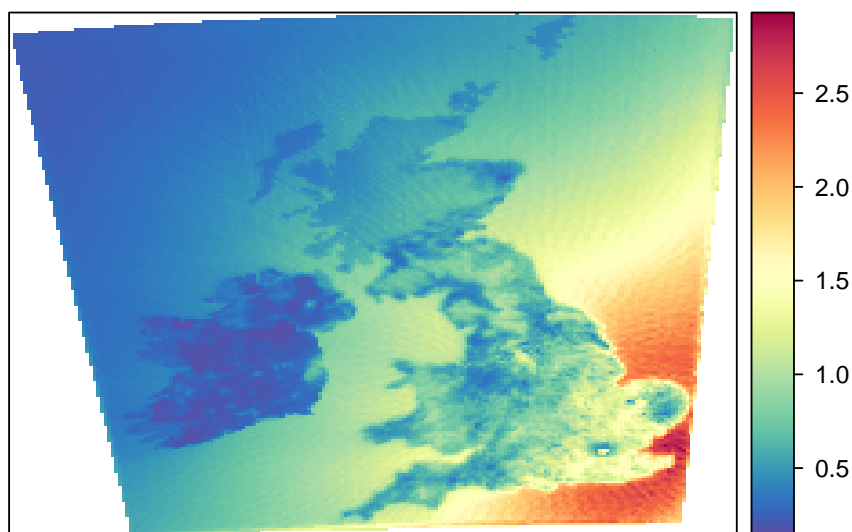
group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
CMAQ.JEP	12.00	1.00	-0.31	0.39	-0.26	0.33	0.58	0.91
CMAQ.UH	12.00	0.92	0.15	0.50	0.12	0.42	0.54	0.78
EMEP4UK	12.00	0.75	-0.45	0.45	-0.38	0.38	0.70	0.84
EMEPUnified	12.00	0.83	-0.35	0.42	-0.29	0.35	0.68	0.69
FRAME	12.00	0.83	-0.38	0.50	-0.32	0.42	0.78	0.61
HARM	12.00	0.83	-0.23	0.45	-0.19	0.38	0.68	0.76
NAME	12.00	1.00	-0.13	0.30	-0.11	0.25	0.47	0.89

```
scatterPlot(hno3.results, x = "measured", y = "predicted", type = "group", mod.line = TRUE,
            smooth = FALSE, pch = 16, key = FALSE)
```

```
makeMap(mapNAME, pollutant = "hno3", aspect = "iso")
```



**Figure 26:** Annual mean nitric acid concentrations from the NAME model.



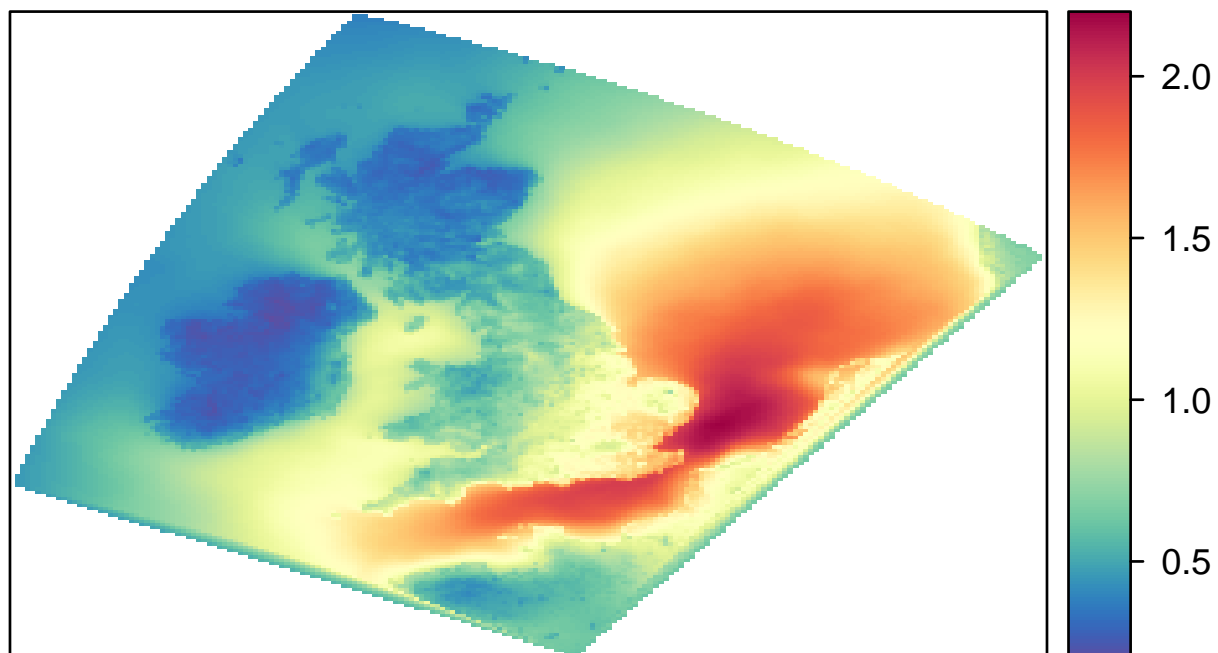
**Figure 27:** Annual mean nitric acid concentrations from the FRAME model.

```
FRAMEHNO3 <- prepareGrid(mapFRAME, pollutant = "HNO3")
makeMap(FRAMEHNO3, pollutant = "HNO3", aspect = "iso")
```

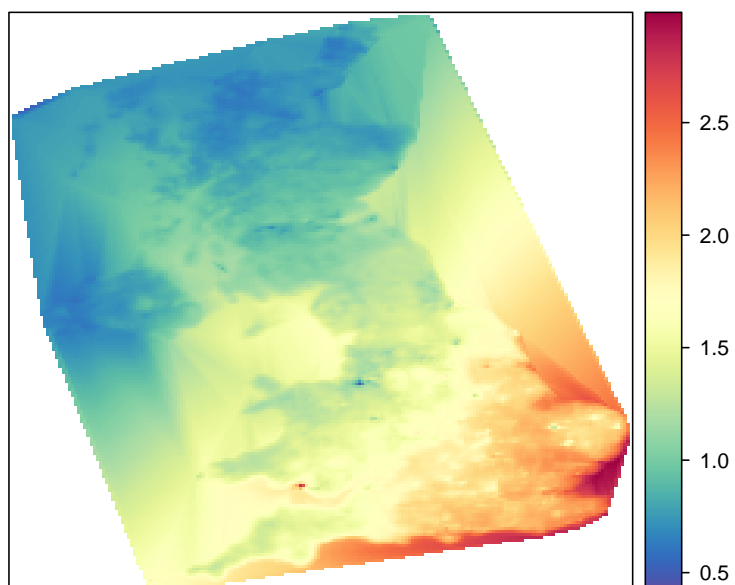
```
EMEPHNO3 <- read.csv("depositionTemplateV1.0_EMEP4UK_rv3.7_final_SURFACE_MAP_HNO3_ugm3.csv",
  header = TRUE, na.strings = "missing")
EMEPHNO3 <- na.omit(EMEPHNO3) ## remove missing data
EMEPHNO3 <- prepareGrid(EMEPHNO3, pollutant = "HNO3.ugm3")
makeMap(EMEPHNO3, pollu="HNO3.ugm3", aspect = "iso")
```

```
mapUHHNO3 <- prepareGrid(mapUH, pollutant = "HNO3")
makeMap(mapUHHNO3, pollutant = "HNO3", aspect = "iso")
```

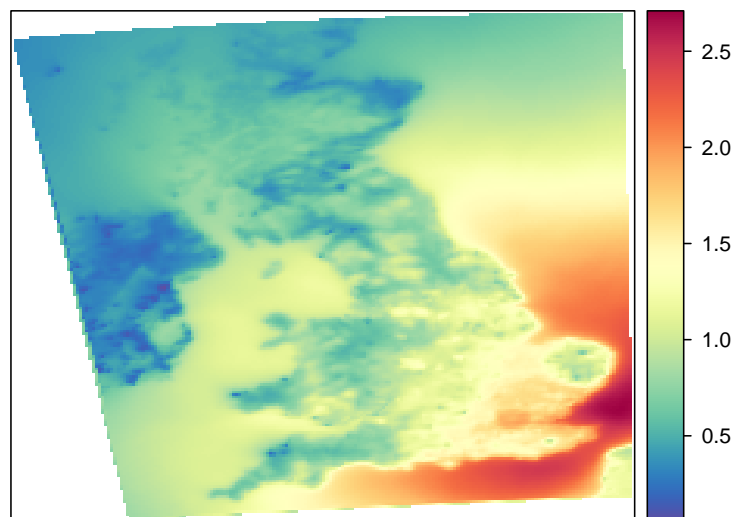
```
mapJEPHNO3 <- prepareGrid(mapJEP, pollutant = "hno3")
makeMap(mapJEPHNO3, pollutant = "hno3", aspect = "iso")
```



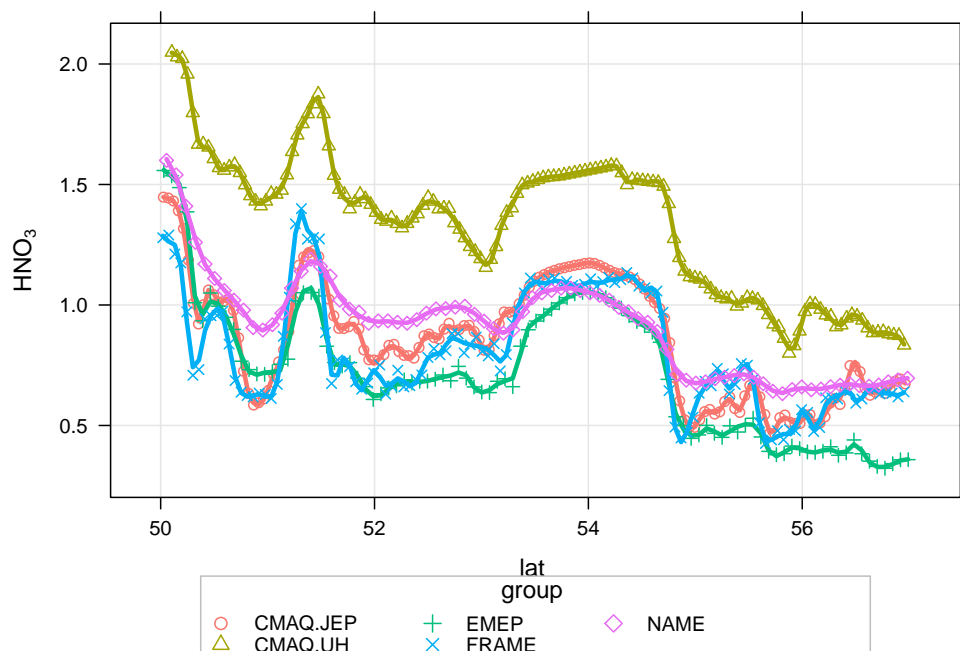
**Figure 28:** Annual mean nitric acid concentrations from the EMEP4UK model.



**Figure 29:** Annual mean nitric acid concentrations from the CMAQ University of Hertfordshire model.



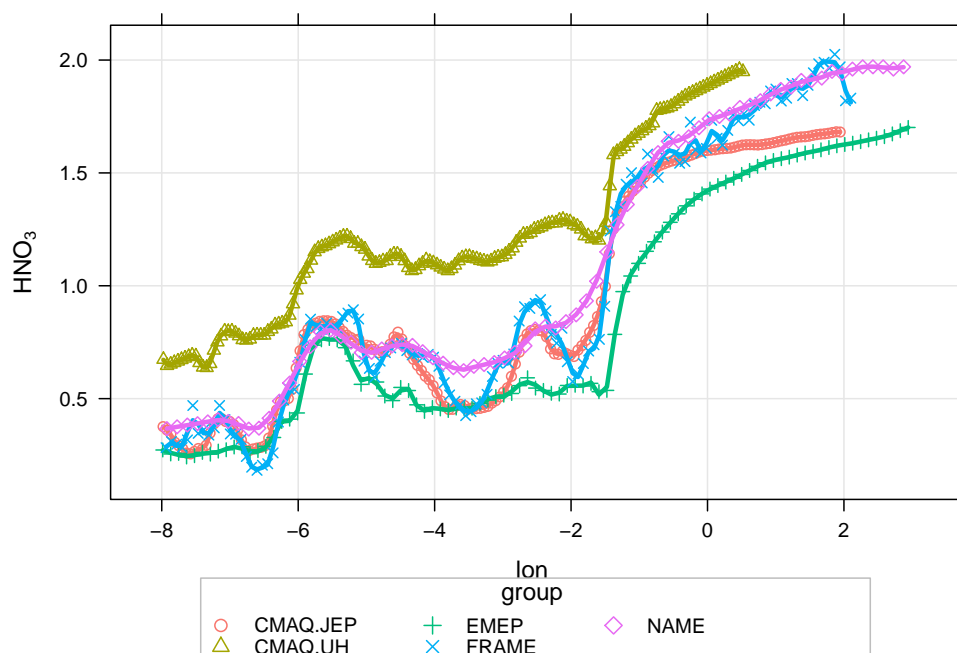
**Figure 30:** Annual mean nitric acid concentrations from the CMAQ JEP model.



**Figure 31:** Transect of nitric acid concentrations along  $-4.05$  longitude.

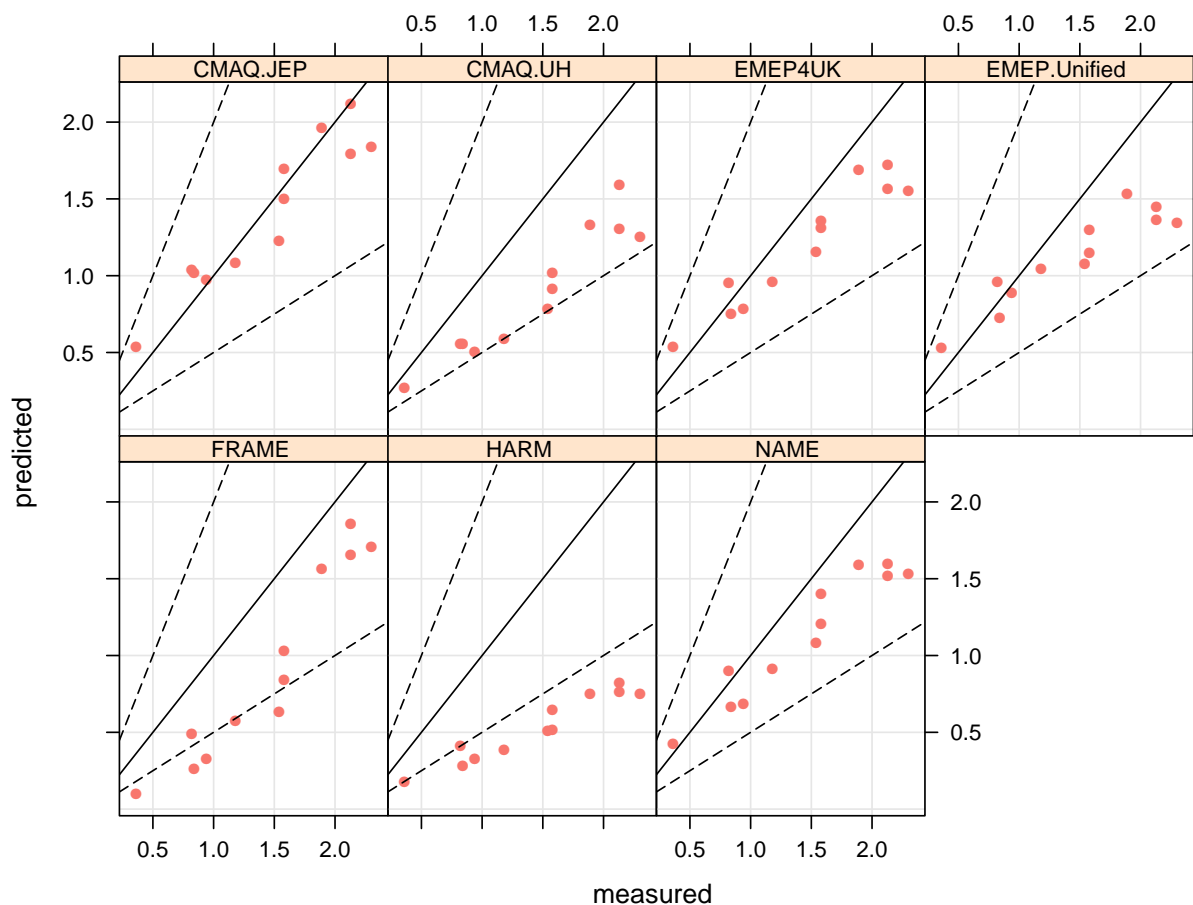
The transects require some work to extract from each of these maps.

```
## NAME
id <- nearest(mapNAME, lon = -4.05)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, hno3))
names(transNAME)[3] <- "HNO3"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPHNO3, lon = -4.05)
transEMEP <- EMEPHNO3[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, HNO3.ugm3))
names(transEMEP)[3] <- "HNO3"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMEHNO3, lon = -4.05)
transFRAME <- FRAMEHNO3[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, HNO3))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHHNO3, lon = -4.05)
transUH <- mapUHHNO3[id , ]
transUH <- subset(transUH, select = c(lat, lon, HNO3))
names(transUH)[3] <- "HNO3"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPHNO3, lon = -4.05)
transJEP <- mapJEPHNO3[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, hno3))
names(transJEP)[3] <- "HNO3"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transHNO3 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transHNO3, lat > 50 & lat < 57), x = "lat", y = "HNO3", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 32:** Transect of nitric acid concentrations along 55.065 latitude.

```
## NAME
id <- nearest(mapNAME, lat = 55.065)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, hno3))
names(transNAME)[3] <- "HNO3"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPHNO3, lat = 55.065)
transEMEP <- EMEPHNO3[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, HNO3.ugm3))
names(transEMEP)[3] <- "HNO3"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMEHNO3, lat = 55.065)
transFRAME <- FRAMEHNO3[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, HNO3))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHHNO3, lat = 55.065)
transUH <- mapUHHNO3[id , ]
transUH <- subset(transUH, select = c(lat, lon, HNO3))
names(transUH)[3] <- "HNO3"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPHNO3, lat = 55.065)
transJEP <- mapJEPHNO3[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, hno3))
names(transJEP)[3] <- "HNO3"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transHNO3 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transHNO3, lon > -8 & lon < 3), x = "lon", y = "HNO3", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 33:** Measured versus predicted annual mean  $\text{NH}_4^+$  concentrations.

### 3.5 Ammonium

First we will extract the ammonia data.

```
nh4.results <- subset(all.results, species == "NH4+")
```

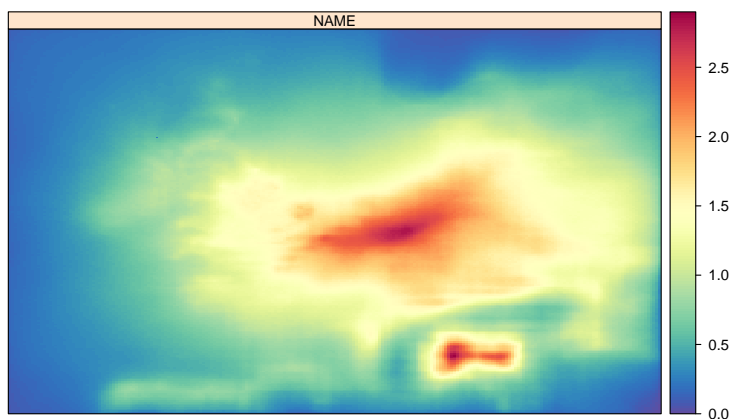
```
NH4stats <- modStats(nh4.results, type = "group", mod = "predicted", obs = "measured")
```

**Table 6:** Summary model evaluation statistics for annual mean  $\text{NH}_4^+$  concentrations.

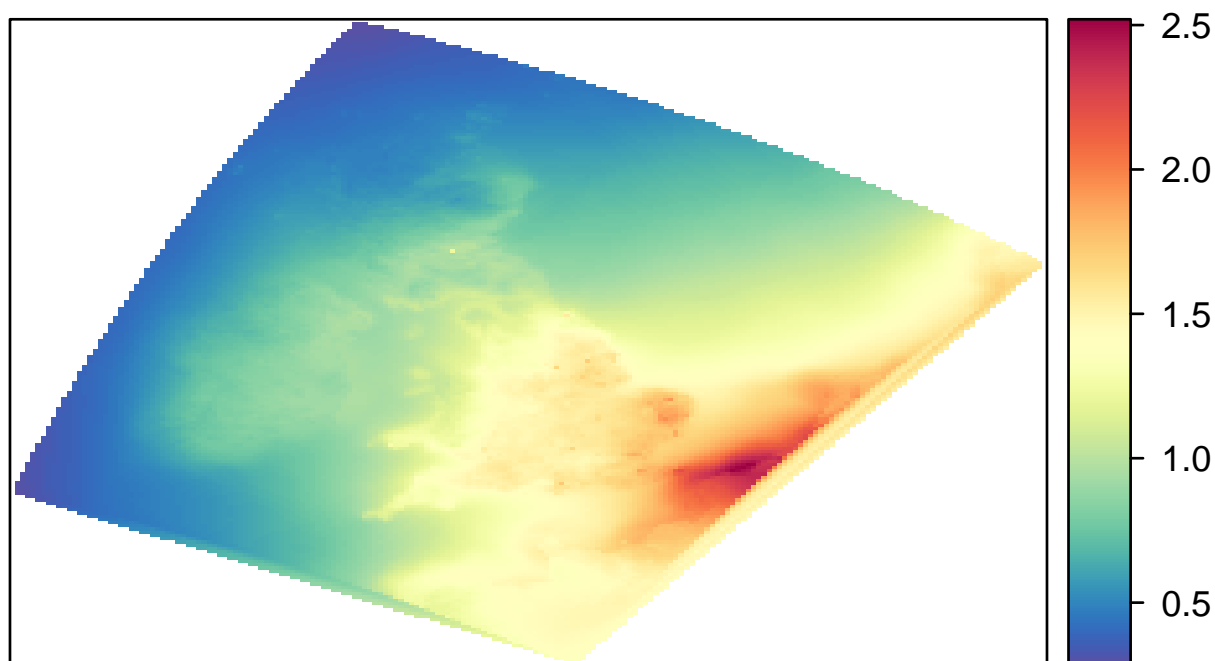
group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
CMAQ.JEP	12.00	1.00	-0.04	0.17	-0.03	0.12	0.22	0.94
CMAQ.UH	12.00	0.92	-0.55	0.55	-0.38	0.38	0.61	0.95
EMEP4UK	12.00	1.00	-0.25	0.30	-0.17	0.21	0.35	0.96
EMEPUnified	12.00	1.00	-0.33	0.38	-0.23	0.26	0.47	0.93
FRAME	12.00	0.58	-0.52	0.52	-0.36	0.36	0.55	0.95
HARM	12.00	0.08	-0.91	0.91	-0.63	0.63	0.99	0.96
NAME	12.00	1.00	-0.31	0.34	-0.22	0.24	0.40	0.96

```
scatterPlot(nh4.results, x = "measured", y = "predicted", type = "group", mod.line = TRUE,
            smooth = FALSE, pch = 16, key = FALSE)
```

```
makeMap(mapNAME, pollutant = "nh4", aspect = "iso")
```



**Figure 34:** Annual mean ammonium concentrations from the NAME model.



**Figure 35:** Annual mean ammonium concentrations from the EMEP4UK model.

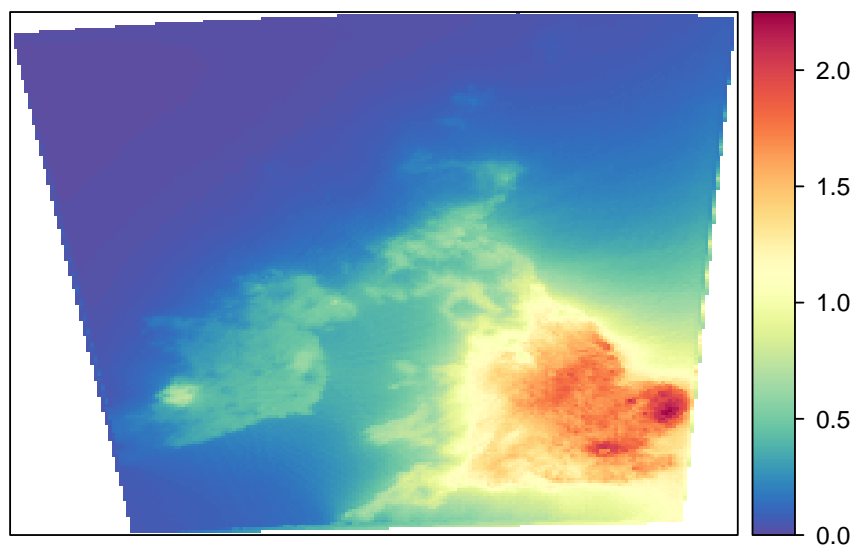
```
EMEPNH4plus <- read.csv("depositionTemplateV1.0_EMEP4UK_rv3.7_final_SURFACE_MAP_NH4+_ugm3.csv",
  header = TRUE, na.strings = "missing")
EMEPNH4plus <- na.omit(EMEPNH4plus) ## remove missing data
EMEPNH4plus <- prepareGrid(EMEPNH4plus, pollutant = "NH4..ugm3")
makeMap(EMEPNH4plus, pollu="NH4..ugm3", aspect = "iso")
```

```
FRAMENH4 <- prepareGrid(mapFRAME, pollutant = "NH4")
makeMap(FRAMENH4, pollutant = "NH4", aspect = "iso")
```

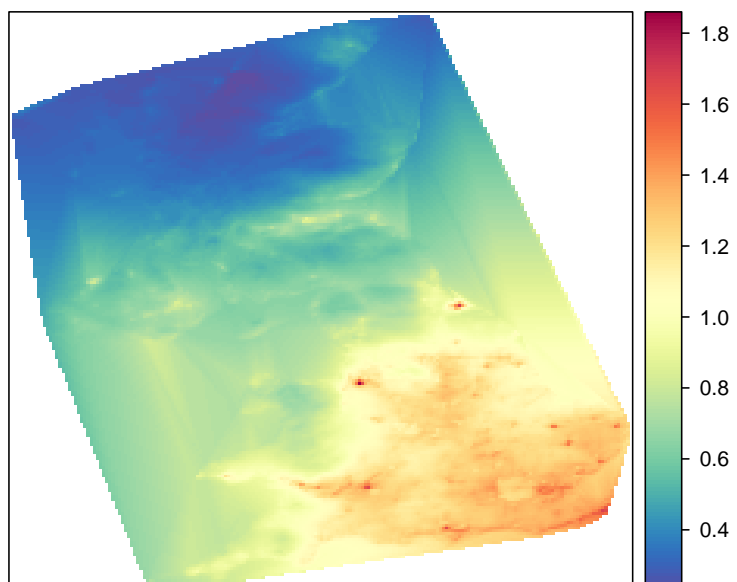
```
mapUHNH4 <- prepareGrid(mapUH, pollutant = "NH4.")
makeMap(mapUHNH4, pollu="NH4.", aspect = "iso")
```

```
mapJEPNH4 <- prepareGrid(mapJEP, pollutant = "nh4")
makeMap(mapJEPNH4, pollu="nh4", aspect = "iso")
```

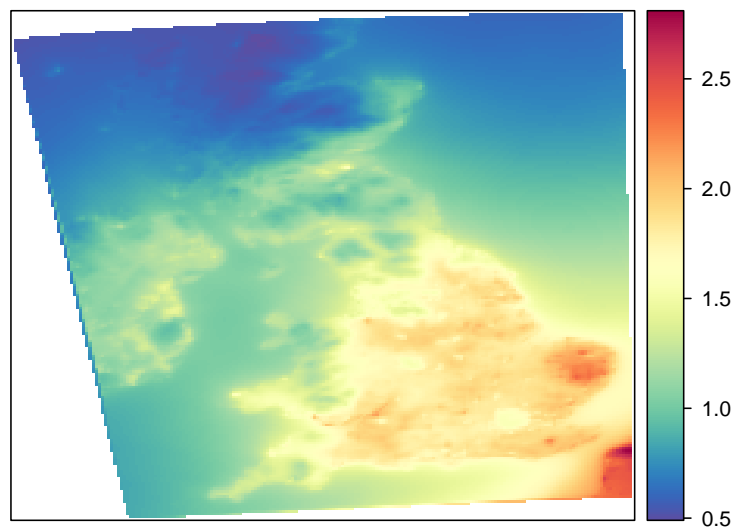




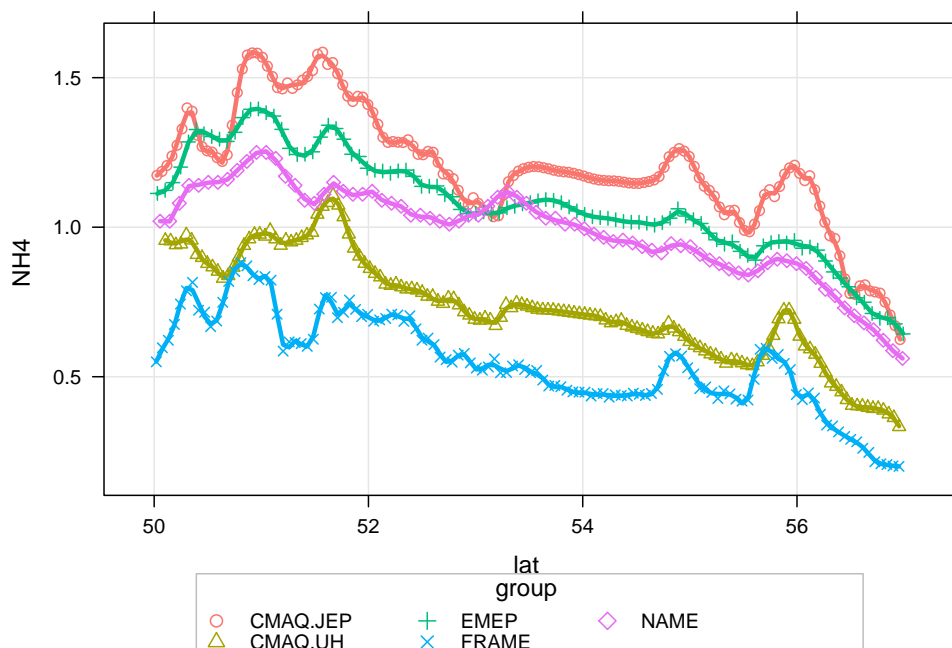
**Figure 36:** Annual mean ammonium concentrations from the FRAME model.



**Figure 37:** Annual mean ammonium concentrations from the CMAQ UH model.



**Figure 38:** Annual mean ammonium concentrations from the CMAQ JEP model.



**Figure 39:** Transect of ammonium concentrations along  $-4.05$  longitude.

The transects require some work to extract from each of these maps.

```
## NAME
id <- nearest(mapNAME, lon = -4.05)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, nh4))
names(transNAME)[3] <- "NH4"
transNAME$group <- "NAME"

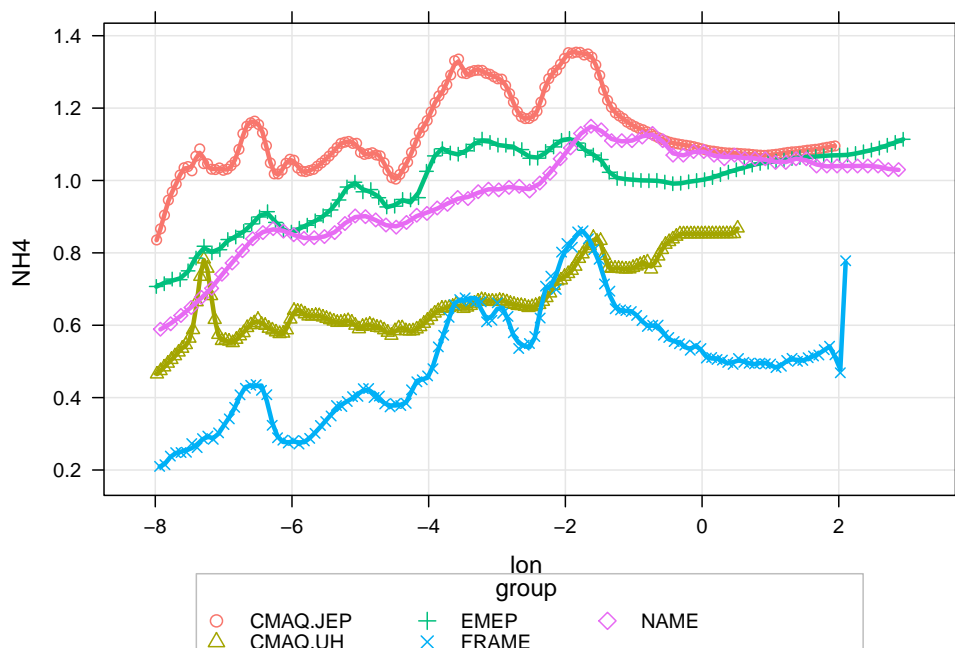
## EMEP
id <- nearest(EMEPNH4plus, lon = -4.05)
transEMEP <- EMEPNH4plus[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, NH4..ugm3))
names(transEMEP)[3] <- "NH4"
transEMEP$group <- "EMEP"

## FRAME
id <- nearest(FRAMENH4, lon = -4.05)
transFRAME <- FRAMENH4[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, NH4))
transFRAME$group <- "FRAME"

## CMAQ UH
id <- nearest(mapUHNH4, lon = -4.05)
transUH <- mapUHNH4[id , ]
transUH <- subset(transUH, select = c(lat, lon, NH4.))
names(transUH)[3] <- "NH4"
transUH$group <- "CMAQ.UH"

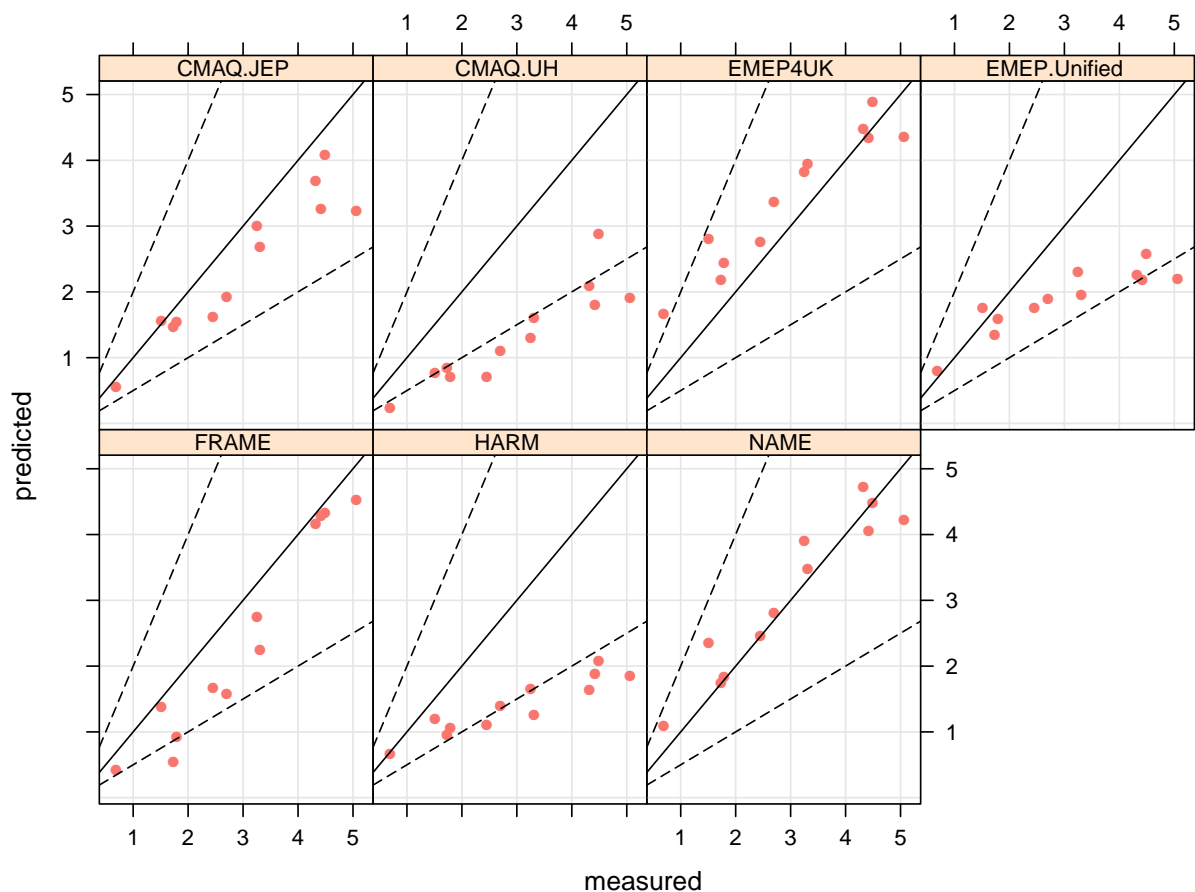
## CMAQ JEP
id <- nearest(mapJEPNH4, lon = -4.05)
transJEP <- mapJEPNH4[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, nh4))
names(transJEP)[3] <- "NH4"
transJEP$group <- "CMAQ.JEP"

## now combine all the results
transNH4 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transNH4, lat > 50 & lat < 57), x = "lat", y = "NH4", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 40:** Transect of Ammonium concentrations along 55.065 latitude.

```
## NAME
id <- nearest(mapNAME, lat = 55.065)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, nh4))
names(transNAME)[3] <- "NH4"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPNH4plus, lat = 55.065)
transEMEP <- EMEPNH4plus[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, NH4..ugm3))
names(transEMEP)[3] <- "NH4"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMENH4, lat = 55.065)
transFRAME <- FRAMENH4[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, NH4))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHNH4, lat = 55.065)
transUH <- mapUHNH4[id , ]
transUH <- subset(transUH, select = c(lat, lon, NH4.))
names(transUH)[3] <- "NH4"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPNH4, lat = 55.065)
transJEP <- mapJEPNH4[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, nh4))
names(transJEP)[3] <- "NH4"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transNH4 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transNH4, lon > -8 & lon < 3), x = "lon", y = "NH4", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 41:** Measured versus predicted annual mean  $\text{NO}_3^-$  concentrations.

### 3.6 Nitrate

First we will extract the  $\text{NO}_3^-$  data.

```
nitrate.results <- subset(all.results, species == "NO3-")
```

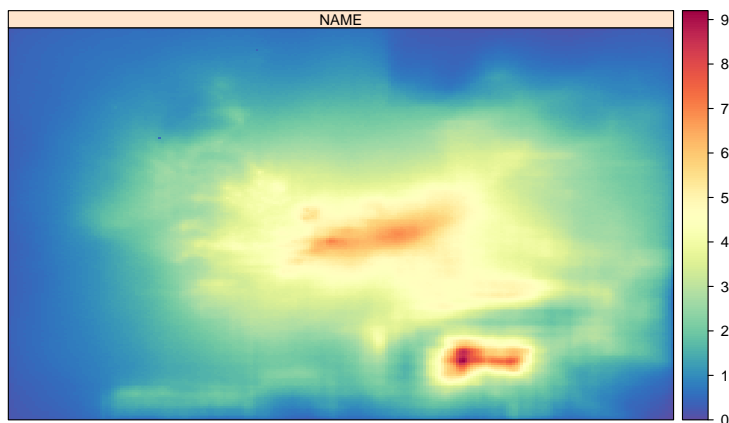
```
nitrateStats <- modStats(nitrate.results, type = "group", mod = "predicted", obs = "measured")
```

**Table 7:** Summary model evaluation statistics for annual mean  $\text{NO}_3^-$  concentrations.

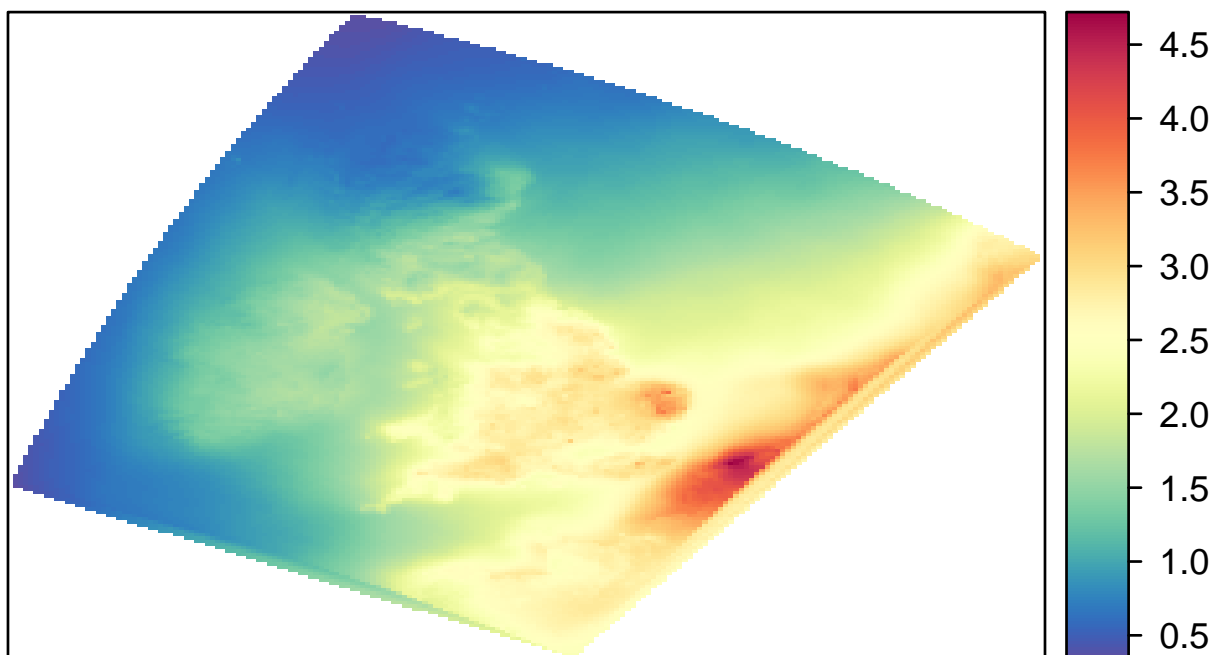
group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
CMAQ.JEP	12.00	1.00	-0.59	0.60	-0.20	0.20	0.77	0.94
CMAQ.UH	12.00	0.17	-1.65	1.65	-0.55	0.55	1.81	0.90
EMEP4UK	12.00	0.92	0.44	0.57	0.15	0.19	0.66	0.95
EMEPUnified	12.00	0.83	-1.09	1.15	-0.37	0.39	1.45	0.88
FRAME	12.00	0.92	-0.58	0.58	-0.19	0.19	0.70	0.97
HARM	12.00	0.50	-1.58	1.58	-0.53	0.53	1.85	0.93
NAME	12.00	1.00	0.12	0.32	0.04	0.11	0.44	0.95

```
scatterPlot(nitrate.results, x = "measured", y = "predicted", type = "group", mod.line = TRUE,
            smooth = FALSE, pch = 16, key = FALSE)
```

```
makeMap(mapNAME, pollutant = "no3", aspect = "iso")
```



**Figure 42:** Annual mean nitrate concentrations from the NAME model



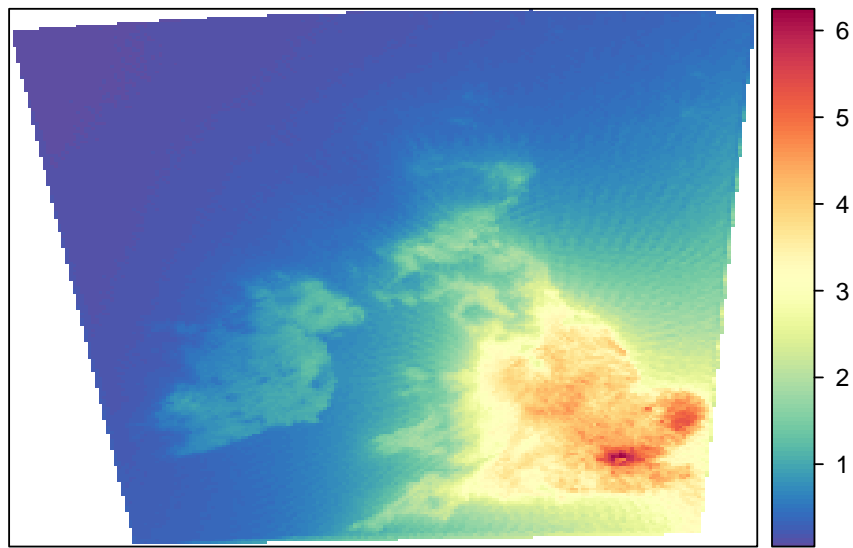
**Figure 43:** Annual mean nitrate concentrations from the EMEP4UK model.

```
EMEPN03minus <- read.csv("depositionTemplateV1.0_EMEP4UK_rv3.7_final_SURFACE_MAP_N03-_ugm3.csv",
  header = TRUE, na.strings = "missing")
EMEPN03minus <- na.omit(EMEPN03minus) ## remove missing data
EMEPN03minus <- prepareGrid(EMEPN03minus, pollutant = "NO3..ugm3")
makeMap(EMEPN03minus, pollu="NO3..ugm3", aspect = "iso")
```

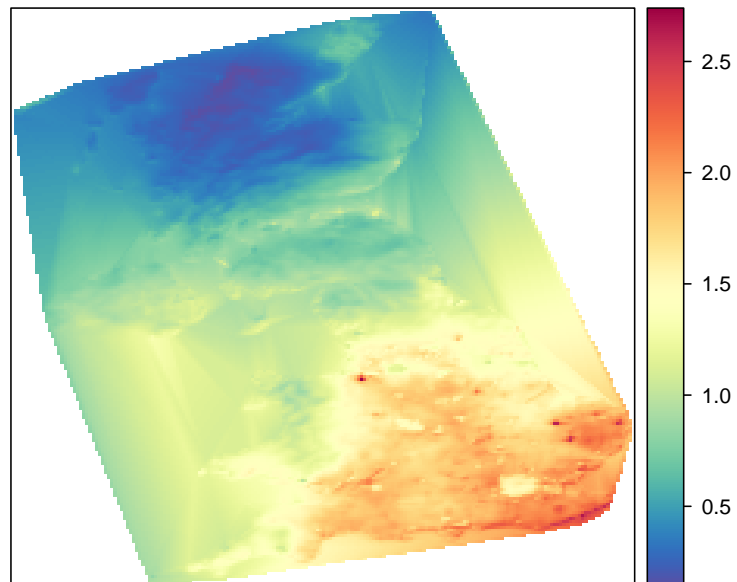
```
FRAMEN03 <- prepareGrid(mapFRAME, pollutant = "NO3")
makeMap(FRAMEN03, pollutant = "NO3", aspect = "iso")
```

```
mapUHN03 <- prepareGrid(mapUH, pollutant = "NO3.")
makeMap(mapUHN03, pollu="NO3.", aspect = "iso")
```

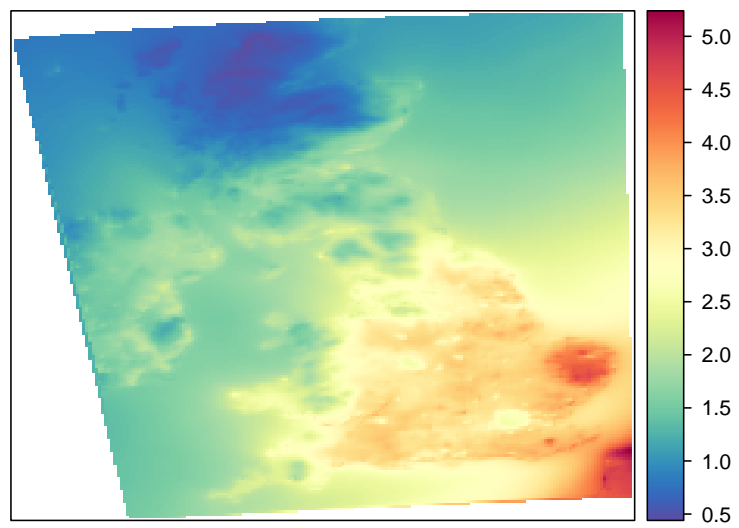
```
mapJEPN03 <- prepareGrid(mapJEP, pollutant = "no3")
makeMap(mapJEPN03, pollu="no3", aspect = "iso")
```



**Figure 44:** Annual mean nitrate concentrations from the FRAME model.

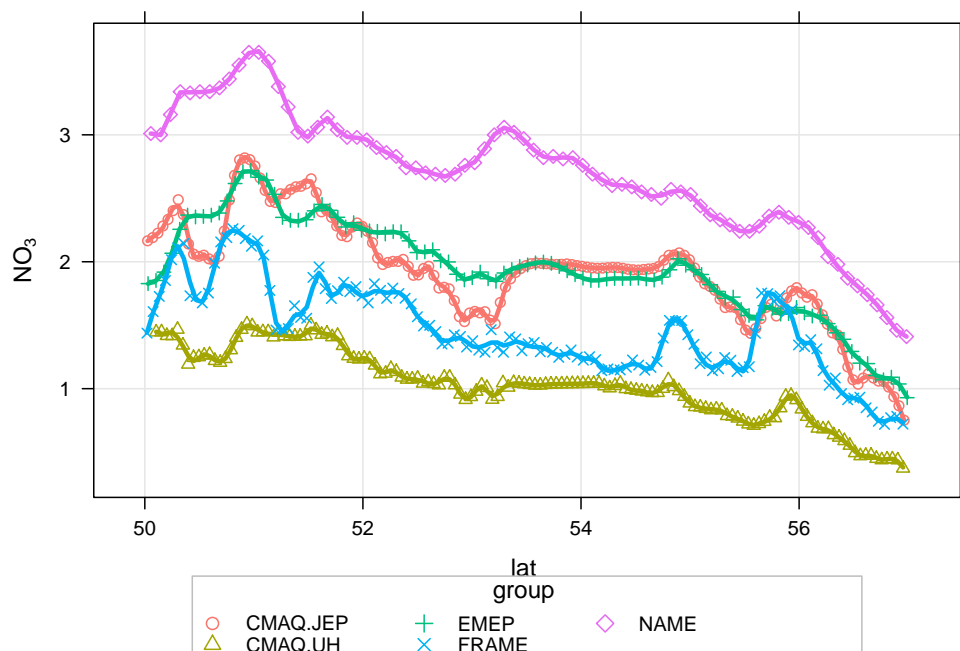


**Figure 45:** Annual mean nitrate concentrations from the CMAQ University of Hertfordshire model.



**Figure 46:** Annual mean nitrate concentrations from the CMAQ JEP model.

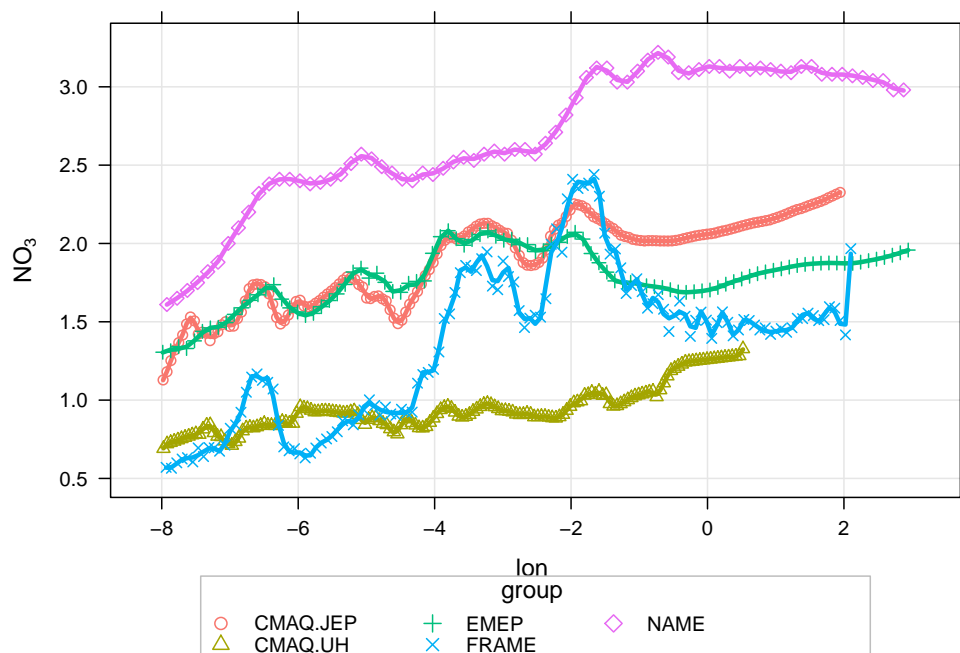




**Figure 47:** Transect of nitrate concentrations along  $-4.05$  longitude.

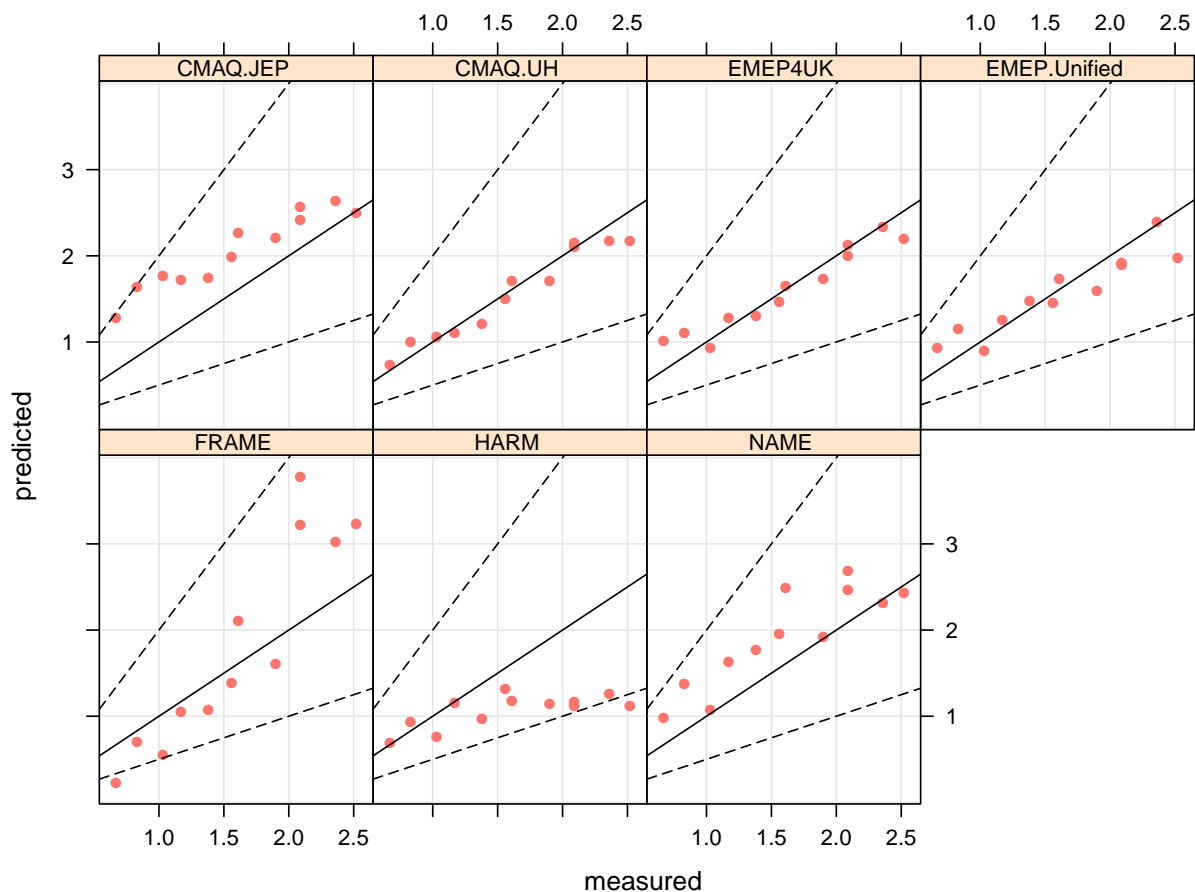
The transects require some work to extract from each of these maps.

```
## NAME
id <- nearest(mapNAME, lon = -4.05)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, no3))
names(transNAME)[3] <- "NO3"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPNO3minus, lon = -4.05)
transEMEP <- EMEPNO3minus[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, NO3..ugm3))
names(transEMEP)[3] <- "NO3"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMENO3, lon = -4.05)
transFRAME <- FRAMENO3[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, NO3))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHN03, lon = -4.05)
transUH <- mapUHN03[id , ]
transUH <- subset(transUH, select = c(lat, lon, NO3.))
names(transUH)[3] <- "NO3"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPNO3, lon = -4.05)
transJEP <- mapJEPNO3[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, no3))
names(transJEP)[3] <- "NO3"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transNO3 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transNO3, lat > 50 & lat < 57), x = "lat", y = "NO3", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 48:** Transect of nitrate concentrations along 55.065 latitude.

```
## NAME
id <- nearest(mapNAME, lat = 55.065)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, no3))
names(transNAME)[3] <- "NO3"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPNO3minus, lat = 55.065)
transEMEP <- EMEPNO3minus[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, NO3..ugm3))
names(transEMEP)[3] <- "NO3"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMENO3, lat = 55.065)
transFRAME <- FRAMENO3[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, NO3))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHN03, lat = 55.065)
transUH <- mapUHN03[id , ]
transUH <- subset(transUH, select = c(lat, lon, NO3.))
names(transUH)[3] <- "NO3"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPNO3, lat = 55.065)
transJEP <- mapJEPNO3[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, no3))
names(transJEP)[3] <- "NO3"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transNO3 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transNO3, lon > -8 & lon < 3), x = "lon", y = "NO3", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 49:** Measured versus predicted annual mean non-sea salt  $\text{SO}_4$  concentrations.

### 3.7 Non-sea salt sulphate

First we will extract the nns  $\text{SO}_4$  data.

```
nssSO4.results <- subset(all.results, species == "nss SO4")
```

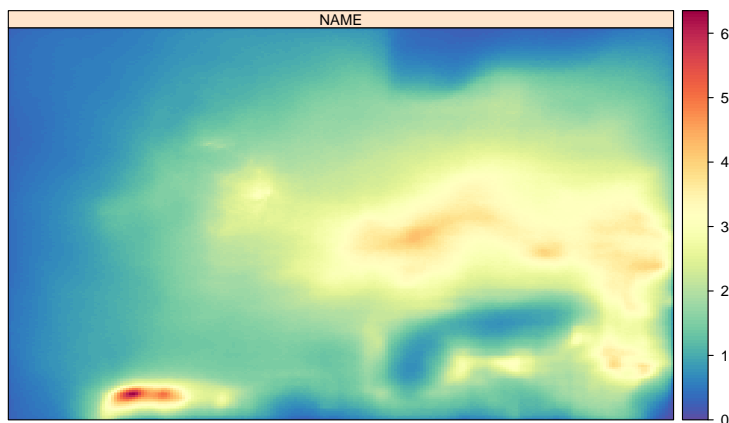
```
nsssStats <- modStats(nssSO4.results, type = "group", mod = "predicted", obs = "measured")
```

**Table 8:** Summary model evaluation statistics for annual mean nns  $\text{SO}_4$  concentrations.

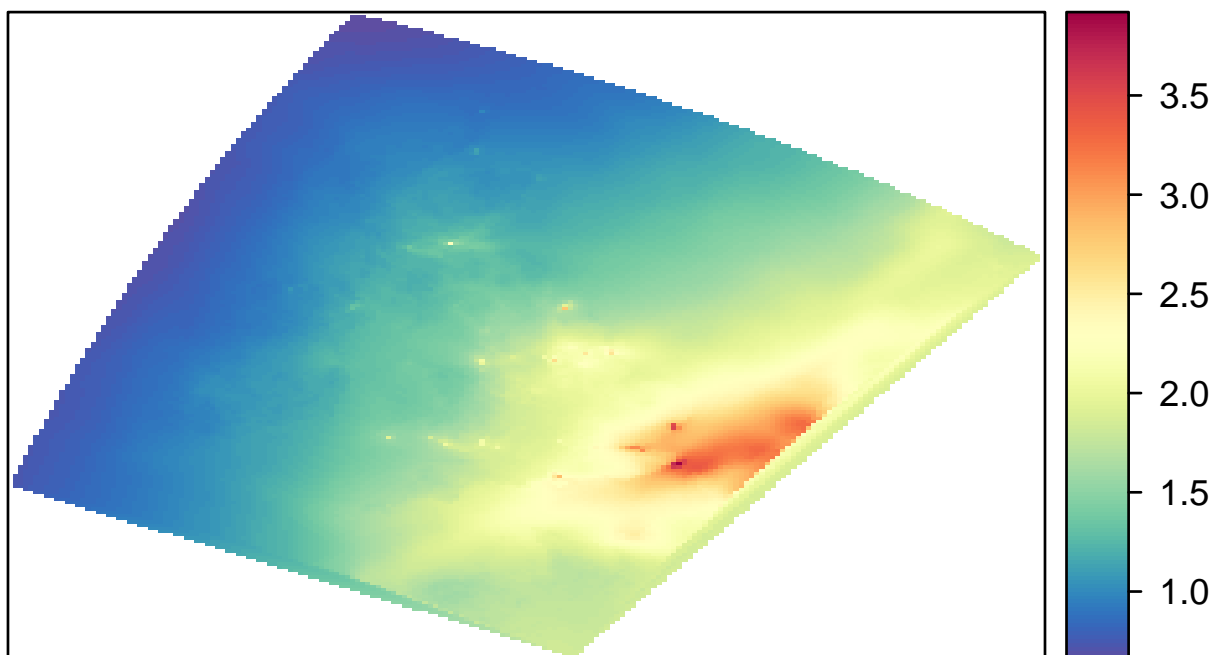
group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
CMAQ.JEP	12.00	1.00	0.46	0.46	0.29	0.29	0.51	0.95
CMAQ.UH	12.00	1.00	-0.05	0.12	-0.03	0.08	0.15	0.97
EMEP4UK	12.00	1.00	-0.01	0.14	-0.00	0.09	0.18	0.97
EMEPUnified	12.00	1.00	-0.04	0.20	-0.03	0.12	0.24	0.93
FRAME	12.00	0.92	0.23	0.55	0.14	0.34	0.71	0.92
HARM	12.00	0.92	-0.53	0.55	-0.33	0.35	0.71	0.71
NAME	12.00	1.00	0.33	0.35	0.20	0.22	0.43	0.88

```
scatterPlot(nssSO4.results, x = "measured", y = "predicted", type = "group", mod.line = TRUE,
            smooth = FALSE, pch = 16, key = FALSE)
```

```
makeMap(mapNAME, pollutant = "so4", aspect = "iso")
```



**Figure 50:** Annual mean sulphate concentrations from the NAME model



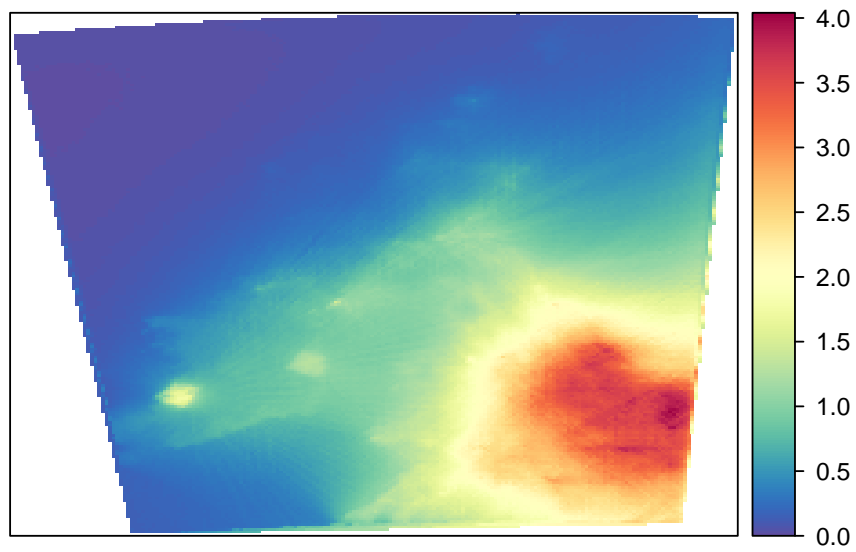
**Figure 51:** Annual mean sulphate concentrations from the EMEP4UK model.

```
EMEPnss_S04 <- read.csv("depositionTemplateV1.0_EMEP4UK_rv3.7_final_SURFACE_MAP_nss_S04_ugm3.csv",
  header = TRUE, na.strings = "missing")
EMEPnss_S04 <- na.omit(EMEPnss_S04) ## remove missing data
EMEPnss_S04 <- prepareGrid(EMEPnss_S04, pollutant = "nss.S04.ugm3")
makeMap(EMEPnss_S04, pollu="nss.S04.ugm3", aspect = "iso")
```

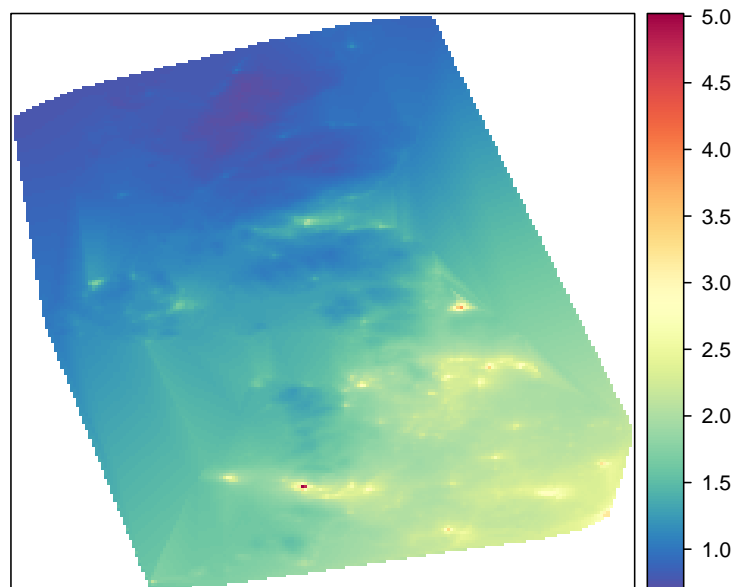
```
FRAMES04 <- prepareGrid(mapFRAME, pollutant = "S04")
makeMap(FRAMES04, pollutant = "S04", aspect = "iso")
```

```
mapUHnssS04 <- prepareGrid(mapUH, pollutant = "nss.S04")
makeMap(mapUHnssS04, pollutant = "nss.S04", aspect = "iso")
```

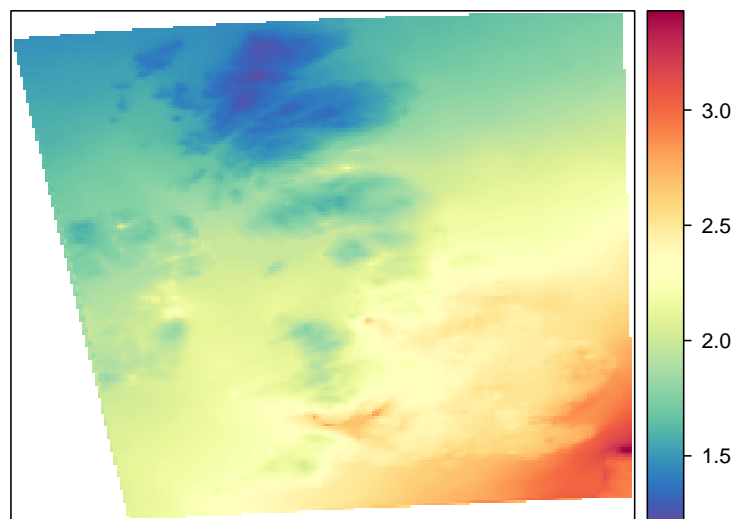
```
mapJEPnssS04 <- prepareGrid(mapJEP, pollutant = "nssS04")
makeMap(mapJEPnssS04, pollutant = "nssS04", aspect = "iso")
```



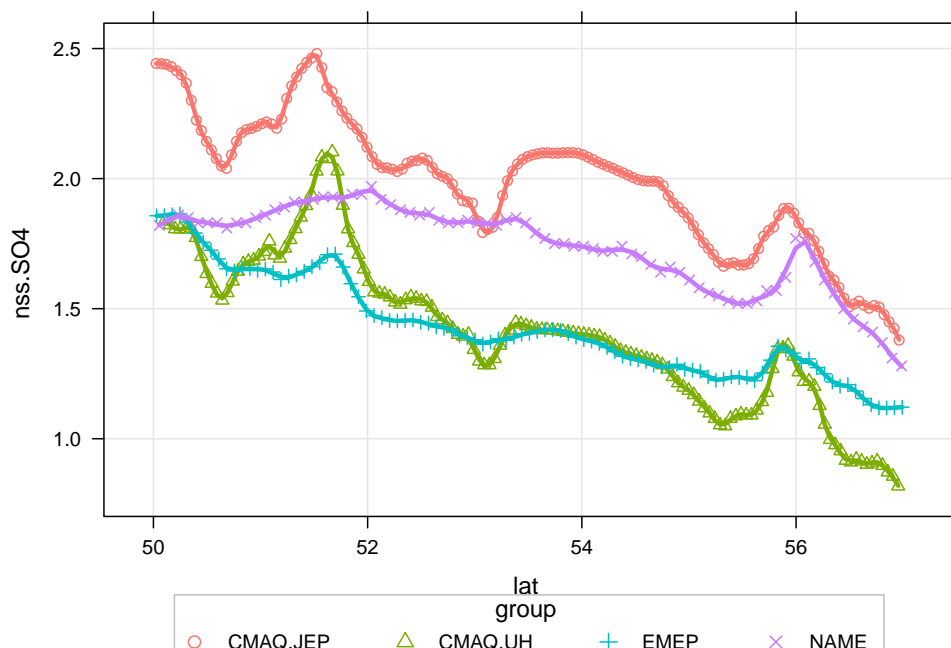
**Figure 52:** Annual mean sulphate concentrations from the FRAME model.



**Figure 53:** Annual mean sulphate concentrations from the CMAQ University of Hertfordshire model.



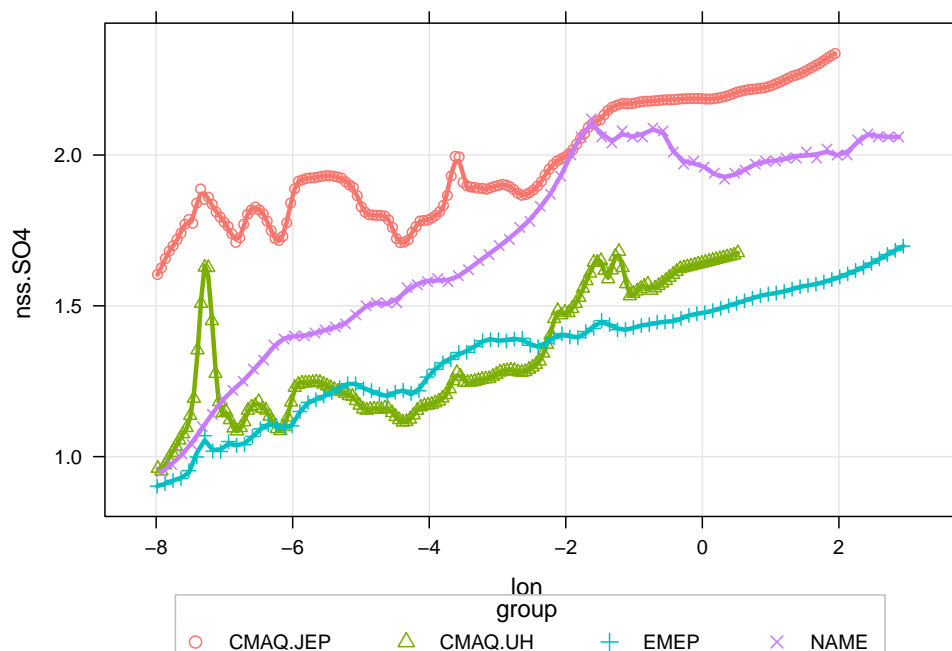
**Figure 54:** Annual mean sulphate concentrations from the CMAQ JEP model.



**Figure 55:** Transect of nss sulphate concentrations along  $-4.05$  longitude.

The transects require some work to extract from each of these maps.

```
## NAME
id <- nearest(mapNAME, lon = -4.05)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, so4))
names(transNAME)[3] <- "nss.SO4"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPnss_S04, lon = -4.05)
transEMEP <- EMEPnss_S04[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, nss.SO4.ugm3))
names(transEMEP)[3] <- "nss.SO4"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMES04, lon = -4.05)
transFRAME <- FRAMES04[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, S04))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHnssS04, lon = -4.05)
transUH <- mapUHnssS04[id , ]
transUH <- subset(transUH, select = c(lat, lon, nss.SO4))
names(transUH)[3] <- "nss.SO4"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPnssS04, lon = -4.05)
transJEP <- mapJEPnssS04[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, nssS04))
names(transJEP)[3] <- "nss.SO4"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transnssS04 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transnssS04, lat > 50 & lat < 57), x = "lat", y = "nss.SO4", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 56:** Transect of nss sulphate along 55.065 latitude.

```
## NAME
id <- nearest(mapNAME, lat = 55.065)
transNAME <- mapNAME[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, so4))
names(transNAME)[3] <- "nss.SO4"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPnss_S04, lat = 55.065)
transEMEP <- EMEPnss_S04[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, nss.SO4.ugm3))
names(transEMEP)[3] <- "nss.SO4"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMES04, lat = 55.065)
transFRAME <- FRAMES04[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, S04))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHnssS04, lat = 55.065)
transUH <- mapUHnssS04[id , ]
transUH <- subset(transUH, select = c(lat, lon, nss.SO4))
names(transUH)[3] <- "nss.SO4"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPnssS04, lat = 55.065)
transJEP <- mapJEPnssS04[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, nssS04))
names(transJEP)[3] <- "nss.SO4"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transnssS04 <- rbind.fill(transNAME, transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transnssS04, lon > -8 & lon < 3), x = "lon", y = "nss.SO4", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



### 3.8 Non-sea salt sulphate in precipitation

Note the following text from the Met Office with regard to the NAME model:

The NAME deposition runs done for this study have highlighted two issues with the NAME wet deposition scheme. Firstly the wet deposition field has a blocky appearance, with the blocks denoting the resolution of the NWP data and secondly there are distinct lines appearing in the field. The first issue has arisen from the use of the nearest NWP gridpoint values for precipitation rather than interpolation between the NWP gridpoint values. This was done to ensure that precipitation information was in agreement with cloud information. In order to produce smooth wet deposition fields which have a better appearance and do not show the resolution of the underlying met data used, NAME will be revised to use both interpolated precipitation and cloud data. The second issue is arising from the orographic enhancement scheme which cuts in at a fixed height above sea level. This scheme will be reviewed in light of these results.

For now we have not added the transects for the NAME model, but have plotted the maps. Additional refinements can be made as necessary in Phase 2.

First we will extract the nns SO<sub>4</sub> in precipitation data.

```
nssS04precip.results <- subset(all.results, species == "nss sulphate")
```

```
modStats(nssS04precip.results, type = "group", mod = "predicted", obs = "measured")
```

**Table 9:** Summary model evaluation statistics for annual mean nns SO<sub>4</sub> concentrations.

group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
CMAQ.JEP	37.00	0.89	2.19	7.30	0.10	0.32	8.26	0.80
CMAQ.UH	37.00	0.97	-5.96	6.89	-0.26	0.30	9.08	0.84
EMEP4UK	37.00	1.00	-2.83	5.09	-0.12	0.22	7.13	0.83
EMEPUnified	37.00	1.00	0.76	4.00	0.03	0.18	5.39	0.91
FRAME	37.00	0.84	6.40	9.56	0.28	0.42	13.94	0.75
HARM	37.00	1.00	-3.62	6.23	-0.16	0.27	8.35	0.86
NAME	37.00	0.57	-10.21	11.51	-0.45	0.50	14.91	0.33

```
scatterPlot(nssS04precip.results, x = "measured", y = "predicted", type = "group", mod.line = TRUE,
            smooth = FALSE, pch = 16, key = FALSE)
```

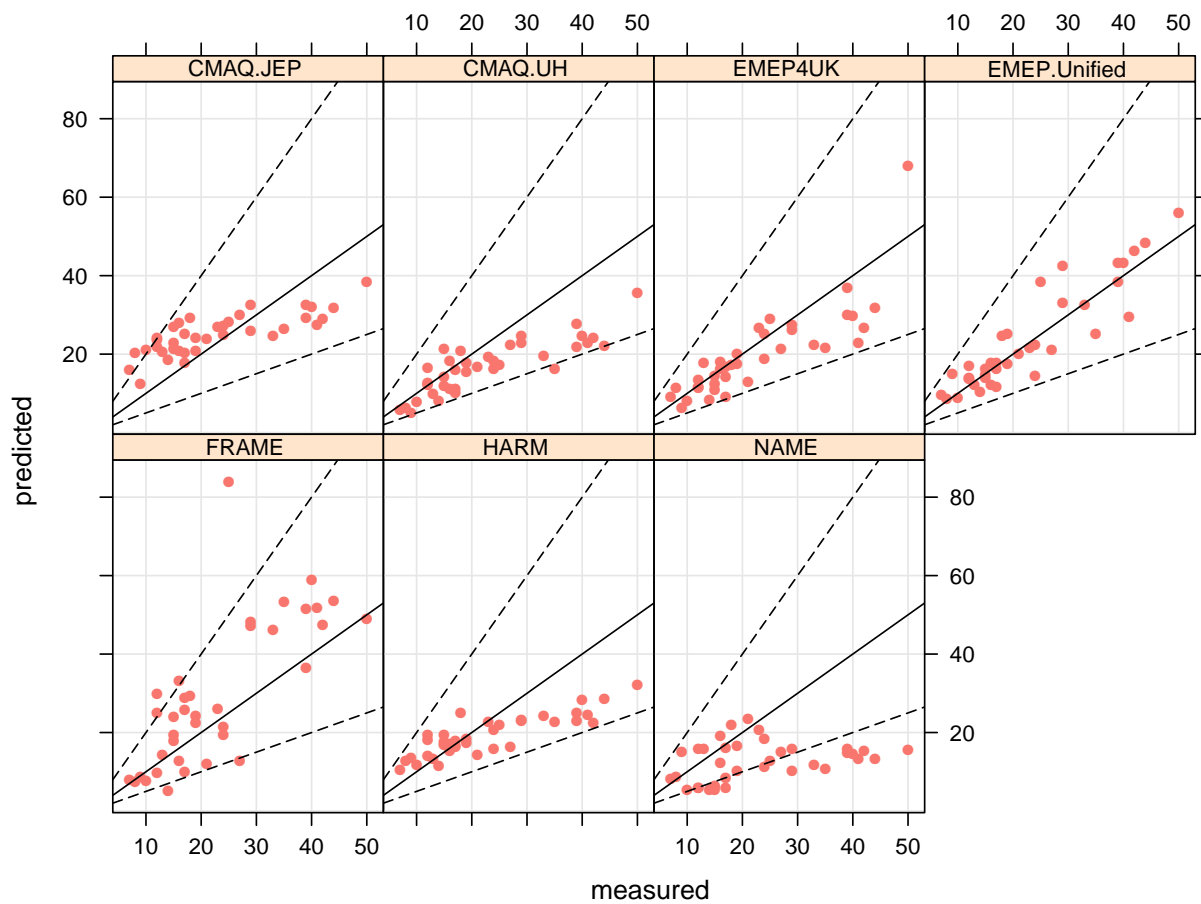
```
makeMap(mapNAMEwet, pollutant = "sulphatePrecip", aspect = "iso")
```

```
EMEPnss_sulphate <- read.csv("depositionTemplateV1.0_EMEP4UK_rv3.7_final_SURFACE_MAP_nss_sulphate_ueq1-1.csv",
                           header = TRUE, na.strings = "missing")
EMEPnss_sulphate <- na.omit(EMEPnss_sulphate) ## remove missing data
EMEPnss_sulphate <- prepareGrid(EMEPnss_sulphate, pollutant = "nss.sulphate.ueq.1.1")
makeMap(EMEPnss_sulphate, pollu="nss.sulphate.ueq.1.1", aspect = "iso")
```

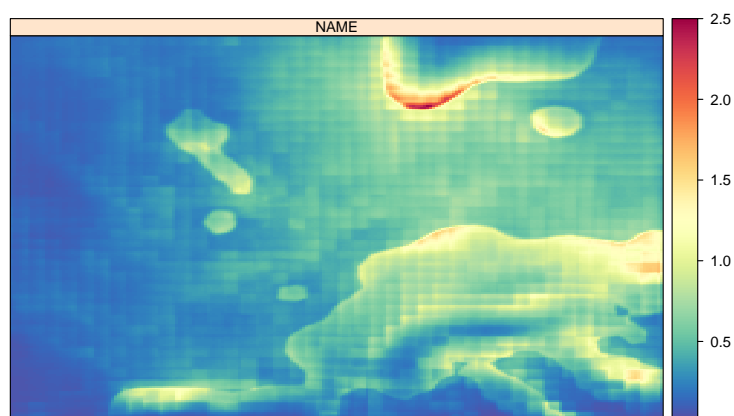
```
mapUHnssSulphate <- prepareGrid(mapUH, pollutant = "nss.sulphate")
makeMap(mapUHnssSulphate, pollutant = "nss.sulphate", aspect = "iso")
```

```
mapJEPnssSulphate <- prepareGrid(mapJEP, pollutant = "S04precip")
makeMap(mapJEPnssSulphate, pollutant = "S04precip", aspect = "iso")
```

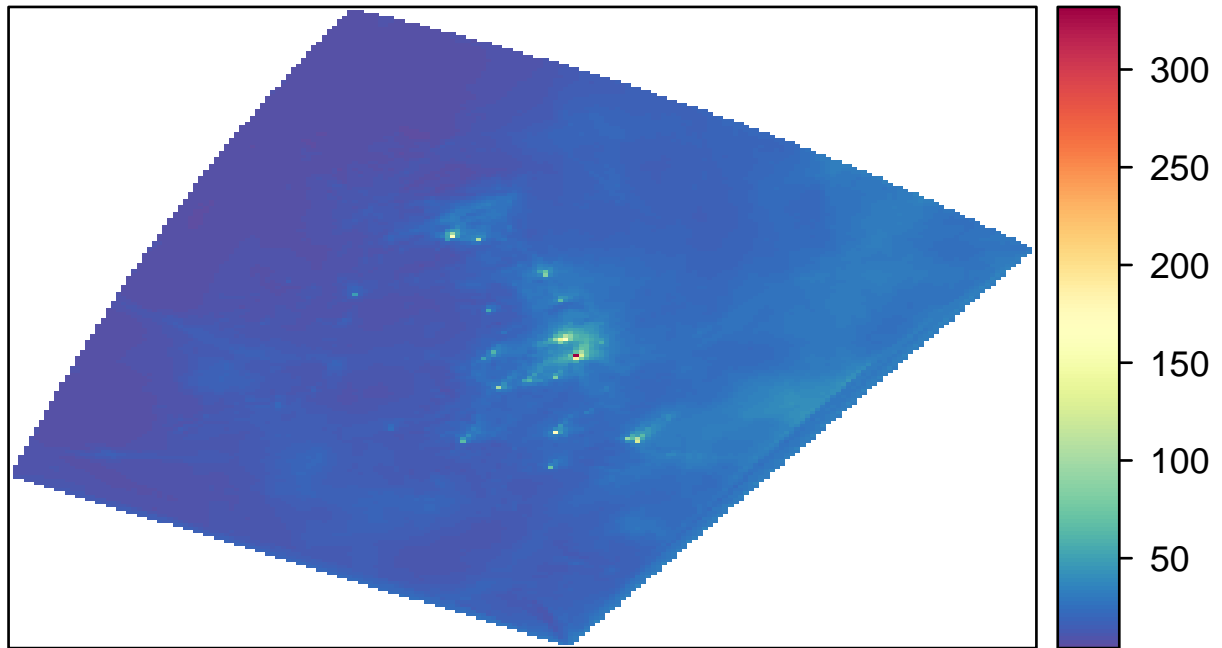
```
FRAMESOyWet <- prepareGrid(mapFRAMEwet, pollutant = "grd_S0y_wet")
makeMap(FRAMESOyWet, pollutant = "grd_S0y_wet", aspect = "iso")
```



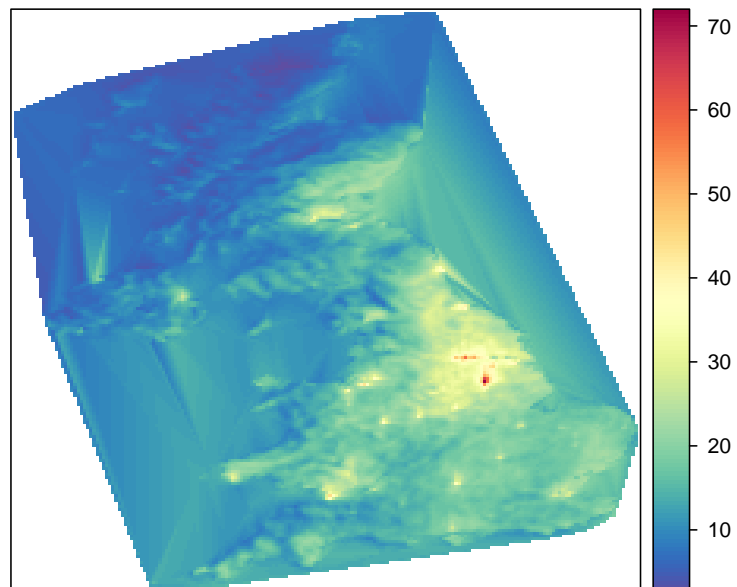
**Figure 57:** Measured versus predicted annual mean non-sea salt  $\text{SO}_4$  in precipitation concentrations.



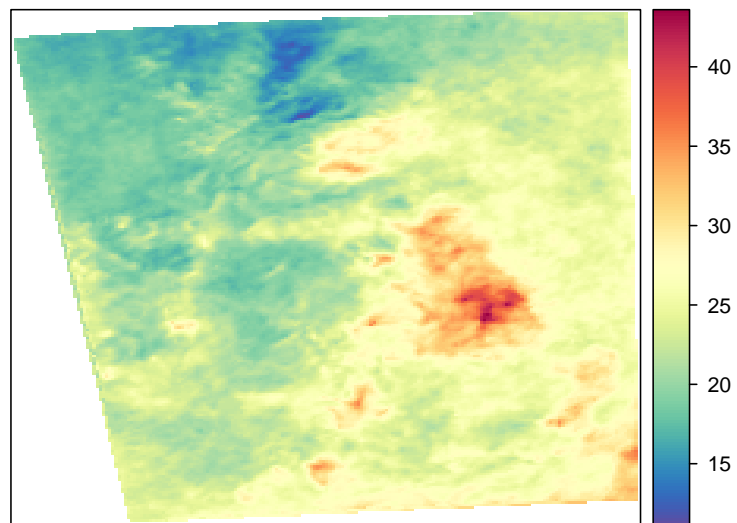
**Figure 58:** Annual mean sulphate from wet deposition using the NAME model (in  $\text{g m}^2 \text{yr}^{-1}$ ).



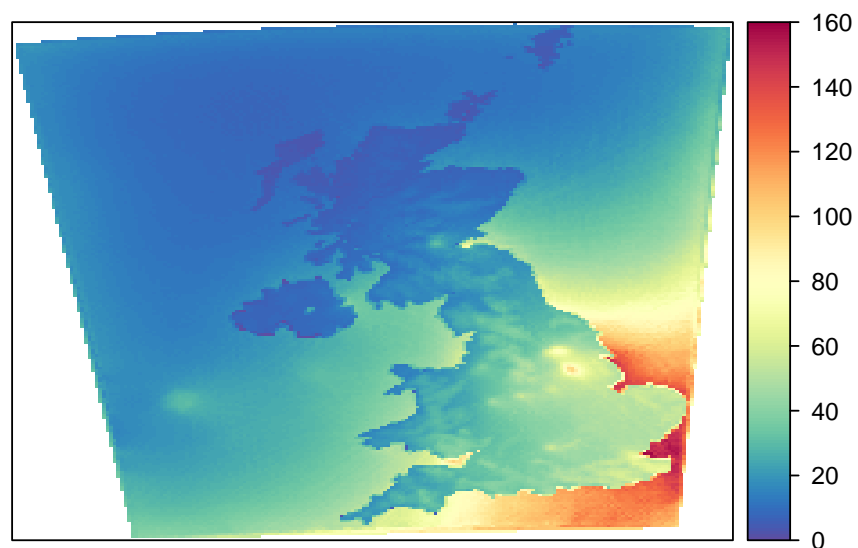
**Figure 59:** Annual mean sulphate in precipitation from the EMEP4UK model.



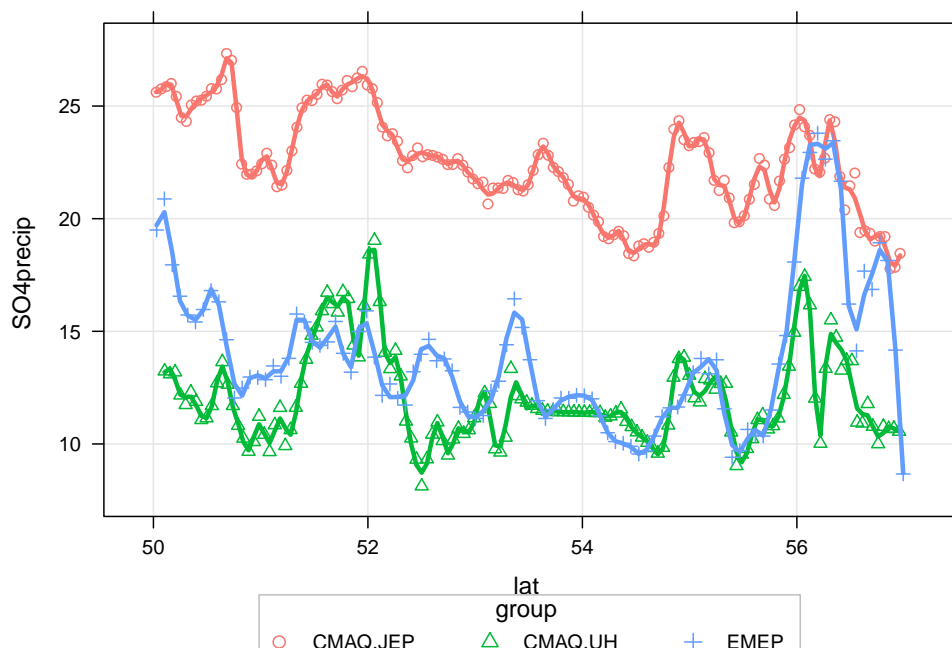
**Figure 60:** Annual mean sulphate in precipitation from the CMAQ University of Hertfordshire model.



**Figure 61:** Annual mean sulphate in precipitation from the CMAQ JEP model.



**Figure 62:** Annual mean sulphate in precipitation from the FRAME model.



**Figure 63:** Transect of sulphate in precipitation concentrations along  $-4.05$  longitude.

The transects require some work to extract from each of these maps.

```
## NAME
id <- nearest(mapNAMEwet, lon = -4.05)
transNAME <- mapNAMEwet[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, sulphatePrecip))
names(transNAME)[3] <- "SO4precip"
transNAME$group <- "NAME"

## EMEP
id <- nearest(EMEPnss_sulphate, lon = -4.05)
transEMEP <- EMEPnss_sulphate[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, nss.sulphate.ueq.l.1))
names(transEMEP)[3] <- "SO4precip"
transEMEP$group <- "EMEP"

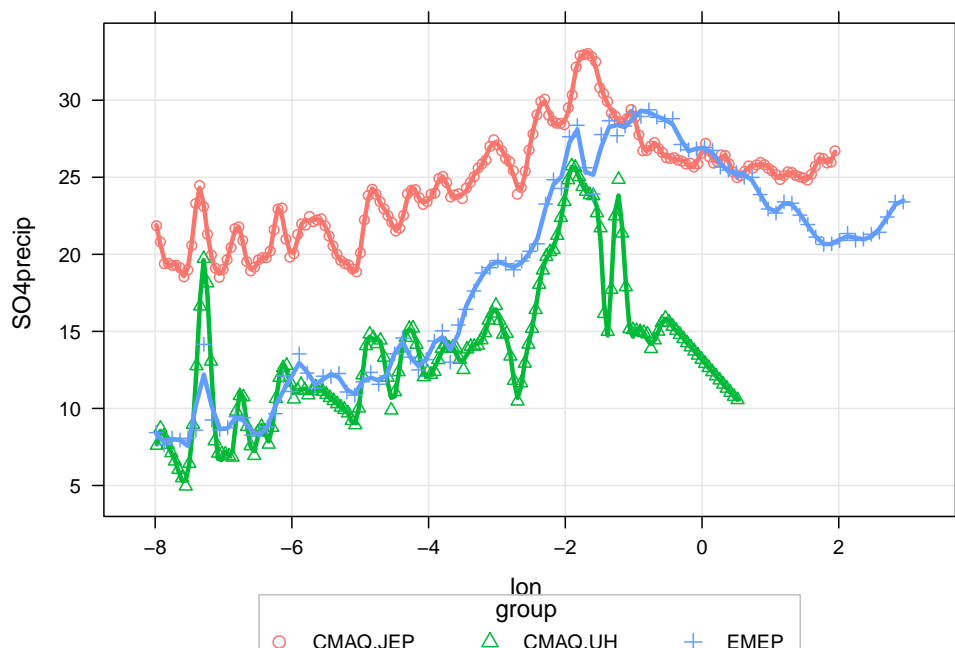
## FRAME
id <- nearest(FRAMESOyWet, lon = -4.05)
transFRAME <- FRAMESOyWet[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, grd_S0y_wet))
transFRAME$group <- "FRAME"

## CMAQ UH
id <- nearest(mapUHnssSulphate, lon = -4.05)
transUH <- mapUHnssSulphate[id , ]
transUH <- subset(transUH, select = c(lat, lon, nss.sulphate))
names(transUH)[3] <- "SO4precip"
transUH$group <- "CMAQ.UH"

## CMAQ JEP
id <- nearest(mapJEPnssSulphate, lon = -4.05)
transJEP <- mapJEPnssSulphate[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, S04precip))
names(transJEP)[3] <- "SO4precip"
transJEP$group <- "CMAQ.JEP"

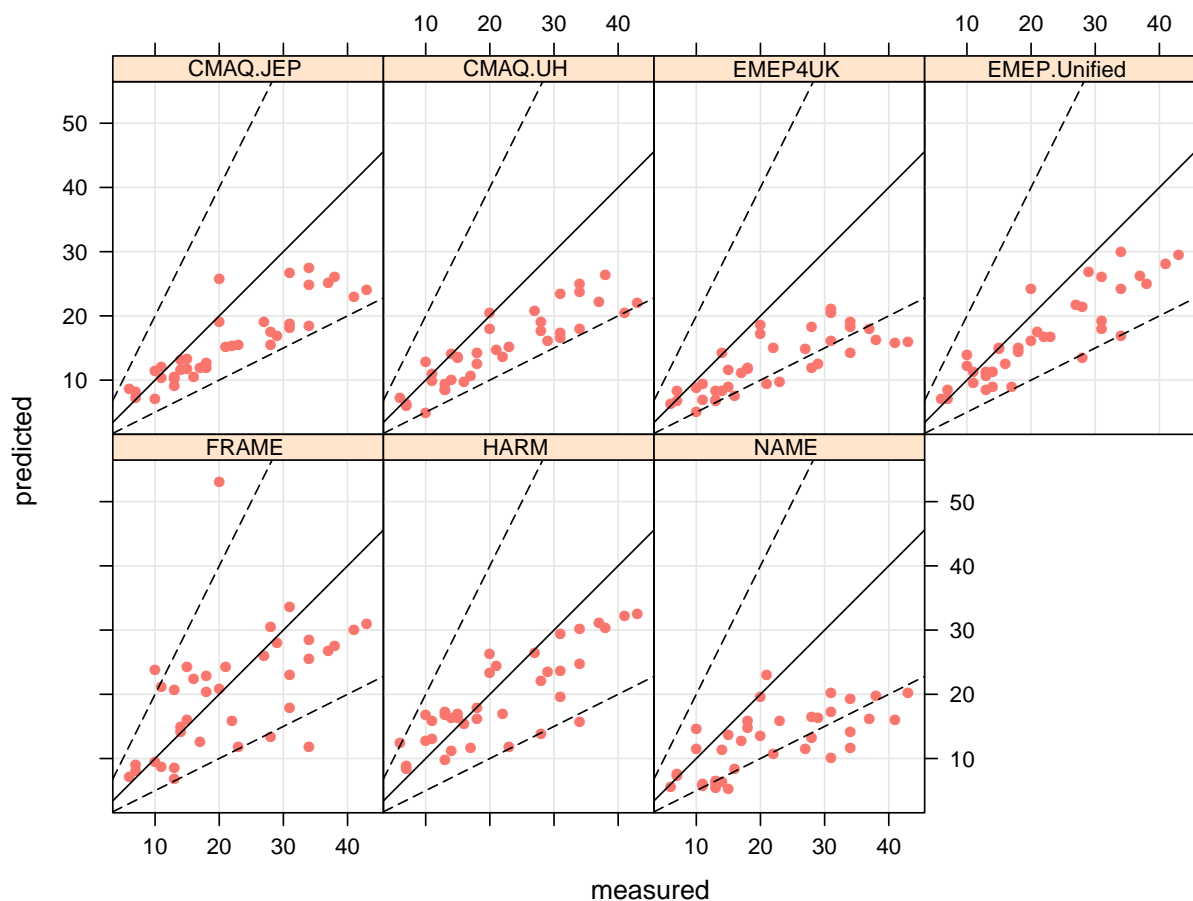
## now combine all the results
transnssSulphate <- rbind.fill(transEMEP, transUH, transJEP, transFRAME)

## now we can plot it
scatterPlot(subset(transnssSulphate, lat > 50 & lat < 57), x = "lat", y = "SO4precip", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 64:** Transect of sulphate in precipitation along 55.065 latitude.

```
## NAME
id <- nearest(mapNAMEwet, lat = 55.065)
transNAME <- mapNAMEwet[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, sulphatePrecip))
names(transNAME)[3] <- "SO4precip"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPnss_sulphate, lat = 55.065)
transEMEP <- EMEPnss_sulphate[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, nss.sulphate.ueq.l.1))
names(transEMEP)[3] <- "SO4precip"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMESOyWet, lat = 55.065)
transFRAME <- FRAMESOyWet[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, grd_S0y_wet))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHnssSulphate, lat = 55.065)
transUH <- mapUHnssSulphate[id , ]
transUH <- subset(transUH, select = c(lat, lon, nss.sulphate))
names(transUH)[3] <- "SO4precip"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPnssSulphate, lat = 55.065)
transJEP <- mapJEPnssSulphate[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, S04precip))
names(transJEP)[3] <- "SO4precip"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transnssSulphate <- rbind.fill(transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transnssSulphate, lon > -8 & lon < 3), x = "lon", y = "SO4precip", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 65:** Measured versus predicted annual mean nitrate in precipitation concentrations.

### 3.9 Nitrate in precipitation

First we will extract the nitrate in precipitation data.

```
nitratePrecip.results <- subset(all.results, species == "nitrate")
```

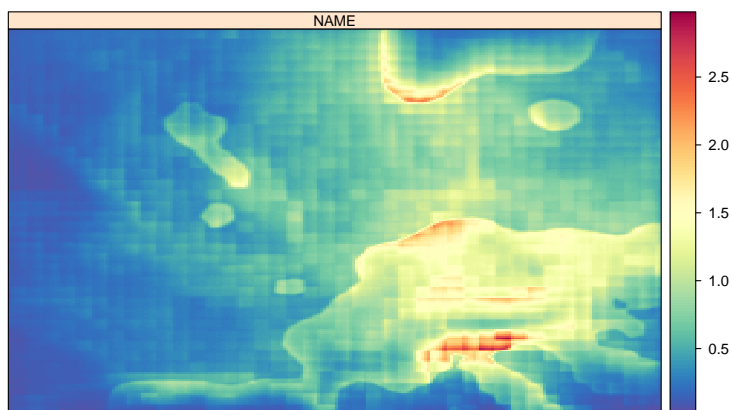
```
modStats(nitratePrecip.results, type = "group", mod = "predicted", obs = "measured")
```

**Table 10:** Summary model evaluation statistics for annual mean nitrate in precipitation concentrations.

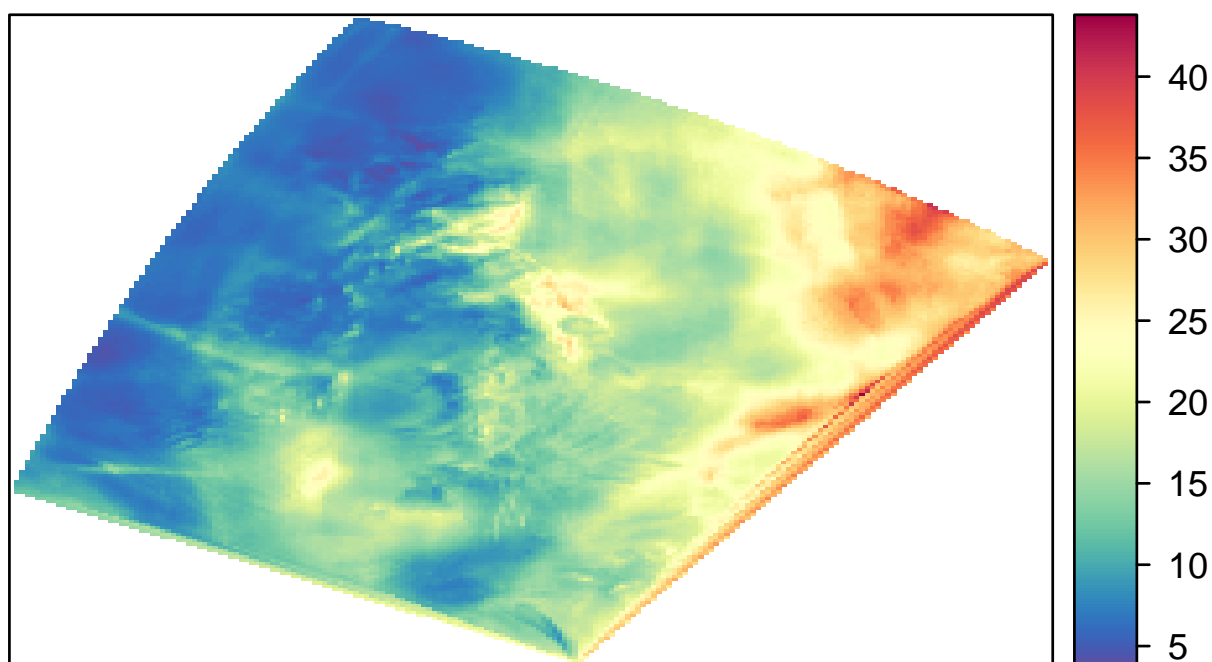
group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
CMAQ.JEP	37.00	1.00	-5.84	6.51	-0.27	0.30	8.22	0.88
CMAQ.UH	37.00	0.95	-6.65	6.91	-0.31	0.32	8.87	0.89
EMEP4UK	37.00	0.73	-9.13	9.24	-0.42	0.43	11.67	0.79
EMEPUnified	37.00	0.95	-4.87	5.60	-0.23	0.26	7.26	0.88
FRAME	37.00	0.89	-1.34	6.92	-0.06	0.32	9.60	0.54
HARM	37.00	0.92	-2.37	5.23	-0.11	0.24	6.57	0.81
NAME	37.00	0.65	-8.92	9.41	-0.41	0.44	11.87	0.67

```
scatterPlot(nitratePrecip.results, x = "measured", y = "predicted", type = "group", mod.line = TRUE,
            smooth = FALSE, pch = 16, key = FALSE)
```

```
makeMap(mapNAMEwet, pollutant = "nitratePrecip", aspect = "iso")
```



**Figure 66:** Annual mean nitrate from wet deposition using the NAME model (in  $\text{g m}^2 \text{yr}^{-1}$ ).



**Figure 67:** Annual mean nitrate in precipitation from the EMEP4UK model.

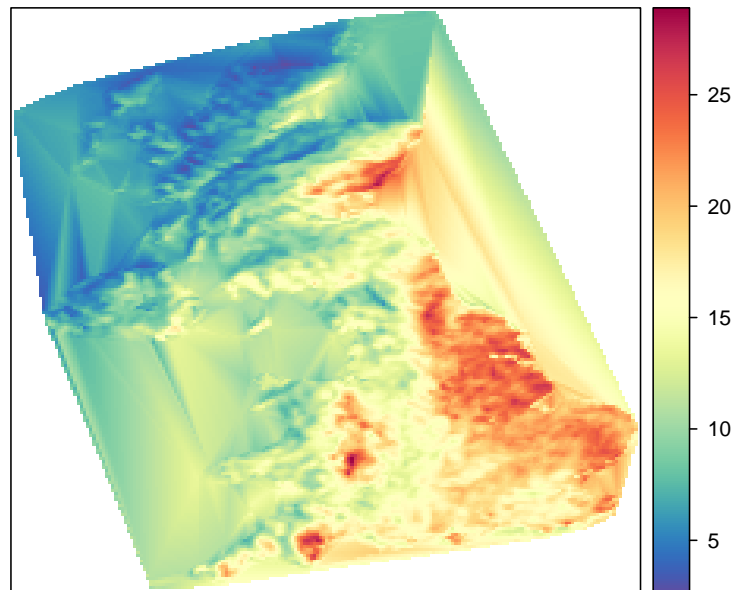
```
EMEPnss_nitrate <- read.csv("depositionTemplateV1.0_EMEP4UK_rv3.7_final_SURFACE_MAP_nitrate_ueq1-1.csv",
                           header = TRUE, na.strings = "missing")
EMEPnss_nitrate <- na.omit(EMEPnss_nitrate) ## remove missing data
EMEPnss_nitrate <- prepareGrid(EMEPnss_nitrate, pollutant = "nitrate.ueq.1.1")
makeMap(EMEPnss_nitrate, pollu="nitrate.ueq.1.1", aspect = "iso")
```

```
mapUHnssNitrate <- prepareGrid(mapUH, pollutant = "nitrate")
makeMap(mapUHnssNitrate, pollutant = "nitrate", aspect = "iso")
```

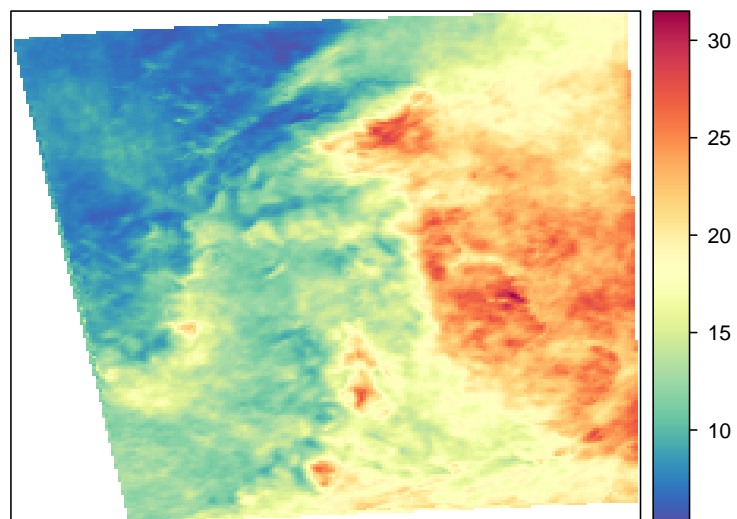
```
mapJEPnssNitrate <- prepareGrid(mapJEP, pollutant = "N03precip")
makeMap(mapJEPnssNitrate, pollutant = "N03precip", aspect = "iso")
```

```
FRAMENOyWet <- prepareGrid(mapFRAMEwet, pollutant = "grd_N0y_wet")
makeMap(FRAMENOyWet, pollutant = "grd_N0y_wet", aspect = "iso")
```

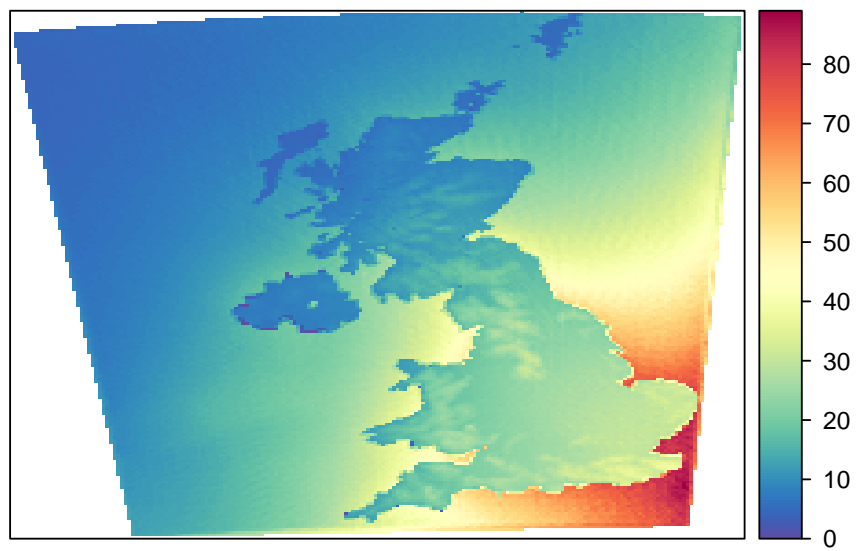




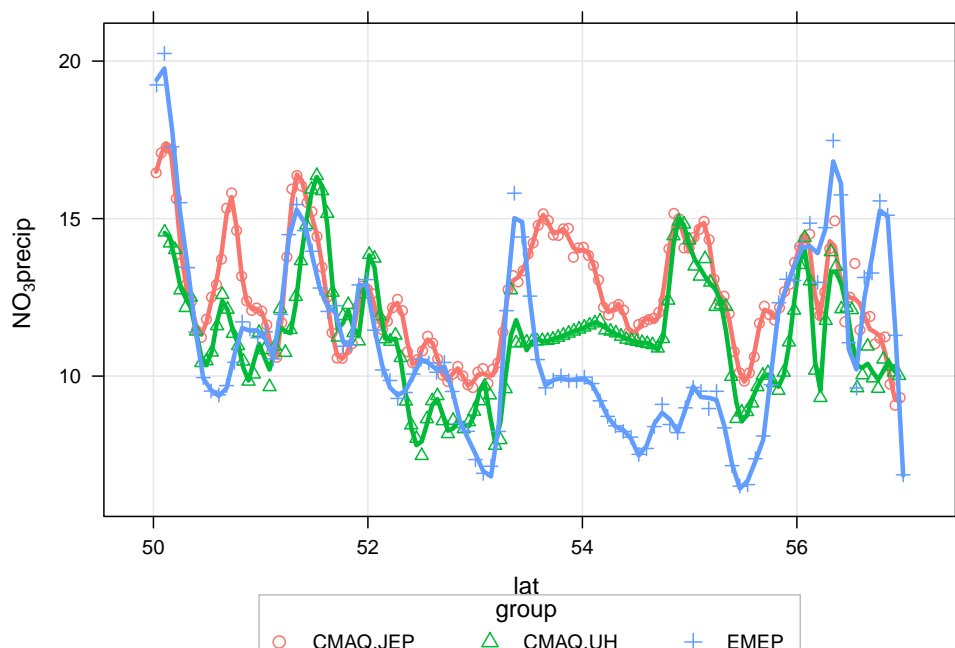
**Figure 68:** Annual mean nitrate in precipitation from the CMAQ University of Hertfordshire model.



**Figure 69:** Annual mean nitrate in precipitation from the CMAQ JEP model.

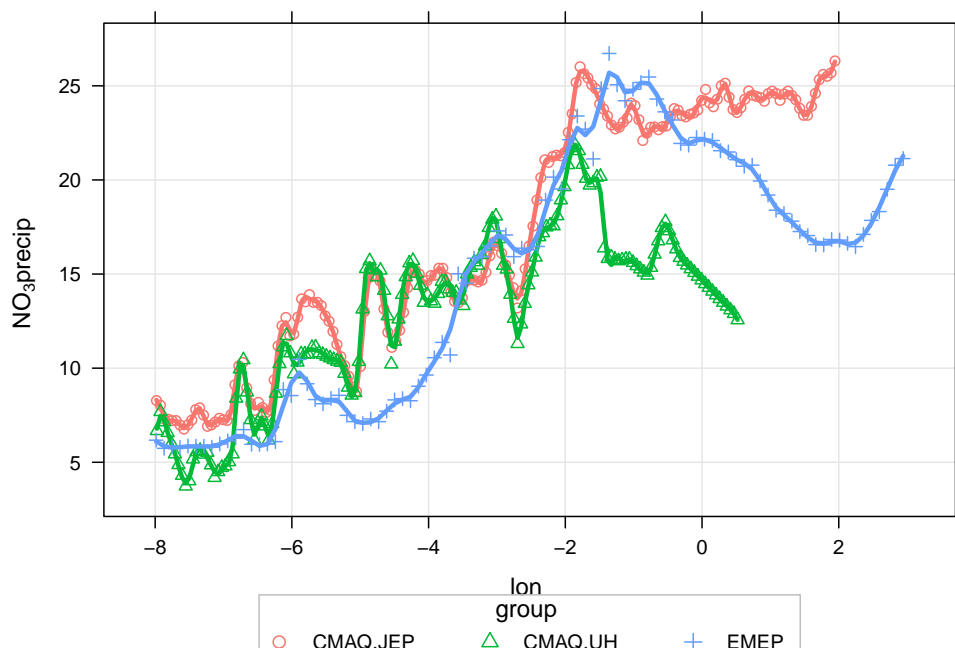


**Figure 70:** Annual mean nitrate in precipitation from the FRAME model.



**Figure 71:** Transect of nitrate in precipitation concentrations along  $-4.05$  longitude.

```
## NAME
id <- nearest(mapNAMEwet, lon = -4.05)
transNAME <- mapNAMEwet[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, nitratePrecip))
names(transNAME)[3] <- "NO3precip"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPnss_nitrate, lon = -4.05)
transEMEP <- EMEPnss_nitrate[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, nitrate.ueq.1.1))
names(transEMEP)[3] <- "NO3precip"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMENOyWet, lon = -4.05)
transFRAME <- FRAMENOyWet[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, grd_NOy_wet))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHnssNitrate, lon = -4.05)
transUH <- mapUHnssNitrate[id , ]
transUH <- subset(transUH, select = c(lat, lon, nitrate))
names(transUH)[3] <- "NO3precip"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPnssNitrate, lon = -4.05)
transJEP <- mapJEPnssNitrate[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, NO3precip))
names(transJEP)[3] <- "NO3precip"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transnssNitrate <- rbind.fill(transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transnssNitrate, lat > 50 & lat < 57), x = "lat", y = "NO3precip", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 72:** Transect of nitrate in precipitation along 55.065 latitude.

```
## NAME
id <- nearest(mapNAMEwet, lat = 55.065)
transNAME <- mapNAMEwet[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, nitratePrecip))
names(transNAME)[3] <- "NO3precip"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPnss_nitrate, lat = 55.065)
transEMEP <- EMEPnss_nitrate[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, nitrate.ueq.1.1))
names(transEMEP)[3] <- "NO3precip"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMENOyWet, lat = 55.065)
transFRAME <- FRAMENOyWet[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, grd_NOy_wet))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHnssNitrate, lat = 55.065)
transUH <- mapUHnssNitrate[id , ]
transUH <- subset(transUH, select = c(lat, lon, nitrate))
names(transUH)[3] <- "NO3precip"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPnssNitrate, lat = 55.065)
transJEP <- mapJEPnssNitrate[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, NO3precip))
names(transJEP)[3] <- "NO3precip"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transnssNitrate <- rbind.fill(transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transnssNitrate, lon > -8 & lon < 3), x = "lon", y = "NO3precip", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```

### 3.10 Ammonium in precipitation

First we will extract the ammonium in precipitation data.

```
ammoniumPrecip.results <- subset(all.results, species == "ammonium")
```

Save the basic results for post-processing if necessary.

```
save(so2.results, no2.results, nh3.results, hno3.results, nh4.results, nitrate.results, nssS04.results,
     nssS04precip.results, nitratePrecip.results, ammoniumPrecip.results, file = "depositionResults.RData")
```

```
modStats(ammoniumPrecip.results, type = "group", mod = "predicted", obs = "measured")
```

**Table 11:** Summary model evaluation statistics for annual mean ammonium in precipitation concentrations.

group	n	FAC2	MB	MGE	NMB	NMGE	RMSE	r
CMAQ.JEP	37.00	0.89	-1.26	8.28	-0.05	0.34	9.72	0.70
CMAQ.UH	37.00	0.84	-8.61	9.62	-0.36	0.40	12.00	0.79
EMEP4UK	37.00	0.84	-5.66	8.52	-0.23	0.35	10.62	0.70
EMEPUnified	37.00	0.89	-4.01	6.67	-0.17	0.28	8.78	0.79
FRAME	37.00	0.78	-1.73	9.08	-0.07	0.38	11.17	0.57
HARM	37.00	0.86	-4.67	7.73	-0.19	0.32	9.43	0.75
NAME	37.00	0.78	-3.98	9.39	-0.16	0.39	11.17	0.52

```
scatterPlot(ammoniumPrecip.results, x = "measured", y = "predicted", type = "group", mod.line = TRUE,
            smooth = FALSE, pch = 16, key = FALSE)
```

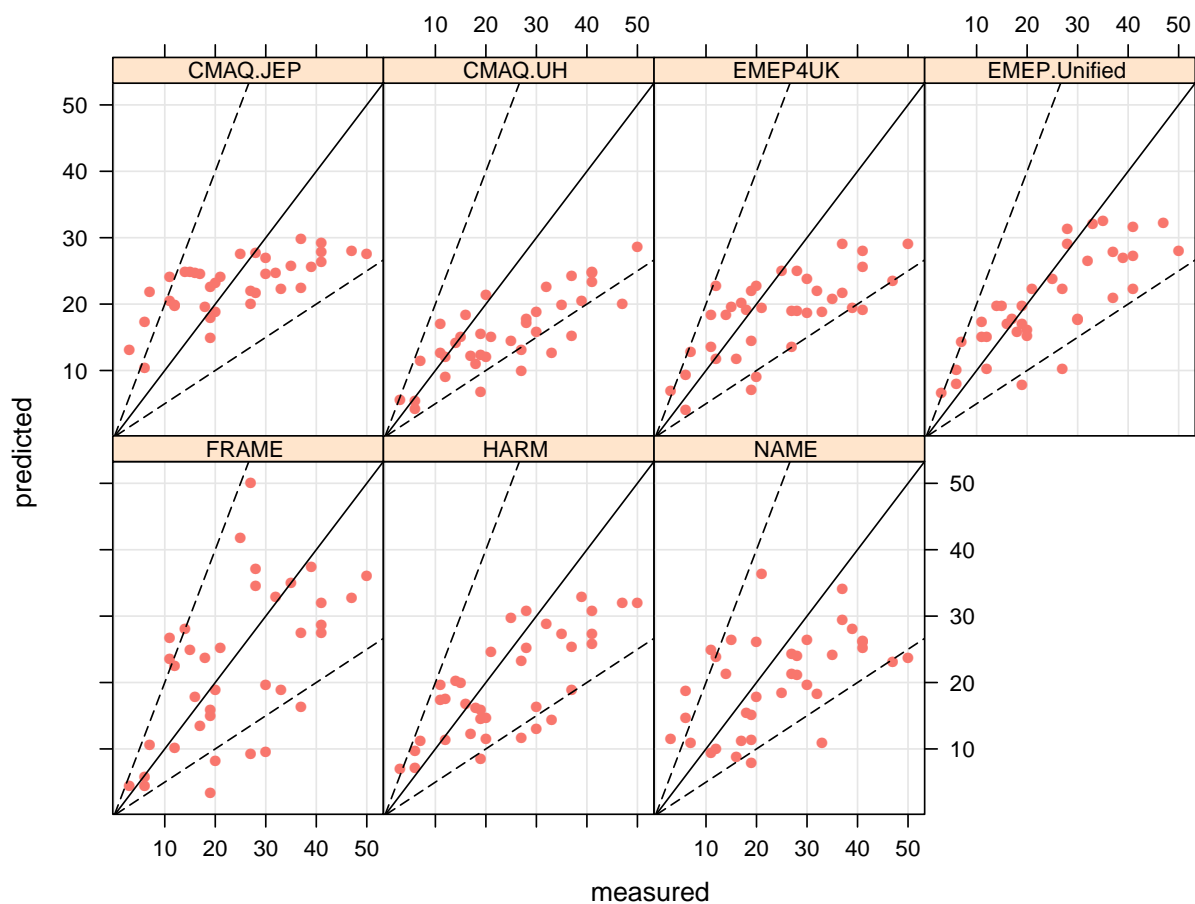
```
makeMap(mapNAMEwet, pollutant = "ammoniumPrecip", aspect = "iso")
```

```
EMEPnss_ammonium <- read.csv("depositionTemplateV1.0_EMEP4UK_rv3.7_final_SURFACE_MAP_ammonium_ueq1-1.csv",
                           header = TRUE, na.strings = "missing")
EMEPnss_ammonium <- na.omit(EMEPnss_ammonium) ## remove missing data
EMEPnss_ammonium <- prepareGrid(EMEPnss_ammonium, pollutant = "ammonium.ueq.1.1")
makeMap(EMEPnss_ammonium, pollu="ammonium.ueq.1.1", aspect = "iso")
```

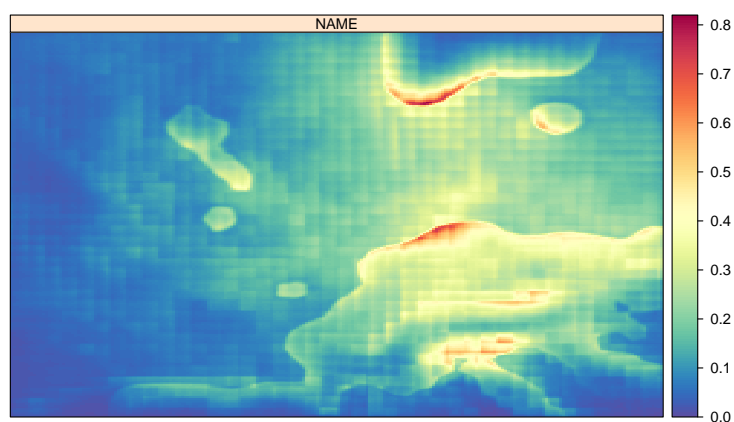
```
mapUHAmmonium <- prepareGrid(mapUH, pollutant = "ammonium")
makeMap(mapUHAmmonium, pollutant = "ammonium", aspect = "iso")
```

```
mapJEPAmmonium <- prepareGrid(mapJEP, pollutant = "NH4precip")
makeMap(mapJEPAmmonium, pollutant = "NH4precip", aspect = "iso")
```

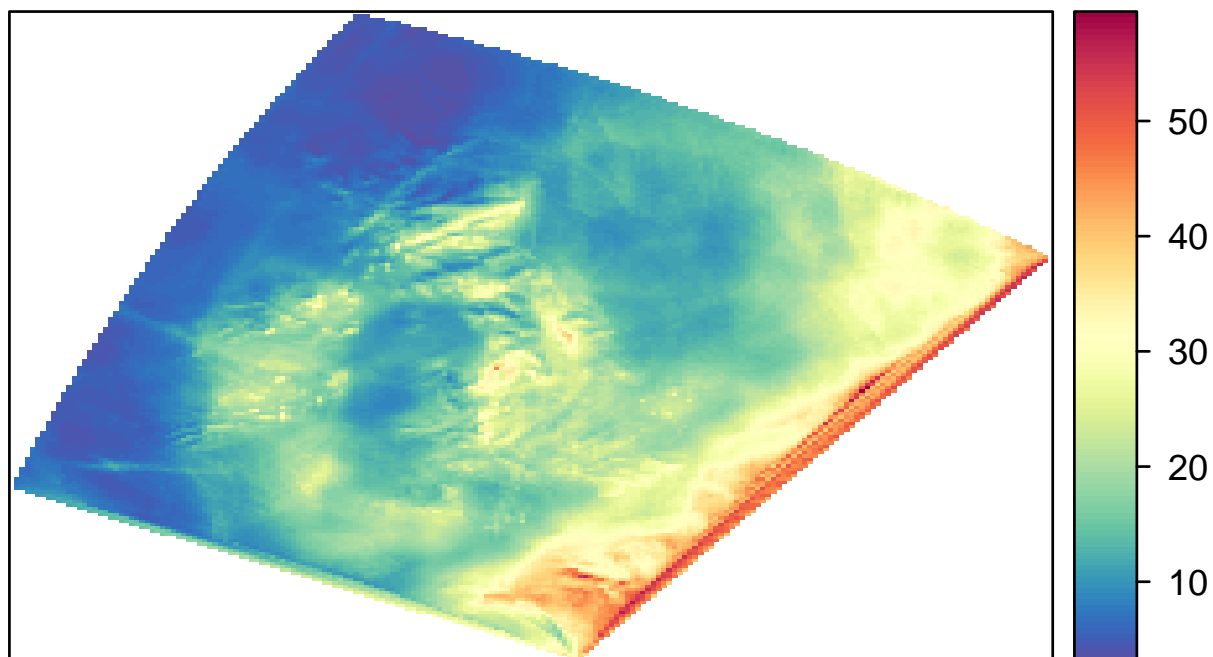
```
FRAMENHxWet <- prepareGrid(mapFRAMEwet, pollutant = "grd_NHx_wet")
makeMap(FRAMENHxWet, pollutant = "grd_NHx_wet", aspect = "iso")
```



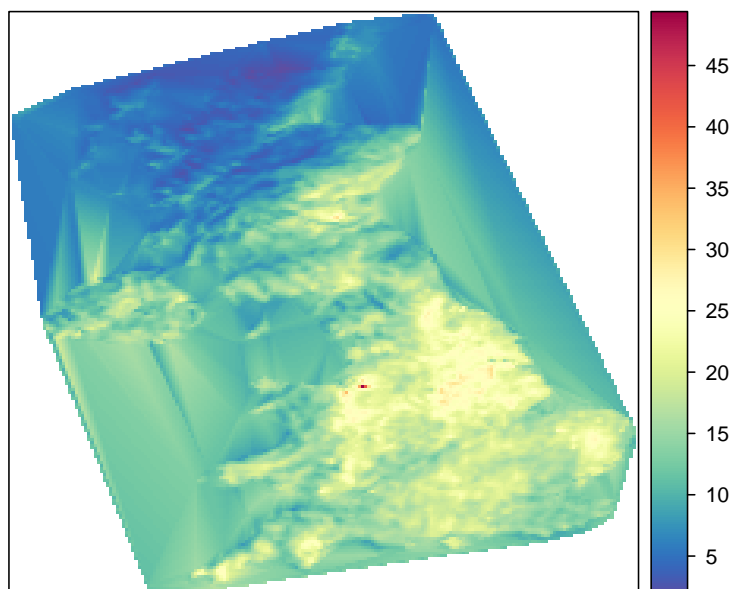
**Figure 73:** Measured versus predicted annual mean ammonium in precipitation concentrations.



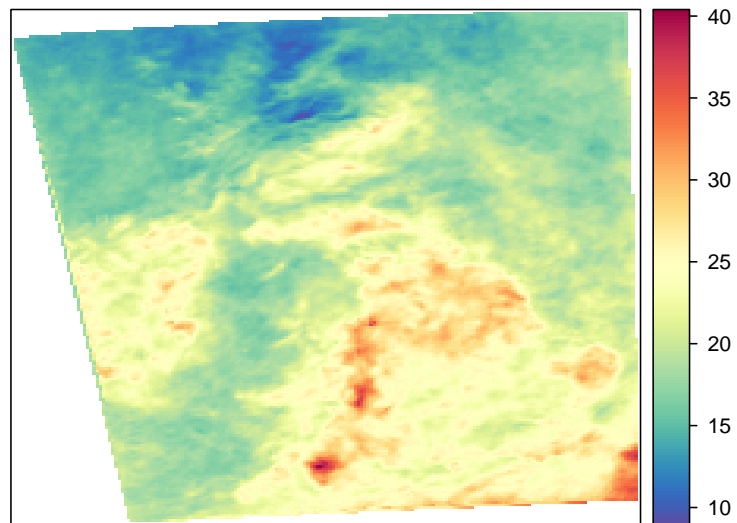
**Figure 74:** Annual mean ammonium from wet deposition using the NAME model (in  $\text{g m}^2 \text{yr}^{-1}$ ).



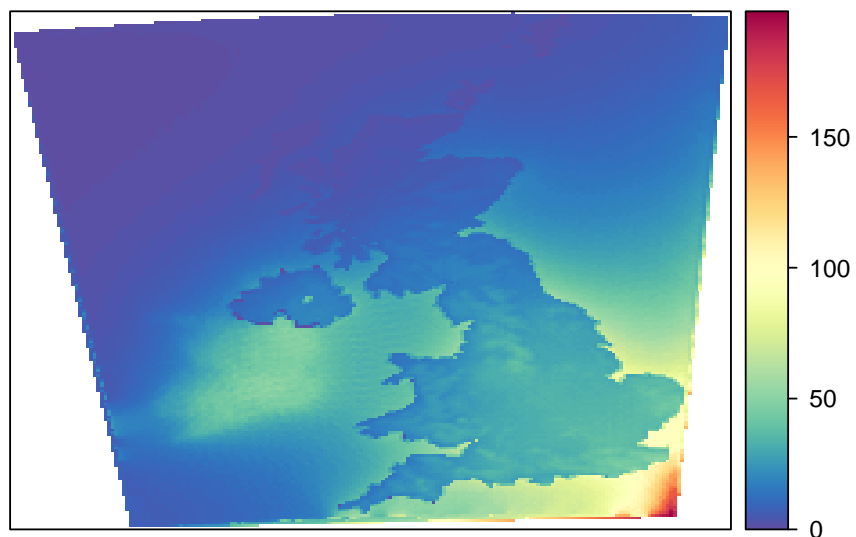
**Figure 75:** Annual mean ammonium in precipitation from the EMEP4UK model.



**Figure 76:** Annual mean ammonium in precipitation from the CMAQ University of Hertfordshire model.

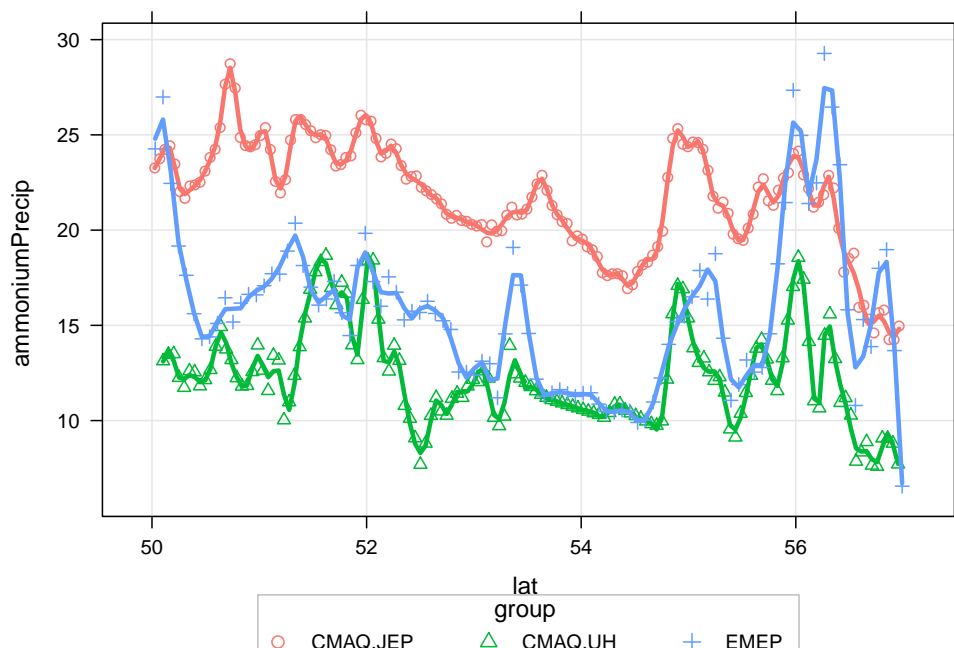


**Figure 77:** Annual mean ammonium in precipitation from the CMAQ JEP model.



**Figure 78:** Annual mean ammonium in precipitation from the FRAME model.





**Figure 79:** Transect of ammonium in precipitation concentrations along  $-4.05$  longitude.

The transects are calculated by:

```
## NAME
id <- nearest(mapNAMEwet, lon = -4.05)
transNAME <- mapNAMEwet[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, ammoniumPrecip))
names(transNAME)[3] <- "ammoniumPrecip"
transNAME$group <- "NAME"

## EMEP
id <- nearest(EMEPnss_ammonium, lon = -4.05)
transEMEP <- EMEPnss_ammonium[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, ammonium.ueq.l.1))
names(transEMEP)[3] <- "ammoniumPrecip"
transEMEP$group <- "EMEP"

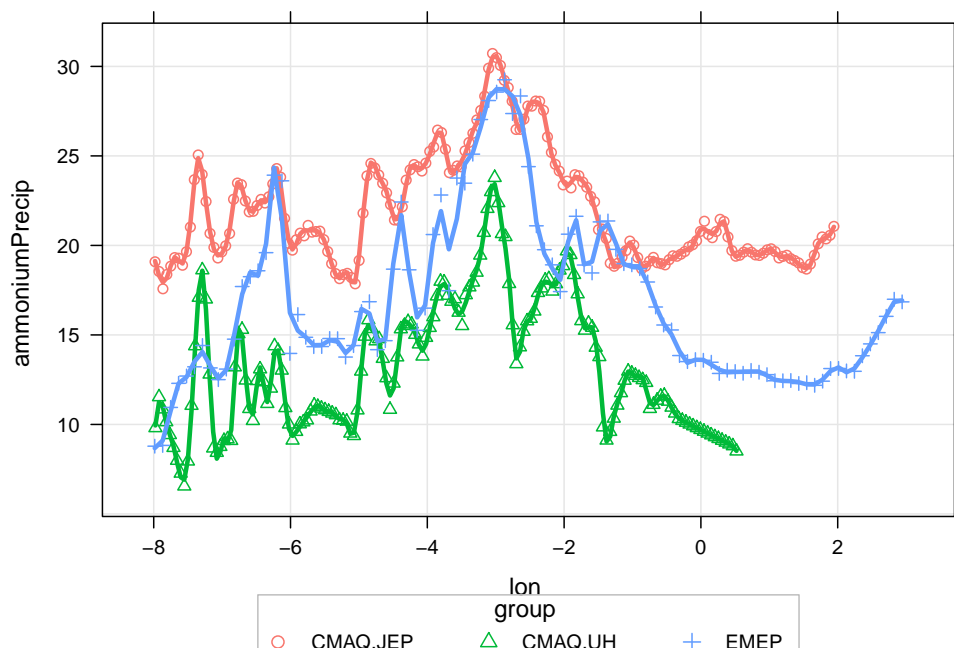
## FRAME
id <- nearest(FRAMENHxWet, lon = -4.05)
transFRAME <- FRAMENHxWet[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, grd_NHx_wet))
transFRAME$group <- "FRAME"

## CMAQ UH
id <- nearest(mapUHAmmonium, lon = -4.05)
transUH <- mapUHAmmonium[id , ]
transUH <- subset(transUH, select = c(lat, lon, ammonium))
names(transUH)[3] <- "ammoniumPrecip"
transUH$group <- "CMAQ.UH"

## CMAQ JEP
id <- nearest(mapJEPAmmonium, lon = -4.05)
transJEP <- mapJEPAmmonium[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, NH4precip))
names(transJEP)[3] <- "ammoniumPrecip"
transJEP$group <- "CMAQ.JEP"

## now combine all the results
transnssAmmonium <- rbind.fill(transEMEP, transUH, transJEP, transFRAME)

## now we can plot it
scatterPlot(subset(transnssAmmonium, lat > 50 & lat < 57), x = "lat", y = "ammoniumPrecip", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```



**Figure 80:** Transect of ammonium in precipitation along 55.065 latitude.

```
## NAME
id <- nearest(mapNAMEwet, lat = 55.065)
transNAME <- mapNAMEwet[id , ]
transNAME <- subset(transNAME, select = c(lat, lon, ammoniumPrecip))
names(transNAME)[3] <- "ammoniumPrecip"
transNAME$group <- "NAME"
## EMEP
id <- nearest(EMEPnss_ammonium, lat = 55.065)
transEMEP <- EMEPnss_ammonium[id , ]
transEMEP <- subset(transEMEP, select = c(lat, lon, ammonium.ueq.l.1))
names(transEMEP)[3] <- "ammoniumPrecip"
transEMEP$group <- "EMEP"
## FRAME
id <- nearest(FRAMENHxWet, lat = 55.065)
transFRAME <- FRAMENHxWet[id , ]
transFRAME <- subset(transFRAME, select = c(lat, lon, grd_NHx_wet))
transFRAME$group <- "FRAME"
## CMAQ UH
id <- nearest(mapUHAMmonium, lat = 55.065)
transUH <- mapUHAMmonium[id , ]
transUH <- subset(transUH, select = c(lat, lon, ammonium))
names(transUH)[3] <- "ammoniumPrecip"
transUH$group <- "CMAQ.UH"
## CMAQ JEP
id <- nearest(mapJEPAmmonium, lat = 55.065)
transJEP <- mapJEPAmmonium[id , ]
transJEP <- subset(transJEP, select = c(lat, lon, NH4precip))
names(transJEP)[3] <- "ammoniumPrecip"
transJEP$group <- "CMAQ.JEP"
## now combine all the results
transsssAmmonium <- rbind.fill(transEMEP, transUH, transJEP, transFRAME)
## now we can plot it
scatterPlot(subset(transsssAmmonium, lon > -8 & lon < 3), x = "lon", y = "ammoniumPrecip", group = "group",
            smooth = FALSE, spline = TRUE, lwd = 3)
```

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## A Model performance evaluation statistics

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

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

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

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

$$0.5 \leq \frac{M_i}{O_i} \leq 2.0 \quad (1)$$

### 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.

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

### 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.

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

### 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.

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

### Normalised mean gross error, *NMGE*

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

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

**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.

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

**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.

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