



UK Research  
and Innovation



UK-SCAPE

UK Status, Change and Projections of the Environment

# Local Physical Chemistry Statements for Low cost sensor added value

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TFMM Warsaw 07.05.2024



UK Centre for  
Ecology & Hydrology

MANCHESTER  
1824

The University of Manchester



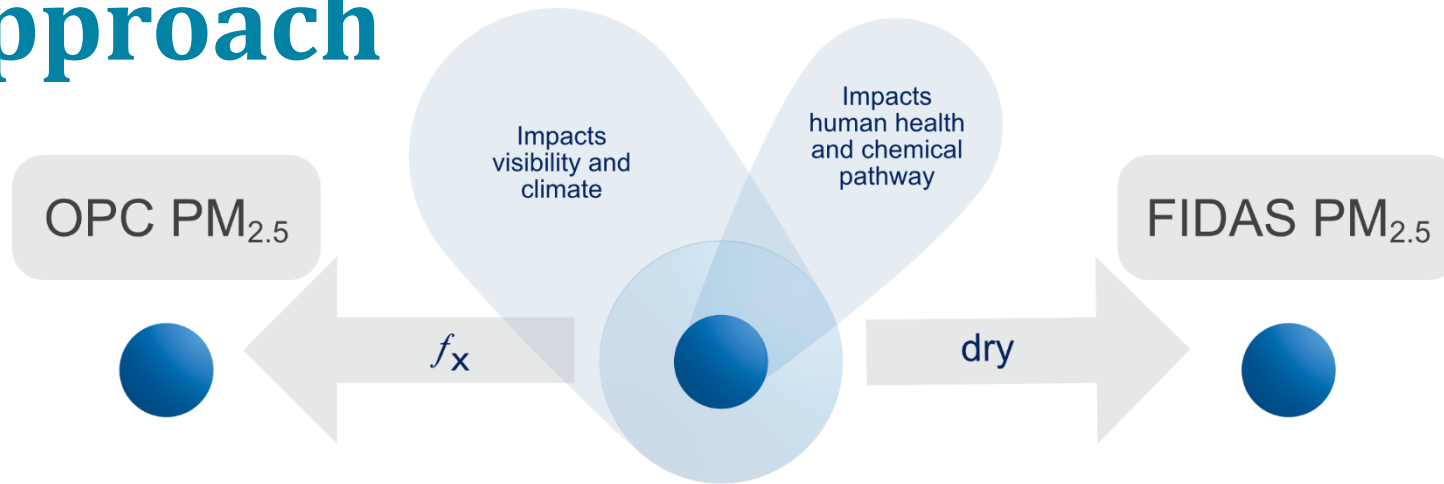
UNIVERSITY  
*of York*



UNIVERSITY OF  
BIRMINGHAM



# Approach



*Snider et al. (2016)* use  $\kappa$ -Köhler theory with hygroscopicity parameter  $\kappa$  (*Petters and Kreidenweis, 2007*) to calculate diameter  $D$  growth factors  $GF$  for chemicals depending on relative humidity

Calculate water mass for organics and inorganic salts  
BC and metal oxides assumed to be insoluble

$$GF = \left( a + k_v \frac{RH}{100 - RH} \right)^{1/3}$$

# Manchester supersite (20/02/2021 to 08/03/2021)

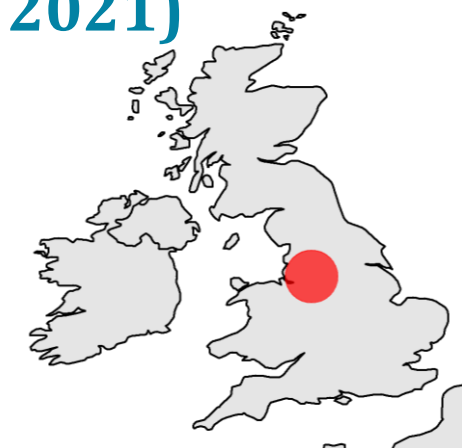
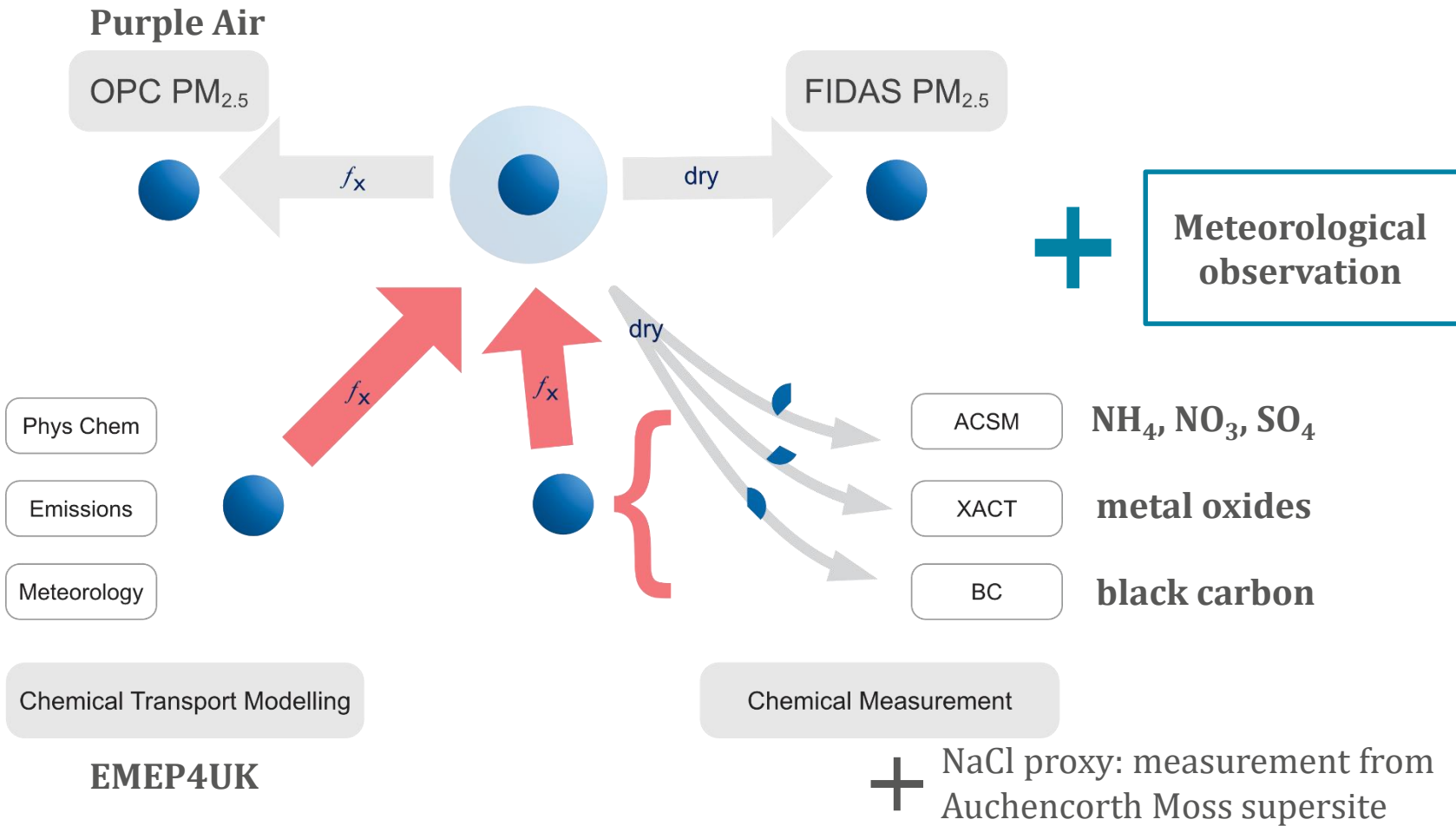
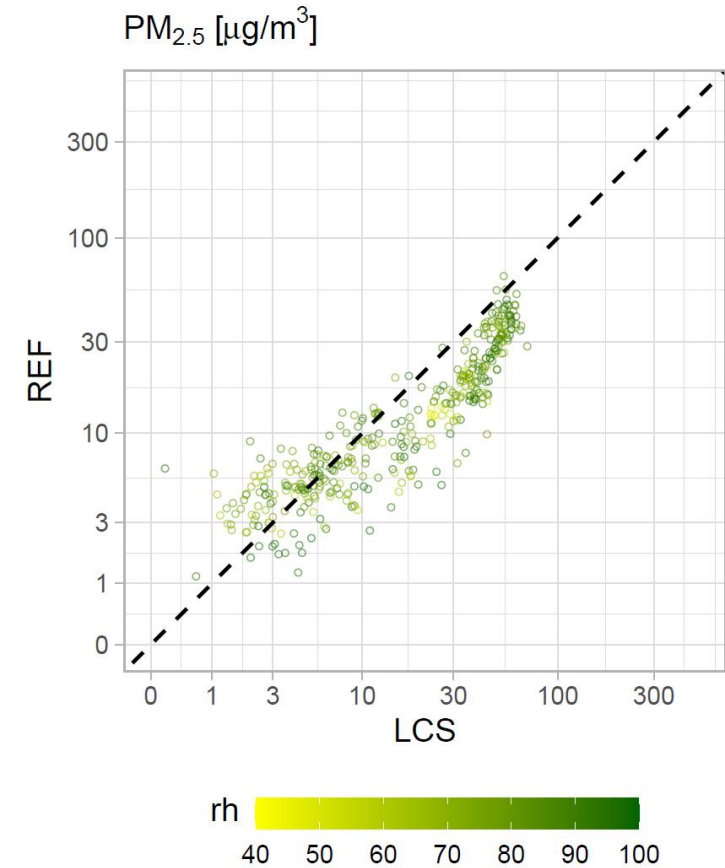
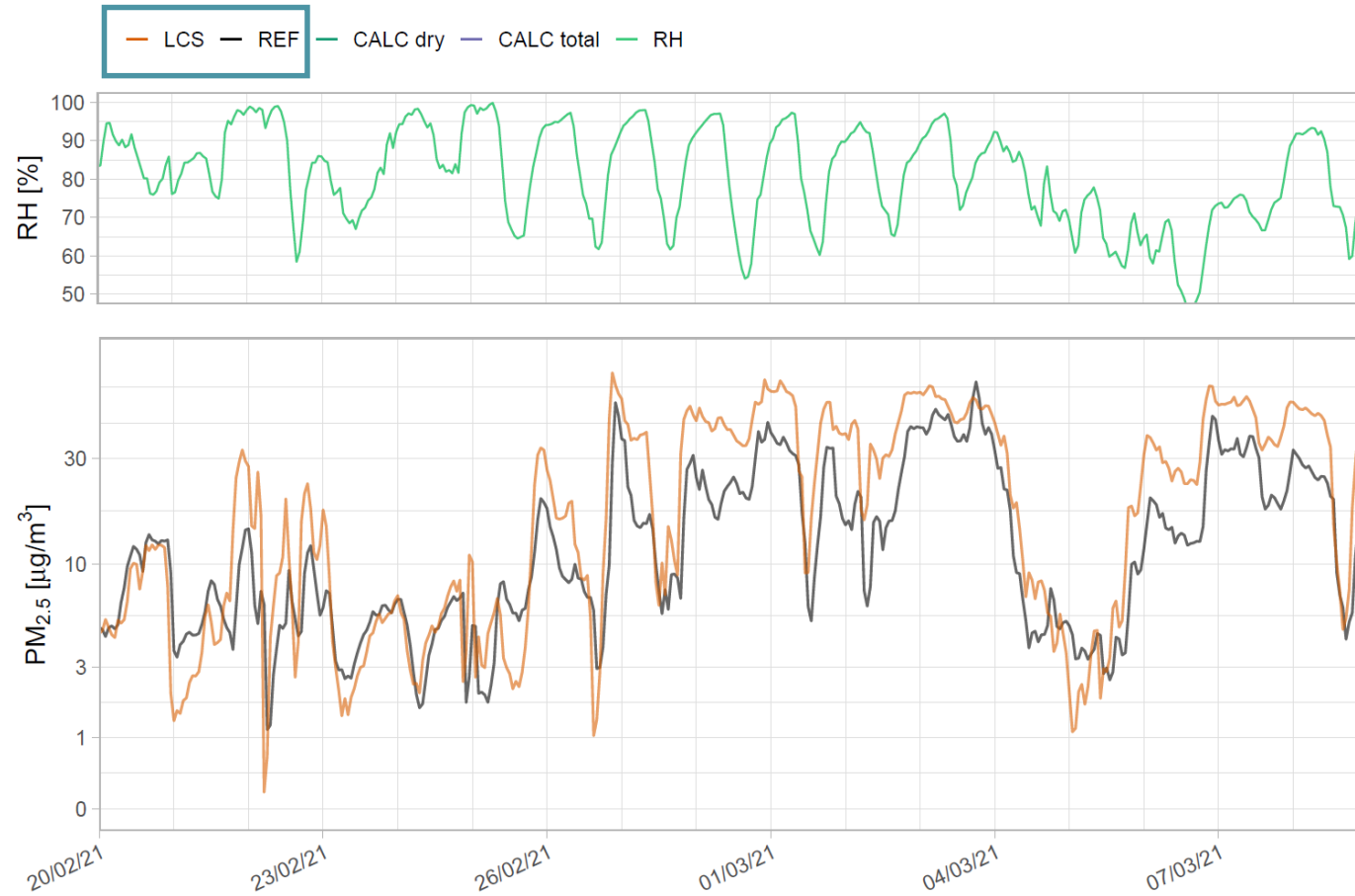


Photo: Michael Flynn

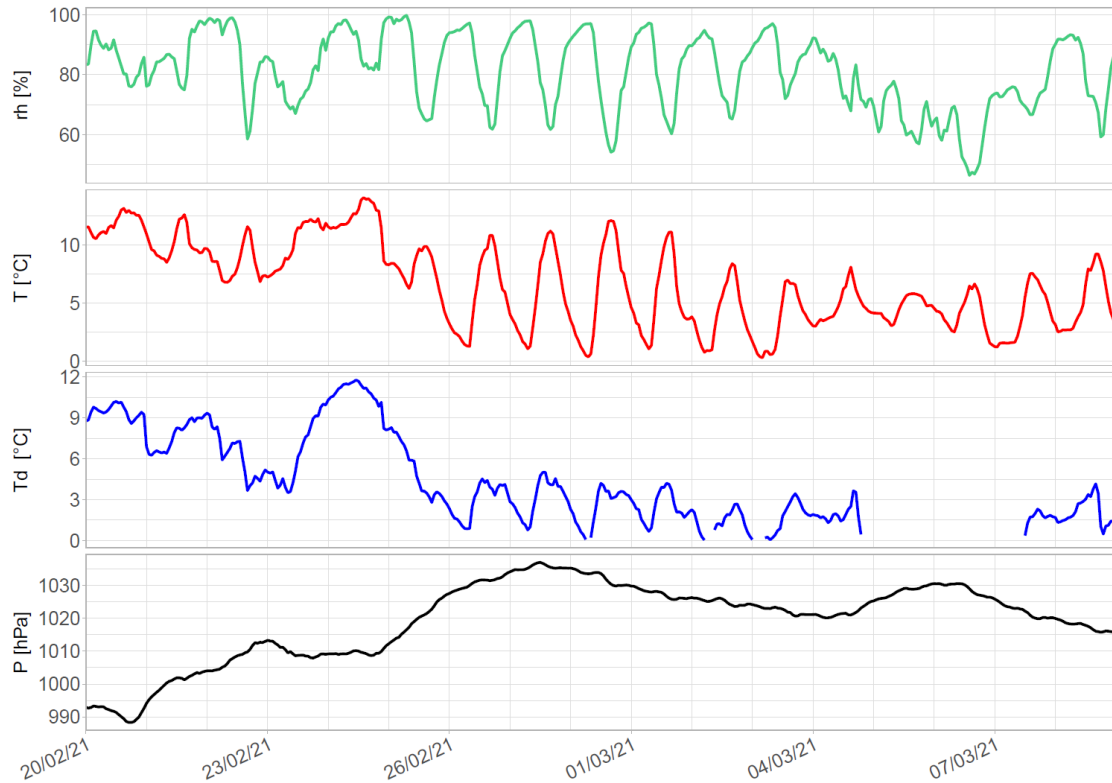
# Traditional approach



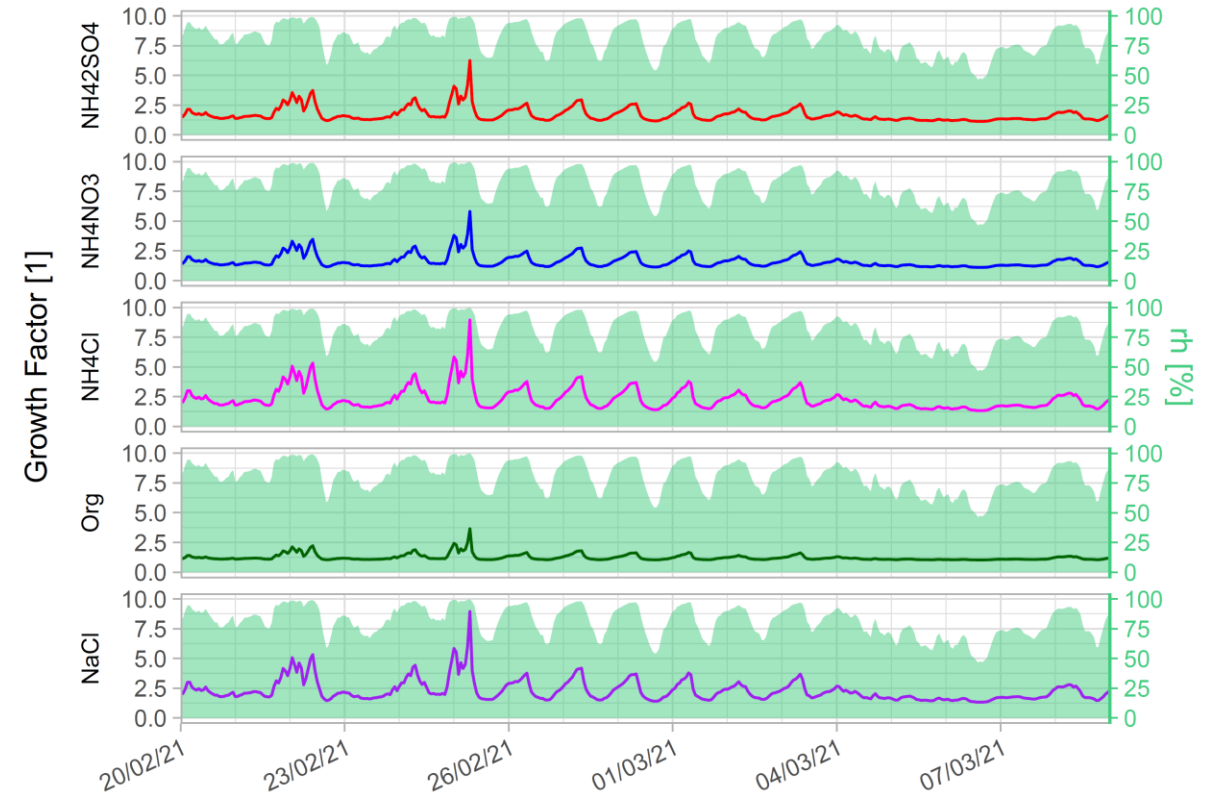


# Local Physical Chemistry Statement (LPCS) approach

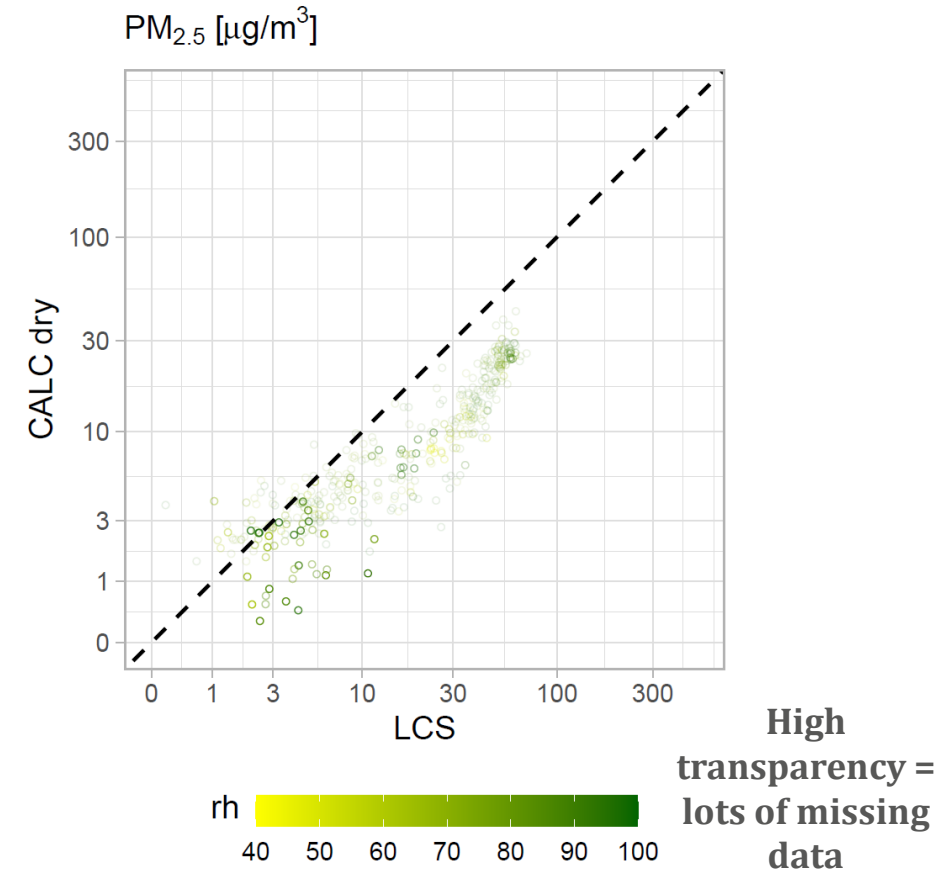
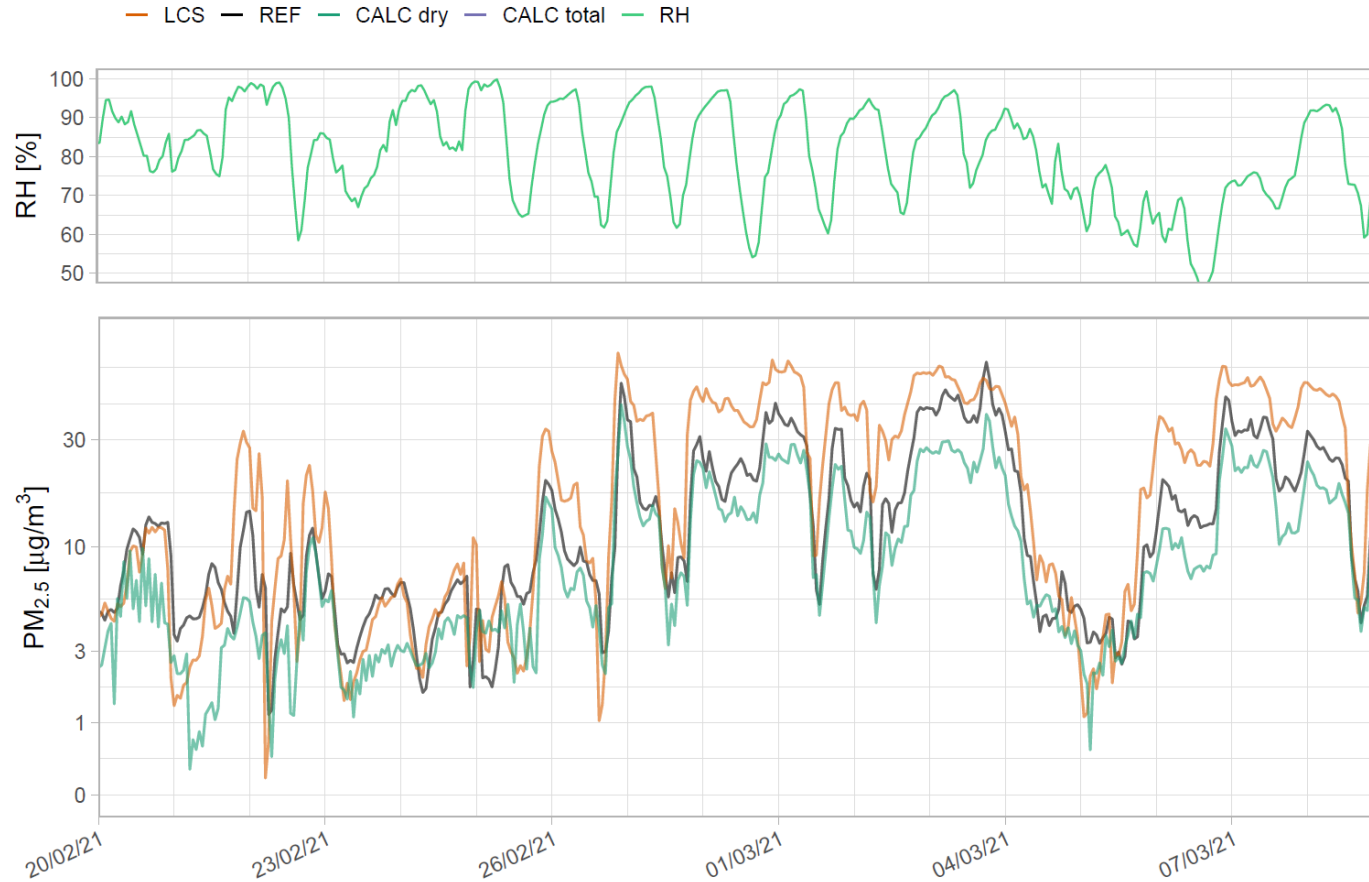
## Weather



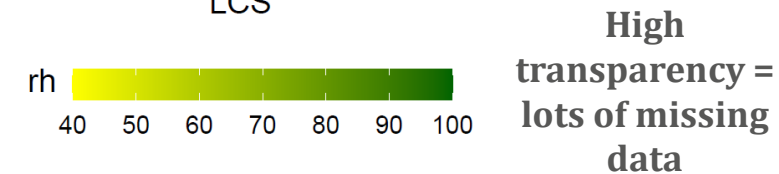
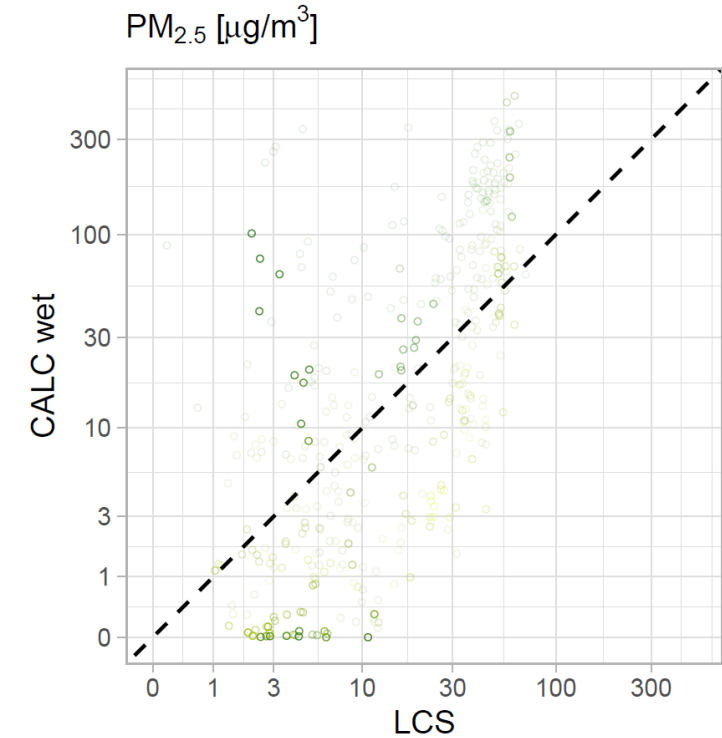
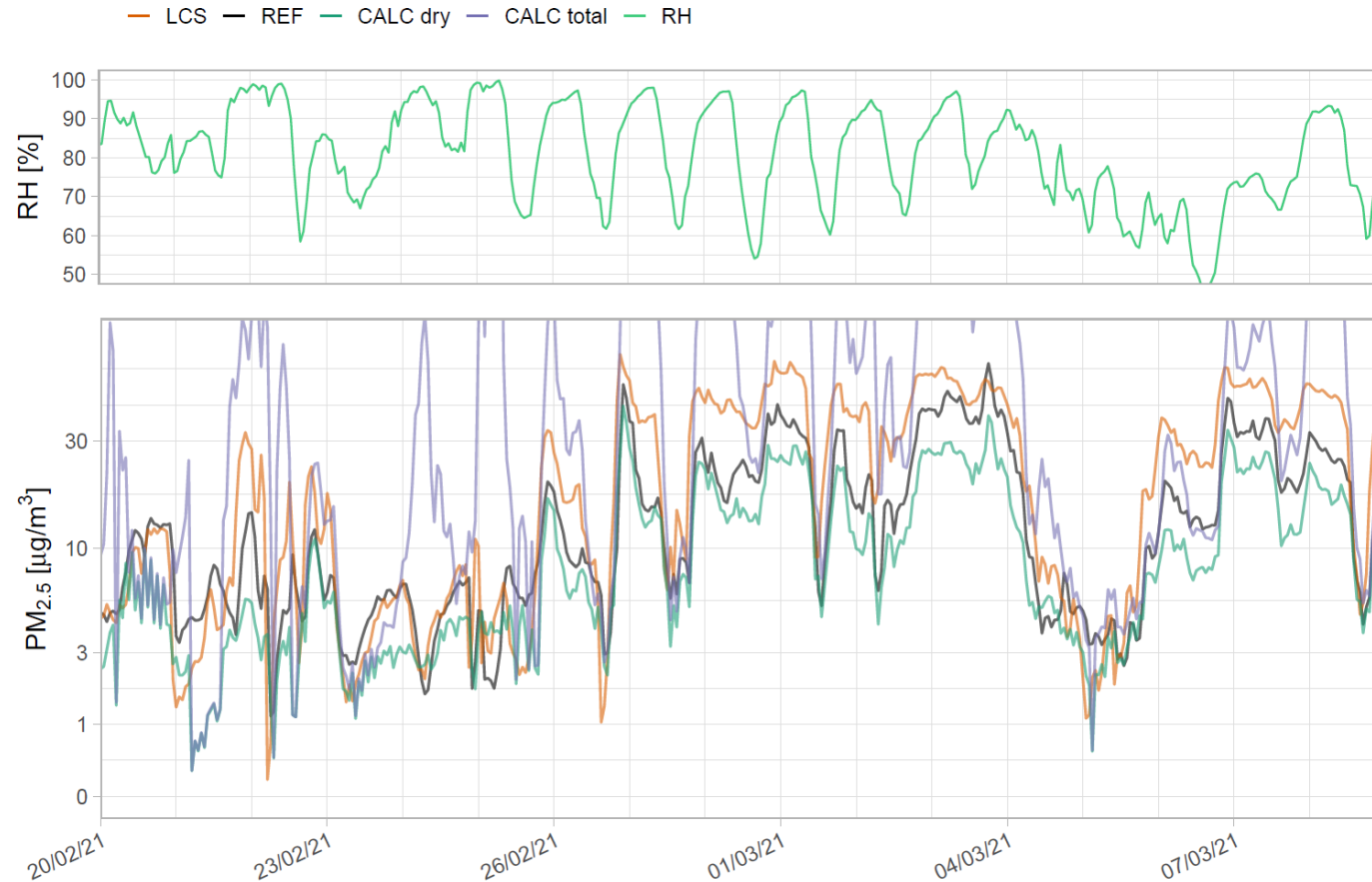
## Growth factors



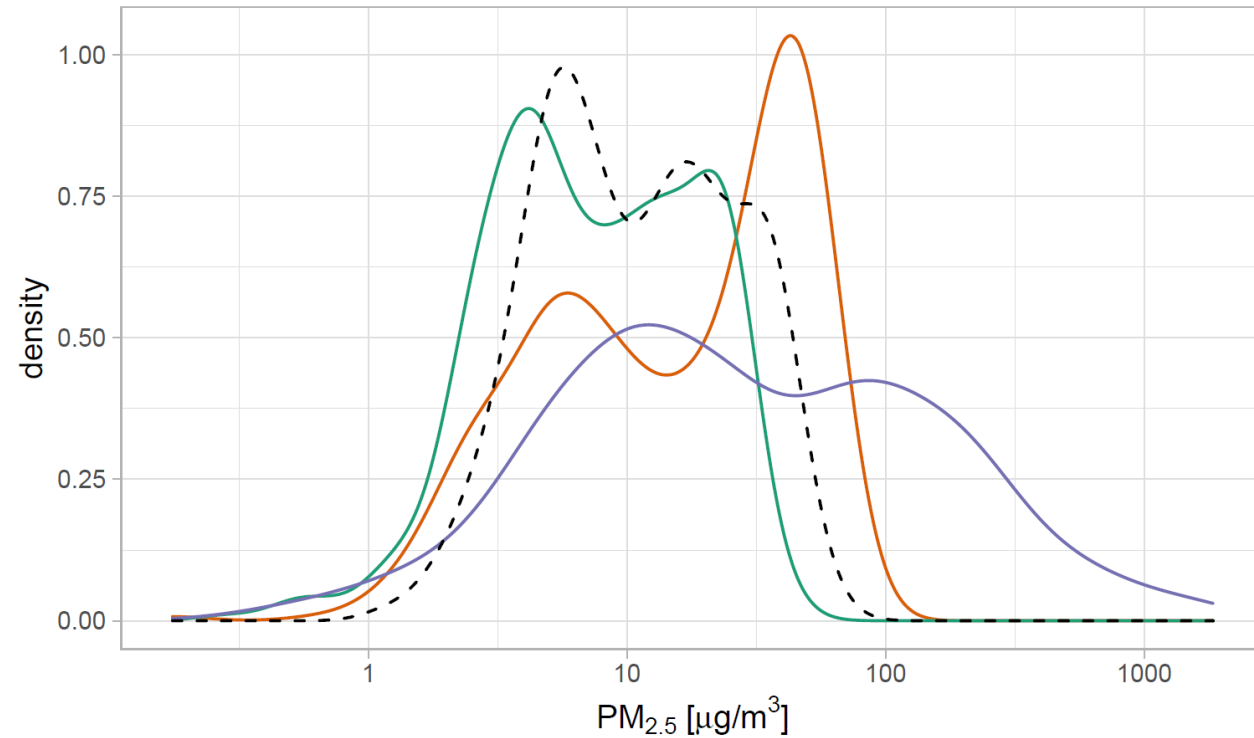
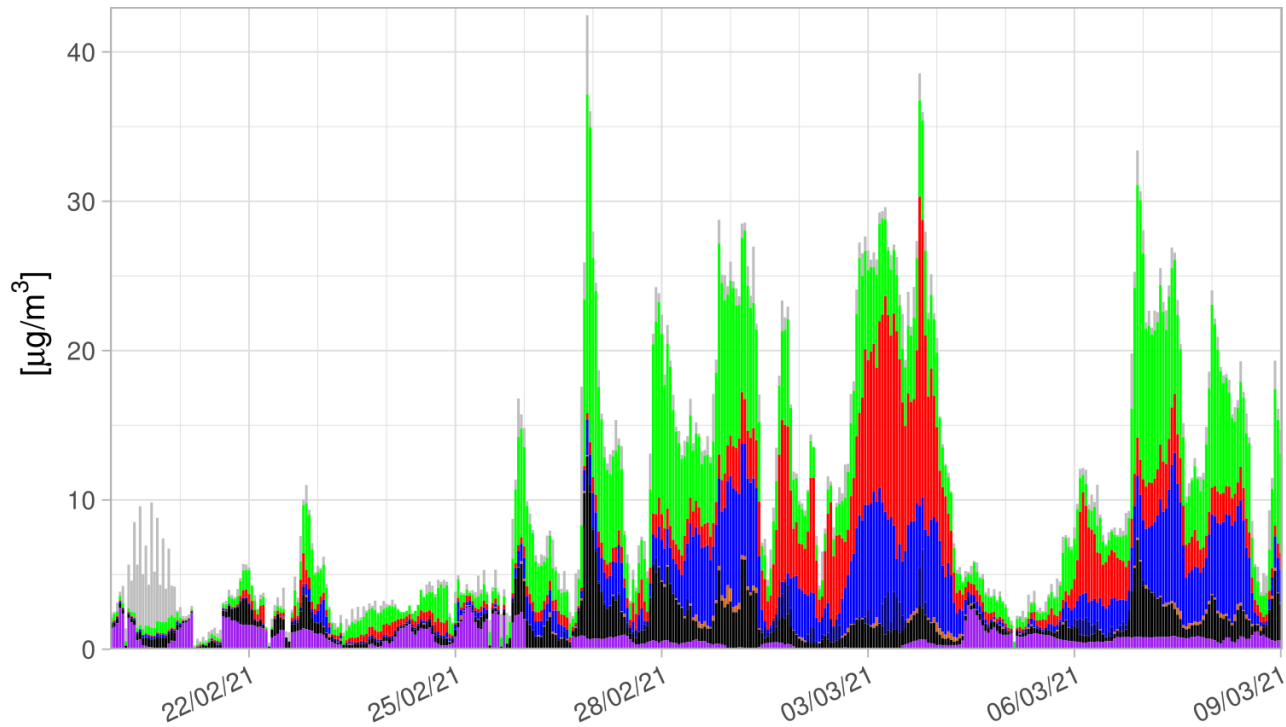
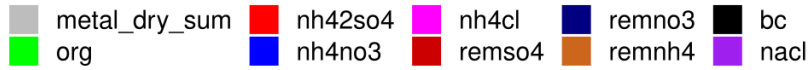
# Local Physical Chemistry Statement (LPCS) approach



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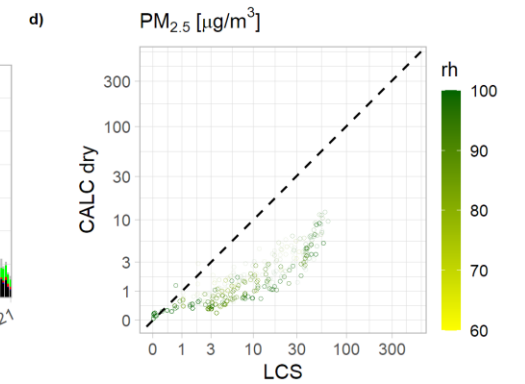
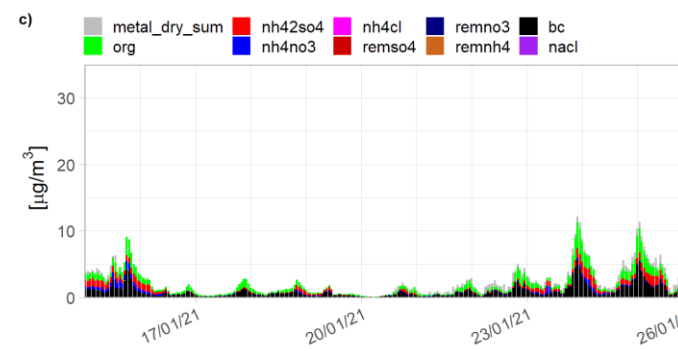
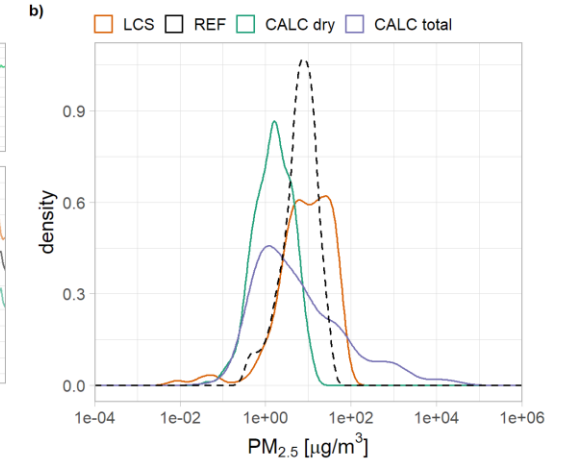
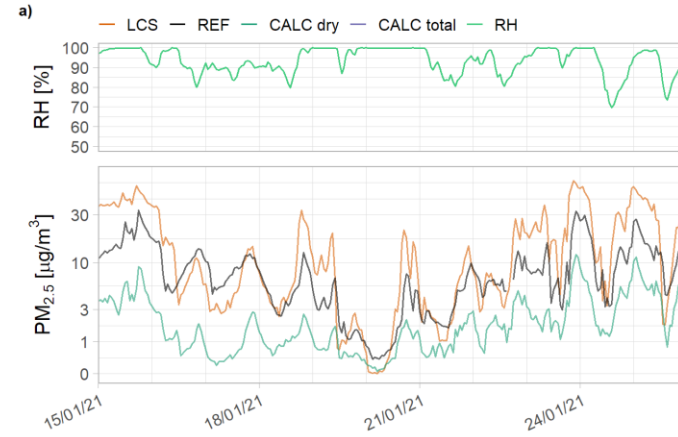
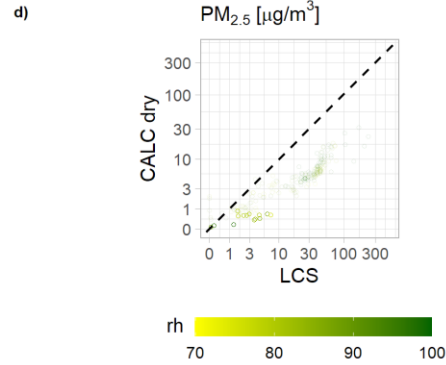
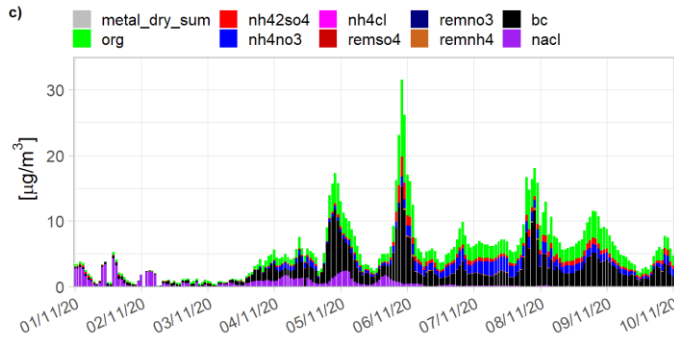
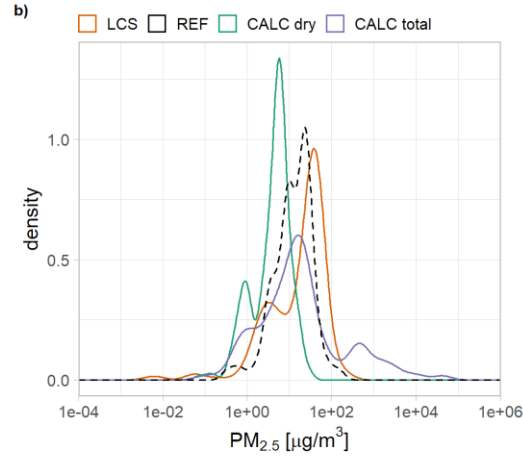
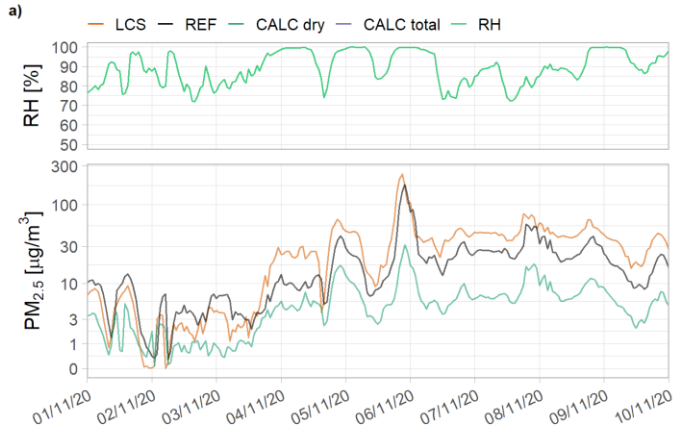




# Bonfire night

# winter storm

Storm Christoph 18-20/01/2021



# Local Physical Chemistry Statement

## Background of Tool

- modelled or forecast PM composition, RH, T
- Information about unusual conditions for location or time period

## User upload:

- Location of measurements
- Type of location
- LCS data (csv)

## Data report contains:

- Time series of mass concentration for LCS and chemicals
- Density distribution
- Correlation of predicted vs measured PM<sub>2.5</sub> mass concentration
- Information about local sources or conditions

- **gives power to non-expert user to interpret results of their LCS**
- **chemically sense-checks why and when the algorithm is working**

**Not everyone has super site, but EMEP4UK data -> tool**

# QUANT local sensor information

User input

Results

## Location selected

Click on the map or type in your coordinates, using the projection of your choice

### Projection

- WGS84 / EPSG:3857
- BNG / EPSG:27700

### Coordinates (Lng, Lat)

-1.71651000585488,54.7182750183023

Validate



Leaflet | Tiles © Esri — Source: Esri, i-cubed, USDA, USGS, AEX, GeoEye, Getmapping, Aerogrid, IGN, IGP, UPR-EGP, and the GIS User Community

## Location type selected

Please select one location type

- Farm
- Road site
- Other

## Local sensor raw data uploaded

Please select your local sensor type; this affects the raw data file format

- Purple Air
- Other

Upload your time series and local sensor type file formatted as specified on the right-hand side

Browse... MAN\_obs\_hm\_2021-02-20-2021-03-09\_total\_sum - Copy.csv

Upload complete

Select a subset of your time series (defaults to the whole time series)

2021-02-20

to

2021-03-09

Validate and go to Results

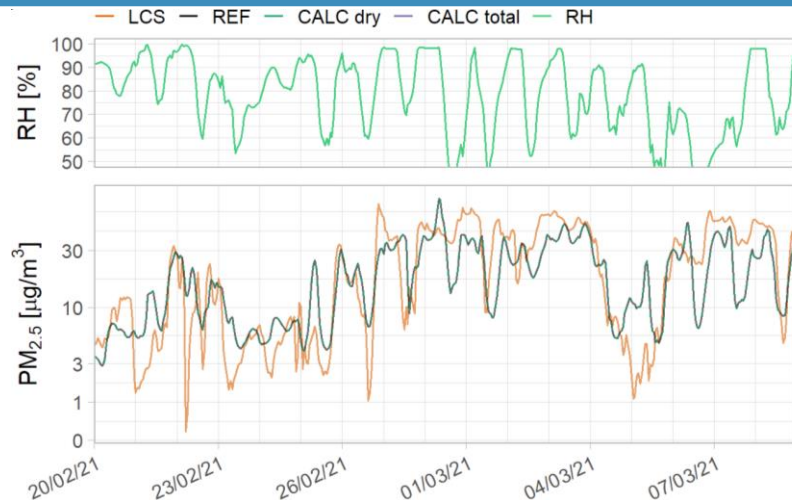
Your raw data file is formatted as specified below

The file total\_sum.csv should contain 1 row per measurement

The first column, date, contains a date, formatted as follows (beware of letters T and Z): "YYYY-MM-DDTHH:MM:SSZ". The second column, pm25\_lcs, contains PM25 measurements, as a numeric. The third column, lcs, describes the local sensor type, as a character

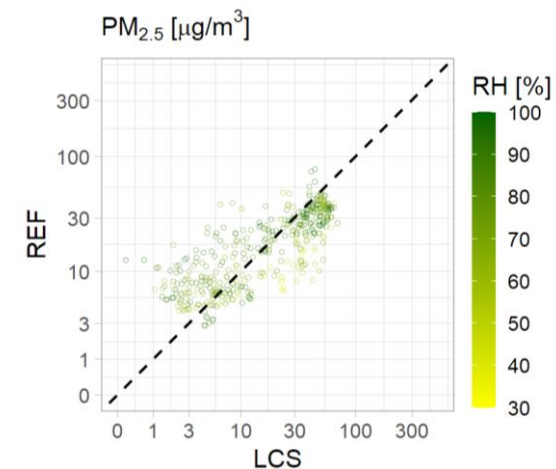
date	pm25_lcs	lcs
2021-02-20T00:00:00Z	4.568	Purple Air
2021-02-20T01:00:00Z	4.72266666666667	Purple Air
2021-02-20T02:00:00Z	5.3848275862069	Purple Air

## PM25 time series



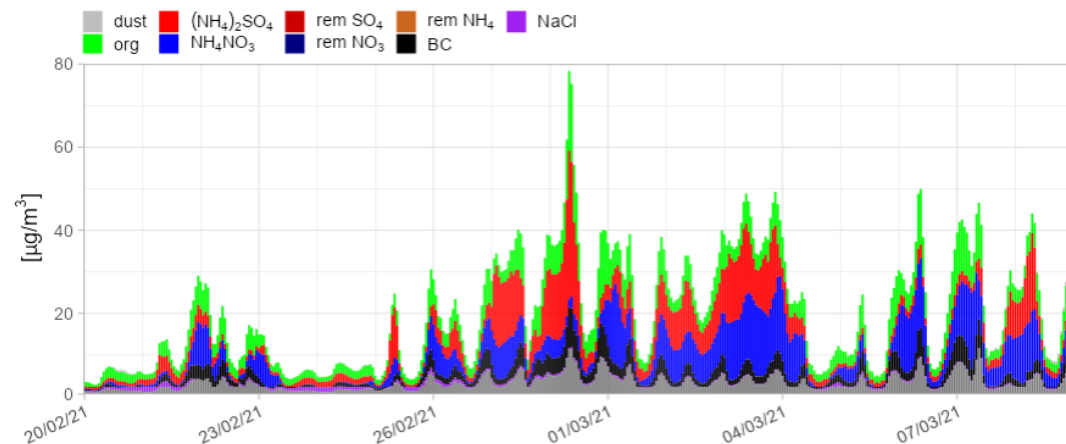
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## Scatter plot fit to reference



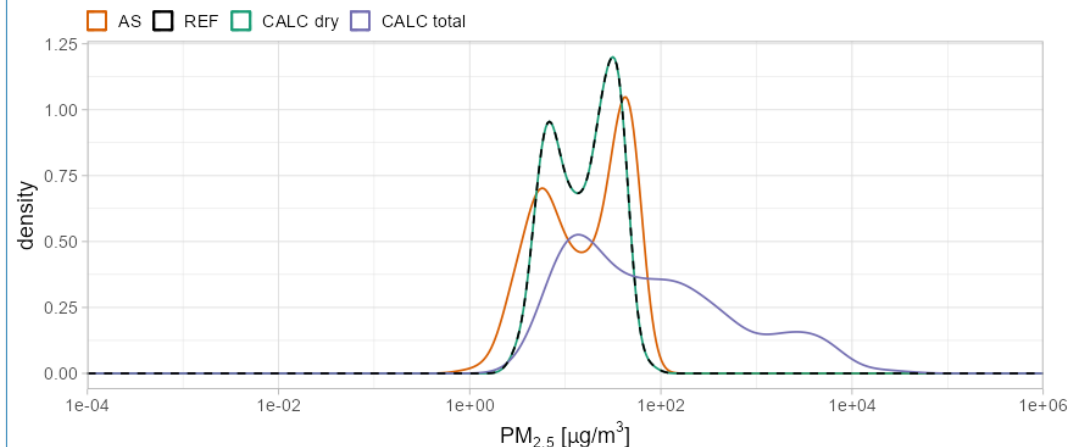
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## PM25 composition bar plot



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## Probability densities plot



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# Summary

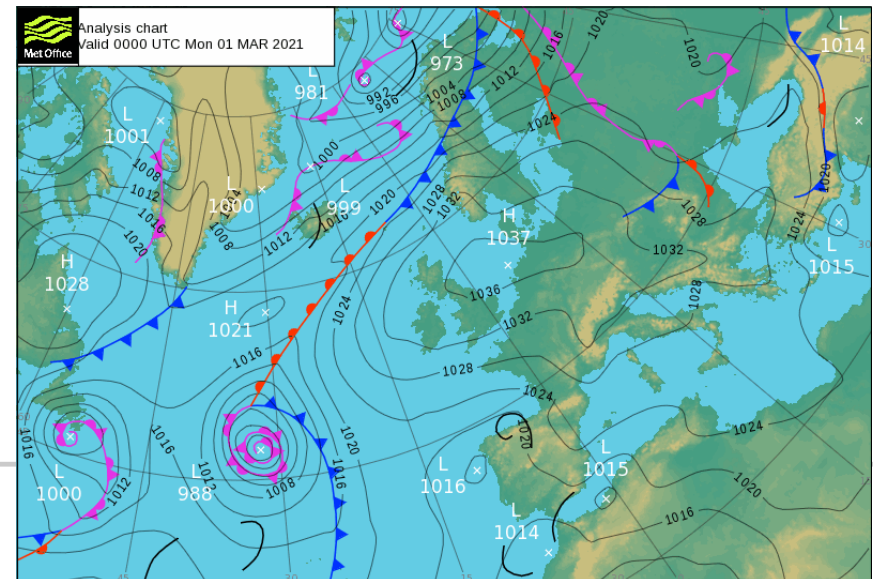
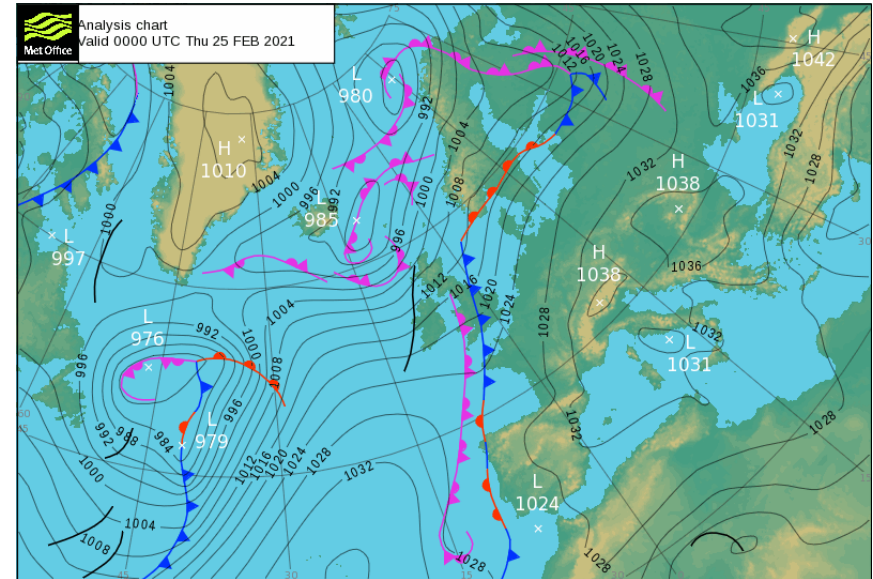
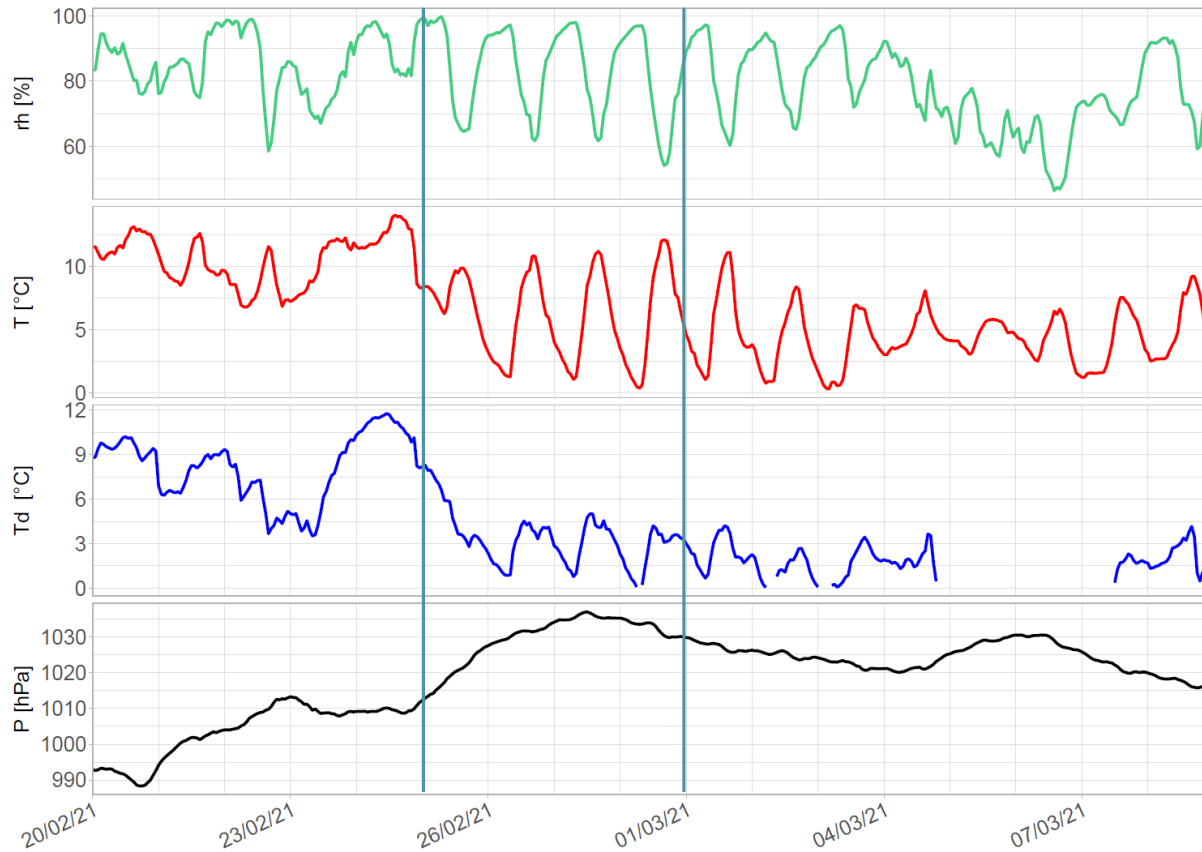
- Local Physical Chemistry statement developed
- App for using modelled EMEP4UK data to compare against measured air PM sensor data prototyped
- Given PM<sub>2.5</sub> chemical composition from global EMEP run, the LPCS may be a useful tool to non-specialist sensor users
- Next steps: develop app further for the UK and explore global options
- Approach is complementary to AI/ machine learning approaches



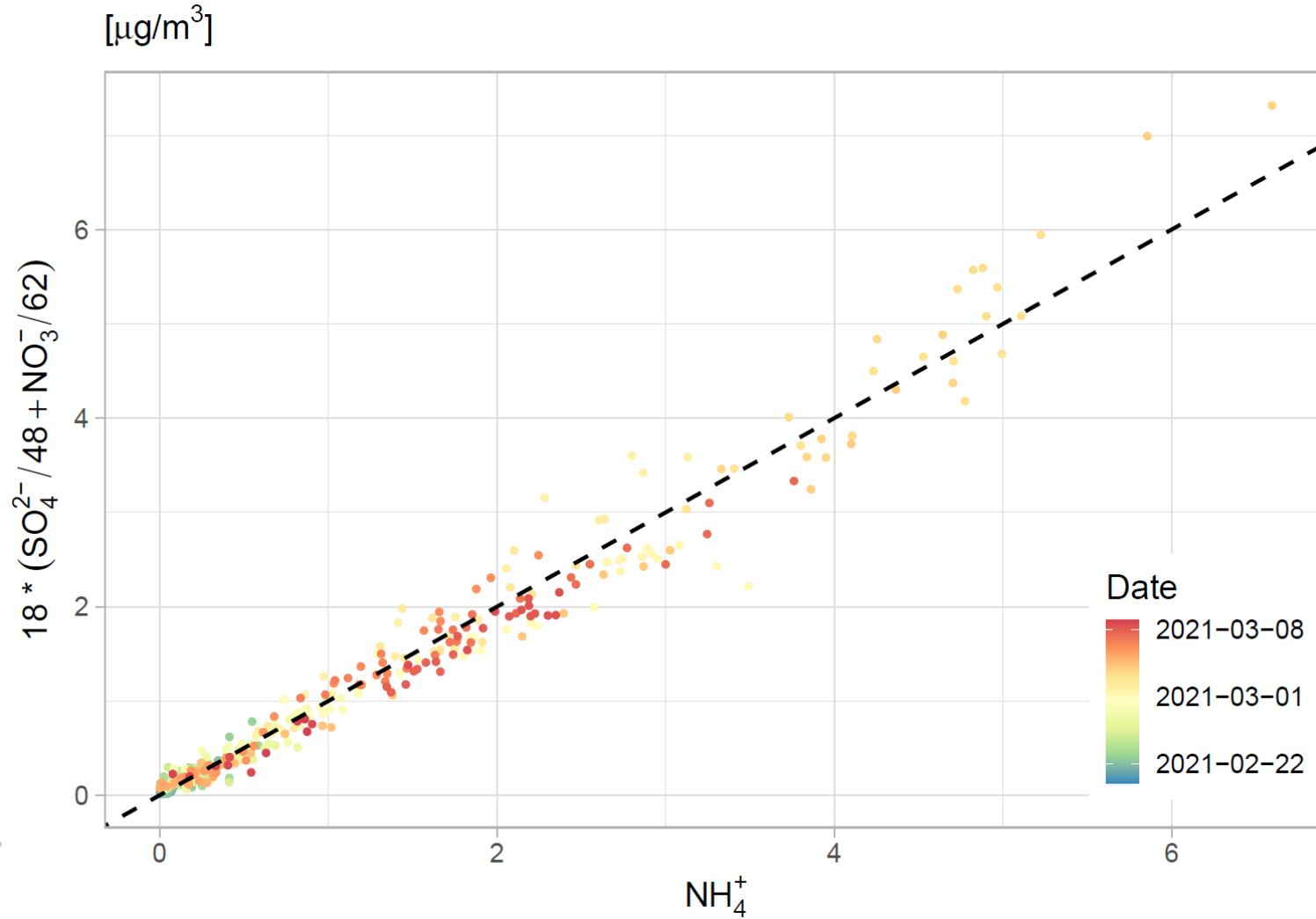
# Additional slides

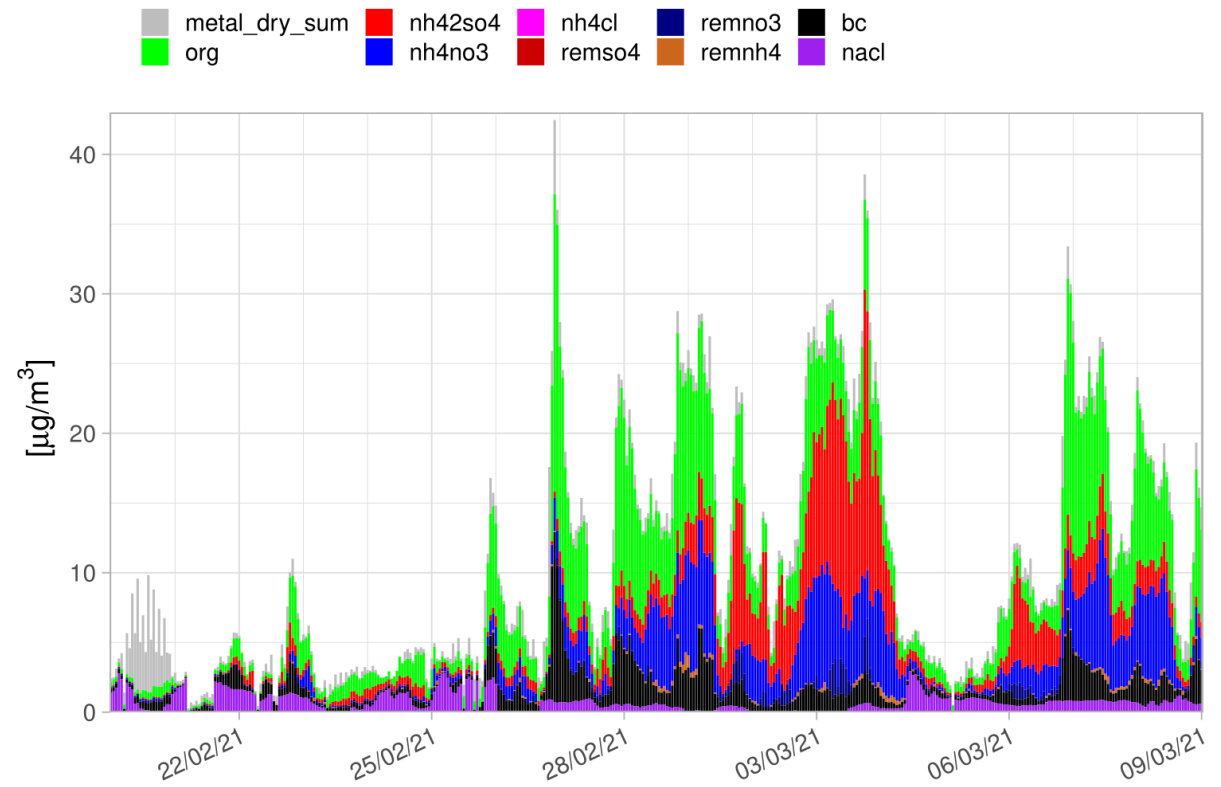
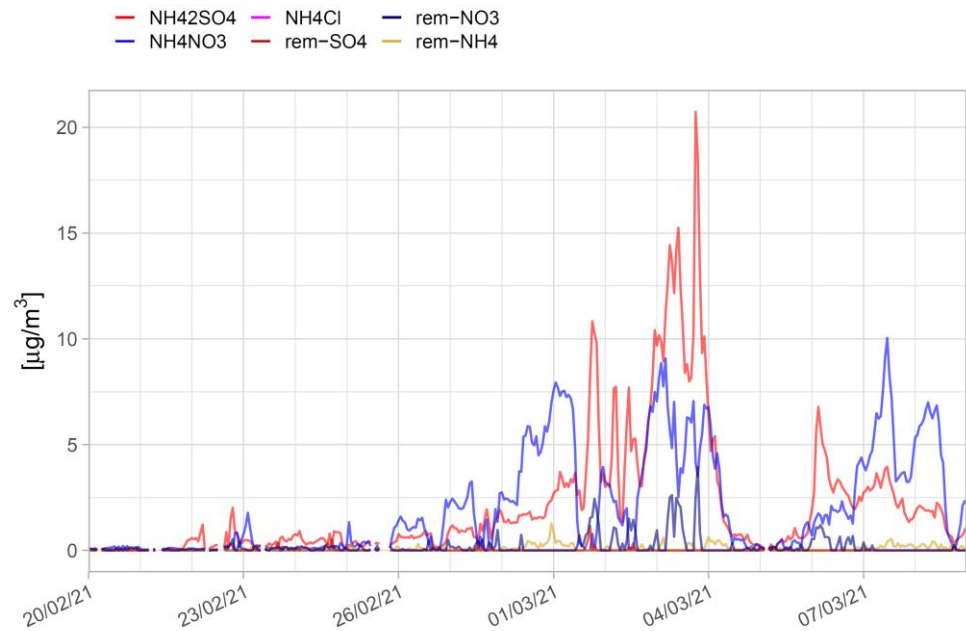
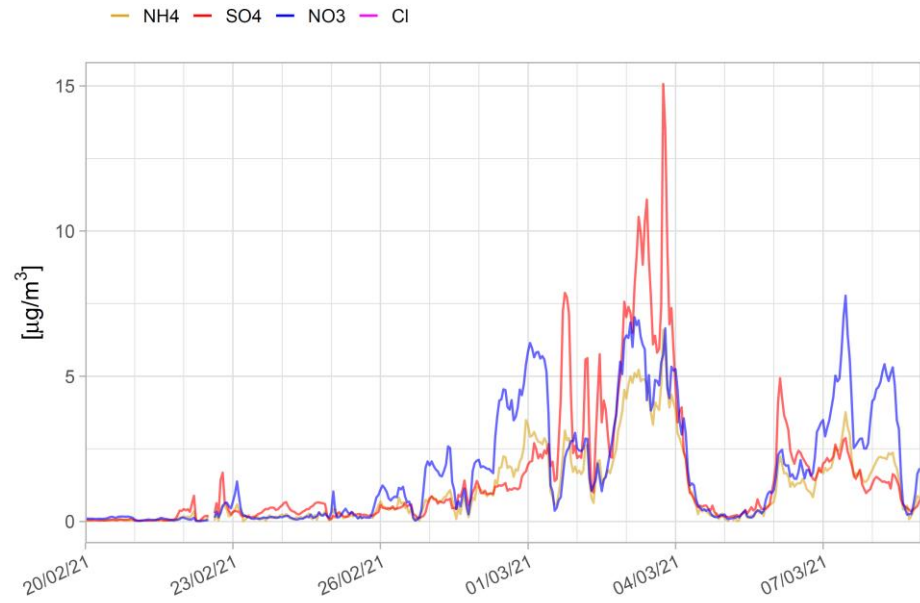
# Example period – Manchester – 20/02/2021 to 08/03/2021

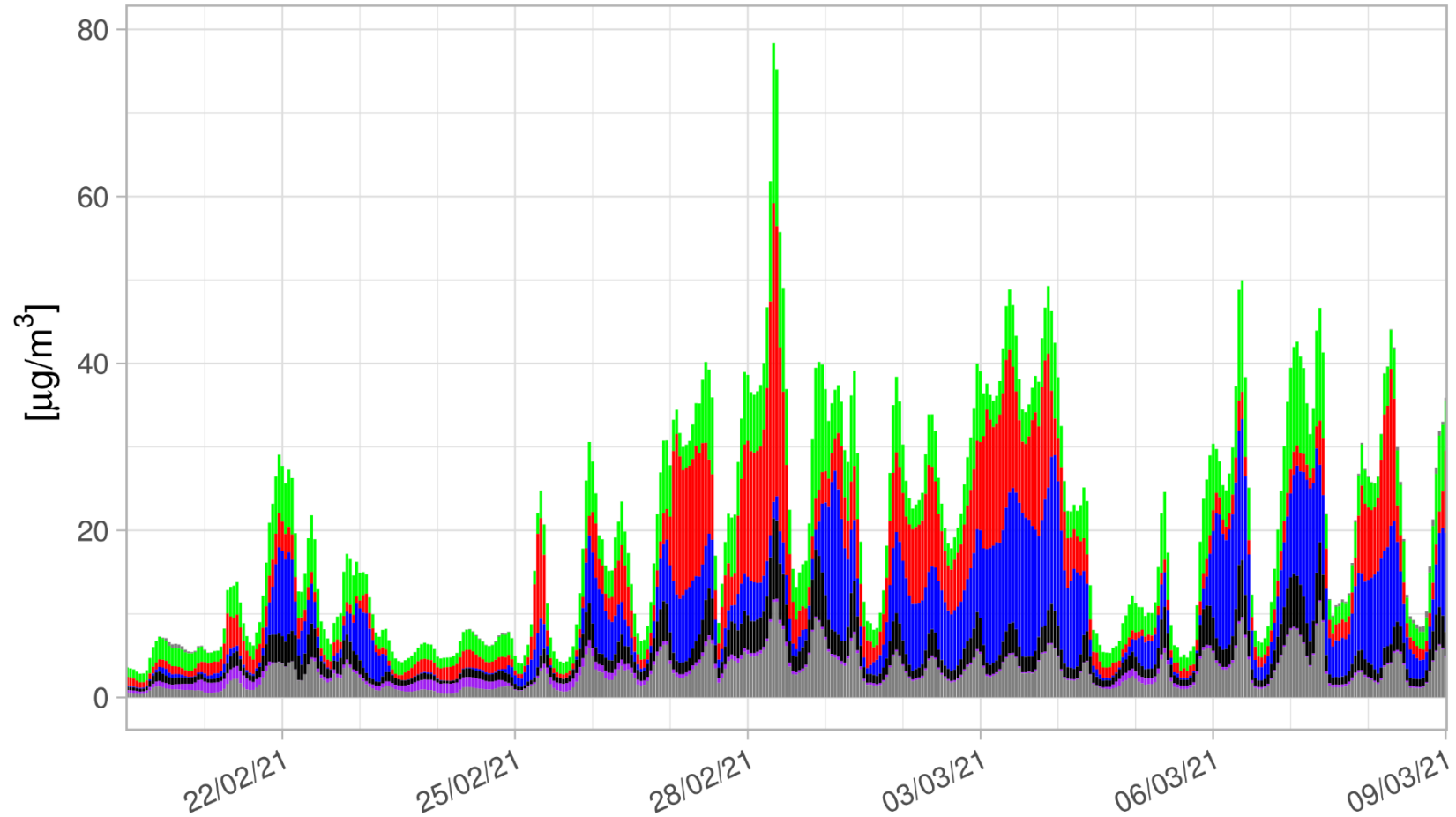
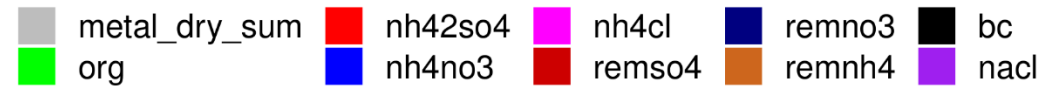
## Weather



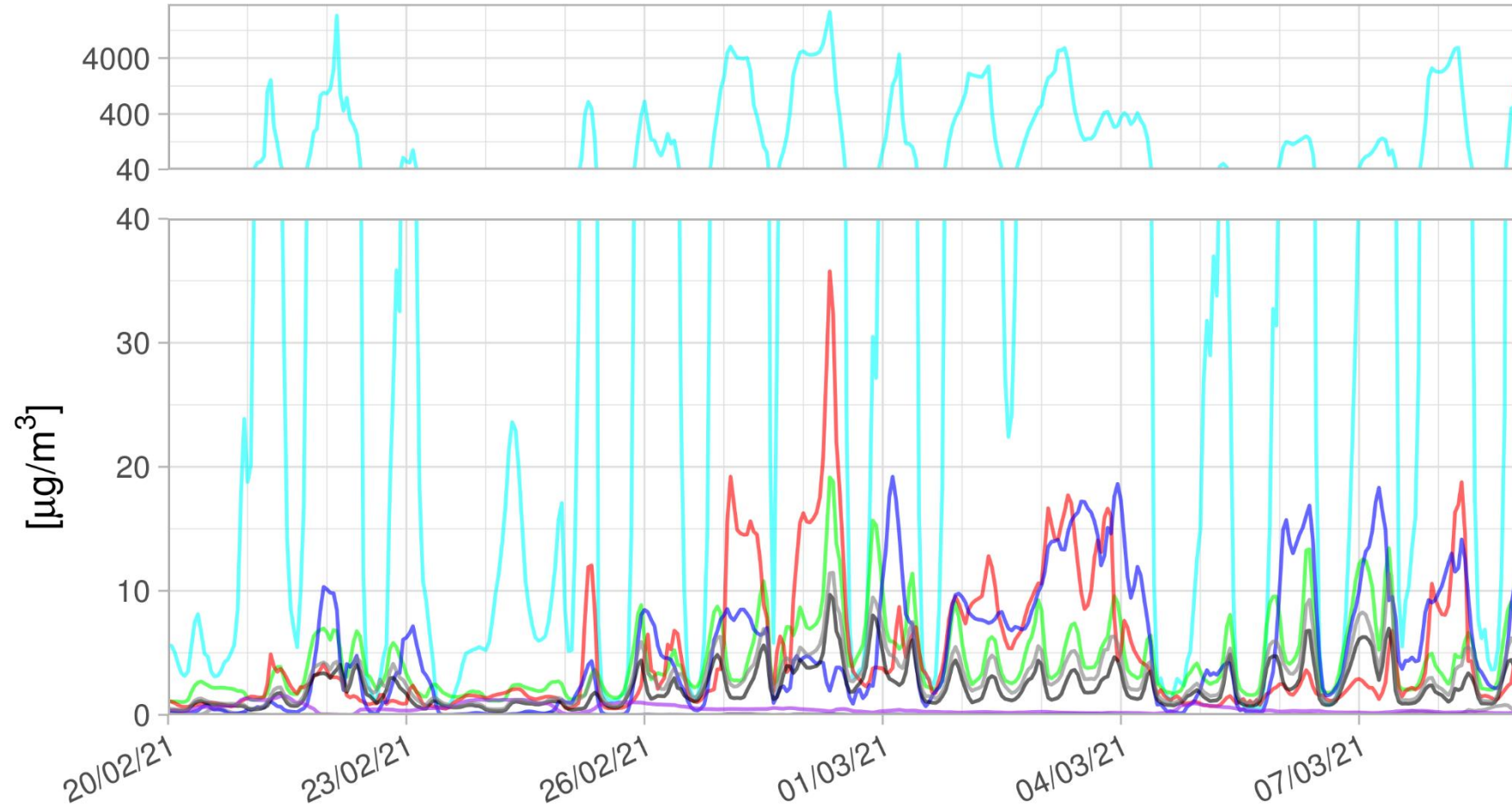
# Ion balance

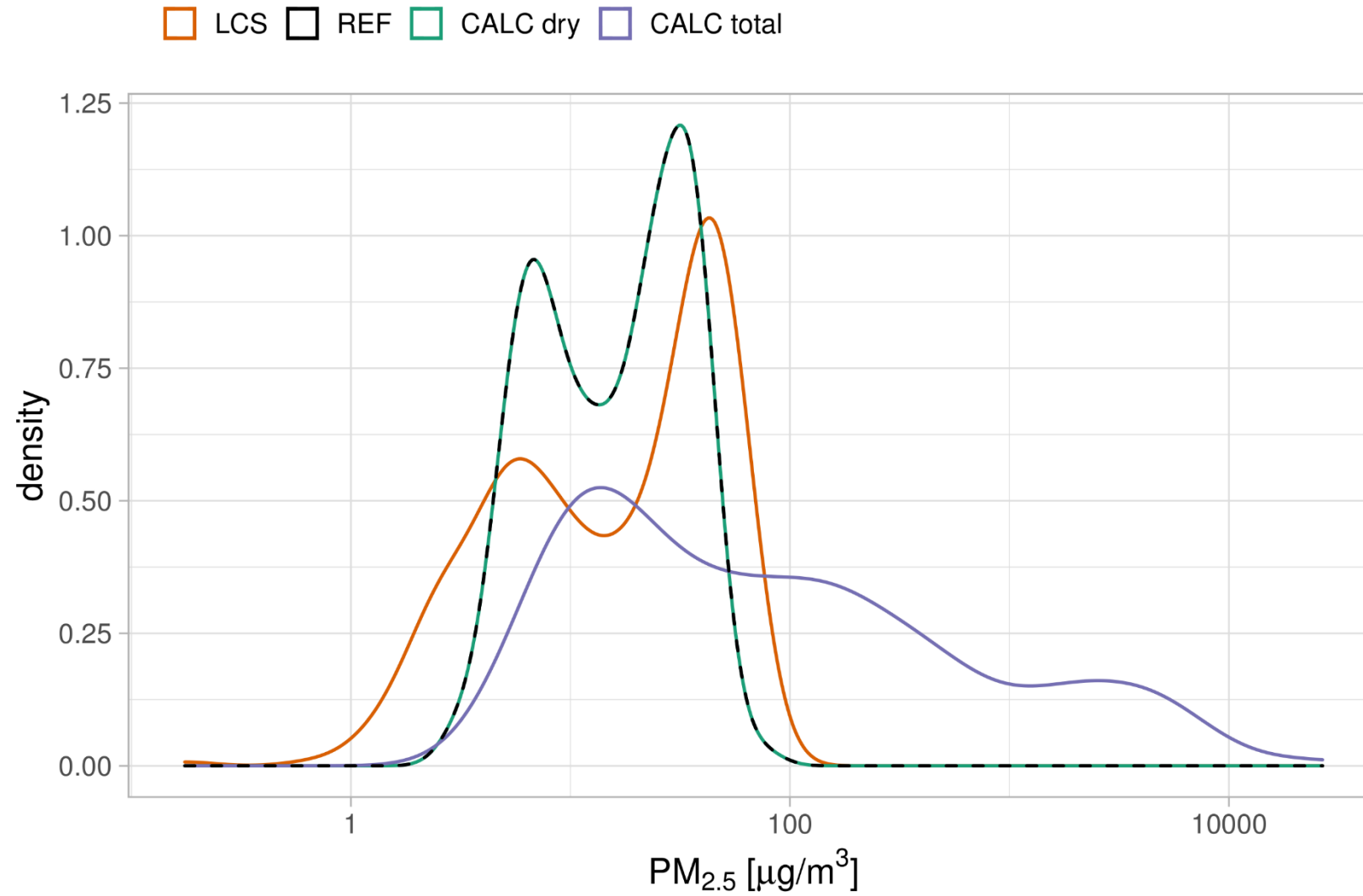


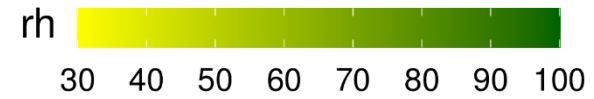
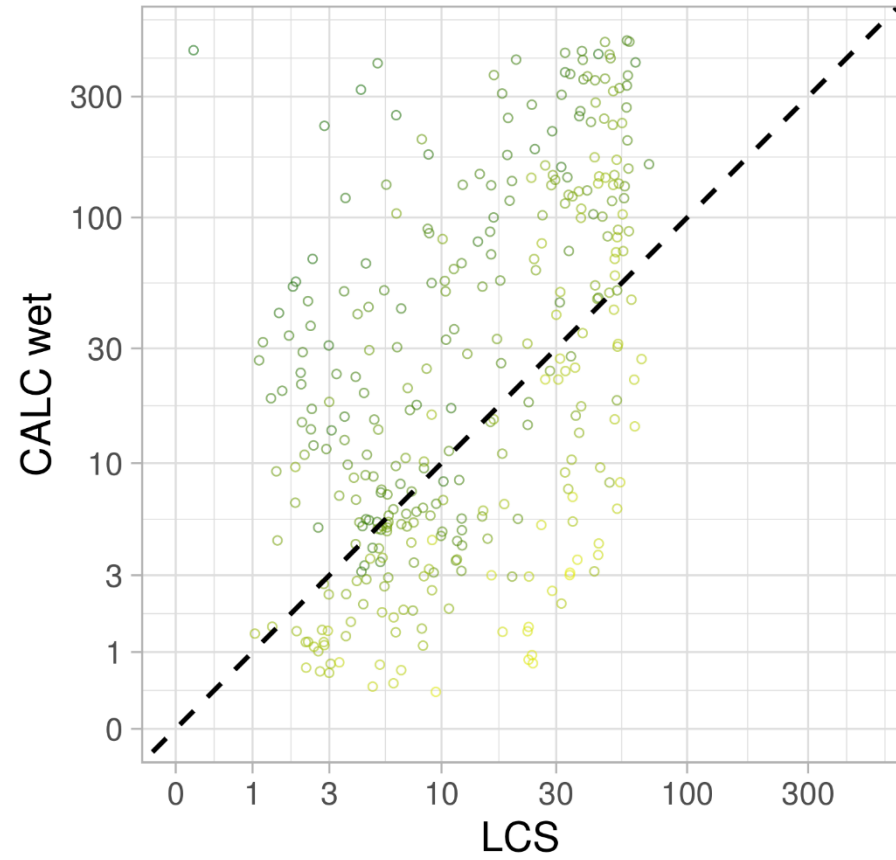
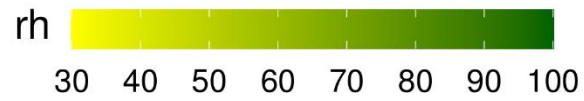
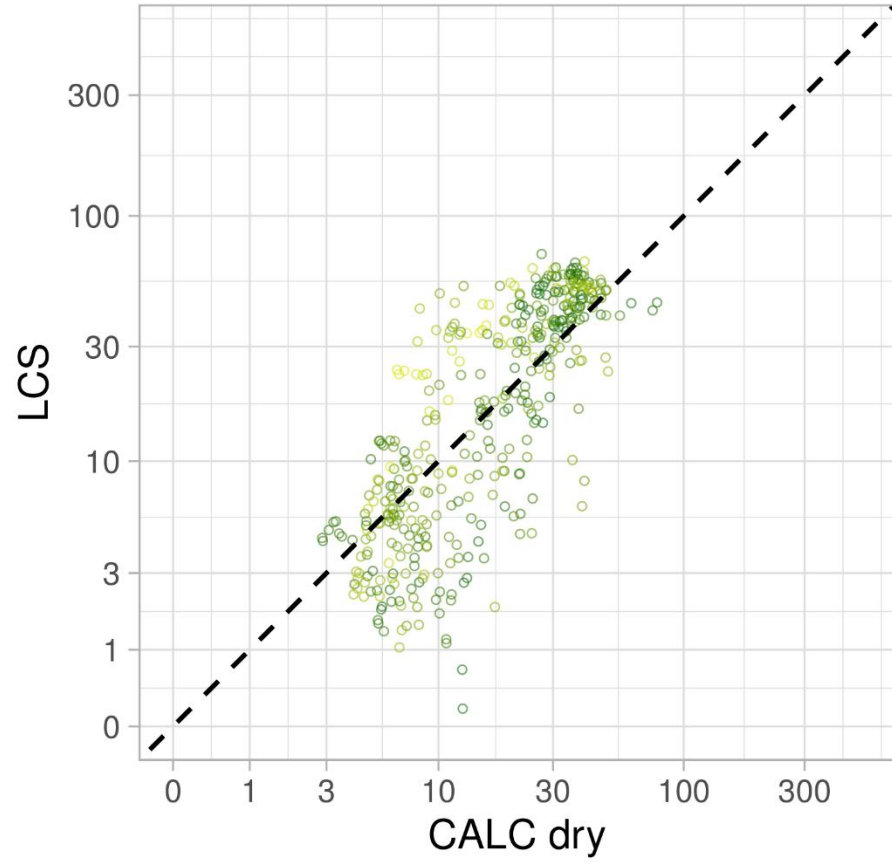












# Datalabs

Developed by Iain Walmsley within UKSCAPE

EMEP

<https://emep-emep4uk.datalabs.ceh.ac.uk/example-panel-app>

WRF

<https://emep-wrfddata.datalabs.ceh.ac.uk/wrf-data>

We'll use the underlying API for the Quant App