International Conference on Air Quality – Science and Application

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www.airqualityconference.org

Model Output and Data Management, Evaluating a forecast and its applications

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University of Hertfordshire

Resources

WMO/GAW Training Materials and Best Practices for Chemical Weather/Air Quality Forecasting (CW-AQF)
Version 1 Scientific Editors: Yang Zhang and Alexander Baklanov
CW-AQF guide can be downloaded from:
https://elioscloud.wmo.int/share/s/WB9UoQ5kQK-dmgERjSAqIA
Chapter 8. Model Output and Data Management, Christoph A. Keller
Chapter 9. Model Evaluation, K. Wyat Appel, Johannes Flemming, and Yang Zhang

Mesoscale Modelling for Meteorological and Air Pollution Applications
Edited by Ranjeet S. Sokhi, Alexander Baklanov, K. Heinke Schlünzen
Published by Anthem Press

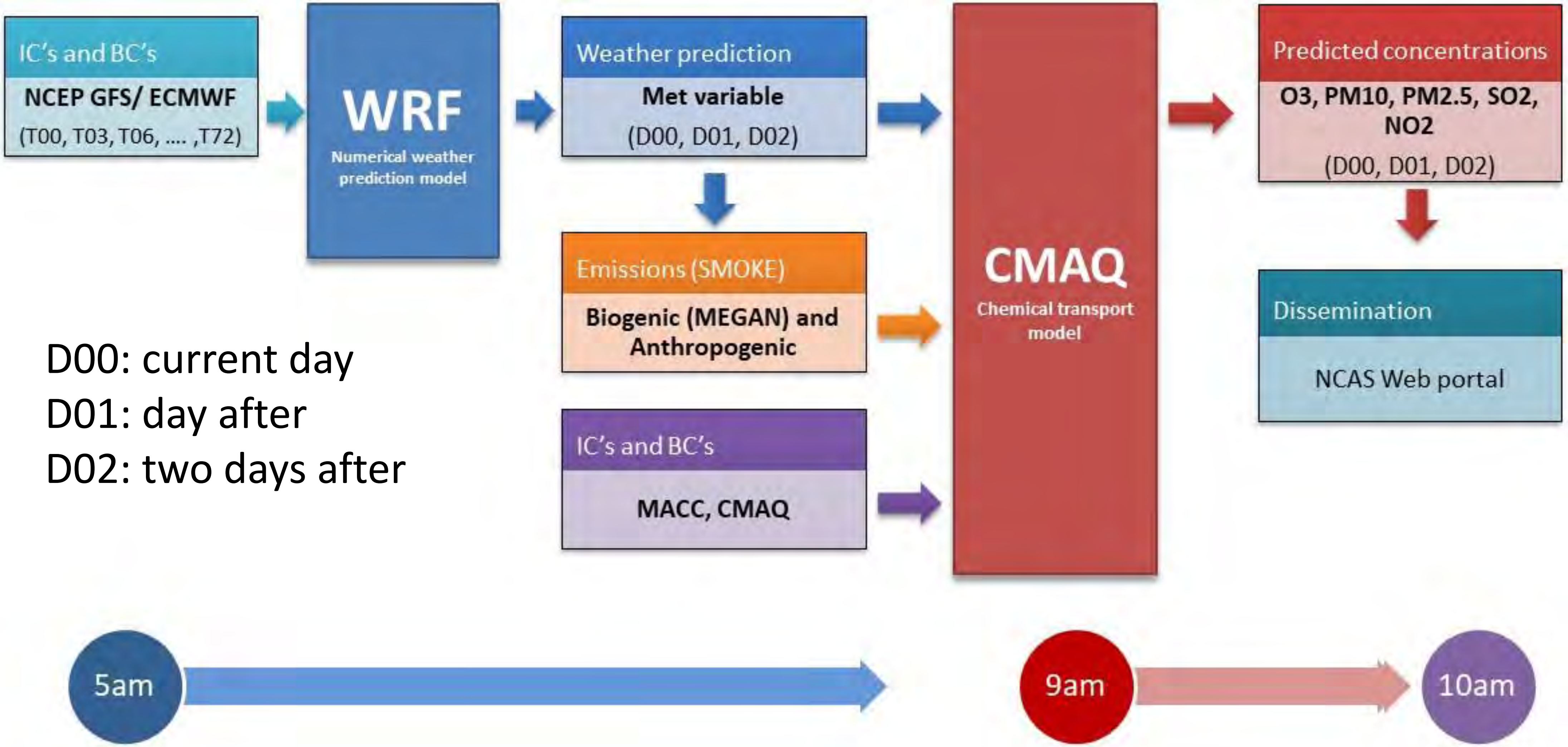
The book can be purchased, for example from Amazon

Selected chapters 2, 5, 6 and 7 made available for the trainees who attend the Training course.
These chapters are only for personal use and should not be copied or circulated.

COST 728/WMO reports https://library.wmo.int/index.php?lvl=more_results&autolevel1=1

Overview of Tools And Methods For Meteorological And Air Pollution Mesoscale Model Evaluation and User Training Editors: K. Heinke Schlünzen and Ranjeet S Sokhi (2008)

University of Hertfordshire AQF System for NCAS



Model outputs

Large amount of data is produced by advanced AQ models (Chemical Weather AQ models or chemical Transport Models) ~ 10s TB

3D Concentrations for a large number of species ~ 100 species at every averaging time interval (e.g. hourly) over the domain at the specified grid resolution

Meteorological fields over the domain at the specified grid resolution at every averaging time interval e.g. wind speed and direction, precipitation, RH, temperature, boundary layer height and many more

Emissions data that is spatially and temporally distributed over the 3D domain and time (e.g. hourly)

Data management considerations

Many considerations:
Types of outputs and variables
Horizontal grip resolution
Vertical levels, resolution
Frequency of output – averaging times
Data format
Access tools

Data management considerations

Types of outputs and variables

concentrations for a number of species, meteorological conditions, process diagnostics, and customized

regulatory species (e.g. PM2.5, O3, NO2, CO, SO2

process related species e.g. HONO (source of OH), Aerosol Optical Depth (AOD), Aerosol Optical Thickness (AOT)

Horizontal grip resolution

high horizontal grid resolution is important to capture air pollutant spatial gradients, e.g. for NOx/NO2 and CO (pollutants that have major local sources)

Data management considerations

Vertical levels, resolution

- output at the first lowest model level is usually sufficient for many air quality applications
- 3D fields are important to understand processes e.g. entrainment and to capture the vertical structure e.g. for BL processes/dynamics and long range transport

Frequency of output

- averaging times sufficient to capture diurnal variabilities of air pollutants which is dependent on meteorology and source activity e.g those near roads or downwind of point sources
- Hourly outputs allow longer averaging statistics (e.g. daily, annual means and percentiles) to be generated

Data format

Access tools

Implications for data storage and archiving

Data management considerations

Meteorological variables

- Critical for interpreting the variations in modelled and observed pollutant species concentration
- For source profiling and apportionment analysis
- To convert output units ppb < > $\mu g/m^3$)
- Important modelled 2m surface temperature (and vertical profile), relative humidity, pressure, and 10m wind speed (u and v direction), boundary layer height
- Others e.g. precipitation, cloud cover, radiation, thermal stability (e.g., buoyancy)
- Coupled chemistry-meteorology models - variables need to be available on each time step and can be output if needed

Data management considerations

Process Diagnostics

- Most common process diagnostics are flux diagnostics e.g. emission, dry and wet deposition fluxes
- Other process diagnostics include chemical processes, e.g. reaction and photolysis rates or chemical production and loss rates
- Important for:
  - Interpretation of species concentrations
  - Explain the differences among models
  - Differences between model and observations

Data management considerations

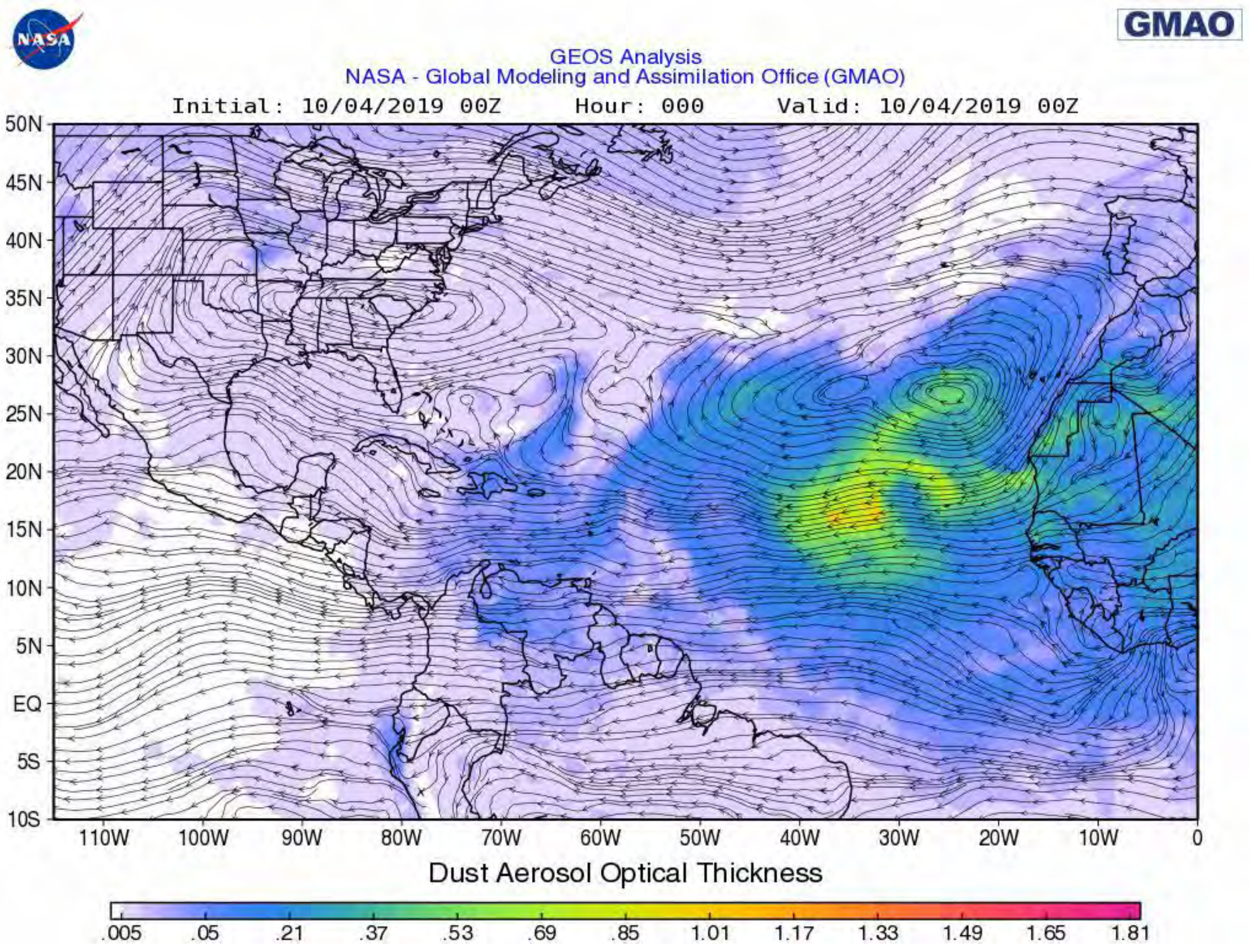
Customized Diagnostics – Post processing
Using model input and output variables to understand air quality and resulting impacts, for example,

- Population exposure studies
- Health impact studies
- Deriving source-receptor relationships
- Understanding particle for mation and evolution
- Deriving metrics, such as, Daily means, accumulated ozone exposure over 40 ppbv (AOT40), or sum of all hourly average concentrations at or above 60 ppbv (SUM60), percentiles, maximum daily average 8-h (MDA8)
- Air Quality Index (AQI) or Air Quality Health Index (AQHI)
  - 1-10 in the UK (10 is worst AQ)
  - 0-500 in the USA (500 is worst AQ)

Data Access

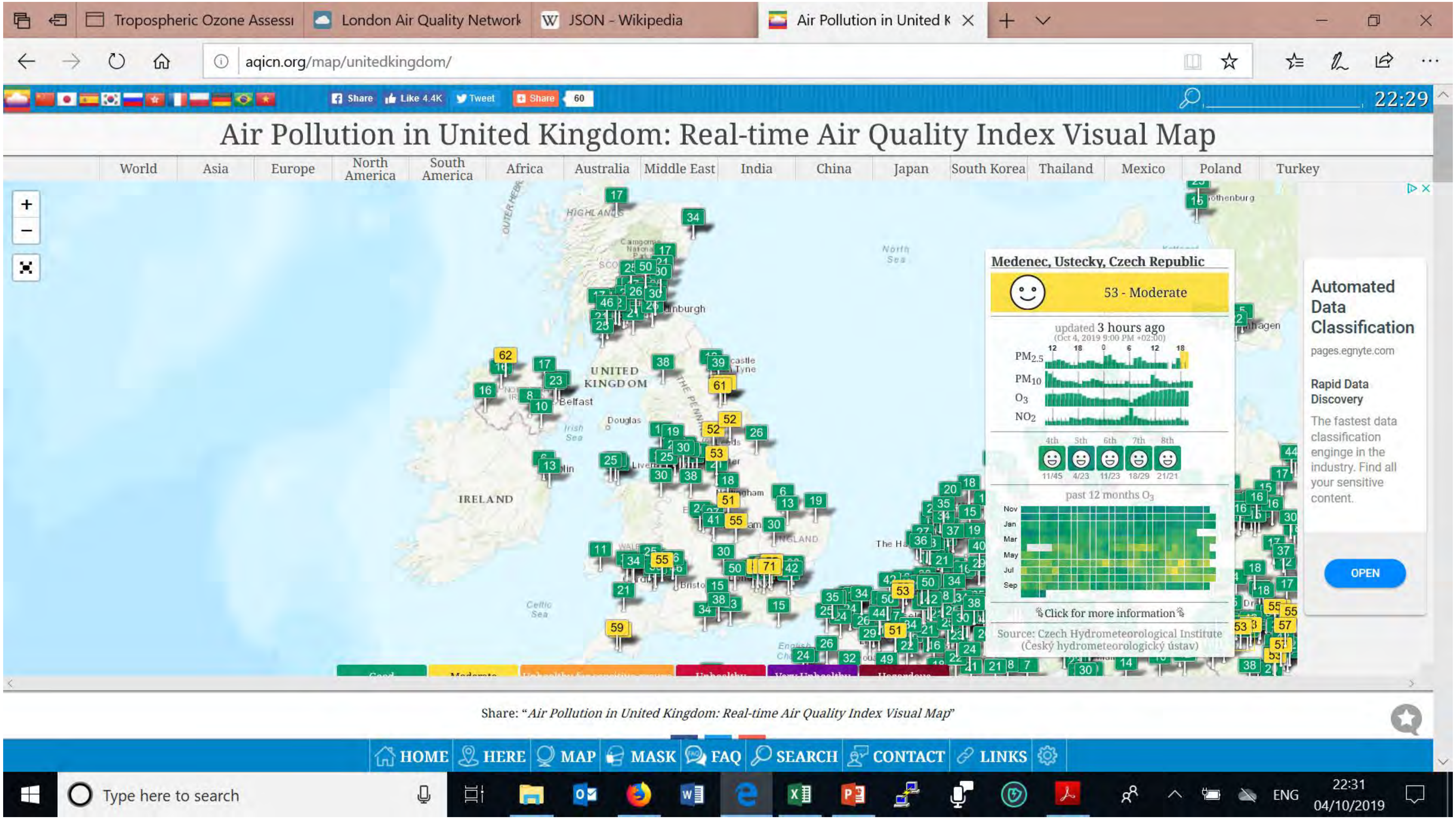
Needs to be application and user orientated

Many online platforms globally e.g. visualizations of surface concentration maps of air pollutants such as ozone and PM2.5. e.g., from the **Copernicus Atmosphere Monitoring Service (CAMS)** or **the NASA Global Modeling and Assimilation Office (GMAO), UK Air** and many others



Model output data

- From download tools for the full (3-dimensional) output files
- Use of **Application Programming Interface (API)**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London Air Quality Network
JSON - Wikipedia
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Share
Like 4.4K
Tweet
Share
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Air Pollution in United Kingdom: Real-time Air Quality Index Visual Map
World
Asia
Europe
North America
South America
Africa
Australia
Middle East
India
China
Japan
South Korea
Thailand
Mexico
Poland
Turkey
UNITED KINGDOM
IRELAND
Belfast
Douglas
Irish Sea
Celtic Sea
North Sea
Medenec, Ustecky, Czech Republic
53 - Moderate
updated 3 hours ago
(Oct 4, 2019 9:00 PM +02:00)
PM2.5
PM10
O3
NO2
4th
5th
6th
7th
8th
11/45
4/23
11/23
18/29
21/21
past 12 months O3
Nov
Jan
Mar
May
Jul
Sep
Click for more information
Source: Czech Hydrometeorological Institute
(Český hydrometeorologický ústav)
Automated Data Classification
pages.egnyte.com
Rapid Data Discovery
The fastest data classification enginge in the industry. Find all your sensitive content.
OPEN
Share: "Air Pollution in United Kingdom: Real-time Air Quality Index Visual Map"
HOME
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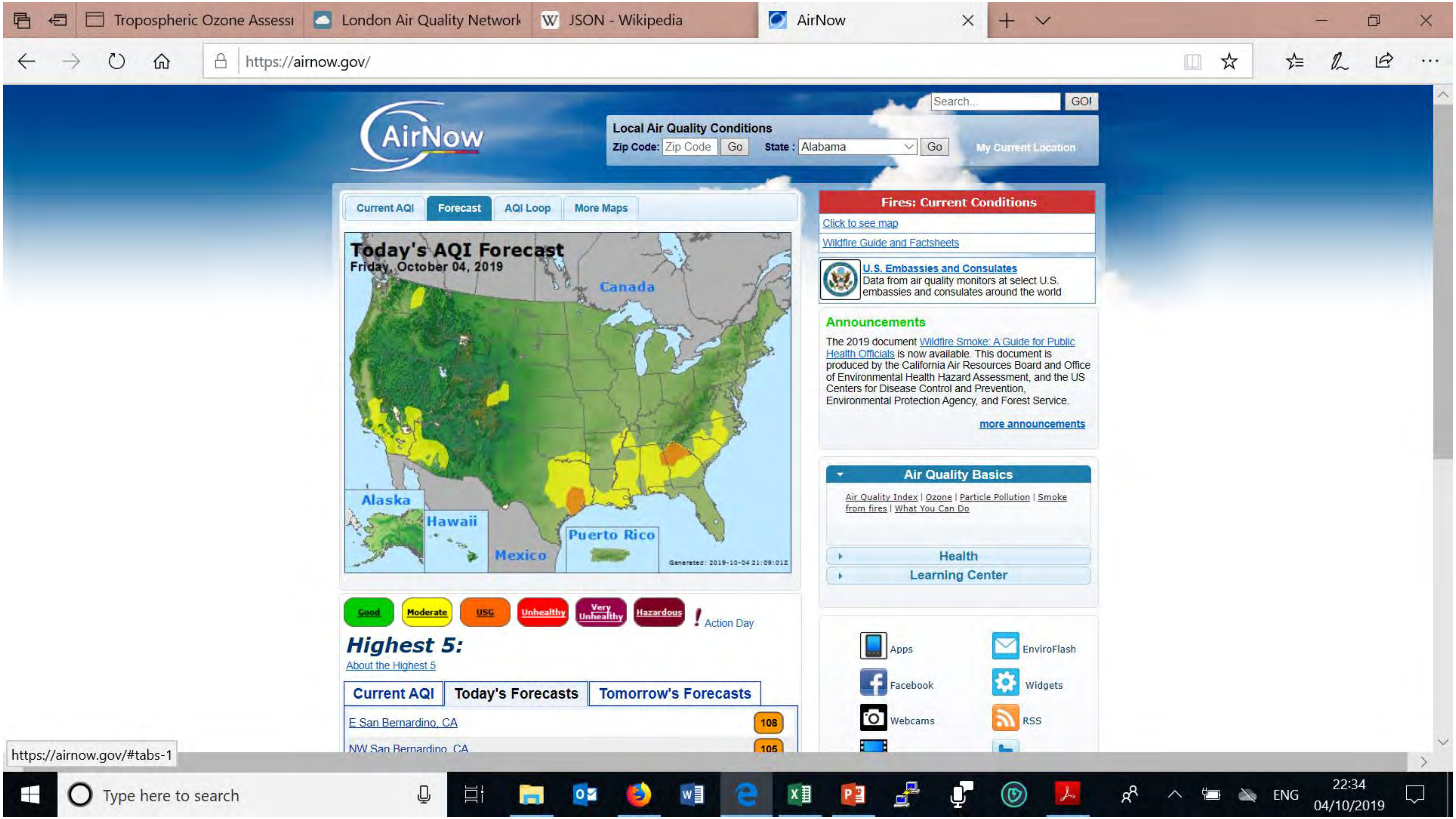
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London Air Quality Network
JSON - Wikipedia
AirNow
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Search...
GO!
AirNow
Local Air Quality Conditions
Zip Code: Zip Code Go
State : Alabama Go
My Current Location
Current AQI
Forecast
AQI Loop
More Maps
Today's AQI Forecast
Friday, October 04, 2019
Canada
Alaska
Hawaii
Mexico
Puerto Rico
Fires: Current Conditions
Click to see map
Wildfire Guide and Factsheets
U.S. Embassies and Consulates
Data from air quality monitors at select U.S. embassies and consulates around the world
Announcements
The 2019 document Wildfire Smoke: A Guide for Public Health Officials is now available. This document is produced by the California Air Resources Board and Office of Environmental Health Hazard Assessment, and the US Centers for Disease Control and Prevention, Environmental Protection Agency, and Forest Service.
more announcements
Air Quality Basics
Air Quality Index | Ozone | Particle Pollution | Smoke from fires | What You Can Do
Health
Learning Center
Good
Moderate
USG
Unhealthy
Very Unhealthy
Hazardous
Action Day
Highest 5:
About the Highest 5
Current AQI
Today's Forecasts
Tomorrow's Forecasts
E San Bernardino, CA 108
NW San Bernardino, CA 105
Apps
EnviroFlash
Facebook
Widgets
Webcams
RSS
https://airnow.gov/#tabs-1
Type here to search
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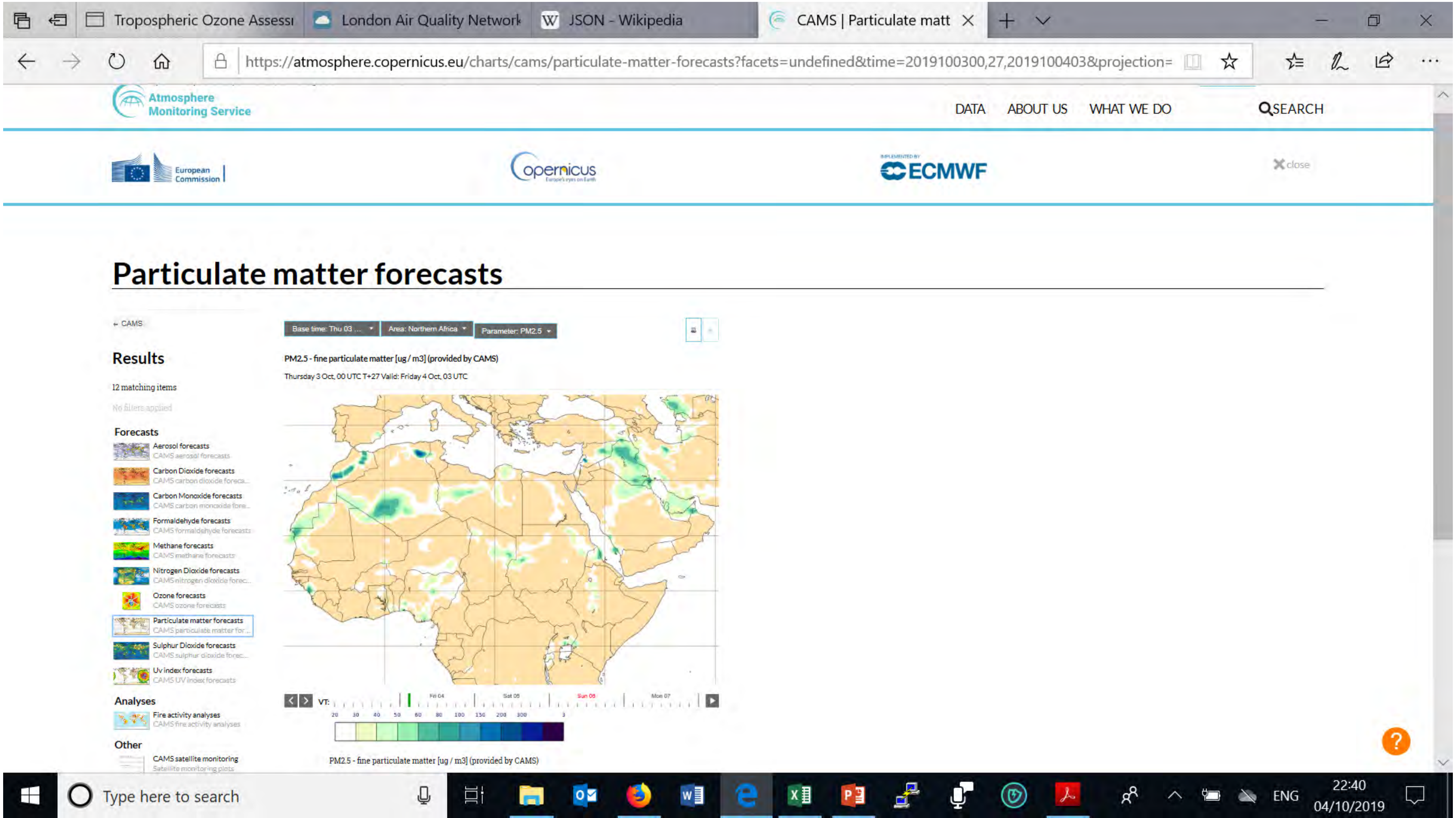
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London Air Quality Network
JSON - Wikipedia
CAMS | Particulate matt
https://atmosphere.copernicus.eu/charts/cams/particulate-matter-forecasts?facets=undefined&time=2019100300,27,2019100403&projection=
Atmosphere
Monitoring Service
DATA
ABOUT US
WHAT WE DO
SEARCH
European Commission
Copernicus
ECMWF
close
Particulate matter forecasts
← CAMS
Results
12 matching items
No filters applied
Forecasts
Aerosol forecasts
CAMS aerosol forecasts
Carbon Dioxide forecasts
Carbon Monoxide forecasts
Formaldehyde forecasts
Methane forecasts
Nitrogen Dioxide forecasts
Ozone forecasts
CAMS ozone forecasts
Particulate matter forecasts
Sulphur Dioxide forecasts
Uv index forecasts
CAMS UV index forecasts
Analyses
Fire activity analyses
CAMS fire activity analyses
Other
CAMS satellite monitoring
Satellite monitoring plots
Base time: Thu 03 ...
Area: Northern Africa
Parameter: PM2.5
PM2.5 - fine particulate matter [ug / m3] (provided by CAMS)
Thursday 3 Oct, 00 UTC T+27 Valid: Friday 4 Oct, 03 UTC
VT:
Fri 04
Sat 05
Sun 06
Mon 07
20 30 40 50 60 80 100 150 200 300
PM2.5 - fine particulate matter [ug / m3] (provided by CAMS)
Type here to search
ENG
22:40
04/10/2019

Data Format

Size of air quality data files can be of large size – 100sTB !!

File formats should allow geospatial information to be handled efficiently

Examples: Network Common Data Form (netCDF), Hierarchical Data Format 5 (HDF5), and GRIdded Binary or General Regularly-distributed Information in Binary form (GRIB, GRIB2)

These formats can be handled by **common scientific data analysis software languages**, such as IDL, MATLAB, Python, or R

Data Format

For processed **data of smaller volume** other model outputs can be used - comma separated values (csv) or text format (txt) e.g., surface concentrations of selected species.

Meta data

Detailed description of the model output should be included in every data file (meta data)

e.g. location (lat/long/altitude),
time in Coordinated Universal *Time* (*UTC*),
and units for each value

Purpose of model evaluation

Overall purpose: To assess and benchmark the performance of the model through comparison with observations, process sensitivity studies and diagnostic analysis

How do you decide which evaluation approaches to use:
Know the nature of application of the model (e.g. assessment, forecasting, scenario analysis, research process analysis etc..)

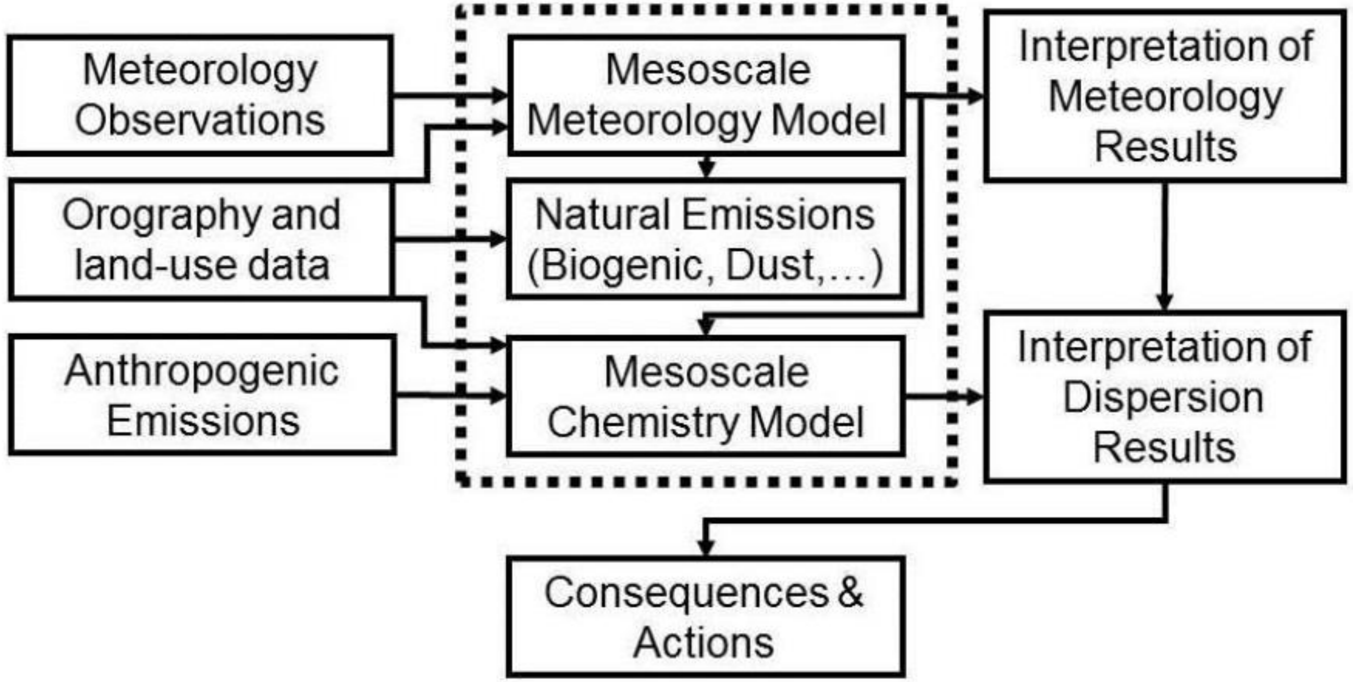
Consult available experience and methodologies e.g.
COST 728 – Reports on WMO Publications
FAIRMODE
AQMEII

Evaluation of model performance

Evaluating concentrations only is not enough for advanced, Eulerian models e.g. all key components should be evaluated including input datasets and pre-processing procedures

How do you decide which evaluation approaches to use?

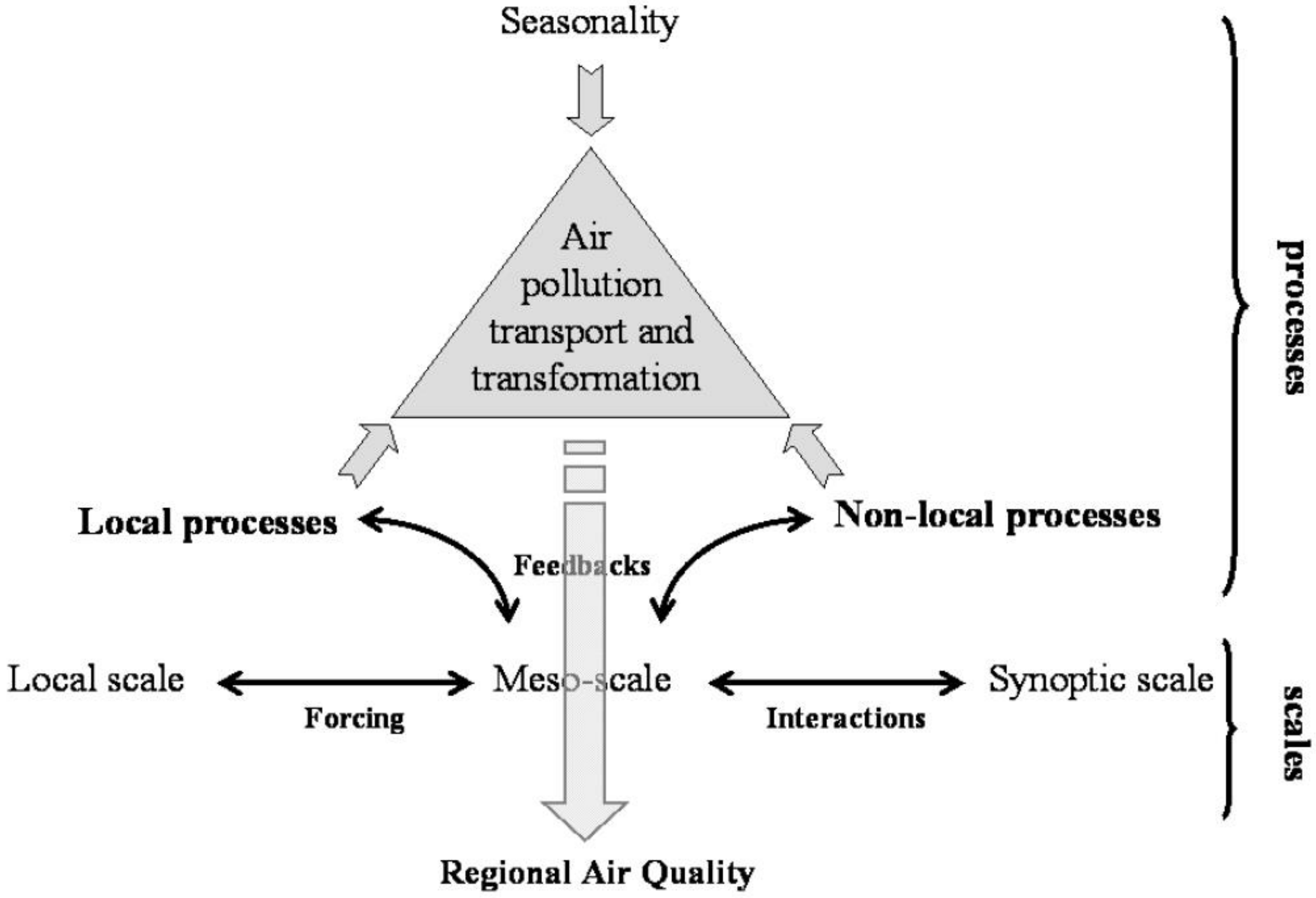
Know the nature of application of the model (e.g. assessment, forecasting, scenario analysis, research process analysis etc..)



AQ simulation chain; the models can either be online coupled (dotted square) or chemistry and meteorology are offline coupled

Sokhi et al., 2019

Atmospheric processes and scales



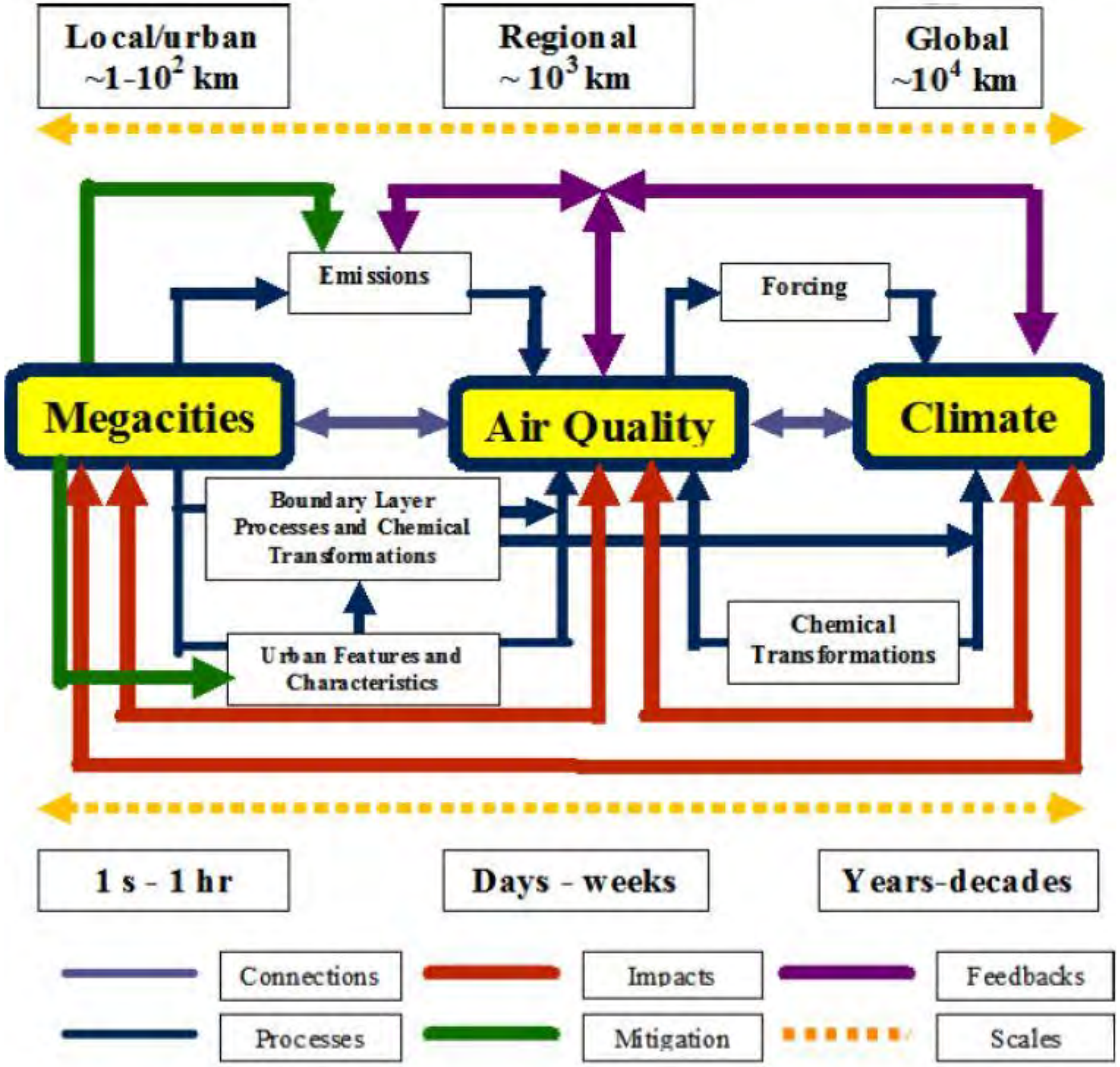
Coupling between the different processes and scales relevant for air pollution transport and transformation.
The synergy of all these components (processes plus meteorological scales) results in the “Regional Air Quality”.

See Chapter 7 of Sokhi et al (2019)

Connections of Megacities, AQ, Weather and Climate

main feedbacks, ecosystem, health & weather impact pathways, mitigations

- Science - nonlinear interactions and feedbacks between emissions, chemistry, meteorology and climate
- Multiple spatial and temporal scales
- Complex mixture of pollutants from large sources
- Interacting effects of urban features and emissions
- Chain of meteo-hazards domino effects on city safety and social activities



Nature, 455, 142-143 (2008)

Relevance of better knowledge on specific processes to improve simulation of meteorological, chemical, biological variables

Processes (clouds, aerosols)	For variables in			For applications		
	Met.	Chem.	Biol.	NWP	AQ	Clim.
Cloud processes						
• Microphysics, dynamics,	X	X	X	X	X	X
• In-cloud and below-cloud scavenging,		X	X		X	X
• Aqueous-phase chemistry		X	X		X	X
Aerosol processes						
• Chemistry		X			X	X
• Thermodynamics	(X)	X		(X)	X	X
• Dynamics		X		(X)	X	X
Representation of aerosol–radiation–cloud–chemistry interactions (improve indirect estimates of aerosol effect)	**X**	**X**	**X**	**X**	**X**	**X**

EuMetChem: Baklanov, Schlünzen et al.

Relevance of better process descriptions to improve simulation of meteorological, chemical, biological variables

Process (emissions)	For variables in			For applications		
	Met.	Chem.	Biol.	NWP	AQ	Clim.
Meteorology-dependent emission processes to be described more accurately:						
• Biogenic		X	X		X	X
• Sea spray		X			X	X
• Windblown dust	(X)	X		(X)	X	X
• Lightning		X			X	X
Anthropogenic emission data in urgent need for improvement:						
• Ships		X			X	X
• Wild fires		X			X	X
• Volcanic eruptions	X	X		X		X
Heat fluxes sources needing better knowledge:	X	X		X	X	X
• Wild fires	X	X		X	X	X
• Volcanic eruptions						

EuMetChem: Baklanov, Schlünzen et al.

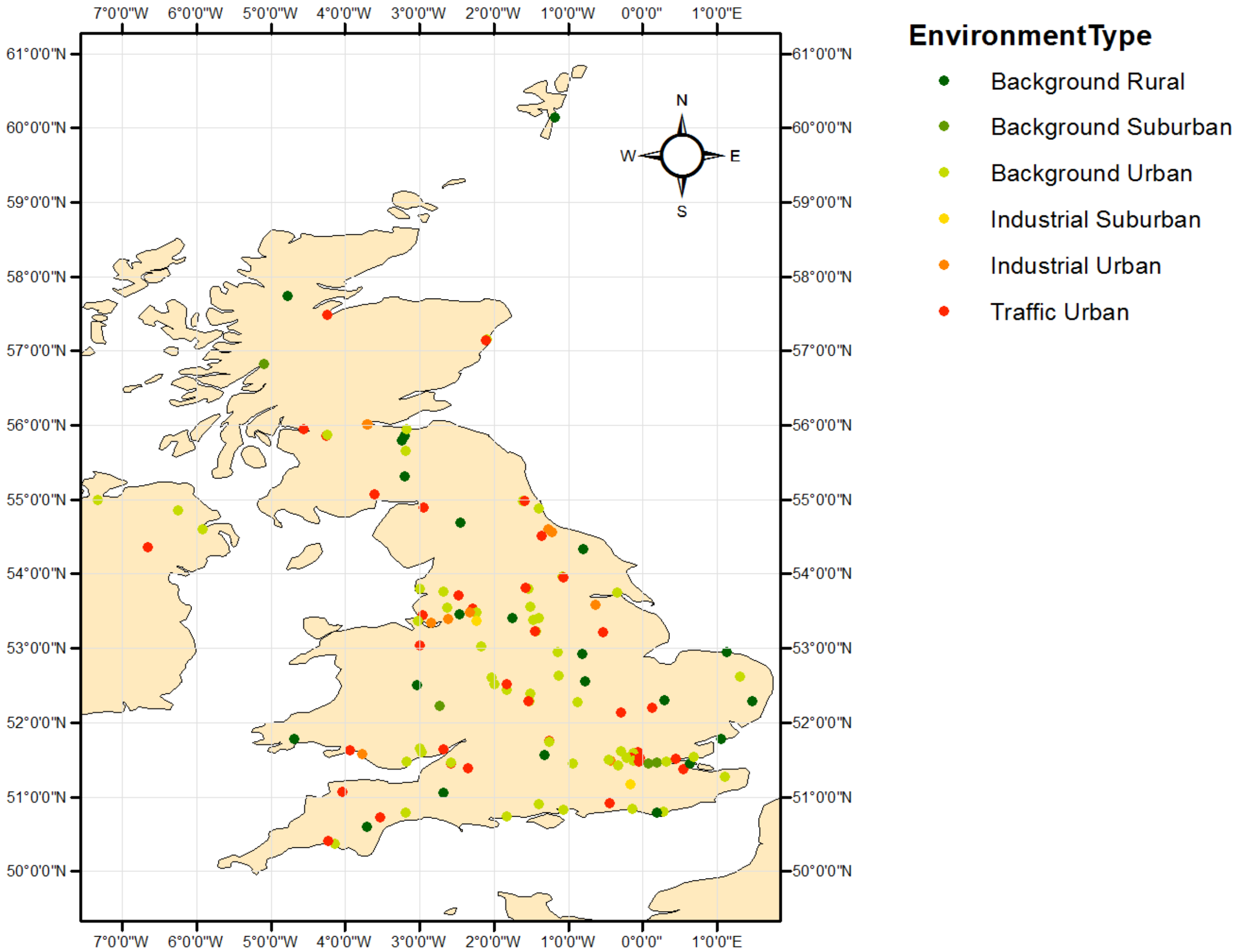
Evaluation of model performance

Availability of observations:
Routine surface networks,
field campaigns,
Satellites
aircrafts,
other models

Consider:
Type of stations – urban, rural, remote, traffic, industrial, residential etc…
- location and height of stations – is it appropriate for the model?
Model Grid resolution
Model Temporal resolution
Output species

UH AQ Forecast evaluation

AURN Network (2014)



Total stations for all pollutants
135

	PM2.5
Background Rural	**3**
Background Suburban	**2**
Background Urban	**37**
Industrial Suburban	0
Industrial Urban	7
Traffic Urban	18
Total	**67**

Evaluation of model performance

Station Representative of the location

Related to surrounding of station and grid size of the model

Urban stations – spatial representativeness is generally less

Rural stations – spatial representativeness is generally greater

Evaluation of model performance

Available measurements – ideally we need long term hourly datasets of

air pollutant concentrations
meteorological parameters e.g. wind speed, direction, temperature, PBL height, RH, pressure, precipitation

Model output variables and metrics to be evaluated:

Routine gaseous species e.g. O3, NO, NO2, CO and SO2.

Particle matter Total mass – PM10, PM2.5
Particulate species e.g. SO42-, NO3- and NH4+, EC, OC

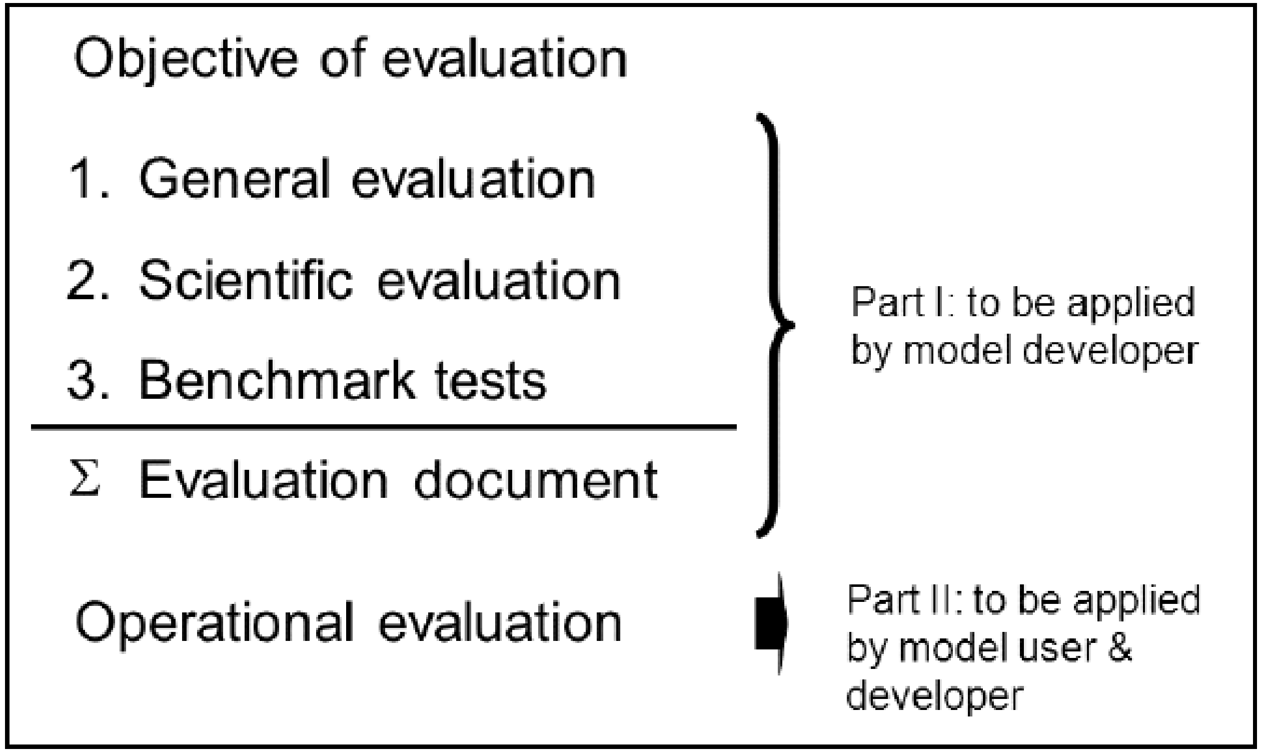
Deposition species e.g.
wet and dry deposition of SO42-, NO3- and NH4+, Cl-, Na+, and O3.

Structure of evaluation of model performance

Evaluation approaches depends on the detail of evaluation that is required:

Purpose - Science or assessment

Types of evaluation,
operational,
dynamic,
diagnostic,
probabilistic



Structure of a generic evaluation protocol

Chapter 7 of Sokhi et al (2019)

Types of model performance metrics

Discrete metrics – commonly used for operational evaluation e.g. bias, error, and correlation

Categorical metrics – used for evaluating a model in a forecast capacity

Usually **absolute** and **relative** evaluation metrics are used in combination for a more comprehensive evaluation of model performance.

Evaluation of model performance

Model performance discrete metrics

Bias/error (the deviation of the forecast value from the observed value)
Large values → **large deviation** between the observed and forecast values
Overestimation (+ve) or underestimation (–ve)

Correlation (assessment of the linear relationship between observed and forecast values). Typically 0 (no correlation) to 1 (perfect correlation)

Should be used in context e.g.
Different species
Diurnal variations
Seasonal e.g. summer vs winter
Annual
Urban, rural

Discrete Model performance metrics

Metric	Definition	Unit	Range
Mean Bias (MB)	$\frac{1}{N}\sum_{i=1}^{N}(C_m - C_o)$	Absolute	$\pm\infty$
Mean Error (ME)	$\frac{1}{N}\sum_{i=1}^{N}\lvert C_m - C_o\rvert$	Absolute	$+\infty$
Root Mean Square Error (RMSE)	$\sqrt{\frac{\sum_{i=1}^{N}(C_m - C_o)^2}{N}}$	Absolute	$+\infty$

Discrete Model performance metrics

Metric	Definition	Unit	Range
Normalized Mean Bias (NMB)	$\frac{1}{N}\sum_{i=1}^{N}\frac{(C_m - C_o)}{\sum_{i=1}^{N} C_o}$	%	-100% to +∞
Normalized Mean Error (NME)	$\frac{1}{N}\sum_{i=1}^{N}\frac{\lvert C_m - C_o\rvert}{\sum_{i=1}^{N} C_o}$	%	0% to +∞
Mean Normalized Bias (MNB)	$\frac{1}{N}\sum_{i=1}^{N}(\frac{C_m - C_o}{C_o})$	%	-100% to +∞
Mean Normalized Error (MNE)	$\frac{1}{N}\sum_{i=1}^{N}\lvert\frac{C_m - C_o}{C_o}\rvert$	%	0% to +∞
Mean Fractional Bias (MFB)	$\frac{1}{N}\sum_{i=1}^{N}\frac{(C_m - C_o)}{\left(\frac{C_o + C_m}{2}\right)}$	%	-200% to +200%
Mean Fractional Error (MFE)	$\frac{1}{N}\sum_{i=1}^{N}\frac{\lvert C_m - C_o\rvert}{\left(\frac{C_o + C_m}{2}\right)}$	%	0% to +200%
Correlation (r)	$\frac{n(\sum C_m C_o) - (\sum C_m)(\sum C_o)}{\sqrt{[n\sum {C_m}^2 - (\sum C_m)^2][n\sum {C_o}^2 - (\sum C_o)^2]}}$	None	-1 to 1

Categorical Model Evaluation Metrics

Metric	Definition	Unit	Range
Hit Rate (HR)	(True Positives + True Negatives) / All Values	%	0% to 100%
False Alarm Rate (FAR)	False Positives/(False Positives + True Positives)	%	0% to 100%
Probability of Detection (POD)	True Positives/(True Positives + False Positives)	%	0% to 100%
Critical Success Index (CSI) (Threat Score)	True Positives/(True Positives + False Positives + False Negatives)	None	0 to 1
Brier Score (BS)	The mean square error of probabilistic two-category forecasts where the observations are either 0 (no occurrence) or 1 (occurrence) and forecast probability may be arbitrarily distributed between occurrence and non-occurrence	None	BS=0 for perfect (deterministic) forecasts. BS=1 for forecasts that are always incorrect.
Skill Score	A measure of the relative improvement of the forecast over some (usually 'low-skilled') benchmark forecast. Commonly used reference forecasts include climatology, persistence, or output from an earlier version of the forecast	%	Typically, skill scores are the percentage difference between verification scores for two sets of forecasts (e.g., operational forecasts versus climatology). Perfect score: 1
Uncertainty	The degree of variability in the observations. Most simply measured by the variance of the observations (e.g.): $\frac{\sum(C-\bar{C})^2}{N-1}$	Absolute	0 to +∞

Typical operational evaluation statistics

Forecast performance indexes

- Correlation Coefficient (CORR)
- Mean error (MERR)
- Mean absolute error (MAE)
- Normalised mean error (NME)
- Root mean square error (RMSE)

- Scatter plots

Performance as compared to reference model

- **Skill score** (-∞ ≤ SK ≤ 1)

$$SK = 1 - \frac{MSE(forecast)}{MSE(reference.forecast)}$$

Typical questions

- How many pollution episodes occurring during the test period were correctly forecast (“Hit rate”)?
- For what percentage of times does the AQ index forecast predicting worse AQ with respect to observations?
- Exceedances – how many times did the system forecast exceedances, and how does this compare with the percentage shown in the observations?
- What percentage of observed exceedances were hit/missed by the forecast?

Exceedance forecast performance indices (binary events)

True Positive rate (Hit Rate)
TPR=A/M

False Positive rate
FPR=(F-A)/(N-M)

False Alarms
FA=(F-A)/F

Success index (-1 to +1)
SI=TPR-FPR

N = Total number of days considered
M = Observed exceedances
F = Forecasted / predicted exceedances
A = correctly predicted exceedances

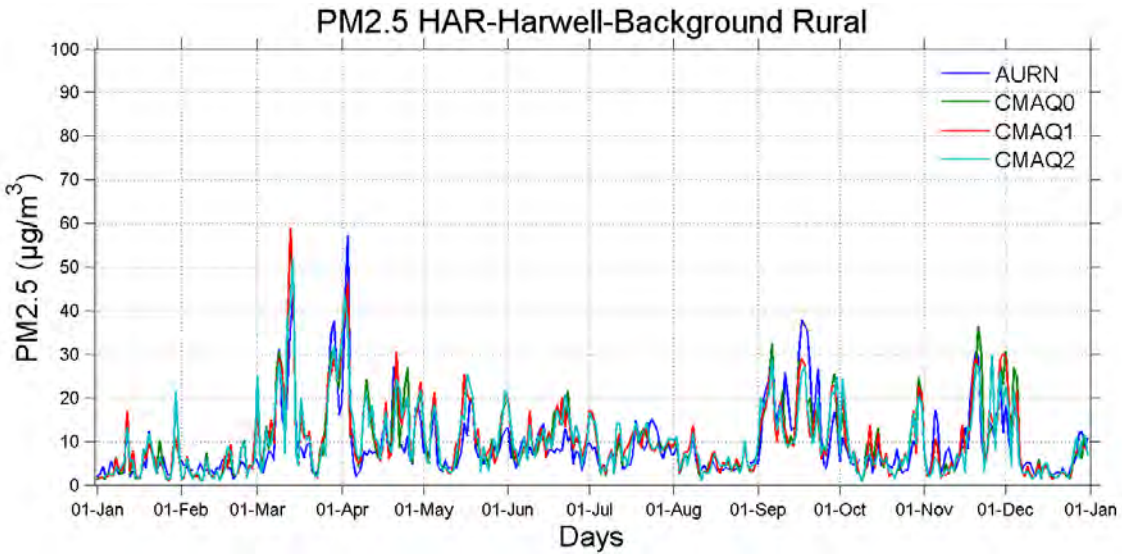
Measured

Forecast	Yes	No	Total
Yes	A	F-A	F
No	M-A	(N-M)-(F-A)	N-F
Total	M	N-M	N

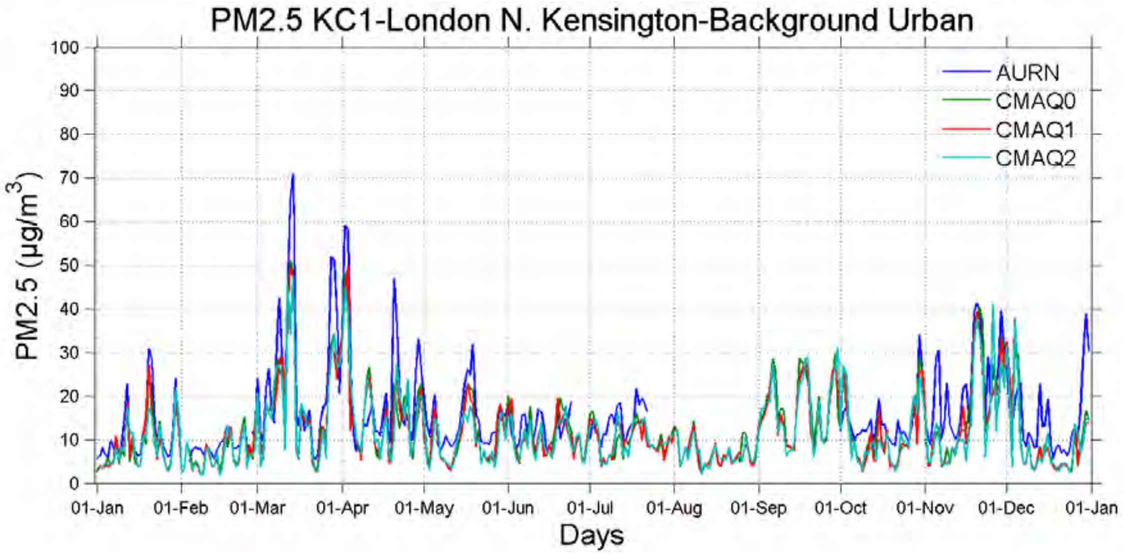
Threshold Limits
Daily mean PM2.5 = 25 μg/m³

Daily mean PM2.5 time series

Time series analysis
Diurnal variations
Visual inspection

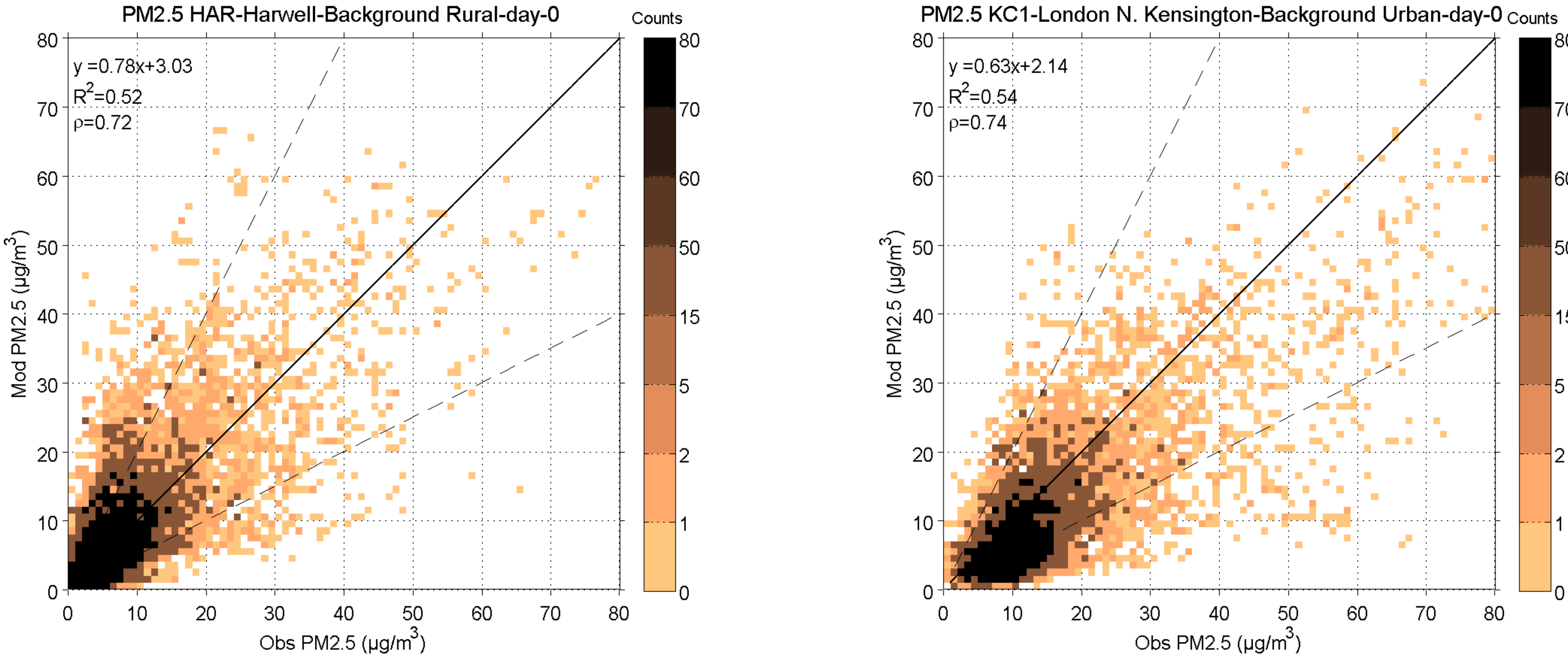


Rural

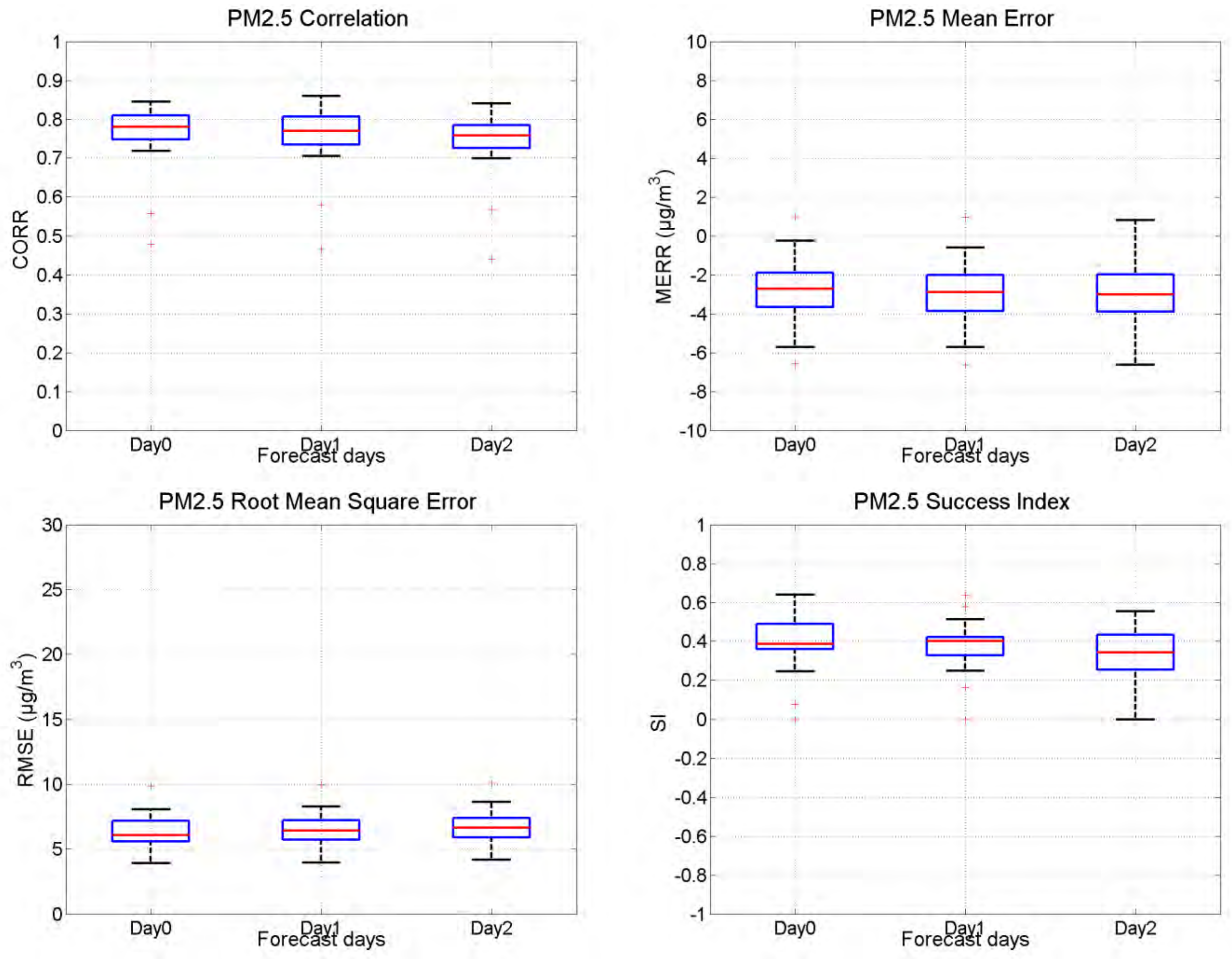


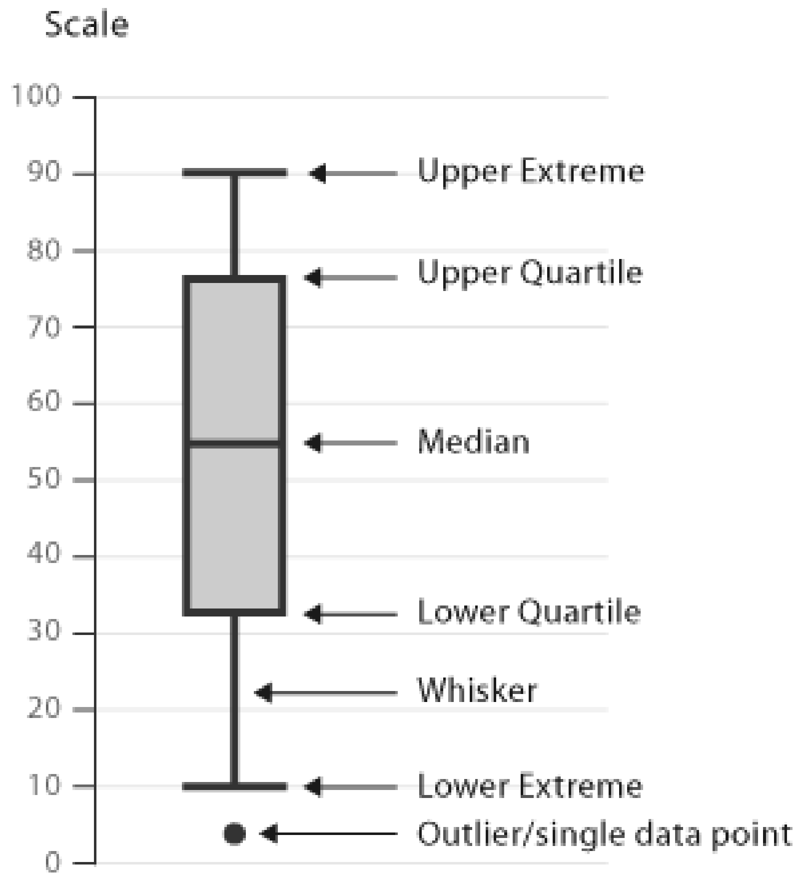
Urban

Typical scatter plot (Hourly PM2.5)

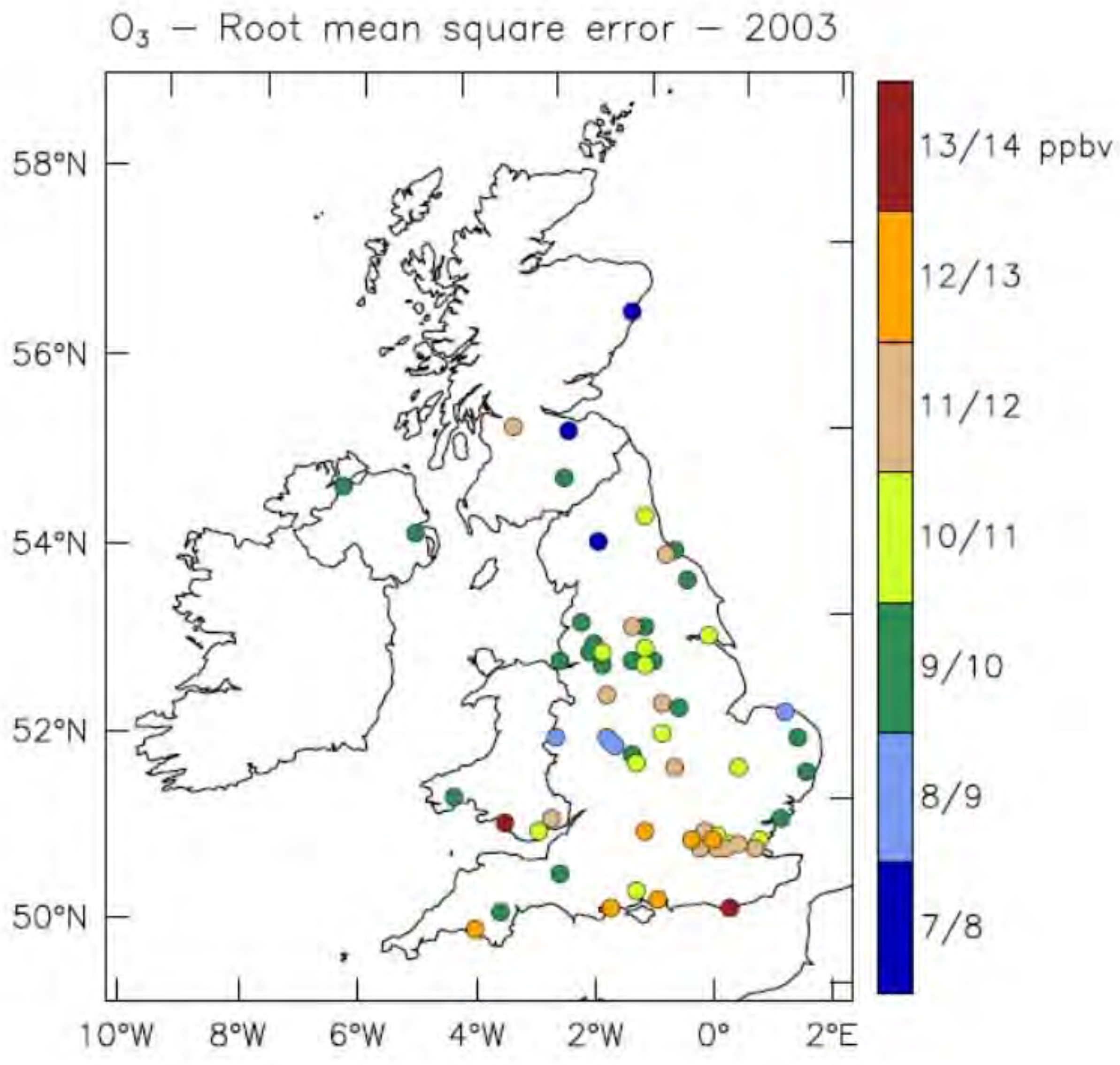


PM2.5 comparison statistics
Box whisker plots



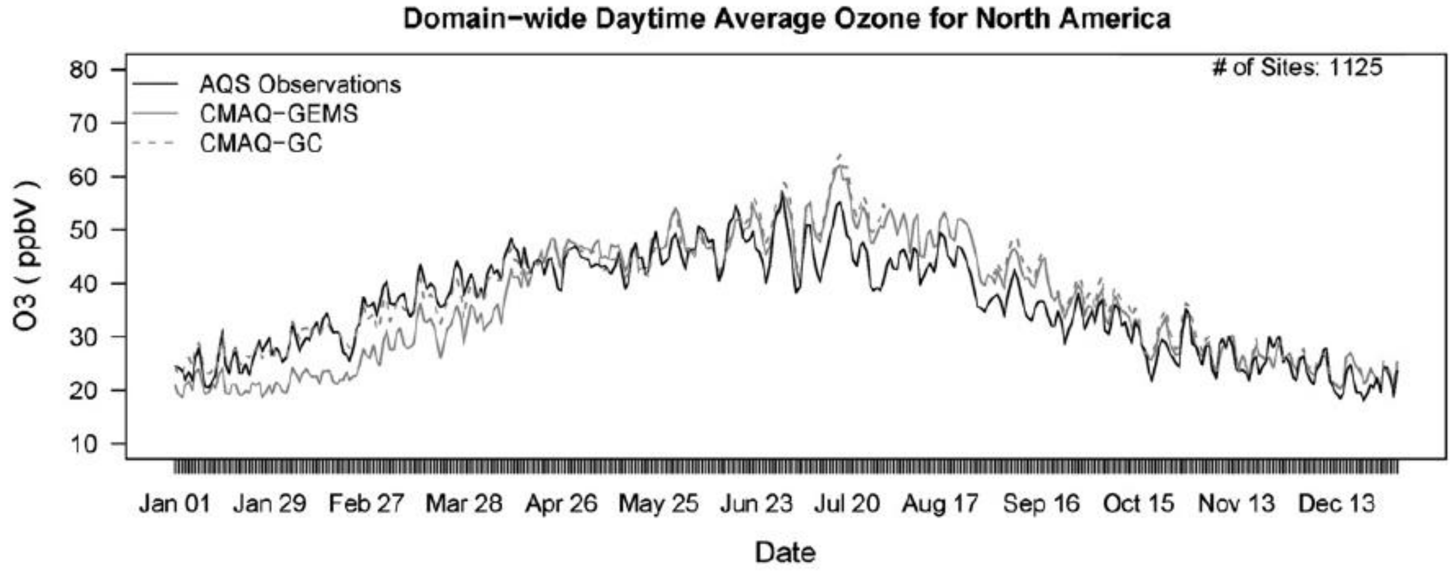


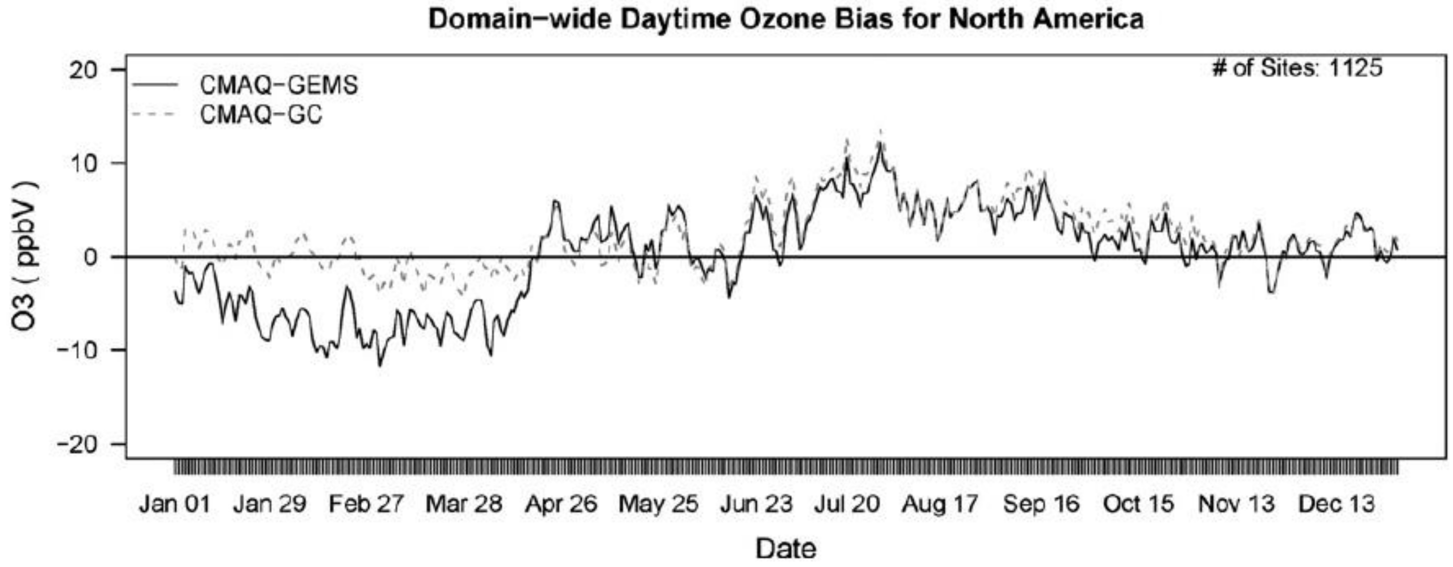
Representing discrete metrics spatially



Example of CMAQ run over the UK

Sensitivity analysis for two different boundary conditions with CMAQ over the USA





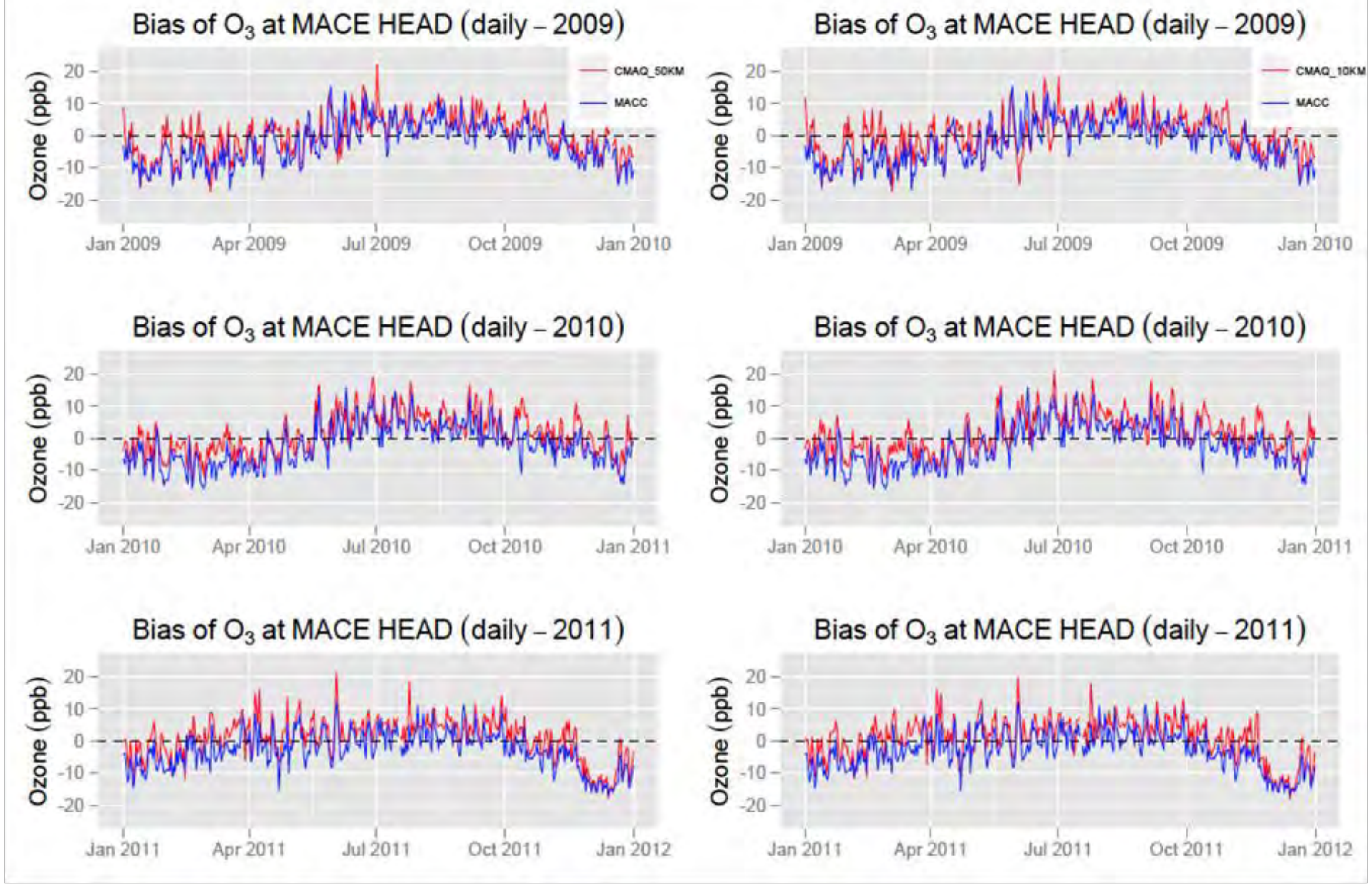
Global and regional Earth-system Monitoring (GEMS)

GEOS-Chem (GC)

Bias of O_3 at Mace Head: MACC vs CMAQ

Sensitivity analysis
BC for two different grid resolutions

50 km **10 km**

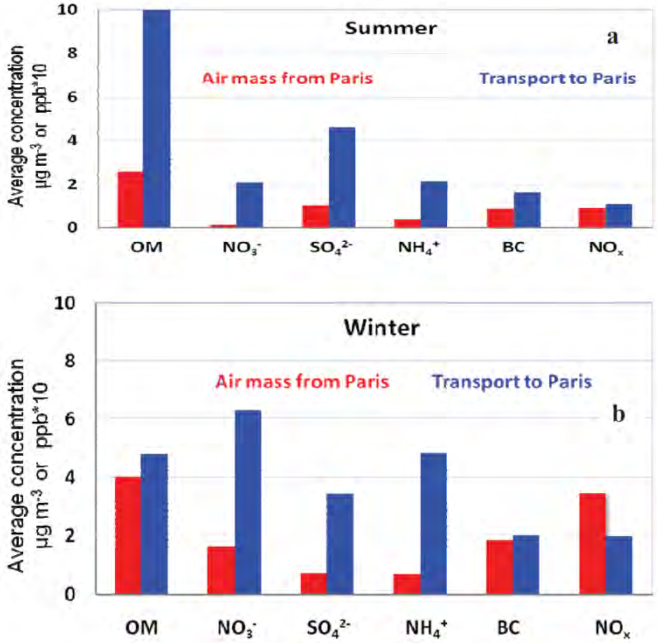


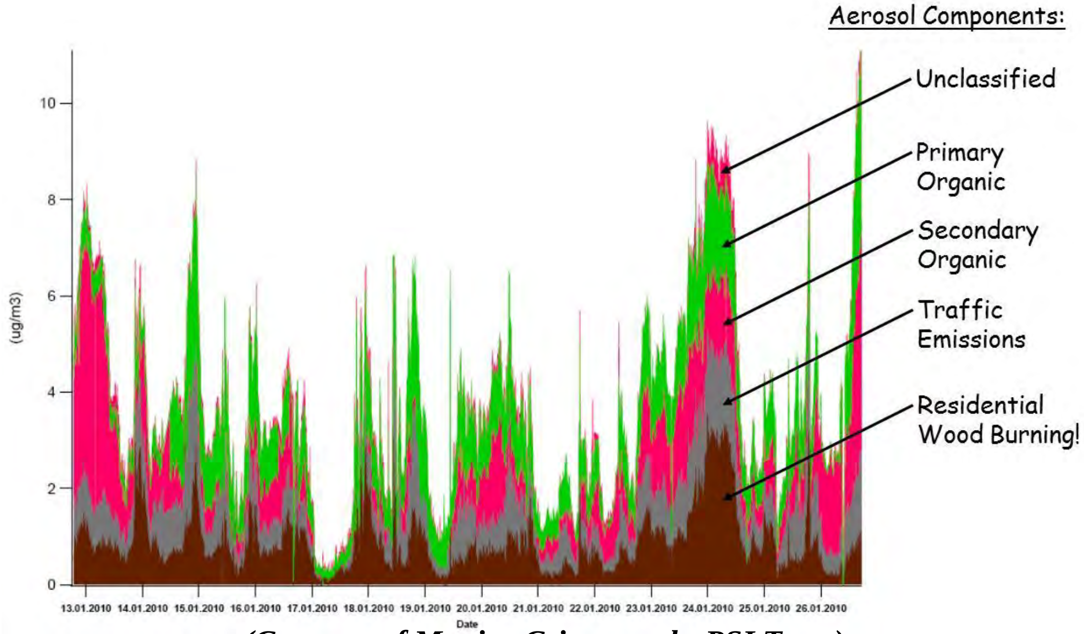
With Ricardo and KCL

MEGAPOLI Paris Measurement Campaigns

Chemical species

- Aim: Provide new experimental data to better quantify sources of primary and secondary carbonaceous aerosol in a megacity and its plume. Duration: Summer – 1-31 Jul 2009, Winter – 15Jan-15Feb 2010
- 30 research institutions from France and other European countries, MEGAPOLI Teams & Collaborators





(Courtesy of Monica Crippa et al.; PSI Team)

- Surprisingly low fine PM levels
- 70% of fine PM mass is transported into megacity from continental Europe
- Fossil fuel combustion contributes only little to organic fine PM
- Large fraction of carbonaceous aerosol is of secondary biogenic origin
- Cooking and, during winter, residential woodburning are the major primary OA
- BC concentrations are on the lower end of values encountered in megacities worldwide.

(Beekmann et al., ACP, 2015)

Model Evaluation - New Developments

Satellite data

Biggest advantage

Spatial coverage
Can provide data where in-situ measurements are not available
Information from the entire column of the atmosphere
useful for AOD, NO, NO2, O3, dust, fire plumes etc….

Disadvantages

Sometimes satellites only produce data on narrow swaths and can take several days to cover an area
Lack of sensitivity to ground level concentrations
Concentrations based on algorithms and hence not a direct measurements
Hence satellite data can be treated a ‘model data’ with their own uncertainty and bias
Problems with deep clouds

Model Evaluation -
Ensemble Evaluation Approaches

Multiple simulations for a single time period and location, while varying other aspects of the model simulation e.g.

Meteorology (different meteorology models, different meteorology configuration options, etc.)
Different emission inputs,
Different boundary conditions, or
Different CW-AQ model configuration options

Model Evaluation -
Ensemble Evaluation Approaches

Approaches

Brute force - where the model is simply run many times, each time varying some aspects of the model simulation

Decoupled direct method (DDM)

Sensitivity analysis technique for computing sensitivity coefficients simultaneously while air pollutant concentrations are being computed

Allows for the computation of the impact (sensitivity) of the model to an input perturbation (typically emission perturbations) using a single model simulation

More efficient computationally efficient than running the equivalent brute-force simulations

Model Evaluation -
Ensemble Evaluation Approaches

Ensembles can help in understanding:

Structure uncertainty - lack of knowledge regarding the fundamental mechanisms underlying an environmental process (i.e. ensembles by varying a single process

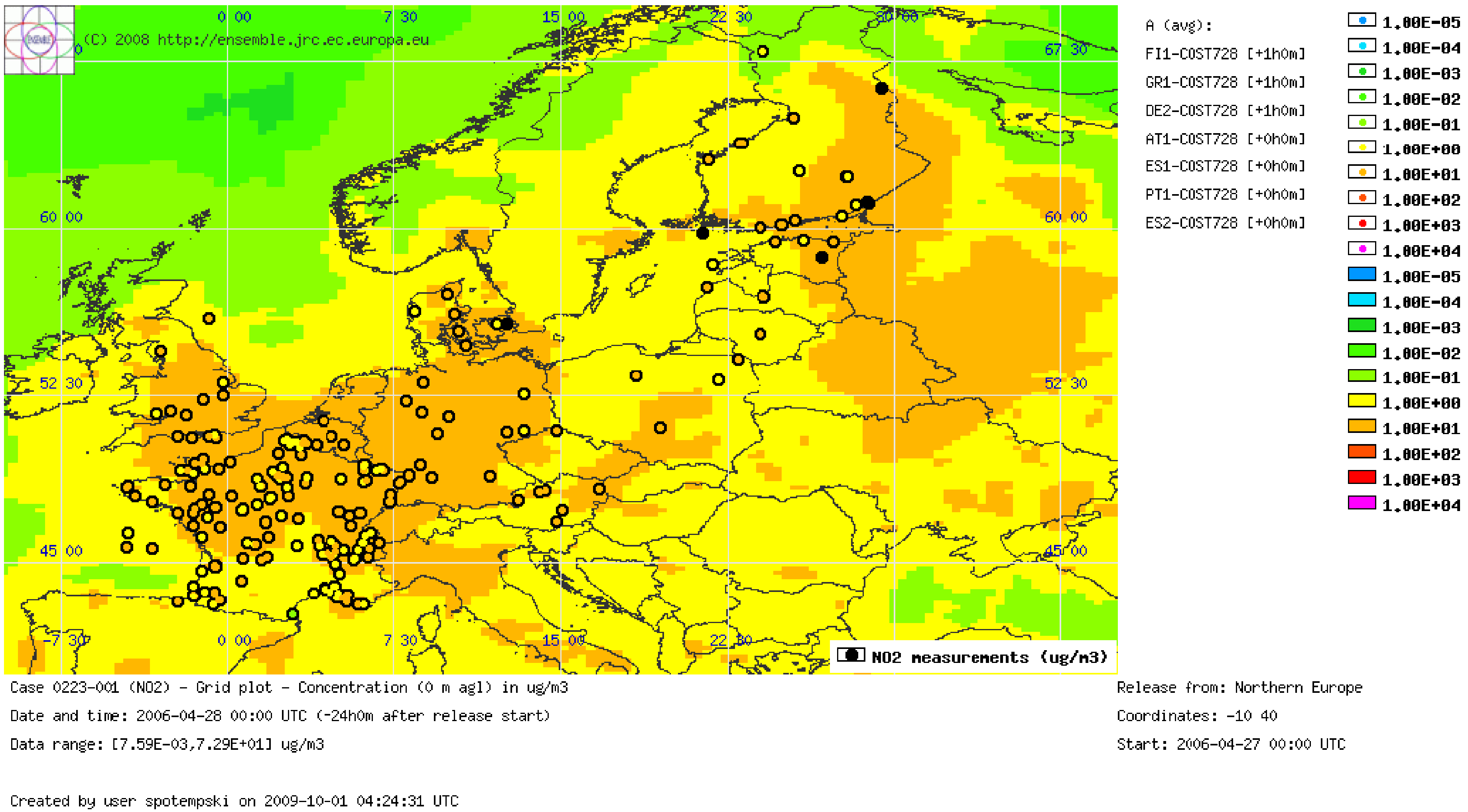
Parametric uncertainty - uncertainty in the inputs and parameter values (ensembles by varying an input or parameter used)

Example:

Pinder et al., 2009

Model Evaluation - Ensemble Evaluation Approaches

Average ensemble for NO_2 from five models



Chapter 7 of Sokhi et al (2019)

Model Evaluation Tools

Software Name	Developer	Application	Supported Models	Availability	Website	Reference
AMET	EPA	Meteorology, Air Quality	CMAQ directly, other models indirectly	Open Source	https://www.cmascenter.org/amet/	Appel et al., 2010
MET	NCAR	Meteorology, Air Quality	WRF, MPAS	Open Source	https://dtcenter.org/met/users/index.php	
ENSEMBLE	JRC	Meteorology, Air Quality	Multiple models indirectly	Online	https://ec.europa.eu/jrc/en/scientific-tool/model-evaluation-platform-ensemble	Galmarini et al., 2012
OPENAIR	NERC	Air Quality	Model independent	Open Source (R package)	http://davidcarslaw.github.io/openair/	Carslaw and Ropkins, 2011
MONET	NOAA	Air Quality	CMAQ directly	Open Source	https://github.com/noaa-oar-arl/MONET	Baker and Pan, 2017

Example references

Im, U., et al., 2014a, Evaluation of operational on-line-coupled regional air quality models over Europe and North America in the context of AQMEII phase 2. Part I: Ozone, 115, 404-420, *Atmospheric Environment*, doi: 10.1016/j.atmosenv.2014.09.042.

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Examination of the Community Multiscale Air Quality (CMAQ) model performance over the North American and European domains. Atmospheric Environment 53 (2012) 142-155

Pinder, R.W., R.C. Gilliam**,** K.W. Appel, S.L. Napelenok, A.B. Gilliland. Efficient probabilistic estimates of surface ozone concentration using an ensemble of model configurations and direct sensitivity calculations, *Environ. Sci. Technol*., 2009, 43 (7), pp 2388-2393, DOI: 10.1021/es8025402