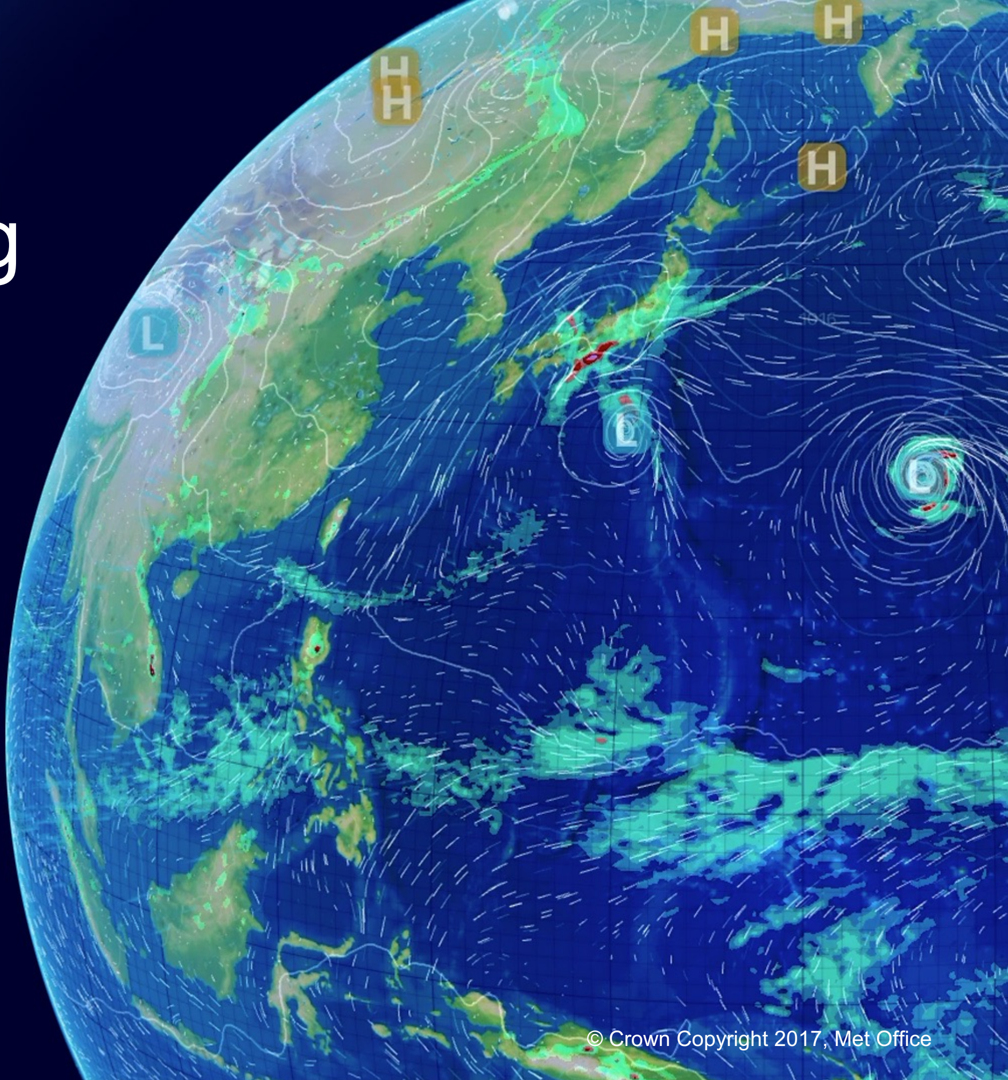
Met Office

Air Quality Forecasting Applications of UKCA

Paul Agnew
Cambridge
December 2022



Met Office

Air Quality

- Presence of naturally or anthropogenically emitted chemical species and particles in the air breathed by people
  - NO_2, (CO), SO_2, O_3, $PM_{10/2.5}$
- Elevated concentrations can affect human health
- Acceptable concentrations are prescribed by national and international law
- Governments are required to warn people of elevated levels

Met Office

Background

DIRECTIVE 2008/50/EC OF THE EUROPEAN PARLIAMENT AND OF THE COUNCIL of 21 May 2008 on ambient air quality and cleaner air for Europe

- **Detailed specification of regulations for ambient AQ pollutants: sulphur dioxides, nitrogen oxides, ozone, particulate matter, lead, benzene, carbon monoxide**

Review of the UK Air Quality Index

- **A report by the Committee on the Medical Effects of Air Pollutants**

Met Office

Daily AQ Index

- Index computed from concentrations of ozone, NO_2, SO_2, PM_{10}, $PM_{2.5}$
- CO no longer contributes
- Ozone computed from 8-hrly rolling mean
- Different averaging period for PM: daily 24 hour mean instead of rolling 24 hour mean
- Introduction of $PM_{2.5}$

Daily Air Quality Index

The new bandings for the Daily Air quality Index are detailed in Table 1.

Band	Index	Ozone Running 8 hourly mean μgm^{-3}	Nitrogen Dioxide hourly mean μgm^{-3}	Sulphur Dioxide 15 minute mean μgm^{-3}	$PM_{2.5}$ Particles 24 hour mean μgm^{-3}	PM_{10} Particles 24 hour mean μgm^{-3}
LOW						
	1	0-33	0-66	0-88	0-11	0-16
	2	34-65	67-133	89-176	12-23	17-33
	3	66-99	134-199	177-265	24-34	34-49
MODERATE						
	4	100-120	200-267	266-354	35-41	50-58
	5	121-140	268-334	355-442	42-46	59-66
	6	141-159	335-399	443-531	47-52	67-74
HIGH						
	7	160-187	400-467	532-708	53-58	75-83
	8	188-213	468-534	709-886	59-64	84-91
	9	214-239	535-599	887-1063	65-69	92-99
VERY HIGH						
	10	240 or more	600 or more	1064 or more	70 or more	100 or more

Table 1: Daily Air Quality Index bands

The new daily air quality index comes in three parts and includes additional advice for susceptible individuals, alongside advice for the general population:

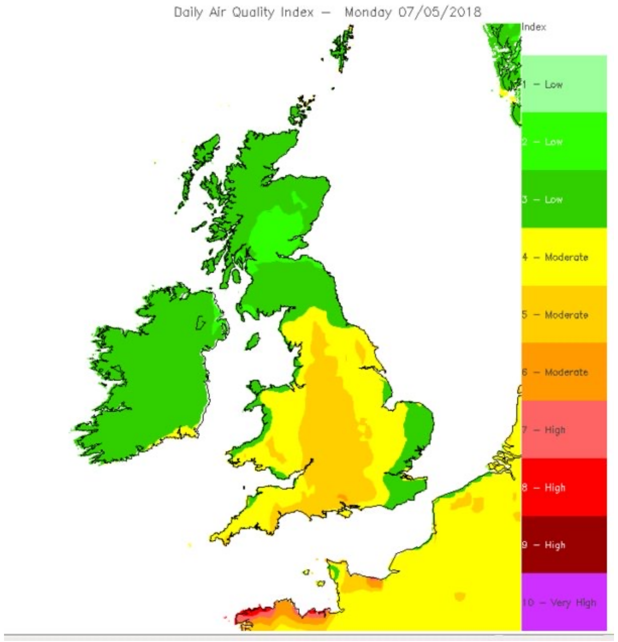
A. Instructions on how the index should be used;
B. The short-term health effects of air pollution and action that can be taken to reduce impacts;
C. Health advice linked to each band to accompany the air quality index.

These are detailed below:

What is forecast? Daily Air Quality Index

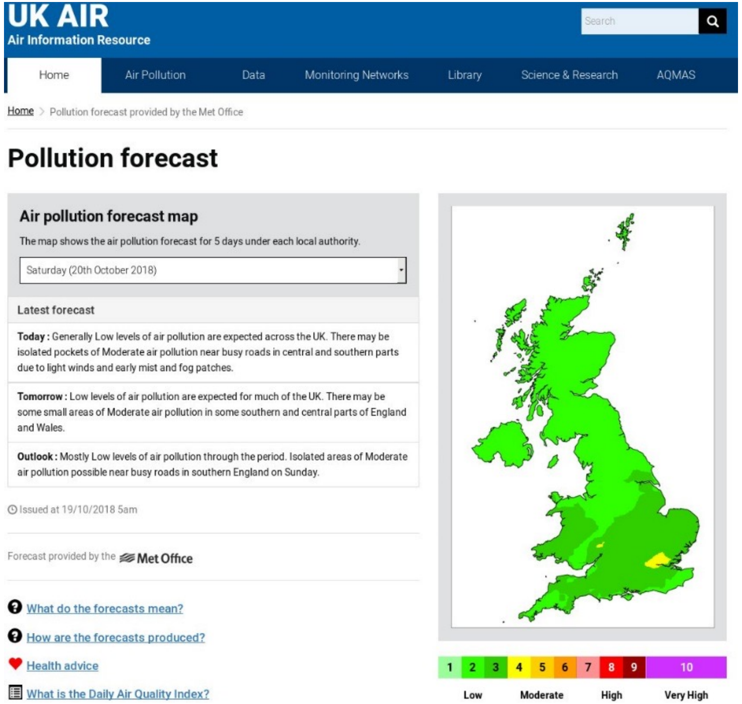
- 10-point index scale depending on time-averaged concentrations
  - O_3: maximum 8-hour rolling mean
  - NO_2: maximum hourly rolling mean
  - SO_2: maximum 15-min rolling mean
  - $PM_{2.5}$, PM_{10} : daily mean

- Partial index calculated for each species and greatest index is assigned to DAQI value



UK Air Quality Forecasting: Defra Website

- A Regional forecast
- ‘Daily Air Quality Index’ Maps issued once per day for current day and 4 days ahead
- Supplemented by a text commentary (and a tweet): Allows for:
    - Forecaster added-value (e.g. local influences, reason for elevations when appropriate etc.)
    - Qualification in cases of a poor forecast



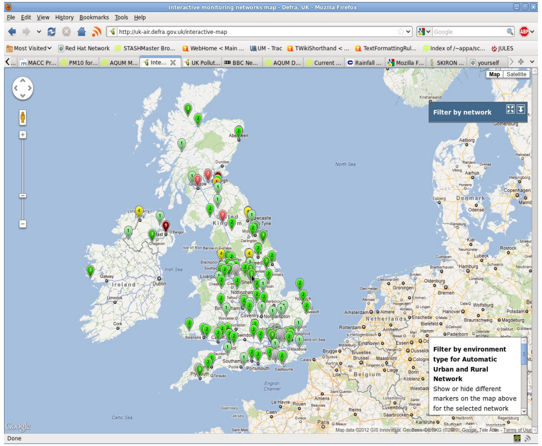
Routine air quality observations

- Defra fund the Automatic Urban and Rural Network (AURN)
- Network of sites spanning roadside, urban background and rural locations across the country
- Hourly measurements available in near-real-time at

http://uk-air.defra.gov.uk

- Measurements for London provided by Imperial College at

http://www.londonair.org.uk/London Air/Default.aspx

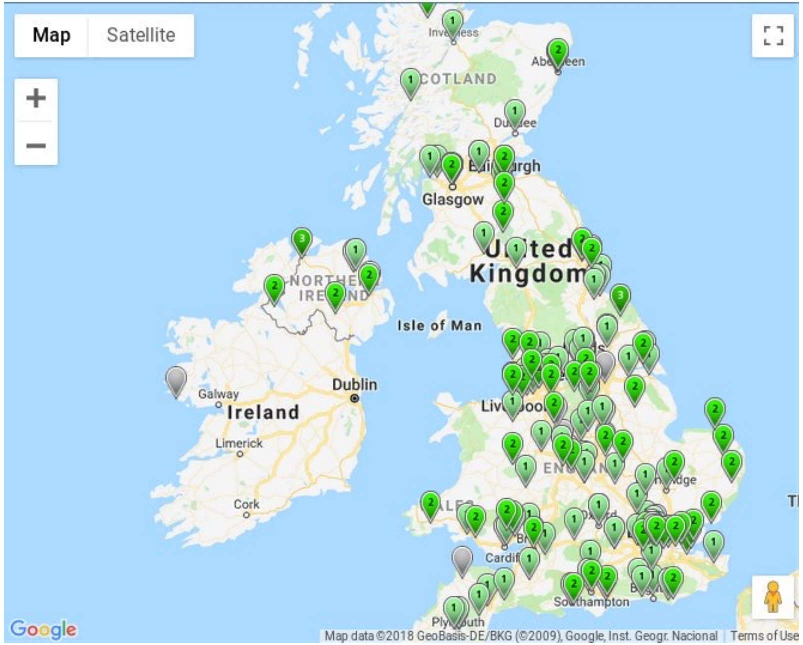


Routine Observation Network

- AURN site classifications:
  - Rural, suburban, urban Background
  - Suburban, urban Industrial
  - Urban Traffic

- Not all sites measure all pollutants
  - Ozone: 66 background + 8 others
  - $PM_{2.5}$: 49 background + 29 others

Routine measurement network

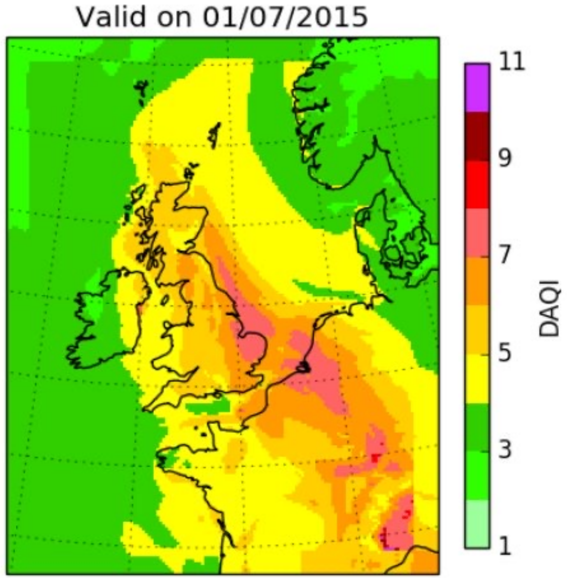


Overview of UK air quality characteristics

- Regional ambient air pollution levels are generally ‘Low’
- Typically ~10-15 episodes of elevated pollution per year
- Almost all episodes driven by one or both of two key pollutants: O_3 and $PM_{2.5}$

- Ozone episodes typically May to September
  - These episodes generally somewhat less intense in UK than continental Europe

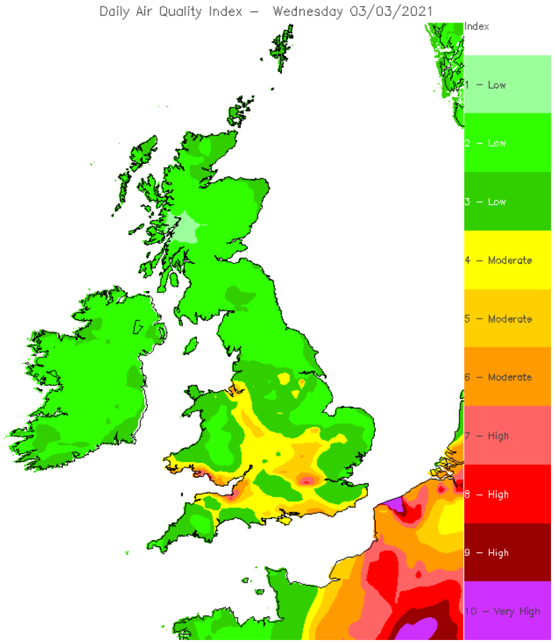
Typical UK summer O_3 episode



Met Office

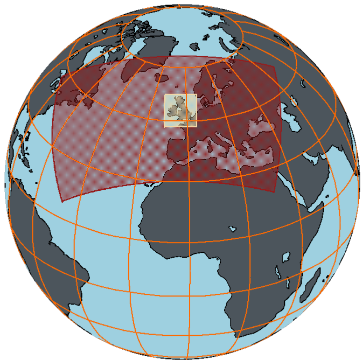
PM episodes

- $PM_{2.5}$ episodes typically spring (Mar/Apr/May) and autumn (Sep/Oct)
  - Usually driven by high pressure synoptic system to east/south-east of UK
  - Major component usually secondary inorganic aerosol
  - dominant species usually ammonium nitrate
- Contributions from both UK emitted precursors and precursors/aerosol imported from continental Europe



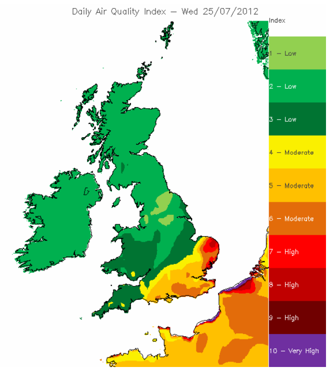
Forecast system

Model: AQUM

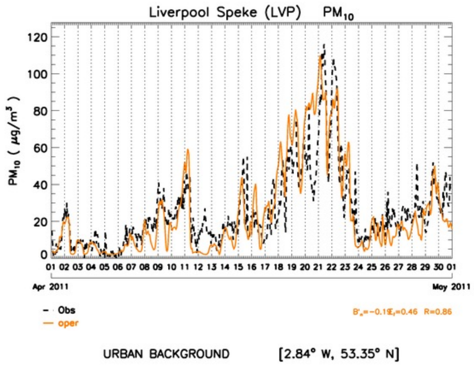


Observations

Forecast and post-processing



Verification

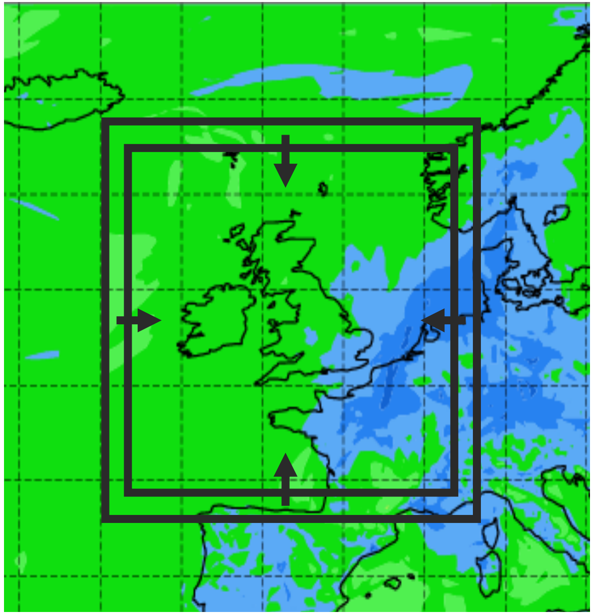


Met Office

AQUM

Air Quality Modelling in the UM

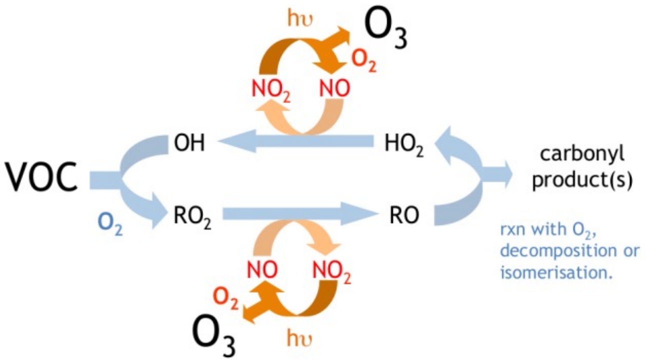
- Limited area configuration of the UM + UKCA
- First Operational 2010
  - 0.1 degree (~11km) horizontal resolution
  - 63 model levels (surface-39km)
- NWP LBCs from Met Office global forecast model
- Composition LBCs from CAMS global model (C-IFS)



Met Office

AQUM – Composition Modelling

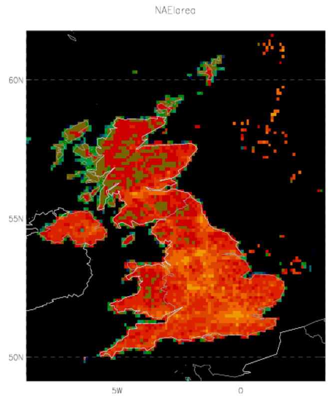
- Chemistry: RAQ (Regional Air Quality)
  - 40 transported species (16 emitted) + 18 non-advected
  - 116 gas-phase reactions + 23 photolysis reactions (FAST-JX)
  - Representative alkanes, alkenes and arenes
- Aerosol: CLASSIC
  - Single moment scheme
  - Sulphate, Black Carbon, Organic Carbon, Biomass burning, Dust (6 bins), Nitrate



National Centre for Atmospheric Science

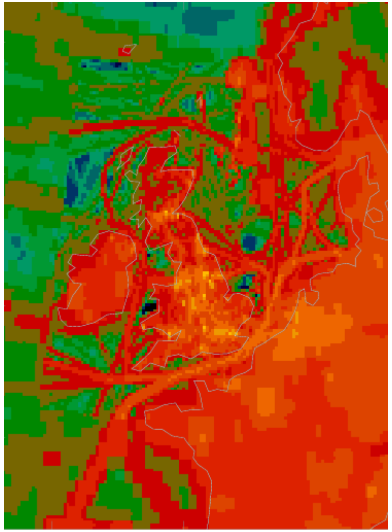
Savage et al. [GMD, 2013]

Air Quality Emissions



National Atmospheric Emissions Inventory @ 1km

https://naei.beis.gov.uk/



EMEP European emissions @ 10km

https://www.emep.int/

- Annual average inventories
- Emissions generated via a set of sophisticated python libraries
- Merging multiple inventory datasets in variety of formats
- Updated on an annual basis
- Additional temporal and vertical profiles from variety of sources are used

Met Office

AQUM Forecast Configuration

- Runs under a cycling Rose suite
- Forecast model is free-running: no data assimilation
- Initial conditions:
  - Meteorology: Met Office global weather model
  - Composition: previous T+24 forecast fields are ‘transplanted’ into the start dump
- Lateral boundary conditions:
  - Meteorology: Met Office global weather model
  - Composition: CAMS C-IFS global compositions model
- Forecast length: T+120; relaxation to climatological LBCS from T+72

Approach to model evaluation and verification

- ‘Mean field’ metrics: bias, rmse, correlation
  - Provide an ‘average’ (over space or time) indication of model vs obs
  - Favour more smoothly varying model fields (or time series)
  - Penalise more inhomogeneous model (potential for ‘double penalty’)

- Categorical metrics
  - Employ 2x2 contingency table
  - Test model skill in predicting exceedance of a threshold: *this is a key performance indicator for a model used to issue alerts*

Aside: Comparing pollutants: use of normalised metrics

Need to employ some form of normalisation when comparing pollutants. Traditional measures

- Normalised mean bias
- Normalised rmse

- Asymmetry problem: asymptotically limited to -1 for under-prediction; unlimited for over prediction

$$B_n = \frac{1}{N}\sum_i \frac{(f_i - o_i)}{o_i}$$

$$E_n = \left(\frac{1}{N}\sum_i \left(\frac{f_i - o_i}{o_i} \right)^2 \right)^{1/2}$$

Met Office

Comparing pollutants: use of normalised metrics

Employ measures which are symmetrical with respect to under/over prediction

- Modified mean bias

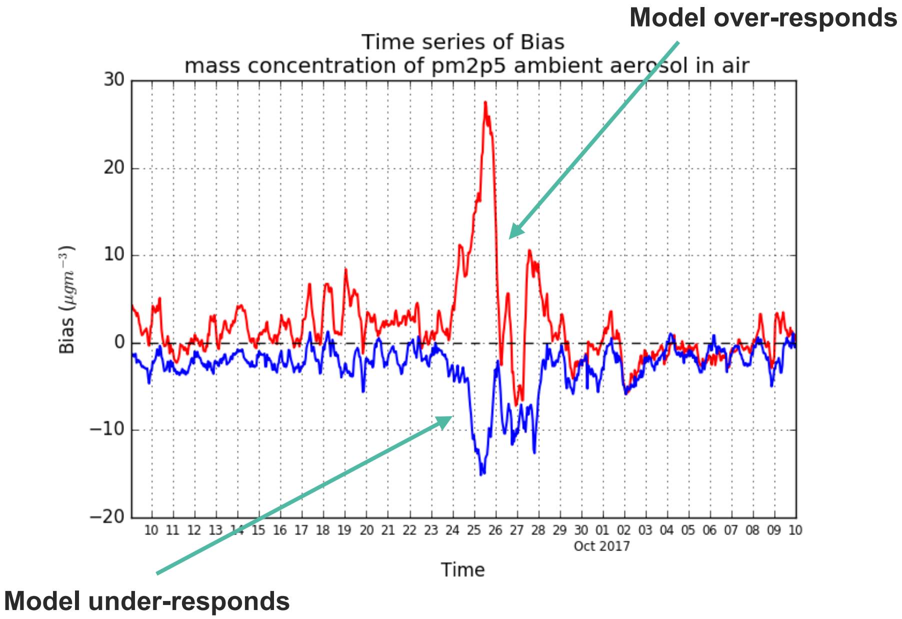
$$B'_n = \frac{2}{N}\sum_i \left(\frac{f_i - o_i}{f_i + o_i} \right)$$

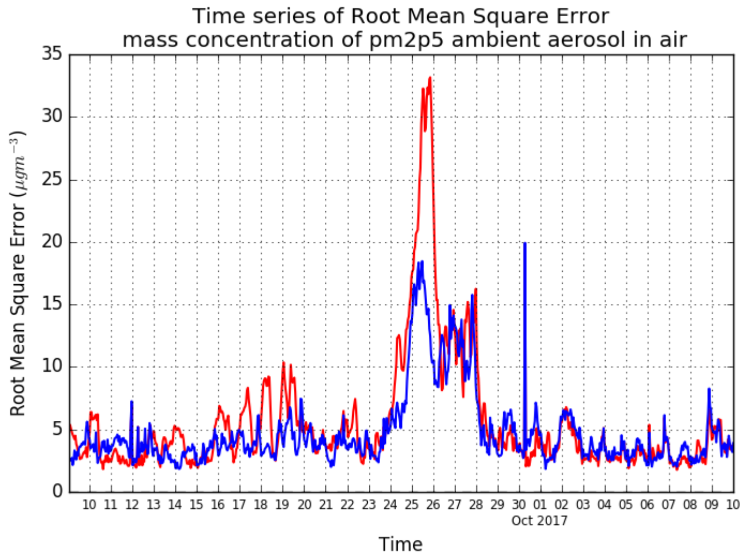
- Fractional gross error

$$E_f = \frac{2}{N}\sum_i \left| \frac{f_i - o_i}{f_i + o_i} \right|$$

- Vary symmetrically between ±2

Verification: mean field metrics
e.g. comparing two model configurations: Red,Blue

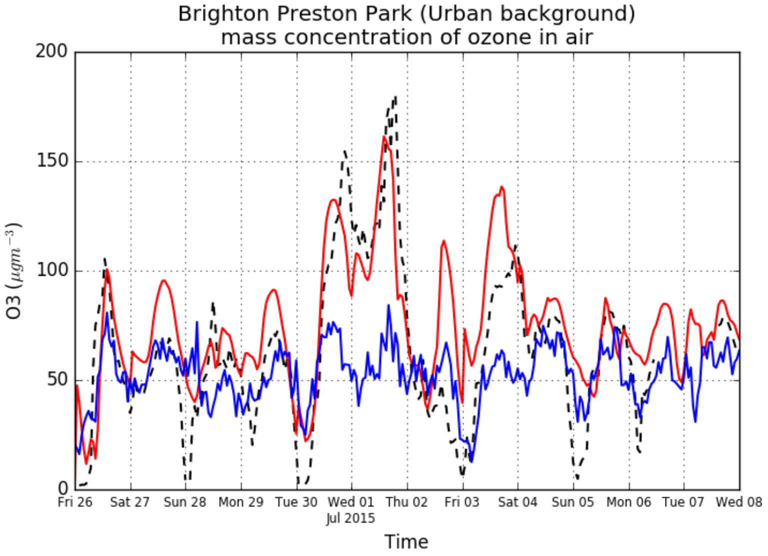




Model responsiveness to episode conditions

Mean over all sites	Red	Blue
Bias (µg/m³)	19.4	-4.6
RMSE (µg/m³)	26.1	24.7
FAC2	0.86	0.87

- These metrics don't capture the lack of responsiveness of **Blue** to episode conditions



Categorical Evaluation

		Events	Observed
		Yes	No
Events	Yes	a	b
Forecast	No	c	d

- Assess model skill for prediction of threshold exceedance
- Compute Hit & False Alarm rate
  - conditional probabilities
  - $H = p(f \mid o)$; $FAR = p(f \mid \bar{o})$
- The Odds Ratio is a useful and robust overall metric*:

  OR = odds of hit / odds of false alarm
  = ad/bc

*D. Stephenson, Weather and Forecasting, 15 (2), 221 (2000)

Properties:

- Only weakly dependent on threshold value used
- Independent of event forecast frequency bias=(a+b)/(a+c)
- Distribution of log(OR) is approximately Gaussian with Standard Error*:

$$SE = (1/a + 1/b + 1/c + 1/d)^{1/2}$$

- Can be tested for significance against null hypothesis that forecast/obs are independent (i.e. log(OR)=0)
  - (require all counts >~5)

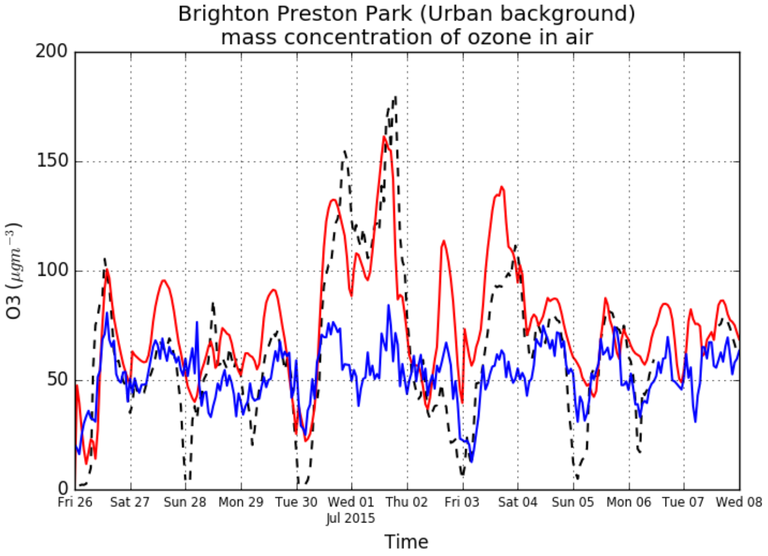
*A. Agresti, *An Introduction to categorical data analysis*, 2007

Met Office

Model responsiveness

Mean over all sites	Red	Blue
Bias (µg/m³)	19.4	-4.6
RMSE (µg/m³)	26.1	24.7
FAC2	0.86	0.87

Hit rate	0.76	<10^{-3}
False alarm rate	0.08	0.00
Odds Ratio	34.8	-----

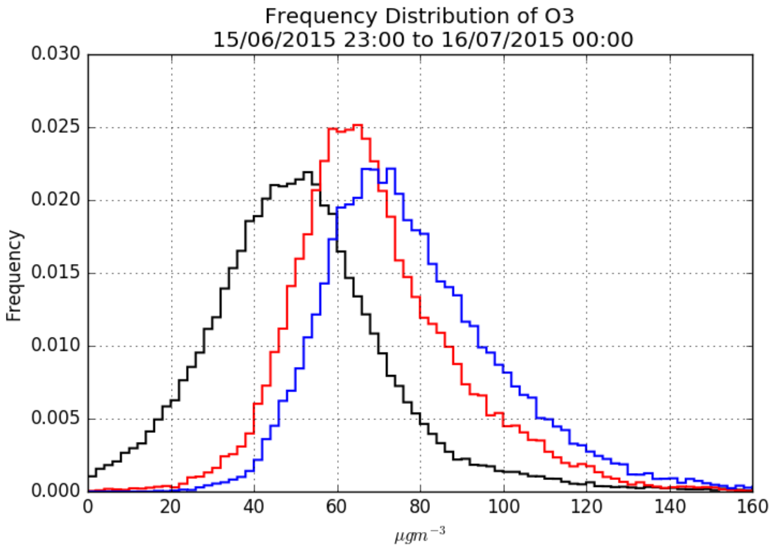


Met Office

Example: comparing performance

	Red	Blue
Bias (μg/m^3)	18.11	27.47
Hit rate	0.78	0.72
False alarm rate	0.06	0.13
Odds Ratio	57.9	16.4

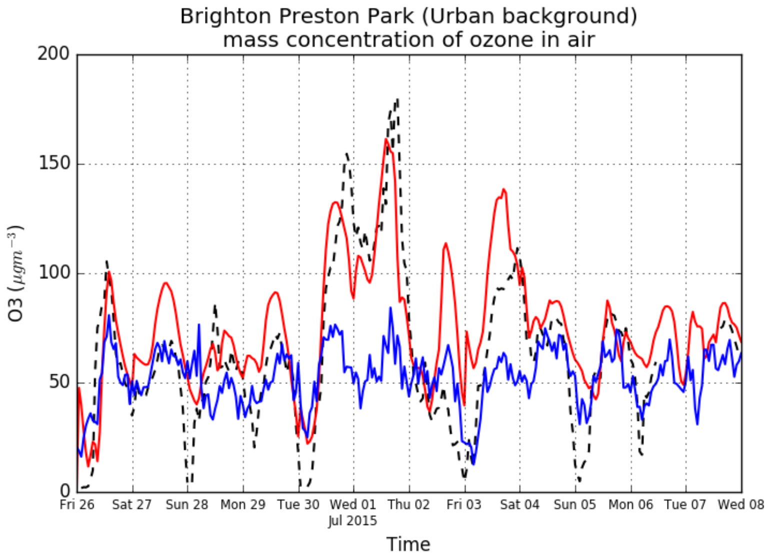
- Mean field plus categorical metrics give a more complete overview of model performance



Met Office

Summary

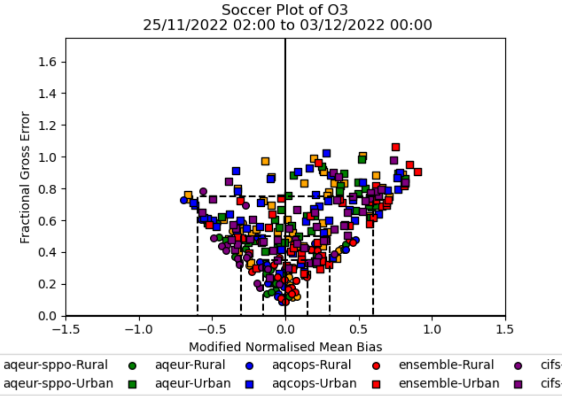
- Model responsiveness to episode conditions is a key characteristic for an air quality forecast/warning system
- Categorical metrics are better suited to capturing this aspect of model performance
- The Odds Ratio is a useful and robust summary metric for evaluating performance

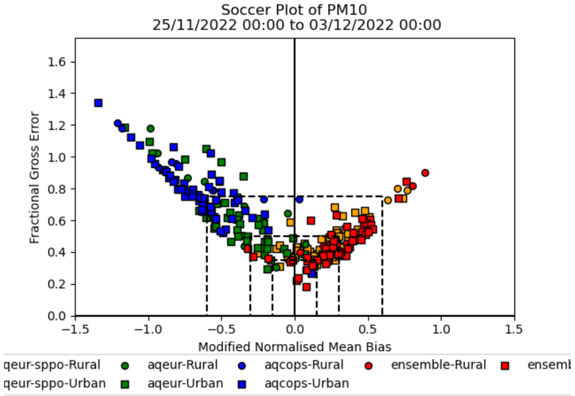


Met Office

Comparing pollutants: visualisation of characteristics

- Soccer plots based on ‘modified normalised metrics’ allow comparison of pollutants
- offer useful and rapid visualisation of key characteristics
- Easy assessment of contribution of bias and random errors to overall errors

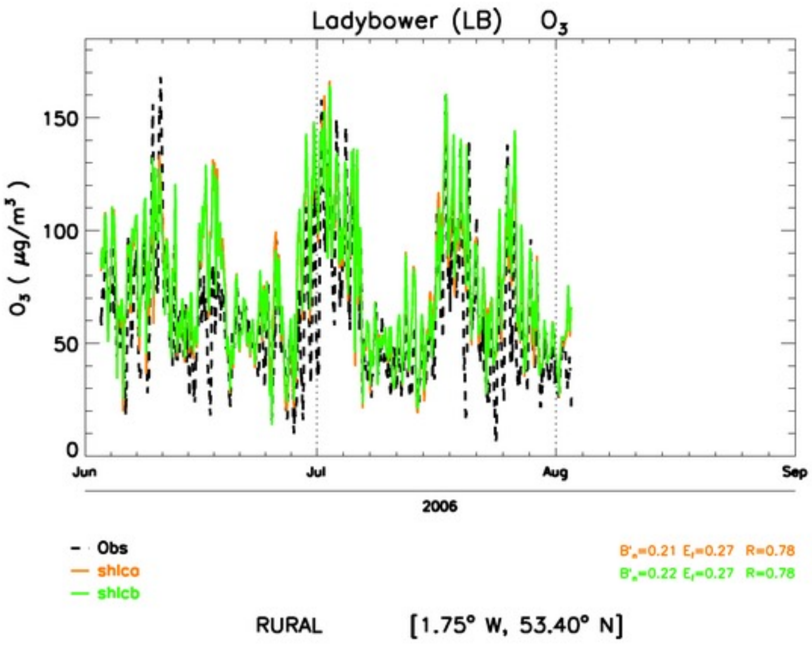




Met Office

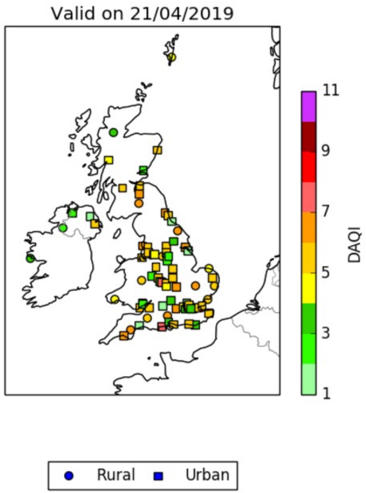
Near-real-time verification: site specific

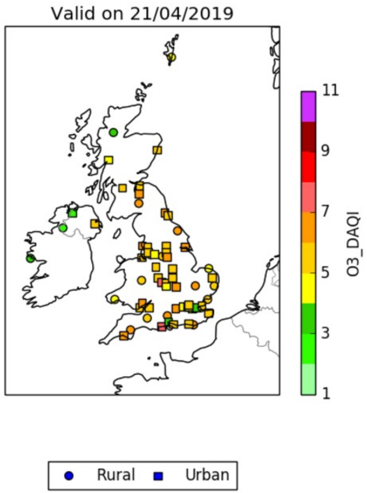
- Routine verification of AQUM against observations from the UK Automatic Urban and Rural Network (AURN)
  - Surface measurements of SO2,O3, NO2, NO, CO and PM10 and PM2.5 are available

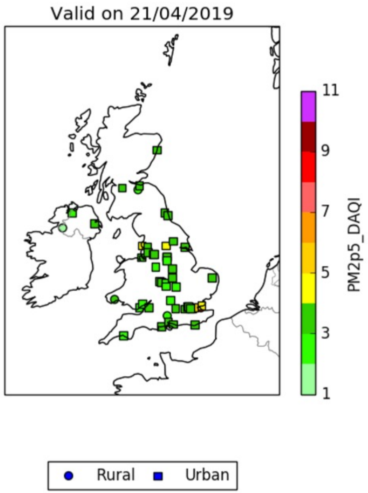


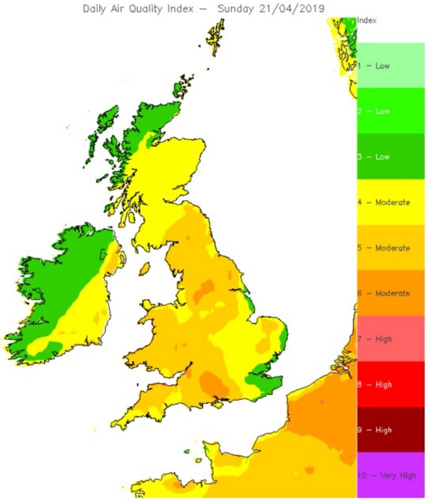
Met Office

Near-real-time verification: field plots





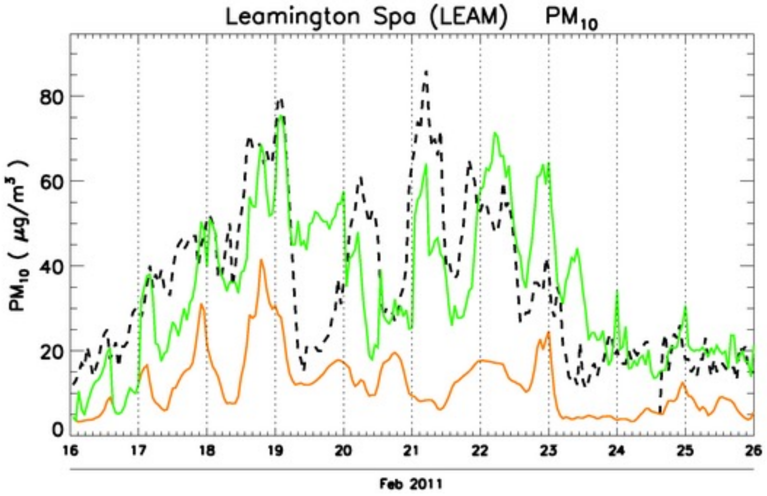




Met Office

Statistical post-processing of observations

- Recent pollutant measurements from the national network can be used to improve forecasts
- We have developed a methodology to adjust the current AQUM forecast, according to local observations
- Large improvements in forecast skill have been demonstrated, especially for PM



--Observed PM10

--Raw model forecast

--Adjusted forecast

Impact of post-processing (simulation of 2007)

Ozone

	Raw Model	Post-Processed
Correlation	0.72	0.91
Bias (μgm^{-3})	14.93	0.50
RMSE (μgm^{-3})	25.38	10.30
FAC2	0.78	0.91
Hit rate	0.49	0.60
False alarm ratio	0.90	0.33
ORSS	0.85	0.99

$PM_{2.5}$

	Raw Model	Post-Processed
Correlation	0.56	0.88
Bias (μgm^{-3})	2.62	0.46
RMSE (μgm^{-3})	9.51	3.64
FAC2	0.63	0.86
Hit rate	0.46	0.73
False alarm ratio	0.89	0.28
ORSS	0.89	1.00

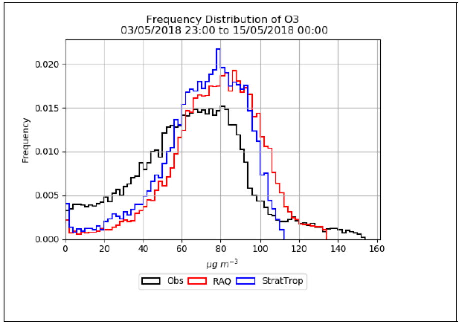
Chemistry for air quality

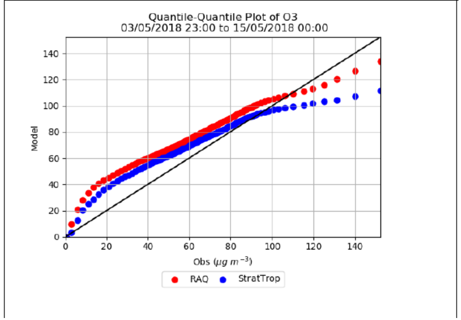
Requirements of a chemistry mechanism differ according to application

- Future climate modelling:
  - Needs to represent well the longer-term average state of the atmosphere – short-term peak values less relevant
- Air quality:
  - Concerned with representing the higher concentrations of pollutants on shorter timescales: short-term peak values essential

Met Office

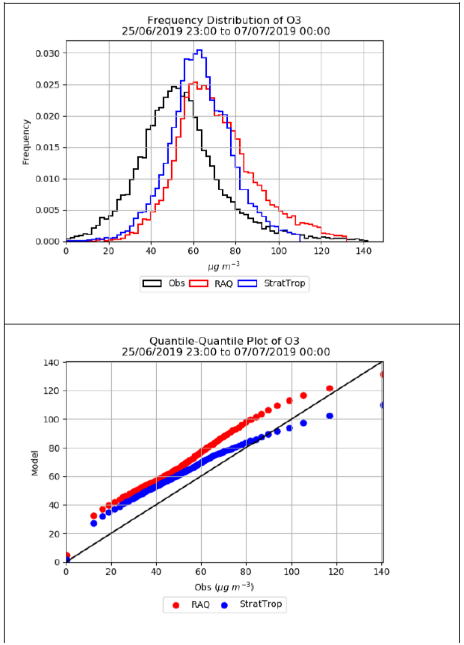
Ozone Episode May 2018





	RAQ	Strat-Trop
DAQI		
Correlation	0.82	0.72
Bias	0.11	-0.18
RMSE	0.73	0.87
Odds Ratio	11.09	4.24
ORSS	0.83	0.62
Hit Rate	0.76	0.26
False Alarm Rate	0.22	0.08
O_3		
Correlation	0.69	0.57
Bias (μg/m^3)	12.66	6.00
RMSE (μg/m^3)	25.13	25.64
Odds Ratio	15.43	8.20
ORSS	0.88	0.78
Hit Rate	0.62	0.23
False Alarm Rate	0.10	0.03

Ozone Episode June 2019



	RAQ	Strat-Trop
DAQI		
Correlation	0.81	0.73
Bias	0.38	0.14
RMSE	0.77	0.72
Odds Ratio	25.96	3.15
ORSS	0.93	0.52
Hit Rate	0.79	0.09
False Alarm Rate	0.13	0.03
O_3		
Correlation	0.72	0.61
Bias ($\mu g/m^3$)	16.79	9.41
RMSE ($\mu g/m^3$)	22.60	19.37
Odds Ratio	45.86	14.94
ORSS	0.96	0.87
Hit Rate	0.74	0.17
False Alarm Rate	0.06	0.01

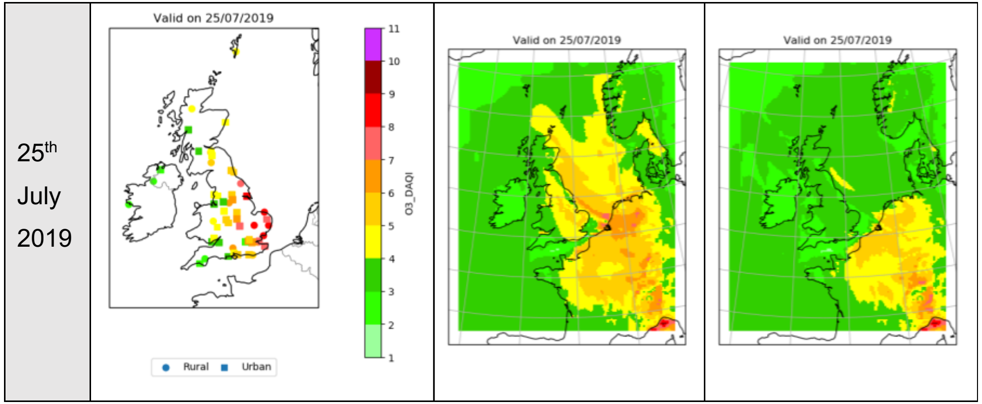
Met Office

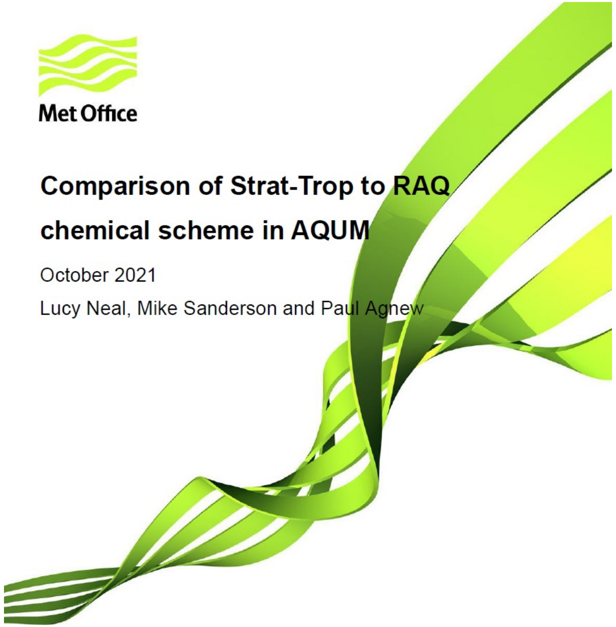
Comparing chemistry mechanisms

StratTrop

- *“Overall, the StratTrop scheme struggled under air quality episode conditions, often failing to show any indication of an episode which the RAQ scheme generally captures.”*

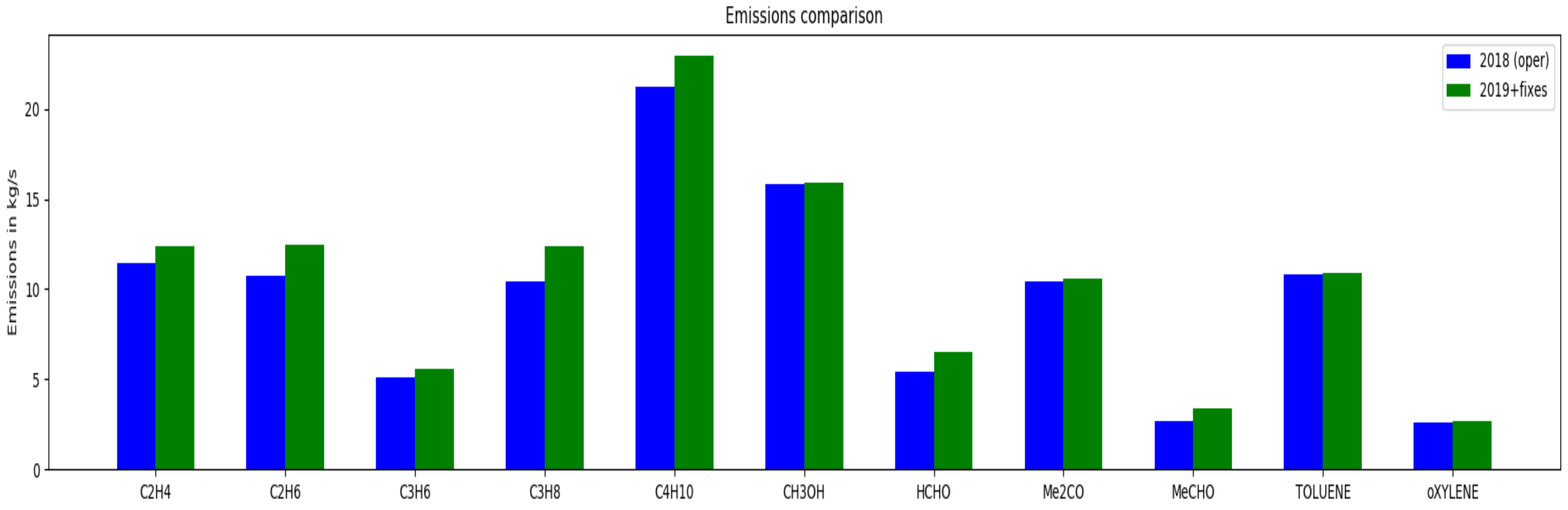
RAQ **StratTrop**





Met Office

NAEI (UK) Emissions



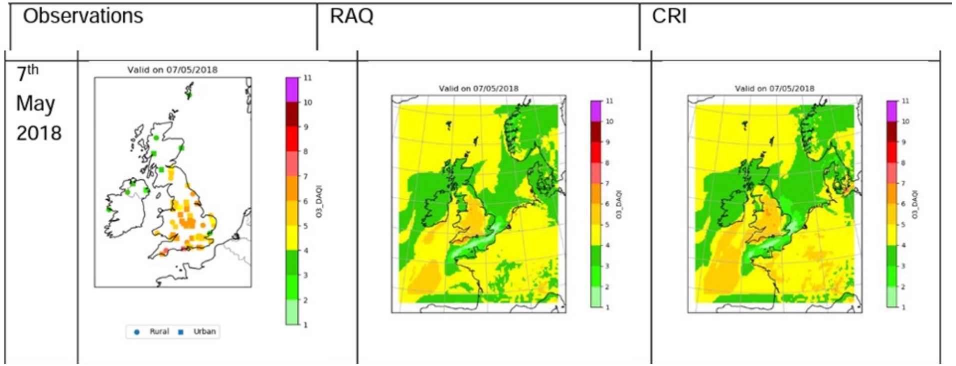
Met Office

WP1: Chemical Mechanism

CRI

- *"Overall – RAQ and CRI give very similar results for ozone episodes"*
- *"CRI more expensive than RAQ (~3.5 x)"*

RAQ **CRI**



Met Office

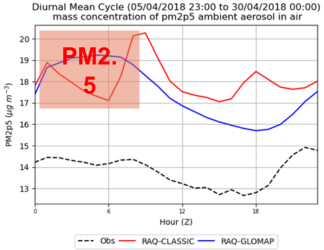
Assessment of the UKCA CRI - Strat2 chemical mechanism for air quality modelling in AQUM

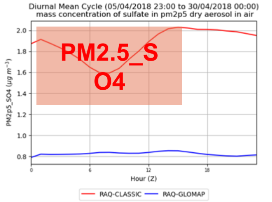
Benjamin Drummond, Lucy Neal, Barnaby Sherratt, and Paul Agnew

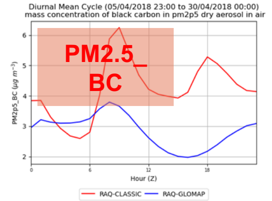
January 2022

Aerosol Modelling

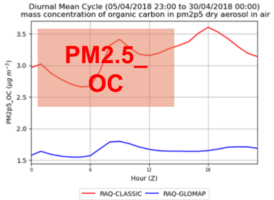
- AQUM currently relies on the CLASSIC aerosol scheme to predict Particulate Mater.
- CLASSIC is being phased out as UKCA is becoming a standalone model.
- NUAQ will replace AQUM and be based on UKCA. Aerosols in UKCA are handled by GLOMAP.
- Until recently, GLOMAP was lacking a representation of Nitrate aerosol limiting is suitability for AQ forecasting. This has been addressed recently.

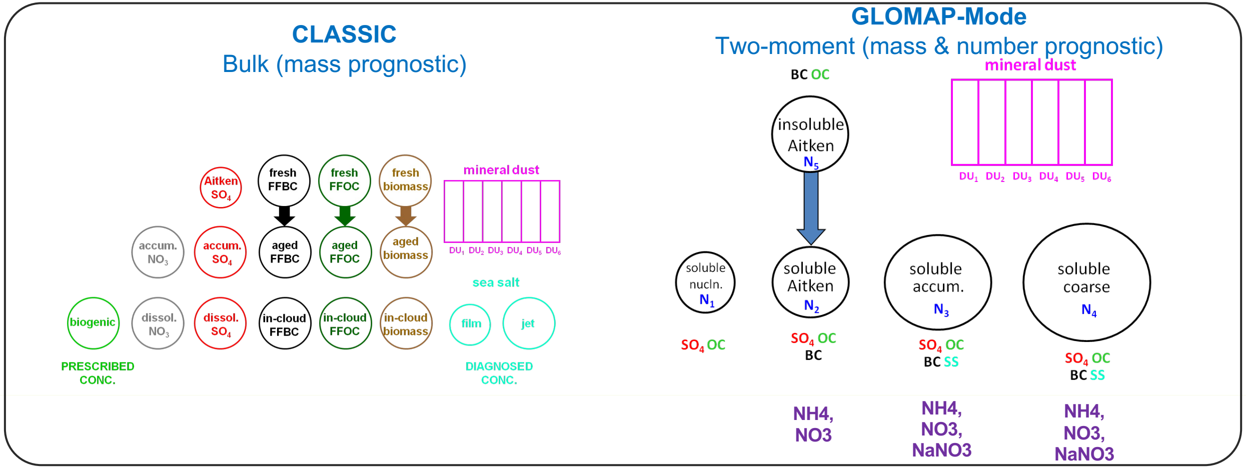


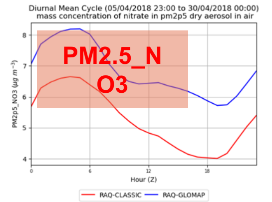




- GLOMAP fully resolves the aerosol size distribution, potential for better prediction of PM.
- Internally mixed (GLOMAP-mode) versus externally mixed (CLASSIC) aerosols.
- Different parameterisation for aerosol processes (e.g. dry and wet removal).
- Prognostic Sea Salt.



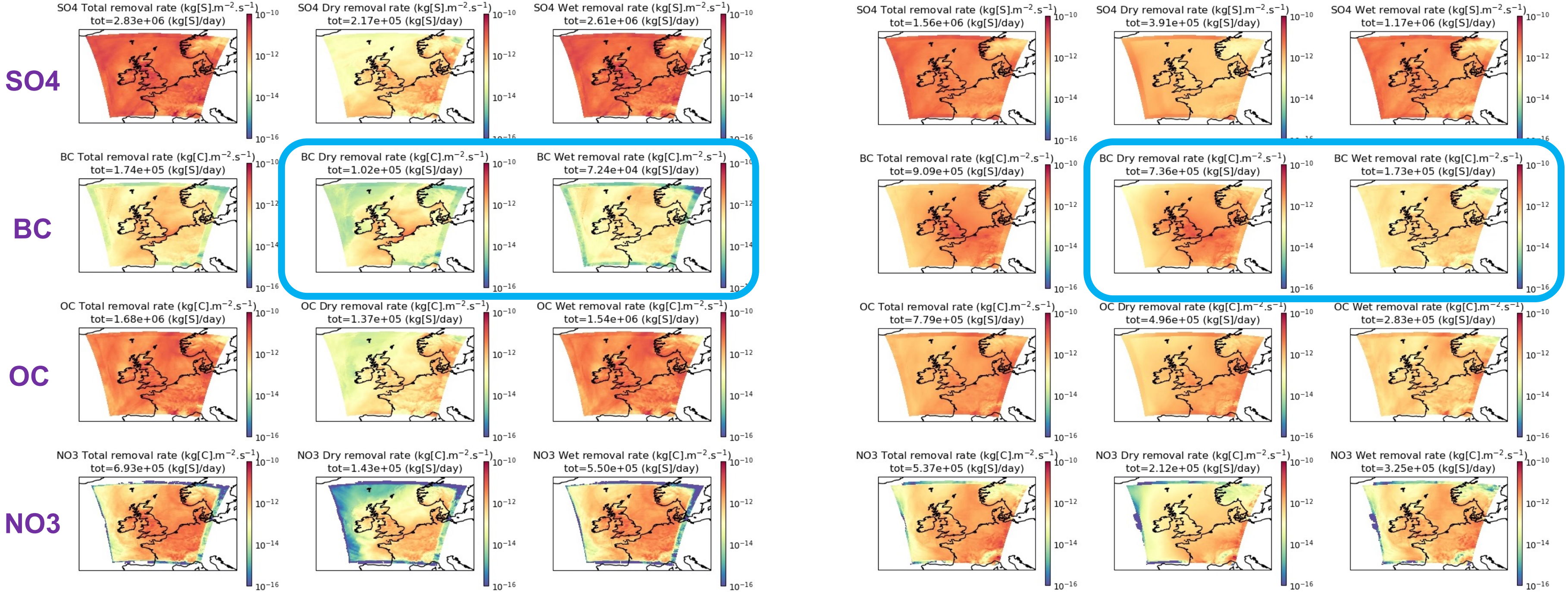




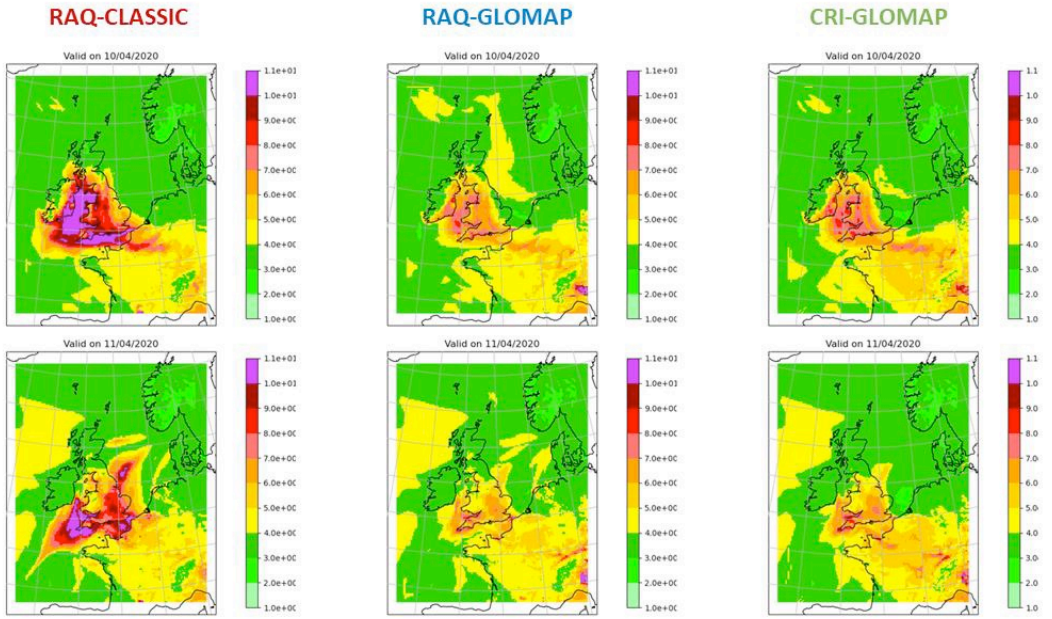
Met Office

CLASSIC (15 Jan – 15 Feb 2017 mean) | GLOMAP (15 Jan – 15 Feb 2017 mean)

Total deposition | **Dry deposition** | **Wet deposition** | **Total deposition** | **Dry deposition** | **Wet deposition**



GLOMAP


RAQ-CLASSIC
RAQ-GLOMAP
CRI-GLOMAP
Valid on 10/04/2020
Valid on 11/04/2020
1.1e+01
1.0e+01
9.0e+0C
8.0e+0C
7.0e+0C
6.0e+0C
5.0e+0C
4.0e+0C
3.0e+0C
2.0e+0C
1.0e+0C

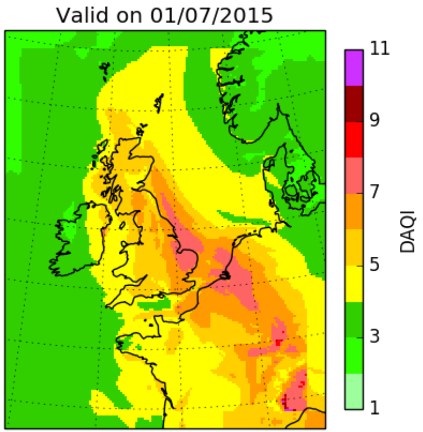
Met Office

Summary of findings of Glomap AQ evaluation

- During non-episode conditions, the GLOMAP-based simulations are capable of simulating fine particulate matter levels that are in good agreement with CLASSIC-based simulations. Compared to a previous evaluation, this is a significant improvement in performance from GLOMAP-mode and mostly stems from the addition of a representation of nitrate aerosol.
- During episode conditions, the GLOMAP-based simulations are less prone to excessive production of nitrate aerosols than the CLASSIC-based simulations, reducing the risk of over-forecasting PM concentrations.
- For the primary (emitted) components of the fine particulate matter, which are represented by the carbonaceous aerosol tracers (BC and OC) in AQUM, the current GLOMAP-based setups systematically simulate lesser contributions from BC and OC than the CLASSIC-based setup. Several factors may be contributing to this situation to a varying degree, including differences in how particulate matter concentrations are derived, the rates of aerosol removal, aerosol modes properties, or how emissions are implemented.
- Rates of aerosol removal differ significantly between the two aerosol schemes. This is particularly noticeable for the BC species with GLOMAP-mode simulating much higher removal, addressing a tendency of CLASSIC to keep BC airborne for too long. This however has a detrimental impact in the current AQUM framework for effectively representing the contribution of primary sources in the particulate matter.
- The emission vertical and temporal scaling assumptions used in the GLOMAP-mode and CLASSIC AQUM setups currently differ. This can affect the simulated particulate matter surface concentrations, with the largest impacts for the carbonaceous species which are essential in modelling PM episodes dominated by local sources.
- Compared to CLASSIC, GLOMAP gives a much-improved representation of the coarse component of aerosol (i.e. PM_{10} - $PM_{2.5}$) thanks to the introduction of prognostic sea salt.
- The choice of chemistry mechanism (RAQ or CRI) did not significantly affect the particulate matter concentrations simulated by GLOMAP. VOC chemistry which differs between the two mechanisms did not contribute to aerosol formation in our simulations but it is not expected to be a dominating aerosol source over the UK.
- Despite the addition of new tracers and a full nitrate scheme, the overhead from using GLOMAP-mode compared to CLASSIC results in a ~40 to 50% increase in model runtime, consistent with previous evaluation GLOMAP-mode cost.
- It is concluded that the GLOMAP scheme is a viable replacement for CLASSIC for air quality forecasting applications and has the potential to be superior in some respects. However further work is required to understand the substantial differing estimates of aerosol removal compared to CLASSIC and the impacts of applying revised aerosol vertical injection heights. *In the longer term, it is recommended that GLOMAP be further developed for short-term air quality applications by the addition of an insoluble coarse aerosol mode.*

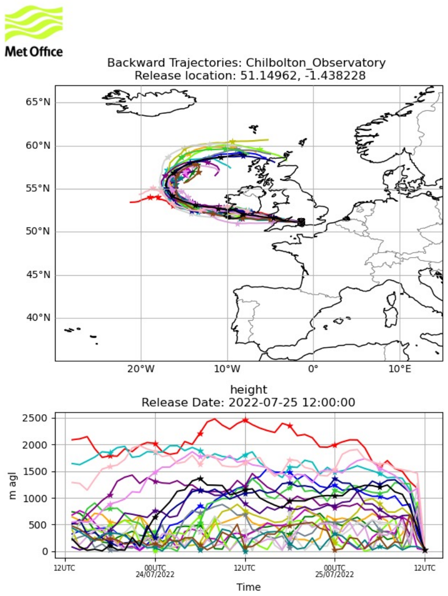
NAME Dispersion, AQ and Trajectory Model

- NAME can be configured as a Lagrangian or Eulerian model
- It is being developed for air quality forecasting applications
- It can be run backwards in time to show where air has come from



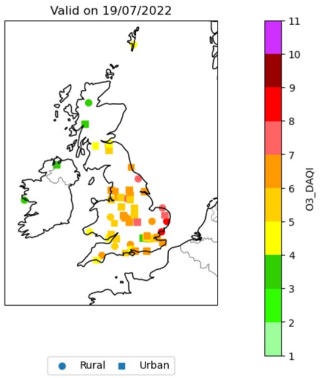
DAQI map during ozone episode – produced by NAME

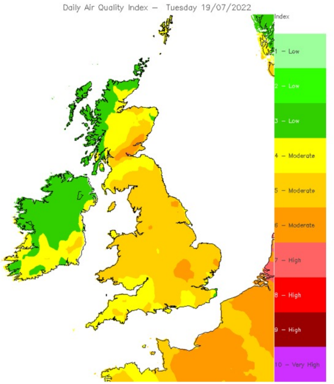
Air back trajectories produced by NAME running backwards in time



Datasets: T+24 AQ Forecast

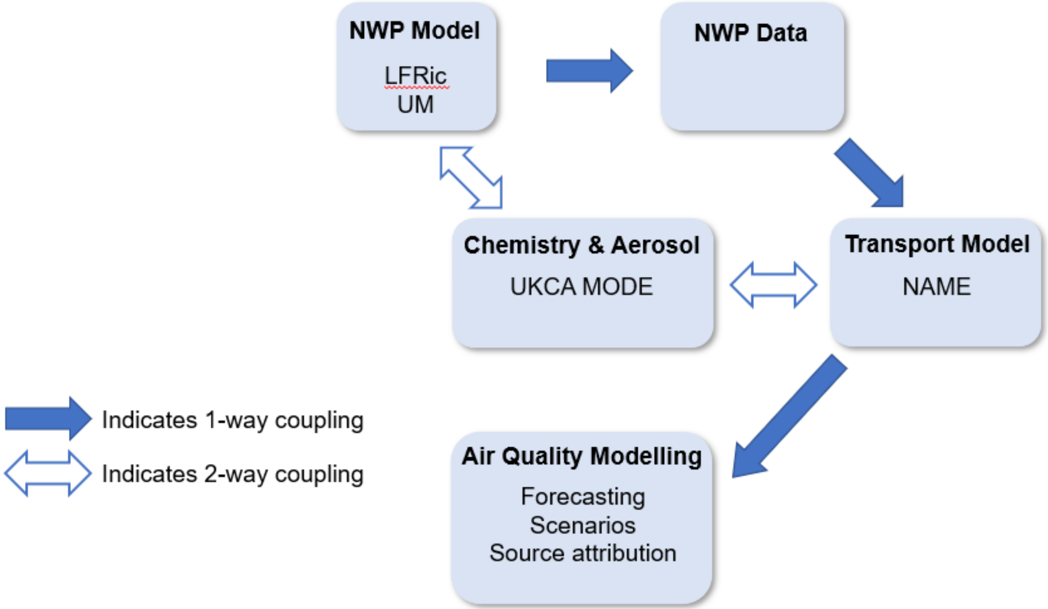
- We maintain an archive of our air quality forecasts
- Covers ~ 2012 to present day
- Predicted hourly surface air concentrations of AQ pollutants on a 2km grid over the whole UK
- A high quality dataset of historic UK pollution levels
- Also available on Jasmin





Met Office

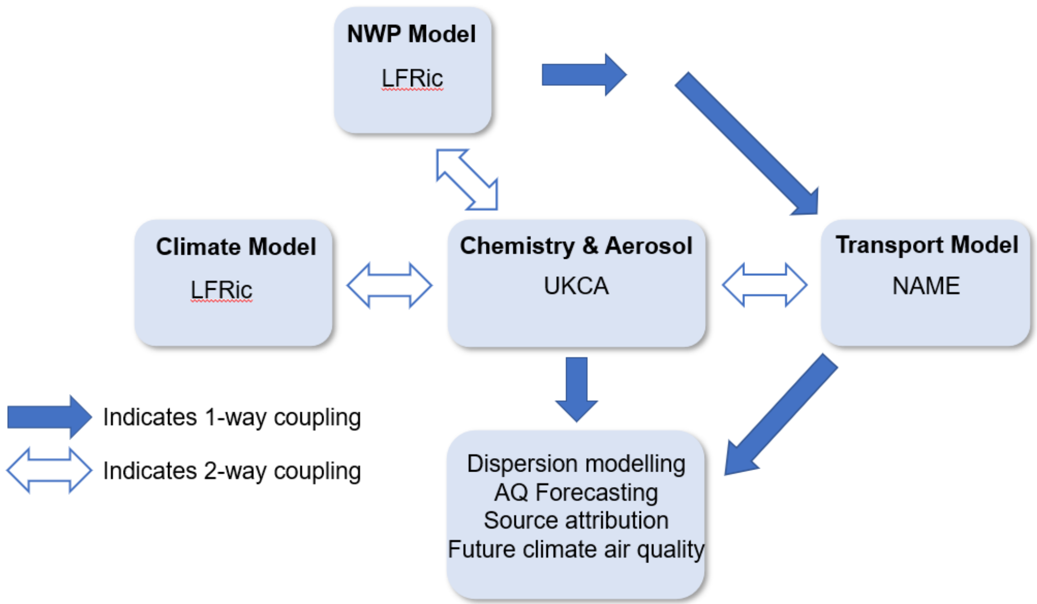
NU-AQ



- NU-AQ Project
    - NAME-UKCA Air Quality
    - “New-A-Q”
- NAME-NGMS
    - Enable efficient use of LFRic meteorology data
- Support both Lagrangian and Eulerian NAME configurations

Met Office

Future Possible NAME Configuration

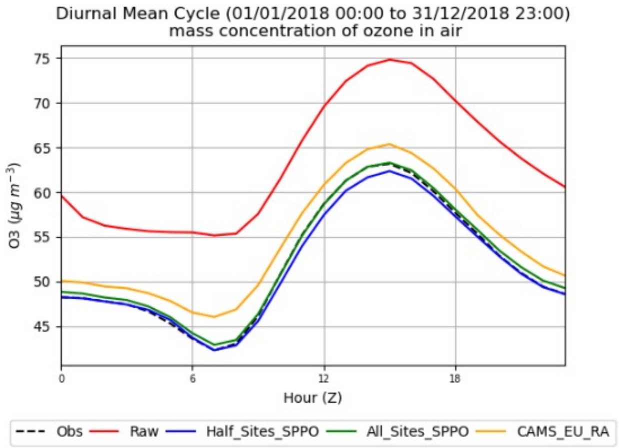


- Closer coupling to driving NWP model brings many benefits
  - No need for met archive
  - Timestep-resolution met
  - Wider range of NWP model parameters

Met Office

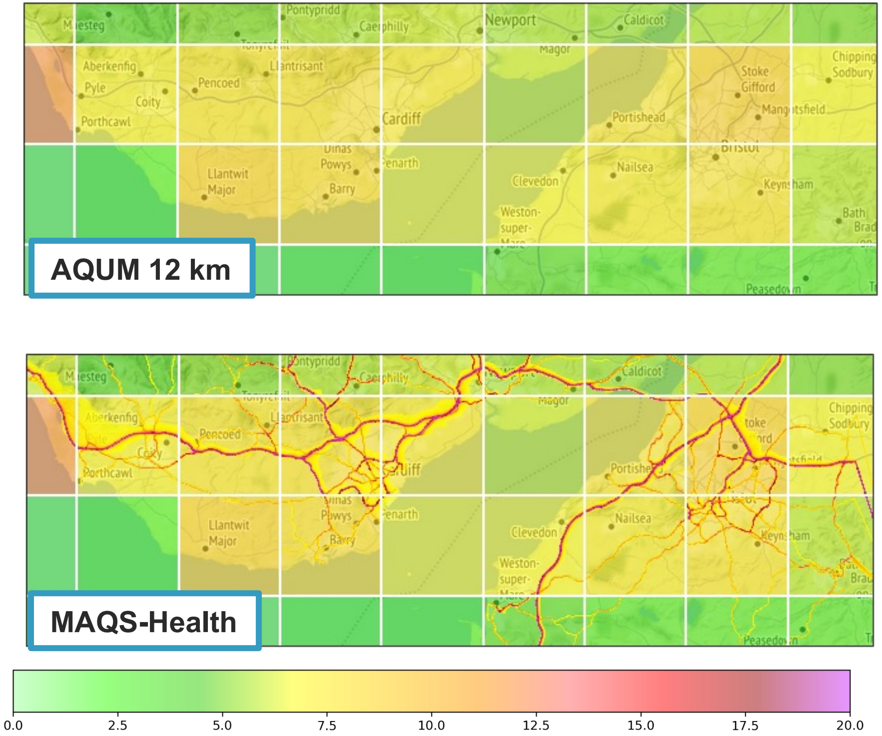
Datasets: Air Quality Reanalysis

- We are producing a reanalysis over the UK of air quality pollutants
- Dataset covers 2003-current day at hourly resolution
- Also includes meteorological parameters
- Uses boundary conditions from a global reanalysis (by ECMWF) assimilating satellite obs
- Surface pollutant concentrations bias-corrected by UK surface network (AURN)
- *A consistent, long-term dataset which can be used for health impact studies*



Lucy Neal, Eleanor Smith, Paul Agnew

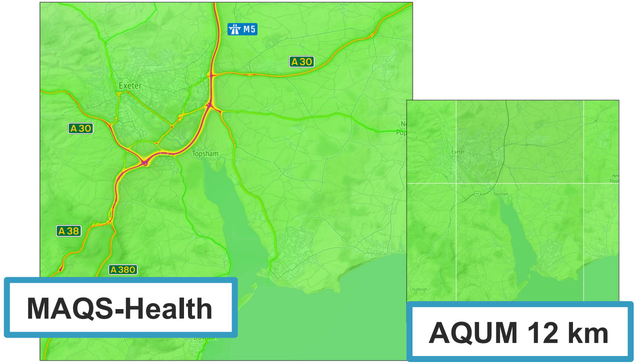
Current research activities: High Resolution Modelling



Nitrogen dioxide (NO_2) concentration µg m^{-3}

MAQS-Health:

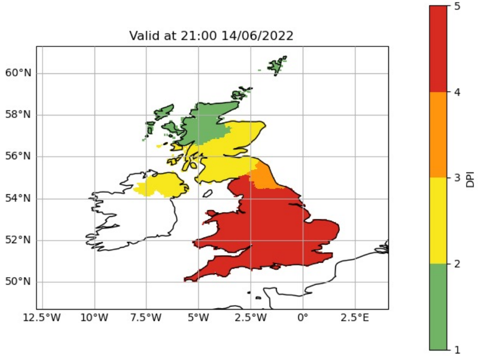
- Multi-Model Air Quality System for Health Research
- Consistently couple **regional** and **local** air quality model
- Regional model
  - 1-10 km spatial resolution
  - Large spatial and long time scales
  - WRF-Chem, CMAQ, CHIMERE, …, AQUM
- Local model:
  - Explicitly model local emissions; road sources
  - Small spatial and short time scales
  - ADMS-Local (freely available) or ADMS-Urban (licensed)

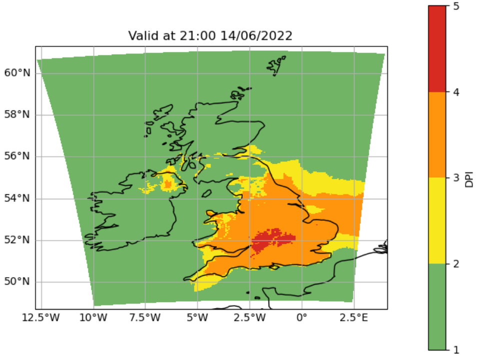


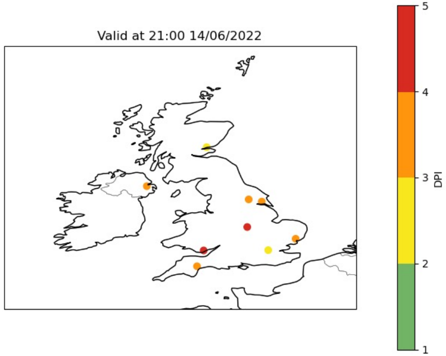
The Clean Air (W1) programme is led by NERC and the Met Office, with Innovate UK, EPSRC, ESRC, MRC, NPL & Defra as delivery partners.

Thanks to Ben Drummond

NAME pollen forecast







Existing pollen forecast

- Uses observations
- Expert judgement
- Forecast changes in weather conditions
- 16 regions

NAME model

- Seasonal cycle uses heat sum
- Short-term: wind, rain, VPD
- 5km, hourly resolution
- Species specific – grass, birch, oak, alder, hazel, nettle

Observations

- Grains manually counted
- Full verification capability

Thanks to Lucy Neal

Thank you for your attention: Any Questions?