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## Statistical evaluation of the input meteorological data used for the UK air quality forecast (UK-AQF)

RMP/1902: Defra Air Quality Forecasting

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**Report for Defra and the Devolved Administrations**

Unrestricted  
RICARDO-AEA/R/ 3388 Issue 1  
01/10/2013



Llywodraeth Cymru  
Welsh Government



**Customer:**

The Department for Environment, Food and Rural Affairs, Welsh Assembly Government, the Scottish Government and the Department of the Environment for Northern Ireland

**Customer reference:**

RMP/1902

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**Ricardo-AEA reference:**

Report no. RICARDO-AEA/R/3388- Issue 1

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# Executive summary

This report summarises the statistical measures used to evaluate the meteorological data, derived from the Weather Research and Forecasting (WRF) v3.0.1 Model, and collapsed using the Meteorology Chemistry Interface Processor (MCIP) v3.4.1, which is used to produce the UK air quality forecast (UK-AQF). **It should be noted that this report evaluates the modelled meteorological parameters (input data) used for the UK-AQF and not the modelled meteorological output from WRF.**

WRF is run daily to provide 72-hour forecasts for Europe and for the UK. The standard configuration for this project is composed of two grids: the first is a European-wide domain and the second is a nested UK grid. The European model is run using a coarse resolution grid of 50 km x 50 km, whilst a finer resolution grid of 10 km x 10 km is used for modelling UK meteorological conditions.

For summer 2012 an even finer 2 km x 2 km resolution grid has also been introduced for London and SE England, but this is not part of the evaluation study described here.

The WRF model provides regional synoptic meteorological conditions which are used as the meteorological driver (input data) for the Community Multi-scale Air Quality (CMAQ) v4.7.1 Model. The daily output from the CMAQ model provides 72-hour forecasts of ground-level air pollutant mass concentrations (NO<sub>x</sub>, NO<sub>2</sub>, O<sub>3</sub>, PM<sub>10</sub>, PM<sub>2.5</sub>, and SO<sub>2</sub>) for Europe and the UK.

Statistical evaluation of the meteorological data used for air quality modelling is achieved by comparing the modelled or forecast meteorological parameters to UK ground-based meteorological station observations of ambient temperature (2 m), wind speed and wind direction. Statistical evaluation involves the derivation of the following parameters through comparison of the observed and modelled values:

- Correlation,
- Standard deviation,
- Mean absolute error,
- Mean bias,
- Mean fractional bias,
- Mean normalised bias,
- Mean normalised error,
- Normalised mean bias,
- Normalised mean error,
- Root mean square error, and
- Index of agreement.

The evaluation of the modelled meteorological input data used for the UK-AQF is an on-going process. Operational statistical evaluation of the modelled meteorological parameters, with observed values, is undertaken daily on a rolling 14-day and calendar month basis. The aim of the evaluation is to provide supplementary information and guidance to assist the air quality forecaster. Statistical evaluation provides a qualitative comparison of how the surface meteorological parameters, used to provide the UK-AQF, reproduce the ambient temperature, wind speed and wind direction for a range of locations distributed throughout the UK-AQF domain. For example, air mass movements within the boundary layer are of particular importance within air quality forecasting models as they determine the rate at which primary air pollutants are dispersed, secondary air pollutants are formed, and the

extent to which air pollutants are transferred to and from the lower atmosphere to earth's surface.

The UK-AQF modelled ambient temperature (2 m) and wind speed compares well with the range of models discussed in the MIE2, particularly against other WRF model-based UK air quality forecasting models. There is a positive bias in the UK-AQF modelled wind direction when compared to the ground-station observations. This bias has been noted by previous researchers. Work has been undertaken by the developers of the WRF model to limit this bias in more recent versions of the WRF modelling software.

This initial evaluation shows that the modelled meteorology input data is suitable for use in the 10 km x 10 km resolution UK-AQF. Whilst the modelled meteorological parameters are representative of regional synoptic conditions at the location of each UK air quality monitoring station, it should be noted that they do not account for local meteorological features, e.g., wind (direction) flow reversal in "street canyons" which can occur at roadside air quality monitoring stations.

The UK-AQF modelled meteorological parameters provide a useful alternative to commercially available meteorological observations which can be measured some distance from the local air quality monitoring station. Therefore whilst the modelled meteorology input data are suitable for use with the openair tools, users should be aware of the above cautionary disclaimer when using them with these tools, or in any local data analysis or modelling studies.

The evaluation of the UK-AQF modelled meteorological parameters is an on-going process: further progress and refinements to the statistical evaluation procedures will be made, with a focus on providing information to the duty forecaster and improving the accuracy of the UK-AQF.

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# 1 Overview of the WRF-CMAQ forecast system used to produce the UK air quality forecast (UK-AQF)

## 1.1 Overview of the UK air quality forecast (UK-AQF)

The UK air quality forecast (UK-AQF) is prepared and published daily on behalf of Defra and the Devolved Administrations (<http://uk-air.defra.gov.uk/forecasting/summary>). The UK-AQF is prepared with reference to all available information and on the basis of many years of 'hands-on' experience of UK air pollution monitoring and forecasting. Ultimately it is the expert judgement of the duty forecaster which determines how the available data are combined to form the forecast issued to the public.

Two key inputs to the UK-AQF are the:

1. Weather forecast from the Weather Research and Forecasting v3.0.1 Model, hereafter simply referred to as the WRF model, and
2. Ground-level air pollutant mass concentrations ( $\text{NO}_x$ ,  $\text{NO}_2$ ,  $\text{O}_3$ ,  $\text{PM}_{10}$ ,  $\text{PM}_{2.5}$ , and  $\text{SO}_2$ ) derived from the Community Multi-scale Air Quality v4.7.1 Model, hereafter simply referred to as the CMAQ air quality forecast model.

The WRF model provides regional synoptic meteorological conditions which are used as the meteorological driver (input data) for the CMAQ chemical transport model. Both models are run daily using multiple grids composed of a European-wide domain and a nested UK grid. The European model is run using a coarse grid with a horizontal resolution of 50 km x 50 km (2500 km<sup>2</sup>), whilst a finer grid, with a horizontal resolution of 10 km x 10 km (100 km<sup>2</sup>), is used for modelling UK conditions.

For summer 2012 an even finer resolution 2 km x 2 km (4 km<sup>2</sup>) grid has been introduced for London and SE England, but this is not part of the evaluation study described here.

An ensemble of other standard UK, European and global meteorological and air quality forecast model results are used to inform the UK-AQF (as detailed on <http://uk-air.defra.gov.uk/forecasting/how-forecasts-are-produced?view=tools>), as well as near real-time air pollutant measurements from the UK's AURN air quality monitoring network (<http://uk-air.defra.gov.uk/interactive-map>).

## 1.2 Setup of WRF-CMAQ system

The overall structure of the WRF-CMAQ forecast system used for the UK-AQF, including the key model inputs and outputs, is illustrated in Figure 1.1. The WRF and CMAQ models themselves are summarised in Sections 1.2.1 and 1.2.2.

### 1.2.1 WRF model

The WRF model (Skamarock et al., 2008<sup>1</sup>) is a next-generation mesoscale numerical weather prediction system designed to serve both operational forecasting and atmospheric research needs. Development of the WRF model, along with a detailed description of the underlining computational methods; chemical and physical components contained within the model; and, a list of publications detailing its extensive use, can be found on the Weather Research and Forecasting Model website homepage (<http://www.wrf-model.org/index.php>). Briefly, WRF features multiple dynamical cores, a 3-dimensional variational (3DVAR) data assimilation system, and a software architecture allowing for computational parallelism and system extensibility. WRF is suitable for a broad spectrum of applications across scales ranging from meters to thousands of kilometres.

Initial meteorological and lateral boundary conditions are derived from the US National Centers for Environmental Prediction (NCEP) Global Forecast System (GFS, <http://www.emc.ncep.noaa.gov/GFS/>). These are used to initiate the outer (coarse-gridded) European domain of the WRF model in order to provide the meteorological forecast for Europe, and subsequently the UK. Gridded GFS analyses are available at intervals of 3 hours with a horizontal resolution of 0.5° on operational pressure levels up to 50hPa for vertically distributed data, and surface and soil levels for surface and deep-soil data.

Table 1.1 and Table 1.2 summarise the WRF model setup and the WRF model physics and operational setup, respectively. The WRF model is run daily to provide 72-hour forecasts, for the current and following day, for Europe and for the UK. For this study the model is composed of two grids: the first is a European-wide domain and a second, nested UK grid. The European model is run using a coarse resolution grid of 50 km x 50 km, whilst a finer resolution grid of 10 km x 10 km is used for modelling UK meteorological conditions, as shown in Figure 1.2. In Figure 1.2 the light grey shaded area bounded by the dashed line denotes the limit of spatial coverage of the outer coarser European domain used in the WRF model using a horizontal resolution of 50 km x 50 km. The un-shaded area bounded by the solid black line denotes the boundary of the finer, nested UK domain, which uses a horizontal resolution of 10 km x 10 km. The WRF model outputs are used as the meteorological driver for the CMAQ air quality forecasting model (described in Section 1.2.2).

**Table 1.1 WRF model setup.**

Parameter	Description	
Domain settings	Coordinate system	Lambert-conformal True latitude 1: 36° True latitude 2: 60° Standard longitude: 10°
	Horizontal setting	50 km x 50 km 10 km x 10 km
	Vertical setting	49 layers
	Nesting	One way, run using adaptive time steps
Input data	Land use	WPS geogrid with 30s resolution
	Land use availability	Distributed with WRF
Initial and boundary conditions	Name of model	NCAR-GFS
	Grid resolution	(48 levels + 5 soil levels)

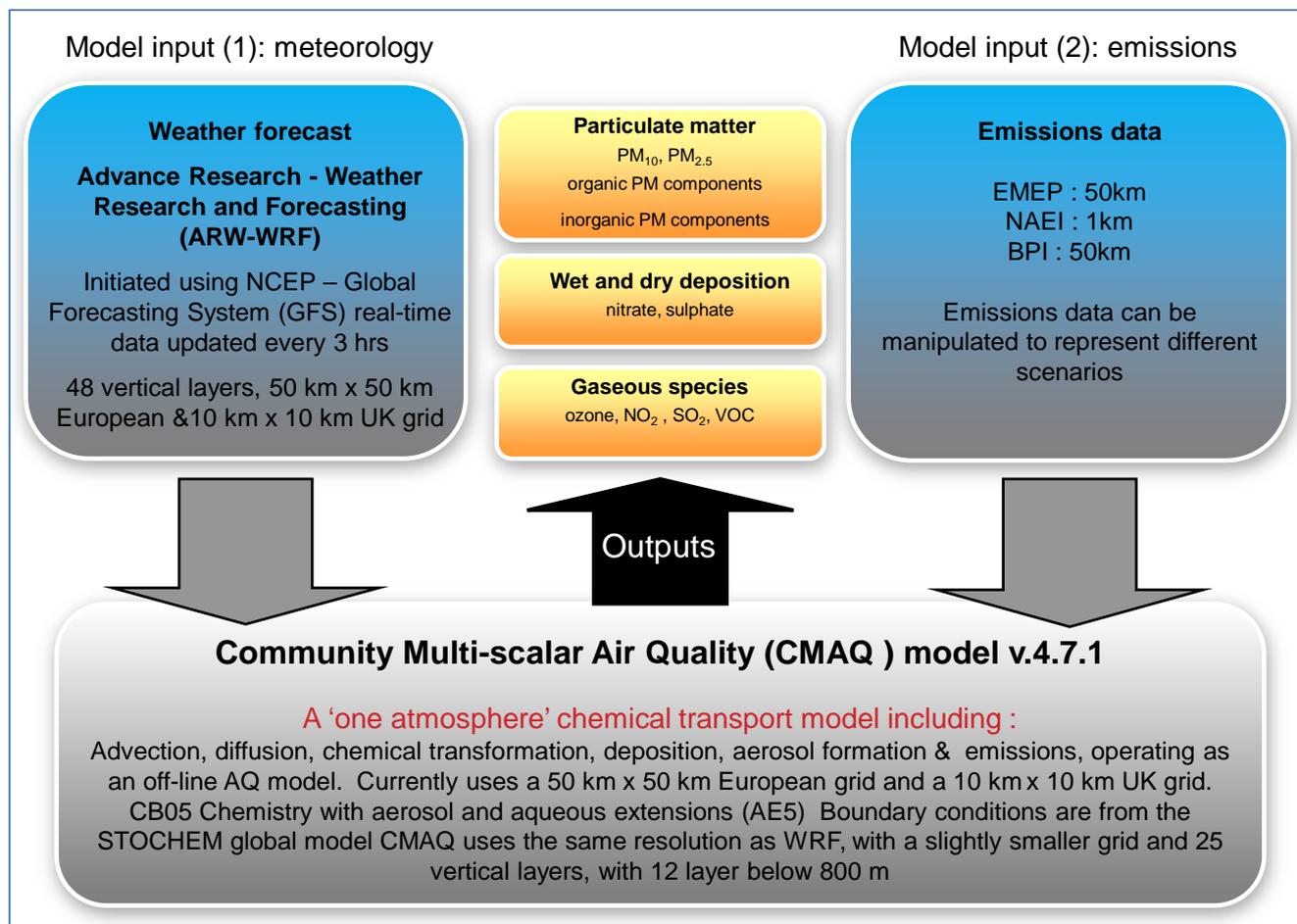
<sup>1</sup> Skamarock, W.C., Klemp, J.B., Dudhia, J., Gill, D.O., Barker, D.M., Duda, M.G., Huang, X.-Y., Wang, W., Powers, J.G. (2008). A description of the Advanced Research WRF Version 3. NCAR Technical Note NCAR/TN-475pSTR. NCAR, Boulder, CO, USA. [http://www.mmm.ucar.edu/wrf/users/docs/arw\\_v3.pdf](http://www.mmm.ucar.edu/wrf/users/docs/arw_v3.pdf)

**Table 1.2 WRF model physics and operational setup.**

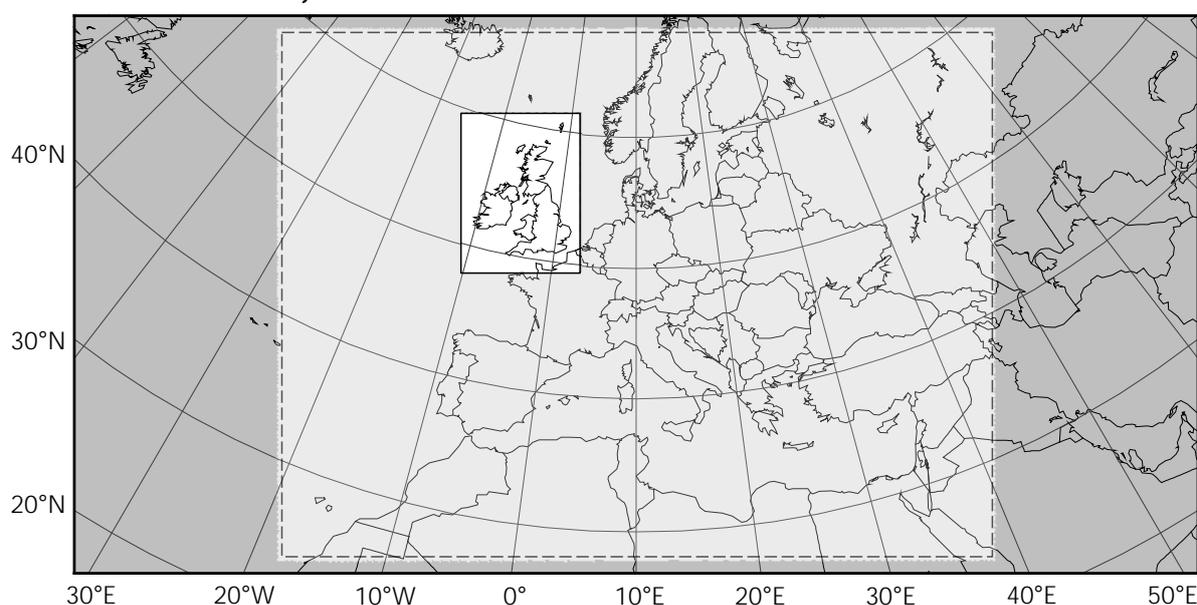
Parameter		Description (WRF option number)
Physics settings	Radiation scheme	Default (1)
	Microphysics	Lin et al. (2)
	Surface layer options	Surface layer physics (1), Monin-Obukhov scheme.  Surface physics = thermal diffusion scheme (1)
	Land surface option	Surface heat and moisture flux and 5 soil moisture layers
	PBL scheme	YSU scheme (1), BLDT = 0
	Cumulus option	Kain-Fritsch (1), CUTD = 0
Nudging and data assimilation	Observational or analysis nudging	Analysis nudging
	Nudging configuration	Nudging in the PBL (uv, t, q), no nudging below layer 10 for (zfrac_uv, t, q)
	Data assimilation method	None
	Input data used in nudging or data assimilation	NCEP-GFS

The final daily WRF output is presented as a series of animated maps which the UK-AQF team use to review the expected weather situation. The mapped output from the WRF forecast is made publicly available each day and can be found on the Defra website (<http://uk-air.defra.gov.uk/forecasting/wrf-summary>).

Figure 1.1 Overview of the WRF-CMAQ forecast system used for daily UK air quality forecasting.



**Figure 1.2 Spatial coverage of the outer coarser European domain used for the WRF model using a horizontal resolution of 50 km x 50 km and the finer, nested UK domain, which uses a horizontal resolution of 10 km x 10 km<sup>2</sup>.**



### 1.2.2 CMAQ air quality forecast model

The CMAQ air quality forecast model (<http://www.cmaq-model.org/>) is a comprehensive air quality model that permits simultaneous modelling of multiple gaseous- and particulate-phase air pollutants, and species contributing to acidic and nitrogenous deposition (US Environment Protection Agency, 1999<sup>3</sup>; Byun and Schere, 2006<sup>4</sup>). Evaluation of the use of CMAQ, and moreover a coupled WRF-CMAQ model, to produce air quality forecasts for the UK has been the focus of previous work (Chemel et al., 2010<sup>5</sup>, Carslaw, 2011<sup>6</sup>) and is the focus of on-going work.

Briefly, CMAQ is based on the 'one atmosphere' concept in which complex interactions between atmospheric pollutants on urban, regional and hemispheric scales are treated in a consistent framework. It can simulate complex atmospheric processes that transport and transform these pollutants in a dynamic environment over a broad range of time scales from minutes to days and weeks. The CMAQ modelling system contains three core modelling components:

- A meteorological modelling system providing adequate representation of key atmospheric chemical and physical processes,
- Anthropogenic and natural emission models, and
- A chemistry-transport modelling system to simulate key atmospheric chemical transformations.

<sup>2</sup> Produced using Panoply v3.1.1 netCDF, HDF and GRIB Data Viewer, <http://www.giss.nasa.gov/tools/panoply/>. The projection is centred on 10°E and 48°N.

<sup>3</sup> Byun, D.W., Ching, J.K.S. (Eds.) (1999). Science Algorithms of the EPA Models-3 Community Multiscale Air Quality Modeling System. Technical Report EPA/600/R-99/030. US Environment Protection Agency, Research Triangle Park, NC, USA. [http://www.epa.gov/AMD/CMAQ/Q00\\_cover\\_exec.pdf](http://www.epa.gov/AMD/CMAQ/Q00_cover_exec.pdf)

<sup>4</sup> Byun, D., Schere, K.L. (2006). Review of the governing equations, computational algorithms, and other components of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. Applied Mechanics Reviews, 59(2), 51-77, doi:10.1115/1.2128636.

<sup>5</sup> Chemel, C., Sokhi, R.S., Yu, Y., Hayman, G.D., Vincent, K.J., Dore, A.J., Tang, Y.S., Prain, H.D., Fisher, B.E.A. (2010). Evaluation of a CMAQ simulation at high resolution over the UK for the calendar year 2003. Atmospheric Environment, 44(24), 2927-2939, doi:10.1016/j.atmosenv.2010.03.029.

<sup>6</sup> Carslaw, D. (2011). Defra regional and transboundary model evaluation analysis - Phase 1. Final Report to Department of Environment, Fisheries and Rural Affairs (Defra) and the Devolved Administrations, London, UK, [http://uk-air.defra.gov.uk/reports/cat20/1105091514\\_RegionalFinal.pdf](http://uk-air.defra.gov.uk/reports/cat20/1105091514_RegionalFinal.pdf)

In addition to the meteorological inputs from the WRF meteorological model, CMAQ requires accurate and up-to-date emissions data to run. Annual UK, European anthropogenic and biogenic emission inventories of NO<sub>x</sub>, PM<sub>10</sub>, PM<sub>2.5</sub>, NH<sub>3</sub>, VOC and SO<sub>2</sub>, are processed using standard temporal factors into hourly emissions data ready for the air quality model, including:

- UK National Atmospheric Emissions Inventory (NAEI, <http://naei.defra.gov.uk/>) available at 1 km<sup>2</sup> resolution,
- EMEP emissions for Europe, available at 50 km x 50 km resolution, and
- Natural emissions calculated using a Biogenic Potential Inventory.

For this study the CMAQ model is run daily to provide 72-hour air quality forecasts for Europe, at a resolution of 50 km x 50 km, and for the UK, at a resolution of 10 km x 10 km. The results for NO<sub>2</sub>, ozone, PM<sub>10</sub>, PM<sub>2.5</sub>, and SO<sub>2</sub> are mapped and animated for the forecasting team to review.

### 1.3 Extraction of the meteorological data used for the UK-AQF

The output of the WRF model is used as the meteorological driver for the CMAQ modelling system: the Meteorology Chemistry Interface Processor v3.4.1. (MCIP, <http://www.cmascenter.org/download/>, Otte and Pleim, 2010<sup>7</sup>) links the modelled meteorological data with the CMAQ model.

Meteorological initial and lateral boundary conditions of the outer domain were derived from the NCEP-GFS gridded forecast available every 3 hours with a horizontal resolution of 0.5° on operational pressure levels up to 50 hPa for vertically distributed data, and surface and soil levels for surface and deep-soil data. A grid nudging technique (Four-Dimensional Data Assimilation, FDDA, Stauffer and Seaman, 1990<sup>8</sup>) is employed for the upper layers of the outer domain every 3 hours in order to constrain the model towards the analyses (Otte, 2008a<sup>9</sup>; Otte, 2008b<sup>10</sup>). The MCIP process prepares the data ready for CMAQ. This includes collapsing the original 49 vertical layers in WRF to 19 layers for CMAQ and discarding the 3 grid cells around each domain to smooth gradients near the lateral boundaries. Finally, the MCIP translated modelled meteorological data, which is used in the UK-AQF, is passed into a MySQL relational database for a series of paired AURN and ground-based meteorological stations. The process by which sites are paired is described in Section 1.5.

**It should be noted that this report evaluates the modelled meteorological parameters (input data) used for the UK-AQF and not the modelled meteorological output from WRF.**

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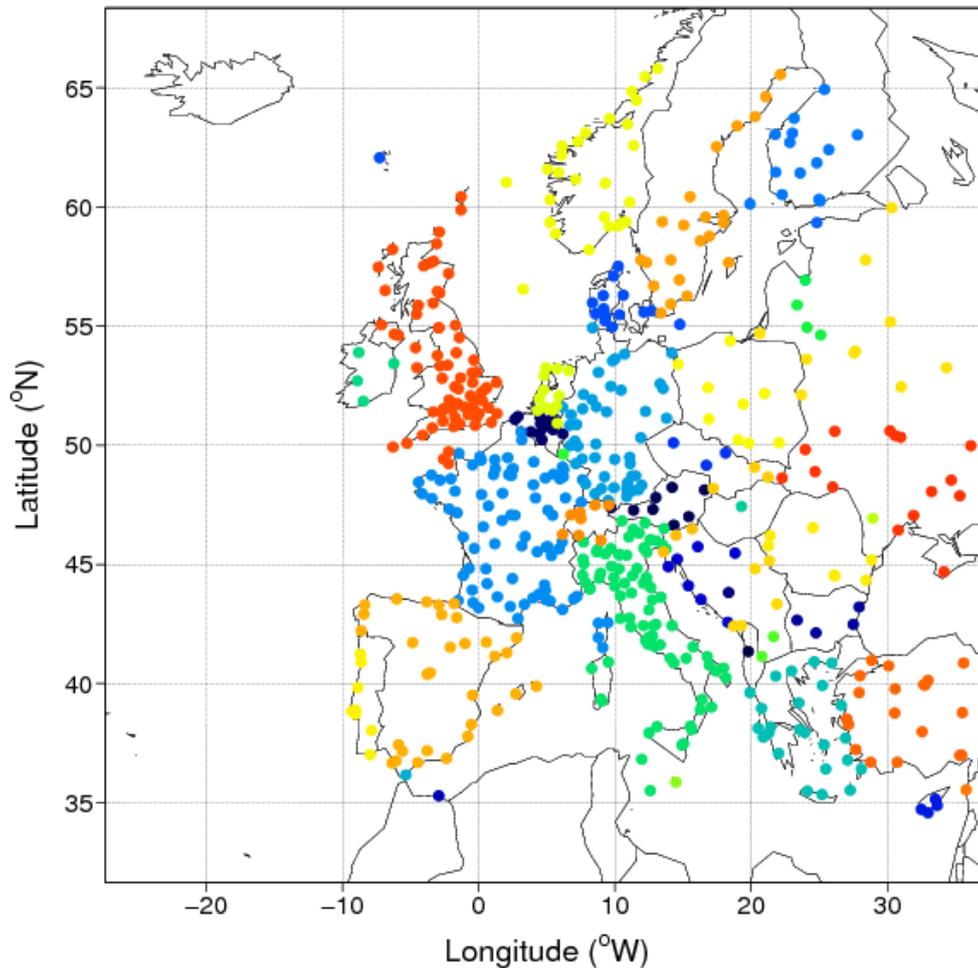
<sup>7</sup> Otte, T.L., Pleim, J.E. (2010). The Meteorology-Chemistry Interface Processor (MCIP) for the CMAQ modeling system: updates through MCIPv3.4.1. *Geoscientific Model Development*, 3, 243-256, doi: 10.5194/gmd-3-243-2010.

<sup>8</sup> Stauffer, D.R., Seaman, N. (1990). Use of Four-Dimensional Data Assimilation in a limited-area mesoscale model. Part I: experiments with synoptic-scale data. *Monthly Weather Review*, 118(6), 1250-1277, doi: 10.1175/1520-0493(1990)118<1250:UOFDDA>2.0.CO;2.

<sup>9</sup> Otte, T.L. (2008a). The impact of nudging in the meteorological model for retrospective air quality simulations. Part I: evaluation against national observation networks. *Journal of Applied Meteorology and Climatology*, 47(7), 1853-1867, doi: 10.1175/2007JAMC1790.1.

<sup>10</sup> Otte, T.L. (2008b). The impact of nudging in the meteorological model for retrospective air quality simulations. Part II: evaluating collocated meteorological and air quality observations. *Journal of Applied Meteorology and Climatology*, 47(7), 1868-1887, doi: 10.1175/2007JAMC1791.1.

**Figure 1.3** The location of the Europe-wide ground based meteorological observation stations used to evaluate the WRF model data.



## 1.4 Ground-based meteorological station observations

The WRF model has been extensively validated over the USA and for some parts of Europe (<http://www.mmm.ucar.edu/wrf/users/forecasts.html>). Statistical evaluation of the meteorological data used for the UK-AQF is achieved by comparing the reduced modelled meteorological parameters from MCIP to ground-based meteorological station observations of:

- Ambient temperature (2 m),
- Wind speed, and
- Wind direction.

These three meteorological parameters are downloaded daily from the University of Wyoming website (<http://weather.uwyo.edu/surface/meteogram/>). The website also provides barometric pressure, dew point, and relative humidity observations. The University of Wyoming website holds meteorological observations from approximately 600 sites, located throughout the UK and mainland Europe, as shown in Figure 1.3. These observations are then passed into a MySQL relational database.

## 1.5 Observation-model matching

AURN stations and ground-based meteorological stations were paired and assigned grid-cell co-ordinates within the CMAQ UK modelling domain using the site comparison function (SITECMP) taken from the AMET toolset. Atmospheric Model Evaluation Tool (AMET, <http://www.cmascenter.org/help/documentation.cfm?MODEL=amet&VERSION=1.1>, Gilliam et al., 2005<sup>11</sup>) is an open-source toolkit that allows error and uncertainty in the model simulations to be examined. AMET matches observations with the corresponding model-estimated values in space and time. It also provides a range of analysis programs to permit user specified data to be extracted from the database to generate statistical plots and tables.

Table 1.3 lists the AURN air quality monitoring stations and corresponding ground-based meteorological observation station (based on International Civil Aviation Organization, ICAO, name and id) used to evaluate the meteorological data used for the UK-AQF.

## 1.6 Performance reports

Performance reports, showing both statistical evaluation plots and results tables, are produced on a rolling 14-day and calendar month basis. These provide a comparison of the forecast meteorological data used for the UK-AQF and the observations from the ground-based meteorological stations. Performance reports are produced comparing observed and modelled:

- Ambient temperature (2 m),
- Wind speed, and
- Wind direction.

Examples of the performance report for each meteorological parameter can be found in Section 3. The ground-based meteorological stations were paired with AURN air quality monitoring stations on the basis of whether the site co-ordinates of the both sites place them within the same grid cell within the UK-AQF domain, as shown in Figure 1.2.

The performance reports are currently produced for the paired ground-based meteorological stations and AURN air quality monitoring stations listed in Table 1.3. This pairing provides a simple contextual reference of the modelled meteorological parameters analogous with the national air quality monitoring station network. The current operational pairings of ground-based meteorological stations and AURN air quality monitoring stations are given in Table 1.3. The pairing of sites is dynamic and is dependent on two key factors:

- a) The availability of meteorological observations at the ground-based meteorological station, and
- b) The operational status of AURN air quality monitoring stations. The number of AURN air quality monitoring stations is dynamic: the number of air quality monitoring stations within the AURN is principally governed by the compliance monitoring requirements of the Air Quality Directive(s), and to a lesser extent, site operational factors, e.g., site accessibility, location, and so on.

Therefore it is possible that the number of paired sites may vary with time.

The performance plots are produced using a modified version of AMETPLOT function distributed with the AMET toolkit and run in R v2.14.1<sup>12</sup>. The performance plot script utilises a MySQL query to dynamically select the ground-based meteorological stations and AURN air quality monitoring stations to be compared. Section 2 summarises the statistical measures presented in the performance reports.

<sup>11</sup> Gilliam, R. C., Appel, W., Phillips, S. (2005). The Atmospheric Model Evaluation Tool: meteorology module. Presented at 4<sup>th</sup> Annual CMAQ Models-3 User's Conference, Chapel Hill, NC, USA, September 26-28, [http://www.cmascenter.org/conference/2005/abstracts/6\\_1.pdf](http://www.cmascenter.org/conference/2005/abstracts/6_1.pdf).

<sup>12</sup> R Development Core Team (2005). R: A Language and Environment for Statistical Computing, R Foundation for Statistical Computing, Vienna, Austria, <http://www.R-project.org>.

**Table 1.3** *Ground-based meteorological observation station (based on ICAO name and site id) and corresponding AURN air quality stations.*

ICAO				AURN	
Site name	Site ID	Latitude (°N)	Longitude (°E)	Site name	Site ID
Belfast Harbour	EGAC	54.60	-5.88	Belfast Centre	BEL2
Birmingham	EGBB	52.45	-1.73	Birmingham Acocks Green	AGRN
Shoreham-By-Sea	EGKA	50.83	-0.28	Brighton Preston Park	BEL2
Filton (Bristol)	EGTG	51.52	-2.58	Bristol Old Market and Bristol St. Paul's	BRS2 and BRS8
Carlisle	EGNC	54.93	-2.95	Carlisle Roadside	CARL
Yeovilton	EGDY	51.00	-2.63	Charlton Mackrell	MACK
London Gatwick	EGKK	51.15	-0.18	Horley	HORE
Liverpool	EGGP	53.33	-2.85	Liverpool Speke	LVP
London Heathrow	EGLL	51.48	-0.45	London Harlington and London Hillingdon	HRL and HIL
Newcastle	EGNT	55.03	-1.70	Newcastle Centre and Newcastle Cradlewell Roadside	NEWC and NCA3
Southampton Airport	EGHI	50.90	-1.40	Southampton Centre	SOUT
Teeside	EGNV	54.52	-1.42	Stockton-on-Tees Eaglescliffe	EAGL

## 2 Statistical evaluation

### 2.1 Overview of the evaluation method

Generally speaking, statistics used to evaluate the performance of meteorological models tend to be presented in absolute terms (e.g., wind speed in  $\text{m s}^{-1}$ ) rather than relative terms (i.e., as a percentage error) as is the case for air quality assessments. The reason for this is that a very different significance is associated with a given relative error for meteorological parameters. For example a 10% error for wind speed measured at  $10 \text{ m s}^{-1}$  is an absolute error of  $1 \text{ m s}^{-1}$ , a minor error. Yet a 10% error for barometric pressure measured at 1002 mbar is an absolute error of 100 mbar, an abnormally large error. On the other hand, it should be noted that the relative error (also termed the “normalised” error) provides a means by which to compare the bias (or error) of different meteorological parameters which may vary to different extents.

**Table 2.1 Model performance statistics calculated for each modelled meteorological parameter.**

Model performance statistic	Meteorological parameter		
	Temperature	Wind speed	Wind direction
Data count (the total number of paired values considered, $N$ )	●	●	●
Correlation (also termed the Pearson Correlation Coefficient, $R$ )	●	●	○
Standard deviation ( $St. Dev$ )	●	●	●
Mean absolute error ( $MAE$ )	●	●	●
Mean bias ( $BIAS$ )	●	●	●
*Mean fractional bias (%)	●	●	○
*Mean normalised bias (%)	●	●	○
*Mean normalised error (%)	●	●	○
*Normalised mean bias (%)	●	●	○
*Normalised mean error (%)	●	●	○
Root mean square error ( $RMSE$ , Root-Mean-Sqr-Error)	●	●	●
Index of agreement	●	●	○

● calculated, ○ not calculated.

The table on the left-hand side of the performance plots presented in Section 3 provides eleven model performance statistics, also termed model-to-observation indicators (MOIs). The eleven statistical indices calculated are given in Sections 2.2 to 2.12. The model performance statistics express the quality of the modelled meteorological data used for the

UK-AQF, namely the ambient surface (2 m) temperature, wind speed and direction, with respect to observed values, derived from the ground-based stations. It should be noted that not all statistical indices are calculated for each meteorological parameter. Generally speaking, relative model performance statistics do not tend to be calculated for wind direction. The eleven statistical indices detailed in Table 2.1 are calculated as described in Sections 2.2 to 2.12.

It should be noted that the statistical measures described below are not exhaustive and there are a wide-range of statistical measures that can be used to evaluate both meteorological, and air quality, model performance<sup>13,14</sup>.

## 2.2 Correlation (also termed the Pearson Correlation Coefficient, $R$ )

The Correlation (also termed the Pearson Correlation Coefficient,  $R$ ) is calculated thus:

$$R = \frac{\sum_{i=1}^N (M_i - \bar{M}) \times (O_i - \bar{O})}{\sqrt{\sum_{i=1}^N (M_i - \bar{M})^2} \sqrt{\sum_{i=1}^N (O_i - \bar{O})^2}}, \quad (1)$$

where:

$M$	=	modelled value,
$\bar{M}$	=	mean of modelled value,
$O$	=	observed value,
$\bar{O}$	=	mean of observed value, and
$N$	=	number of paired values considered (termed “data count”).

$R$  ranges from -1 to +1 and indicates the strength of the linear relationship between the modelled and observed datasets. A value of +1 indicates a positive correlation and corresponds to all pairs lying on a straight line with positive slope in the scatter diagram (Panel B). As  $R \rightarrow 0$ , this indicates a lack of a linear correlation between the modelled and observed datasets. It should be noted that the value of  $R$  is sensitive to extreme pairs (statistical outliers).

## 2.3 Standard deviation (St. Dev)

The standard deviation (square root of the variance) is a measure of the spread of the individual modelled values from the mean of the modelled values:

$$\sigma = \sqrt{1/N \left( \sum_{i=1}^N (M_i - \bar{M})^2 \right)}, \quad (2)$$

where:  $\sigma$  = standard deviation.

## 2.4 Mean absolute error (MAE)

The mean absolute error (MAE) is used to measure the closeness of modelled and observed values. It is calculated from the absolute of the difference between a modelled and an

<sup>13</sup> Thunis, P., Georgieva, E., Galmarini, S. (2011). A procedure for air quality models benchmarking. [http://fairmode.ew.eea.europa.eu/models-benchmarking-sq4/wq2\\_sq4\\_benchmarking\\_v2.pdf/download](http://fairmode.ew.eea.europa.eu/models-benchmarking-sq4/wq2_sq4_benchmarking_v2.pdf/download)

<sup>14</sup> Agnew, P., Mittermaier, M.P., Honore, C., Elbern, H., Coll, I., Vatuard, R., Peuch, V.-H. (2007). Evaluation of GEMS regional air quality forecasts. European Centre for Medium-Range Weather Forecasts (ECMWF) <http://gems.ecmwf.int/do/get/PublicDocuments/1533/1402?showfile=true>

observed value, or bias, as described in Section 2.5, or  $|M_i - O_i|$ . Therefore the mean absolute error is always positive.

The absolute value (or modulus)  $|a|$  of a real number  $a$ , is the numerical value of  $a$  without regard to its sign. So, for example, the absolute value of 3 is 3, and the absolute value of -3 is also 3. The absolute value of a number may be thought of as its distance from zero.

The mean absolute error is simply the average bias between the modelled and observed values measured throughout a domain and/or over a specified time period (hour, day, etc).

$$MAE = 1/N \sum_{i=1}^N |M_i - O_i|, \quad (3)$$

## 2.5 Mean bias

The difference between a modelled and an observed value,  $M_i - O_i$ , is referred to as the bias. If the difference between the modelled and an observed value is zero, i.e., the predictions and the observations exactly cancel each other out, the modelled value is said to be unbiased. Otherwise the modelled value is said to be biased.

The mean bias is simply the average bias between the modelled and observed values measured throughout a domain.

$$BIAS = 1/N \sum_{i=1}^N (M_i - O_i), \quad (4)$$

## 2.6 Mean fractional bias (%)

The mean fractional bias (MFB) is used as a substitute for the mean normalised bias, discussed in the next Section, when the mean normalised bias becomes large. The mean normalised bias can become very large when a minimum threshold is not used for the observations.

The fractional bias for cases with factors of 2 under- and over-prediction are -67 and +67%, respectively (as opposed to -50 and +100%, when using normalised bias).

The mean fractional bias is a useful indicator because it has the advantage of equally weighting positive and negative bias estimates. It has also the advantage of not considering observations as the true value. The mean fractional bias can range in value from -200% to +200%.

$$MFB = 1/N \sum_{i=1}^N \frac{(M_i - O_i)}{[(M_i + O_i)/2]}, \quad (5)$$

## 2.7 Mean normalised bias (%),

The mean normalised bias (MNB) is calculated in a similar fashion to the mean bias. The mean normalised bias is calculated from the difference between the modelled and observed values (i.e., the bias,  $M_i - O_i$ ) is normalised (divided) by the observed value ( $O_i$ ). The mean normalised bias is reported as a percentage.

$$MNB = 1/N \sum_{i=1}^N \left( \frac{M_i - O_i}{O_i} \right), \quad (6)$$

## 2.8 Mean normalised error (%),

The mean normalised error (MNE) is calculated in a similar fashion to the mean absolute error. The mean normalised error is calculated from the absolute of the bias,  $M_i - O_i$ ,

normalised by the observed value,  $O_i$ . Therefore the mean normalised error is always positive. The mean normalised error is reported as a percentage.

$$MNE = 1/N \sum_{i=1}^N \frac{|M_i - O_i|}{O_i}, \quad (7)$$

## 2.9 Normalised mean bias (%)

The normalised mean bias (NMB) is calculated by summing the difference between the modelled and observed values,  $\sum_{i=1}^N (M_i - O_i)$ , and normalising by the sum of the observed values,  $\sum_{i=1}^N O_i$ . The NMB is reported as a percentage.

$$NMB = \frac{\sum_{i=1}^N (M_i - O_i)}{\sum_{i=1}^N O_i}, \quad (8)$$

## 2.10 Normalised mean error (%)

The normalised mean error (NME) is calculated by summing the absolute of the bias,  $\sum_{i=1}^N |M_i - O_i|$ , and normalising by the sum of the observed values,  $\sum_{i=1}^N O_i$ . Therefore the normalised mean error is always positive. The NME is reported as a percentage.

$$NME = \frac{\sum_{i=1}^N |M_i - O_i|}{\sum_{i=1}^N O_i}, \quad (9)$$

## 2.11 Root mean square error (RMSE, Root-Mean-Sqr-Error)

The Root Mean Square Error (*RMSE*) is calculated as the square root of the mean squared difference in modelled-observed values with valid data within a given analysis region and for a given time period. It is commonly used as a measure of the **overall** model performance. The rationale for employing the *RMSE* as an indicator of overall forecast error is two-fold (Agnew et al., 2007<sup>14</sup>):

- i. By squaring the errors before combining, this measure removes any cancellation of under and over-prediction, and
- ii. In cases where the spread of errors approximates to a well-known distribution (e.g., normal, binomial, poison, etc) the *RMSE* can be attributed with a physical significance.

The *RMSE* is calculated from the square root of the mean squared difference in the model-observation pairings (N) within a given analysis region and for a given time period:

$$RMSE = \sqrt{\left( \frac{\sum_{i=0}^N (M_i - O_i)^2}{N} \right)}, \quad (10)$$

The ideal value of the *RMSE* is zero. It should be noted that since large errors are heavily weighted (due to squaring), therefore a few large errors (for example in a small sub-region) may produce a large *RMSE* even though errors may be small and quite acceptable elsewhere.

## 2.12 Index of agreement

The index of agreement condenses the differences between modelled and observed values within a given analysis region and for a given time period (hourly or daily) into one statistical quantity. The index of agreement is the ratio of the total RMSE to the sum of two differences

– between each modelled value, or predicted value, and the observed mean, and each observation and the observed mean.

$$IOA = 1 - \frac{N \times RMSE^2}{\sum_{i=1}^N (|M_i - \bar{o}| + |O_i - \bar{o}|)^2}, \quad (11)$$

The index of agreement provides a measure of the match between the departure of each prediction from the observed mean and the departure of each observation from the observed mean. Determination of the index of agreement allows quantification of the correspondence between the predicted and observed values across the UK domain at a given time. The IOA can subsequently be plotted as a time series. The index of agreement has a theoretical range of 0 to 1, with a value of 1 suggesting ‘perfect’ agreement.

## 3 Operational evaluation

Statistical evaluation of the meteorological data used for the UK-AQF is achieved by comparing the modelled or forecast meteorological parameters to UK ground-based meteorological station observations of ambient temperature (2 m), wind speed and wind direction.

Operational statistical evaluation of the modelled meteorological parameters, with observed values, is undertaken daily on a rolling 14-day, calendar month, and annual basis. The statistical evaluation provides a qualitative comparison of how the meteorological parameters used for the purposes of providing the UK-AQF reproduce the ambient temperature, wind speed and wind direction for a range of locations distributed throughout the UK modelling domain. Figure 3.1, Figure 3.2, and Figure 3.3 present performance reports for 2011 comparing the modelled and forecast ambient temperature, wind speed and wind direction, respectively.

An initial statistical evaluation of the UK-AQF meteorological input data for the sites described in Table 1.3 was undertaken. The results were compared with the statistical evaluation of 2006 modelled meteorology used in the six UK air quality models (as described in Carslaw, 2011<sup>6</sup>) reported in Defra's Model Intercomparison Exercise Phase 2 (MIE2) (Carslaw, 2012<sup>15</sup>). It should be noted that the two-sets of evaluations are not directly comparable. This is because the modelled meteorological data is for two separate modelling years: 2006 and 2011, and the two comparisons were undertaken for different groups of ground-based meteorological observation sites. On the other hand, this comparison can be used to qualitatively assess the extent to which the meteorological data used for the UK-AQF accurately describes the measured meteorological parameters.

### 3.1 Ambient temperature (2 m)

Figure 3.1 shows the performance report comparing the UK-AQF modelled ambient temperature against observed values for 2011. The scatter plot in the top left of the report demonstrates that the modelled values compare well with the observed ambient temperatures well although there is a small degree of scatter. The UK-AQF modelled values of ambient temperature tend to be lower than the observed values, falling below the solid blue line denoting  $y=x$  on the scatter plot. This is supported by the value of the mean bias ( $MB$ ) which is -0.62, as shown in the model performance statistics presented on the right-hand side of the performance report. The model performance statistics show that the correlation coefficient ( $R$ ) between the two dataset is 0.91,  $n = 101088$ . The box and whisker plot in the bottom right of the performance report compares the median and quartile ranges of the modelled and observed values. This plot demonstrates that a good correlation exists between the modelled and observed median and quartiles. The modelled values are just slightly lower than the observed values, which corresponds well with the comparison presented in the scatter plot and the negative mean bias.

Table 3.1 summarises the other key statistical parameters: root mean squared error ( $RMSE$ ) and index of agreement (IOA), which are discussed in the previous section of this report. The three statistical parameters for the UK-AQF are well inside the range of values reported in the MIE2 for WRF-based models. The statistical parameters compare less favourably

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<sup>15</sup> Carslaw, D. (2012). DEFRA Phase 2 Regional Model Evaluation. Draft Working Document (version 10th May 2012). [http://www.erg.kcl.ac.uk/downloads/Policy\\_Reports/regionalPhase2.pdf](http://www.erg.kcl.ac.uk/downloads/Policy_Reports/regionalPhase2.pdf)

with the two Met Office models considered as part of the MIE2, namely AQUM and NAME. The two met office models show the best (highest) values of  $R$  and IOA of all six UK air quality models considered in the MIE2 and the lowest  $RMSE$  values.

**Table 3.1 Summary of the statistical parameters comparing of the UK-AQF modelled ambient temperature and the six UK air quality models reported in MIE2.**

Model	Mean bias (°)	$RMSE$	$R$	IOA
UK-AQF	-0.62	2.32	0.91	0.71
<b>WRF-based models</b>				
KCL-CMAQ	-0.30	2.0	0.95	0.85
Hert-CMAQ	0.81	2.12	0.95	0.84
EMEP4UK	-0.80	2.39	0.93	0.82
AEA-CMAQ	0.42	2.48	0.92	0.81
WRF-Chem	-0.30	2.0	0.95	0.85
<b>Met Office models</b>				
AQUM	-0.07	1.63	0.97	0.88
NAME	-0.45	1.72	0.96	0.87

### 3.2 Wind speed

Figure 3.2 shows the performance report comparing the UK-AQF modelled ambient wind speed against observed values for 2011. The model performance statistics presented on the right-hand side of the performance report show that the correlation coefficient ( $R$ ) between the UK-AQF modelled wind speed and the observed values is 0.73, indicating a reasonable agreement between the two sets of values. While some degree of scatter can be seen in the scatter plot in the top-left corner, this results in a comparatively very small mean bias of 0.72 m s<sup>-1</sup> in the modelled wind speed.

The box and whisker plots in the lower right corner of the performance report, comparing the modelled and observed values, indicate very good agreement between the model results and the observations. The observed values show a much higher range of values, whilst the modelled median and quartiles are slightly above the observed values, reflecting the positive  $MB$ . Table 3.2 shows the statistical parameters comparing the UK-AQF modelled wind speed for the range of UK air quality models considered in the MIE2. From the table, it can be seen that the modelled wind speed used in the UK-AQF compares well for the values of  $R$  and  $RMSE$  against most of the other models except KCL-CMAQ, AQUM and NAME.

**Table 3.2 Summary of the statistical parameters comparing of the UK-AQF modelled wind speed and the six UK air quality models reported in MIE2.**

Model	Mean bias (°)	RMSE	R	IOA
UK-AQF	-0.72	2.18	0.73	0.54
<b>WRF-based models</b>				
KCL-CMAQ	-0.15	1.79	0.80	0.70
Hert-CMAQ	0.97	2.39	0.75	0.60
EMEP4UK	-0.41	2.03	0.76	0.66
AEA-CMAQ	1.23	2.59	0.72	0.56
WRF-Chem	-0.15	1.79	0.80	0.70
<b>Met Office models</b>				
AQUM	0.00	1.82	0.79	0.70
NAME	0.13	1.87	0.78	0.70

### 3.3 Wind direction

Comparison of the UK-AQF modelled wind direction with observations reveals a noticeable positive bias. Figure 3.3 shows that over the whole of 2011, the modelled wind direction mean bias was +15.8° (positive being clockwise from north). Table 3.3 shows the statistical parameters comparing the UK-AQF modelled wind direction against the six UK air quality models evaluated in the MIE2. The wind direction mean bias for all models ranges from +3.95° to +15.81°. Similar observations have recently been reported by Gillam et al., 2012<sup>16</sup>. While the wind direction mean bias in the UK-AQF is the greatest of all models, the corresponding value of the *RMSE* is also the lowest.

**Table 3.3 Summary of the statistical parameters comparing of the UK-AQF modelled wind direction and the six UK air quality models reported in MIE2.**

Model	Mean bias (°)	RMSE	R	IOA
UK-AQF	15.81	45.76	-	-
<b>WRF-based models</b>				
KCL-CMAQ	10.07	77.58	0.64	0.73
Hert-CMAQ	4.28	70.34	0.70	0.77
EMEP4UK	3.95	142.79	-0.04	0.23
AEA-CMAQ	13.47	77.82	0.64	0.70
WRF-Chem	3.76	83.02	0.56	0.69
<b>Met Office models</b>				
AQUM	4.22	70.76	0.69	0.77
NAME	6.36	71.00	0.69	0.77

<sup>16</sup> Gilliam, R.C., Godowitch, J.M., Rao, S.T. (2012). Improving the horizontal transport in the lower troposphere with four dimensional data assimilation. *Atmospheric Environment*, 53, 186-201, doi:10.1016/j.atmosenv.2011.10.064.

**Figure 3.1 Observed ambient temperature vs. forecast ambient temperature performance report for 2011.**

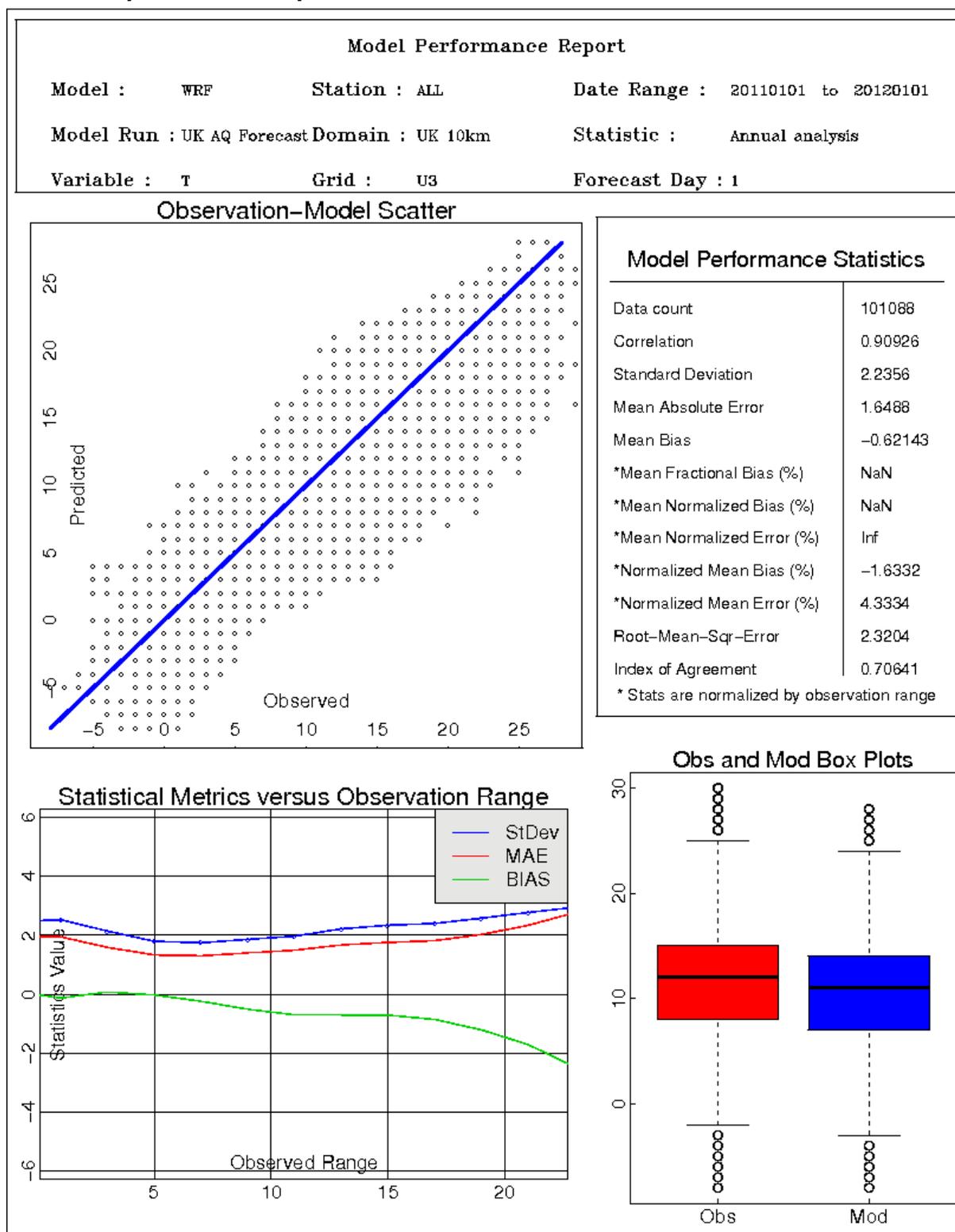
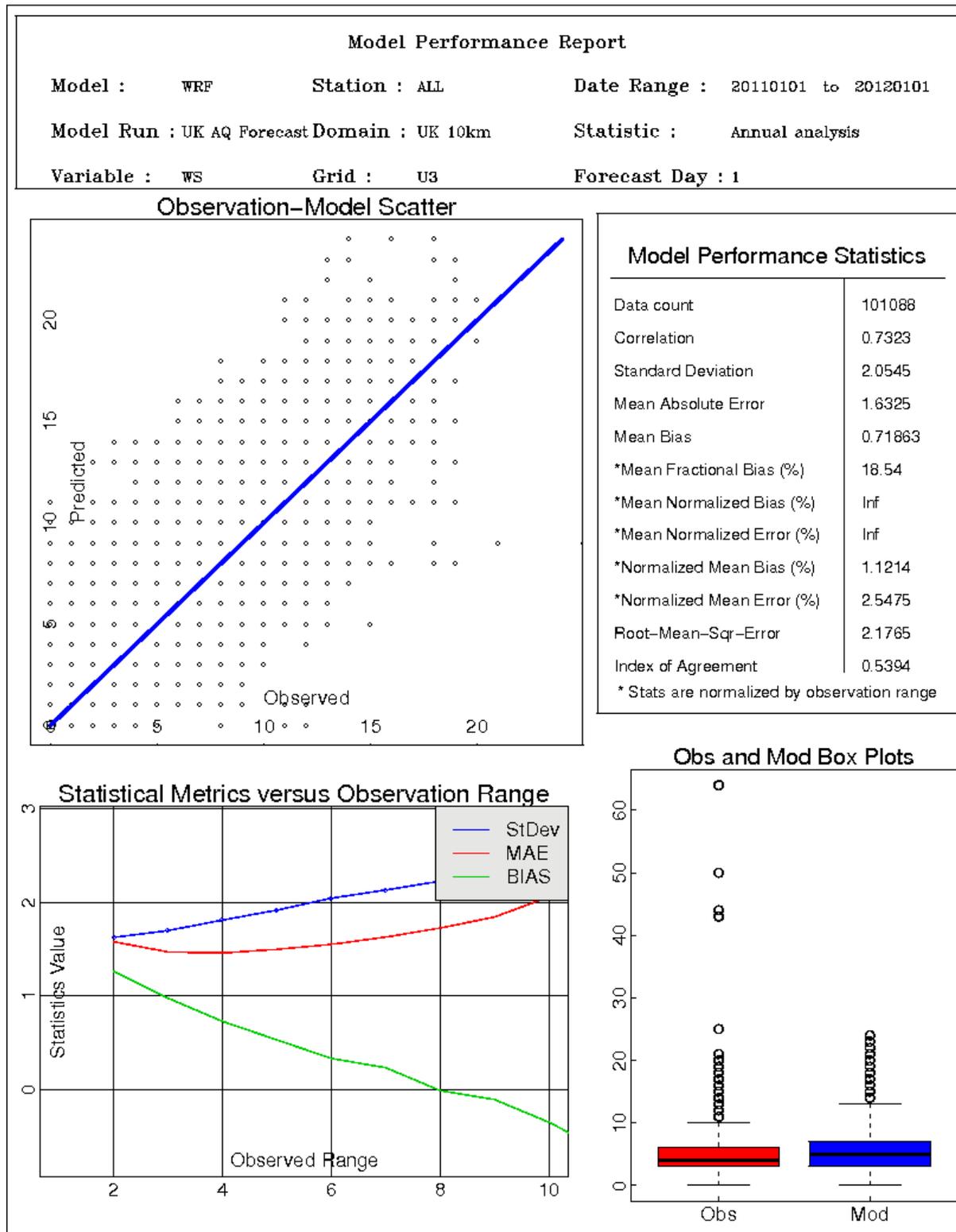


Figure 3.2 Observed wind speed vs. forecast wind speed performance report for 2011.



**Figure 3.3 Observed ambient temperature vs. forecast wind direction performance report for 2011.**

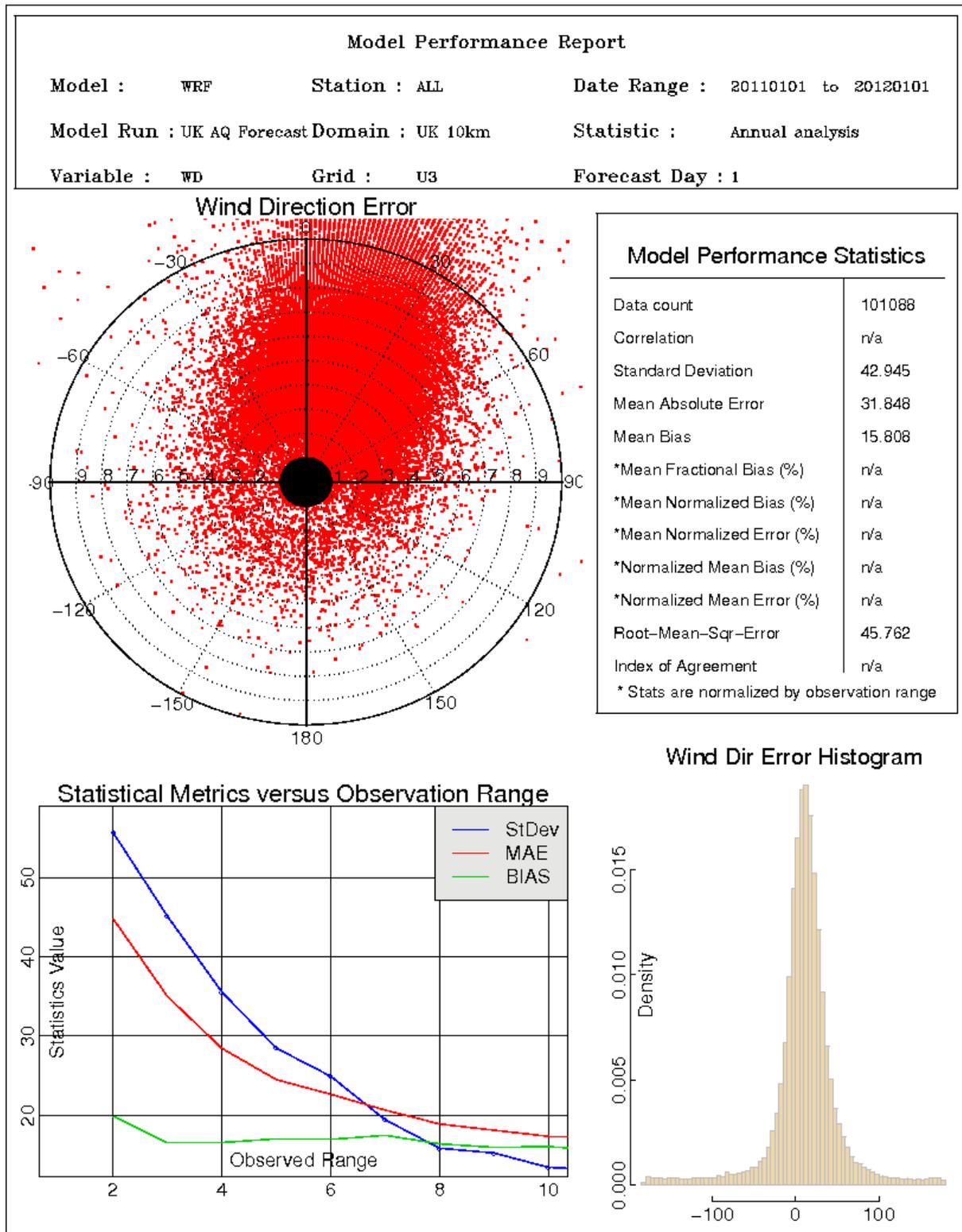


Figure 3.4 shows the variation in the UK-AQF modelled wind direction bias for selected ground-based AURN sites for condition of 2011. The plot shows that the monthly wind direction mean bias varies from site-to-site over the year. No clear trend was obvious throughout 2011, except that the mean bias in wind direction during spring and summer was generally lower, when compared to autumn and winter months. Further analysis revealed that there was no discernible trend based on relative geographic location, i.e., whether the site under consideration, where the UK-AQF modelled and observed wind direction were being compared, was located in the east or west, north or south of the UK. Neither was the mean bias in wind direction shown to be dependent on the prevailing wind direction.

**Figure 3.4 Comparison of monthly averaged UK-AQF modelled wind direction mean bias for selected AURN air quality monitoring sites in 2011.**

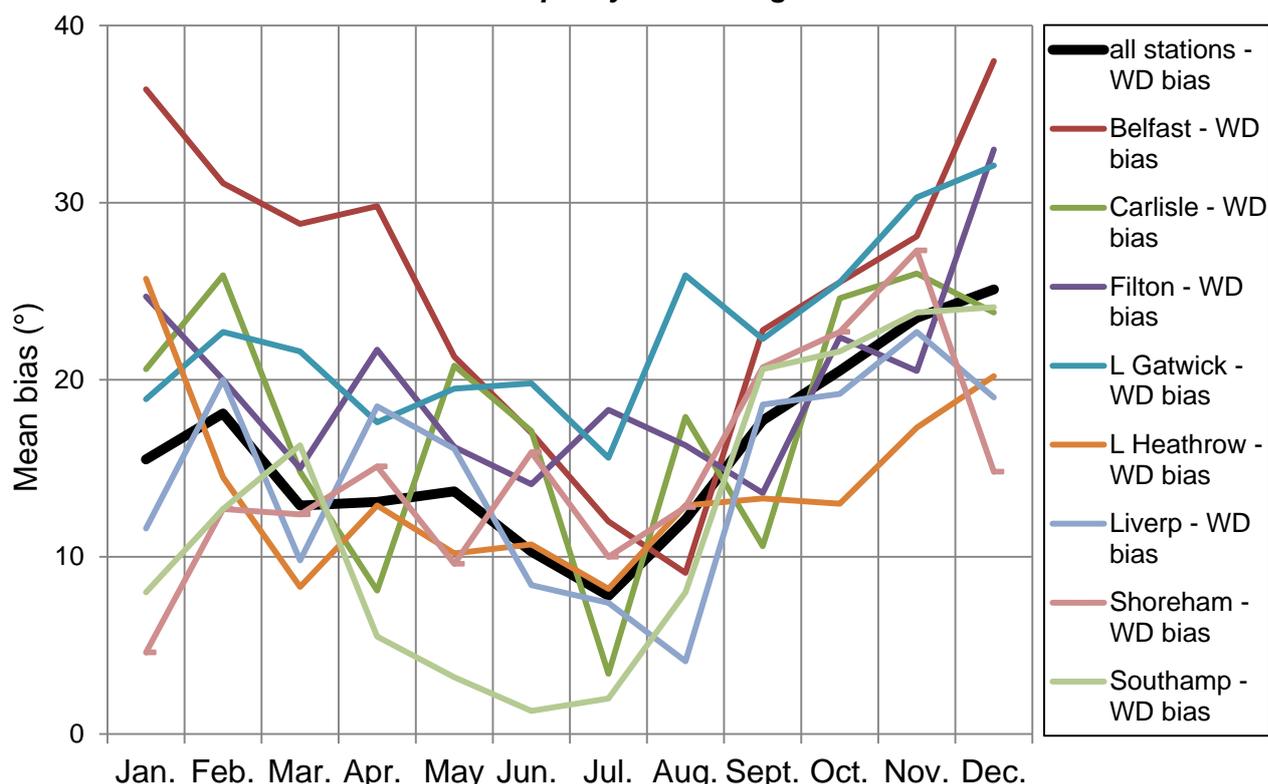


Table 3.4 shows the altitude above sea level (asl) of selected meteorological observation stations and the associated modelled mean wind direction bias. In general, the sites with the highest altitude (i.e., Filton, Carlisle, and London Gatwick) resulted in the highest magnitude of the modelled mean wind direction bias. The relatively high elevation of these sites points to a generally complex terrain topography. Recent work by Owens and Mass (2011)<sup>17</sup> indicated that the complexity of the terrain being modelled may be at the heart of biases in wind direction in WRF. On a 10 km x 10 km grid terrain complexity cannot be accurately represented, effects on wind direction/speed still may occur between neighbouring grid cells to some degree. This issue is under investigation. Upgrading the current version of WRF to the latest release could be a first step in addressing and correcting the modelled wind direction mean bias observed. This upgrade is planned to be implemented from January 2013.

<sup>17</sup> Mass, C., Owens, D. (2011). Fixing WRF's high speed wind bias: a new sub-grid scale drag parameterization and the role of detailed verification. 91<sup>st</sup> American Meteorological Society Annual Meeting, 615-617 (Washington State Convention Centre).

**Table 3.4 Summary of monthly-averaged modelled wind direction bias for 2011 and elevation for selected stations.**

ICAO station name	Altitude above sea level (m)	Wind direction mean bias (°)
Shoreham-By-Sea	2	14.9
Belfast Harbour	5	25.0
London Heathrow	23	13.9
Liverpool	25	14.6
Carlisle	58	17.8
London Gatwick	62	22.5
Filton (Bristol)	69	19.7
Newcastle	81	-6.3
<b>Mean</b>		<b>15.8</b>

## 4 Use of UK-AQF modelled meteorological parameters with openair data analysis tools

### 4.1 Introduction to openair

[openair](#)<sup>18</sup> provides free, open-source and innovative tools to analyse interpret and understand air pollution data using R<sup>19</sup>; a free and open-source programming language designed for the analysis of data. The openair package was primarily developed for the analysis of air pollution datasets with the ability to handle high volumes of data; the AURN, with its long data record lends itself to this. A further strength of the openair tools is that they also allow data to be conditioned by one or more variables. For example, plots can be produced that show the inter-relationships between air pollutants and meteorological parameters, or temporal trends.

UK-AIR provides simplified web access to a customised selection of the openair tools, including tools that require meteorological measurements to run. To implement tools requiring meteorological data, the UK-AQF modelled wind speed and wind direction are available along with air pollutant concentrations measured at AURN air quality monitoring stations. This is in-line with the findings of the MIE2 report<sup>15</sup> which remarks that *‘the generally good quality meteorological predictions suggest that modelled values could usefully be substituted for surface observations or help predict in locations without surface measurements’*. The UK-AQF modelled meteorological parameters on the UK-AIR website are available for download and should be used in accordance with the following cautionary disclaimer:

**Box 1: An example of a highlight box with a caption**

**Please Note: The modelled meteorological parameters provided on the UK-AIR website for use with the openair tools have been created under the Defra & Devolved Administrations UK air quality forecasting (UK-AQF) contract. The modelled meteorological parameters are updated daily and are evaluated against meteorological observations.**

The UK-AQF uses a 10 km x 10 km grid resolution for modelling UK meteorology. Therefore the modelled meteorological parameters are representative of regional synoptic conditions at the location of each UK air quality monitoring station. It should be noted that they ***do not*** account for local meteorological features, e.g., wind (direction) flow reversal in “street canyons” which can occur at roadside air quality monitoring stations. The UK-AQF modelled meteorological parameters should therefore be used with caution in local data analysis or modelling studies. The UK-AQF modelled meteorological parameters do provide an alternative to commercially available meteorological observations which can be measured some distance from the local air quality monitoring station.

**Any use of these data is at the users own risk and should be made in accordance with the terms and conditions of the website.**

<sup>18</sup> Carslaw, D.C., Ropkins, K. (2012). Openair: Open-source tools for the analysis of air pollution data. R package version 0.6-0. <http://www.openair-project.org/>

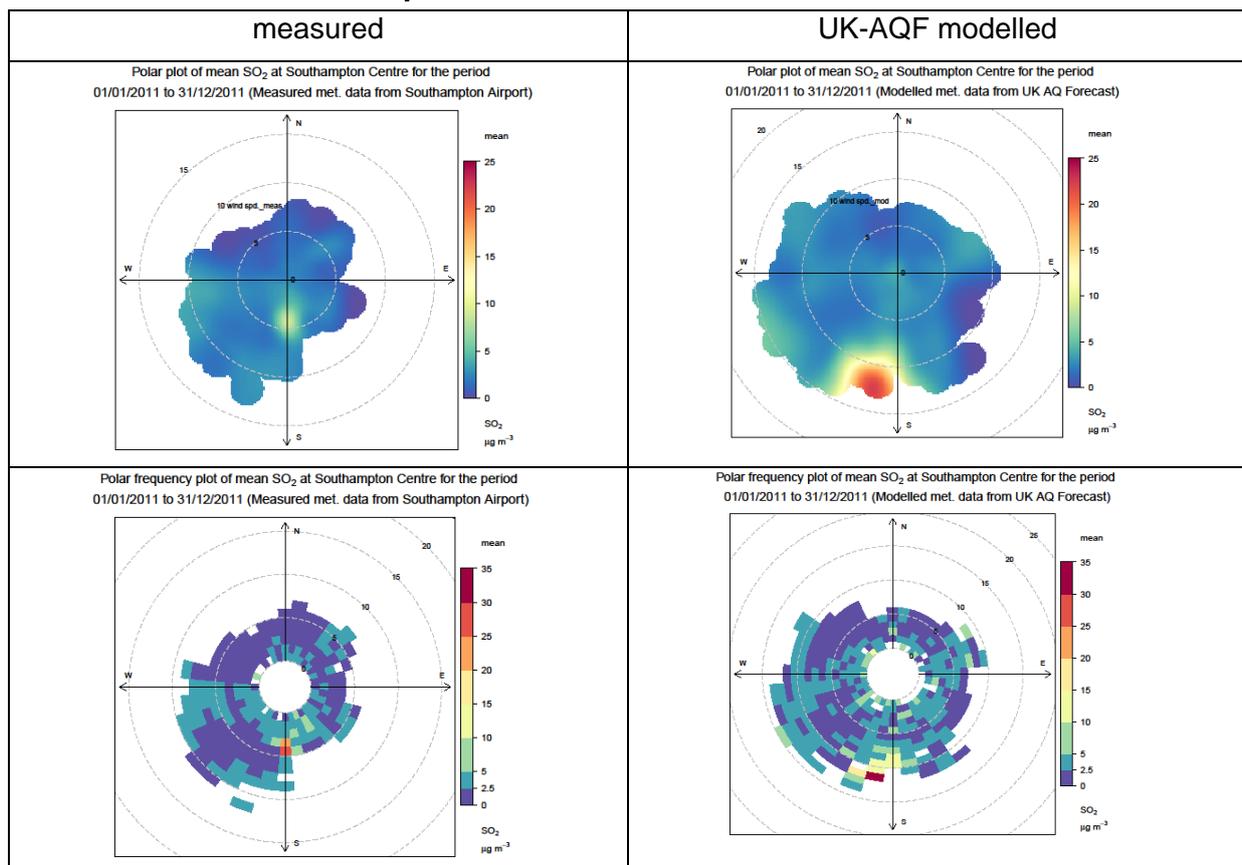
<sup>19</sup> R Development Core Team (2010). R: A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria. ISBN 3-900051-07-0. <http://www.R-project.org>

## 4.2 Example comparison

Below are two examples (Figure 4.1 and Figure 4.2) comparing bivariate plots of 2011 air pollutant concentrations ( $\text{SO}_2$  and  $\text{NO}_2$ , respectively) conditioned by wind speed and wind direction. In both cases the air pollutant concentrations are from Southampton Centre (Figure 4.1) and London Hillingdon (Figure 4.2) AURN air quality monitoring stations.

The plots in Figure 4.1 and Figure 4.2 were generated using the openair tools available on the UK-AIR website. The air pollutant concentrations presented in Figure 4.1 and Figure 4.2 were conditioned using measured and UK-AQF modelled wind speed and wind direction. Measured meteorological observations were taken from ground-based meteorological stations located in the same grid square as the AURN air quality monitoring stations as shown in Table 1.3. Therefore  $\text{SO}_2$  measurements from Southampton Centre were conditioned against the wind speed and wind direction measured at Southampton Airport and the UK-AQF modelled values, while the  $\text{NO}_2$  measurements from London Hillingdon were conditioned against the wind speed and wind direction measured at Heathrow Airport and the UK-AQF modelled values. The data presented is **only** for times when air pollutant concentrations, and measured and UK-AQF modelled wind speed and wind direction measurements were available.

**Figure 4.1 Example openair bivariate plots of 2011  $\text{SO}_2$  concentrations conditioned by wind speed and direction at Southampton Centre AURN air quality monitoring station using measured (Southampton Airport) and UK-AQF modelled wind speed and wind direction.**



The top two panes of Figure 4.1 show polar plots of the 2011  $\text{SO}_2$  concentrations measured at Southampton Centre AURN air quality monitoring station. By comparing the plots in the top left and top right panes there are some obvious differences, namely the peak  $\text{SO}_2$  concentration occurs to a greater extent and at higher wind speed speeds when plotted against the UK-AQF modelled wind speed and wind direction, than when compared the

observed values. Comparison of the plots in the top two panes with the corresponding polar frequency plots in the lower two panes provides an insight as to why this is occurring. When the UK-AQF modelled meteorological parameters are conditioned in openair, prior to plotting, the highest SO<sub>2</sub> concentrations are placed (binned) into a narrow range in terms of wind speed and direction. Hence when averaged, it results in the highest SO<sub>2</sub> concentration occurring at the edge of the polar plot: thus when smoothing is applied, the plot shows a steep SO<sub>2</sub> concentration gradient.

By comparison, the measured meteorological data appears to put the highest SO<sub>2</sub> concentrations at lower wind speeds. openair also places the highest SO<sub>2</sub> concentrations mid-way within the range of wind speeds. Hence when smoothed and averaged by openair, this feature is ameliorated. For this example, the UK-AQF modelled wind speed and wind direction appear to be a better representation of the situation at the Southampton Centre AURN air quality monitoring station. Stronger coastal winds would be expected to cause exhaust plumes emitted from activities at Fawley refinery to ground at the AURN air quality monitoring station. Conversely, the meteorological observations from Southampton Airport, which is further inland, would not be a good representation of the coastal winds at the AURN monitoring air quality station location.

**Figure 4.2 Example openair bivariate plots of 2011 NO<sub>2</sub> concentrations conditioned by wind speed and direction at London Hillingdon (top row) and London Harlington (bottom row) AURN air quality monitoring station using measured (Heathrow Airport) and UK-AQF modelled wind speed and wind direction**

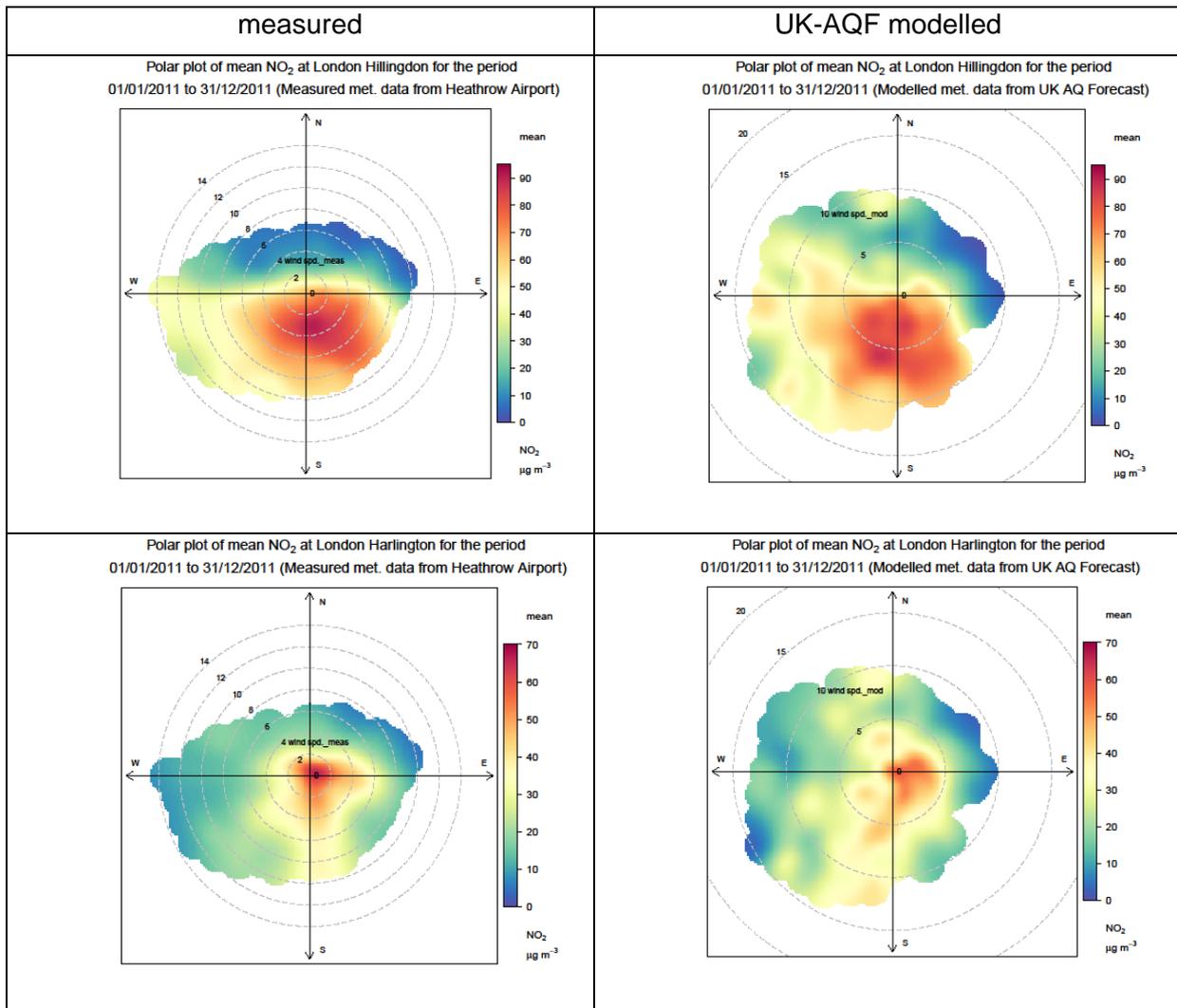


Figure 4.2 shows polar plots of 2011 NO<sub>2</sub> concentrations measured at London Hillingdon and London Harlington AURN air quality monitoring stations. These two AURN air quality monitoring sites are within the same 10 km x 10 km grid cell as Heathrow Airport as indicated by Table 1.3. In this example, the UK-AQF modelled wind speed and wind direction are more varied than the observations from Heathrow Airport. A positive bias in the UK-AQF modelled wind direction is apparent which appears to increase with wind speed. Overall, the distribution of NO<sub>2</sub> with wind speed is consistent between the UK-AQF modelled and measured meteorological data. The patterns in the 2011 NO<sub>2</sub> concentrations are also realistic with London Hillingdon located north of the M4 motorway and Heathrow Airport, whilst London Harlington is situated to the south of the M4 motorway and north of Heathrow Airport.

The initial evaluation of the UK-AQF modelled meteorological indicates that they perform in-line with the range reported in the MIE2. The examples above indicate that the UK-AQF modelled meteorological parameters are suitable for use with the openair tools within the context of the cautionary disclaimer.

## 5 Conclusions

This report summarises the findings of the initial statistical evaluation of the UK-AQF modelled meteorological parameters, namely: ambient temperature (2 m), wind speed and wind direction. These meteorological parameters were derived from the WRF v3.0.1 and prepared for the CMAQ v4.7.1 air quality modelling using the MCIP v3.4.1 for the UK-AQF.

Operational evaluation of the modelled meteorological parameters, with observed values, is undertaken daily on a rolling 14-day and calendar month basis. The evaluation provides a qualitative comparison of how the meteorological parameters used for UK-AQF reproduces the ambient temperature, wind speed and wind direction for a range of locations distributed throughout the UK air quality modelling domain. This evaluation is automated and performed daily on a daily basis. It is used to provide information and guidance to the duty air quality forecaster.

The UK-AQF modelled ambient temperature (2 m) and wind speed compares well with the range of models discussed in the MIE2, particularly against other WRF model-based UK air quality forecasting models. There is a positive bias in the UK-AQF modelled wind direction when compared to the ground-station observations. This bias has been noted by previous researchers. Work has been undertaken by the developers of the WRF model to limit this bias in more recent versions of the WRF modelling software. T

This initial evaluation shows that the modelled meteorology input data is suitable for use in the 10 km x 10 km resolution UK-AQF. Whilst the modelled meteorological parameters are representative of regional synoptic conditions at the location of each UK air quality monitoring station, it should be noted that they do not account for local meteorological features, e.g., wind (direction) flow reversal in “street canyons” which can occur at roadside air quality monitoring stations.

The UK-AQF modelled meteorological parameters provide a useful alternative to commercially available meteorological observations which can be measured some distance from the local air quality monitoring station. Therefore whilst the modelled meteorology input data are suitable for use with the openair tools, users should be aware of the above cautionary disclaimer when using them with these tools, or in any local data analysis or modelling studies.

The evaluation of the UK-AQF modelled meteorological parameters is an on-going process: further progress and refinements to the statistical evaluation procedures will be made, with a focus on providing information to the duty forecaster and improving the accuracy of the UK-AQF. The statistical evaluation presented here only considers surface observations and does not examine UK-AQF modelled atmospheric profiles against atmospheric soundings. The accurate representation of air mass movements above ground and the representation of the planetary boundary layer are important for air quality models. Comparison of UK-AQF modelled atmospheric profiles and atmospheric soundings should be considered at a later date.



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