CMAQ Development for UK National Modelling:

WRF Optimisation

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Executive Summary

To establish the role that WRF meteorological forecasts play in CMAQ's over prediction of observed NO_x (and an under prediction of O_3) during the late afternoon and overnight periods and in response to stakeholder comments, this report summarises an extended analysis of WRF to include a number of parameters which have an important influence on air pollution: Planetary Boundary Layer (PBL) height, friction velocity (u_*), atmospheric stability (z/L), sensible and latent heat flux as well as those that are important in the calculation of wet deposition (cloud amount and precipitation) and may influence WRF's performance (number of model layers and nudging). The aim has been to provide recommendations for the use of WRF in CMAQ-UK policy applications.

Recommended WRF set-up for CMAQ-UK

Based on statistical performance of WRF and CMAQ, the recommended surface layer, land surface and PBL schemes, grid nudging settings and vertical layer structure for WRF is as follows:

- **Surface layer scheme**: PX
- **Land surface scheme**: RUC
- **PBL**: ACM2
- **Grid nudging**: Grid analysis nudging with nudging coefficients of $3x10^{-4}$ s^{-1} for U,V,Q and T, 6h nudging time interval throughout a simulation period, and nudging within PBL and above.
- **Vertical layer structure**: 23 layers

Although the use of ACM2 scheme improved the performance of WRF and CMAQ predictions, there was no clear cut "best" model for all conditions and in all locations. In summary the recommended scheme tended to work best in urban areas which is important for $PM_{2.5}$ exposure and less well in rural locations.

The ACM2 WRF-CMAQ model improved the prediction of NO_X, NO_2 and O_3 during the evening and overnight periods, although the problem has not been fully resolved. It proved difficult to interpret the new NO_X results using the model's turbulence and surface meteorological performance alone. As a consequence, an additional set of diagnostic analysis was undertaken, using vertical mixing intensity (Kz) and ethane observations.

The use of Kz and ethane proved to be beneficial in interpreting the modelled concentrations and in resolving the relative role of emissions and dispersion in the performance of the model. The new diagnostic analysis suggested that NO_X emissions played an important role in the model's performance in January and that dispersion was important in July. It is therefore recommended that the use of these two diagnostics be incorporated into any further model evaluation.

The analysis of cloud and precipitation observations showed that all models under predict cloud cover by 50-60% and under predict precipitation by a factor of two in winter and at night time in summer. To improve the model's performance, further sensitivity analysis would be required to investigate the performance of different microphysics and cumulus schemes within the CMAQ-UK model.

The grid nudging analysis indicated that the phase 1 CMAQ-UK provisional configuration: nudging all model layers every 6h, with a nudging coefficient of $3x10^{-4}$ s^{-1} for u and v wind component, temperature (T) and water vapour mixing ratio (Q), is most suitable for retrospective modelling.

Sensitivity tests of the model using different layer structures showed that only the 35 layer scheme improved the model performance, but at the same time increased run times by factor of two compared with the phase 1 recommended scheme. With such small improvements it is recommended that the phase 1 layer settings be retained.

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1. Background and phase 2 aims

During phase 1 of the DEFRA CMAQ-UK project, a comparison of the performance of CMAQ air quality predictions against UK measurements showed an over prediction of NO_x (and an under prediction of O_3) during the late afternoon and overnight periods. One possible explanation for this was the negative bias observed in WRF's wind speed and temperature predictions for this period and possibly an underestimation of PBL height. The aim of this work is to identify the factors responsible for the deficiency of WRF/CMAQ during these (and other) periods and to recommend a new WRF configuration. Furthermore, in response to stakeholder comments, the phase 2 WRF analysis has been extended to include a number of parameters which have an important influence on air pollution: Planetary Boundary Layer (PBL) height, friction velocity (u_*), atmospheric stability (z/L), sensible and latent heat flux as well as those that are important in the calculation of wet deposition (cloud amount and precipitation) and may influence WRF's performance (number of model layers).

The specific project objectives include:

- To quantify the effect of PBL and surface schemes on PBL height, atmospheric stability and turbulent parameters in WRF.
- To identify factors affecting late afternoon and overnight wind speed, temperature and relative humidity predictions and their effects on predicting NO_X, NO_2 and O_3.
- To analyse WRF performance on cloud and precipitation predictions.
- To quantify the effect of vertical layer structure and nudging on WRF's performance.

In section 2 we provide information on our experimental design, in section 3 a summary of WRF results, in section 4 we analyse CMAQ's predictions of NO_X, NO_2 and O_3, and in section 5 we analyse WRF's cloud and precipitation predictions. In section 6 we compare the performance of WRF using alternative layer structures and in section 7 we discuss the influence of grid nudging configuration. Finally, in section 8 we provide the conclusions of this work.

2. WRF and CMAQ experimental design

In this report we summarise a number of alternative planetary boundary layer (PBL), surface layer and land surface parameterisations, used to investigate WRF's negative wind speed and temperature bias, observed during the late afternoon and evening. The reason for running WRF assuming different surface layer, land surface and PBL parameterisations is that these schemes are important in determining the transfer of heat, moisture and momentum between the surface and the PBL (Skamarock, et al. 2008, Hu, et al. 2010) and have an important influence the prediction of air quality using CMAQ.

The PBL schemes tested in this report include two first order nonlocal closure schemes YSU (Hong, et al., 2006) and ACM2 (Pleim, 2007a,b) and two 1.5 order local closure or Turbulent Kinetic Energy (TKE) schemes MYNN (Nakanishi and Niino, 2004) and BouLac (Bougeault and Lacarrére, 1989). The PBL schemes have also been combined with a number of surface layer schemes including: MYNN (Pagowski, 2008), P-X (Pleim, 2006) and MM5 similarity (Zhang and Anthes, 1982). Finally, the combination of PBL and surface layer schemes have been combined with alternative land surface models (LSM) including: 5-layer thermal diffusion (Skamarock, et al., 2008), PX (Pleim and Xiu, 1995, Xiu and Pleim, 2001), Noah (Chen and Dudhia, 2001) and RUC (Smirnova, et al., 1997 and Smirnova, et al., 2000). The combination of model tests is summarised in Table 1.

Table 1 The assumptions used in the PBL, surface layer and land surface parameterisation sensitivity tests

Test	**WRF Version**	**Land use**	**Number of layers**	**Surface Layer**	**Land Surface**	**PBL**	**Nudging**
MYNN3.3.1 (Provisional version)	3.3.1	MODIS	23	MYNN	NOAH	**MYNN2.5**	Grid
YSU	3.4	USGS	23	MM5	NOAH	**YSU**	Grid
MYNN3.4	3.4	USGS	23	MYNN	NOAH	**MYNN2.5**	Grid
PXACM2	3.4	USGS	23	P-X	P-X	**ACM2**	Grid
BouLac	3.4	USGS	23	MM5	NOAH	**BouLac**	Grid
MM5MYNN	3.4	USGS	23	**MM5**	NOAH	MYNN2.5	Grid
MM5ACM2	3.4	USGS	23	**MM5**	P-X	ACM2	Grid
EtaBoulac	3.4	USGS	23	**Eta**	NOAH	BouLac	Grid
TherACM2	3.4	USGS	23	P-X	**5-layer**	ACM2	Grid
NoahACM2	3.4	USGS	23	P-X	**NOAH**	ACM2	Grid
RucACM2	3.4	USGS	23	P-X	**RUC**	ACM2	Grid

For direct comparison, simulations of the different PBL schemes were undertaken using the same WRF version (v3.4), domain configuration, USGS land use data and GFS lateral boundary conditions. The MYNN v3.3.1 results were taken from the Phase 1 CMAQ-UK simulation. The sensitivity tests were undertaken for the months January and July 2006, consistent with Phase 1 of the project, and widely studied within the DEFRA MIE (Carslaw, et al., 2013) and AQMEII project (http://aqmeii.jrc.ec.europa.eu/). This period was chosen due to the variety of weather conditions, for example, in 2006 the temperature varied from -11 °C on the 31st January at a few sites in the north of England and Scotland up to approximately 35 °C on the 19th July at sites across the UK. In addition, the summer heat wave in June and July lead to an O_3 episode in the UK and Europe.

All of the sensitivity tests in this study were undertaken using the same nudging configuration, described in the DEFRA Phase 1 report, and the model results from the UK domain (10km grids) compared against the measurements from 169 UK Meteorological Office surface stations and 8 Global radiosonde sites (Figure 1a). The UKMO surface sites provided the measurements of wind speed and direction at 10m, temperature and relative humidity at 2m, cloud cover and precipitation, while the radiosonde sites provided wind speed and temperature vertically in the atmosphere. Due to the lack of measurements of PBL height and other turbulence parameters, model to model comparisons were made for PBL height, u_*, z/L, sensible and latent heat flux. In addition, each WRF model run was used in concert with the CMAQ model and a comparison made against NO_x, NO_2, and O_3 measurements at 22 DEFRA MIE sites (Figure 1b). NO_X, NO_2, and O_3 were chosen, rather than PM, to ease interpretation of the CMAQ results, despite the importance of $PM_{2.5}$ for the core demonstration work.

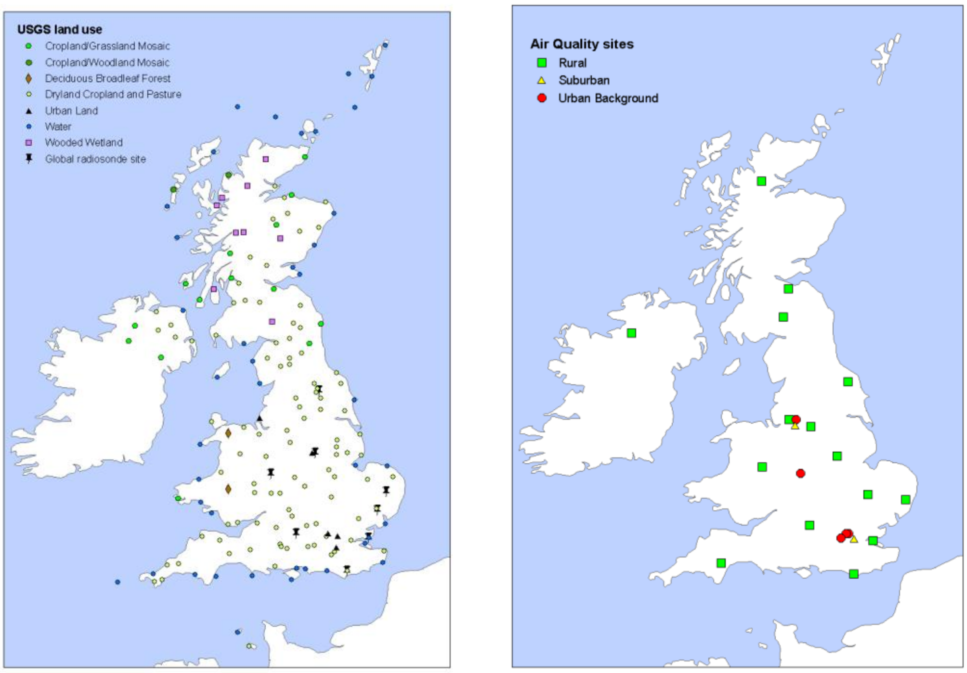


Figure 1 a) The 169 surface meteorological stations by USGS land use and 8 UK MO global radiosonde stations used for the WRF evaluation, b) The 22 air quality monitoring sites used for comparison with NO_X, NO_2 and O_3.

A further set of sensitivity tests has been undertaken to compare WRF predictions of wind speed, temperature and relative humidity to different layer structure assumptions in the model. The layer height chosen for each sensitivity test is shown in Figure 2 , Table 2 and in Table 6 (Appendix 1).

Table 2 A description of alternative layer tests and grid nudging configurations

Test	WRF Version	Land use	Number of layers	Surface Layer	Land Surface	PBL	Nudging
23new	3.4	USGS	**23**	P-X	P-X	ACM2	Grid
27new	3.4	USGS	**27**	P-X	P-X	ACM2	Grid
35	3.4	USGS	**35**	P-X	P-x	ACM2	Grid
35smooth	3.4	USGS	**35**	P-X	P-X	ACM2	Grid
PBL nudging	3.4	USGS	23	P-X	P-X	ACM2	**no PBL nudging**
Nudging frequency	3.3.1	MODIS	23	MYNN	NOAH	MYNN2.5	**Only first 24h**
Nudging time interval	3.4	USGS	23	P-X	P-X	ACM2	**168h**
	3.4	USGS	23	P-X	P-X	ACM2	**72h**
Nudging Coefficients	3.4	USGS	23	P-X	P-X	ACM2	**$Q = 1 \times 10^{-5}$ s^{-1}**

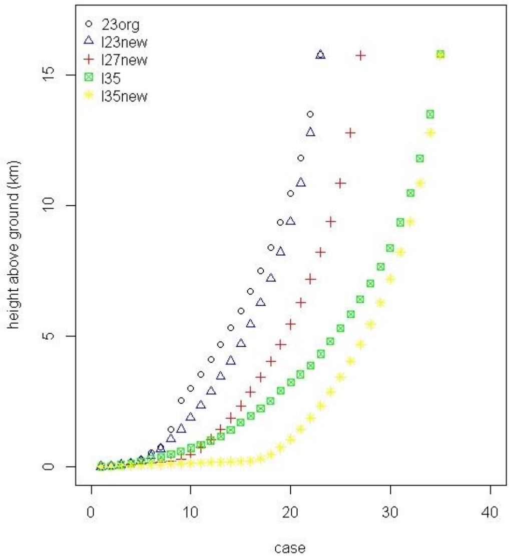


Figure 2 Top model layer heights above ground for structure sensitivity

In addition, Table 2 also provides details of the tests undertaken to assess different grid nudging strategies, including: with and without PBL nudging, the effects of nudging frequency, use of different nudging time intervals, and the effect of using different nudging coefficients.

Finally, the results of a number of WRF-CMAQ combinations were compared with NO_X, NO_2 and O_3 concentrations. In all cases v5.0.1 of the CMAQ model has been used and use made of emissions from TNO (Europe), NAEI (UK) and King's traffic emissions (GB). Although the EMEP emissions were recommended in Phase 1 due to its publicly availability, the TNO emissions were used in this study due to its finer spatial grid resolution (i.e., ~7km grid resolution as compared with 50km grid resolution of EMEP).

3. WRF results at UKMO sites

A comparison between the five alternative WRF schemes and UKMO sites has been made for January and July 2006, for wind speed at 10m height (ws10), temperature at 2 m height (ta2), surface temperature (tag) and relative humidity at 2 m height (rh2). Because there remains a lack of measurements of some parameters, the assessment of PBL height, friction velocity (u_*), atmospheric stability (z/L) and sensible and latent heat fluxes remains qualitative, through comparison between models. The results of these tests are given in Figure 3.

By comparing the results of each PBL scheme, a number of important results are evident. There is poor agreement between the YSU (and Boulac) schemes and observed wind speed during evening and night time periods and this translates to the highest values of u_* during these periods. In the middle of the day all of the schemes, including YSU and Boulac, agree reasonably well with wind speed measurements. All schemes are in better agreement with temperature (ta2) with the two MYNN schemes (v3.3.1 and 3.4) tending to under predict overnight (~1° C). Sensible heat flux values are in close agreement between each scheme with ACM2 having the highest estimate during the afternoon period, which is reflected in the different partitioning between latent (qfx) and sensible heat fluxes (hfx). ACM2 is the only scheme that runs with the PX LSM, which may explain this difference. Any differences in heat flux partitioning between the schemes, and in particular the ACM2 model, are not reflected in the relative humidity estimates (rh2) which are also in reasonable agreement with observations. YSU and Boulac are in closest agreement with measurements of relative humidity, with the three remaining schemes having a positive bias, especially during the night. There is a close agreement between all of the schemes for ground level temperature (tag). For wind direction (not shown here), the frequency of winds in the north-south, east-west, southeast-northwest and southwest-northeast sectors are also well predicted for all models, with a small bias of ±5% for individual wind direction sectors.

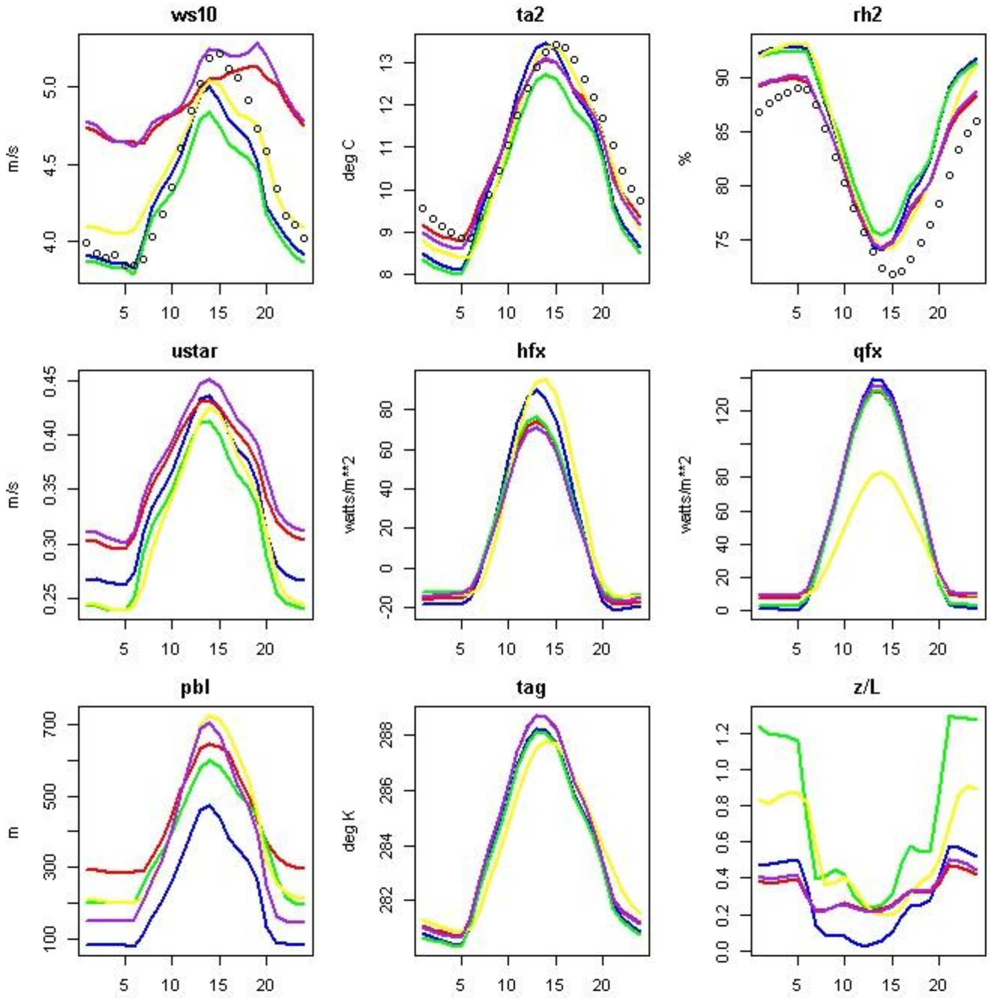


Figure 3 All sites and the Jan06 and Jul 06 period average of diurnal profiles of surface meteorological data, including wind speed at 10m (ws10), temperature at 2m (ta2), relative humidity at 2m (rh2), friction velocity (ustar or u*), sensible heat flux (hfx), latent heat flux (qfx), PBL height (pbl), ground temperature (tag) and atmospheric stability (z/L) (blue= MYNN3.3.1, red = YSU, green = MYNN3.4, yellow = ACM2, purple = BouLac, black circle = observation)

Estimates of atmospheric stability (z/L) are classified as stable if they are greater than 0.2, neutral between 0.2 and -0.2 and unstable if they are less than -0.2. The YSU, Boulac and MYNN (v3.3.1) schemes show a small range in stability during the period (neutral to stable) and this is reflected in the YSU and Boulac wind speed results which also show a small diurnal variation. However, for MYNN (v3.3.1) this small range is not apparent either in the ws10 or ta2 results but is reflected in the diurnal profile of u*. MYNN 3.4 and ACM2 predict the most stable meteorology and although in reasonable agreement with the other schemes towards midday and early afternoon, both models are more stable overnight with the MYNN3.4 scheme the most stable of all five tested.

In summary the Phase 2 comparison between WRF meteorological forecasts and UKMO observations (wind speed, temperature and relative humidity) and model to model comparisons of Planetary Boundary Layer (PBL) height, friction velocity (u*), atmospheric stability (z/L), sensible and latent heat flux) have shown that:

- The model Boulac provides similar results to those of YSU, i.e. good temperature predictions but wind speed estimates that show considerable over prediction during the evening and night time periods;
- The new version of MYNN (v3.4), (the MYNN (v3.3.1) scheme was recommended at the end of phase 1), gives results which are similar to ACM2. Both schemes show similar PBL heights, u_* predictions and a greater range of stability (z/L);
- During phase 1 of the DEFRA CMAQ project, concerns were raised over predicting late afternoon and evening concentrations of NO_X. Phase 2 results show that ACM2 on average predicts both wind speed and temperature well during that period and also provides PBL predictions and stability estimates that are in the middle of the range of the models tested. The PBL results from ACM2 qualitatively agree with measurements such as those of Barlow, et al. (2011) who reported PBL heights over London in autumn 2007 from Lidar measurements which were typically between 200-400m at night and ~700-850m during daytime. Furthermore, the PBL heights from ACM2 are similar to results of the non-WRF models in the DEFRA MIE (e.g., NAME and AQUM);
- In LSM sensitivity analysis (not shown), indicates that LSM schemes have a strong influence on all surface variables.
- However, this analysis has shown that it is not simple to decide on the "best" WRF model to put forward for use with CMAQ and in these tests no model achieves a "best" estimate for all parameters and for all periods. The continued lack of measurements such as PBL heights and flux estimates also hinder a more comprehensive comparison of the 5 schemes' performance. However, we have recommended ACM2 as the scheme for use with WRF/CMAQ as it provides good results across a range of parameters. Furthermore, use of ACM2 is recommended by the USEPA (Foley, et al., 2010 and Appel, et al., 2010).

4. CMAQ evaluation

This section aims to quantify the response of CMAQ to PBL height, u_*, surface heat fluxes and z/L and to provide an insight into the factors responsible for the diurnal biases of NO_x, NO_2 and O_3 concentrations that we see. For the sake of clarity we have only compared the results from CMAQ using the ACM2 variants (ACM2-PX, ACM2-MM5, ACM2-RUC) and those of MYNN (recommended in phase 1).

4.1 CMAQ results - NO_X, NO_2 and O_3

To establish the performance of different combinations of WRF-CMAQ, the average NO_X predictions, separated by model version, month and site type, and ordered by Coefficient of Efficiency (COE) has been summarised in Table 3. Given that COE is the best overall estimate of model performance (Carslaw et al, 2013), the results show that the model using the WRF-RUC variant provides the best results in Jan for suburban, urban background and rural sites. And that in July the WRF-RUC model provides the highest COE values for suburban sites and the second highest results for urban background and rural sites. The MYNN model has the highest COE results for urban background and rural sites in July, however it is notable that there isn't a consistent "best" model for both urban and rural locations and that in rural locations all models perform less well against NO_X than in within urban areas.

Table 3 NO_X results for alternative WRF-CMAQ combinations during Jan and Jul 2006, split by month and site type and ordered by Coefficient of Efficiency (COE)

WRF version	Month	Site type	n	r	COE
ACM2-RUC	**Jan**	**Suburban**	**739**	**0.78**	**0.21**
ACM2-RUC	**Jan**	**Urban Background**	**3538**	**0.66**	**0.17**
MYNN	Jan	Suburban	739	0.80	0.14
ACM2-PX	Jan	Suburban	739	0.77	0.14
ACM2-PX	Jan	Urban Background	3538	0.64	0.13
MYNN	Jan	Urban Background	3538	0.67	0.13
ACM2-RUC	**Jan**	**Rural**	**7288**	**0.73**	**-0.07**
ACM2-PX	Jan	Rural	7288	0.73	-0.26
MYNN	Jan	Rural	7288	0.74	-0.29
ACM2-RUC	**July**	**Suburban**	**1481**	**0.63**	**0.23**
MYNN	July	Suburban	1481	0.66	0.22
ACM2-PX	July	Suburban	1481	0.64	0.19
MYNN	July	Urban Background	3499	0.54	0.17
ACM2-RUC	**July**	**Urban Background**	**3499**	**0.50**	**0.11**
ACM2-PX	July	Urban Background	3499	0.49	0.09
MYNN	July	Rural	5959	0.59	-0.04
ACM2-RUC	**July**	**Rural**	**5959**	**0.61**	**-0.06**
ACM2-PX	July	Rural	5959	0.61	-0.12

The meteorological and air quality performance presented so far suggests that ACM2 is an appropriate choice for use with CMAQ. However, testing ACM2 with different surface layer and land surface schemes (not shown) has highlighted a number of important differences in the WRF model's predictive capability. It is important to understand how these differences affect the WRF-CMAQ model's performance against air quality measurements, and this has been undertaken by combining ACM2 (RUC, MM5 and PX) with CMAQ v5.0.1. A summary of the results for each comparison (NO_X, NO_2, O_3), separated into January and July 2006, is given in Table 4. Once again the COE results have been ordered and this shows that the ACM2-RUC version of the model provides a consistently better agreement between modelled and measured results.

Table 4 Statistical measures of CMAQ performance for NO_2, NO_x and O_3 simulations (Jan and Jul 2006) across all sites

Period	Pollutants	case	n	FAC2	MB	NMB	RMSE	r	COE
JAN	**NO2**	**ACM2-RUC**	**11565**	**0.64**	**4.03**	**0.31**	**8.95**	**0.78**	**0.33**
	NO2	ACM2-MM5	11565	0.59	6.03	0.47	10.65	0.76	0.19
	NO2	ACM2-PX	11565	0.59	6.09	0.47	10.71	0.76	0.18
	NOx	**ACM2-RUC**	**11565**	**0.58**	**4.38**	**0.19**	**28.59**	**0.64**	**0.34**
	NOx	ACM2-MM5	11565	0.55	6.84	0.29	29.80	0.64	0.28
	NOx	ACM2-PX	11565	0.54	6.92	0.29	29.87	0.64	0.27

	O3	**ACM2-RUC**	**15165**	**0.65**	**-0.21**	**-0.01**	**8.00**	**0.79**	**0.43**
	O3	ACM2-MM5	15165	0.65	0.56	0.03	8.23	0.79	0.42
	O3	ACM2-PX	15165	0.64	0.51	0.03	8.27	0.79	0.41
JUL	**NO2**	**ACM2-RUC**	**10939**	**0.57**	**0.67**	**0.07**	**8.91**	**0.65**	**0.30**
	NO2	ACM2-MM5	10939	0.56	1.49	0.16	9.56	0.64	0.25
	NO2	ACM2-PX	10939	0.56	1.46	0.15	9.53	0.64	0.25
	NOx	**ACM2-RUC**	**10939**	**0.57**	**-0.43**	**-0.04**	**12.13**	**0.60**	**0.30**
	NOx	ACM2-MM5	10939	0.57	0.28	0.02	12.52	0.60	0.27
	NOx	ACM2-PX	10939	0.57	0.24	0.02	12.47	0.60	0.27
	O3	**ACM2-RUC**	**16081**	**0.88**	**-0.53**	**-0.02**	**12.94**	**0.76**	**0.38**
	O3	ACM2-MM5	16081	0.86	4.01	0.12	14.23	0.75	0.32
	O3	ACM2-PX	16081	0.85	4.32	0.13	14.51	0.74	0.31

4.2 Diurnal errors in NO_X, NO_2 and O_3 predictions

Whilst the use of ACM2 has demonstrated good performance compared with other meteorological model schemes, two questions remain: has ACM2 reduced the positive bias in the late afternoon and evening NO_X predictions, identified in Phase1? and can we explain why such a problem exists. In Figure 4, a comparison has been made between the Phase 1 WRF provisional version (MYNN v 3.3.1) and ACM2 RUC (the Phase 2 recommended scheme) for NO_X and NO_2. It is immediately apparent that over prediction of NO_X during the evening has not been solved, however using ACM2-RUC the positive bias has been reduced and the model's predictive performance has improved compared with MYNN v 3.3.1.

The second question relates to our interpretation of the results. Two of the most likely causes of the positive bias are either total emissions that are too great or the assumed diurnal variation, which incorrectly placing too much of each days emissions into the evening period. The second explanation is whether the model is not dispersing the emissions sufficiently, leading to higher predicted concentrations than is observed. However, from section 3, we have shown that it is difficult to interpret the influence of alternative WRF schemes on CMAQ using wind speed, temperature, z/L and PBL alone. We have therefore used an additional parameter, Kz which represents the intensity of vertical mixing within the PBL.

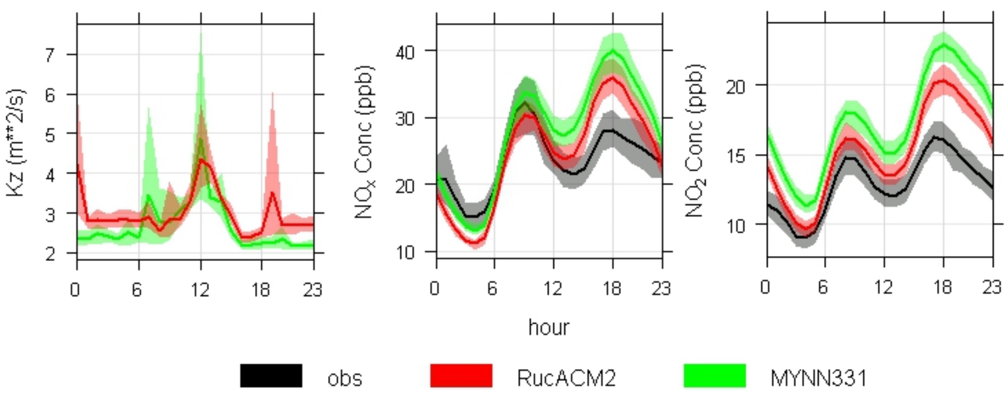


Figure 4 A comparison between the CMAQ NO_X and NO_2 average diurnal profiles and observations from the DEFRA MIE sites (Jan 2006), plus the average value of the vertical eddy diffusivity (Kz) using the two WRF schemes, ACM2 RUC and MYNN v 3.3.1. Kz represents the intensity of vertical mixing within the surface layer.

From Figure 4, the CMAQ Kz values, using ACM2 RUC, are higher than MYNN during the periods midnight to 08:00 hrs, are similar for both schemes between 08:00hrs and 16:00hrs, and higher for the remainder of the day. One would expect a larger Kz value to reduce ground level concentrations of a primary pollutant such NO_X (in January) and looking next at the NO_X diurnal profile this seems to be the case. Between midnight and 06:00 the CMAQ predictions using ACM2 RUC are lower than the MYNN equivalent, are in reasonable agreement albeit slightly lower during the day and lower during the evening period. The model under predicts observations (in black) between midnight and 06:00 hrs, over predicts observations by a small margin between 06:00hrs and ~14:00hrs and by a larger margin for the evening period.

In this brief example Kz promises to add to our ability to judge the meteorological influence of WRF predictions on CMAQ. However, crucially we are still unable to disentangle the emissions and meteorological effects which in combination may be causing the positive evening bias. As a consequence we have undertaken an additional analysis using atmospheric ethane concentrations.

The reason for choosing ethane is that it is a ground level and constant emissions source (eliminating any diurnal uncertainty) and it has no complex chemistry. Therefore ethane acts as a primary tracer gas with which to compare against NO_X.

CMAQ-ACM2 PX has been tested with constant ethane emissions for Eltham in January 2006 (

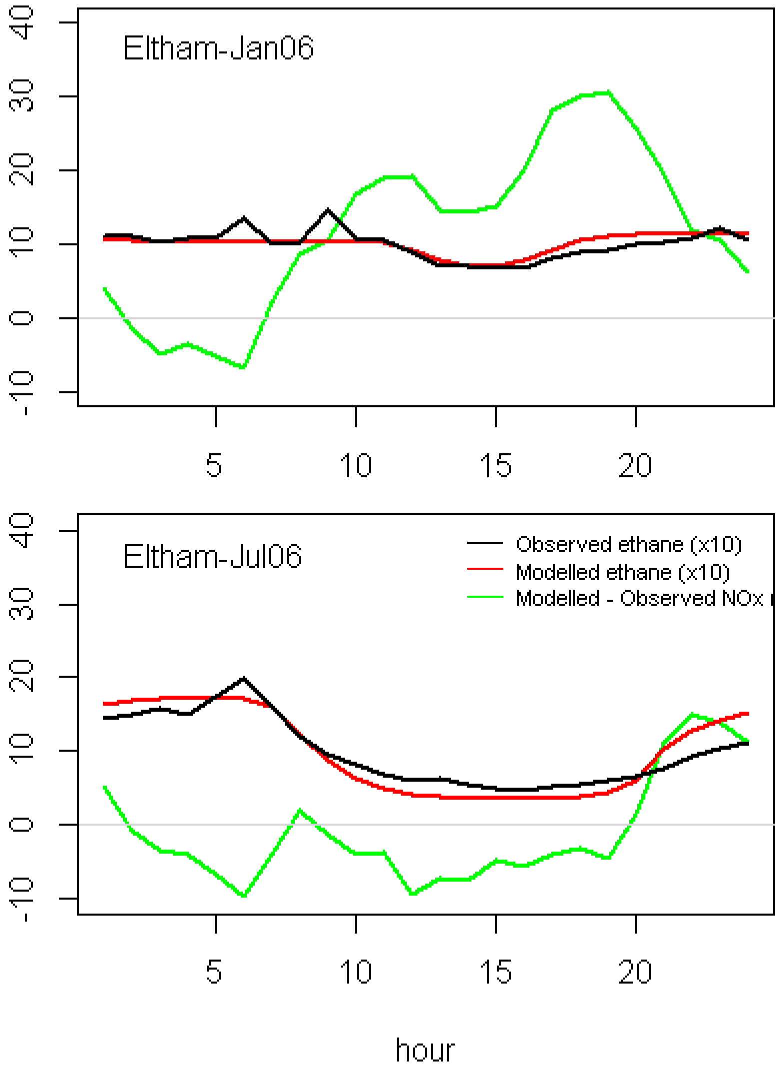


Figure 5 - top) and July 2006 (

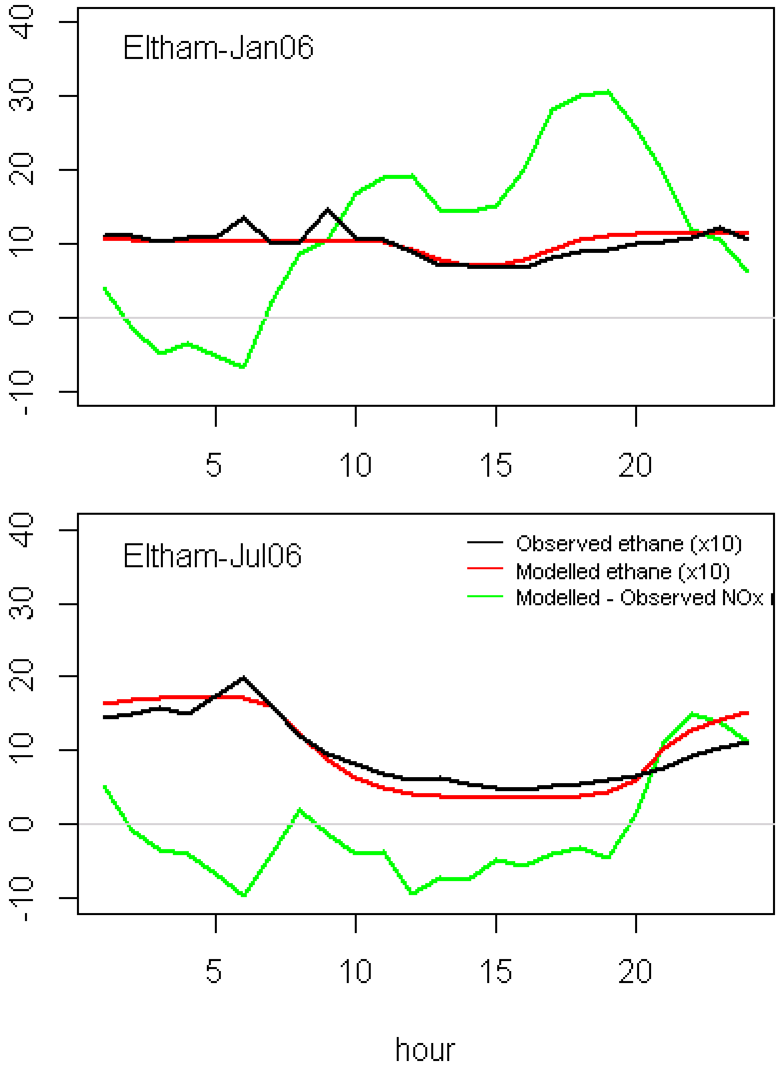


Figure 5 - bottom). Both the model and observed results were then normalised, to eliminate the influence of emissions totals and leaving only the influence of dispersion. For the period in January 2006, there is good agreement between the modelled ethane (red) and observed ethane (blue) averaged across all hours of the day. The two observed early morning peaks are associated with periods of very high ethane concentrations overnight which are not predicted by the CMAQ model. The figure for January also includes the model minus observed NO_X concentrations (green line) for the same period, and by comparison there is a negative bias in the early morning hours (midnight-5am) and an increasingly large positive bias during the rest of the day peaking at about 7pm.

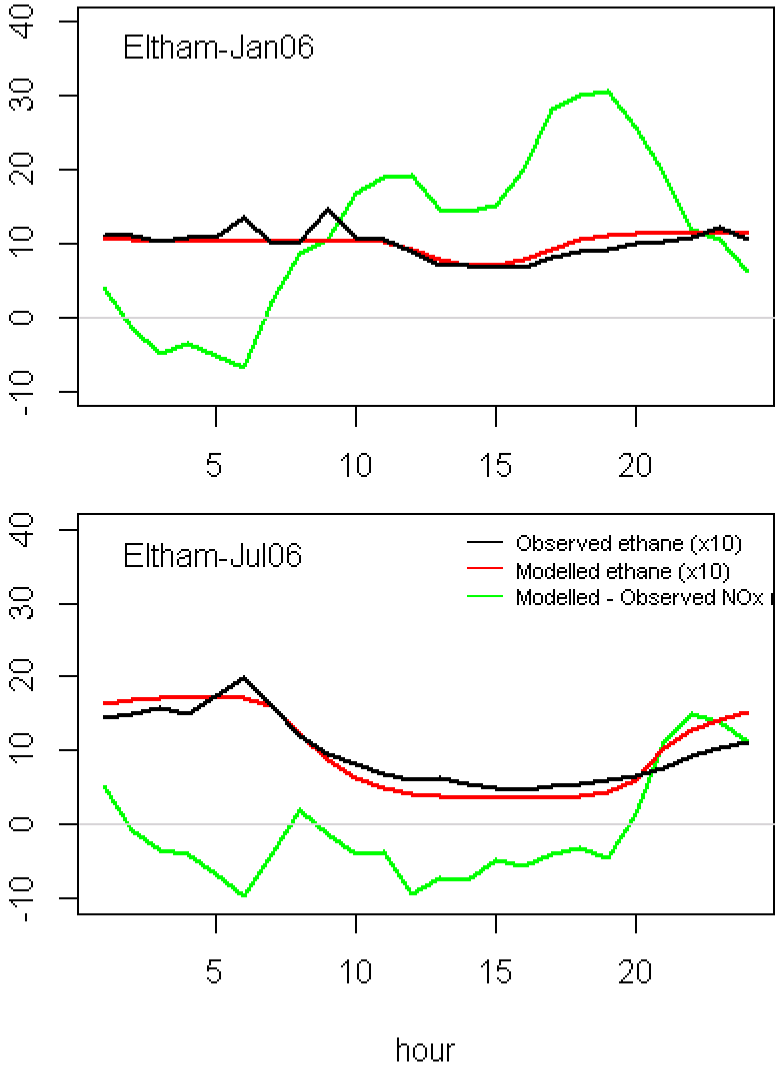


Figure 5 Normalized ethane concentrations at the Eltham measurement site for Jan 2006 (top) and July 2006 (bottom) and the CMAQ PxACM2 constant ethane model. Model – Observed NO_X concentrations (ppb)

To interpret the good agreement between modelled and observed ethane, whilst having a large over prediction of NO_X, would suggests that NO_X emissions have played an important role in the models' positive bias. For example, during the afternoon period (13:00 to 21:00) the overestimation between modelled and observed ethane concentrations is ~14%, yet for NO_X is ~100% and suggests that the emissions for January 2006 are much greater than one would expect.

There is similar good agreement between the modelled and observed ethane during July, with the model slightly over predicting dilution during the late morning and afternoon period and under predicting dilution overnight. The model-observed NO_X concentrations are also in reasonable agreement with the measurements for July, having a small negative bias during the day and a late evening positive bias which seems to be as a consequence of too little dilution in the model during this period rather than an emissions effect.

5. WRF results - cloud and precipitation

The microphysics in WRF parameterises water vapour, cloud water/ice and precipitation, while the cumulus parameterisation is responsible for the sub grid scale effects of convective or shallow clouds and to represent vertical fluxes due to updrafts and downdrafts and compensating motion outside the clouds (Skarmarock, et al., 2008).

A comprehensive test of the sensitivity to different microphysics and cumulus schemes is beyond the scope of this study and so only results from the previously described sensitivity tests are discussed. During all of the tests use was made of the Single-Moment 3-class (WSM 3) microphysics scheme (Hong et al., 2004) and the Kain-Fritsch (KF) cumulus scheme (Kain, 2004).

The monthly mean cloud fractions derived from five PBL simulations have been compared with the NOAA satellite AVHRR derived cloud fractions, from the EUMETSAT (Figure 6). The satellite derived cloud fractions have been expressed as a percent and defined as the fraction of cloudy pixels compared to the total number of pixels in that 15x15 km grid square (Karlsson et al, 2011).

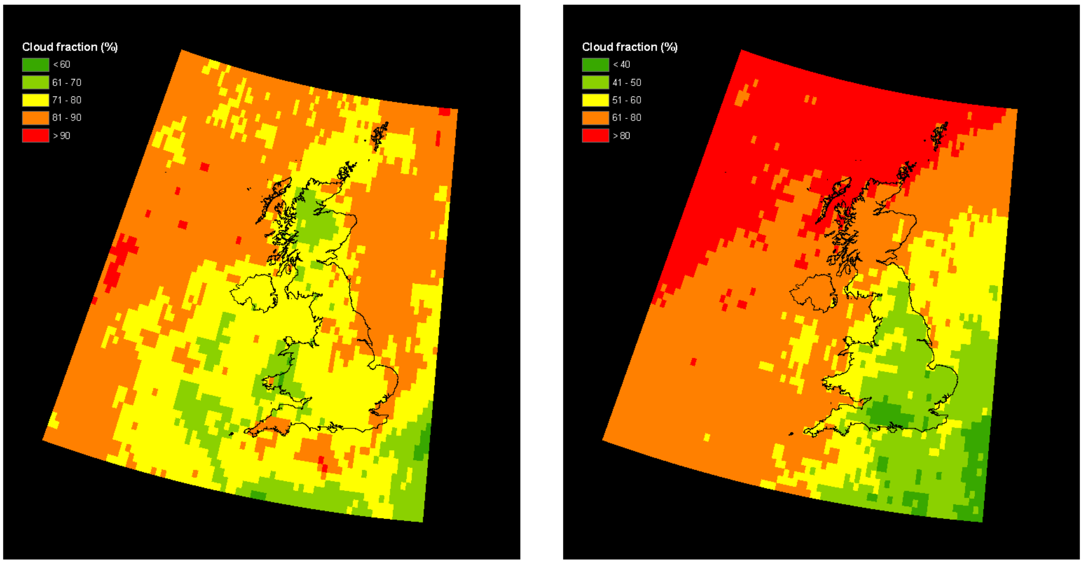
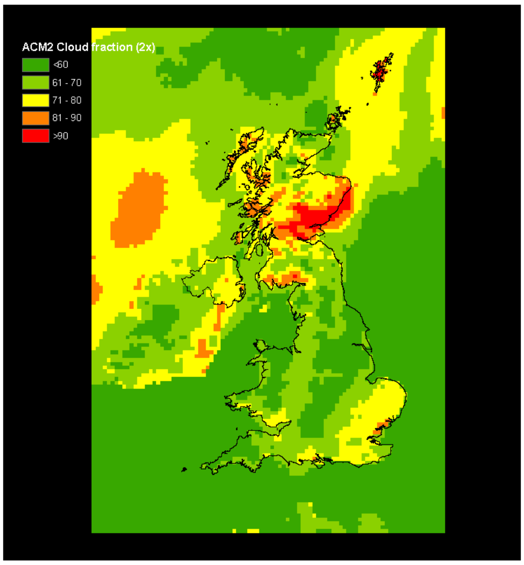


Figure 6 NOAA satellite AVHRR derived monthly mean cloud fractions (%) for Jan and July 2006

The satellite shows large fraction of cloud over the Midlands and coastal areas of the UK in January and a NW-SE gradient for July 2006. By comparison the spatial distribution of modelled cloud



fractions in July (

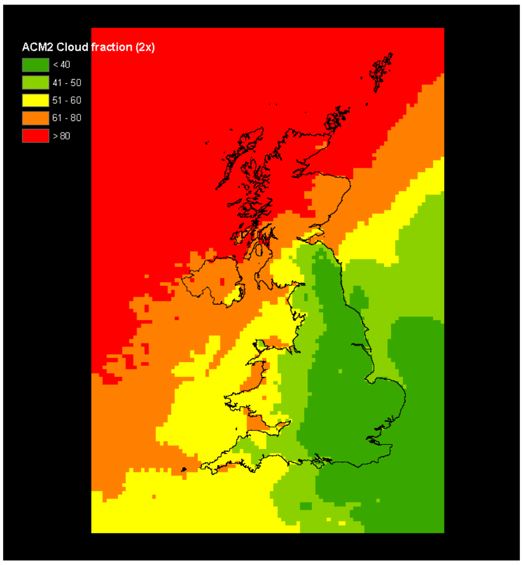


Figure 7) are close to the satellite derived data while larger biases are observed in January.

Comparison between the PBL schemes shows that the between scheme differences are approximately -1 to 3 oktas in January and ±1 okta in July. However, comparison against the surface measurements from UK Met Office shows that all models underestimate observations by approximately 50-60%, with YSU under predicting cloud cover by the largest margin.

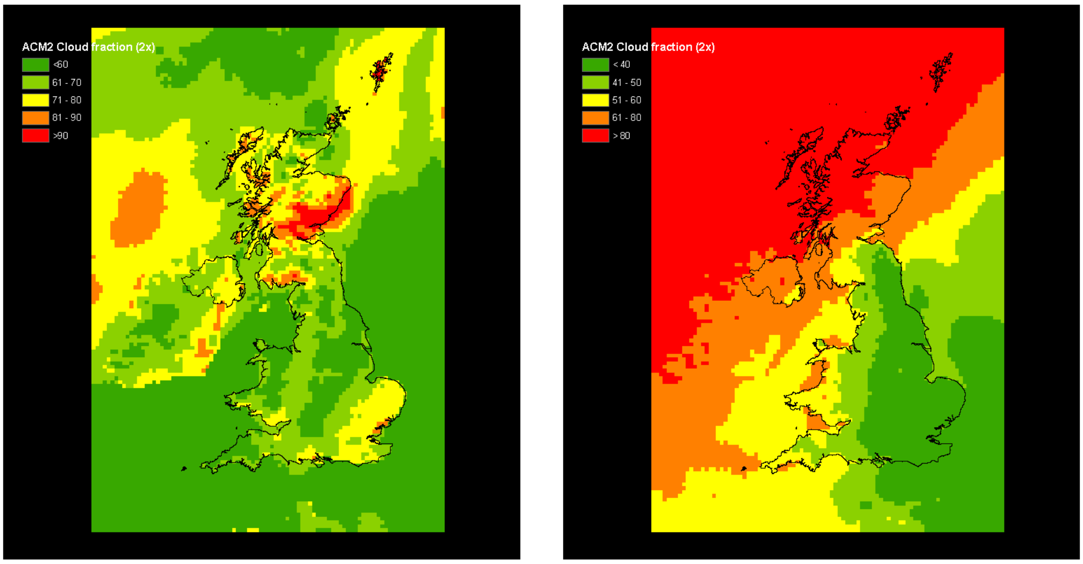


Figure 7 Mapping of monthly means cloud fraction (%) (scaled by factor of 2) from ACM2 PBL simulations for January and July 2006

In addition, the spatial distribution of modelled precipitation has been compared with the UK MO gridded rainfall maps with 5km grid spacing (Figure 8). The monthly total rainfall maps have been interpolated from over 2500 stations using a combination of multiple regression and inverse-distance weighted interpolation. The effects of geographic and topographic factors such as easting and northing, terrain height and shape, and urban and coastal effects were included in the model (Perry and Hollis, 2004).

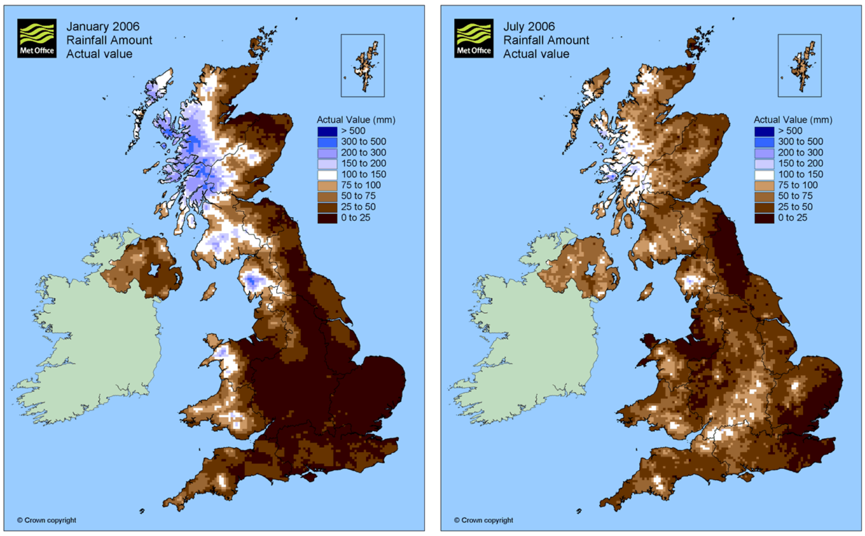


Figure 8 Interpolated rainfall maps (5 km grid resolution) over the UK in January and July 2006 from the UK MO (http://www.metoffice.gov.uk/climate/uk/anomacts/).

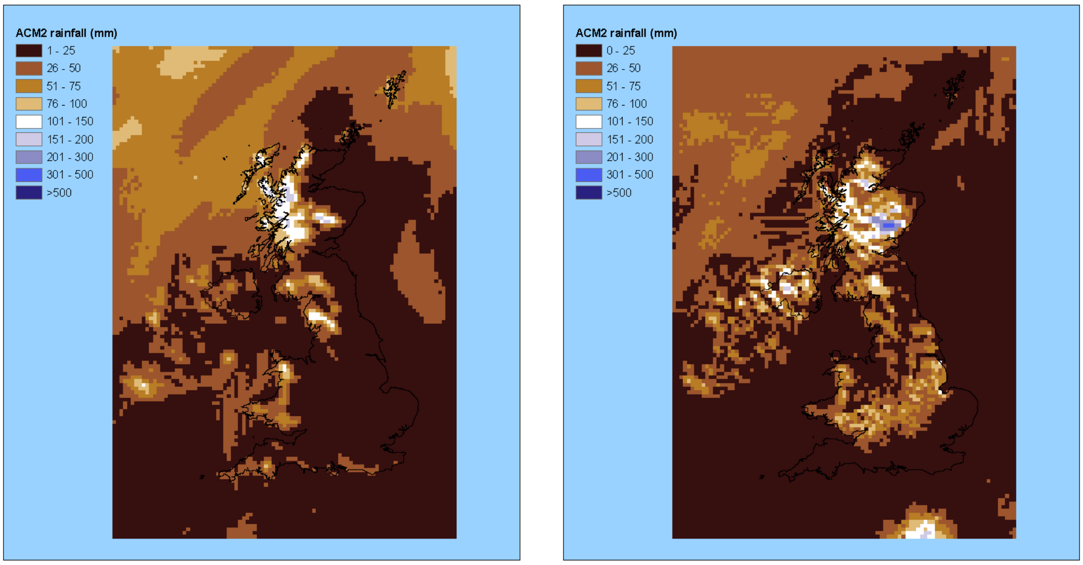
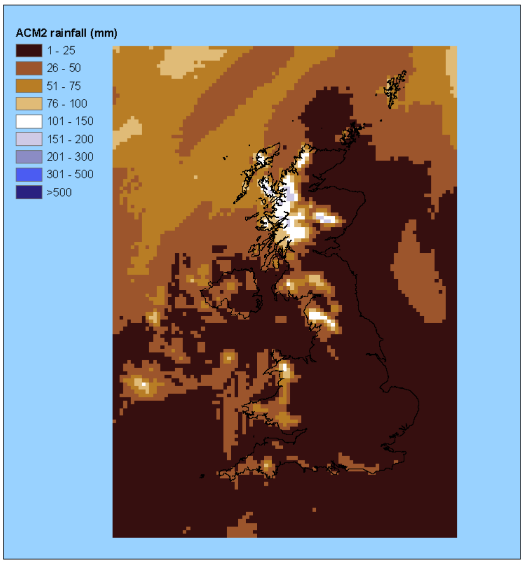


Figure 9 Mapping of total precipitation from ACM2 during January and July 2006



The results from ACM2 in

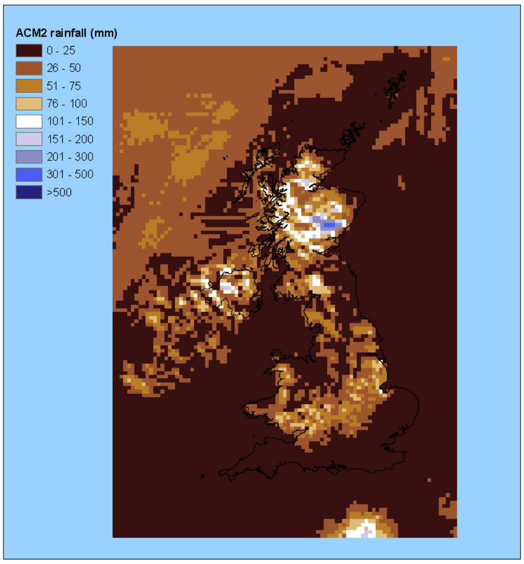


Figure 9 exhibit the observed northwest to southeast gradient in precipitation. In January, the model predicts precipitation in western Scotland and north west England of between 100mm and 300mm and low precipitation in the midlands and the south, where both measurements and model predictions are less than 25mm. In summer, the model replicates the observed spatial patterns of rainfall well, predicting high rainfall rates around western Scotland, the western side of England (especially in Lake District and Snowdonia) and in the midlands, where rainfall varies between 75-200mm.

The between model differences are as high as 80mm at some locations, but within ±20mm across the country as a whole. However all models under predict the rainfall observations by a factor of two in January. In July the models predict the magnitude of the observations well during day but under predict precipitation by ~60% during the night.

6. The sensitivity of WRF to layer structure assumptions

To test the influence on WRF to assumptions regarding vertical layer structure we have included the following sensitivity analysis: (i) The 23 layer phase 1 WRF settings (7 layers below 1.5 km), (ii) l23new (8 layers below 1.5 km), (iii) l27new (12 layers below 1.5 km), (iv) l35 (13 layers below 1.5km), and (v) l35 new (20 layers below 1.5 km). A comparison against observed wind speed, temperature and relative humidity (Table 5), shows that the layer structure has a relatively small influence and is most important for ws10 with a more limited influence on ta2 and rh2. The maximum difference in the between model predictions is ~0.2 m s^{-1} (or 3%) for ws10. The phase 1 WRF settings perform best for ws10 in winter and in summer although the l35new has the best results for ta2 and rh2. However, the largest difference between MB (NMB) from five runs is only -0.1 °C for ta2 and 0.35% for rh2 giving a small performance benefit for a factor of two increase in runtimes.

Table 5 Statistics measures of ws10, ta2, and rh2 results derived from layer stricture sensitivity tests

scenario	PARAM	PERIOD	n	FAC2	MB	NMB	RMSE	r	COE
23org	**ws10**	**JAN**	**115015**	**0.807**	**0.181**	**0.037**	**2.460**	**0.762**	**0.393**
l23new			115015	0.807	0.225	0.046	2.460	0.763	0.391
l35			115015	0.806	0.243	0.049	2.460	0.763	0.390
l35new			115015	0.805	0.336	0.068	2.480	0.763	0.384
l27new			115015	0.805	0.281	0.057	2.490	0.760	0.383
23org	**ws10**	**JUL**	**109732**	**0.779**	**-0.128**	**-0.033**	**1.910**	**0.681**	**0.291**
l35			109732	0.780	-0.085	-0.022	1.910	0.681	0.290
l23new			109732	0.779	-0.097	-0.025	1.910	0.680	0.290
l35new			109732	0.779	-0.003	-0.001	1.920	0.678	0.285
l27new			109732	0.779	-0.029	-0.008	1.920	0.676	0.284
l35new	**ta2**	**JAN**	**114594**	**0.703**	**-0.507**	**-0.112**	**2.14**	**0.818**	**0.363**
l23new			114594	0.697	-0.538	-0.119	2.17	0.814	0.35
l35			114594	0.696	-0.555	-0.122	2.17	0.815	0.35
l27new			114594	0.694	-0.561	-0.124	2.17	0.815	0.349
23org			114594	0.691	-0.561	-0.124	2.2	0.813	0.344
l35new	**ta2**	**JUL**	**110376**	**0.998**	**-0.471**	**-0.027**	**2.24**	**0.885**	**0.534**
l27new			110376	0.998	-0.492	-0.028	2.25	0.884	0.53
l35			110376	0.998	-0.45	-0.026	2.27	0.882	0.524
l23new			110376	0.997	-0.444	-0.025	2.28	0.881	0.522
23org			110376	0.997	-0.371	-0.021	2.32	0.878	0.513
l35new	**rh2**	**JAN**	**111209**	**0.998**	**4.44**	**0.052**	**9.88**	**0.553**	**0.054**
l23new			111209	0.998	4.7	0.055	10.01	0.548	0.039
l35			111209	0.998	4.76	0.056	10	0.552	0.039
l27new			111209	0.998	4.62	0.054	10.02	0.548	0.038
23org			111209	0.998	4.79	0.056	10.05	0.547	0.034
l35new	**rh2**	**JUL**	**108832**	**0.997**	**2.83**	**0.037**	**11.8**	**0.795**	**0.392**
l27new			108832	0.997	2.93	0.038	11.9	0.795	0.388
l35			108832	0.997	2.95	0.039	11.9	0.793	0.386

l23new	108832	0.997	2.86	0.038	12	0.791	0.383
23org	108832	0.997	2.53	0.033	12.1	0.79	0.378

Given that the effect of nudging is influential on the results in Table 5, limiting any differences seen, it is important to compare the results vertically through the atmosphere. Comparison has also shown that the vertical profiles of these variables also remains unchanged between model variants and for clarity are not shown here.

7. The sensitivity of WRF to grid nudging assumptions

In Phase 1 we recommended the use of grid nudging when using WRF, with nudging applied to all model layers every 6 hours, and a nudging coefficient of $3x10^{-4}$ s^{-1} for u and v wind component, temperature (T) and water vapour mixing ratio (Q).

To test the influence of grid nudging assumptions, four differences grid nudging configurations have been compared including: (i) with or without PBL nudging for all parameters, (ii) nudging time intervals of 6h, 72h and 168h, (iii) nudging coefficients for Q of $1x10^{-5}$ s^{-1} c.f. $3x10^{-4}$ s^{-1}, and (iv) only nudging for the first 24 hours of the simulation period.

The ‘with and without PBL nudging’ analysis shows the greatest effect on model performance with nudging u and v, T and Q within the PBL producing better results than ‘without nudging in the PBL’. For ws10, the IOA values are 0.68 (<1% bias) and 0.67 (8% bias) for all layers nudging and without nudging in the PBL, respectively. Similarly for ta2, the IOA values are 0.87 (4% bias) for all layers nudging and 0.84 (10% bias) without PBL nudging and for rh2, the IOA values are 0.65 (10% bias) and 0.58 (12% bias), respectively. In addition, the diurnal trends of ws10, ta2 and rh2 from ‘nudging all layers’ are also better than ‘no nudging in the PBL’ case.

Using a new nudging coefficient for Q of $1x10^{-5}$ s^{-1} introduces insignificant changes to ws10, ta2 and rh2 and for nudging interval sensitivity analysis, the 6h nudging interval delivered the best results when compared with 72h and 168h intervals. Using nudging for the first 24h of the simulation period only, results in model performance which declines after 72 hours. This is demonstrated in Figure 10 for ws10, wind direction and ta2 at Heathrow during July 2006, and significant biases are observed during send half of the month. Overall, there is no substantial improvement WRF performance using the alternative nudging settings tested and therefore the phase 1 recommended settings have been retained.

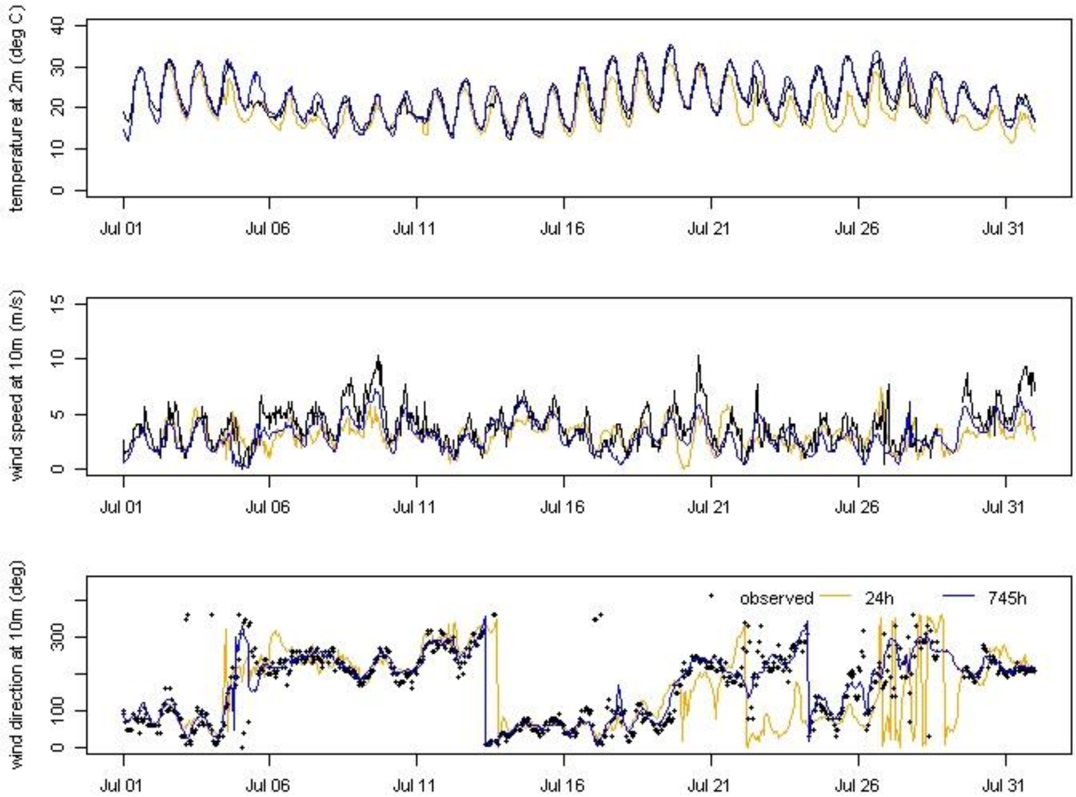


Figure 10 Time series of hourly wind speed, temperature and wind direction in July 2006 period derived from grid nudging sensitivity tests; (i) first 24h (24h) and (ii) throughout the simulation period (745h)

8. Conclusions and discussion

The analysis of results indicate that surface layer and land surface parameterisations are important in predicting Planetary Boundary Layer (PBL) height, friction velocity (u_*), atmospheric stability (z/L), sensible and latent heat flux, wind speed, temperature, relative humidity and ultimately air quality concentrations. Across all of the meteorological parameters considered the ACM2 PBL scheme (with RUC LSM) performed better than the MYNN, YSU and BouLac schemes both in terms of the magnitude of predictions compared with observations and in providing realistic diurnal profiles.

However, in analysing WRF results it has been difficult to reconcile the different PBL predictions with the other model parameters (see Figure 3). Examples include the comparison of z/L values and PBL height which for MYNN 3.4 and ACM2 are the most stable schemes overnight (have low u_* values and similar hfx values) yet provide PBL heights which are in the middle range (200m) of all the schemes tested. The YSU and Boulac schemes have a very small range of ws10 and z/L yet the overnight range of PBL is between 300m (YSU) and ~160m (Boulac), an important difference. Finally, MYNN 3.3.1 provides z/L values that are more neutral during the day than all the schemes tested, are more stable at night than YSU/Boulac and less stable than MYN3.4/ACM2. Likewise MYNN 3.3.1 has intermediate u_* values, the smallest hfx values over night (albeit by a small margin) and some of the highest during the day (similar to ACM2), yet it provides consistently low PBL heights with overnight averages of ~90m, c.f. ~200m for ACM2 and afternoon maximum PBL heights of ~460m c.f. ~700m for ACM2.

One explanation is that a different definition of PBL height is used within each scheme adding to the difficulty in interpreting the prediction of this important parameter and that this in turn limits our ability to interpret PBL height in terms of air quality predictions, as has been found in the DEFRA MIE analysis. Furthermore, some schemes include a lower limit for other parameters, for example a lower limit of 0.1 m s^{-1} is imposed in the MM5 surface layer scheme (used in YSU and BouLac simulations) for u_* (Jemenez, et al., 2012) which adds further difficulty in interpreting the results.

When combined with the CMAQ model ACM2 also improves the predictions of surface NO_2, NO_x and O_3 concentrations, although the over prediction of NO_X during the evening and night time has still not been fully resolved.

It also proved difficult to interpret the NO_X results against observations using the model's turbulence and surface meteorological performance and so an additional diagnostic analysis was undertaken, using vertical mixing intensity (Kz). Interpreting the model's air quality results using Kz has some advantages in that it is a single physical quantity, which has direct relevance to surface air quality concentrations and it is recommended that more extensive investigation of the model's performance using Kz diagnostics be undertaken.

Our ability to separate the relative importance that emissions and dispersion play in predicting surface NO_X concentrations also limits interpretation of the model's performance. In an attempt to remedy this situation we used ethane concentrations as a diagnostic tool. Using ethane improved our ability to split the two important factors in model performance and suggested that for January 2006 the emissions were much greater than one would expect but that in July the late evening positive bias seemed to be as a consequence of too little dilution in the model during this period, rather than an emissions effect. On the basis of these first tests using ethane we would recommend further investigation of ethane as a diagnostic tool, although with the proviso that ethane measurements are currently very limited in the UK.

The analysis of cloud and precipitation observations shows that PBL and surface schemes alter the spatial patterns of cloud cover and rainfall rates. Overall, all models under predict cloud cover by 50-60% when compared with NOAA satellite based cloud fractions and the measurements from the UKMO surface stations. For precipitation, the models are able to capture the diurnal profile of the observations well but under predict the magnitude by factor of two in winter and at night time in summer. To improve the model's performance, further sensitivity analysis would be required to investigate the performance of different microphysics and cumulus schemes within the CMAQ-UK model.

The grid nudging analysis indicated that the phase 1 CMAQ-UK provisional configuration: nudging all model layers every 6h, with a nudging coefficient of $3x10^{-4}$ s^{-1} for u and v wind component, temperature (T) and water vapour mixing ratio (Q), is most suitable for retrospective modelling.

Sensitivity tests of the model using different layer structures showed that using 35 layers (with 20 layers below 1.5 km), compared with the phase 1 recommended 23 layers, showed a slight improvement in some of the surface meteorological fields, but no significant difference in the vertical profiles of the mean variables. However, running WRF with 35 layers increased the CPU run times by factor of two compared and as a consequence provided little benefit over the phase 1 recommended scheme.

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10. Appendix 1 Model vertical layer heights

Table 6 Model full layer heights

layer	zf_23org	zf_l23new	zf_l27new	zf_l35	zf_l35new
1	14.85	14.86	14.85	14.86	14.86
2	52.17	44.69	29.74	44.69	29.75
3	104.69	89.66	59.64	89.64	44.69
4	180.20	149.95	89.65	149.91	59.65
5	302.22	248.72	119.74	225.79	74.64
6	535.01	425.96	149.94	302.24	89.65
7	774.16	701.37	180.23	379.28	104.69
8	**1439.49**	1068.51	241.09	495.96	119.75
9	2534.21	**1448.80**	317.68	614.02	134.83
10	3029.71	1890.52	472.69	733.40	149.94
11	3552.51	2353.60	749.43	854.14	165.07
12	4105.67	2889.74	1068.44	1017.89	180.23
13	4692.82	3457.50	**1448.77**	1184.57	195.41
14	5319.40	4061.45	1890.51	**1440.01**	210.61
15	5993.19	4706.15	2353.60	1702.44	225.84
16	6723.42	5464.36	2889.74	1972.36	241.09
17	7518.95	6293.55	3457.51	2249.96	317.68
18	8393.18	7208.85	4061.46	2535.76	472.71
19	9370.23	8229.41	4706.16	2930.15	749.45
20	10483.33	9390.80	5464.36	3236.95	1068.46
21	11817.47	10873.73	6293.55	3554.15	**1448.80**
22	13507.76	12796.52	7208.84	3882.26	1890.55
23	15811.02	15772.56	8229.40	4337.99	2353.64
24			9390.78	4816.57	2889.79
25			10873.71	5321.25	3457.57
26			12796.50	5856.12	4061.51
27			15772.50	6426.21	4706.21
28				7035.36	5464.41
29				7689.27	6293.59
30				8395.96	7208.87
31				9373.05	8229.42
32				10486.10	9390.79
33				11820.20	10873.73
34				13510.58	12796.53
35				15813.95	15772.51