Comprehensive Analysis of Annual 2005/2008 Simulation of WRF/CMAQ over Southeast of England

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Outline

1. CMAQ modelling system
2. Model domain, physics and chemistry setting
3. Model evaluation framework
4. Results and discussion
5. Summary and future work
CMAQ modelling system at the ERG

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Applications

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Emissions processor for CMAQ

EMEP: 50x50 km²
NAEI and LAEI: 1x1km²

Erna and mobile sources

ERG Emissions Processor and SMOKE
Temporal and speciation profiles

Met Driver

EPER/Point sources
CLC2000/Biogenic sources

Power station – Innogy, Cement non-decarbonising

Layer 1 Hourly NOx Emissions
3 x 3 km, 1 - 14 June 2006

Dover

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WRF/CMAQ model setup

Model Version: WRF V3.0.1 and CMAQ 4.6
WRF Initial and boundary conditions: GFS model (1x1 deg)
CMAQ Initial and boundary conditions: STOCHEM
Radiation Scheme: RRTM scheme
Microphysics: Kain-Fritsch (new Eta) scheme
PBL Scheme: YSU scheme
Surface Scheme: Monin-Obukhov scheme
Land Surface Scheme: Noah scheme
Chemical scheme: CB-05 with aqueous and aerosols chemistry
Emissions: EMEP, NAEI, LAEI, EPER
Study period: 2005 (CMAQ and MET) and 2008 (MET)

2005 is a year with no extreme weather condition
2008 is a wetter year

CMAQ Domain Setting:
- Dom1: 81km grid spacing, 47 x 44 cells
- Dom2: 27km grid spacing, 39x39 cells
- Dom3: 9km grid spacing, 66x108 cells
- Dom4: 3km grid spacing, 72x72 cells
- Dom5: 1km grid spacing, 61x51 cells

Vertical Domain:
- 23 Layers with 7 layers under 800 m above ground

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WRF/CMAQ evaluation framework

**WRF/CMAQ Output**

**Dynamic Evaluation**
- Can the model capture changes related to meteorological events or variations?
- Can the model capture changes related to emission reductions?

**Diagnostic Evaluation**
- Are model errors or biases caused by model inputs or by modeled processes?
- Can we identify the specific modeled process(es) responsible?

**Operation Evaluation**
- How do the model predicted concentrations compare to observed concentration data?
- Are there large temporal or spatial prediction errors or biases?

**Applications**
- Are we getting the right answer?
- Can we capture observed air quality changes?
- Are we getting the right answer for the right (or wrong) reason?

**Probabilistic Evaluation**
- How should uncertainty in model inputs and options be quantified?
- What is the best way to propagate uncertainty through the model?
- What are the best ways to communicate the confidence in the model-predicted values?

Source: ST RAO (USEPA)
AMET and Openair: Model Evaluation Tools

AMET (USEPA): http://www.cmascenter.org/
Openair project (David Carslaw, NERC-funded project): http://www.openair-project.org/
Evaluation of WRF model
Synoptic scale: sea level pressure at 0 UTC, 3 Feb 2005

Low Pressure system

High Pressure system

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Evaluation of WRF model
Synoptic scale: sea level pressure at 0 UTC, 3 Jul 2005

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Vertical profiles of met. at Hermonceux
23 UTC, Jan 2005

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Vertical profiles of met. at Hermonceux
12 UTC, Jan 2005

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Operational evaluations
Meteorological and air quality monitoring networks

26 met sites, 120 air quality monitoring sites
(76 urban background, 24 suburban and 20 rural sites)

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Time series and scatter plots of surface meteorology 2005

Temperature at 2m

Wind Direction at 10m

Wind Speed at 10m

Relative Humidity at 2m

Black = Observed  Red = Modelled  * (-1)

Average of 26 met sites

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Diurnal variations of surface meteorology
Average of 26 sites (2005)

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Horizontal distribution of surface pollutants
2005 annual average of NO$_2$ and O$_3$ concentration

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Time series and scatter plots of NO$_2$ and O$_3$ concentration (2005)
Diurnal error of NO$_2$, NO$_x$ and O$_3$
Average of all sites (2005)

Residual = modelled - observed

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Operational Evaluation
Diurnal error of wind speed at 10m

Residual = modelled - observed
Statistical measures
Met, NO$_2$, NO$_x$ and O$_3$ concentrations (2005)

<table>
<thead>
<tr>
<th>Parameters</th>
<th>IA</th>
<th>CORR</th>
<th>RMSE</th>
<th>NMB</th>
<th>MB</th>
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<tbody>
<tr>
<td>WSPD10</td>
<td>0.73</td>
<td>0.58</td>
<td>2.73</td>
<td>27.4</td>
<td>1.15</td>
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<td>TEMP2</td>
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<td>0.61</td>
<td>11.08</td>
<td>13</td>
<td>2.17</td>
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<td>NO$_x$</td>
<td>0.68</td>
<td>0.52</td>
<td>34.23</td>
<td>-6</td>
<td>-1.77</td>
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<tr>
<td>O$_3$</td>
<td>0.75</td>
<td>0.56</td>
<td>12.4</td>
<td>14</td>
<td>2.84</td>
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UK DEFRA acceptable values (+/- 20%)

IA = Index of Agreement, CORR = correlation coefficient, RMSE = root mean square error, NMB = normalised mean bias, MB = mean bias

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Operational Evaluation
Taylor Diagram: Site representativeness

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Comparison of point measurements and grid models ($\text{NO}_x$) - site representativeness

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Dynamic Evaluation
Surface meteorology prediction of 2005 and 2008

- Statically predict temperature and relative humidity well
- Overpredicts night time wind speed especially in winter

Residual = modelled - observed

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## Dynamic evaluation
Meteorological prediction 2005 vs 2008

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IA = Index of Agreement, CORR = correlation coefficient, RMSE = root mean square error, NMB = normalised mean bias, MB = mean bias
Time series and scatter plots of NO$_2$ and O$_3$

Average of all sites – 2008

**NO$_2$ 2008**

Black = Observed  
Red = Modelled * (-1)

**O$_3$ 2008**
### Statistical measures for NO$_2$ and O$_3$

2005 and 2008

Note! 2005 simulation uses CMAQ 4.6 while 2008 uses CMAQ 4.7
NO$_x$ emissions are also different between 2005 and 2008, hence incomparable

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IA = index of agreement, CORR = correlation coefficient, RMSE = root mean square error, NMB = normalised mean bias, MB = mean bias

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Dynamic evaluation
30% NO\textsubscript{x} and VOC emission reductions (1-14 July 2005)

Percentage changes of O3
\((O3_{\text{nox}}-O3_{\text{base}})\times 100/O3_{\text{base}}\)

July 1, 2005 0:00:00
Min = -3.88 at (48.97), Max = 31.67 at (51.20)

Percentage changes of O3
\((O3_{\text{voc}}-O3_{\text{base}})\times 100/O3_{\text{base}}\)

July 1, 2005 0:00:00
Min = -3.16 at (38.40), Max = 0.07 at (48.98)

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Diagnostic evaluation - 2005
CMAQ NO₂-NOₓ-O₃ chemistry: daytime in winter and summer

Winter

OX = O₃ + NO₂

Summer

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Diagnostic evaluation - 2005
CMAQ NO$_2$-NO$_x$-O$_3$ chemistry:

Observed and modelled daytime local and regional contribution to oxidant at all sites

<table>
<thead>
<tr>
<th>Season</th>
<th>Observed local OX (ppb ppb-1 NO$_x$)</th>
<th>Modelled local OX (ppb ppb-1 NO$_x$)</th>
<th>Observed regional OX (ppb)</th>
<th>Modelled regional OX (ppb)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Winter</td>
<td>0.07</td>
<td>0.06</td>
<td>34.02</td>
<td>39.68</td>
</tr>
<tr>
<td>Spring</td>
<td>0.05</td>
<td>0.03</td>
<td>42.55</td>
<td>42.85</td>
</tr>
<tr>
<td>Summer</td>
<td>0.13</td>
<td>0.01</td>
<td>37.33</td>
<td>42.16</td>
</tr>
<tr>
<td>Autumn</td>
<td>0.09</td>
<td>0.07</td>
<td>33.33</td>
<td>40.05</td>
</tr>
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</table>

**OX = O3 + NO2**

**OX = localOX*NOx + regionalOX**

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Summary of model evaluation

Operational evaluation:
- WRF predicts some bias on vertical profiles of wind speed and relative humidity
- WRF predicts synoptic scale features and surface meteorological conditions well but over-predicts night-time wind speed especially in winter
- CMAQ overestimates night-time O₃ which may be due to over-prediction of wind speed and dilution of NOₓ
- Bias of the model may also be due to site representativeness issue

Dynamic evaluation:
- WRF/CMAQ is able to capture changes of meteorology and emissions

Diagnostic evaluation:
- The model predicts the correlation between NO₂, NOₓ and O₃ well
- This evaluation indicates that the model under-predicts local NOₓ and over-predicts O₃. The reasons may be the same as explained in operational evaluation

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Future Work

- To further investigate and hopefully improve night-time wind speed prediction
- To assess the model performance on PMs prediction
- To develop further model evaluation techniques such as spectral time series analysis to quantify the model performance on temporal and spatial variation
- To resolve site representativeness issues using technique such as spectral time series analysis
- To identify uncertainty of the model through the probabilistic evaluation
Acknowledgement

NCAR, BADC for providing meteorological data,
EEA, DEFRA/AEA for providing emission and air quality monitoring data,
Gary Hayman and Dick Derwent for NMVOC species speciation profiles
Thank you for your attention...