EMEP/MSC-W model performance
for acidifying and eutrophying components,
photo-oxidants and particulate matter in 2014

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This report is a supplement to the EMEP Status Report 1/2016 and presents a more detailed evaluation of the EMEP/MSC-W model. This report is available from the EMEP website (www.emep.int).

The EMEP/MSC-W model is evaluated with respect to acidifying and eutrophying components, photo-oxidants and particulate matter. Model results for 2014 are validated against measurements that have been collected from the EMEP monitoring network for 2014.

Tables of model skill and time series plots are presented for different chemical species at individual EMEP measurement stations, along with scatter-plots and maps covering the EMEP domain.

As in previous evaluation reports, data from some measurement stations have been excluded from this evaluation for either of the following reasons:

- Problems have been identified in regard to the measurements (during Quality Control by EMEP-CCC).

- The measurement site is located in a mountain area, and the difference between its height above sea level and the mean elevation in the respective EMEP/MSC-W model grid cell is larger than 500m.

The agreement between model results and observations depends on a combination of several factors - the measurement accuracy (sampling and analysis), the representativeness of the measurement sites, the adequacy of emissions, and the model performance. Thus, any model underestimation or overestimation in the evaluation presented in the following chapters only implies that the modelled values are different from the observations, but is not necessarily an indication of model deficiency.

Chapter 2 deals with acidifying and eutrophying components (sulphur and nitrogen species), Chapter 3 with photo-oxidants (ozone and nitrogen dioxide), and Chapter 4 with particulate matter.
In this chapter the EMEP/MSC-W model is evaluated with respect to acidifying and eutrophying components. Section 2.1 includes an overview table of the model performance and scatter plots for acidifying and eutrophying components. In Section 2.2 we present time series plots for all EMEP stations with measurements in year 2014, while Section 2.3 contains combined maps of modelled and measured air concentrations and of concentrations in precipitation for selected species in 2014.

2.1 Scatter plots and tables

Evaluations of the EMEP/MSC-W model performance for acidifying and eutrophying components have been presented earlier in numerous EMEP reports (e.g. Gauss et al. 2015, Gauss et al. 2014, Fagerli and Hjellbrekke 2008, Fagerli and Aas 2008).

In addition, an overview study of how the model performance has changed over the years was presented in Chapter 3 of EMEP Status Report 1/2013 (Simpson et al. 2013). The main conclusions of that study were:

- Year-to-year variations in evaluations of model performance can be large when all EMEP measurements available are used. This is mainly caused by the varying number of measurement sites available from year to year. Furthermore, changes in instrumentation, protocols and personnel may influence the quality of measurements.

- Model performance varies strongly among pollutants.

- Model performance is (as expected) generally better for secondary than for primary pollutants;

- A more systematic evaluation is needed, with all inputs and observations held constant while the model version is changed, in order to identify key factors behind changes in model performance (benchmarking);
<table>
<thead>
<tr>
<th>Component</th>
<th>N&lt;sub&gt;stat&lt;/sub&gt;</th>
<th>Obs.</th>
<th>Mod.</th>
<th>Bias (%)</th>
<th>RMSE</th>
<th>Corr.</th>
<th>IOA</th>
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<tr>
<td>NO&lt;sub&gt;2&lt;/sub&gt; (µg(N) m&lt;sup&gt;-3&lt;/sup&gt;)</td>
<td>63</td>
<td>1.76</td>
<td>1.48</td>
<td>-16</td>
<td>0.75</td>
<td>0.84</td>
<td>0.90</td>
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<td>SO&lt;sub&gt;2&lt;/sub&gt; (µg(S) m&lt;sup&gt;-3&lt;/sup&gt;)</td>
<td>53</td>
<td>0.43</td>
<td>0.43</td>
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<td>0.64</td>
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<td>SO&lt;sub&gt;2&lt;/sub&gt;&lt;sup&gt;-&lt;/sup&gt;, sea salt corrected (µg(S) m&lt;sup&gt;-3&lt;/sup&gt;)</td>
<td>20</td>
<td>0.52</td>
<td>0.34</td>
<td>-35</td>
<td>0.26</td>
<td>0.83</td>
<td>0.74</td>
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<tr>
<td>SO&lt;sub&gt;2&lt;/sub&gt;&lt;sup&gt;-&lt;/sup&gt;, including sea salt (µg(S) m&lt;sup&gt;-3&lt;/sup&gt;)</td>
<td>28</td>
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<td>0.38</td>
<td>-35</td>
<td>0.27</td>
<td>0.76</td>
<td>0.72</td>
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<td>0.45</td>
<td>0.38</td>
<td>-17</td>
<td>0.33</td>
<td>0.71</td>
<td>0.81</td>
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<td>NH&lt;sub&gt;4&lt;/sub&gt; (µg(N) m&lt;sup&gt;-3&lt;/sup&gt;)</td>
<td>19</td>
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<td>-4</td>
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<td>0.87</td>
<td>0.93</td>
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<td>NH&lt;sub&gt;3&lt;/sub&gt;+NH&lt;sub&gt;4&lt;/sub&gt; (µg(N) m&lt;sup&gt;-3&lt;/sup&gt;)</td>
<td>30</td>
<td>1.18</td>
<td>1.17</td>
<td>-1</td>
<td>0.49</td>
<td>0.84</td>
<td>0.91</td>
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<tr>
<td>NO&lt;sub&gt;3&lt;/sub&gt; (µg(N) m&lt;sup&gt;-3&lt;/sup&gt;)</td>
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<td>HNO&lt;sub&gt;3&lt;/sub&gt; (µg(N) m&lt;sup&gt;-3&lt;/sup&gt;)</td>
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<td>0.12</td>
<td>0.12</td>
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<td>0.11</td>
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<tr>
<td>NO&lt;sub&gt;3&lt;/sub&gt;+HNO&lt;sub&gt;3&lt;/sub&gt; (µg(N) m&lt;sup&gt;-3&lt;/sup&gt;)</td>
<td>31</td>
<td>0.44</td>
<td>0.48</td>
<td>10</td>
<td>0.14</td>
<td>0.86</td>
<td>0.91</td>
</tr>
<tr>
<td>SO&lt;sub&gt;2&lt;/sub&gt;&lt;sup&gt;-&lt;/sup&gt; wd (µg(S)m&lt;sup&gt;-2&lt;/sup&gt;)</td>
<td>47</td>
<td>10653</td>
<td>8908</td>
<td>-16</td>
<td>125</td>
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<td>0.74</td>
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<td>SO&lt;sub&gt;4&lt;/sub&gt;&lt;sup&gt;-&lt;/sup&gt; cp (µg(S)l&lt;sup&gt;-1&lt;/sup&gt;)</td>
<td>49</td>
<td>0.29</td>
<td>0.24</td>
<td>-18</td>
<td>0.16</td>
<td>0.61</td>
<td>0.76</td>
</tr>
<tr>
<td>NH&lt;sub&gt;3&lt;/sub&gt; wd (µg(N)m&lt;sup&gt;-2&lt;/sup&gt;)</td>
<td>47</td>
<td>12554</td>
<td>14080</td>
<td>12</td>
<td>140</td>
<td>0.75</td>
<td>0.85</td>
</tr>
<tr>
<td>NH&lt;sub&gt;4&lt;/sub&gt; cp (µg(N)l&lt;sup&gt;-1&lt;/sup&gt;)</td>
<td>47</td>
<td>0.33</td>
<td>0.36</td>
<td>9</td>
<td>0.18</td>
<td>0.56</td>
<td>0.75</td>
</tr>
<tr>
<td>NO&lt;sub&gt;3&lt;/sub&gt; wd (µg(N)m&lt;sup&gt;-2&lt;/sup&gt;)</td>
<td>48</td>
<td>10661</td>
<td>10778</td>
<td>1</td>
<td>136</td>
<td>0.70</td>
<td>0.82</td>
</tr>
<tr>
<td>NO&lt;sub&gt;3&lt;/sub&gt; cp (µg(N)l&lt;sup&gt;-1&lt;/sup&gt;)</td>
<td>48</td>
<td>0.26</td>
<td>0.27</td>
<td>4</td>
<td>0.12</td>
<td>0.64</td>
<td>0.79</td>
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<tr>
<td>precipitation (mm)</td>
<td>49</td>
<td>44641</td>
<td>45401</td>
<td>2</td>
<td>258</td>
<td>0.86</td>
<td>0.91</td>
</tr>
</tbody>
</table>

Table 2.1: Comparison of model results and observations for 2014. Annual averages over all EMEP sites with measurements. N<sub>stat</sub> = number of stations, wd=wet deposition, cp= concentration in precipitation, Corr. = spatial correlation coefficient, RMSE = root mean square error, IOA = index of agreement.

This year we present results from EMEP/MSC-W model version rv4.9, which is slightly different from model version rv4.7, which was used for last year’s evaluation (Gauss et al. 2015). Recent changes in the model are described in Simpson et al. (2016). As last year, the meteorological input data are based on data from the ECMWF-IFS model.

Table 2.1 shows for each component the number of stations where measurements were available and data coverage criteria were satisfied (N<sub>stat</sub>), measured yearly average over all stations (Obs), modelled yearly average over all stations (Mod), bias (\(\frac{\text{Mod} - \text{Obs}}{\text{Obs}} \times 100\%\)), correlation between observation and model for station yearly averages (Corr), root mean square error, \(\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (m_i - o_i)^2}\), where \(m_i\) and \(o_i\) are modelled and measured concentration at monitoring station \(i\), and index of agreement (Willmott 1981, 1982). The index of agreement is calculated as follows: \(\text{IOA} = 1 - \frac{\sum_{i=1}^{N\text{stat}} (m_i - o_i)^2}{\sum_{i=1}^{N\text{stat}} (|m_i - \text{Obs}| + |o_i - \text{Obs}|)^2}\). It varies between 0 (theoretical minimum) and 1 (perfect agreement between observed and predicted values) and gives the degree to which model predictions are error free.

The scatter plots in Figures 2.1–2.3 are based on yearly averages of observed data at EMEP stations with measurements in 2014. The lines on the scatter plots display deviations in the scatter of 30% (‘30% line’) and 50% (‘50% line’) relative bias, respectively. Relative bias is defined here as \(\frac{\text{Mod} - \text{Obs}}{0.5 \times (\text{Mod} + \text{Obs})} \times 100\%\), where ‘Mod’ refers to yearly averaged modelled concentrations, while ‘Obs’ refers to yearly averaged measured concentrations.
**Sulphur dioxide in air**

Indeed, SO\textsubscript{2} is, on annual average, unbiased compared to measurements in 2014. In 2012, several modifications to reduce the overestimation during the cold season were implemented (Fagerli et al. 2012). One of these was improved seasonal variation of the emissions implying a 10\% displacement per decade from winter to summer in the model (Simpson et al. 2012) to better account for the fact that nowadays a larger part of emissions is released during the summer time with increasing use of air condition, and more importantly, the growth of telecommunications and computer hardware use.

Figure 2.1(a) shows largest overestimations for SO\textsubscript{2} occurring at stations GB36, IT04, and NO15, and large underestimations at AT05 and many Spanish sites.

**Sulphate in air**

Figures 2.1(b)–2.1(c) show EMEP model results compared to measurements for, respectively, sea salt-corrected sulphate, and sulphate including sea salt. In comparisons with measurements including sea salt, 7\% of modelled sea salt\textsuperscript{1} have been added to modelled sulphate. The modelled and observed sulphate levels are in somewhat better agreement when sea salt sulphate is taken into account. The bias is the same for this year’s evaluation, but the correlation is better for for sea salt corrected sulphate than for sulphate without sea salt (0.83 vs. 0.76).

In 2012 a change in the scheme for the oxidation of SO\textsubscript{2} to SO\textsubscript{4}\textsuperscript{2-} was implemented in the EMEP model (Fagerli et al. 2012, Simpson et al. 2012) resulting in higher oxidation rate and, consequently, less underestimation of sulphate concentrations in air. But the underestimation remains, as visible from the scatter plots.

Time series for sulphate in air are shown in Figures 2.11–2.17.

**Nitrate and nitric acid in air**

Measurements of airborne nitrate are expected to have a rather large uncertainty due to the very different physical characteristics of the compounds making up total nitrate. Whilst nitric acid is a spatially variable volatile gas with fast dry deposition, particulate nitrate dry deposits only slowly and hence concentrations are more determined by long range transport.

In Figure 2.2 we show scatter plots for total nitrate, particulate nitrate and nitric acid in air. Time series for total nitrate in air are shown in Figures 2.18–2.21.

Normally, the results for nitrate aerosol and nitric acid are somewhat worse than for total nitrate, because the monitoring data quality for these components are in general not as good as for total nitrate. The reason for this is that the individual concentrations of nitrate and nitric acid are biased when using the common filter-pack method. This has also been shown in the evaluation of the EMEP model performance for nitrogen compounds using intensive measurement data from two sampling periods, June 2006 and January 2007 (Fagerli and Aas 2008).

In this year’s model results, HNO\textsubscript{3} is overestimated by only 3\%, while NO\textsubscript{3} is overestimated by 11\%. The sum of NO\textsubscript{3}+HNO\textsubscript{3} is slightly overestimated by 10\%. The spatial correlation is best for nitrate aerosol (Corr = 0.81), slightly better for the sum of aerosol and gas (Corr = 0.86) and the lowest for nitric acid (Corr = 0.32). However, one should keep in

\textsuperscript{1}Sea salt is assumed to consist of approximately 7\% sulphate.
Figure 2.1: Scatter plots of model results versus observations of a) sulphur dioxide [$\mu g(S) \text{ m}^{-3}$], b+c) sulphate [$\mu g(S) \text{ m}^{-3}$], d) wet deposition of sulphur [$\mu g(S)\text{m}^{-2}$], and e) precipitation [mm]. For sulphate concentrations, panel (b) shows a comparison of model results to sea salt corrected sulphate measurements, while panel (c) shows model results of sulphate plus 7% sea salt in comparison to non-corrected measurement data.
mind that the stations used in the comparison for the different components are not exactly the same, thus the results are only indicative and not strictly comparable.

Due to changes in the parameterization of sea salt and uptake rates on aerosol surfaces (Simpson et al. 2016), the N\textsubscript{2}O\textsubscript{5} hydrolysis now leads to more HNO\textsubscript{3} (and more NO\textsubscript{3}⁻/total nitrate).

**Ammonia and ammonium aerosol in air**

In order to evaluate the model performance for NH\textsubscript{x} (NH\textsubscript{3}+NH\textsubscript{4}\textsuperscript{+}) properly, ammonia and ammonium should be studied separately. However, the number of measurements for 2014 where the gaseous and particle phase are analyzed both separately and at the same time is limited, e.g. NH\textsubscript{3} measurements are available only from 13 sites (one less than last year).

Normally, individual results for NH\textsubscript{3} and NH\textsubscript{4}\textsuperscript{+} are somewhat worse than for total reduced nitrogen (NH\textsubscript{x}), because the monitoring data quantity and quality for these components are in general not as good as for NH\textsubscript{3}+NH\textsubscript{4}\textsuperscript{+}. The reason for this is that the individual concentrations of ammonia and ammonium are biased when using the common filter-pack method due to the volatile nature of ammonium nitrate. Separation of these gases and particles by a simple
Figure 2.3: Scatter plots of modelled versus observed concentrations of total ammonium+ammonia, aerosol ammonium and ammonia in air [µg(N) m\(^{-3}\)] and wet deposition of reduced nitrogen [µg(N)m\(^{-2}\)].

The aerosol filter is unreliable, and to obtain better quality data it is necessary to use denuders. However, this is a much more demanding method and several sites in the EMEP network are still using the filter-pack method and report the individual concentrations of ammonia and ammonium based on this.

The modelled yearly averages of the concentrations of ammonia, ammonium and the sum of ammonia and ammonium have biases of -17%, -4% and -1%, respectively, compared to the monitoring data. The spatial correlations for NH\(_4^+\) and NH\(_3\)+NH\(_4^+\) are high (0.87 and 0.84), while NH\(_3\) has a lower spatial correlation (Corr=0.71).

The new parameterization of sea salt and uptake rates on aerosol surfaces mentioned above also affects NH\(_4^+\) and NH\(_3\)+NH\(_4^+\) and partly explains the improvement since last year.

Scatter plots for modelled versus measured concentrations for total ammonium+ammonia, aerosol ammonium and ammonia in air in 2014 are presented in Figures 2.3(a), 2.3(b) and 2.3(c), respectively, while time series for NH\(_3\)+NH\(_4^+\) are shown in Figures 2.22–2.25.
Concentrations in precipitation / wet depositions

The ability of the model to predict concentrations in precipitations and wet depositions is limited by the accuracy of the precipitation fields used in the model. The precipitation field pattern is very patchy (e.g. influenced by local topographic effects), and the regional scale model is unable to resolve this sub grid scale distribution. A typical problem arises with small scale showers. In reality precipitation is high in a small area of a given grid, but a large fraction of the grid should remain dry. Within the model, however, this precipitation is averaged out to cover the whole grid at a lower intensity. Thus, even though average precipitation amounts may be simulated well, the model experiences precipitation more often, but in lower amounts than in reality. On a shorter time scale, e.g. on daily basis, this may lead to too high concentrations in precipitation for episodes when it rains only in a small part of the grid square. For a regional scale model it is more sensible to compare the bulk concentrations, i.e. the sum of the wet deposited compounds divided by the sum of precipitation.

The correlation between model and measurements for concentrations in precipitation and wet depositions will to a large extent depend on the model precipitation field.

A scatter plot for modelled versus observed precipitation is shown in Figure 2.1(e). On average, the observed and modelled precipitation is very similar (bias=+2%) and the spatial correlation coefficient is high (0.86). This also contributes to the relatively good model performance in terms of reduced nitrogen in precipitation and sulphur in precipitation (low biases and good correlations).

Scatter plots for modelled versus observed wet depositions of sulphur, oxidized nitrogen and reduced nitrogen are shown in Figures 2.1(d), 2.2(d) and 2.3(d), respectively.

Time series for wet deposition of sulphur, oxidized nitrogen and reduced nitrogen are shown in Figures 2.26–2.31, Figures 2.32–2.37 and Figures 2.38–2.43, respectively.

2.2 Time series

In this section we present time series plots for a selection of stations that have supplied data on acidifying and eutrophying components to EMEP CCC for 2014. The plots show daily model results and measurements, where available. Time series for sulphur dioxide in air are shown in Figures 2.4–2.10, for sulphate in air in Figures 2.11–2.17, for total nitrate in air in Figures 2.18–2.21 and for ammonia+ammonium in air in Figures 2.22–2.25. In addition, time series are shown for wet deposition of sulphur, oxidized nitrogen and reduced nitrogen in Figures 2.26–2.31, Figures 2.32–2.37 and Figures 2.38–2.43, respectively.
Sulphur dioxide in air

Figure 2.4: Comparison of model results and measurements (daily) for SO$_2$ in air [ugS] for stations that have measured SO$_2$ in 2014.
Figure 2.5: Comparison of model results and measurements (daily) for SO$_2$ in air [ugS] for stations that have measured SO$_2$ in 2014.
Figure 2.6: Comparison of model results and measurements (daily) for SO$_2$ in air [ugS] for stations that have measured SO$_2$ in 2014.
Figure 2.7: Comparison of model results and measurements (daily) for SO$_2$ in air [ugS] for stations that have measured SO$_2$ in 2014.
Figure 2.8: Comparison of model results and measurements (daily) for SO$_2$ in air [ugS] for stations that have measured SO$_2$ in 2014.
Figure 2.9: Comparison of model results and measurements (daily) for SO$_2$ in air [ugS] for stations that have measured SO$_2$ in 2014.
Figure 2.10: Comparison of model results and measurements (daily) for SO$_2$ in air [ugS] for stations that have measured SO$_2$ in 2014.
Sulphate in air – sea salt corrected

Figure 2.11: Comparison of model results and measurements (daily) for sea salt corrected sulphate in air [ugS] for stations that have measured sulphate in 2014.
Figure 2.12: Comparison of model results and measurements (daily) for sea salt corrected sulphate in air [ugS] for stations that have measured sulphate in 2014.
Figure 2.13: Comparison of model results and measurements (daily) for sea salt corrected sulphate in air [ugS] for stations that have measured sulphate in 2014.
Sulphate in air – sea salt included

Figure 2.14: Comparison of model results and measurements (daily) for sulphate (including sea salt) in air [µgS] for stations that have measured sulphate in 2014.

Figure 2.14: Comparison of model results and measurements (daily) for sulphate (including sea salt) in air [µgS] for stations that have measured sulphate in 2014.
Figure 2.15: Comparison of model results and measurements (daily) for sulphate (including sea salt) in air [ugS] for stations that have measured sulphate in 2014.
Figure 2.16: Comparison of model results and measurements (daily) for sulphate (including sea salt) in air [ugS] for stations that have measured sulphate in 2014.
Figure 2.17: Comparison of model results and measurements (daily) for sulphate (including sea salt) in air [ugS] for stations that have measured sulphate in 2014.
Figure 2.18: Comparison of model results and measurements (daily) total nitrate concentrations $[\text{µg(N) m}^{-3}]$ for stations that have measured total nitrate in 2014.
Figure 2.19: Comparison of model results and measurements (daily) total nitrate concentrations [µg(N) m$^{-3}$] for stations that have measured total nitrate in 2014.
Figure 2.20: Comparison of model results and measurements (daily) total nitrate concentrations (µg(N) m⁻³) for stations that have measured total nitrate in 2014.
Figure 2.21: Comparison of model results and measurements (daily) total nitrate concentrations $[\mu g(N) \, m^{-3}]$ for stations that have measured total nitrate in 2014.
Ammonia+ammonium in air

Figure 2.22: Comparison of model results and measurements (daily) total ammonium+ammonia concentrations [$\mu$g(N) m$^{-3}$] for stations that have measured total ammonium+ammonia in 2014.
Figure 2.23: Comparison of model results and measurements (daily) total ammonium+ammonia concentrations [µg(N) m⁻³] for stations that have measured total ammonium+ammonia in 2014.
Figure 2.24: Comparison of model results and measurements (daily) total ammonium+ammonia concentrations [µg(N) m$^{-3}$] for stations that have measured total ammonium+ammonia in 2014.
Figure 2.25: Comparison of model results and measurements (daily) total ammonium+ammonia concentrations [$\mu g(N) m^{-3}$] for stations that have measured total ammonium+ammonia in 2014.
Sulphur in precipitation

Figure 2.26: Comparison of model results and measurements (daily) for wet deposition of sulphur [mg(S) l\(^{-1}\)] in 2014.
Figure 2.27: Comparison of model results and measurements (daily) for wet deposition of sulphur [mg(S)\(^{-1}\)] in 2014.
Figure 2.28: Comparison of model results and measurements (daily) for wet deposition of sulphur [mg(S)\textsuperscript{-1}] in 2014.
Figure 2.29: Comparison of model results and measurements (daily) for wet deposition of sulphur [mg(S)\textsuperscript{-1}] in 2014.
Figure 2.30: Comparison of model results and measurements (daily) for wet deposition of sulphur [mg(S)\(^{-1}\)] in 2014.
Figure 2.31: Comparison of model results and measurements (daily) for wet deposition of sulphur [mg(S)l$^{-1}$] in 2014.
Oxidized nitrogen in precipitation

Figure 2.32: Comparison of model results and measurements (daily) for wet deposition of oxidized nitrogen [mg(N)l$^{-1}$] in 2014.
Figure 2.33: Comparison of model results and measurements (daily) for wet deposition of oxidized nitrogen $[\text{mg(N)}l^{-1}]$ in 2014.
Figure 2.34: Comparison of model results and measurements (daily) for wet deposition of oxidized nitrogen [mg(N)/l] in 2014.
Figure 2.35: Comparison of model results and measurements (daily) for wet deposition of oxidized nitrogen [mg(N)l\(^{-1}\)] in 2014.
Figure 2.36: Comparison of model results and measurements (daily) for wet deposition of oxidized nitrogen \([\text{mg(N)l}^{-1}]\) in 2014.

...
Figure 2.37: Comparison of model results and measurements (daily) for wet deposition of oxidized nitrogen [mg(N)l$^{-1}$] in 2014.
Reduced nitrogen in precipitation

Figure 2.38: Comparison of model results and measurements (daily) for wet deposition of reduced nitrogen [mg(N)l$^{-1}$] in 2014.

Figure 2.38: Comparison of model results and measurements (daily) for wet deposition of reduced nitrogen [mg(N)l$^{-1}$] in 2014.
Figure 2.39: Comparison of model results and measurements (daily) for wet deposition of reduced nitrogen [mg(N)l$^{-1}$] in 2014.
Figure 2.40: Comparison of model results and measurements (daily) for wet deposition of reduced nitrogen [mg(N)l$^{-1}$] in 2014.
Figure 2.41: Comparison of model results and measurements (daily) for wet deposition of reduced nitrogen [mg(N)l$^{-1}$] in 2014.
Figure 2.42: Comparison of model results and measurements (daily) for wet deposition of reduced nitrogen [mg(N)l$^{-1}$] in 2014.
Figure 2.43: Comparison of model results and measurements (daily) for wet deposition of reduced nitrogen \([\text{mg(N)}\text{l}^{-1}]\) in 2014.
Figure 2.44: Yearly averaged concentrations of SO$_2$, SO$_4^{2-}$, and SO$_4^{2-}$ sea salt corrected, in air for 2014 [µg(S) m$^{-3}$]. The maps show model results, with observations superimposed by triangles.

2.3 Combined maps of model results and observations

In this section we present maps (Figures 2.44–2.46) showing both modelled and observed concentrations in air and concentrations in precipitation for selected sulphur and nitrogen species. In general, there is good agreement between model results and observations in 2014.
Figure 2.45: Yearly averaged concentrations of oxidized nitrogen (OXN), reduced nitrogen (RDN), ammonium (NH$_4^+$), and total nitrate (TNO$_3^-$), in air for 2014 [$\mu$g(N) m$^{-3}$]. The maps show model results, with observations superimposed by triangles.
Figure 2.46: Yearly wet deposition of oxidized nitrogen (OXN), reduced nitrogen (RDN), oxides of sulphur (SOX), in 2014 [µgN/m² or µgS/m²]. The maps show model results, with observations superimposed by triangles.
CHAPTER 2. SULPHUR AND NITROGEN

References


In this chapter the EMEP/MSC-W model is evaluated with respect to surface ozone concentrations in air. In the following section we present tables of mean values and model performance indicators, and in Sections 3.2 and 3.3 time series are plotted for selected stations to illustrate the performance of the EMEP/MSC-W model for the year 2014 with respect to ozone and NO₂. In Section 3.4 we present maps of ozone for 2014, created by combining measurements and model results.

### 3.1 Tables

Table 3.1 shows for daily maximum ozone and daily mean ozone the number of stations where measurements were available and data coverage criteria were satisfied (N_stat), measured yearly average over all stations (Obs), modelled yearly average over all stations (Mod), bias, correlation between observation and model for station yearly averages, root mean square error, and index of agreement (IOA, as defined in Section 2.1).

The update of the hydrolysis of N₂O₅ (Simpson et al. 2016) is expected to affect ozone performance. Overall, ozone performance is slightly better than last year, but also other factors contribute to model performance, such as the quality of input data, quality of measurements, actual atmospheric conditions, etc.

Model performance for daily maximum ozone is much better than for daily mean ozone, mainly due to the difficulty of reproducing night-time ozone correctly. While the bias in daily mean ozone amounts to +9% it is not biased at all in the case of daily maximum ozone. However, the correlation is slightly lower than last year, and around 0.7 now.

Modelled daily maximum ozone values have been evaluated against measurements from all stations that supply data to EMEP CCC. Table 3.2 summarises these comparisons, and Figures 3.1 to 3.18 show time series plots for selected stations representing the different regions of Europe. To judge model performance, Table 3.2 shows root mean square error (RMSE) and the index of agreement (IOA, defined in Section 2.1).
Similarly to last year (Gauss et al. 2015), the model performance is good for daily maximum ozone. At most of the stations, the index of agreement is between 0.8 and 0.9. In the Nordic countries, correlation and index of agreement have improved at most stations compared to last year, while in Mediterranean countries it has decreased at most stations, although only slightly.

Some more detail is given in the next Section where different regions of the EMEP domain are addressed separately, along with time series plots of model results and observations.
Table 3.2: Comparison of modelled versus observed ozone for year 2014. Concentrations are given as means of daily maximum ozone values [ppb]. Correlation coefficients ($r$), root mean square error (RMSE), and index of agreement (IOA) are included to judge the agreement between model and observations.

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**Mediterranean Countries**

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3.2 Time series for ozone

In this section we present time series plots for a selection of stations that have supplied data on ozone levels to EMEP CCC for 2014. The plots show daily model results and measurements of ozone, where available.

Nordic sites

In addition to the statistics for the Nordic sites listed in Table 3.2, measured and modelled ozone levels are compared for Nordic sites in Figures 3.1–3.3. As seen in the plots the model performs well for ozone, both in terms of levels and seasonality. At the majority of Nordic sites the IOA is between 0.80 and 0.9. Out of the 17 sites, for which data were analyzed both in (Gauss et al. 2015) and this year, the model performance has increased at 9 sites and remained constant at 2 sites, but the magnitude of these changes is very small.

The biases are sometimes positive and sometimes negative with no clear tendency of over- or underestimation. Stations with relatively large (> 3ppb) biases are Nord/Greenland (DK10) and Norra-Kvill (SE32). DK10 is also the only station with an Index of Agreement lower than 0.7.

Eastern European sites

Measured and modelled maximum ozone levels for sites in the Eastern European region are shown in Figures 3.4 to 3.6. These sites are mostly typical continental sites with a clear summer maximum, reflecting local/regional ozone production in summer, and a winter minimum. In general the model performance is rather good, and largely in line with the performance in earlier years (Gauss et al. 2015, 2014).

Out of the 19 sites, for which data were analyzed both in (Gauss et al. 2015) and this year, the model performance, in terms of the index of agreement, has increased at 8 sites, decreased at 8 sites and remained unchanged at 3 sites. The index of agreement is larger than 0.8 at most stations, and below 0.7 only at one station (PL03, 0.68).

Relatively large biases (> 3ppb) are seen at CZ05, CZ07, LT15, LV10, PL03, and SK02, i.e. almost the same stations as last year.
Figure 3.1: Modelled versus Observed Daily Maximum Ozone [ppb] at Swedish sites for 2014. *Note that in some plots the vertical axis does not start at zero.*
Figure 3.2: Modelled versus Observed Daily Maximum Ozone [ppb] at Swedish and Danish sites for 2014. Note that in some plots the vertical axis does not start at zero.
Figure 3.3: Modelled versus Observed Daily Maximum Ozone [ppb] at Norwegian sites for 2014. Note that in some plots the vertical axis does not start at zero.
Figure 3.4: Modelled versus Observed Daily Maximum Ozone [ppb] at Eastern European sites for 2014. Note that in some plots the vertical axis does not start at zero.
Figure 3.5: Modelled versus Observed Daily Maximum Ozone [ppb] at Eastern European sites for 2014. Note that in some plots the vertical axis does not start at zero.
Figure 3.6: Modelled versus Observed Daily Maximum Ozone [ppb] at Eastern European sites for 2014. Note that in some plots the vertical axis does not start at zero.
Central and Northwestern European sites

Measured and modelled maximum ozone levels for selected sites in Central and Northwestern Europe are shown in Figures 3.7–3.15. These sites are mainly typical continental sites with a clear summer maximum, reflecting local/regional ozone production in summer, and a winter minimum. Concentrations at the site Mace Head in Ireland (IE31) are partly used to specify background conditions for the EMEP model, so that good performance, at least for the seasonal cycle, is guaranteed.

The overall model performance is very good in this area with many correlations better than 0.8 and small biases, and the index of agreement is better than last year (Gauss et al. 2015) at a majority of stations.

As usual, the comparison between model and observation has problems in mountainous areas, most notably at Jungfraujoch (CH01), Sonnblick (AT34), Le Casset (FR16), Pic du Midi (FR19), and Puy de Dome (FR30). These are also the only stations (except GB37) with IOA lower than 0.7. Relatively large biases (> 3ppb) biases are found mainly in the Alps, but also at BE01, DE01, FR30, GB06, GB37, and GB38.

Mediterranean sites

Measured and modelled ozone levels for selected sites in the Mediterranean region are shown in Figures 3.16–3.18. The meteorological situation in and around the Mediterranean basin differs considerably from the rest of Europe. This region also receives more solar radiation resulting in conditions favourable for ozone production. Hence these sites have some of the highest ozone levels in Europe.

In general the model performance is good for most sites in this region, with IOA values between 0.71 and 0.90.

Exception with IOA below 0.7 are CY02, ES11, GR02, and SI32 (which has also a large negative bias).

In general, the biases in this region tend to be higher than in other regions (e.g. Ayia Marina, Finokalia, and Krvavec), although the correlation is satisfactory (around 0.7 or higher) even at those stations.
Figure 3.7: Modelled versus Observed Daily Maximum Ozone [ppb] at Austrian sites for 2014. Note that in some plots the vertical axis does not start at zero.
Figure 3.8: Modelled versus Observed Daily Maximum Ozone [ppb] at Austrian sites for 2014.
Figure 3.9: Modelled versus Observed Daily Maximum Ozone [ppb] at sites in Belgium and Switzerland for 2014. Note that in some plots the vertical axis does not start at zero.
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Figure 3.10: Modelled versus Observed Daily Maximum Ozone [ppb] at sites in Germany and France for 2014. Note that in some plots the vertical axis does not start at zero.
Figure 3.11: Modelled versus Observed Daily Maximum Ozone [ppb] at French sites for 2014. Note that in some plots the vertical axis does not start at zero.
Figure 3.12: Modelled versus Observed Daily Maximum Ozone [ppb] at French and British sites for 2014. Note that in some plots the vertical axis does not start at zero.
Figure 3.13: Modelled versus Observed Daily Maximum Ozone [ppb] at British sites for 2014. Note that in some plots the vertical axis does not start at zero.
Figure 3.14: Modelled versus Observed Daily Maximum Ozone [ppb] at British sites for 2014. *Note that in some plots the vertical axis does not start at zero.*
Figure 3.15: Modelled versus Observed Daily Maximum Ozone [ppb] at Irish and Dutch sites for 2014. 
Note that in some plots the vertical axis does not start at zero.
Figure 3.16: Modelled versus Observed Daily Maximum Ozone [ppb] at Mediterranean sites (Cyprus and Spain) for 2014. Note that in some plots the vertical axis does not start at zero.
Figure 3.17: Modelled versus Observed Daily Maximum Ozone [ppb] at Mediterranean Sites (Spain and Greece) for 2014. Note that in some plots the vertical axis does not start at zero.
Figure 3.18: Modelled versus Observed Daily Maximum Ozone [ppb] at Mediterranean Sites for 2014.
3.3 Time series for nitrogen dioxide

In this section we present time series plots for a selection of stations that have supplied data on NO$_2$ levels to EMEP CCC for 2014. The plots show daily model results and measurements of NO$_2$, where available. The plots are arranged in alphabetical order by country code.
Figure 3.20: Modelled versus Observed Daily Mean NO$_2$ (µg(N) m$^{-3}$) for 2014.
Figure 3.21: Modelled versus Observed Daily Mean NO\(_2\) (\(\mu g(N)\) m\(^{-3}\)) for 2014.
Figure 3.22: Modelled versus Observed Daily Mean NO$_2$ (µg(N) m$^{-3}$) for 2014.
Figure 3.23: Modelled versus Observed Daily Mean NO₂ (µg(N) m⁻³) for 2014.
Figure 3.24: Modelled versus Observed Daily Mean NO$_2$ (µg(N) m$^{-3}$) for 2014.
Figure 3.25: Modelled versus Observed Daily Mean NO$_2$ ($\mu$g(N) m$^{-3}$) for 2014.
Figure 3.26: Modelled versus Observed Daily Mean NO$_2$ ($\mu$g(N) m$^{-3}$) for 2014.
Figure 3.27: Modelled versus Observed Daily Mean NO$_2$ ($\mu$g(N) m$^{-3}$) for 2014.
Figure 3.28: Modelled versus Observed Daily Mean NO$_2$ (µg(N) m$^{-3}$) for 2014.
Figure 3.29: SOMO35 (ppb.days) and yearly averaged daily maximum ozone (ppb). The maps show model results, with observations superimposed by triangles.

3.4 Combined maps of model results and observations

In Figure 3.29, maps of modeled SOMO35 and maximum daily ozone are shown. Observations, taken from the EMEP network for 2014, are super-imposed with triangles. By and large, the plots show good agreement between model and observations also for this year.
References


This chapter presents an evaluation of the EMEP/MSC-W model performance in terms of particulate matter. Tables of model skill are presented for the entire EMEP domain and timeseries plots are shown for a large number of individual EMEP measurement stations.

4.1 Tables

Table 4.1 shows for PM and individual components the number of stations where measurements were available and data coverage criteria were satisfied ($N_{stat}$), measured yearly average over all stations (Obs), modelled yearly average over all stations (Mod), bias, correlation between observation and model for station yearly averages, root mean square error, and index of agreement (IOA, as defined in Section 2.1).

On average, the model underestimates annual mean measured PM$_{10}$ by 24% and PM$_{2.5}$ by 13% for 2014. The annual spatial correlations between model results and measurements are 0.74 for PM$_{10}$ and 0.77 for PM$_{2.5}$. The slightly worse model performance in terms of bias and IOA for PM$_{10}$ than for PM$_{2.5}$ is likely due to existing uncertainties in modelling natural PM components, e.g. windblown mineral dust, causing also inaccuracy in coarse NO$_3^-$. In addition, there are yet unaccounted components to PM$_{10}$ (biogenic organic aerosol, agricultural dust). Na$^+$ is also largely underestimated, which partly explains why PM$_{10}$ performance is worse than PM$_{2.5}$ performance.

On an annual basis, the model shows quite variable performance for the individual aerosol components, and also when compared with measurements obtained with different sampling methods (e.g. filter-packs/denuders and high/low volume samples). Calculated SO$_4^-$ is underestimated by around 30% compared to observations. The model overestimates total NO$_3^-$ by 11% and NO$_5^-$ in PM$_{2.5}$ by 19%.

NH$_4^+$ is quite reasonably reproduced by the model, being biased by -4% against total ammonium data (e.g. sampling without size cut-off) and only 2% bias for NH$_4^+$ in PM$_{10}$.

Modelled elemental carbon (EC) in PM$_{2.5}$ is underestimated by 41% on the annual basis,
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<th>(N_{\text{stat}})</th>
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<th>Mod.</th>
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<td>4.89</td>
<td>0.74</td>
<td>0.74</td>
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<td>(\text{PM}_{2.5}) ((\mu g m^{-3}))</td>
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<td>9.47</td>
<td>8.26</td>
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<td>2.92</td>
<td>0.77</td>
<td>0.84</td>
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<td>(\text{SO}_2^{2-}), including sea salt ((\mu g m^{-3}))</td>
<td>28</td>
<td>1.74</td>
<td>1.27</td>
<td>-27</td>
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<td>0.80</td>
<td>0.76</td>
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<td>(\text{SO}_2^{2-}), sea salt corrected ((\mu g m^{-3}))</td>
<td>20</td>
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<td>0.83</td>
<td>0.74</td>
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<td>0.64</td>
<td>0.76</td>
</tr>
<tr>
<td>(\text{OC}) in (\text{PM}_{2.5}) ((\mu g(C) m^{-3})) ⋆</td>
<td>10</td>
<td>2.37</td>
<td>1.07</td>
<td>-55</td>
<td>1.38</td>
<td>0.90</td>
<td>0.53</td>
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<tr>
<td>(\text{Na}^+) ((\mu g m^{-3}))</td>
<td>22</td>
<td>0.69</td>
<td>0.73</td>
<td>5</td>
<td>0.62</td>
<td>0.71</td>
<td>0.83</td>
</tr>
<tr>
<td>(\text{Na}^+) in (\text{PM}_{10}) ((\mu g m^{-3}))</td>
<td>6</td>
<td>0.69</td>
<td>0.20</td>
<td>-71</td>
<td>0.86</td>
<td>0.93</td>
<td>0.45</td>
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</table>

Table 4.1: Comparison of model results and observations for 2014. Annual averages over all EMEP sites with measurements. \(N_{\text{stat}}\) = number of stations, \(wd=\text{wet deposition}\), \(cp=\text{concentration in precipitation}\), Corr. = spatial correlation coefficient, RMSE = root mean square error, IOA = index of agreement. The components marked with ⋆, are relieved of the requirement on 75% common days due to smaller data coverage.

while organic carbon (OC) is underestimated by 52%. However, it has to be noted that these scores are based on only 3 stations.

Tables 4.2 and 4.3 show model performance for \(\text{PM}_{10}\) and \(\text{PM}_{2.5}\) at individual stations, revealing large variability in the model ability to reproduce the observed concentrations in different locations. For most of the sites, the bias vary between -45 and 30 % for \(\text{PM}_{10}\) and between -35 and 30 % for \(\text{PM}_{2.5}\). The temporal correlation is clearly better for \(\text{PM}_{2.5}\), with correlation coefficients ranging mostly between 0.5 and 0.8, whereas they vary between 0.4 and 0.7 for \(\text{PM}_{10}\).

### 4.2 Time series

In this section we present time series plots for a selection of stations that have supplied data on particulate matter to EMEP CCC for 2014.

A comprehensive discussion of model performance at individual stations is not given here, but for reference, the time series plots are shown for different temporal resolutions:

- Figures 4.1–4.4: \(\text{PM}_{2.5}\) daily measurements
- Figures 4.5–4.10: \(\text{PM}_{10}\) daily measurements
- Figures 4.11–4.12: \(\text{PM}_{2.5}\) hourly measurements
- Figures 4.13–4.15: \(\text{PM}_{10}\) hourly measurements
- Figures 4.16: \(\text{PM}_{2.5}\) weekly measurements
- Figures 4.17: \(\text{PM}_{10}\) weekly measurements
### Table 4.2: Statistical analysis of model calculated PM$_{10}$ against daily observations in 2014.

Obs: measured mean, Mod: calculated mean, Bias: calculated as (Mod-Obs)/Obs $\times 100\%$, R: temporal correlation coefficient, and RMSE: Root mean Square Error.

<table>
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<tr>
<th>Site</th>
<th>Name</th>
<th>Obs</th>
<th>Mod</th>
<th>Bias</th>
<th>R</th>
<th>RMSE</th>
<th>IOA</th>
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</table>
Table 4.3: Statistical analysis of model calculated PM$_{2.5}$ against daily observations in 2014. Obs: measured mean, Mod: calculated mean, Bias: calculated as (Mod-Obs)/Obs x100%, R: temporal correlation coefficient, and RMSE: Root mean Square Error.

<table>
<thead>
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<th>Name</th>
<th>Obs</th>
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<th>Bias</th>
<th>R</th>
<th>RMSE</th>
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</tr>
<tr>
<td>SI08</td>
<td>Iskrba</td>
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<td>7.61</td>
<td>-18.0</td>
<td>0.55</td>
<td>5.70</td>
<td>0.71</td>
</tr>
</tbody>
</table>
Figure 4.1: Modelled versus Observed Daily PM$_{2.5}$ [µg m$^{-3}$] in 2014.
Figure 4.2: Modelled versus Observed Daily PM$_{2.5}$ [$\mu$g m$^{-3}$] in 2014.
Figure 4.3: Modelled versus Observed Daily PM$_{2.5}$ [µg m$^{-3}$] in 2014.
Figure 4.4: Modelled versus Observed Daily PM$_{2.5}$ [$\mu g \text{ m}^{-3}$] in 2014.
Figure 4.5: Modelled versus Observed Daily PM$_{10}$ [$\mu$g m$^{-3}$] in 2014.
Figure 4.6: Modelled versus Observed Daily PM$_{10}$ [µg m$^{-3}$] in 2014.
Figure 4.7: Modelled versus Observed Daily PM$_{10}$ [µg m$^{-3}$] in 2014.
Figure 4.8: Modelled versus Observed Daily PM$_{10}$ [µg m$^{-3}$] in 2014.
Figure 4.9: Modelled versus Observed Daily PM$_{10}$ [µg m$^{-3}$] in 2014.
Figure 4.10: Modelled versus Observed Daily PM$_{10}$ [μg m$^{-3}$] in 2014.
Figure 4.11: Modelled versus Observed Hourly PM$_{2.5}$ [$\mu$g m$^{-3}$] in 2014. Note that in some plots the vertical axis does not start at zero.
Figure 4.12: Modelled versus Observed Hourly PM$_{2.5}$ [µg m$^{-3}$] in 2014. Note that in some plots the vertical axis does not start at zero.
Figure 4.13: Modelled versus Observed Hourly PM$_{10}$ [µg m$^{-3}$] in 2014. Note that in some plots the vertical axis does not start at zero.
Figure 4.14: Modelled versus Observed Hourly PM$_{10}$ [$\mu$g m$^{-3}$] in 2014. Note that in some plots the vertical axis does not start at zero.
Figure 4.15: Modelled versus Observed Hourly PM$_{10}$ [$\mu g m^{-3}$] in 2014. Note that in some plots the vertical axis does not start at zero.
Figure 4.16: Modelled versus Observed Weekly PM$_{2.5}$ [$\mu$g m$^{-3}$] in 2014. Note that in some plots the vertical axis does not start at zero.
Figure 4.17: Modelled versus Observed Weekly PM$_{10}$ [µg m$^{-3}$] in 2014. Note that in some plots the vertical axis does not start at zero.
4.3 Combined maps of model results and observations

Combined maps of model results and observations have been produced for nitrogen- and sulphur-containing aerosols only. For details, see Section 2.3 in the chapter on acidifying and eutrophying components.