Validation of LOTOS-EUROS v1.6 against v1.3

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Contents

Versions

- v1.3 +patches 1-10
- v1.6.0

Emission files:
-gems_emissions_13_05_2007.txt
-shipping_rap.txt

Landuse: landuse_tree.txt(v1.3) , landuse_tree.nc (v1.6) (these contain identical information)

Logan boundary conditions
ECMWF meteo
Test period 1-1-2003 00h to 31-12-2003 21h
Basic grid 0.25 lonx0.5 lat 10 E-40W, 35 N-70N

Compilation with optimization.

Functional differences between the versions:
-changes in reaction constants of CBM-IV scheme.
-effect of sea salt added for heterogeneous reaction N_2O_5
-no horizontal diffusion in v1.6
-new emissions grass and crops in v1.6
-rc_gas: statement vpd=0 removed
-output total PM10: sodium converted to sea salt (factor 3.26).

Other differences:
-lerc files not used anymore, only rc files
-parallellisation possible. Cannot be run with isorropia SIA module, needs equisam or mars_modified.
-units of output have changed from ppb to mole mole-1 for gases
-units of output have changed from µg m-3 to kg m-3

There are additional changes for specific purposes. These are not discussed here and are not considered part of the basic LOTOS-EUROS version (bias correction, station output, RACMO coupling, kalman filtering etc).

Timing

The timing is only indicative, runs were done on two different systems (azoren system is about 1/3 faster than linuxma system). Taking this into account, the run time of the two versions is comparable.
v1.3: start time: Jan 25 15h43 end time Jan 30 12.45 (linuxma system)
v1.6: start time: Mar 19 11h22 end time Mar 22 11.17 (azoren system)

Results

The annual mean concentrations are compared, as well as time series on selected EMEP stations. Two episodes are highlighted for illustration: at the end of May 2003 high ozone values were observed in the Netherlands, in March several episodes with high PM concentrations occurred.

Gases

The annual mean concentration of the most important gases over 2003 (Fig 1) show the main emission areas (NO, NO_2, SO_2, NH_3) except for ozone where it mainly illustrates the difference in deposition (land-sea contrast) and titration in areas of high NOx concentrations. The changes all have an effect on the concentrations, in the present set-up they are not treated separately. The changes in chemistry clearly have an impact on the annual mean concentrations (Fig. 2). Setting the horizontal diffusion equal to 0 results in sharper peaks and in timing differences (Fig 3, especially SO_2) but also the change in chemistry plays a role. Table 1 indicates the statistics from a comparison of ozone daily maxima with EMEP observations. Also the emissions of grass and crops contribute to the changes, but their effect was found to be small. The middle section contains scatter plots which indicate the performance for the two model versions for the different components.

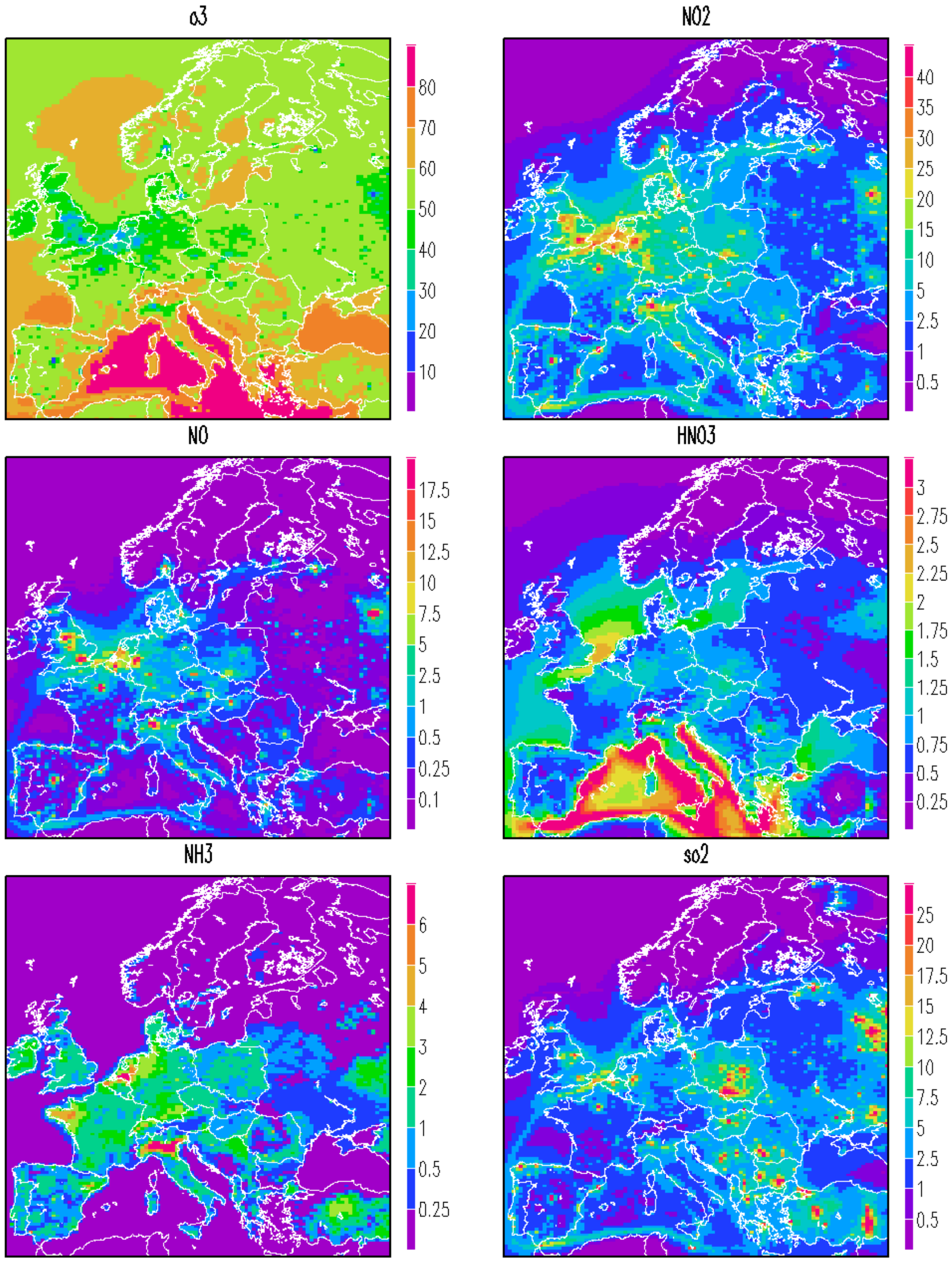


Figure 1: Annual mean concentrations of gases in 2003, v1.6 in ppb

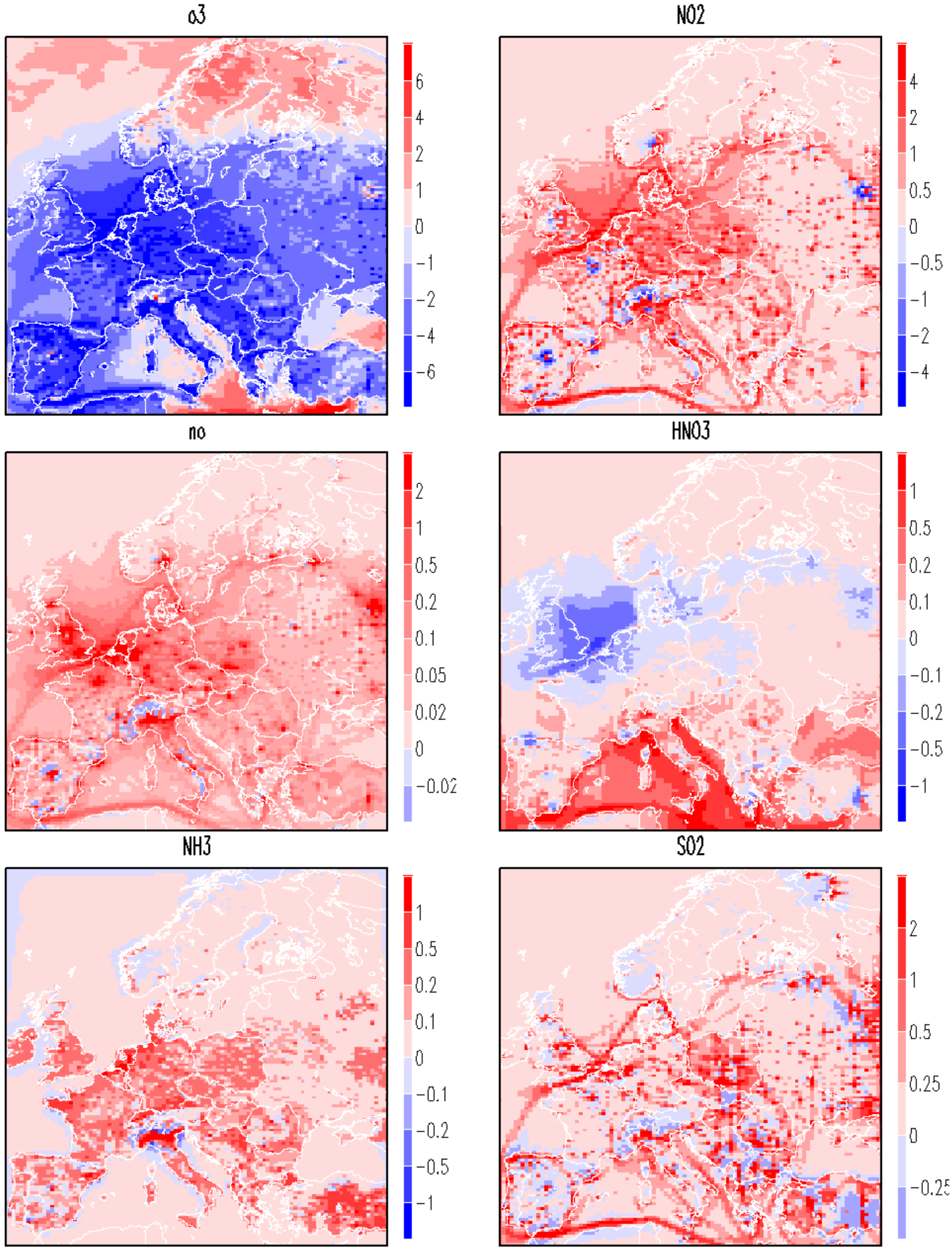


Figure 2: Difference in annual mean concentrations of gases in 2003, v1.6-v1.3 in ppb

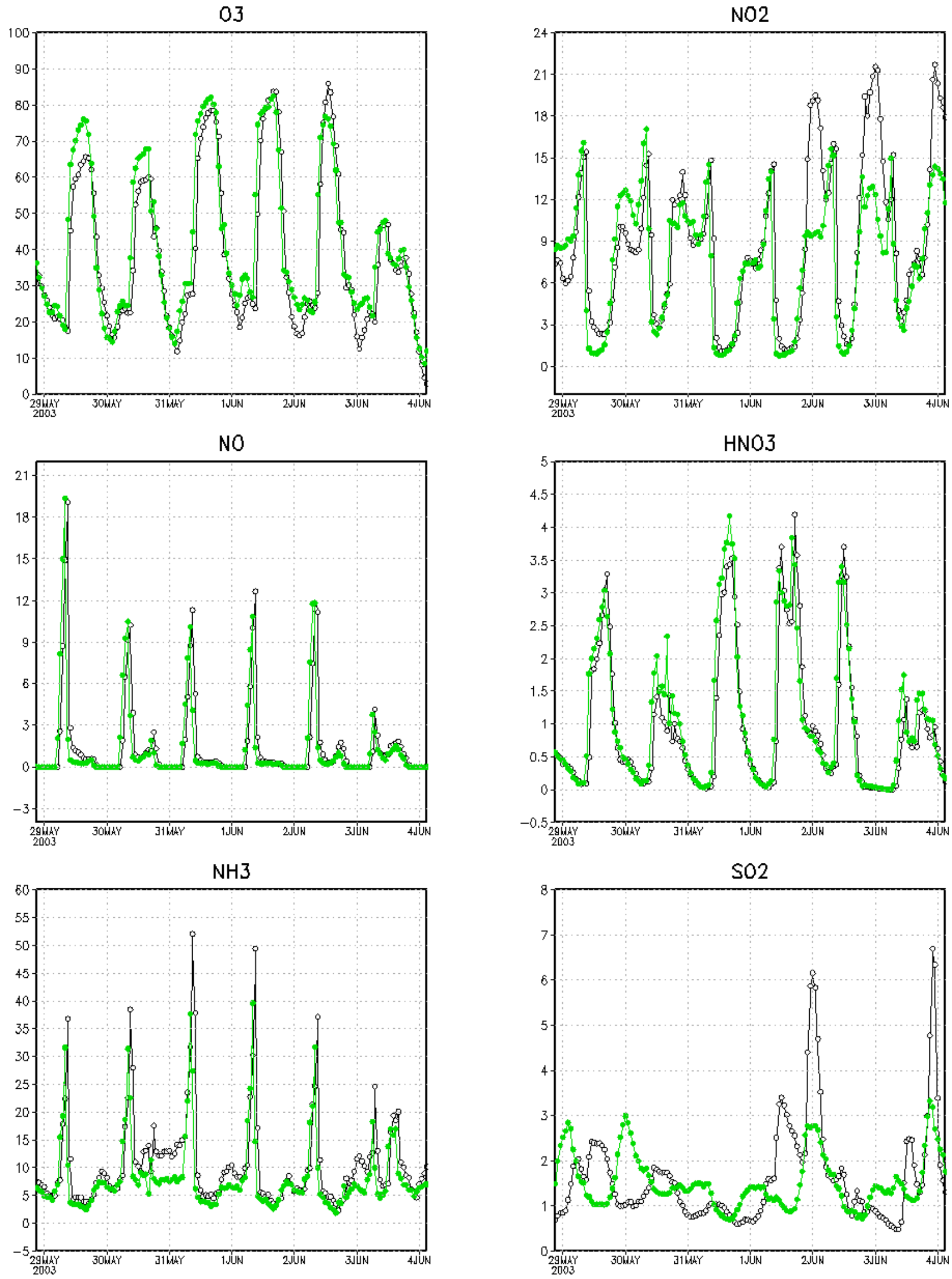


Fig. 3 Time series of v1.3 (green) and v1.6 (black) during a ozone smog episode at Vredepeel. Units: ppb

Table 1 Validation of ozone results with EMEP stations: ozone daily maximum

station	mean	mean	rmse	correl	mean	rmse	correl
	obs	v1.3			v1.6		
NL09	71.34	73.46	18.75	0.83	68.99	16.21	0.84
NL10	73.59	71.09	21.11	0.86	64.70	21.71	0.87
AT41	101.51	84.03	27.99	0.82	77.75	31.94	0.83
BE35	85.62	74.87	21.28	0.89	68.81	25.36	0.89
DE02	88.89	76.08	22.49	0.89	71.71	25.92	0.89
DE35	93.28	80.37	22.73	0.88	74.15	27.03	0.88
DK05	78.75	77.78	17.32	0.86	73.45	16.50	0.84
ES12	100.1	89.06	20.82	0.75	86.02	20.98	0.81
FR10	95.7	79.67	23.91	0.82	76.88	25.57	0.83
IT01	108.96	97.12	29.82	0.86	92.60	27.86	0.89
PL02	84.13	75.55	18.92	0.84	71.76	20.95	0.84
SK04	94.36	82.87	21.5	0.76	79.07	23.27	0.75

Aerosols

Figure 4 displays the annual mean concentrations of several aerosol components. The bottom right plot shows the total PM10 which is the sum over SO_4, NH_4, NO_3, PPM2.5, PPM10, SS(=3.26*Na) and BC. Figure 5 shows the differences between v1.3 and v1.6 per component. Figure 6 illustrates the time series at Vredepeel during a smog episode.

Like for the gases, differences arise because of the changes in chemistry (secondary aerosols) and the change in the horizontal diffusion (inert species like primary PM2.5)

PM10 is underestimated in both model versions, partly due to unmodelled components like secondary organic aerosols and mineral dust. In v1.6 the mean PM10 concentrations are generally slightly higher than in v1.3 but the correlation is slightly lower than for v1.3. Model differences in total PM10 can be mainly attributed to changes in the secondary inorganic aerosols (SIA: SO_4, NH_4, NO_3), with largest differences where the absolute concentrations are largest. These could be ascribed to changes in the chemistry. When calculating total PM10 in the model (tpm10), in v1.6 the fact the factor 3.26 is included for sea salt whereas it was not for v1.3. The postprocessor for the statistics also takes this effect into account, so that it is counted double for v1.6. Therefore we could not show a statistics table like for ozone. In the figures, the output of the model is the sum of the components without conversions. For the statistics, we refer to the scatter plots in the next section.

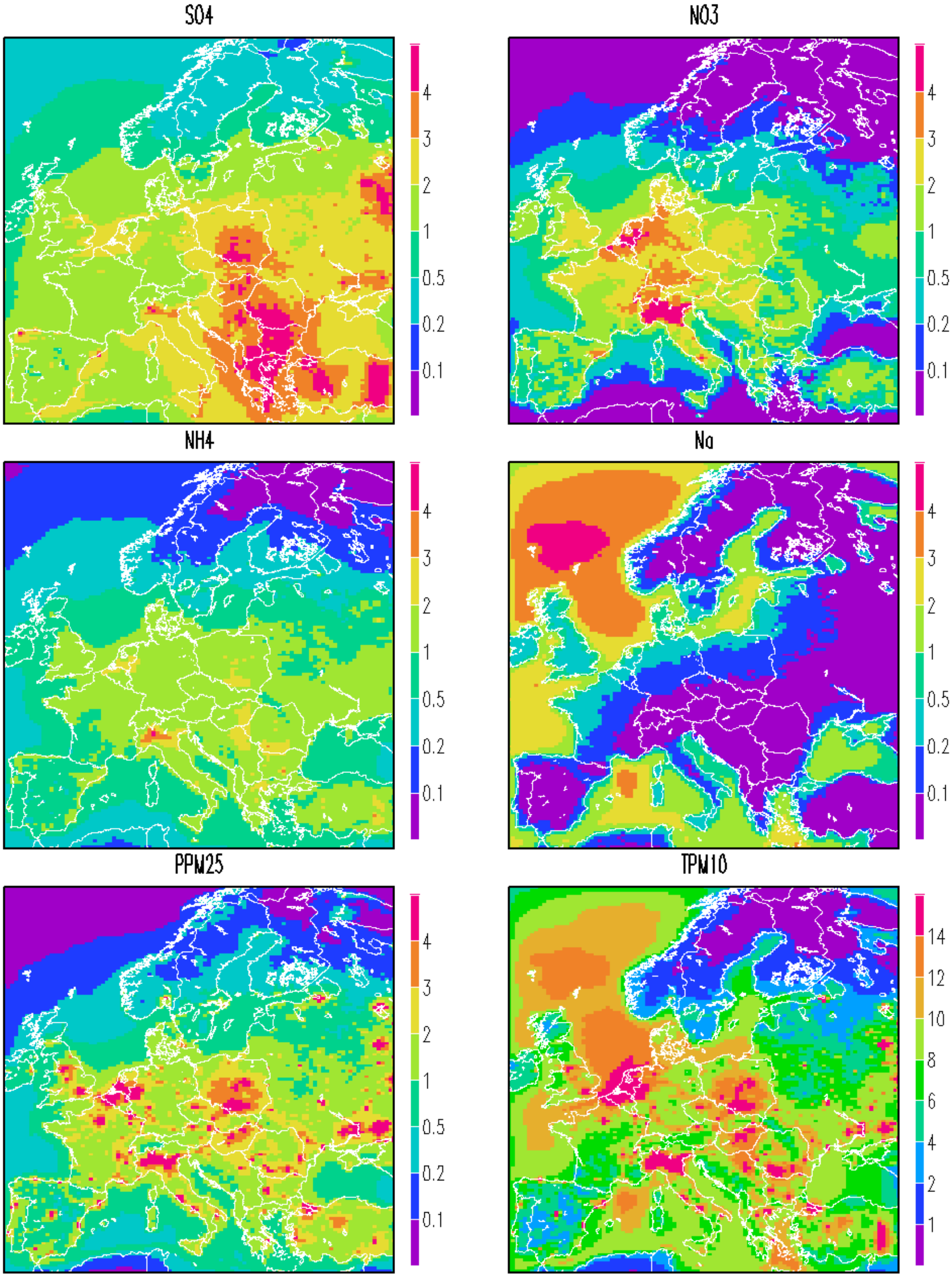


Figure 4 Annual mean concentrations of aerosol in 2003, v1.6 in µg/m3.

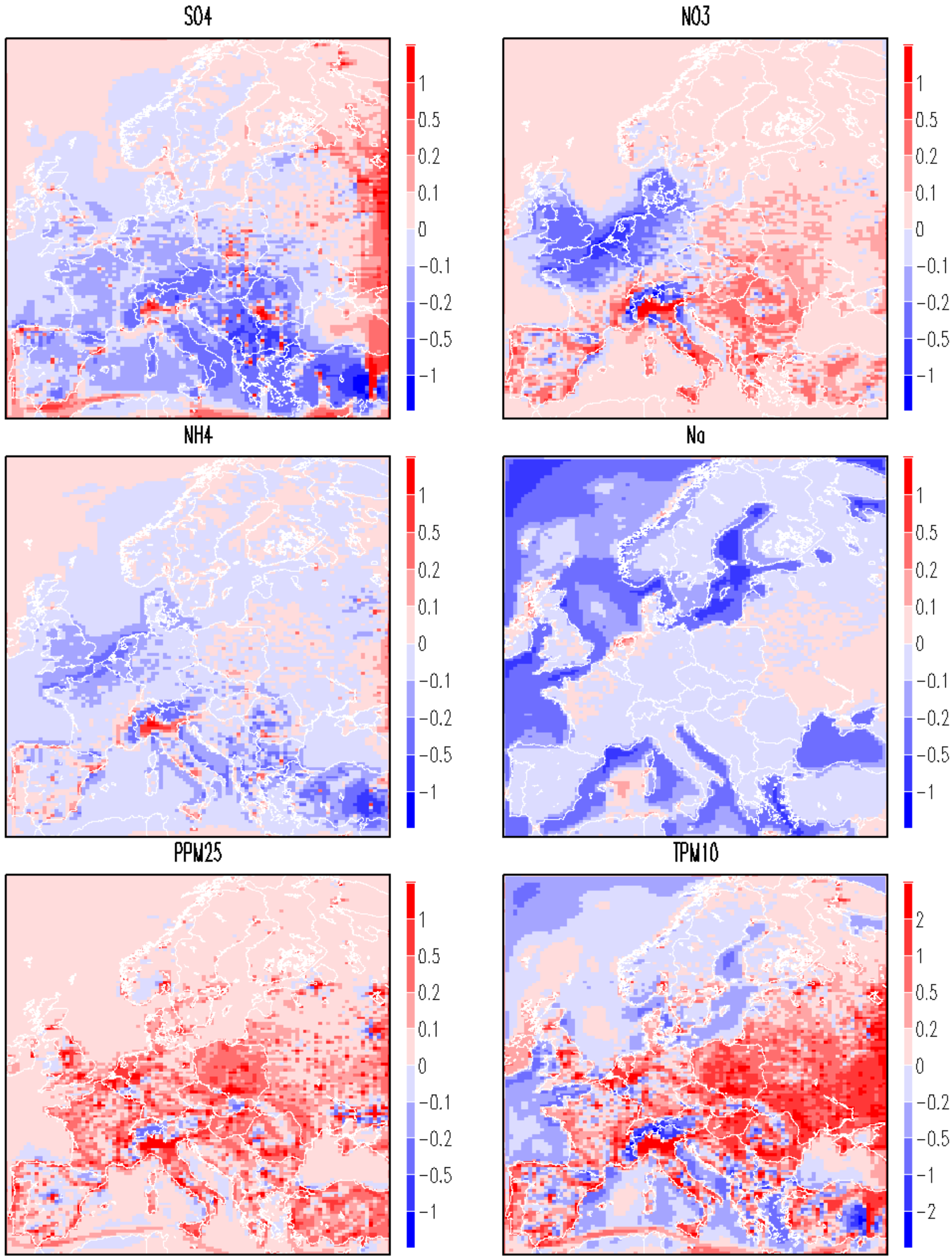


Figure 5: Difference in annual mean concentrations of aerosols in 2003, v1.6-v1.3, in µg/m3

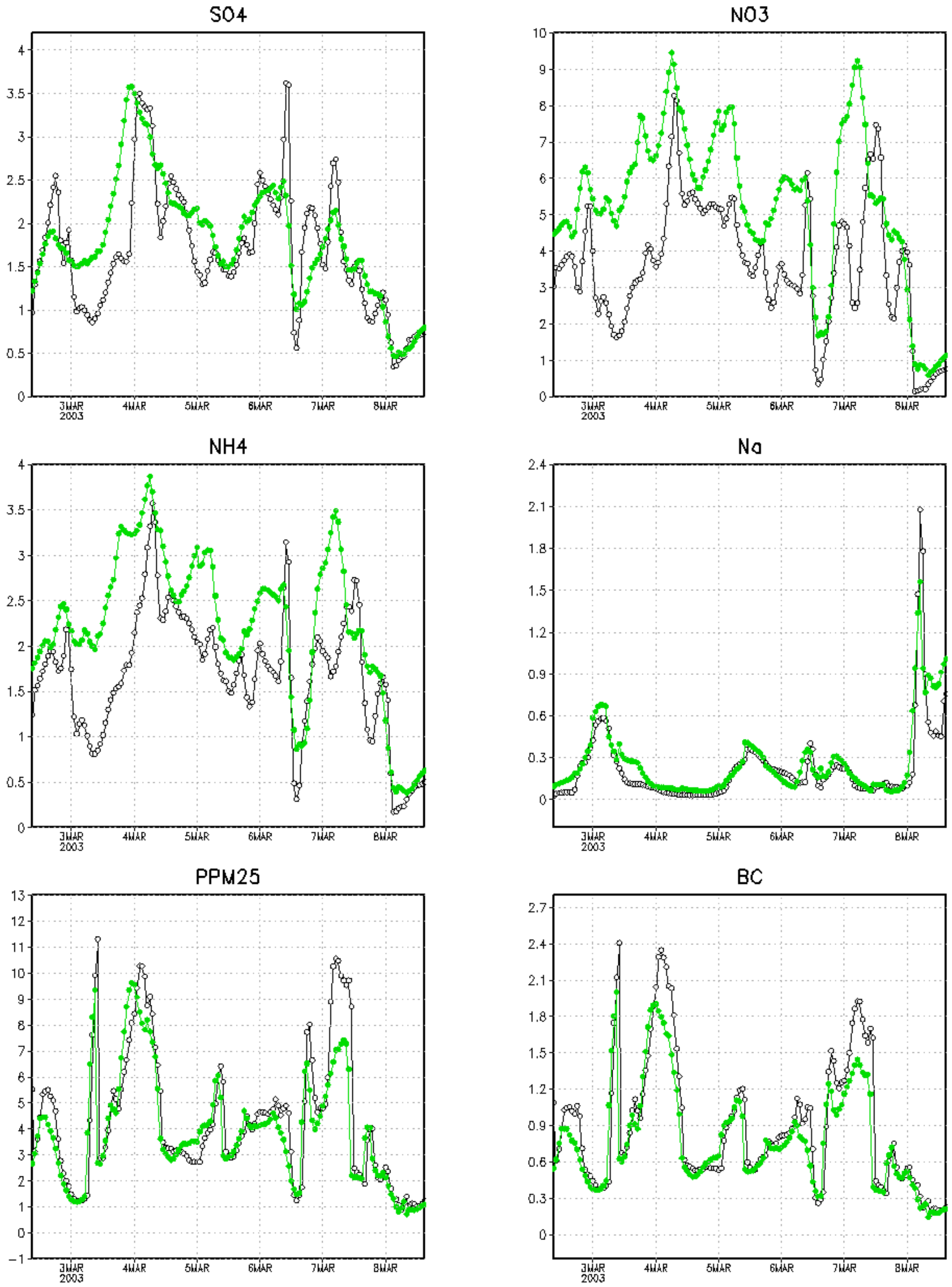
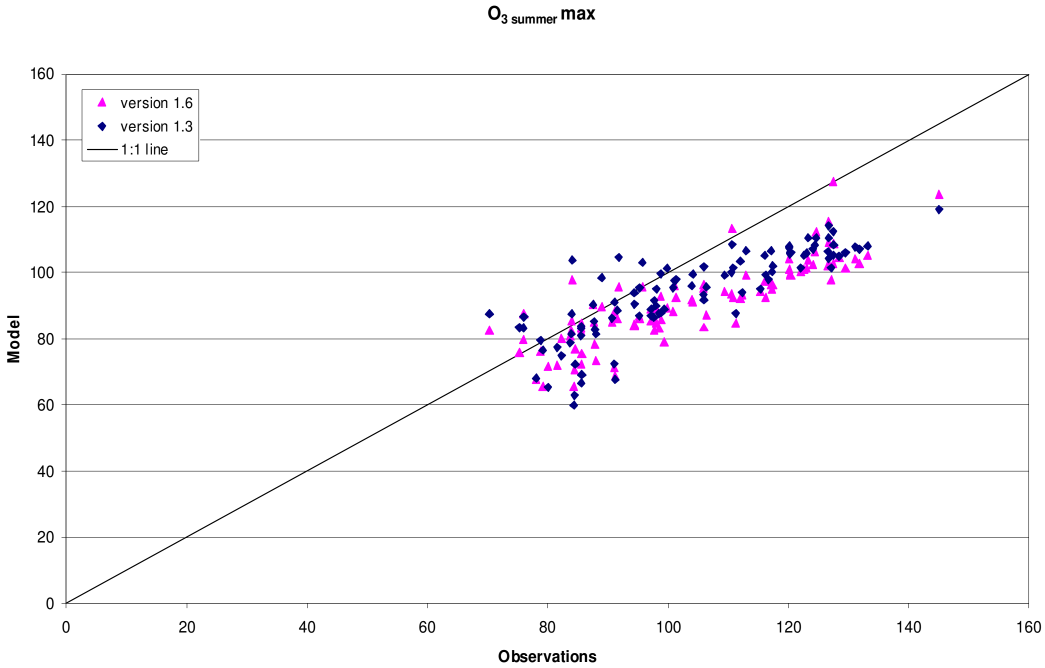


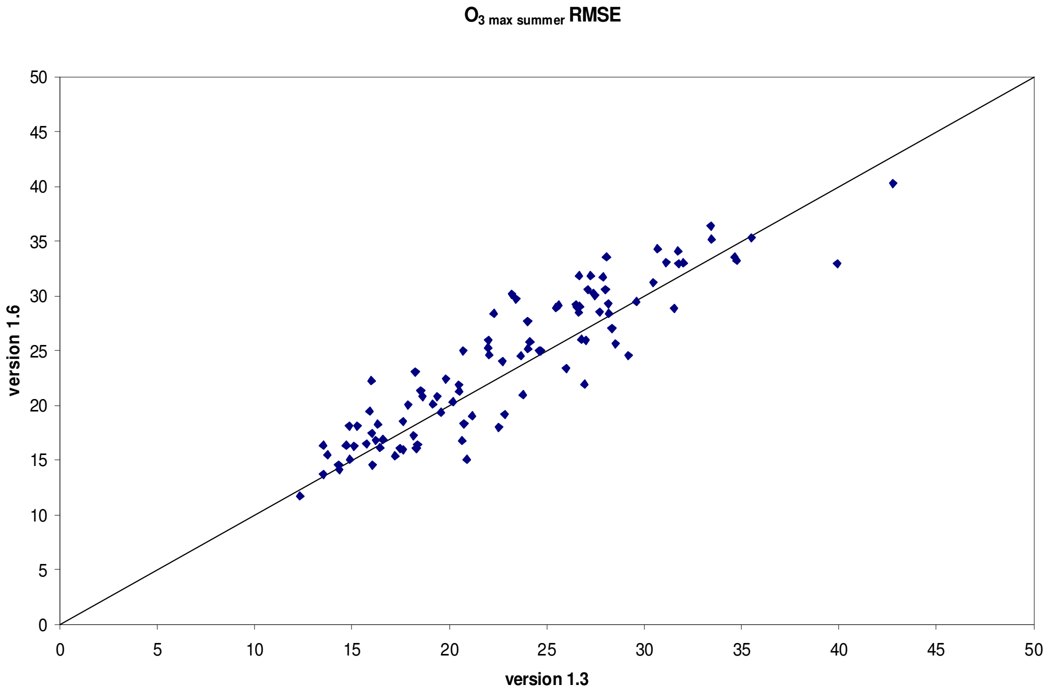
Fig. 6 Time series of v1.3 (green) and v1.6 (black) during a PM10 smog episode. Vertical units: µg/m3

Scatter plots

For the scatter plots, only EMEP stations below 700m a.s.l. were included.

Ozone





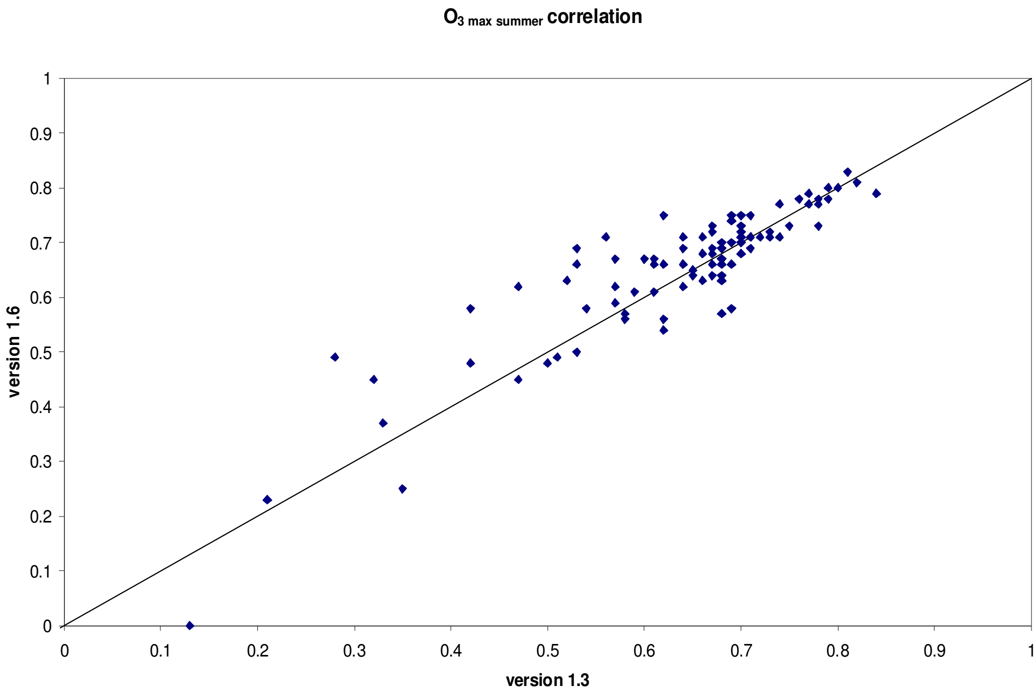
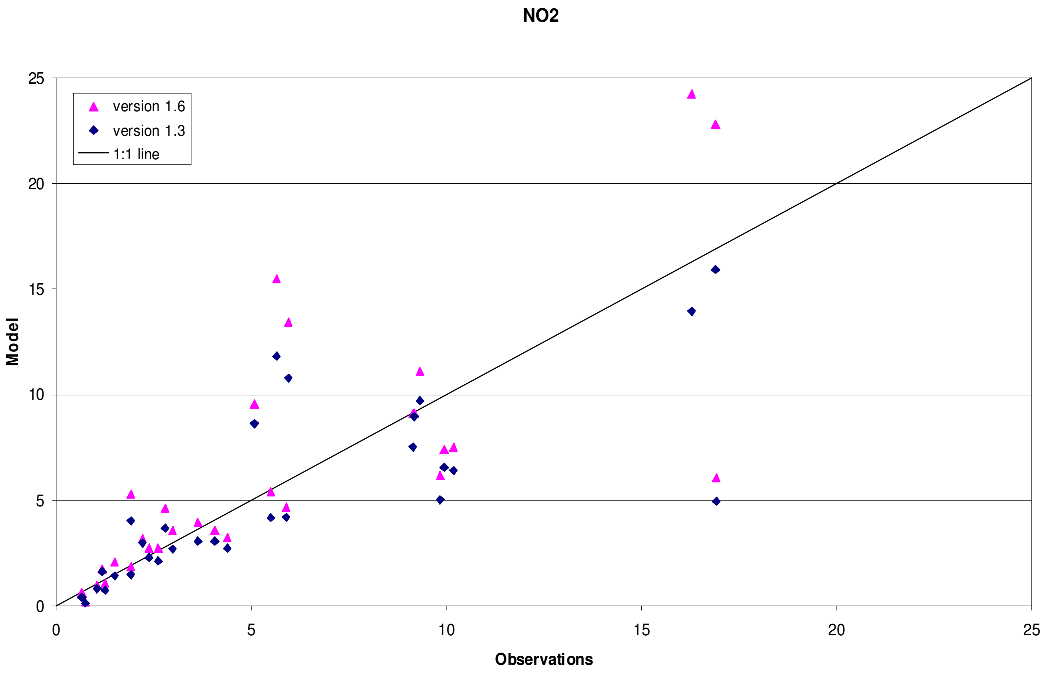


Fig 7. Ozone summer months: daily maxima, models versus observed. RMSE,Correlations.

NO_2



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20
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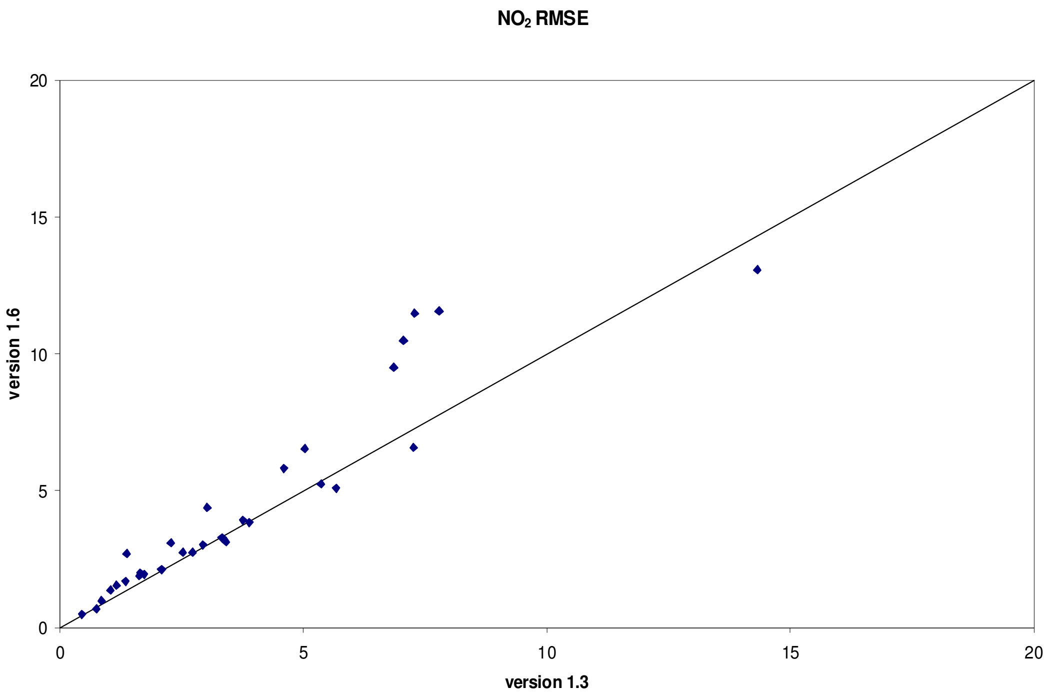
version 1.3
1:1 line
Model
Observations



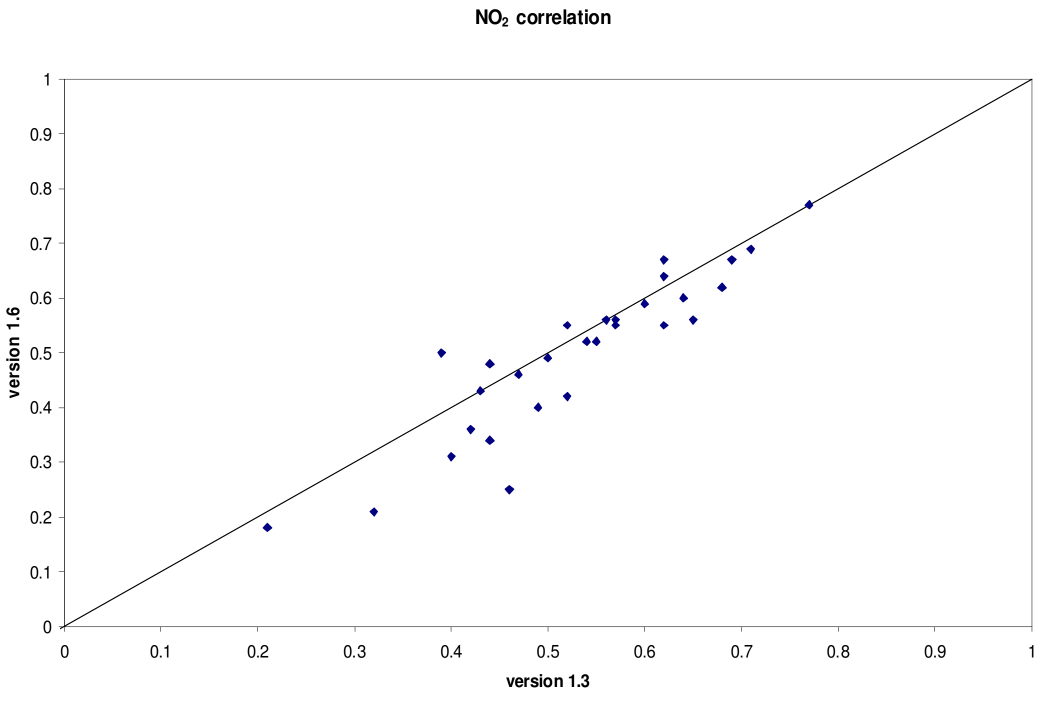
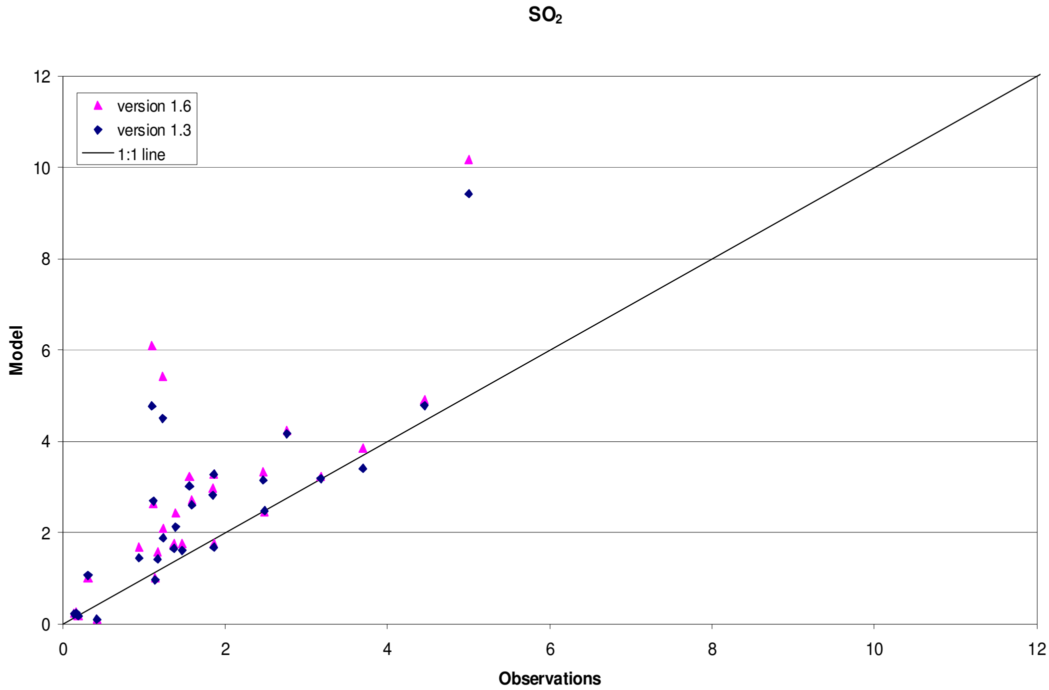


Fig 8.NO_2: Annual statistics: models versus observed. RMSE,Correlations.

SO_2



SO2
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Model
Observations
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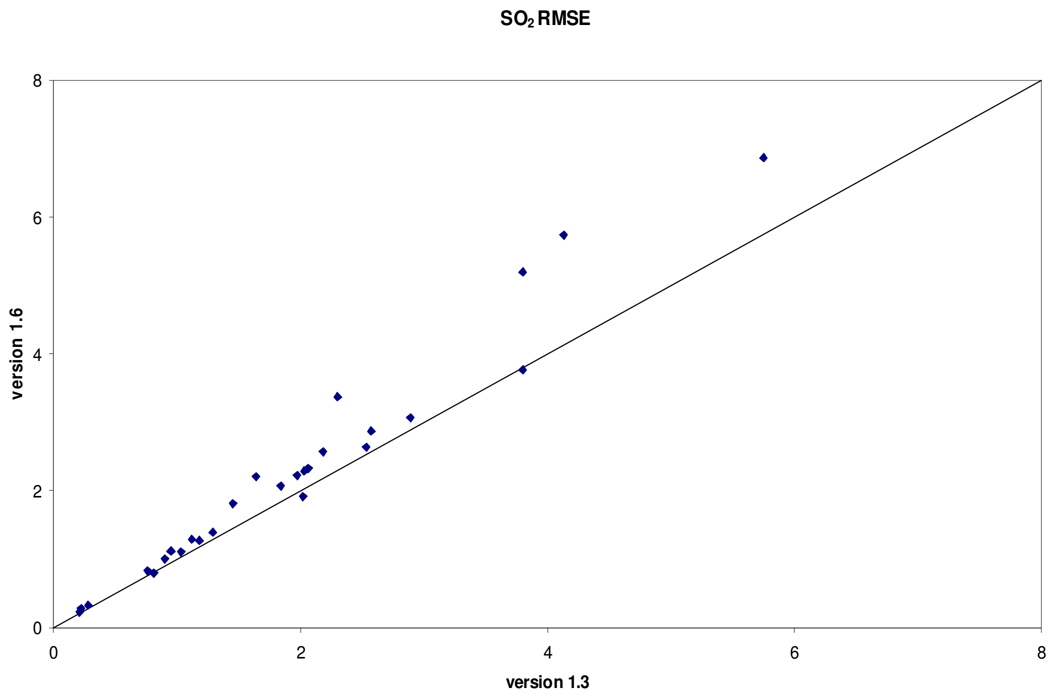
2
4
6
8
10
12



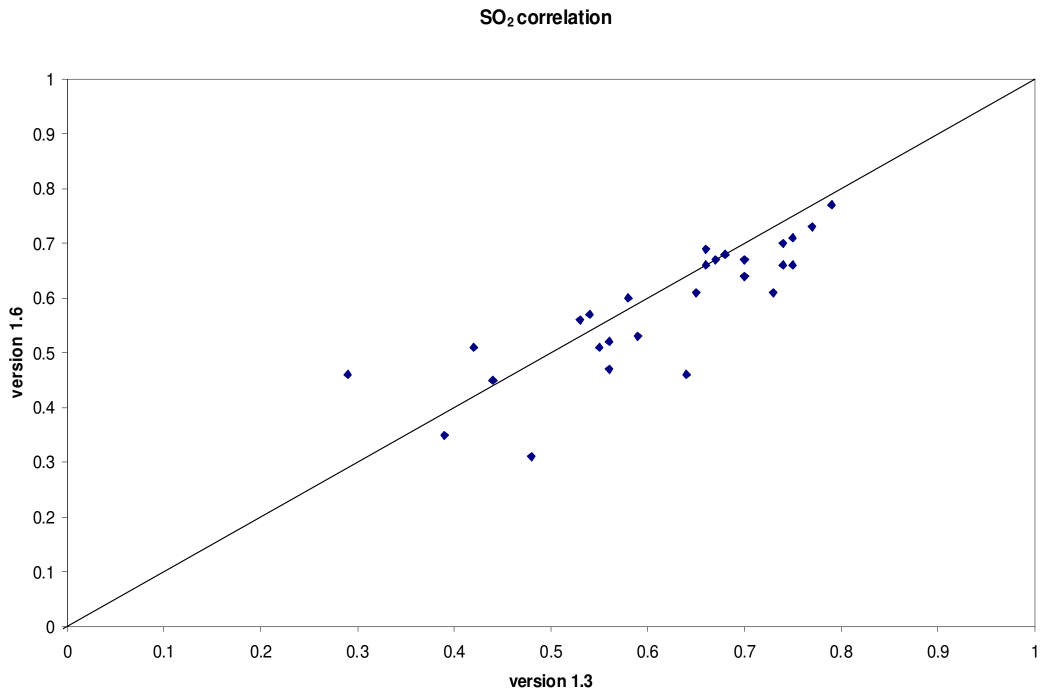
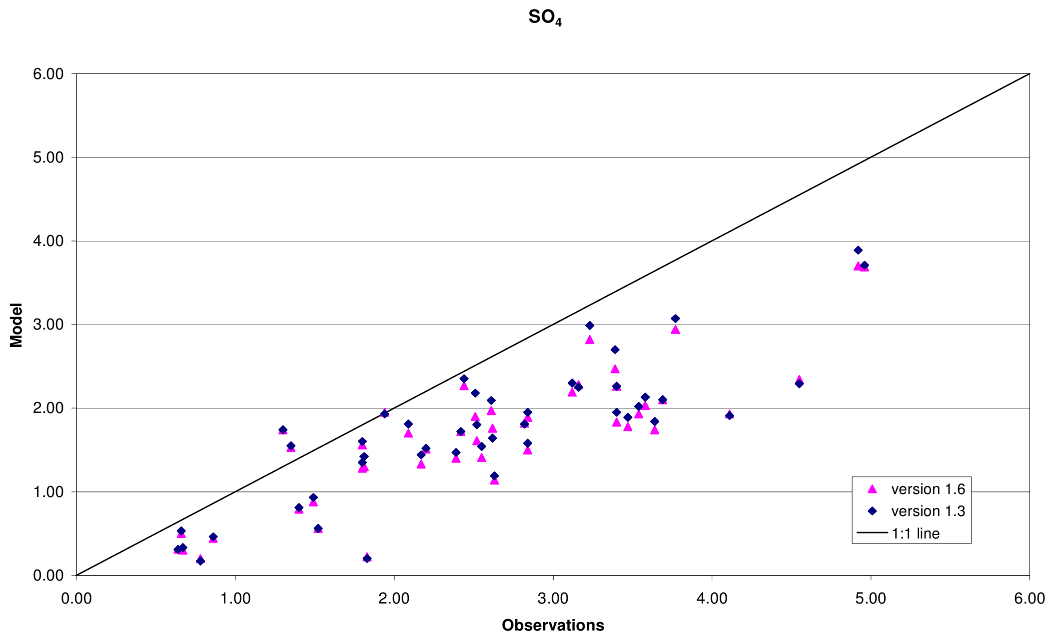


Fig 9.SO_2: Annual statistics: models versus observed. RMSE,Correlations

SO_4



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5.00
4.00
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Model
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5.00
6.00
Observations
version 1.6
version 1.3
1:1 line

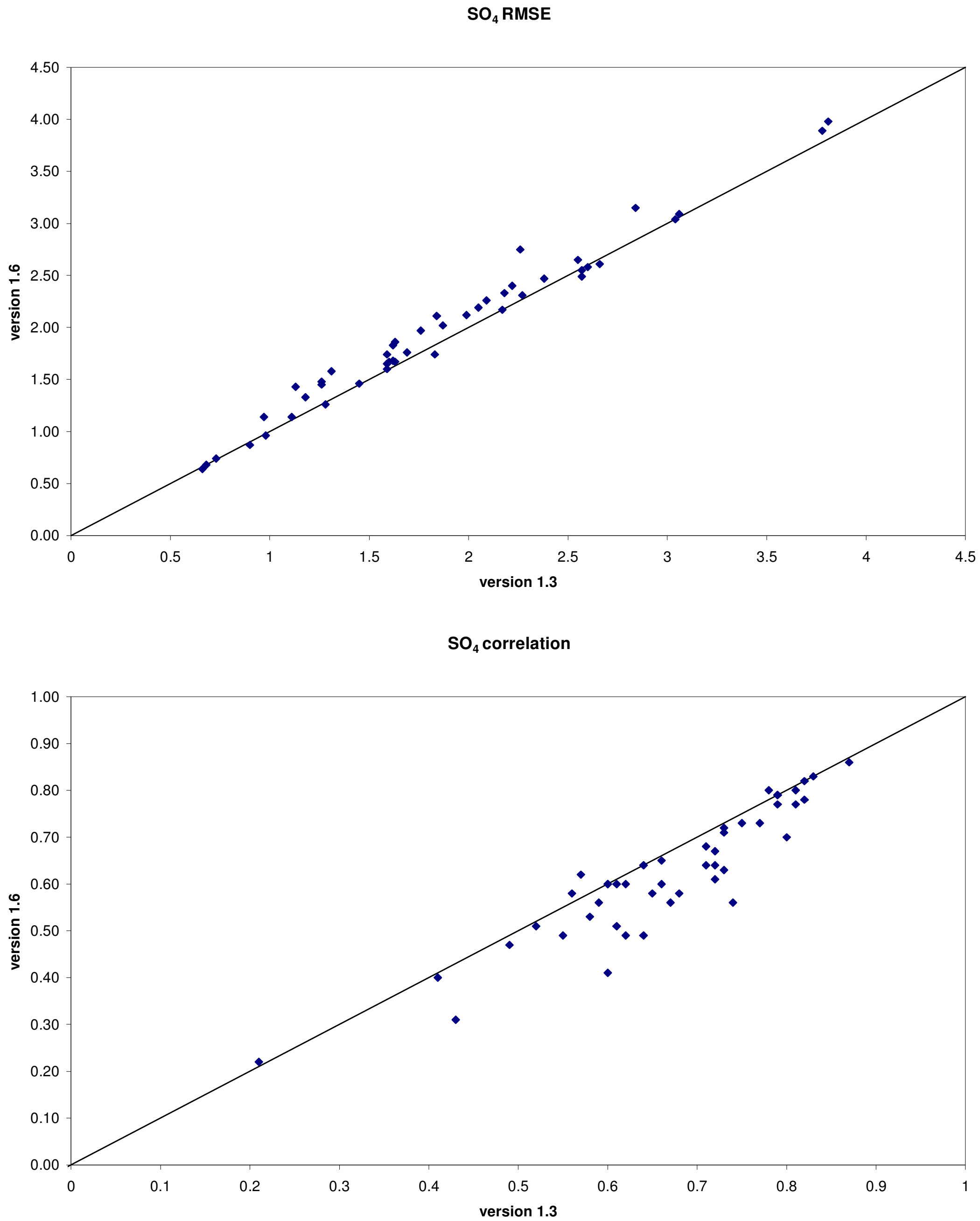
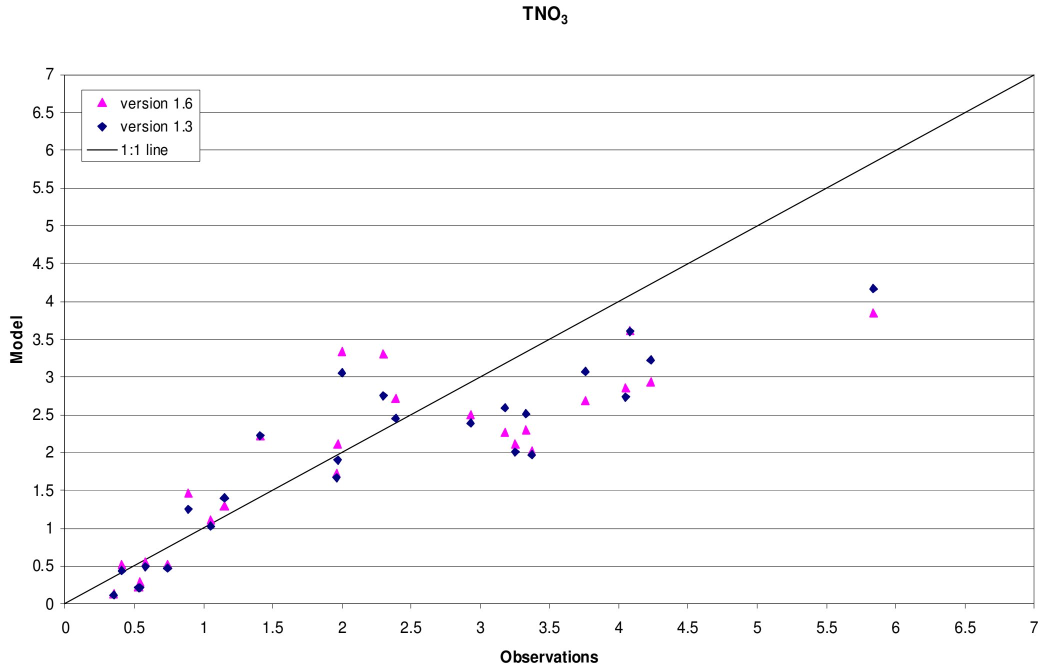


Fig 10.SO_4: Annual statistics: models versus observed. RMSE,Correlations

TNO_3



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Observations
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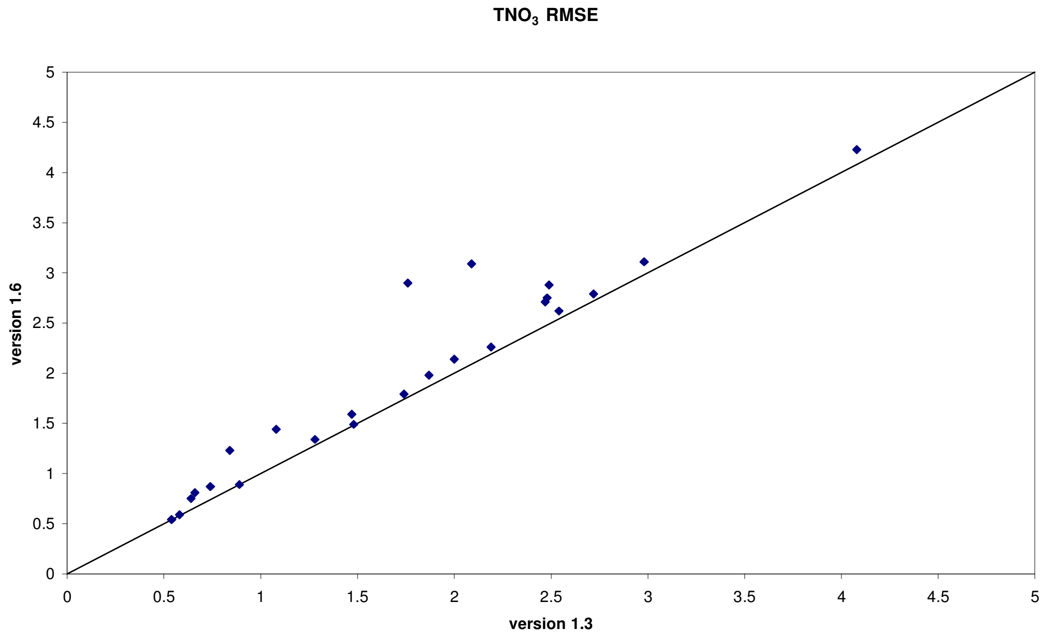
6
6.5
7



TNO_3 RMSE
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4
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5

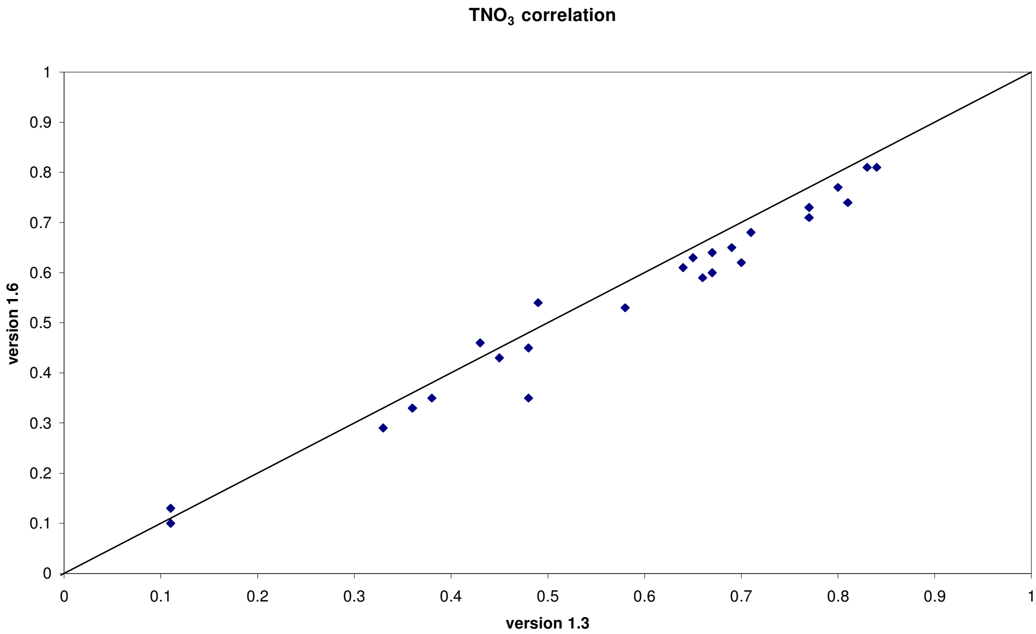
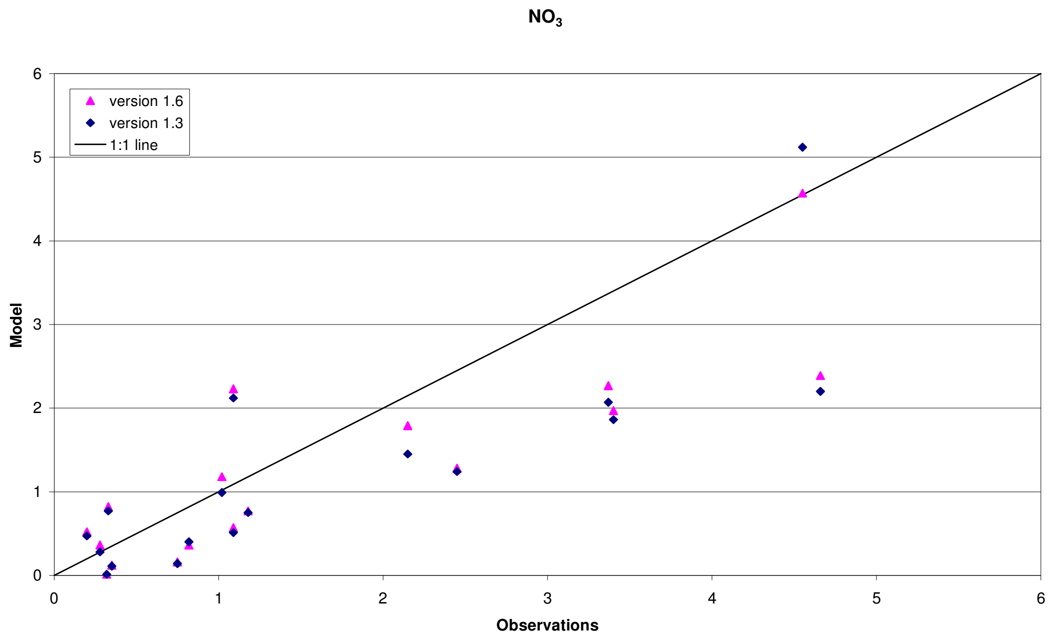


Fig 11.TNO_3: Annual statistics: models versus observed. RMSE,Correlations

NO_3



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version 1.3
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Model
Observations
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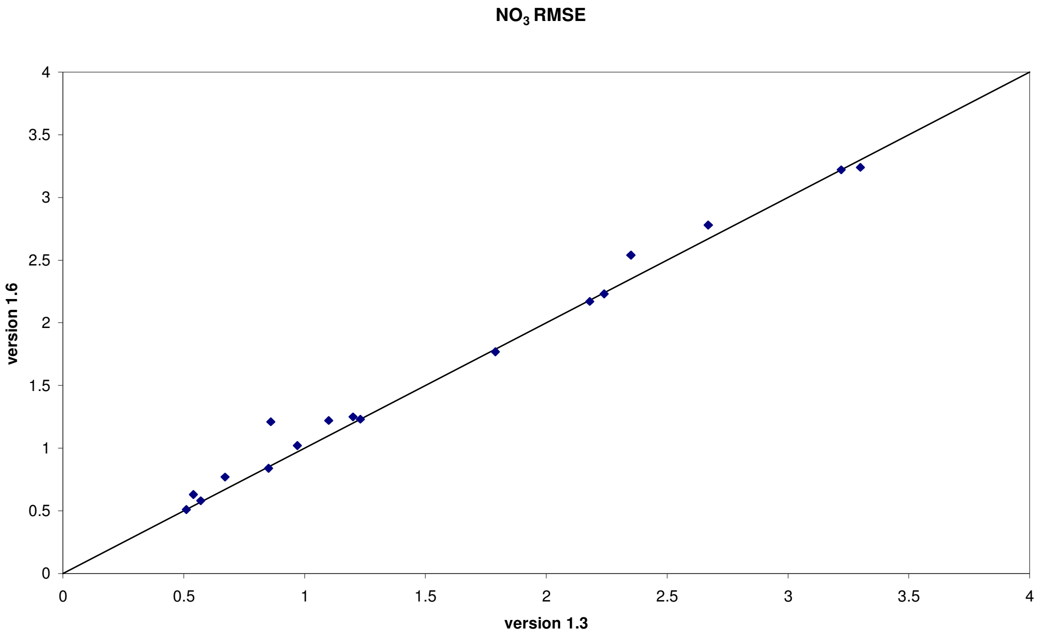
2
3
4
5
6



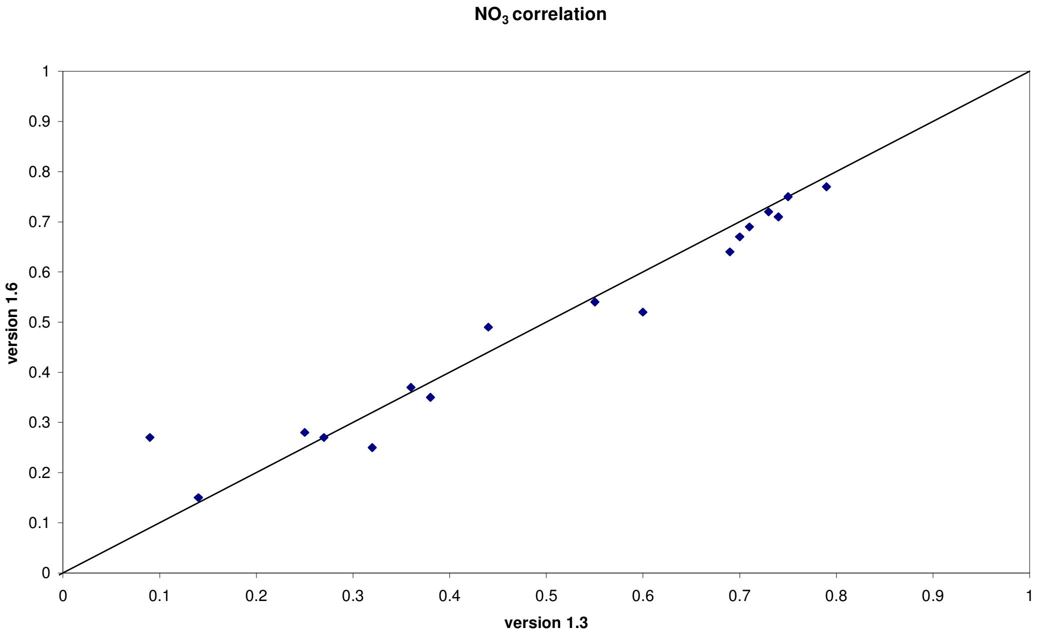
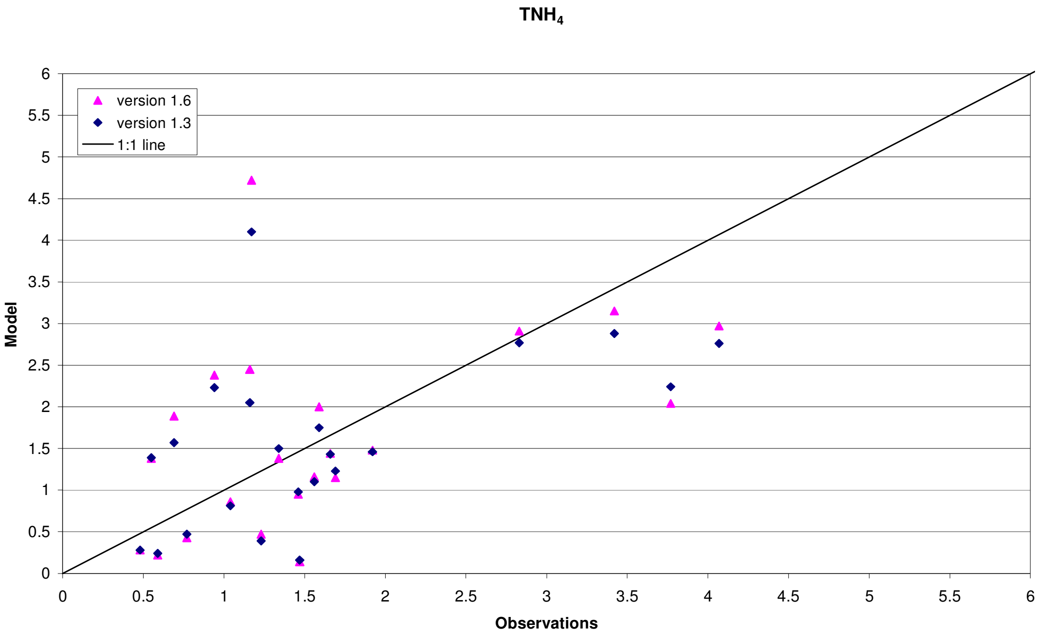


Fig 12 NO_3: Annual statistics: models versus observed. RMSE,Correlations

TNH_4



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5.5
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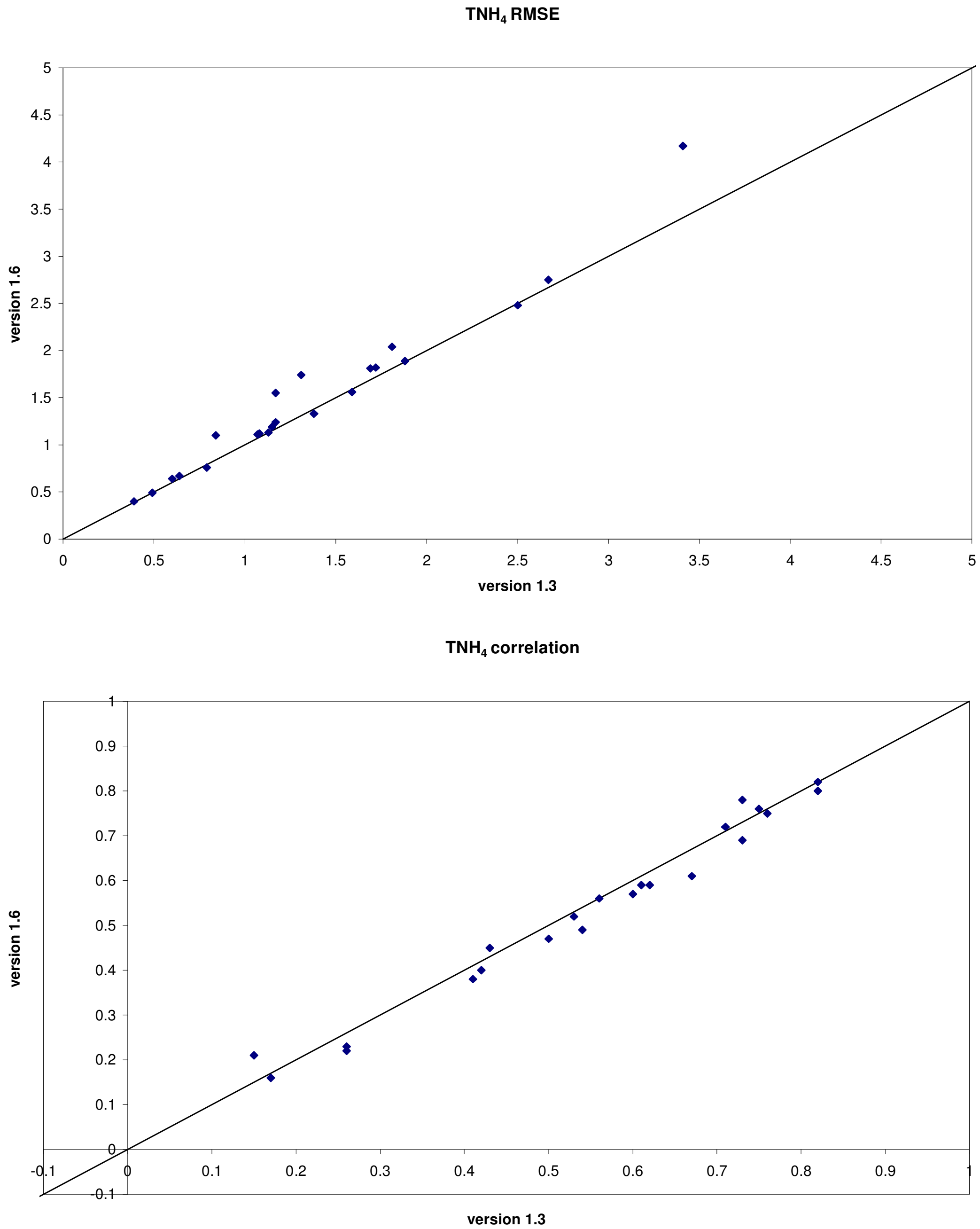
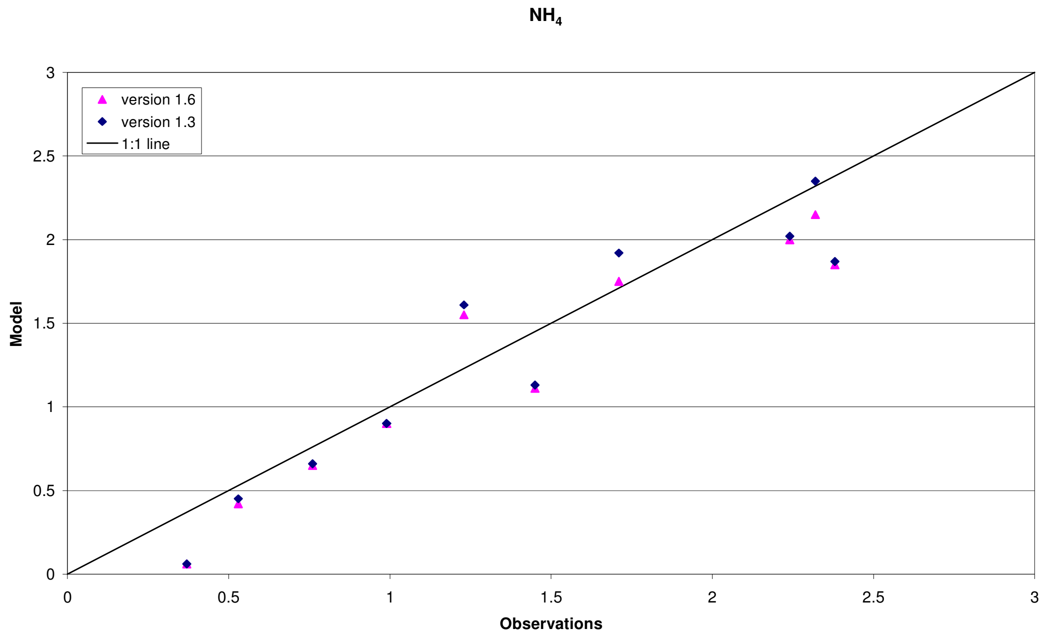


Fig 13 TNH_4: Annual statistics: models versus observed. RMSE,Correlations

NH_4



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Model
Observations
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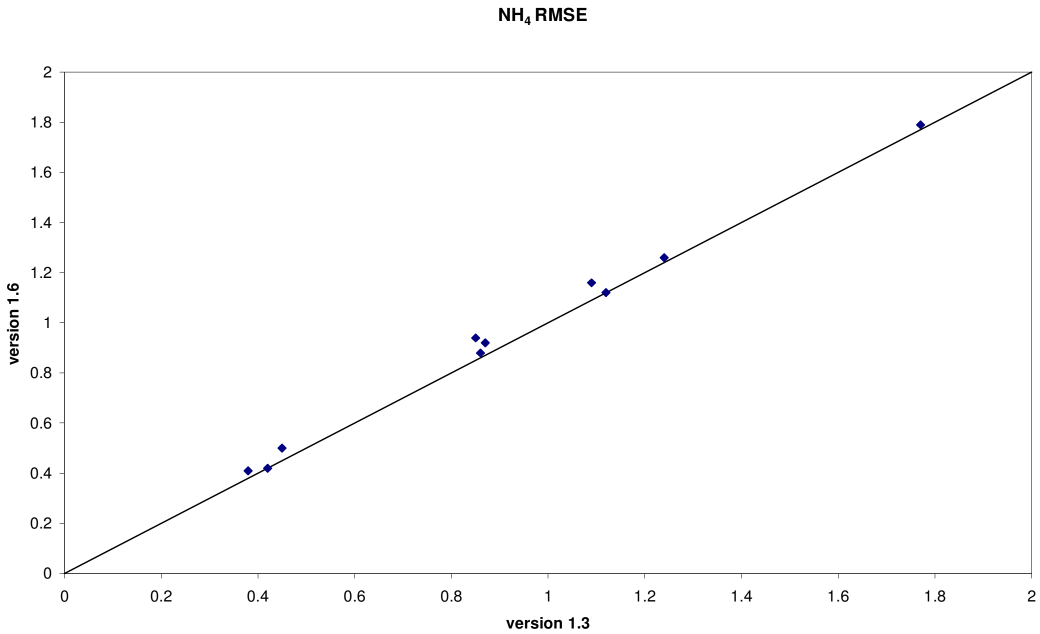
3



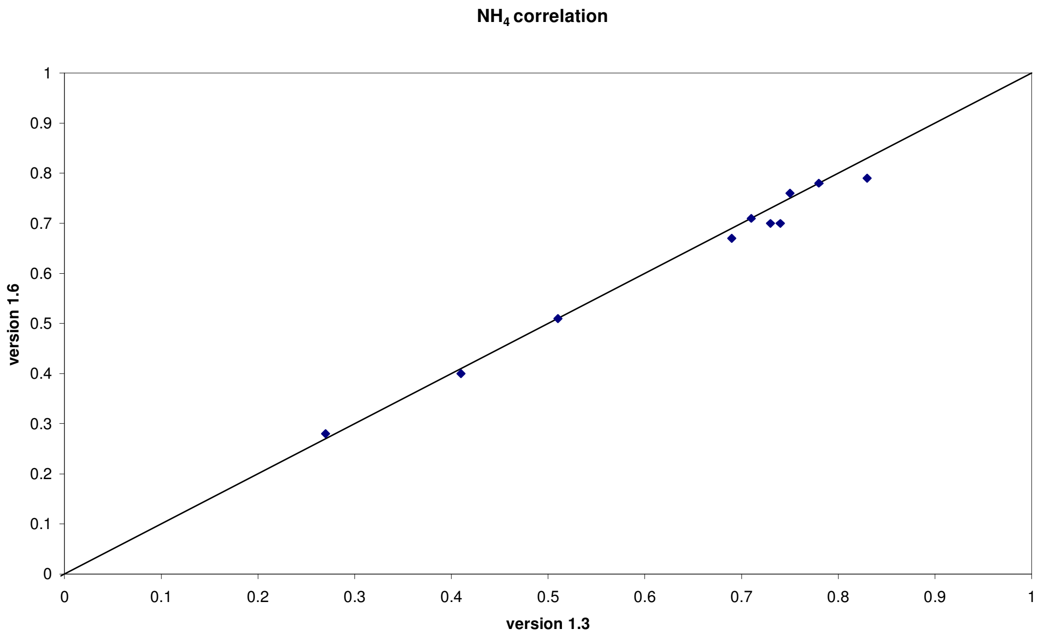


Fig 14 NH_4: Annual statistics: models versus observed. RMSE,Correlations

Zoom tests

Zoom domain: lon: -3-17, lat 42-57, zoom factor 4, test 1 day (17 June) . There is a smooth transition from the standard resolution to the zoom domain. A halo option is available in the rc file, which automatically writes the grid cells surrounding the zoom area to the output files, but this does not work properly yet.

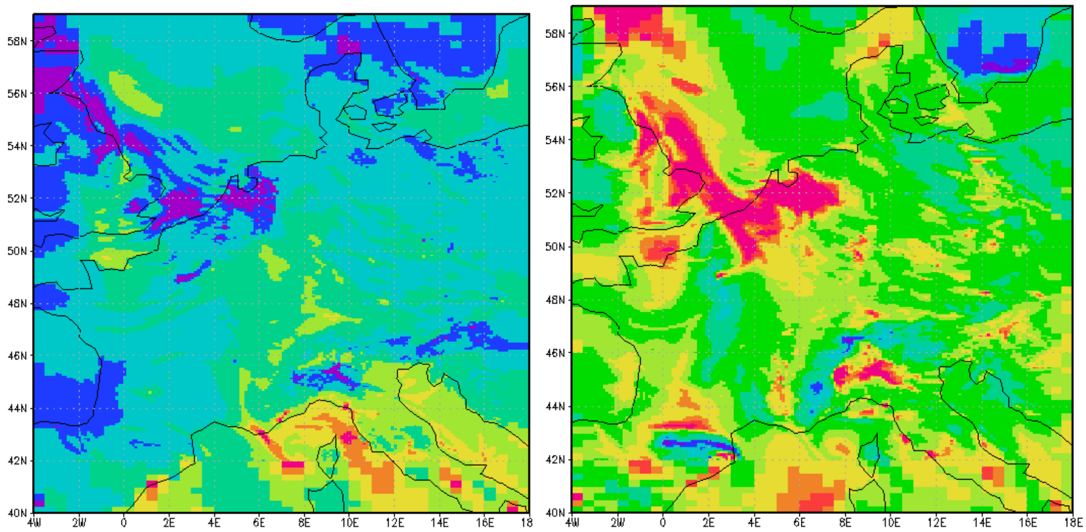


Fig.15 Snapshots 17 june 2003, 16 h: O_3 (left) and tPM10 (right)

Delta test

To investigate the sensitivity of the chemistry scheme with respect to NOx and VOC, two test runs were applied. In one run, the German NOx emissions were reduced by 33%, in the same run the Spanish VOC emissions were reduced by 33%.

Results are sensitive to both VOC and NOx emissions reductions, as expected (Figures 16-19). Due to the complex equilibrium between NOx, VOC and O_3, the effect depends on the region. The NOx reduction has not only an effect on NOx and O_3 concentrations, but also on NH_4 and NO_3 concentrations. Note that the effect on ozone in Germany is rather small, apparently the ozone chemistry is not in a NOx limited regime. The VOC reduction in Spain clearly results in smaller O_3 concentrations.

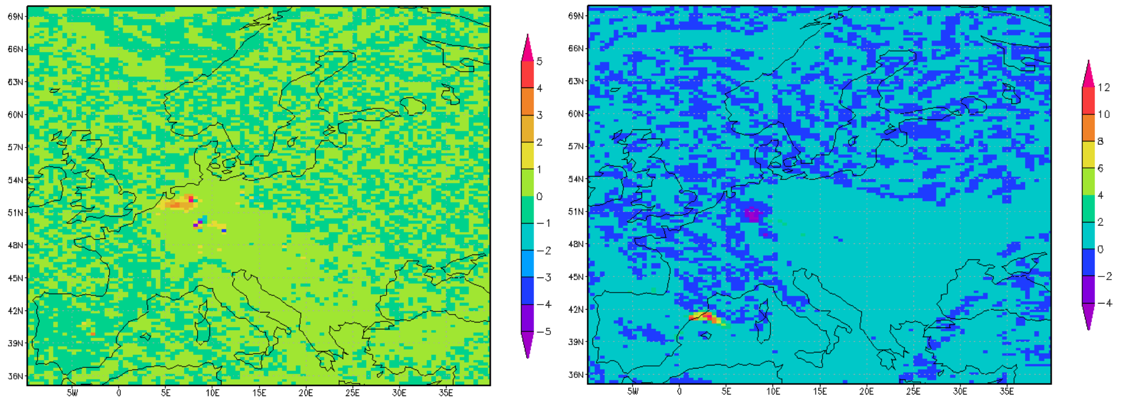


Figure 16 Difference in O_3 concentration with original run , June 17, 15 (left) and June 21 (right)

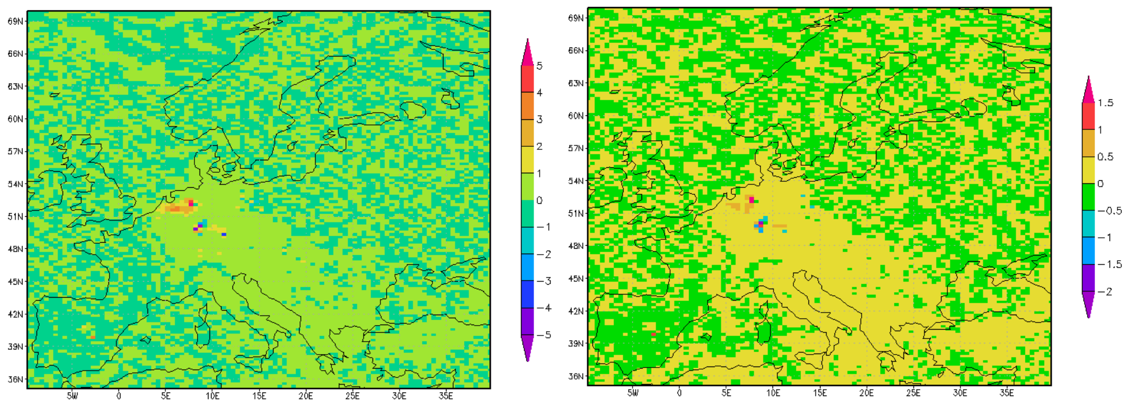


Figure 17 Difference in NO_3 (left) and NH_4 (right) concentration with original run, June 17, 15 h.

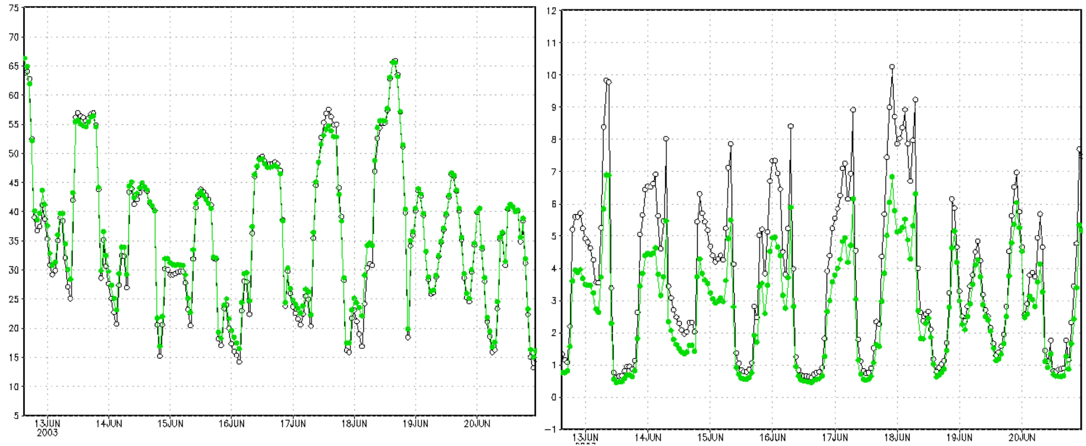


Figure 18 Ozone (left) and NO2 (right) for 52 N 8 E, black=default, green=33% reduction NOx emission

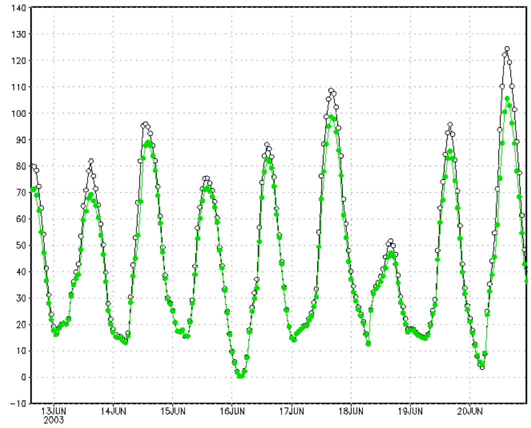


Figure 19 Ozone concentrations for 41 N 1 E. Black=default, green=33% reduction VOC emissions.

Discussion and conclusions

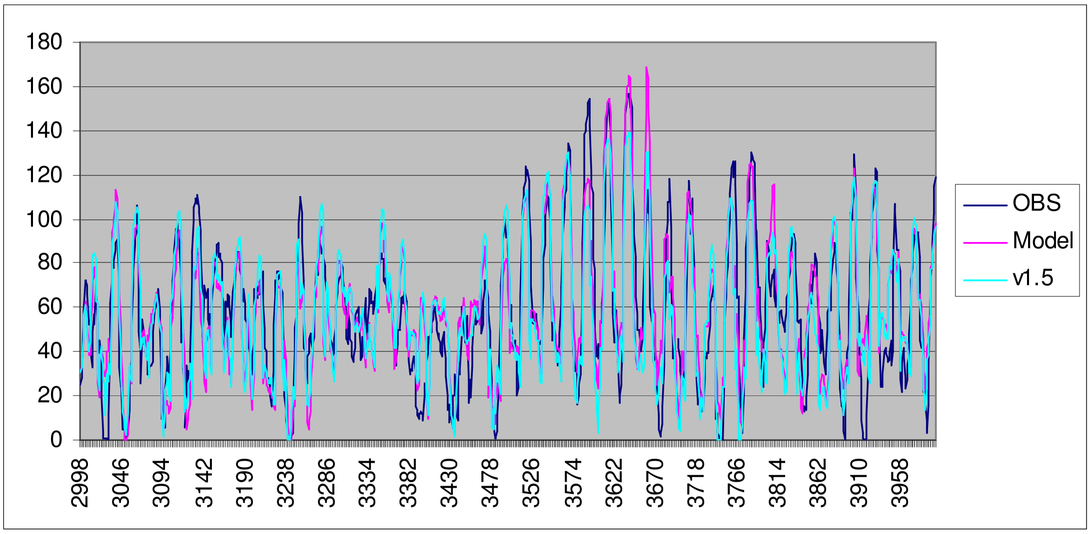
The present version, v1.6, has a performance which is comparable to v1.3.10. Statistics indicate that for some species, the correlation has decreased slightly, but this is at least in part the result of sharper gradients and peaks in v1.6, which give a larger difference in case of a slight mismatch between observations and model results. We consider the sharper gradients and peaks as a model improvement.

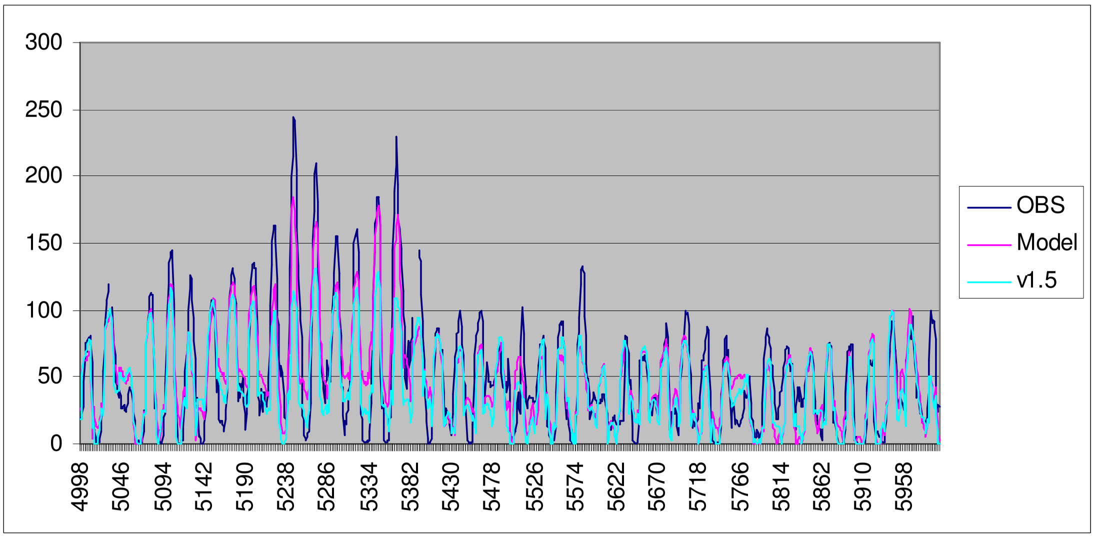
Another improvement is the chemistry. Several reaction constants were updated. This has restored the VOC sensitivity of LOTOS-EUROS in the ozone chemistry, which was very poor in v1.3. In a previous subversion (SMOGPROG version, see appendix) the VOC-sensitivity was improved but then the modeled ozone concentrations were too low in smog episodes.

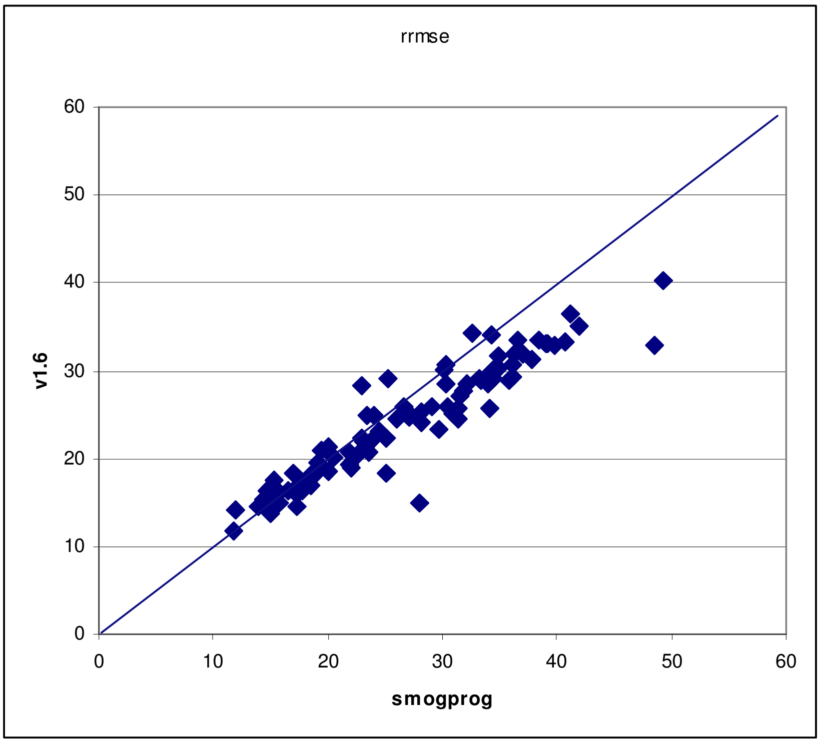
For a future version, the horizontal diffusion may be reconsidered. In v1.3 it was too high but switching it off may be too drastic. Other possible improvements are the SIA chemistry. New SIA observational data have become available to validate the SIA modeling and improve it. Regarding model run time, one may improve on it by streamlining the output.

Appendix

Comparison with SMOGPROG version (v1.5, not oficially released)



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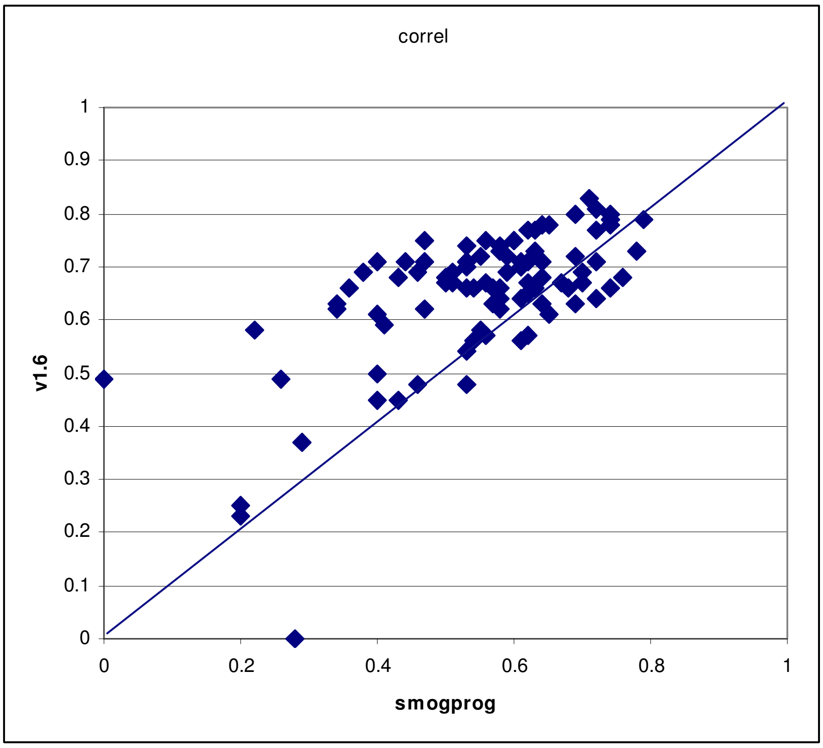
40
50
60
smogprog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0.4
0.3
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0.1
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v1.6
0
0.2
0.4
0.6
0.8
1
smogprog