Inverse modelling of emissions and their time profiles

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Introduction

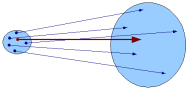
Data assimilation in meteorological models:

- Improvement of the model IC -> forecast improvement.

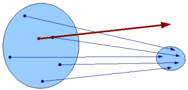
Data asimilation in CTM:

- Improvement of the chemical IC -> small improvement of the forecast
- Forcing by emission inputs and meteorological fields

Meteorological models
deterministic chaos



Ensemble of CTM states
converges to a common solution



Our experience gathered with mesoscale CTM *):
Decrease of the ensemble spread during 24 hours: O_3 to 20%, NO_2 to 10%
Conclusion: we need to improve the inputs and the model itself.

*) *K.Eben et al.: An ensemble Kalman filter for short term forecasting of tropospheric ozone concentrations, Q.J.R.Meteorol.Soc.(2005)*

4DVar with the CMAQ model

Pilot assimilation experiment with simplified design:

- 4DVar based on the CMAQ adjoint model.
- In-situ and satellite observations of NO_2.
- Optimization of IC and emissions of NO and NO_2.
- Corrections of emissions parametrized by one coefficient per gridcell.
- Correction coefficients from one day used for the forecast of the next day (persistent statistical predictor).

Conclusions:

- Emission corrections quite stable from day to day.
- Forecast improved for NO_2 but not for O_3.

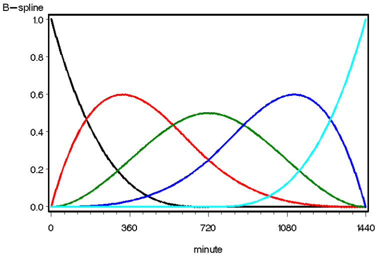
Enhanced assimilation design

Enhancements in the assimilation method:

- Optimization of diurnal emission profiles.
- Implementation of the adjoint for SAPRC99 mechanism.
- Observation of O_3 - stations and satellite columns are assimilated in addition to NO_2
- Optimization of more species.
  - Species with significant backward sensitivity.
  - Radicals and non-reactive species excluded.

Emission profiles optimization

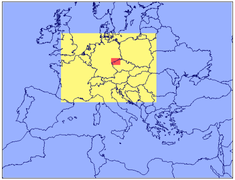
- To avoid an ill-posed problem, emission profile corrections were parameterized using a fixed basis of five splines.
- Emission correction factor calculated as linear combination.
- For every day the 4DVar gives estimates of the coefficients.

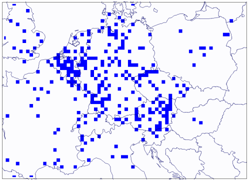


Basis functions used for parametrization of the correction of diurnal emission profile.

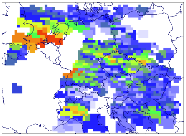
Setup of the experiments

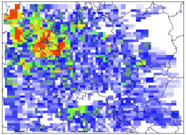
Experiment with all proposed enhancements.

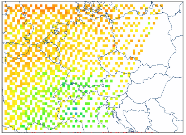




Horizontal domains (left) and in-situ stations (right).





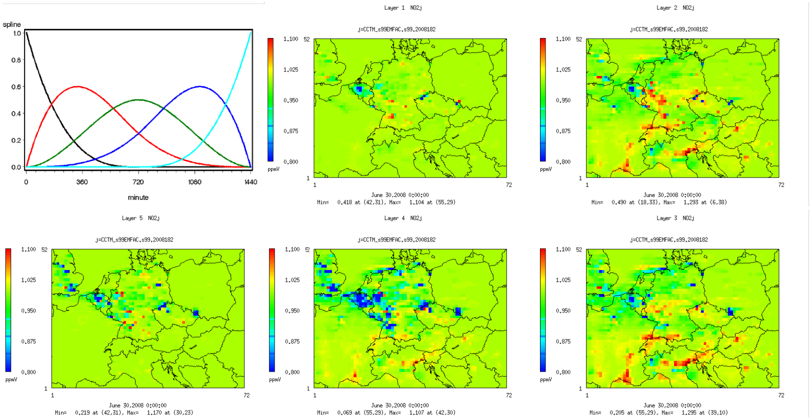


Tropospheric NO_2 columns and O_3 profile layer at July 1 2008.

GOME2 10:24 (left), OMI 13:24 (center), IASI 12:00 (right)

Assimilation episode: June 28 - July 5, 2008.

Emission correction coefficients for the five basis functions

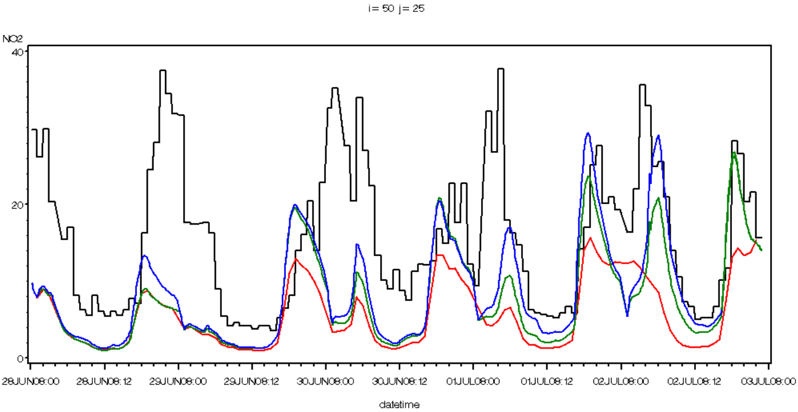


Maps of the optimized emission coefficients for 30.6.2008 for differents parts of the day

Upper from left: night, morning, lower from right: midday, evening, night.

Assimilation shifts emissions from evening peak to morning in some regions.

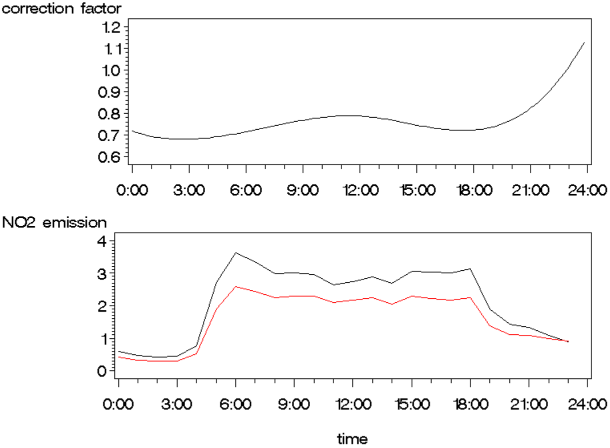
Results - concentration in Brno



Graph of the concentrations of NO_2 in Brno,CZ.

Red: modelled, blue: optimized, green: forecasted, black: observerd (weighted average of background stations).

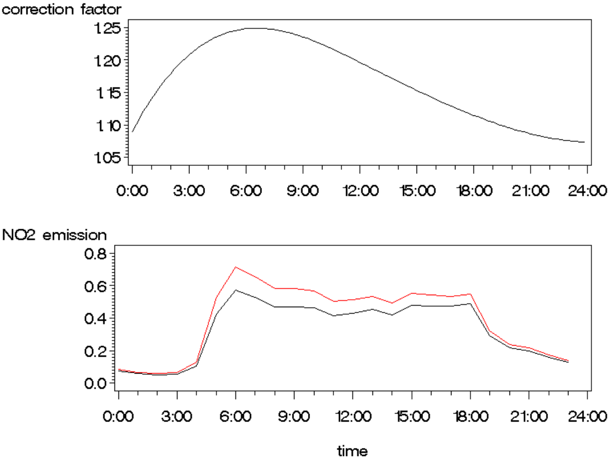
Results - correction factor and emission



Graphs of the daily profile of the correction factor and emission of NO_2 in Prague,CZ for 2.7.2008.

Black: emission modelled by emission model, red: corrected emission.

Results - correction factor and emission



Graphs of the daily profile of the correction factor and emission of NO_2 in Brno,CZ for 2.7.2008.

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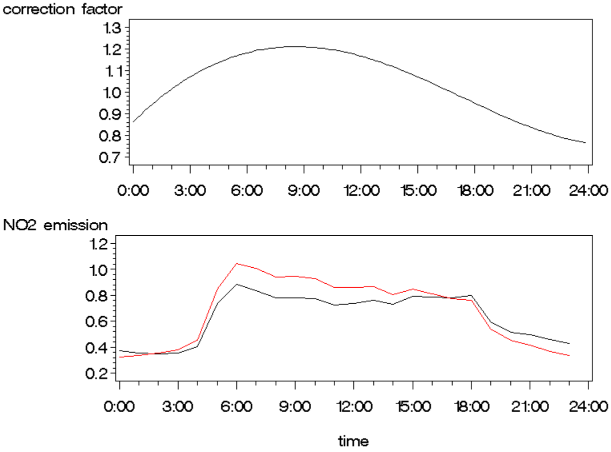
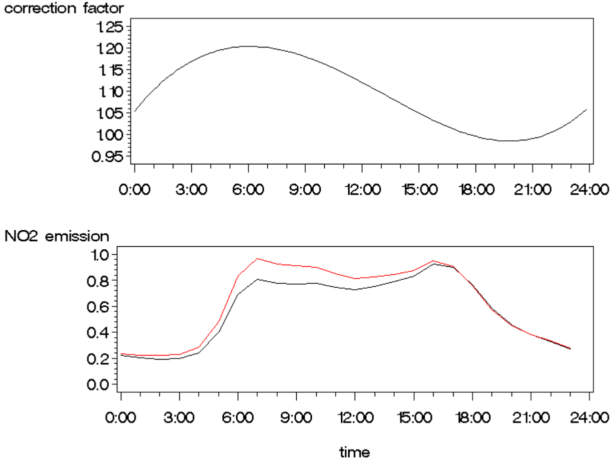
Results - correction factor and emission



Graphs of the daily profile of the correction factor and emission of NO_2 in Usti nad Labem,CZ for 2.7.2008.

Black: emission modelled by emission model, red: corrected emission.

Results - correction factor and emission



Graphs of the daily profile of the correction factor and emission of NO_2 in Koln,DE for 2.7.2008.

Black: emission modelled by emission model, red: corrected emission.

Results - performance of the method

Improvement of the analysis and forecast of the NO_2 and O_3

	NO_2		O_3	
	Analysis	*Forecast*	*Analysis*	*Forecast*
28.6.2008	*27,88*	-	*11,91*	-
29.6.2008	*39,41*	*27,59*	*16,37*	*0,26*
30.6.2008	*26,54*	*14,66*	*24,87*	*1,60*
1.7.2008	*22,02*	*17,26*	*21,39*	*7,83*
2.7.2008	*26,59*	*17,26*	*15,21*	*6,21*
3.7.2008	*26,04*	*18,95*	*18,16*	*6,07*
4.7.2008	*25,61*	*11,00*	*20,80*	*12,08*
5.7.2008	-	*20,84*	-	*9,70*

Relative percentage improvement of analysis and forecast.

A detailed long-term study

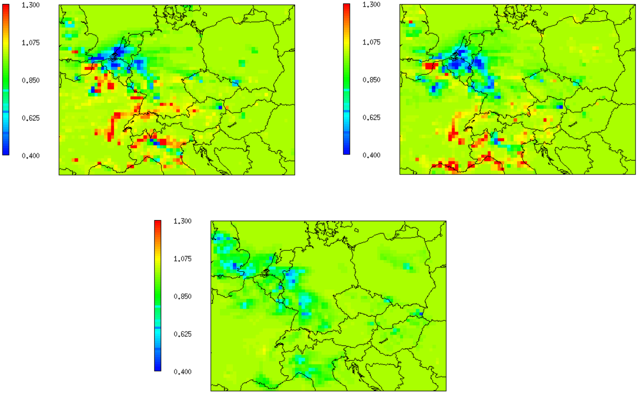
A long-term study of performance of the method is running at present.
(4 months, spring and summer 2007).

The aims of this study:

- To verify the method in a long-term run.
- Investigation of contributions of different kinds of observations and of the extent of their synergy.
- Assessment of influence of different parametrizations of diurnal emission profiles.
- To get statistical characteristics of emission correction.

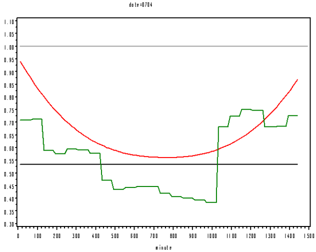
Contributions of different kinds of observations to emission corrections

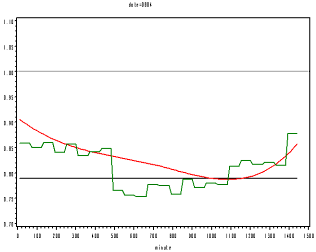
Emission correction factors for NO for midday at Apr 8 2007 induced by ground level resp. satellite observations.

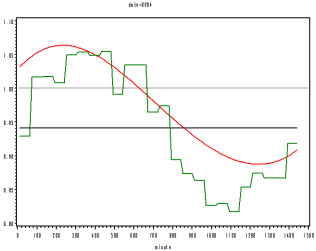


NO_2 observations (upper left), O_3 observations (upper right) and tropospheric collumns of NO_2 from OMI and GOME-2 (down).

Emission profile parametrization







Emission correction factor for Usti nad Labem for daily total correction (black), five b-splines parametrization (red) and independent correction of every hour (green).

Weekly cycles of corrections!

Conclusions

- The 4DVar method proves to be a powerful tool for optimization of emissions and their time profiles.
- Forecast from optimized model corresponds better with observations.
- Many issues still need to be resolved and a long-term validation has to be finalized.
- The proposed method can serve a base for building data-driven emission models.

Thank you for your attention

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