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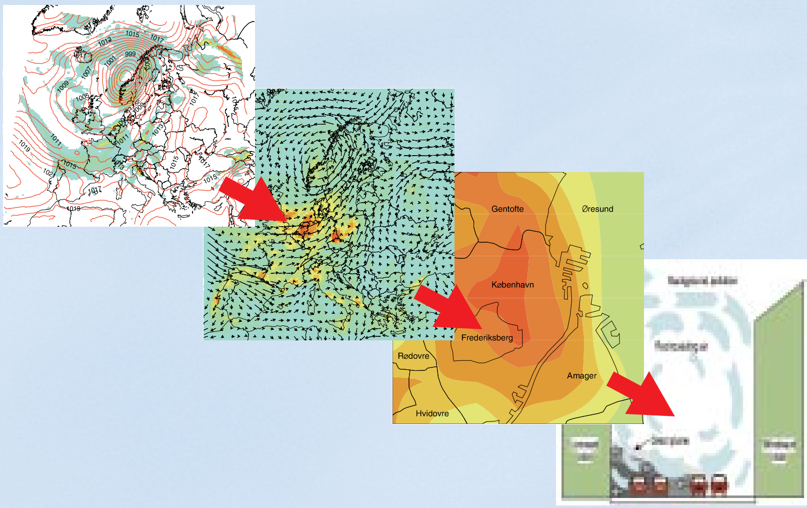
The DMU-ATMI THOR Air Pollution Forecast System

System Description

NERI Technical Report No. 321



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Data sheet

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Department: Department of Atmospheric Environment

Serial title and no.: NERI Technical Report No. 321

Publisher: Ministry of Environment and Energy
National Environmental Research Institute ©

URL: http://www.dmu.dk

Date of publication: June 2000

Referee: Ole Hertel

Layout: Berit Christiansen and Jørgen Brandt

Drawings: Jørgen Brandt and Jesper H. Christensen

Please cite as: Brandt, J., Christensen, J. H., Frohn, L. M., Berkowicz, R. Palmgren, F. (2000): The DMU-ATMI THOR Air Pollution Forecast System - System Description. National Environmental Research Institute, Roskilde, Denmark. 60 pp. - NERI Technical Report No.321

Abstract: A new operational air pollution forecast system, THOR, has been developed at the National Environmental Research Institute, Denmark. The integrated system consists of a series of different air pollution models, which cover a wide range of scales (from European scale to street scale in cities) and applications. The goal of the system is, on continuous basis, to produce 3 days air pollution forecasts of the most important air pollution species on different scales. Furthermore, the system will be an integrated part of the national urban and rural monitoring programmes and will be used for emission reduction scenarios supporting decision-makers.

Keywords: Air pollution forecasting, European, urban background and urban street scales.

Editing complete: May 2000

ISBN: 87-7772-554-9

ISSN (print): 0905-815X

ISSN (electronic): 1600-0048

Paper quality and print: Cyclus Office, 100 % recycled paper. Grønager's Grafisk Produktion AS. This publication has been marked with the Nordic environmental logo "Svanen".

Number of pages: 60

Circulation: 200

Price: DKK 80,- (incl. 25% VAT, excl. freight)

For sale at:

National Environmental Research Institute
P.O. Box 358
Frederiksborgvej 399
DK-4000 Roskilde
Denmark
Tel: +45 46 30 12 00
Fax: +45 46 30 12 14

Miljøbutikken
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Contents

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Abstract

The Thor System

A new operational air pollution forecast system, THOR, has been developed at the National Environmental Research Institute, Denmark. The integrated system consists of a series of different air pollution models, which cover a wide range of scales (from European scale to street scale in cities) and applications. The goal of the system is, on continuous basis, to produce 3 days air pollution forecasts of the most important air pollution species on different scales. Furthermore, the system will be an integrated part of the national urban and rural monitoring programmes and will be used for emission reduction scenarios supporting decision-makers.

Currently, the THOR system consists of a numerical weather forecast model, ETA, a long-range air pollution chemistry-transport model, DEOM, an urban background model, BUM, and an operational street pollution model, OSPM. The ETA model is initialized with global meteorological data from NCEP, USA. Three days air pollution forecasts are produced on operational basis, four times every day. The models create huge amounts of output data from a single run. These data are treated with advanced and fast visualization techniques for easy comprehension.

Automated system

The system is fully automated – meaning that the whole procedure of receiving the data, running the models, producing the visualizations and sending the specified result to the end users is controlled by cron-jobs and Unix scripts. The whole system and the operational procedure have been run, tested and validated since August 1998.

Continuous development

The system is in a state of continuous development and validation. The different models are tested against measurement data and improvements in model concepts, algorithms and visualization techniques are continuously carried out. The improved models, methods and algorithms are implemented if tests show to improve the model output with respect to measurements.

This report

In this report, the different models, the coupling/integration of the models, the input and output, the visualizations and their real time performance on fast workstations with parallel architecture will be described. Some examples of model results and preliminary validations will be shown. Also the end user interface is described. The system has been prepared to include additional cities and streets. However, new implementations also require additional input data such as emission, street configuration and traffic data. These data must be provided by the end user.

1 Introduction

Background

Episodes with high levels of harmful air pollution concentrations, as e.g. ozone, can have damaging effects on human health and plants. In order to minimize the effects of these episodes it is necessary to be able to predict them. An operational air pollution modelling system is an important tool that can be used for air pollution forecasting, monitoring and scenarios. Where critical limit values are exceeded, an operational air pollution forecast system can be used to inform and warn the public. An operational system can be integrated in national urban and rural monitoring networks. Furthermore, it can be used to study the effects from emission reduction scenarios, where emissions from e.g. a part of the traffic are reduced in the model. Such scenarios can be used as guidelines for the authorities for making decisions on restrictions on e.g. traffic, during episodes of high air pollution levels.

The THOR system

Over the last decades, several different air pollution models have been developed at the National Environmental Research Institute, NERI, Department of Atmospheric Environment, ATMI, Denmark. These models cover a wide range of scales (from hemispheric scale to local street scale) and applications. Coupling these models with a weather forecast model in an operational system opens a variety of possible applications. The developed system is called the DMU-ATMI THOR air pollution forecast system.

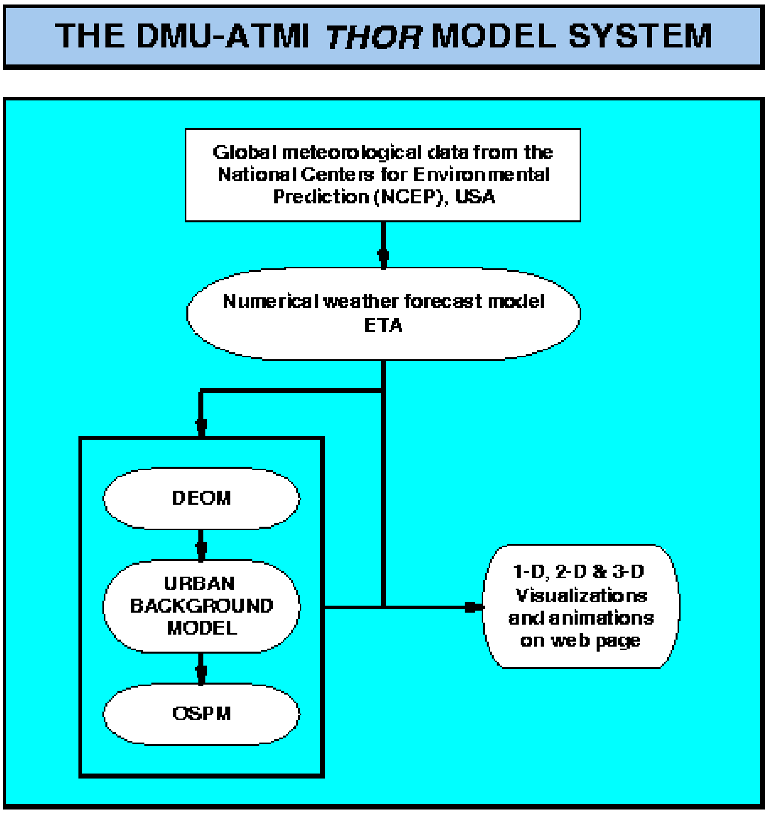


Figure 1. A schematic diagram of the main modules and the data flow in the DMU-ATMI THOR air pollution forecast system.

The ETA model

A schematic diagram of the different modules and the data flow chart of the DMU-ATMI THOR air pollution forecast system is shown in Figure 1. Presently, the model system consists of a coupling of four models. A numerical weather forecast model, ETA is applied (Anadranistakis et al., 1998; Missirlis et al., 1998; Nickovic et al., 1998a; Nickovic et al., 1998b; Papageorgiou et al., 1998). This model is initialized with data from a global circulation model run at the National Centers for Environmental Prediction, NCEP, USA. Data from this global circulation model is the starting point for nearly all weather forecasts in USA.

The DEOM model

The numerical weather forecast is subsequently used as input to a long-range transport air pollution model, the Danish Eulerian Operational Model, DEOM, that calculates air pollution forecasts on European scale. DEOM is an operational version of the Danish Eulerian Model, DEM (Brandt et al., 1996; Zlatev 1995; Zlatev et al., 1992). DEM has been run and validated by comparison to EMEP measurements over a period of 10 years (1989-1998).

The BUM and OSPM models

Meteorological data from ETA and air pollution concentrations from DEOM are used as input to the Background Urban Model, BUM (Berkowicz, 1999b), which calculates the urban background pollution using emissions on a 2 km x 2 km grid covering the whole city of Copenhagen. The output from BUM is used as input to the Operational Street Pollution Model, OSPM, (Berkowicz, 1999a; Berkowicz et al., 1997) which describes the air pollution concentrations on street level, at both sides of the street in major cities.

Four times a day

The weather forecasts, the European air pollution forecasts, the urban background forecast and the street canyon forecast are currently run operationally, four times every day, initiated with data at 00 UTC, 06 UTC, 12 UTC and 18 UTC.

Visualizations

The system produces huge amounts of output data in every run. These data are impossible to comprehend without fast and advanced visualization and animation techniques. For every forecast, nearly 1000 visualizations and animations are produced and systemized so they can be seen with the use of an Internet browser. In this way, it is easy to follow the temporal and spatial development of the air pollution levels and to discover whether critical air pollution limit values will be exceeded. In the case of a predicted exceedance of the critical limit values for e.g. ozone, the population can be informed or alerted. A demonstration of the whole system including visualizations, animations and time series of the weather and air pollution concentrations is available at the web page:

http://www.dmu.dk/AtmosphericEnvironment/thor

Furthermore, operational data are available for Denmark, for the city of Copenhagen and for the street of Jagtvej in Copenhagen. The operational air pollution forecast can be found at the web page:

http://luft.dmu.dk

2 The model system

2.1 The Danish Eulerian Operational Model, DEOM

The DEOM model

The Danish Eulerian Operational Model, DEOM, calculates the regional background pollution levels on European scale. The operational version of the model calculates transport, dispersion, deposition and chemistry of 35 species. Three vertical layers are presently used. The three layers are defined as a mixed layer (below the mixing height), a smog layer (between the present mixing height and the advected mixing height from the previous day) and the top layer that is located between the advected mixing height and the free troposphere. Experiments have been carried out with a fourth layer, the emission layer (close to the ground). However performance improvements were not achieved. The emission data used in DEOM is a combination of data provided by the European Monitoring and Evaluation Programme (EMEP) (with a spatial resolution of 50 km x 50 km) and the Danish emission inventories which have a resolution of down to 1 km x 1 km. The data include emissions of NO_x, SO_2, NH_3 and anthropogenic VOC emissions. Biogenic VOC emissions are calculated from land use data. Examples of NO_x emissions used in the model for Europe and Denmark are shown in Figures 2 and 3.

Equations

The model is based on a system of partial differential equations (PDE's):

$$
\begin{aligned}
\frac{\partial c_s}{\partial t} = & -u\frac{\partial c_s}{\partial x} - v\frac{\partial c_s}{\partial y} \\
& + K_x\frac{\partial^2 c_s}{\partial x^2} + K_y\frac{\partial^2 c_s}{\partial y^2} \\
& - (\kappa_{1s} + \kappa_{2s})\, c_s \\
& + E_s \\
& + Q_s(c_1, c_2, \ldots, c_q) \\
& + V(c_s) \\
s = 1, 2, \ldots, q &
\end{aligned}
$$

where q is the number of the chemical species. The horizontal advection is represented by the first two terms on the right-hand-side of the equation. The third and the fourth terms describe the horizontal dispersion. The dry and wet deposition terms, $-(\kappa_{1s} + \kappa_{2s})c_s$, are linear, while the chemistry term, $Q_s(c_1, c_2, \ldots, c_q)$, introduces non-linearity. The concentrations are denoted by c_s, u, v are wind velocities, K_x, K_y are dispersion coefficients, assumed constant 10000 $m^2\ s^{-1}$, E_s describe the emission sources, κ_{1s} and κ_{2s} are dry and wet deposition coefficients, respectively, and the chemical reactions are denoted by $Q_s(c_1, c_2, \ldots, c_q)$. Different vertical exchange procedures, $V(c_s)$, which are

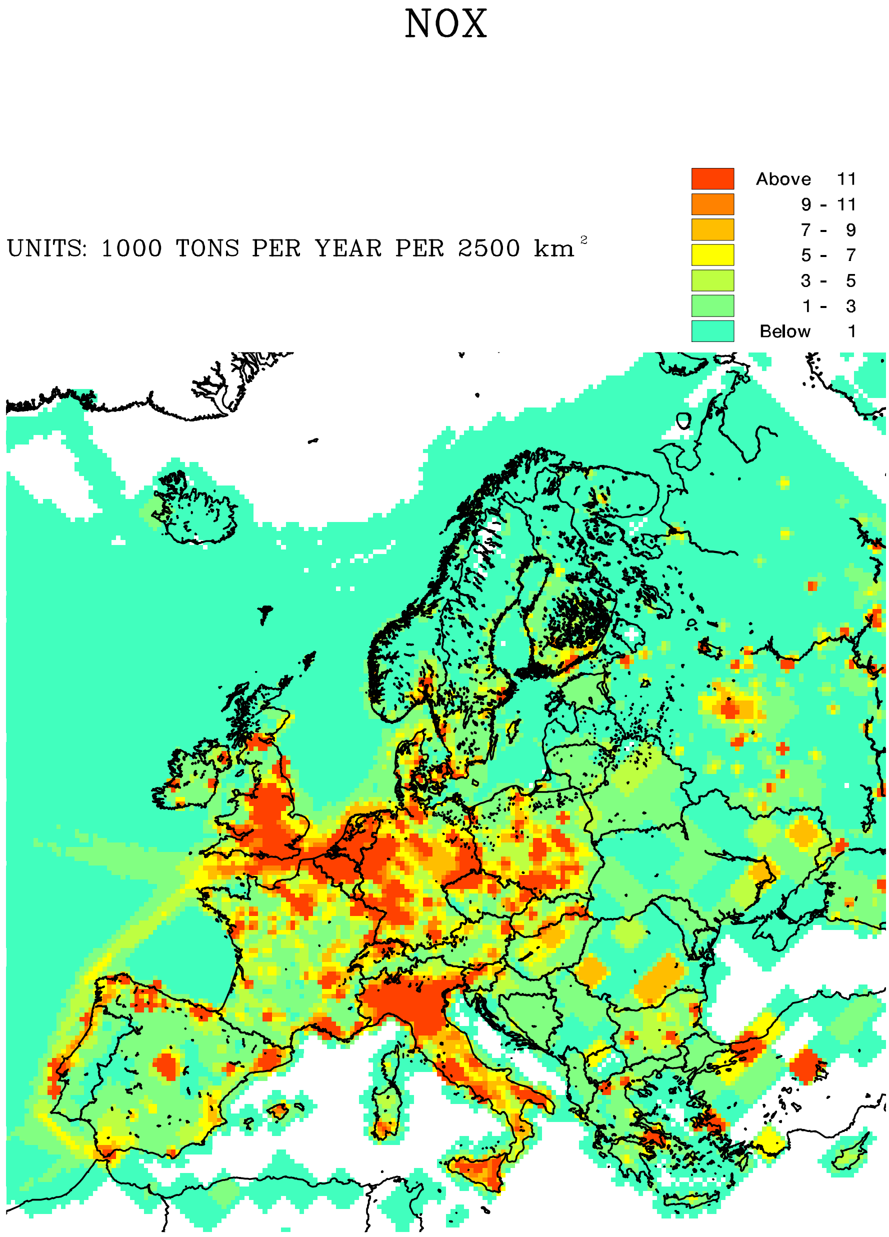


Figure 2. Example of NO_x emissions used in DEOM for Europe. The grid resolution is 25 km x 25 km.

functions depending on the number of layers have been developed, based on ideas in Pankrath (1988).

Numerical methods

It is difficult to treat the system of equations directly. Therefore, the model is split into four sub-models. A simple splitting procedure, based on ideas from Marchuk (1985) and McRae et al. (1984), can be defined. The four sub-models include (1) horizontal transport, (2) horizontal dispersion (3) dry and wet deposition, and (4) emissions and chemistry. An Accurate Space Derivative algorithm is used to handle the transport and dispersion terms in the first sub-model. Time integration for the advection term is performed with a predictor-corrector scheme with several correctors (Zlatev, 1995). For the horizontal dispersion, truncated Fourier series approximate the concentrations. It is then possible to find an analytical solution for each Fourier coefficient in the Fourier space. The deposition terms are solved directly. The chemical scheme used in the model is the CBM-

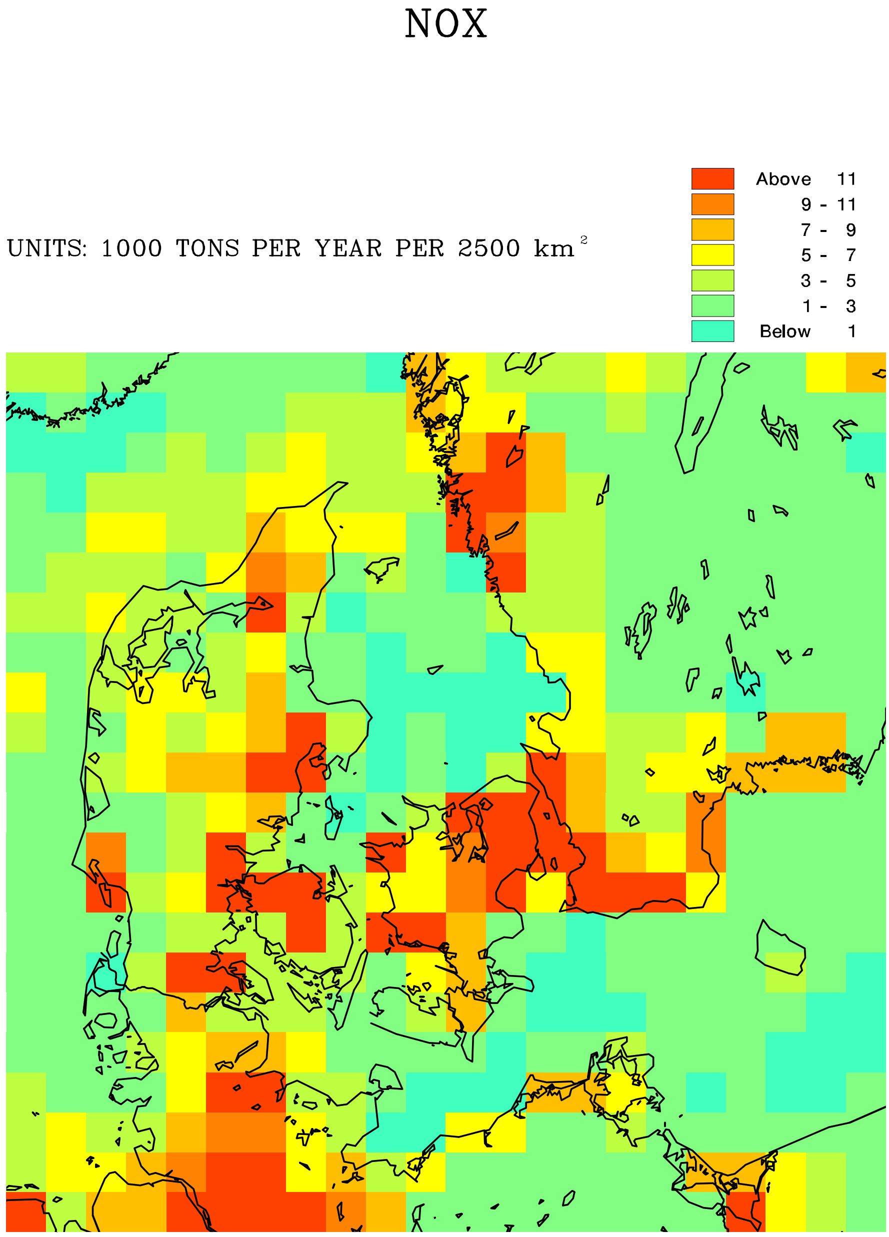


Figure 3. Example of NO_x emissions used in DEOM, for Denmark. The grid resolution is 25 km x 25 km.

IV scheme (Zlatev et al., 1992). Chemistry is solved using the QSSA method (Hesstvedt et al., 1978).

Resolution

It is possible to run the model with up to 4 layers and 2 different horizontal resolutions (25 km x 25 km or 50 km x 50 km). Higher resolution and more layers increase the computing time but can also increase the precision of the results.

2.2 The Background Urban Model, BUM

The BUM model

The BUM model is suitable for calculations of urban background concentrations when the dominating source is the road traffic. For this source the emissions take place at ground level, and a good approximation is to treat the emissions as area sources, but with an initial vertical dispersion determined by the height of the buildings.

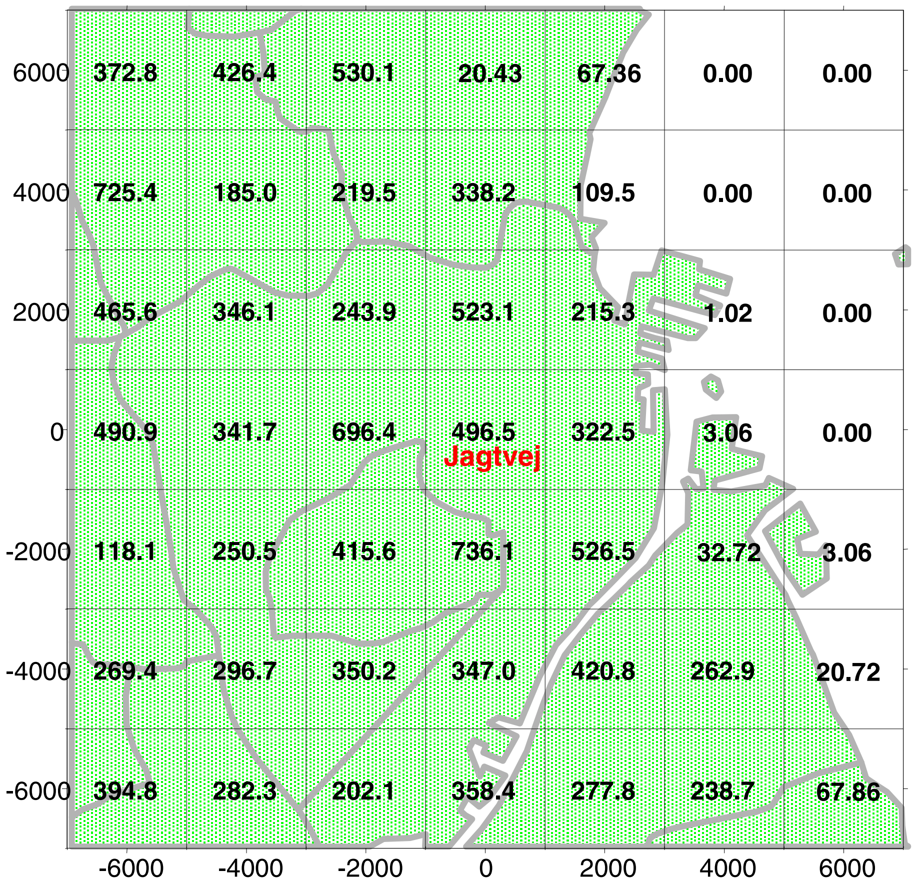


Figure 4. Average daily emissions of NO_x in Copenhagen (in kg/grid/day). Units in the x- and y-axes are distance in m from the centre of the grid (Berkowicz, 1999b).

Model description

Contributions from the individual area sources, subdivided into a grid with a resolution of 2 km x 2 km, are integrated along the wind direction path assuming linear dispersion with the distance to the receptor point. Horizontal dispersion is accounted for by averaging the calculated concentrations over a certain, wind speed dependent, wind direction sector, centred on the average wind direction. Formation of the nitrogen dioxide due to oxidation of NO by ozone is calculated using a simple chemical model based on an assumption of photochemical equilibrium on the time scale of the pollution transport across the city area. This time scale governs the rate of entrainment of fresh rural ozone (Berkowicz, 1999b).

Emission data used in the model have to be provided on a grid with the same resolution as used in the model. An example of NO_x emissions for Copenhagen, Denmark, is given in Figure 4.

2.3 The Operational Street Pollution Model, OSPM

The OSPM model

The OSPM model is a parameterized semi-empirical model making use of a priori assumptions about the flow and dispersion conditions in a street canyon, see Figure 5. In the model, concentrations of exhaust gases are calculated using a combination of a plume model for the direct contribution and a box model for the recirculating part of the pollutants in the street. Parameterization of flow and dispersion conditions in street canyons was deduced from extensive analysis of experimental data and model tests. Results from these tests have been used to improve the model performance, especially with regard to different street configurations and a variety of meteorological conditions. The model calculates air concentrations of NO, NO_2, NO_x, O_3, CO and Benzene in the street canyon at both sides of the street. For a more detailed description of the model, see Berkowicz (1999a).

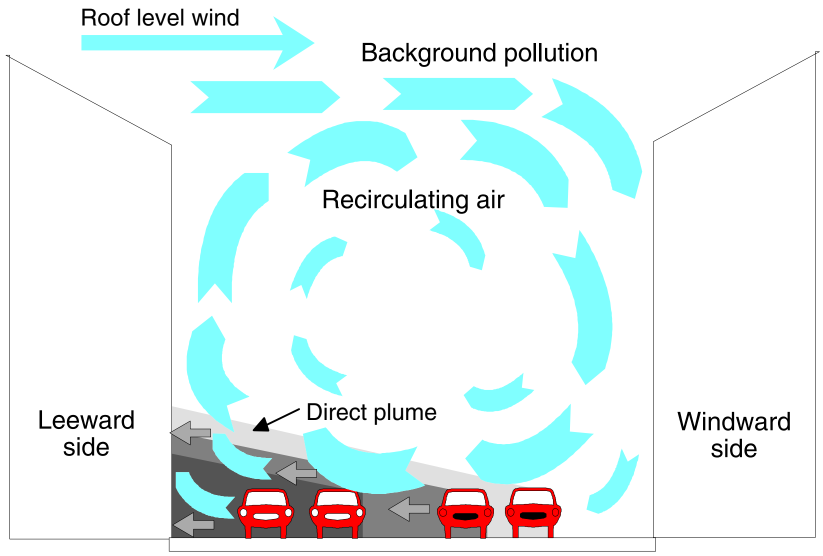


Figure 5. An illustration of the flow and dispersion conditions in a street canyon (Berkowicz, 1999a).

2.4 Model configurations and performance

Optimization on fast computers

When operational air pollution forecasts are produced, it is important that the different models and the model system is optimized on fast computers and that the system is fully automated, in order to ensure available prognoses early in the morning. The THOR system has been optimized to run operationally on two powerful workstations, both SGI Origin 200 with 4 processors. One machine is dedicated to run the models and the other to produce visualizations and animations.

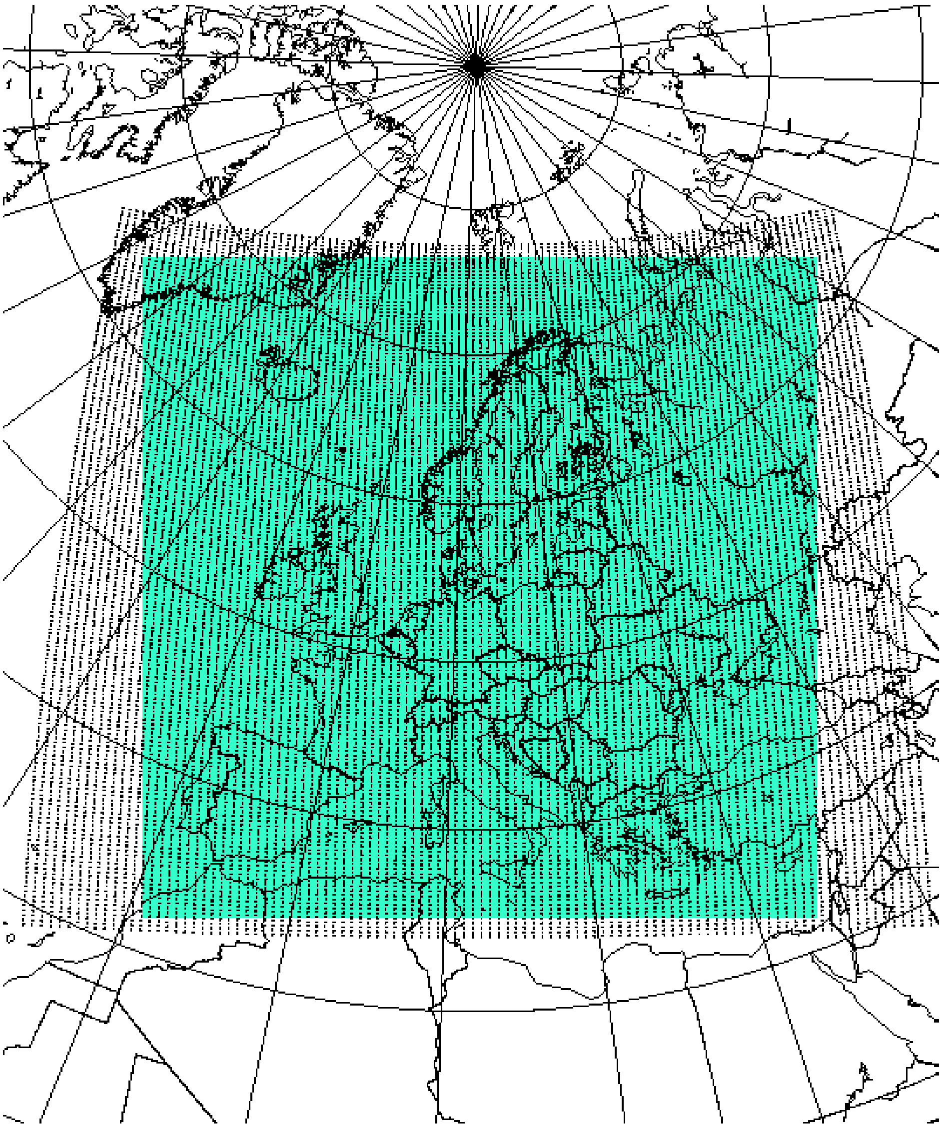


Figure 6. The model domains of the ETA model (dots) and the Danish Eulerian Operation Model (shaded square). The center of the domains is at DMU, Roskilde, Denmark.

Configurations

The production time for one total forecast depends, of course, on the configuration of the models with respect to the number of grid points and the grid resolution. The ETA model is run on a staggered Arakawa E grid using a latitude/longitude system with shifted pole. The horizontal grid resolution is 0.25° x 0.25° corresponding to approximately 39 km at 60° north. The number of horizontal grid points is 104 x 175 and the number of vertical layers is 32. The Danish Eulerian Operational Model is applied on a polar stereographic projection using an Arakawa A grid. The horizontal grid resolution is optional. The model can be run with a 25 km x 25 km or a 50 km x 50 km grid resolution at 60° north, corresponding to 192 x 192 or 96 x 96 horizontal grid points, respectively, when preserving the model domain. The possible greater precision obtained with higher resolution must be weighted against the higher computing time (8 times higher with a change of resolution from 50 km to 25 km). The model domains of the two models are displayed in Figure 6.

Performance

The ETA and DEOM models have been parallellized and are running with a speed-up of approximately 3.5 when 4 processors are used and with a real performance of approximately 350 MFLOPS. The theoretical peak performance of this Origin 200 is 1.8 GFLOPS so the efficiency is 20% of the peak performance. This is generally considered very good on parallel machines. The visualizations and animations are calculated on another similar workstation. By the time the weather forecast is finished, the air pollution forecast will be running simultaneously with the production of the visualizations of the weather forecasts on the two different computers.

Time for one forecast

The time spent on the different operational tasks is shown in Table 1. The total time required for calculating a 3 days forecast is around 3 hours, including the data transfer from NCEP (which takes around 30 min) and the production of the visualizations.

Table 1. Real time performance of the model system for a total forecast on SGI Origin 200 (225 MHz) with 4 processors

Task	Approximate time
Data transfer of global meteorological data from NCEP	30 min
ETA model	130 min
Danish Eulerian Operational Model	9 min (50 km, 3 layers)
BUM and OSPM	< 1 sec
Production of visualization and animations	30 min
Total time for a single forecast	~ 3 hours

2.5 System input

The input data required for the different models are summarized below. Setting up additional cities and additional streets in these cities requires new input files to the models BUM and OSPM. A detailed description of data types, etc. can be found in the section: “System interface for the end users”.

ETA

- Global meteorological data from NCEP.
- Land use data.
- Topography data.

DEOM

- Regional emission data (EMEP and DK emissions).
- Meteorological data from ETA.
- Land use data.

BUM

- Regional air pollution data from DEOM.
- Meteorological data from ETA.
- Local city emission data.

OSPM

- Urban air pollution data from BUM.
- Meteorological data from ETA.
- Local street emission data.
- Local street configuration data (building heights, street width, street orientation, etc.).
- Local street traffic data.
- Yearly traffic factors.

Examples of the input files to OSPM can be found in the appendix.

2.6 System output

Visualization techniques

Not all model results are visualized on a regular basis. In the regional air pollution model, 35 species are included and only a few of these are used for visualization. The output chosen for visualization is summarized in Table 2. There are 3 different visualization techniques:

- Contour plots
- Animated contour plots (animated GIF-files and Java animations)
- Time series

All parameters from ETA and DEOM are visualized using the 3 different techniques. Time series can be chosen from a map showing predefined locations (see Figure 7a and 7b). Two different maps are included: one for Europe and one for Denmark. The output from BUM and OSPM is visualized as time series.

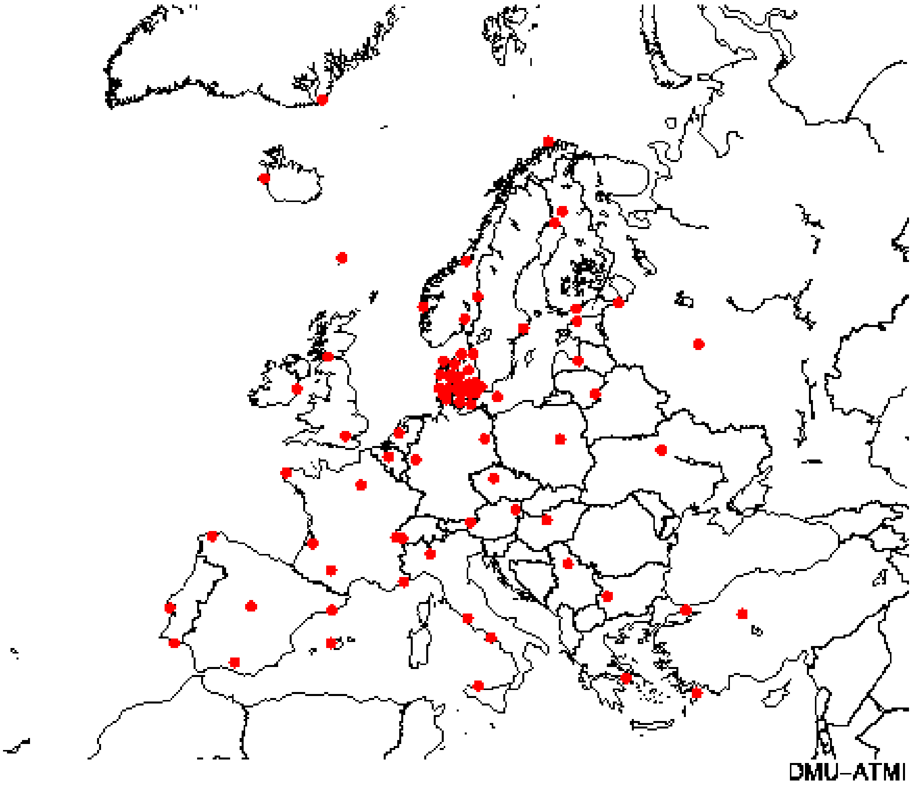


Figure 7a. Predefined locations for time series for the weather forecast and for the regional air pollution forecast. Clicking on Denmark gives a detailed map over the area with surroundings (see Figure 7b). More stations can easily be implemented.

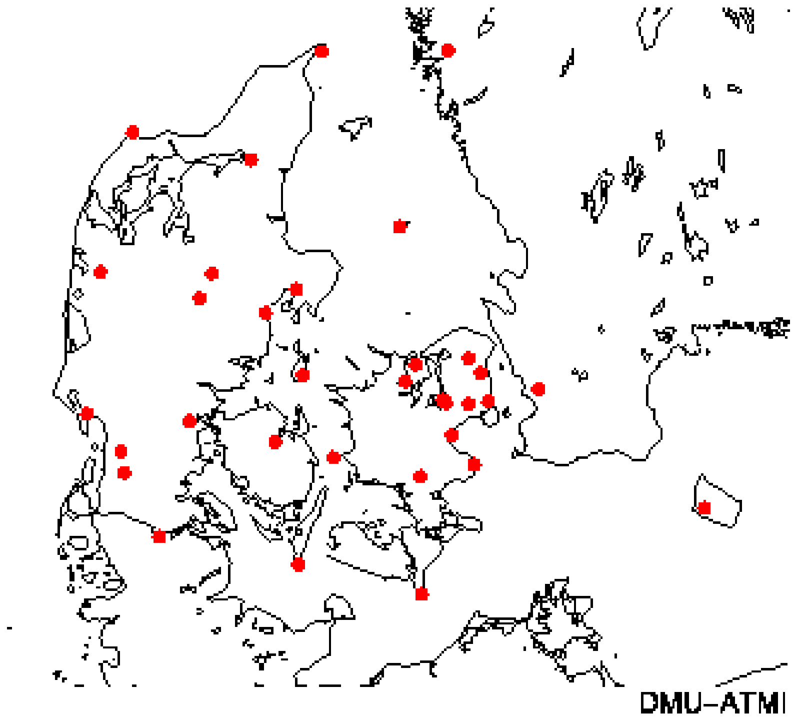


Figure 7b. Predefined locations for time series for the weather forecast and for the regional air pollution forecast in Denmark.

Table 2. summary of the visualized model output from the 4 different models

Model	Parameters	Resolution
ETA	Wind direction (10 m) Wind speed (10, 80 and 800 m) Temperature (2, 80 and 800 m) Mean Sea Level Pressure, MSLP Precipitation (convective, stratisform, snow and total) Snow cover Planetary boundary layer height Friction velocity Surface heat flux Relative humidity (80 and 800 m) Cloud cover fraction (high and low clouds) Cloud volume fraction 850 hPa winds, geopotential heights and temperature 500 hPa winds, geopotential heights and temperature	Spatial resolution: ~ 39 km Temporal resolution: Time series 1 hour Contour and animations: 6 hour
DEOM	O_3, NO, NO_2, NO_x, SO_2 and SO_4	Spatial resolution: ~ 25 km or ~ 50 km Temporal resolution: Time series: 1 hour Contour and animations: 6 hour
BUM	O_3, NO, NO_2 and NO_x	Spatial resolution: 2 km Temporal resolution: Time series: 1 hour
OSPM	NO_x, NO_2, O_3, CO and benzene	Spatial resolution: Both sides of the street Temporal resolution: Time series: 1 hour

3 Model results

3.1 Examples of model results

1000 visualizations

A typical output from a forecast consists of several Gigabytes of data. Different visualization techniques have been developed and implemented in the system. The visualization programmes produce at the moment nearly 1000 postscript files (which are converted to GIF files for use in the web page), 2 to 4 times a day. A demonstration of these results can be seen at the previously mentioned web page.

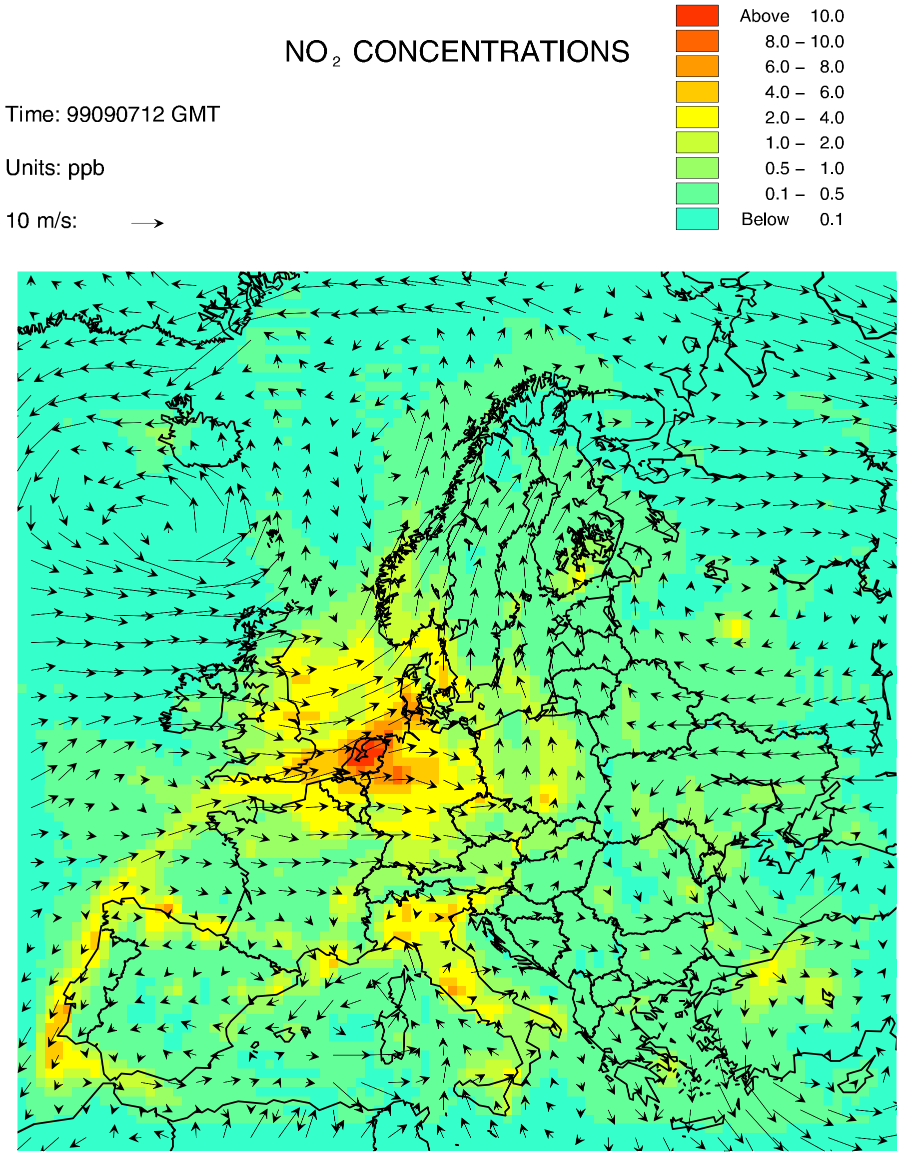


Figure 8. Calculated NO_2 concentrations on September 7th, 12 UTC, 1999.

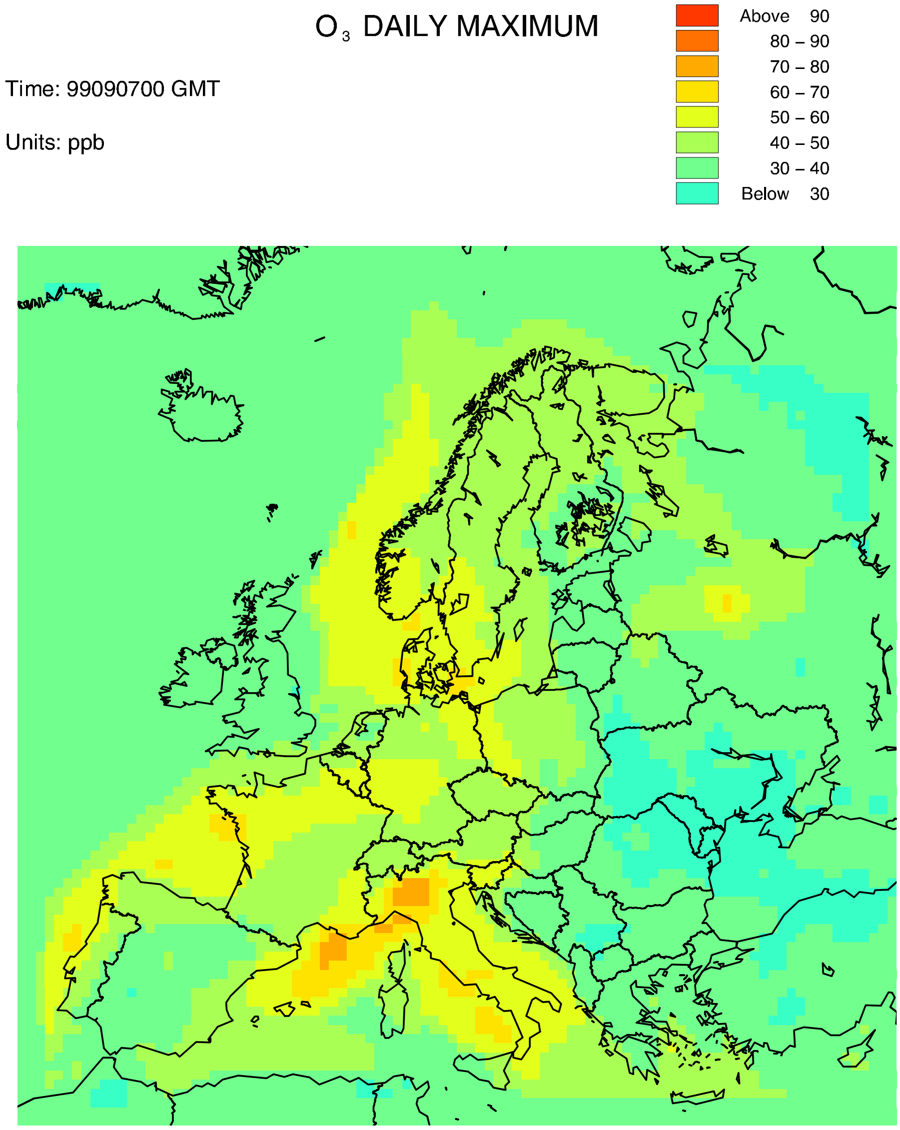


Figure 9. Calculated daily O_3 maximum concentrations on September 7th, 1999.

DEOM examples

In Figure 8 and 9 typical example of an air pollution forecast for Europe is shown. The forecast is initiated at September 7th, 00 UTC, 1999. The figures show the NO_2 concentrations and the daily maximum ozone concentrations over Denmark at September the 7th. At this date there was an ozone episode over Denmark with concentrations just below 90 ppb. The model predicted ozone concentrations between 80 ppb and 90 ppb in the area. Measurements obtained from Ulborg in the western part of Jutland showed maximum values of 85 ppb. The forecast system predicted this ozone episode 3 days in advance of the actual event. The maximum concentrations were predicted to occur at 14.00 hours. This was in total agreement with measurements. The ozone concentrations are given as hourly mean values, representative for the grid-cell with the resolution of 25 km x 25 km (or 50 km x 50 km). According to the last EU directives, the population should be warned when the hourly mean ozone concentration exceeds 90 ppb and alerted when the ozone concentration exceeds 120 ppb.

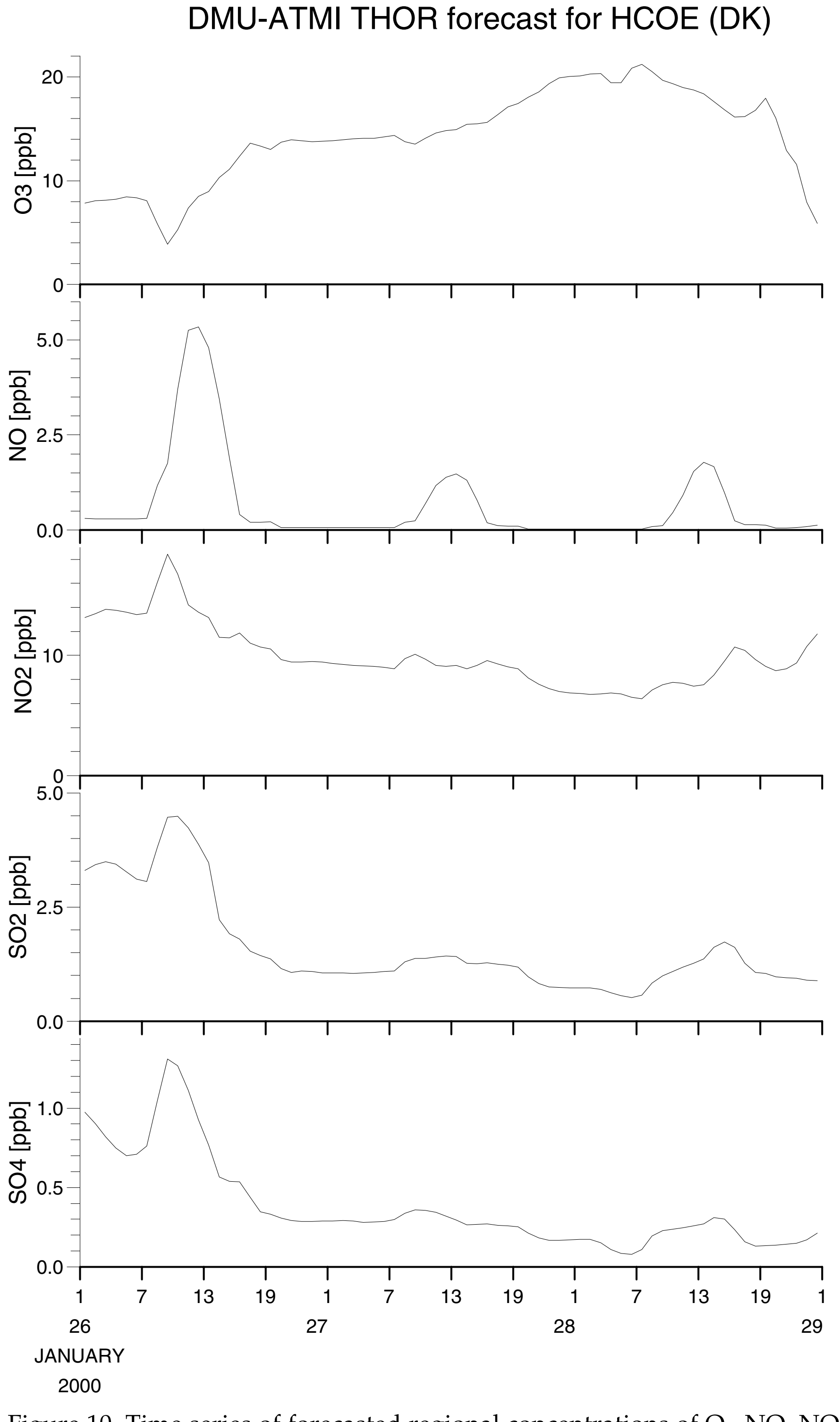


Figure 10. Time series of forecasted regional concentrations of O_3, NO, NO_2, SO_2 and SO_4 over Copenhagen, for the period January 26th, 00 UTC, to January 29th, 00 UTC, 2000. Results are calculated using the regional air pollution model, DEOM.

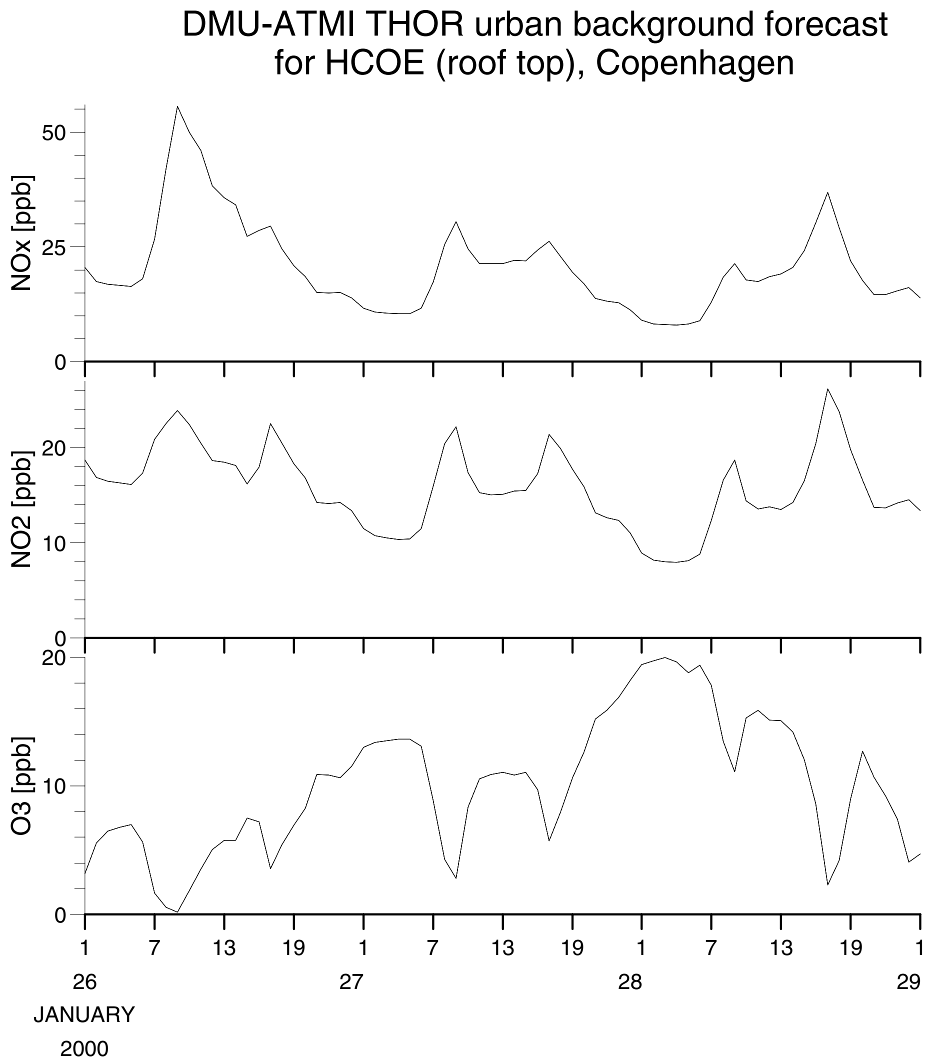


Figure 11. Time series of forecasted urban concentrations of NO_x, NO and O_3 over Copenhagen, for the period January 26th, 00 UTC, to January 29th, 00 UTC, 2000. Results are calculated using the background urban model, BUM.

Time series at specific locations

Visualizations of the daily maximum ozone concentrations over an area provide an effective tool for monitoring such warning or alert situations. More detailed information is available in the THOR system. For nearly one hundred locations in Europe (Figures 7a and 7b), time series are produced for some of the most important species.

Figure 10 shows an example of the regional air pollution time series for Copenhagen, Denmark. The results from the regional forecast and the weather forecast are used as input to the urban background forecast, shown in Figure 11. The model calculates concentrations at roof level. The results are together with the weather forecast used as input to the operational street pollution model, OSPM. This model calculates air concentrations in the street canyon at both sides of the street. An example is seen in Figure 12. Depending on the wind direction, there can be major differences in the air concentrations at the two sides of the street.

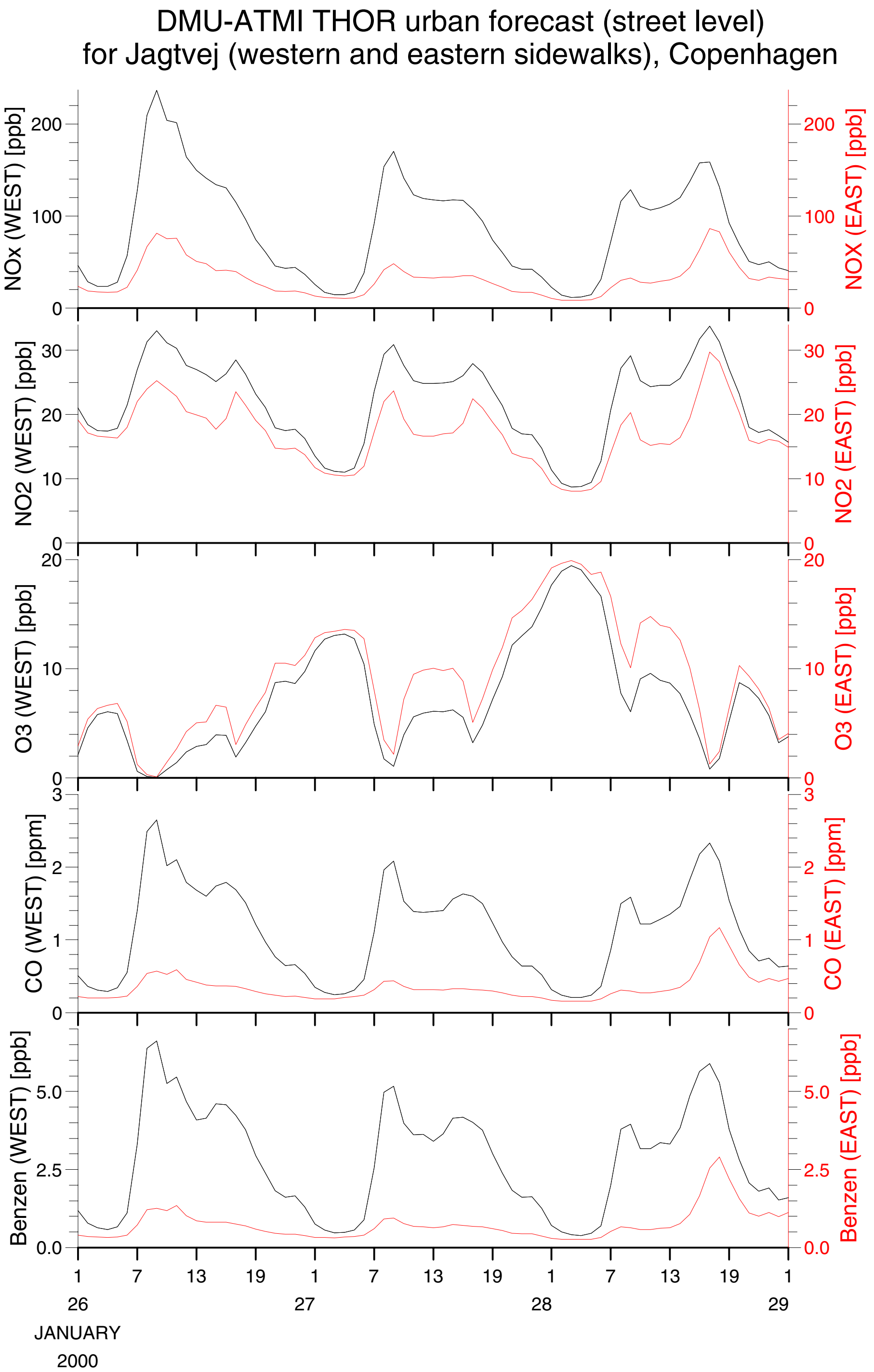


Figure 12. Time series of forecasted street canyon concentrations of NO_x, NO_2, O_3, CO and benzene in the street Jagtvej, Copenhagen, for the period January 17th, 00 UTC, to January 20th, 00 UTC, 2000. The black curves are the concentrations at the western side and the red curves are the concentrations at the eastern side of the street. Results are calculated using the Operational Street Pollution Model, OSPM. Notice the daily double peaks resulting from the two rush hours (in the morning and in the afternoon).

3.2 Data supply statistics

The 3-day weather forecasts have been run operationally since August 10th, 1998. Since that date, data have been obtained twice a day (00 UTC and 12 UTC). From August 12th, 1999 data have additionally been obtained for the 06 UTC and 18 UTC initialization times. Figure 13 shows the number of global meteorological data missing from NCEP per month in the period August 10th, 1998 to December 31st, 1999. Considering only the 00 UTC and 12 UTC forecasts, data have been transferred from NCEP 1018 times in the period August 10th 1998 to December 31st, 1999. In this period it happened only 19 times that data could not be obtained from the American server, corresponding to 1.9%. However, considering the year 1999, the amount of data missing is only 0.8%. This is due to general improvements and developments in the system and in the scripts developed for automatic receiving data. It should be emphasized that whenever data were missing, the forecast from the previous initialization time covered the full period. In this way there are no "holes" in the meteorological data time series. In case of missing data, the previous forecast can be used, and the data supply security is therefore very satisfying.

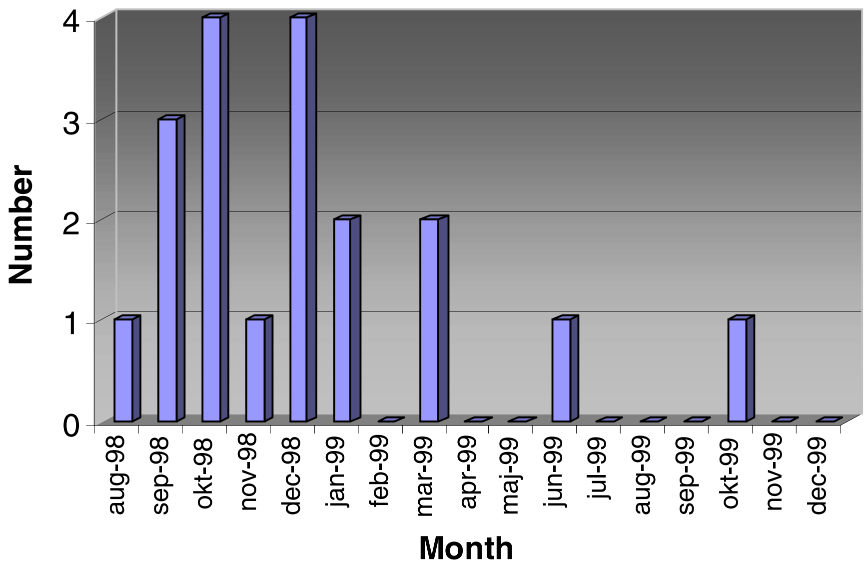


Figure 13. Number of global meteorological data missing from NCEP per month in the period August 10th, 1998 to December 31st, 1999.

3.3 Examples of validations of the different models

The whole model system is continuously being validated against measurements. Measurement data from the Danish rural and urban monitoring networks are used for comparisons (Kemp and Palmgren, 1999; Skov et al., 1999). Furthermore, Risø National Laboratory, Denmark has provided meteorological data from the Risø mast. Some results are shown in Figures 14 to 20.

ETA validation at the Risø mast

In Figure 14 and Table 3 some results from the comparisons of ETA model results (12 hours forecast) and meteorological data from the Risø mast are shown. The parameters include hourly values of surface pressure, wind direction, temperature (2 m), global radiation and precipitation for September, 1998. The cloud cover from the model has been included, since the global radiation and the precipitation depend on this parameter. It should be emphasized that the measured wind direction at 125 m height has been compared to a wind direction in the model representative for the mixing height. Therefore a small bias is seen.

Statistics

In Table 3, statistics for the curves have been calculated. These include the number of data samples, *N*, mean values, standard deviations, correlation coefficient with test for significance, figure of merit, *FM*, the bias with the 95% confidence interval, the fractional bias, *FB*, the fractional standard deviation, *FSD* and the normalized mean square error, *NMSE* with 95% confidence interval. These statistical parameters give a good indication of the system performance concerning both mean values and data variability. Detailed explanations for all these statistical parameters can be found in Appendix 2, see also Brandt (1998).

Comparisons of the measured pressure with the modelled pressure gives a correlation coefficient of 1.00 and mean values of practically the same value. This is extremely good! For the wind direction, temperature and global radiation the statistical tests gives correlation coefficients of above 0.8 and small differences in mean values. The global radiation depends on the cloud cover in the model, so test of this parameter gives an indication of the quality of the modelled cloud cover.

ETA validation at HCØ institute

In Figure 15 and Table 4 similar results from the comparisons of ETA model results (12 hours forecast) and meteorological data from the roof at the HCØ institute located in Copenhagen, Denmark, are shown. The parameters included are hourly values of wind speed (10 m), wind direction (10 m), temperature (2 m), global radiation and relative humidity. However, no measurements are available for the relative humidity. The statistical tests show very good agreement between model results and measurements.

OSPM validations

Figures 16 to 18 give examples of comparisons of OSPM model results (12 hours forecast) and air pollution measurement data at street level (eastern side of the street) for Jagtvej, located in Copenhagen, Denmark. The parameters included are hourly values of O_3, NO, NO_2, CO and NO_x.

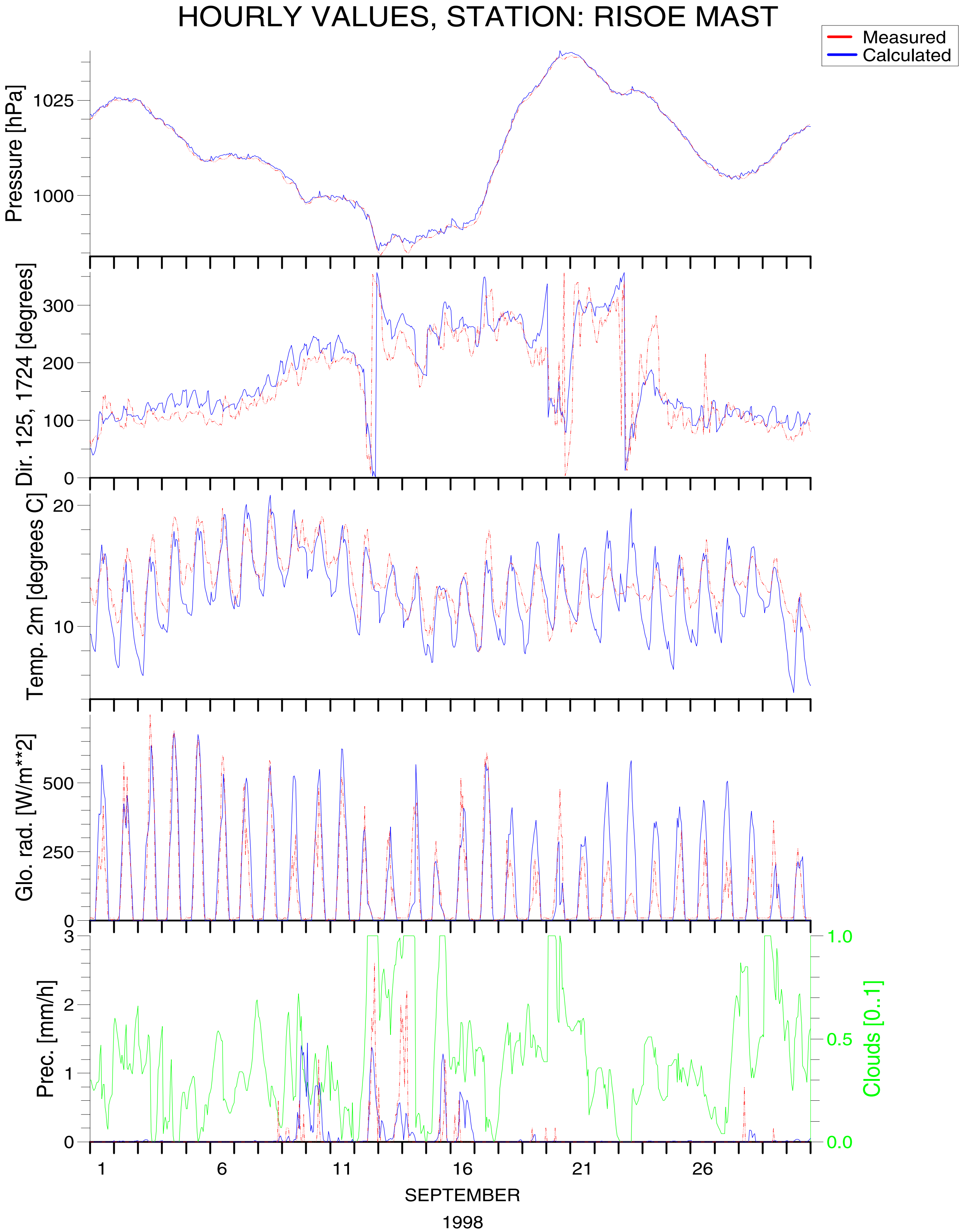


Figure 14. Comparisons of hourly values of measurements (red curves) and 12 hours forecasts using the ETA model (blue curves) for September 1998 at Risø, Denmark. Green curve is the total cloud cover from the ETA model.

Table 3. Statistics for pressure, wind direction, temperature, global radiation and precipitation for the curves in Figure 14. The statistics include the number of points, N, calculated and measured mean values, calculated and measured standard deviations, correlation coefficient with test for significance (values above 3.31 are significant within a significance level of 0.1%), Figure of Merit, FM, bias with 95% confidence interval, fractional bias, FB, Fractional Standard Deviation, FSD, and Normalized Mean Square Error, NMSE, with 95% confidence interval.

Parameter N=720	Surface pressure	Wind direction	Temperature	Global radiation	Precipitation
Calculated mean	1011.59	178.36	12.70	134.68	0.07
Measured mean	1011.25	167.03	13.76	105.88	0.05
Calc. std. deviation	13.63	77.70	3.11	176.03	0.22
Meas. std. deviation	13.78	76.63	2.31	153.37	0.26
Correlation coefficient	1.00	0.84	0.83	0.84	0.48
(test for significance)	(-)	(41.47)	(40.24)	(40.79)	(14.61)
FM	99.95%	84.86%	88.34%	61.10%	24.55%
Bias	0.342	11.334	-1.062	28.807	0.015
(CI 95%)	(0.047)	(3.192)	(0.128)	(7.080)	(0.018)
FB	0.000	0.066	-0.080	0.239	0.249
FSD	-0.021	0.028	0.576	0.274	-0.344
NMSE	0.000	0.068	0.024	0.715	15.993
(CI 95%)	(0.000)	(0.024)	(0.003)	(0.121)	(4.489)

For a description of the measurement data and techniques, see (Kemp and Palmgren, 1999). Figure 16 shows comparisons for September 1998, Figure 17 for October 1998 and Figure 18 for March 1999. The statistical results in Tables 5-7 show correlation coefficients of around 0.8-0.9 for the nitrogen-oxide compounds and CO and 0.6-0.8 for ozone. Ozone depends more on the long-range transported air pollution compared to the nitrogen-oxide compounds which depends more on local sources.

Uncertainties

In Figures 16-18 it is seen that the OSPM model underestimates a few measured peak values with duration of only one hour. The reason for this could be uncertainties in the local emission sources or uncertainties in the wind for low wind speed conditions. Vehicles with higher emissions than assumed in the model or deviations from the traffic data can generate these peak values in the measurements. The emissions in the model are estimated from mean values of traffic data and large deviations from the means can, of course, not be described in such a model.

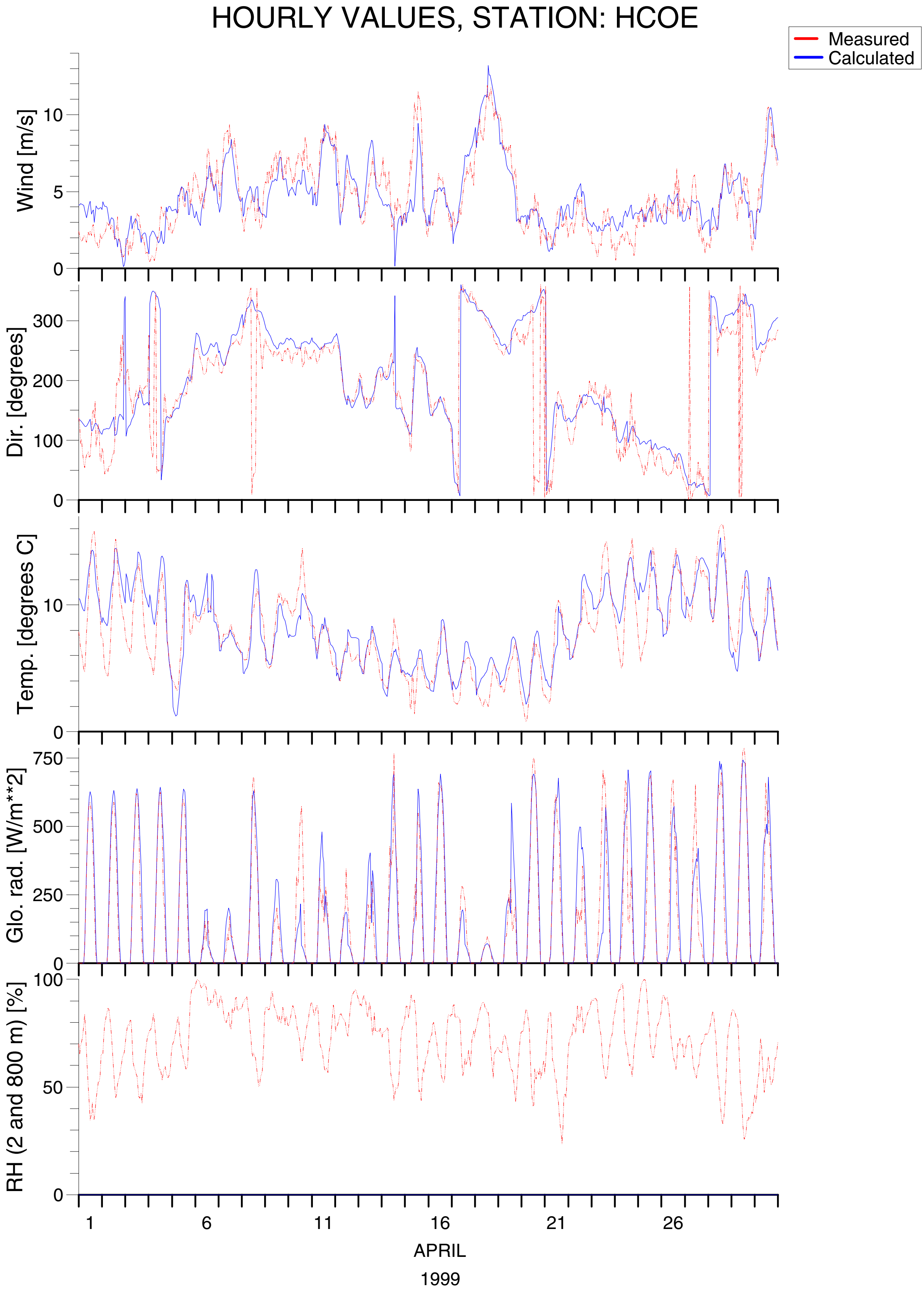


Figure 15. Comparisons of hourly values of measurements (red curves) and 12 hours forecasts using the ETA model (blue curves) for April 1999 at HCØ (roof), Copenhagen, Denmark, (only model results are shown for the relative humidity).

Table 4. Statistics for wind speed (10 m), wind direction (10 m), temperature (2 m), global radiation for the curves in Figure 15. The statistics include the number of points, N, calculated and measured mean values, calculated and measured standard deviations, correlation coefficient with test for significance (values above 3.31 are significant within a significance level of 0.1%), Figure of Merit, FM, bias with 95% confidence interval, fractional bias, FB, Fractional Standard Deviation, FSD, and Normalized Mean Square Error, NMSE, with 95% confidence interval.

Parameter N=720	Wind speed	Wind direction	Temperature	Global radiation
Calculated mean	4.61	203.98	8.28	167.29
Measured mean	4.57	187.05	7.85	152.38
Calc. std. deviation	2.09	90.25	3.07	218.09
Meas. std. deviation	2.39	90.03	3.25	210.30
Correlation coefficient	0.85	0.73	0.87	0.91
(test for significance)	(42.36)	(28.72)	(46.58)	(57.23)
FM	79.82%	84.07%	(85.20)	74.14%
Bias	0.033	16.932	0.428	14.913
(CI 95%)	(0.094)	(4.831)	(0.120)	(6.824)
FB	0.007	0.087	0.053	0.093
FSD	-0.275	0.005	-0.112	0.073
NMSE	0.078	0.122	0.044	0.351
(CI 95%)	(0.010)	(0.034)	(0.005)	(0.075)

Scatter plots

In Fig. 19a-19d comparisons of modelled and measured daily mean values as scatter plots of NO, NO_2, NO_x and CO concentrations at street level at Jagtvej, Copenhagen, Denmark, are shown. The modelled values are daily mean values of the 12 hours forecast, meaning that two forecasts are included in the daily mean. In Figures 20a-20d similar scatter plots are given, however, for these plots the daily maximum values of NO, NO_2, NO_x and CO concentrations at Jagtvej have been compared to measurements. The period is from August 1998 to September 1999. Statistics are given in the figures and indicate that the forecasted concentrations are very close to measurements. Mean values and standard deviations are nearly the same and high correlation coefficients are seen. There is a small bias in the CO plot. The reason for this is that CO at the moment is not included in the BUM model, so the contribution from the urban background is missing. CO and benzene will be included in BUM in the future.

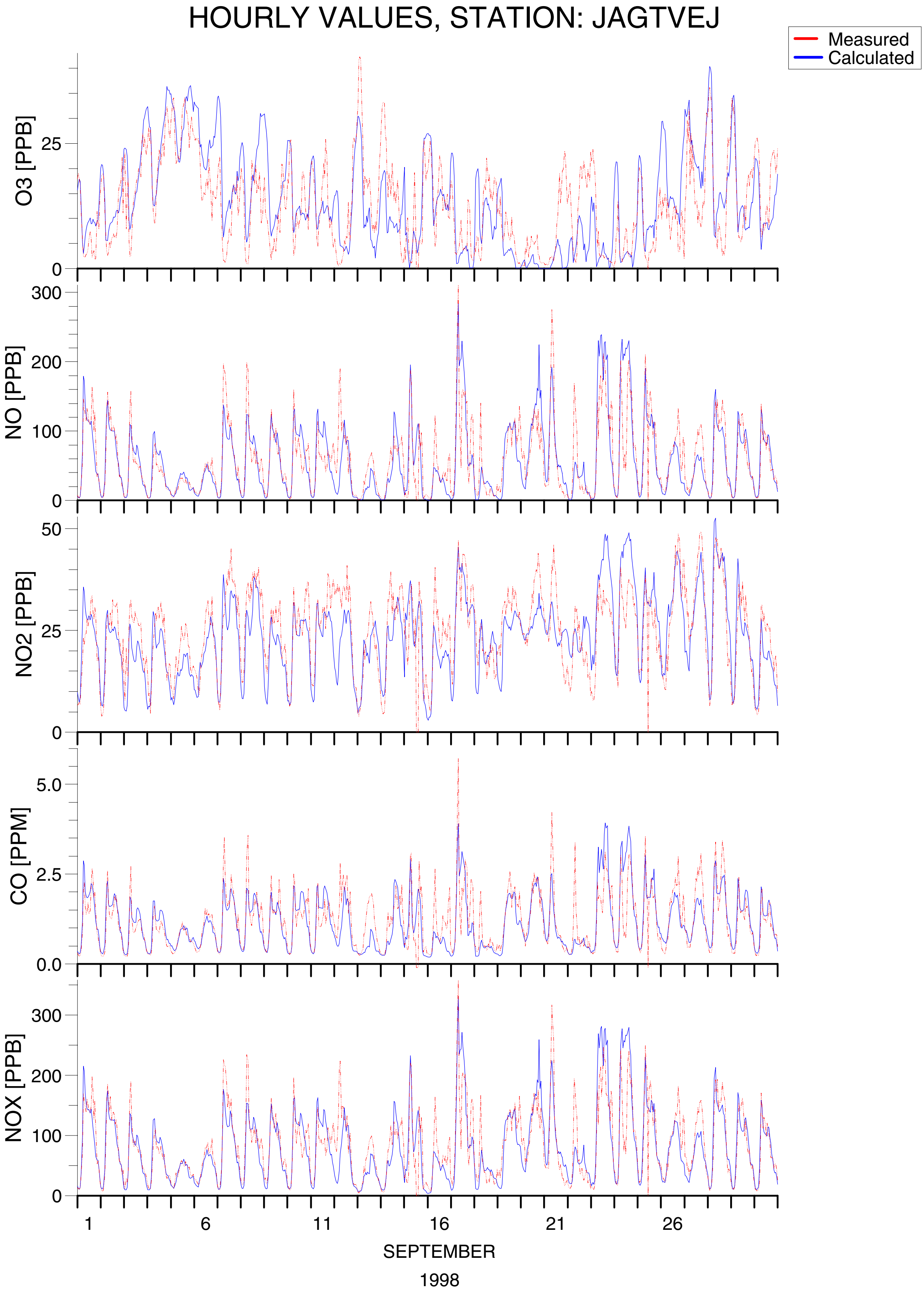


Figure 16. Comparisons of hourly values of measurements (red curves) and 12 hours forecasts using the OSPM model (blue curves) for September 1998 at Jagtvej (eastern side), Copenhagen, Denmark.

Table 5. Statistics for O_3, NO, NO_2, CO and NO_x for the curves in Figure 16. The statistics include the number of points, N, calculated and measured mean values, calculated and measured standard deviations, correlation coefficient with test for significance (values above 3.31 are significant within a significance level of 0.1%), Figure of Merit, FM, bias with 95% confidence interval, fractional bias, FB, Fractional Standard Deviation, FSD, and Normalized Mean Square Error, NMSE, with 95% confidence interval.

Parameter **N=716**	**O_3**	**NO**	**NO_2**	**CO**	**NO_x**
Calculated mean	13.64	57.31	23.51	1.16	80.81
Measured mean	12.89	59.98	25.18	1.22	85.15
Calc. std. deviation	9.54	53.09	9.81	0.76	60.89
Meas. std. deviation	8.76	50.84	9.89	0.79	58.61
Correlation coefficient	0.72	0.81	0.77	0.80	0.83
(test for significance)	(27.65)	(37.26)	(32.73)	(35.14)	(39.41)
FM	66.56%	70.97%	79.96%	75.95%	75.74%
Bias	0.750	-2.670	-1.671	-0.064	-4.341
(CI 95%)	(0.505)	(3.337)	(0.485)	(0.036)	(2.576)
FB	0.056	-0.046	-0.069	-0.054	-0.052
FSD	0.171	0.087	-0.015	-0.061	0.076
NMSE	0.274	0.298	0.079	0.175	0.182
(CI 95%)	(0.037)	(0.060)	(0.006)	(0.039	(0.035)

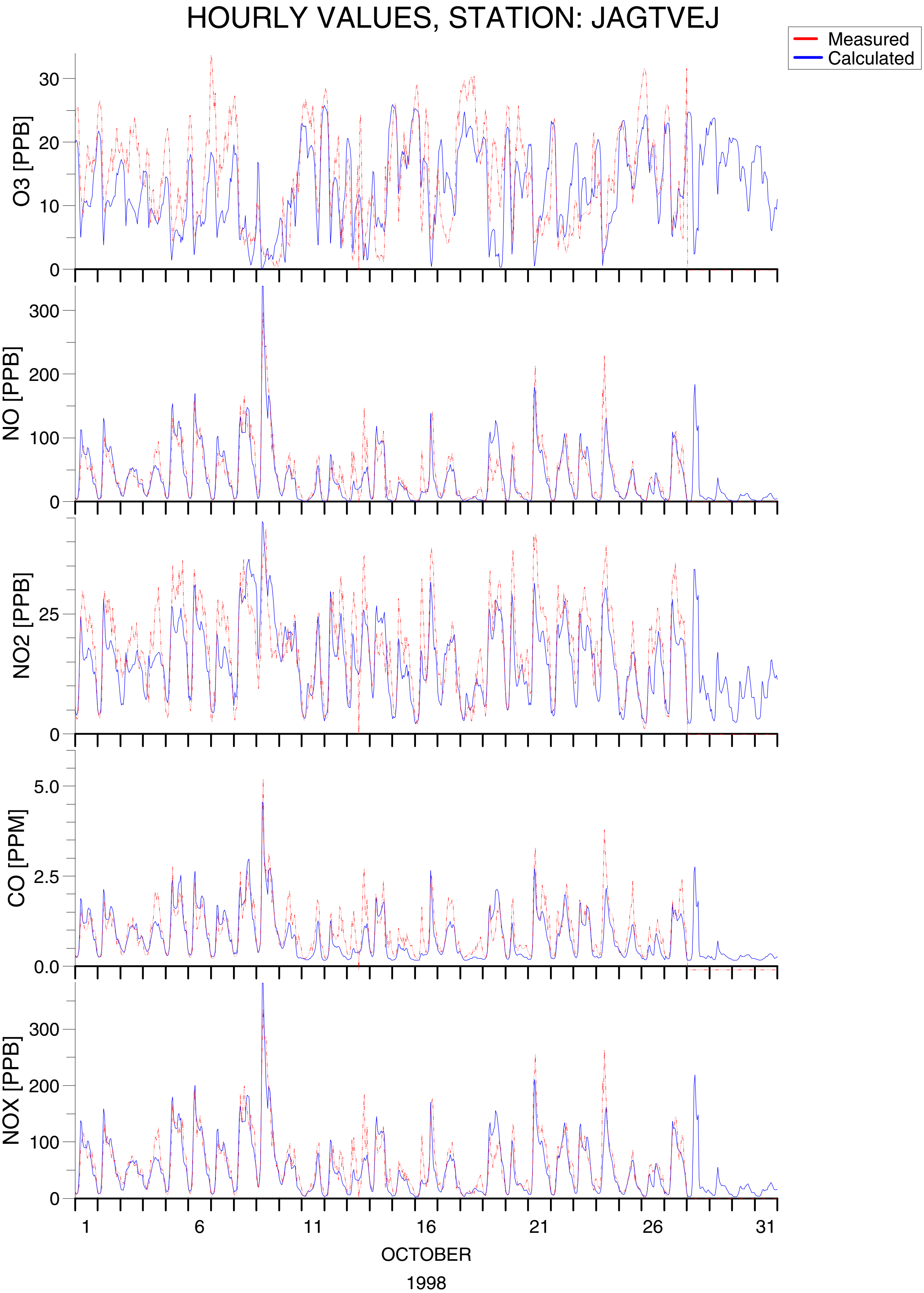


Figure 17. Comparisons of hourly values of measurements (red curves) and 12 hours forecasts using the OSPM model (blue curves) for October 1998 at Jagtvej (eastern side), Copenhagen, Denmark.

Table 6. Statistics for O_3, NO, NO_2, CO and NO_x for the curves in Figure 17. The statistics include the number of points, N, calculated and measured mean values, calculated and measured standard deviations, correlation coefficient with test for significance (values above 3.31 are significant within a significance level of 0.1%), Figure of Merit, FM, bias with 95% confidence interval, fractional bias, FB, Fractional Standard Deviation, FSD, and Normalized Mean Square Error, NMSE, with 95% confidence interval.

Parameter **N=716**	**O_3**	**NO**	**NO_2**	**CO**	**NO_x**
Calculated mean	12.51	41.41	15.59	0.85	57.00
Measured mean	14.54	44.41	18.34	1.01	62.75
Calc. std. deviation	6.45	43.67	7.83	0.65	50.39
Meas. std. deviation	7.77	43.51	9.00	0.67	51.16
Correlation coefficient	0.73	0.88	0.83	0.86	0.90
(test for significance)	(26.88)	(47.88)	(38.03)	(42.73)	(51.23)
FM	70.53%	73.27%	76.07%	74.34%	76.73%
Bias	-2.025	-3.000	-2.751	-0.156	-5.751
(CI 95%)	(0.416)	(1.623)	(0.386)	(0.027)	(1.787)
FB	-0.150	-0.070	-0.162	-0.169	-0.096
FSD	-0.369	0.007	-0.278	-0.036	-0.030
NMSE	0.183	0.246	0.114	0.172	0.159
(CI 95%)	(0.013)	(0.057)	(0.010)	(0.026)	(0.033)

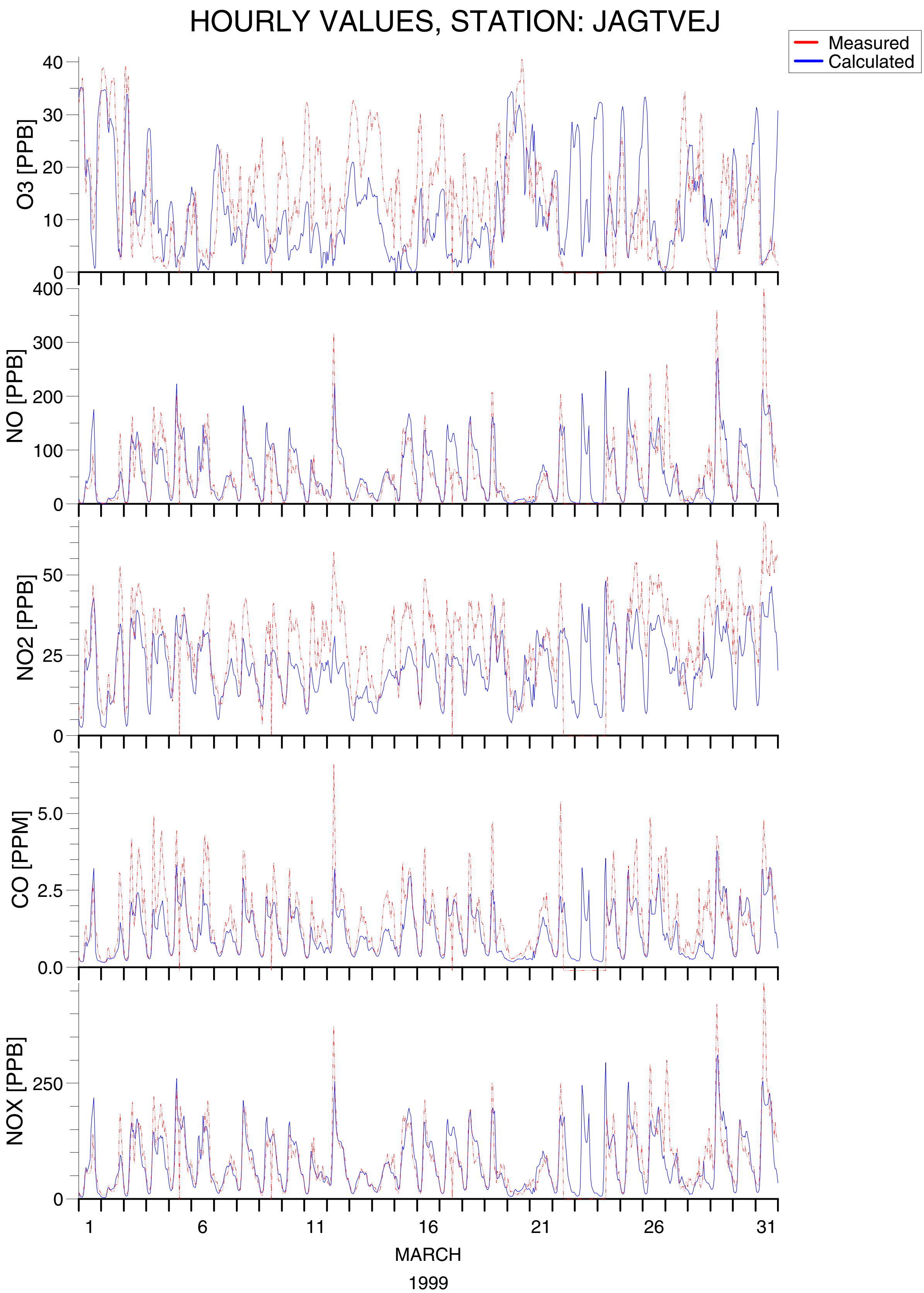
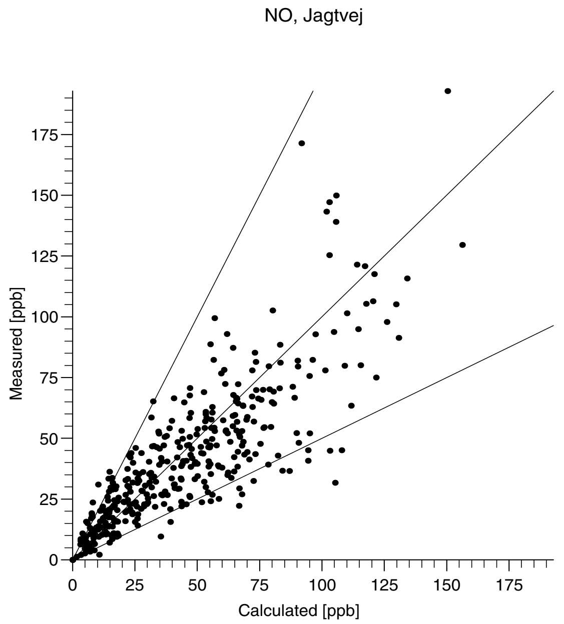


Figure 18. Comparisons of hourly values of measurements (red curves) and 12 hours forecasts using the OSPM model (blue curves) for March 1999 at Jagtvej (eastern side), Copenhagen, Denmark.

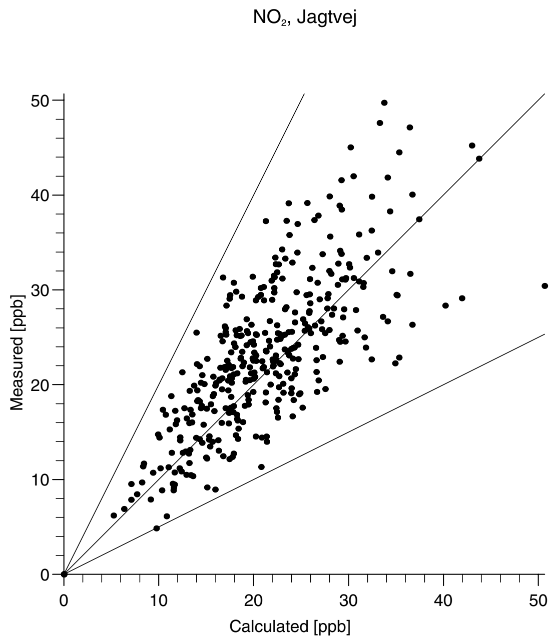
Table 7. Statistics for O_3, NO, NO_2, CO and NO_x for the curves in Figure 18. The statistics include the number of points, N, calculated and measured mean values, calculated and measured standard deviations, correlation coefficient with test for significance (values above 3.31 are significant within a significance level of 0.1%), Figure of Merit, FM, bias with 95% confidence interval, fractional bias, FB, Fractional Standard Deviation, FSD, and Normalized Mean Square Error, NMSE, with 95% confidence interval.

Parameter **N=695**	**O_3**	**NO**	**NO_2**	**CO**	**NO_x**
Calculated mean	11.64	57.08	21.32	1.13	78.39
Measured mean	14.39	55.57	29.35	1.57	84.92
Calc. std. deviation	8.77	51.52	9.25	0.76	58.83
Meas. std. deviation	9.57	57.81	12.20	1.07	67.73
Correlation coefficient	0.60	0.80	0.80	0.83	0.82
(test for significance)	(19.56)	(34.69)	(35.38)	(38.87)	(38.07)
FM	57.37%	67.72%	69.95%	68.29%	73.94%
Bias	-2.748	1.502	-8.030	-0.422	-6.528
(CI 95%)	(0.615)	(2.631)	(0.543)	(0.045)	(2.876)
FB	-0.211	0.027	-0.317	-0.328	-0.080
FSD	-0.176	-0.229	-0.541	-0.654	-0.280
NMSE	0.454	0.395	0.188	0.323	0.231
(CI 95%)	(0.067)	(0.056)	(0.011)	(0.049)	(0.031)



N = 385, means: calculated = 45.86, measured = 42.38
Standard deviations: calculated = 31.07, measured = 28.73
correlation = 0.83, test (H: corr=0) = 28.83, FM = 74.48%
bias = 3.479, ci_{bias}(95%) = +/- 1.771, FB = 0.079, FSD = 0.157
NMSE = 0.168, ci_{NMSE}(95%) = +/- 0.027

Figure 19a. Comparisons of measurements and the daily mean values of the 12 hours forecasted NO, modelled concentrations at Jagtvej, Copenhagen, Denmark for the period August 1998 to September 1999.



N = 385, means: calculated = 21.54, measured = 23.24
Standard deviations: calculated = 7.11, measured = 7.93
correlation = 0.74, test (H: corr=0) = 21.29, FM = 81.73%
bias = -1.699, ci_{bias}(95%) = +/- 0.552, FB = -0.076, FSD = -0.217
NMSE = 0.067, ci_{NMSE}(95%) = +/- 0.007

Figure 19b. Comparisons of measurements and the daily mean values of the 12 hours forecasted NO_2 modelled concentrations at Jagtvej, Copenhagen, Denmark for the period August 1998 to September 1999.

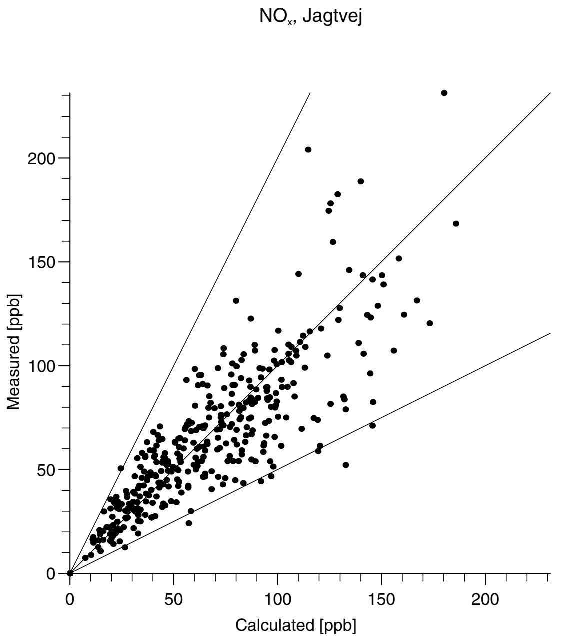


Figure 19c. Comparisons of measurements and the daily mean values of the 12 hours forecasted NO_x modelled concentrations at Jagtvej, Copenhagen, Denmark for the period August 1998 to September 1999.

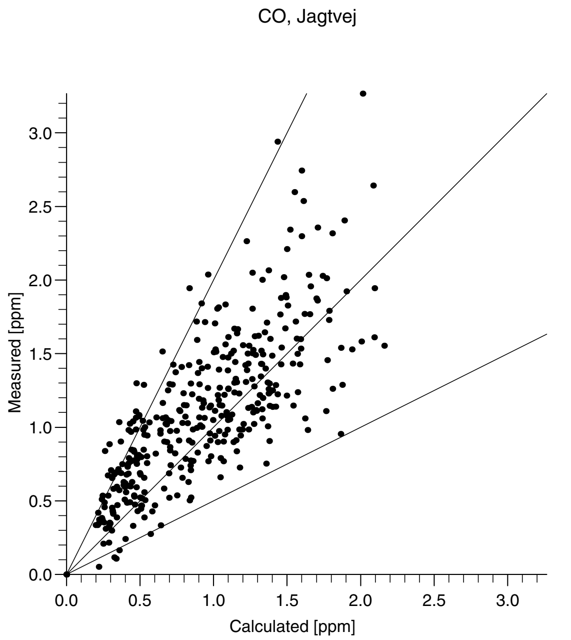
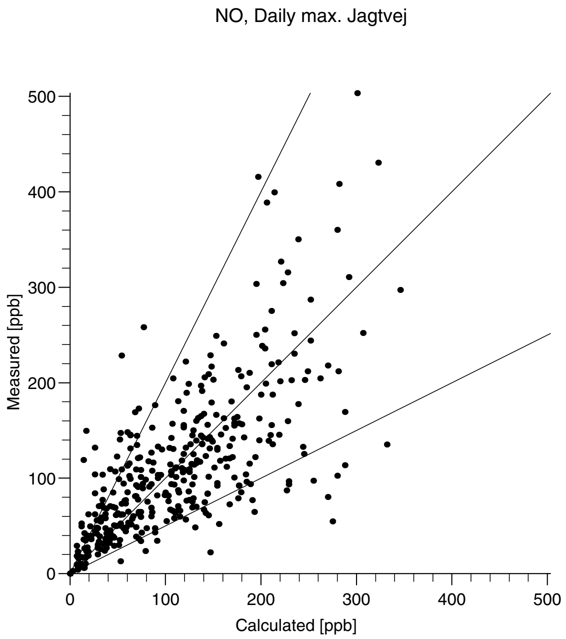
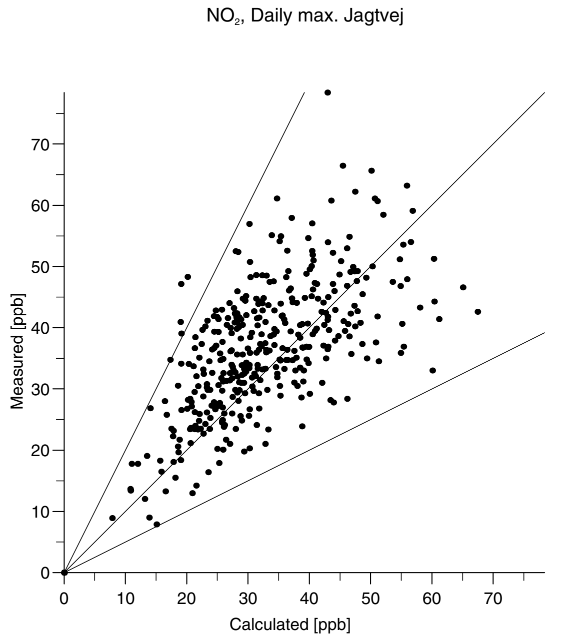


Figure 19d. Comparisons of measurements and the daily mean values of the 12 hours forecasted CO modelled concentrations at Jagtvej, Copenhagen, Denmark for the period August 1998 to September 1999.



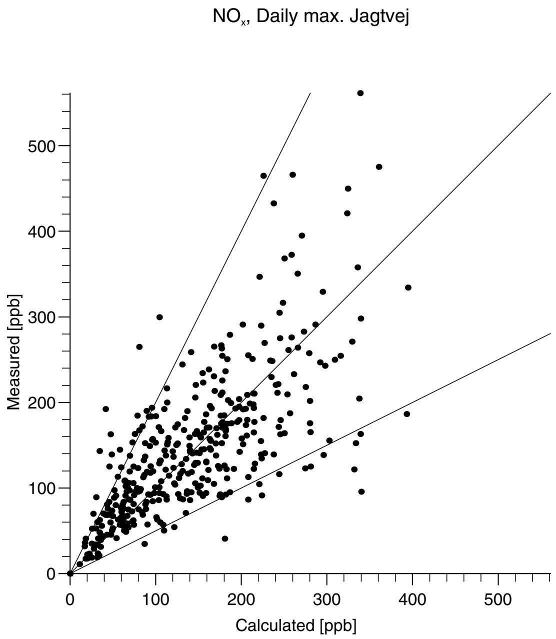
N = 397, means: calculated = 111.16, measured = 110.33
Standard deviations: calculated = 73.54, measured = 76.91
correlation = 0.71, test (H: corr=0) = 20.06, FM = 69.21%
bias = 0.830, $ci_{bias}(95\%)$ = +/- 5.648, FB = 0.007, FSD = -0.089
NMSE = 0.268, $ci_{NMSE}(95\%)$ = +/- 0.059

Figure 20a. Comparisons of measurements and the daily maximum values of the 12 hours forecasted NO modelled concentrations at Jagtvej, Copenhagen, Denmark for the period August 1998 to September 1999.



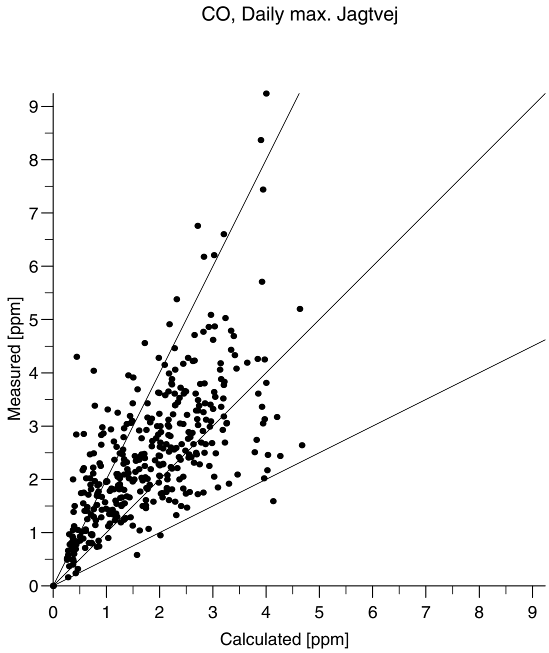
N = 397, means: calculated = 32.81, measured = 36.21
Standard deviations: calculated = 10.36, measured = 10.62
correlation = 0.61, test (H: corr=0) = 15.31, FM = 79.76%
bias = -3.393, $ci_{bias}(95\%)$ = +/- 0.912, FB = -0.098, FSD = -0.049
NMSE = 0.082, $ci_{NMSE}(95\%)$ = +/- 0.011

Figure 20b. Comparisons of measurements and the daily maximum values of the 12 hours forecasted NO_2 modelled concentrations at Jagtvej, Copenhagen, Denmark for the period August 1998 to September 1999.



N = 397, means: calculated = 142.75, measured = 144.71
Standard deviations: calculated = 80.77, measured = 83.29
correlation = 0.71, test (H: corr=0) = 19.98, FM = 73.17%
bias = -1.961, ci_{bias}(95%) = +/- 6.169, FB = -0.014, FSD = -0.061
NMSE = 0.190, ci_{NMSE}(95%) = +/- 0.039

Figure 20c. Comparisons of measurements and the daily maximum values of the 12 hours forecasted NO_x modelled concentrations at Jagtvej, Copenhagen, Denmark for the period August 1998 to September 1999.



N = 396, means: calculated = 1.86, measured = 2.46
Standard deviations: calculated = 1.00, measured = 1.25
correlation = 0.65, test (H: corr=0) = 16.84, FM = 67.17%
bias = -0.604, ci_{bias}(95%) = +/- 0.096, FB = -0.279, FSD = -0.447
NMSE = 0.286, ci_{NMSE}(95%) = +/- 0.043

Figure 20d. Comparisons of measurements and the daily maximum values of the 12 hours forecasted CO modelled concentrations at Jagtvej, Copenhagen, Denmark for the period August 1998 to September 1999.

4 System interface for the end users

Additional cities

The THOR system has been prepared for future implementation of additional cities and streets. However, information for the additional city and street with respect to emissions and traffic has to be provided by the end users.

In order to include new cities, the following information should be provided by the end user:

- A grid with NO_x, CO and benzene emissions covering the city. An example is shown in Figure 4, where the NO_x emissions for Copenhagen, Denmark, is shown. The grid could e.g. have a 2 km x 2 km spatial resolution and should have a temporal resolution of 1 hour for one day. For a grid of e.g. 7 x 7 grid cells, the number of data is 7 x 7 grid cells x 24 hours = 1176 data. The unit of the emission data is [$\mu g\ m^{-2}\ s^{-1}$]. However, emission data can also be generated from the total "traffic work" in the grid cells in the unit of [$km\ hour^{-1}$], meaning the total number of km driven in the grid cell per hour. The diurnal traffic work is required for passenger cars, vans, trucks, buses, and no. of cold starts.

Additional streets

When an additional city has been included an optional number of streets in this city can be included. For every street, the street canyon configuration data as well as traffic data are needed. The street canyon should be defined from the following parameters (examples of input files for the OSPM model can be seen in the appendix):

- Average height of buildings in the street (e.g. 18 m).
- The width of the street (e.g. 25 m).
- The length of the street in the two directions to a main crossroad (e.g. 40 m and 70 m).
- The direction of the street in terms of an angle with respect to north (e.g. 30°). This angle is always in the range from 0° to 180°.
- Exceptions from the average values above. E.g. in the range 215° to 230° the height of the buildings is 25 m. In the range 340° to 350° the height of the buildings is 0 m (a street), etc.

Traffic data

The traffic data are divided into working days, Saturday and Sunday – both for normal conditions and for holiday conditions. The unit of the traffic data is [number of vehicles / hour]. For each of the following temporal periods, traffic data are needed:

- Working days,
- Saturday,
- Sunday,
- Working day, holiday (e.g. in July),
- Saturday, holiday (e.g. in July), and
- Sunday, holiday (e.g. in July).

The traffic data are divided into different groups of vehicles:

- Passenger cars,
- Vans,
- Trucks,
- Buses, and
- Number of cold starts in the street.

Average speed

Furthermore, the average speed of the vehicles is needed for every hour of the day. This average speed is divided on short vehicles (below 7.5 m) and long vehicles (above 7.5 m).

5 Conclusions and future work

5.1 Conclusions

An air pollution forecast system has been developed. At the present, the system includes weather forecasts and air pollution forecasts for the whole of Europe, urban air pollution forecasts for the urban background of Copenhagen, Denmark, and street canyon air pollution forecasts for a single street in Copenhagen. The present system has been optimized and fully automated on local fast workstations. The system is presently being validated against measurements. Some preliminary validation results have been shown. These results indicate very good agreement with measurements.

5.2 Future work

DEHM and DREAM models

Two additional models will furthermore be implemented in the THOR system. These are 1) the Danish Eulerian Hemispheric Model, DEHM, (Christensen, 1995; Christensen 1997) which is used to describe the transport of SO_2, SO_4, Lead and Mercury on hemispheric scale and 2) the Danish Rimpuff and Eulerian Accidental release Model, DREAM, (Brandt 1998; Brandt et al., 1998) which is used to describe the transport, dispersion, deposition and radioactive decay from a nuclear accidental release, as e.g. the Chernobyl accident.

Data assimilation

An important field for further development of the system is data assimilation of real time air pollution measurements, in the same way as is known in weather forecasting. This will require a European corporation concerning exchange of real time measurement data. At the present, data from the Danish monitoring stations are used for real time validation of the system. These measurements will be assimilated into the model for a better estimation of the initial fields in DEOM.

REGINA model

A new high-resolution model, REGINA (REGIonal high resolutioN Air pollution model), is under development for the regional air pollution forecast. The model will be a variable scale model with nesting capabilities, using high-resolution meteorological and land use input data. The model includes 56 chemical species (only 35 species is presently used in DEOM), and will include a full 3-D description of the transport, with an optional number of vertical layers.

MM5 model

It is also planned to include the meteorological meso-scale model, MM5, developed at NCAR/Penn state University, USA, (Grell et al., 1995). Comparisons of results from ETA and MM5 will be carried out. The MM5 model has been used as a meteorological preprocessor for the DREAM model (Brandt 1998; Brandt et al., 1998) and for the DEHM model. MM5 includes nesting capabilities which are useful for a nested version of DEOM. However, preliminary studies indicate that the computing time for MM5 is approximately twice the computing time required for running the ETA model.

In Figure 21, a schematic diagram of the future system is shown (compare with Figure 1). Additional modules are the DEHM, DREAM and MM5 models and data assimilation.

Validation

It is important that the single models and the whole system are validated against operational and historical measurements. At the present, validation of the single models and the whole model system is carried out. Measurements from the Danish urban and rural monitoring network are used.

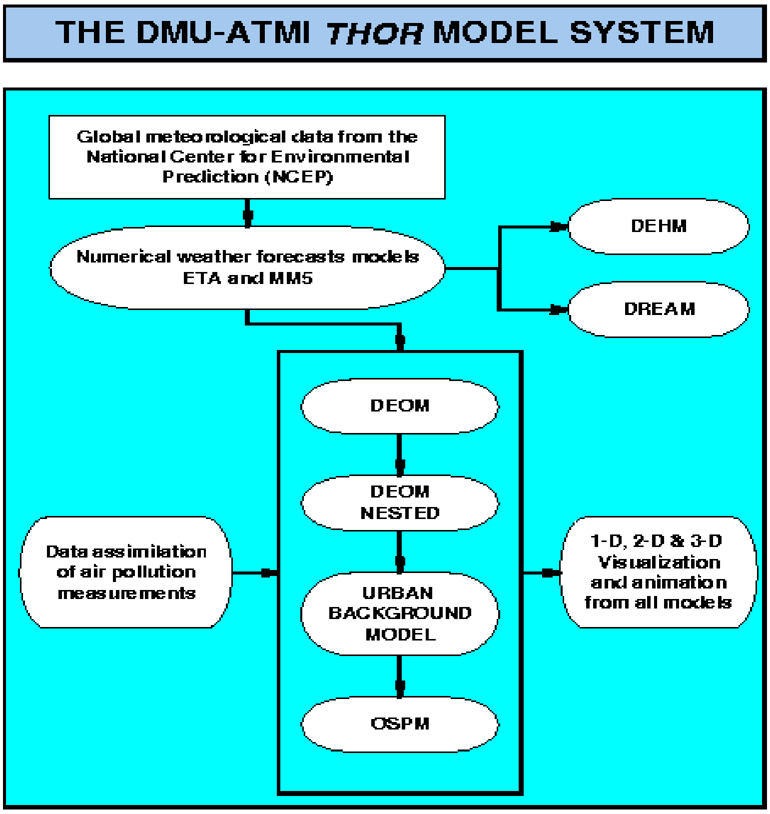


Figure 21a. schematic diagram of the future main modules and the data flow in the DMU-ATMI THOR air pollution forecast system.

5.3 Further information

The operational forecast for Denmark, the City of Copenhagen and for the street of Jagtvej in Copenhagen can be seen at:

http://luft.dmu.dk

A demonstration of the THOR system can be seen at the web page:

http://www.dmu.dk/AtmosphericEnvironment/thor

Some validations of the Danish Eulerian Model can be seen at the page http://www.dmu.dk/AtmosphericEnvironment/dem

Demonstrations of the DREAM model is shown at

http://www.dmu.dk/AtmosphericEnvironment/WEPTEL/DREAM

Online measurement data from the Danish Monitoring Programme can be found at the web page:

http://www.dmu.dk/AtmosphericEnvironment/netw.htm

Acknowledgements

Dr. Kåre Kemp and Dr. Finn Palmgren, National Environmental Research Institute, Department of Atmospheric Environment, Denmark have kindly provided air pollution measurement data. Dr. Hans E. Jørgensen, Risø National Research Center, Department of Wind Energy and Atmospheric Physics has kindly provided meteorological measurement data from the Risø mast. Global meteorological data have been kindly provided by The National Centers for Environmental Prediction, NCEP, USA. Dr. Ole Hertel, National Environmental Research Institute, Department of Atmospheric Environment, Denmark, is acknowledged for useful comments to the manuscript.

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Appendix 1: Input files to the Operational Street Pollution model, OPSM – an example

Street configuration data file

```
'Street name'
**************************************************************
 HEIGHT (m) WIDTH (m) LENGTH1 (m) LENGTH2 (m) DIRECTION (deg)
  18.        25.        40.         70.        30.
**************************************************************
 NUMBER OF EXCEPTIONS (MAX 10)
   3
 RANGES
  355.0 215.0 340.0    !dd_l
   30.0 230.0 350.0    !dd_u
   25.0  25.0   0.0    !Building heights
```

Traffic data file

```
Traffic data
street name, year
Working days
  HOUR PAS_Car Vans  Trucks  Buses  V_short V_long  Cold_start
   1    262     14      4      6     50.0    30.0      0
   2    139      7      4      0     50.0    30.0      0
   3     93      4      2      0     50.0    30.0      0
   4     78      3      3      0     50.0    30.0      0
   5     95      4      5      1     40.0    30.0      0
   6    227     10     12     11     40.0    30.0      0
   7    726     95     49     13     40.0    20.0     10
   8   1426    194     77     18     30.0    20.0     10
   9   1520    191     90     18     30.0    20.0     10
  10   1257    194     79     26     40.0    30.0      5
  11   1250    188     90     20     40.0    40.0      5
  12   1261    194     86     18     40.0    40.0      5
  13   1371    128     72     28     40.0    40.0      5
  14   1363    183     64     29     40.0    40.0      5
  15   1487    178     56     26     30.0    40.0      5
  16   1593    166     39     24     30.0    20.0      5
  17   1646    127     34     15     30.0    20.0      5
  18   1529    110     23     14     30.0    20.0      5
  19   1427     76     14     17     40.0    40.0      5
  20   1061     71     10     15     40.0    40.0      5
  21    795     47      9      9     40.0    40.0      5
  22    784     42      6     10     50.0    40.0      5
  23    858     43      2     13     50.0    40.0      0
```

24	629	23	1	11	50.0	40.0	0

Saturday

HOUR	PAS_Car	Vans	Trucks	Buses	V_short	V_long	Cold_start
1	615	31	2	8	50.0	40.0	0
2	459	23	0	3	50.0	40.0	0
3	337	17	0	0	50.0	40.0	0
4	257	10	0	2	50.0	40.0	0
5	221	11	1	1	50.0	40.0	0
6	186	9	5	4	50.0	40.0	0
7	226	14	11	3	50.0	40.0	10
8	347	52	17	4	50.0	40.0	10
9	520	63	23	5	50.0	40.0	10
10	748	122	22	7	50.0	40.0	5
11	991	160	24	5	50.0	40.0	5
12	1181	216	29	5	50.0	40.0	5
13	1340	140	28	4	50.0	40.0	5
14	1289	196	28	4	50.0	40.0	5
15	1318	186	21	9	50.0	40.0	5
16	1276	132	15	12	50.0	40.0	5
17	1264	101	10	12	50.0	40.0	5
18	1373	97	10	13	50.0	40.0	5
19	1270	65	7	14	50.0	40.0	5
20	829	46	5	11	50.0	40.0	5
21	570	32	4	8	50.0	40.0	5
22	544	30	8	4	50.0	40.0	5
23	631	29	4	8	50.0	40.0	0
24	743	21	2	7	50.0	40.0	0

Sunday

HOUR	PAS_Car	Vans	Trucks	Buses	V_short	V_long	Cold_start
1	684	34	2	9	50.0	40.0	0
2	544	27	0	1	50.0	40.0	0
3	448	22	0	0	50.0	40.0	0
4	336	13	0	1	50.0	40.0	0
5	255	12	1	1	50.0	40.0	0
6	199	10	1	1	50.0	40.0	0
7	185	11	7	1	50.0	40.0	10
8	216	32	8	2	50.0	40.0	10
9	313	38	8	1	50.0	40.0	10
10	532	87	10	3	50.0	40.0	5
11	699	112	15	3	50.0	40.0	5
12	928	170	20	3	50.0	40.0	5
13	1260	132	21	3	50.0	40.0	5
14	1294	196	22	3	50.0	40.0	5
15	1392	197	19	8	50.0	40.0	5
16	1304	135	13	11	50.0	40.0	5
17	1276	101	10	12	50.0	40.0	5
18	1347	95	11	13	50.0	40.0	5
19	1102	56	7	13	50.0	40.0	5
20	942	52	5	12	50.0	40.0	5
21	685	39	6	10	50.0	40.0	5
22	672	37	11	6	50.0	40.0	5
23	688	32	5	9	50.0	40.0	0
24	475	13	2	10	50.0	40.0	0

Working days, July

HOUR	PAS_Car	Vans	Trucks	Buses	V_short	V_long	Cold_start
1	318	16	2	10	50.0	40.0	0
2	171	8	0	2	50.0	40.0	0
3	107	5	0	1	50.0	40.0	0
4	83	3	0	2	50.0	40.0	0
5	82	4	3	2	40.0	40.0	0
6	174	8	11	10	40.0	40.0	0

7	539	33	29	9	40.0	40.0	10
8	944	143	45	18	30.0	40.0	10
9	1109	135	68	20	30.0	40.0	10
10	967	158	64	25	40.0	40.0	5
11	1008	162	76	22	40.0	40.0	5
12	1068	196	78	15	40.0	40.0	5
13	1135	119	72	14	40.0	40.0	5
14	1067	162	67	14	40.0	40.0	5
15	1128	159	45	24	40.0	40.0	5
16	1283	133	26	27	40.0	40.0	5
17	1322	105	17	25	40.0	40.0	5
18	1224	86	13	20	40.0	40.0	5
19	1085	55	8	21	40.0	40.0	5
20	882	49	6	17	40.0	40.0	5
21	723	41	6	11	40.0	40.0	5
22	656	36	8	5	50.0	40.0	5
23	718	33	4	9	50.0	40.0	0
24	603	17	2	10	50.0	40.0	0

Saturday, July

HOUR	PAS_Car	Vans	Trucks	Buses	V_short	V_long	Cold_start
1	478	24	1	6	50	50	0
2	324	16	0	2	50	50	0
3	223	11	0	0	50	50	0
4	188	7	0	2	50	50	0
5	161	8	1	0	50	50	0
6	148	7	4	3	50	50	0
7	202	12	10	2	50	50	10
8	308	46	15	4	50	50	10
9	436	53	19	4	50	50	10
10	625	102	18	5	50	50	5
11	802	129	20	4	50	50	5
12	909	166	22	3	50	50	5
13	1019	107	21	3	50	50	5
14	929	141	20	3	50	50	5
15	848	120	13	5	50	50	5
16	807	83	10	8	50	50	5
17	791	63	6	8	50	50	5
18	883	62	6	8	50	50	5
19	869	44	5	9	50	50	5
20	659	36	4	9	50	50	5
21	557	31	4	7	50	50	5
22	509	28	7	4	50	50	5
23	527	24	3	7	50	50	0
24	630	18	1	6	50	50	0

Sunday, July

HOUR	PAS_Car	Vans	Trucks	Buses	V_short	V_long	Cold_start
1	491	24	1	7	50	50	0
2	331	16	0	0	50	50	0
3	280	14	0	0	50	50	0
4	220	8	0	0	50	50	0
5	180	9	1	0	50	50	0
6	147	7	1	0	50	50	0
7	161	10	6	1	50	50	10
8	192	29	7	2	50	50	10
9	237	29	6	1	50	50	10
10	408	67	7	2	50	50	5
11	580	93	12	3	50	50	5
12	707	129	15	2	50	50	5
13	891	93	15	2	50	50	5
14	883	134	15	2	50	50	5

15	852	120	11	4	50	50	5
16	811	84	8	6	50	50	5
17	825	65	7	8	50	50	5
18	956	67	7	9	50	50	5
19	944	48	6	11	50	50	5
20	891	49	5	11	50	50	5
21	827	47	7	12	50	50	5
22	714	39	12	6	50	50	5
23	622	29	4	8	50	50	0
24	453	13	2	10	50	50	0

Appendix 2: Statistical methodology

Many different statistical methods can be used when comparisons with measurements are performed. The statistical parameters used for validation of the model system using the global analysis are briefly described here. For most of the statistical parameters, the main idea is basically, to find a measure of the distance between observed and calculated values. This distance can be investigated as comparison of different forms of average values in the series (including the bias, the fractional bias, FB, and the figure of merit, FM) or by looking at the variability in the series (including the correlation coefficient, $\hat{r}$, the fractional standard deviation, FSD, and the normalized mean square error, NMSE).

The notation used in this section is as follows: O_i is the ith observed value and P_i is the ith predicted (calculated) value. i can be both temporal in which case $i \in T$ or spatial in which case $i \in S$, where T denotes the temporal points in a fixed space and S denotes the spatial points at a fixed time. The number of points in a series is denoted by N. $\overline{O}$ and $\overline{P}$ are mean values of observed and predicted series, respectively.

The correlation coefficient

An estimate for the correlation coefficient, $\hat{r}$, is given as the covariance between the two series deviation from their respective means divided by their respective standard deviations (Spiegel, 1992)

$$\hat{r} = \frac{\sum_{i=1}^{N}(O_i - \overline{O})(P_i - \overline{P})}{\sqrt{\sum_{i=1}^{N}(O_i - \overline{O})^2 \sum_{i=1}^{N}(P_i - \overline{P})^2}} \qquad \textbf{(1)}$$

By test of significance of the correlation coefficients, the hypothesis, H_1, is that the series O_i and P_i are independent which means that the correlation coefficient is zero:

$$H_1 : \hat{r} = 0 \qquad \textbf{(2)}$$

If the hypothesis can be rejected at a given significance level, it is generally accepted that O_i and P_i are correlated or anti-correlated depending on the sign of $\hat{r}$. Test of the hypothesis is based on the test parameter given by (Spiegel, 1992a; 1992b; Allerup, 1974)

$$t_c = \frac{\hat{r}\sqrt{N-2}}{\sqrt{1-\hat{r}^2}} \qquad \textbf{(3)}$$

which is students t-distributed with N-2 degrees of freedom when the zero-hypothesis is true.

The Bias

Bias is used to examine a tendency for over- or under prediction and defined as (Mosca et al., 1997)

$$bias = \frac{1}{N}\sum_{i=1}^{N}(P_i - O_i) = \overline{P} - \overline{O} \qquad \textbf{(4)}$$

the bias will be negative if the model is generally underpredicting and positive if the model is generally overpredicting with respect to measurements. The confidence interval for the bias can be determined from the standard deviation multiplied by a confidence coefficient (Spiegel, 1992; Mosca et al., 1997)

$$ci = \pm t_\alpha \sqrt{\frac{1}{N(N-1)}\sum_{i=1}^{N}(P_i - O_i - bias)^2} \qquad \textbf{(5)}$$

where t_α is the confidence coefficient found from students t-distribution defined on N-1 degrees of freedom, and given by e.g. 1.96 and 2.58 for the 95% and 99% confidence levels, respectively. Using a confidence level of 95% means that there is 95% probability that a sample is in the confidence interval between bias-ci and bias+ci.

The Normalized Mean Square Error (NMSE)

The normalized mean square error (NMSE) is a measure of the overall deviation between observed and measured values and is defined as (Mosca et al., 1997)

$$NMSE = \frac{1}{N\,\overline{O}\,\overline{P}}\sum_{i=1}^{N}(P_i - O_i)^2 \qquad \textbf{(6)}$$

The NMSE is in general an easy way to compare the differences between different model results. If the NMSE is small the model is performing well both in space and time. To construct a confidence interval for NMSE the bootstrapping technique is used (Efron, 1982) where resampling with replacement is performed a large number of times with recalculation of the NMSE at each iteration. A sampling distribution is then constructed from the histogram of resampled values, which is used to estimate the confidence interval. The confidence level ci can be found from estimation of the probability that a resampled value is below or above appropriate percentiles from the distribution, p_1 and p_2, such that

$$\frac{1 - ci}{2} = Prob(NMSE < p_1) = Prob(NMSE > p_2) \qquad \textbf{(7)}$$

Fractional bias (FB) and fractional standard deviation (FSD)

The absolute values of bias and standard deviation should be used in connection with the fractional bias (FB) and fractional standard deviation (FSD) which give a measure of the relative values. This is important when comparisons are made between different data sets. The fractional bias is defined as (Mosca et al., 1997)

$$FB = 2\,\frac{\overline{P} - \overline{O}}{\overline{P} + \overline{O}} \tag{8}$$

The fractional bias is the difference between the predicted and observed mean values divided by the average value. Unbiased models will have a value of FB close to zero. The fractional standard deviation (FSD) is defined in the same way (Mosca et al., 1997)

$$FSD = 2\,\frac{\hat{\sigma}_P^2 - \hat{\sigma}_O^2}{\hat{\sigma}_P^2 + \hat{\sigma}_O^2} \tag{9}$$

where $\hat{\sigma}_P^2$ and $\hat{\sigma}_O^2$ are the predicted and observed estimated variances, respectively. The FSD should, however, be called the fractional variance instead. A model that gives a good estimation of the spread of the observations will have a FSD close to zero.

Figure of merit (FM)

The figure of merit (FM) is the total percentage agreement between observed and predicted values. It is defined as (Mosca et al., 1997)

$$FM = 100\,\frac{\sum_{i=1}^{N} \mathrm{Min}(P_i, O_i)}{\sum_{i=1}^{N} \mathrm{Max}(P_i, O_i)} \tag{10}$$

The FM evaluates the overlapping concentration histogram, normalized to the time series of the maximum measured or observed concentration. If FM=100%, there is a total overlap between the calculated and measured values. If FM=0% there is no overlapping between calculated and measured values.

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Ministry of Environment and Energy
National Environmental Research Institute

ISBN 87-7772-529-8
ISSN 0905-815x