TOOL FOR EXPLORATORY ANALYSIS OF OSPM MODEL PERFORMANCE FOR LONG TIME SERIES

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Abstract: The Danish Operational Street Pollution Model, OSPM, has for two decades been successfully applied in many cities worldwide as recently reviewed by Kakosimos et al. (2010). However, as a result of the many applications various shortcomings of the model have been identified. This has e.g. made it clear that further development of the model is needed. Such work is now ongoing in order to make the model more widely applicable for non-standard street canyons as often encountered in exposure analysis (Ketzel et al. 2011). Examples of locations for which the model cannot reproduce observed concentrations are very narrow street canyons and street canyons where the traffic is not homogeneously and symmetrically distributed between the building facades. Since the user community of OSPM has been growing in recent years, a combined effort is suggested and outlined in the current paper aiming at addressing the issues.

In order to identify model shortcomings, long-term measured time-series at five Danish monitoring stations, including non-regular street canyons, have been re-calculated with updated emission and traffic data. Results of the evaluation have been analysed with a newly developed validation tool. The validation tool examines trends in observed and modelled annual averages, and produces scatter plots for hourly, diurnal and monthly mean concentrations of NO_x, NO_2, O_3, PM_{10}, $PM_{2.5}$ as well as plots displaying concentrations as function of wind direction. In this paper examples are presented of how this tool facilitates the exploratory data analysis of observations and model results. Further is demonstrated how this tool enables the user to identify both shortcomings in the model parameterisation and possible errors and uncertainties in the measured data. After a thorough validation with measured historic data, the model is applied to predict the development in future NO_2 concentrations as well as the model is used to identify the year when the presently exceeded limit values will be complied with.

***Key words:** model validation, street canyon, urban air pollution, OSPM, exploratory data analysis.*

INTRODUCTION

The OSPM (Operational Street Pollution Model) has been evaluated and applied by a wide range of users worldwide (see: Kakosimos et al. 2010) for modelling urban air pollution at street level. Proper model validation protocols and best modelling practise have been discussed in the scientific community for many years, lately in the COST 732 action (URL 1) and in the Forum for Air quality Modelling in Europe (FAIRMODE, URL 2). A document produced by COST 732 provides general guidance on model evaluation protocols (Britter and Schatzmann, 2007).

Model validation is also relevant in context of the European Air Quality Directive (EC, 2008) that is mentioning models as a method to assess air quality with respect to compliance with limit values. The directive defines some model quality objectives that are now interpreted and discussed within FAIRMODE, and performed tests have revealed some ambiguities in the interpretation of those objectives (e.g. Gidhagen at al. 2011). This paper aims at contributing to the discussion. Model quality objectives are in the directive as in other guidelines formulated in terms of quantitative statistical analysis, e.g. maximum uncertainty presented for the annual average or for percentiles. However this statistical analysis might obscure deficiencies of the model, and model results could be "right for the wrong reason", i.e. the model quality objective might be fulfilled even if the model fails to reproduce some essential features in observations. Therefore Di Sabatini et al. (2008) recommended for the case of CFD models a combination of qualitative (exploratory data analysis) and quantitative (statistical analysis) evaluations. The usefulness in identifying model errors by means of qualitative data analysis using an automated Excel workbook was presented by Olesen et al. (2008). This work focuses on the evaluation of OSPM and presents a similar approach suggesting a combined evaluation strategy of qualitative and quantitative analysis. Even though OSPM is a parameterised semi-empirical model with much simpler physics compared to the CFD models this evaluation strategy is applicable. This approach and the here presented Excel evaluation tool can easily be used also by other models of this type.

MODEL AND DATA DESCRIPTION

Measurements from 5 streets in the 4 largest Danish cities (Copenhagen, Aalborg, Aarhus, and Odense) are exploited with up to 17 years of data. In each city an urban background monitoring station measuring urban background concentrations as well as meteorological parameters is operated. All stations are part of the Danish Air Quality Monitoring Programme (Ellermann et al. 2011).

The street canyon model OSPM (http://OSPM.dmu.dk/) is used to calculate air pollution at 2 m height at the side walks of the selected streets. The model includes various elements:

- emissions from traffic at the selected street,
- simple chemical reactions describing the reactions of air pollutants in the street canyons, and
- the dispersion of the air pollution in the street canyon (due to meteorological conditions and turbulence induced by traffic).

The routine for calculating Danish traffic emission data that are used as input for the calculations with OSPM has been substantially updated with detailed information (average daily traffic, vehicle distribution) obtained from the four Danish municipalities within a project on evaluation of the effects of low emission zones (Jensen at al. 2011). Emission factors are based on the most recent version of the COPERT IV model and are applied for 2010 conditions taking account of the effect of the low emission zones inside the cities. This is done by means of a detailed analysis of the vehicle composition using video licensing plate analysis linked to the National Auto Registry at a street in Copenhagen (for details see Jensen at al. 2011). The input data for the OSPM model on traffic volume and street configurations for the selected urban streets are generated based on various register data and digital maps using the AirGIS system (http://AirGIS.dmu.dk).

MODEL VALIDATION FOR ANNUAL AVERAGES

According to model quality objective described in the Air Quality Directive (EC, 2008) the maximum annual average modelling uncertainty is ±30% for NO_2 and ± 50% for PM_{10}. In Table 1 we present annual averages of measured and modelled NO_x, NO_2, PM_{10} and $PM_{2.5}$ for 5 streets in 2010. All deviations between observed and modelled values for compounds with limit values or target values (NO_2, PM_{10}, $PM_{2.5}$) are within the required +-30% range. The largest deviation is observed in Aalborg where the model under predicts by 22% and 24% for NO_2 and $PM_{2.5}$, respectively. However, if we focus on NO_x (without air quality limits), the under prediction by the model appears to be more pronounced with deviations of 16% to 49%. The ratio between NO_x and NO_2 is obviously not the same in the model results and the measurements. The reason for this difference might be uncertainties in emission data, and especially in the fraction of direct NO_2 emissions (fracNO_2). This shows that just focussing on the annual statistics for the regulated compounds does not provide the full picture regarding the model performance. Model evaluation should be performed for all compounds for which reliable data are available and should furthermore include qualitative data analysis as described in the following section.

Table 1. Comparison of measurements and model results for 5 streets in 4 Danish cities adopted from Jensen et al. 2011. Annual averages for 2010 are given for NO_x, NO_2, $PM_{2.5}$, and PM_{10}. Calculations are carried out using the full THOR model calculation system (Brandt et al. 2003; http://THOR.dmu.dk), including DEHM, UBM, and OSPM models. Coph.=Copenhagen; HCAB=H.C. Andersens Boulevard

Station Name	Measurements		Model results		Relative difference		Absolute Difference	
	NO_x	NO_2	NO_x	NO_2	NO_x	NO_2	NO_x	NO_2
	µg/m^3	µg/m^3	µg/m^3	µg/m^3	(%)	(%)	µg/m^3	µg/m^3
Coph.-HCAB	133	56	88	51	-35%	-10%	-46	-5
Coph.-Jagtvej	86	39	63	39	-26%	-1%	-22	0
Odense	75	32	63	35	-16%	12%	-12	4
Aarhus	87	39	65	36	-25%	-8%	-22	-3
Aalborg	104	39	53	30	-49%	-22%	-50	-9
	PM_{10}	$PM_{2.5}$	PM_{10}	$PM_{2.5}$	PM_{10}	$PM_{2.5}$	PM_{10}	$PM_{2.5}$
Coph.-HCAB	28.1	17.4	30.0	19.4	7%	11%	1.9	2.0
Coph.-Jagtvej	26.7	17.8	27.7	18.3	4%	3%	1.0	0.5
Odense	26.0	-	27.8	17.7	7%	-	1.8	-
Aarhus	24.8	15.3	23.8	15.5	-4%	1%	-1.0	0.2
Aalborg	-	18.3	23.8	13.8	-	-24%	-	-4.5

VALIDATION TOOL

OSPM operates with a time resolution of one hour similar to several models used for air quality assessment. Running this type of model for several compounds, several stations and many years lead to the production of a vast amount of data. Analysing such data in detail is a huge task, and often a shortcut is taken by using simple statistical analysis on annual averages or percentiles. As pointed out above a combination of exploratory data analysis and statistical analysis has been recommended for model evaluation (Di Sabatini et al. 2008) and proofed to be manageable and useful even for complex models producing large amount of outputs (Olesen et al. 2008).

The here presented validation tool is a based on MS Excel (version 2003) and is taking advantage of Excel's plotting facilities, data analysis tools as well as macro language. It is a standard facility in OSPM that the output for several years and compounds may be directly saved in Excel file format (one sheet per year, separate files for each street), avoiding any errors related to import, conversion or transfer of model data. After re-running the model, e.g. with a changed set of emission data, the plots and analysis of differences between the two model runs are available immediately.

The validation tool provides so far three types of plots for the parameters (NO_x, NO_2, fracNO_2, O_3, CO, PM_{10} and $PM_{2.5}$):

1) Scatter plots of hourly values, point by point, measured versus modelled (for one year at the time)
2) Plots of aggregated data showing the measured and modelled concentrations as function of essential parameters like wind direction, hour of the day and month (for one year at the time)
3) Trend plots for annual averages for all calculated years.

An example of the latter type of plots is shown in Figure 1 for one of the streets (HCAB) in Copenhagen included in the current analysis. Besides the historic analysis of previous years, also a forecast for the years 2015 and 2020 is included in the results. This type of plot provides a fast overview of results in an aggregated way and at the same time it indicates e.g. whether the emission model is capturing the development in the concentrations in a correct way.

The first two types of plots are designed for looking deeper into the data, and the plots are here produced for one year at a time. Figure 2 shows an example of the Excel sheet with monthly aggregated values for 2006 at HCAB. Monthly trends will reveal whether the seasonal variation is captured correctly by the model. Some compounds show a pronounced seasonal variation as e.g. O_3 due to the seasonal variation in global radiation or PM_x due to a seasonal variation in emissions (Ketzel et al. 2007).

An additional feature (also visible in Figure 2) is that data filters (for Hour or Month, DayCase, DayOfWeek, Wind speed range) can be applied to consider only parts of the datasets. Changing the option in the filter in one of the plots will automatically synchronise the filters in the other plots. The year for which the data are plotted can be modified easily by a drop-down menu, again being simultaneously synchronised for all plots automatically. Also, filter selections once applied will remain in place after a new year is selected. Such features help to handle the vast amount of data to be plotted and analysed. In the case that unexpected discrepancies or peculiarities are recognised in the data, the user can by means of filters and years selection focus the nature and origin of the discrepancy and thereby identify e.g. periods of malfunctioning measuring devices or errors in model input data.

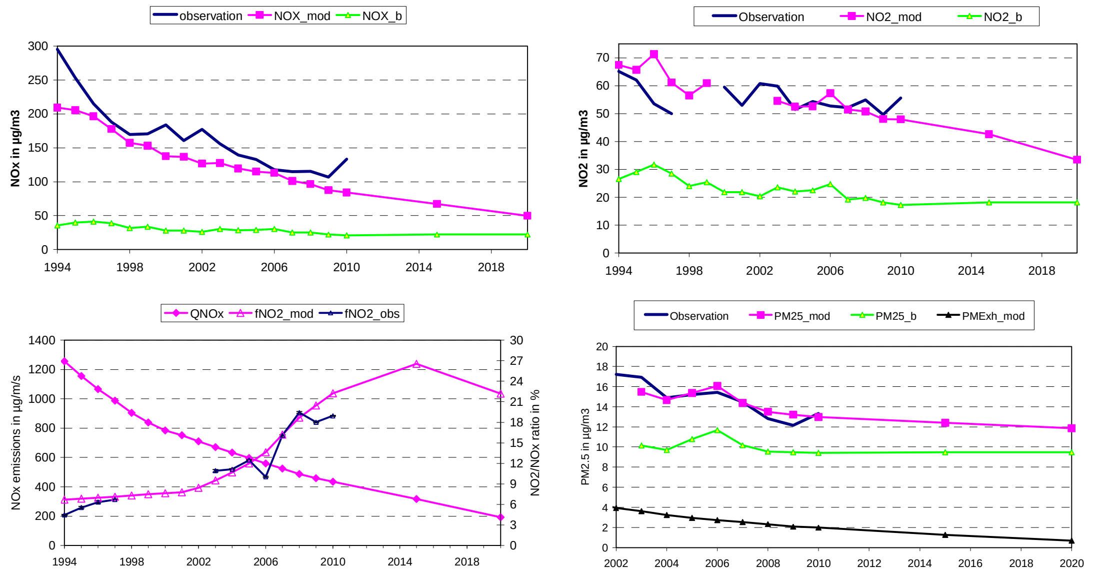

Figure 1. Trend in annual averages (1994-2020) of NO_x, NO_2, fraction of direct emitted NO_2 (fNO_2) and $PM_{2.5}$ at H.C. Andersens Boulevard in Copenhagen. Values for 2015 and 2020 are using forecasted emission, but background and meteorology from 2010. "_mod"=modelled; "_b"=measured background; "QNO_x "=NOx emission density; "PMExh_mod"= Concentration due to exhaust emissions only.

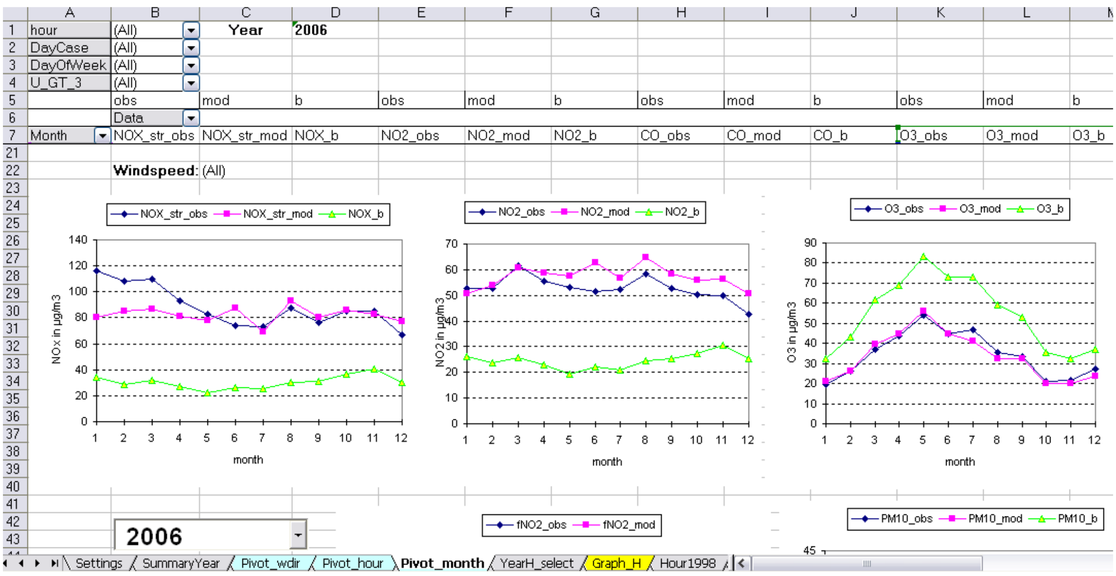

Figure 2. Example of the Excel worksheet presenting the monthly variations of observed and modelled concentrations at HCAB for 2006.

Another example of an aggregated data plot is in Figure 3 showing the average concentration as function of wind direction for two different street canyons. The dependence on wind direction is a sensitive parameter and often not easy to match since it is influenced by several factors such as: the correct simulation of the flow patterns due to the buildings (vortex flow, windward vs. leeward position of receptor point) or the existence of unaccounted sources in the vicinity of the street (larger crossing streets close by or diesel trains) or the fact that the background monitoring station is usually located in some distance of the street station. In Figure 3 the difference between the direction dependence for a street with buildings on both sides and only on one side is clearly visible and well reproduced by the model. For the street with buildings on both sides a sector exists where the monitoring point is placed on the windward side showing significantly reduced concentration (wind directions 240º to 360º). On the other hand, in streets with buildings on one side only, such a sector with reduced concentrations is absent.

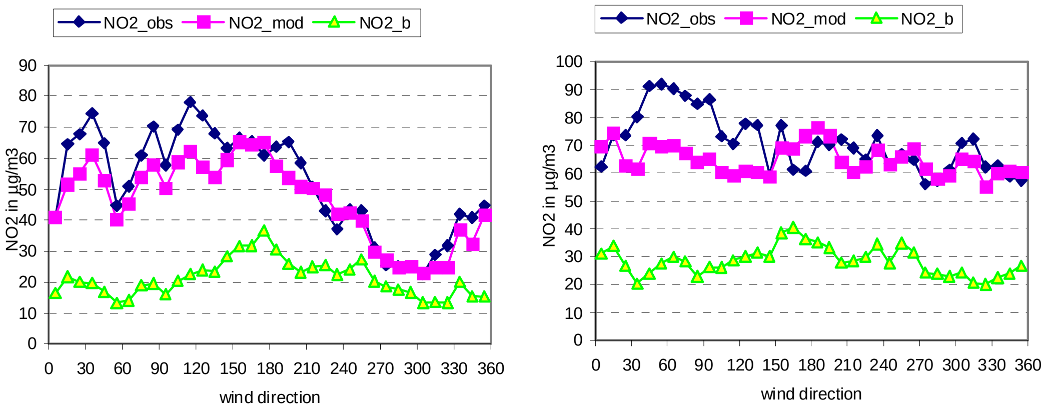

Figure 3. Dependence of measured and modelled street concentrations of NO_2 on wind direction. Plots are based on one full year (2007) of hourly data for two streets in Copenhagen. Left: Jagtvej (street canyon with buildings on both sides), Right: H.C. Andersens Boulevard (buildings on one street side only). "_obs"=measured "_mod"=modelled; "_b"=measured background;

SUMMARY AND CONCLUDING REMARKS

This paper argues for the necessity of exploratory (qualitative) data analysis in addition to widely used statistical model evaluation. An easily applicable evaluation tool to facilitate the qualitative analysis of large datasets has been developed, and the features of this tool have been demonstrated. The tool can help the model developer/user to identify and systematically investigate the nature of discrepancies between model calculations and measurements. Reasons for disagreement could be manifold e.g. shortcomings in the model itself, errors in the model input data (emission factors, traffic information, meteorological data etc.) and also errors in the measurements. The tool is available to the modelling community from the OSPM web page (ospm.dmu.dk). Its application could be extended to other models as well. Also a version of the tool that compares two model performances with each other is in planning. The validation sheet was developed under Excel version 2003, but seems to work well also under Excel 2010.

REFERENCES

Brandt, J., Christensen J.H., Frohn, L.M., Berkowicz R. 2003: Air pollution forecasting from regional to urban street scale – implementation and validation for two cities in Denmark. Physics and Chemistry of the Earth, 28, 335-344.

Britter R. and Schatzmann M. (eds), 2007: Model evaluation guidance and protocol document, COST Action 732: Quality assurance and improvement of micro-scale meteorological models, 27p. http://www.mi.uni-hamburg.de/fileadmin/files/forschung/techmet/cost/cost_732/pdf/GUIDANCE_AND_PROTOCOL_DOCUMENT_1-5-2007_www.pdf

Di Sabatino, Silvana ; Olesen, Helge Rørdam ; Berkowicz, Ruwim ; Franke, Jörg ; Schatzmann, Michael ; Britter, Rex ; Schlünzen, Heinke ; Martilli, Alberto ; Carissimo, Bertrand: A model evaluation protocol for urban scale flow and dispersion models. In: Hrvatski Meteoroloski Casopis, 2008, p. 409-413. http://hrcak.srce.hr/file/96397

EC (2008) Directive 2008/50/EC of the European Parliament and of the Council of 21 May 2008 on ambient air quality and cleaner air for Europe. Official Journal L 152, 11.6.2008, p. 1–44.

Ellermann, T., Nordstrøm, C., Brandt, J., Christensen, J., Ketzel, M. & Jensen, S.S. 2011: The Danish Air Quality Monitoring Programme. Annual Summary for 2010. National Environmental Research Institute, Aarhus University. 55 pp. - NERI Technical Report No. 836. http://www.dmu.dk/Pub/FR836.pdf

Gidhagen, L., Omstedt, G. and Andersen S. (2011): Swedish experiences of applying the Quality Objectives for NO_2 and PM_{10} modelling. Presentation at FAIRMODE meeting June 2011,Norrkjoping. (http://fairmode.ew.eea.europa.eu/)

Jensen, S.S., Ketzel, M., Nøjgaard, J. K. & Becker, T. 2011: Hvad er effekten af miljøzoner for luftkvaliteten? - Vurdering for København, Frederiksberg, Aarhus, Odense, og Aalborg. Slutrapport. Danmarks Miljøundersøgelser, (Danish with English Summary), Aarhus Universitet 110 s. – Faglig rapport nr. 830. http://www.dmu.dk/Pub/FR830.pdf.

Kakosimos K.E., Hertel O., Ketzel M. and Berkowicz R. (2010): "Operational Street Pollution Model (OSPM) - a review of performed validation studies, and future prospects", Environmental Chemistry, 7, 485-503.

Ketzel, M., G. Omstedt, C. Johansson, I. Düring, M. Pohjola, D. Oettl, L. Gidhagen, P. Wåhlin, A. Lohmeyer & R. Berkowicz (2007): Estimation and validation of $PM_{2.5}/PM_{10}$ exhaust and non-exhaust emission factors for practical street pollution modelling, *Atmospheric Environment* **41**: 9370–9385.

Ketzel M, Berkowicz R, Hvidberg M, Jensen SS, Raaschou-Nielsen O. (2011): Evaluation of AirGIS - a GIS-based air pollution and human exposure modelling system. International Journal for Environment and Pollution. In Press.

Olesen, Helge Rørdam ; Baklanov, A. ; Bartzis, J. ; Barmpas, F. ; Berkowicz, Ruwim ; Brzozowski, K. ; Buccolieri, R. ; Carissimo, B. ; Costa, A. ; Di Sabatino, S. ; Efthimiou, G. ; Franke, J. ; Goricsan, I. ; Hellsten, A. ; Ketzel, Matthias ; Leitl, B. ; Nuterman, R. ; Polreich, E. ; Santiago, J. ; Tavares, R..: The MUST model evaluation exercise: Patterns in model performance. In: Hrvatski Meteoroloski Casopis, Vol. 43, No. 1, 2008, p. 403-408. http://hrcak.srce.hr/file/96396

URL1: COST 732: http://www.mi.uni-hamburg.de/Home.484.0.html

URL2: FAIRMODE: http://fairmode.ew.eea.europa.eu/