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EVALUATION OF NUMERICAL MODELS USED TO SIMULATE ATMOSPHERIC POLLUTION NEAR ROADWAYS

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Abstract: Numerical modelling of traffic-related pollution can be useful to check compliance with regulatory thresholds, compare the atmospheric impact of various traffic scenarios or represent roadside concentrations in air quality maps. Because of operational constraints, local actors usually make use of parametrised models which are easy to implement but require caution and rigour in their application. Since 2007 an Internet information base including data sets, technical information and reference methodologies, has been built up by the French Central Laboratory for Air Quality Monitoring (LCSQA) to help local actors in evaluating their modelling tools. In addition, simulations have been performed for different types of streets to provide examples of model evaluation studies and draw some indications about the application framework of a few commonly used models. The results of those tests are presented and discussed for two street canyons and one semi-open street located in the French city of Nantes.

Key words: Traffic-related pollution; street canyon; dispersion modelling; model evaluation

INTRODUCTION

Numerical models used to assess atmospheric concentrations near road traffic have received growing interest as support to air quality monitoring. Indeed many monitoring stations for which exceedances of regulatory limit values (in particular of those related to NO_2 and PM_{10}) have been observed are traffic stations. In compliance with the European Directive on ambient air quality and cleaner air for Europe (2008/50/EC), Member States have to report on those exceedances and in particular give an estimate of their geographical extent. More generally, population exposure not only to average background pollution but also to traffic-related concentrations has raised serious concerns, eliciting the need for small-scale air quality assessment.

In addition to properly designed monitoring surveys, simulation tools may prove very useful in that context, providing their reliability and application framework are well known. This study was mainly aimed towards local actors involved in air quality monitoring. Its objective was to gather experimental data and develop reference methodologies which can help them to evaluate the available models and optimize their use.

A comprehensive inventory of measuring campaigns conducted in France and Europe near streets or roads was first undertaken. Given the campaigns characteristics and potentially retrievable data, a large panel of sites covering different configurations (street canyons, crossroads, open roads...) was selected as suitable for modelling evaluation purposes. Then common tools (ADMS-Urban, CALINE4, OSPM, SIRANE, STREET) were applied to some of those cases to ensure that the proposed data and methodologies were consistent and supply examples of comparison between model output and measurements. All processed data, modelling results, evaluation tools and technical information have been made available to the French air quality monitoring agencies on a website.

In section 1 and 2, the implemented models and three case studies (two street canyons and one semi-open street in the French city of Nantes) are briefly described. The main conclusions of a preliminary sensitivity analysis are then provided (section 3). In section 4, simulation results are presented and discussed for the three test cases. The content of the web site is outlined in section 5. The most significant outcomes and some perspectives are given as conclusion.

MODELS

ADMS-Urban is an advanced Gaussian dispersion model mainly intended to assess air quality in urban areas (CERC, UK, version 2.2, 2006). It can simulate the atmospheric dispersion of pollutants released from industrial, domestic and road traffic sources. It also includes a street canyon model based on OSPM formulation to represent the dynamics and dispersion features expected in roads with street canyon characteristics.

The Operational Street Pollution Model (OSPM) is a parameterised model for flow and dispersion conditions in street canyons (NERI, Denmark, version 5.1.90, 2007). The concentration of a pollutant is described as the sum of two components: a Gaussian plume model for the direct contribution from street traffic, and a box model for the recirculating part of pollutants in the street.

SIRANE is an urban dispersion model developed to simulate pollutant exchanges occurring between interconnected streets and between the streets and the overlying atmosphere (LMFA, France, version 1.16, 2008). In a street section, concentrations are calculated as the result from a mass balance between the incoming and outgoing flows (direct emissions from traffic, exchange at the intersections and at roof level). Dispersion above roofs or in open streets is modelled by a Gaussian plume.

STREET is a parametric model reserved for assessing annual average concentrations in various types of street layouts (TÜV, Oxalis Mobilité, KTT, version 5.2, 2008). It does not simulate dispersion by itself but utilizes a library of simulation results produced by the 3D Eulerian MISKAM model (Institut für Physik der Atmosphäre, Mainz, Germany). Concentration values computed by STREET depend on three main inputs which are the street geometry and orientation, the prevailing wind conditions and the annual average emission rate.

Note that CALINE4 was deliberately not used in the case studies presented here. This Gaussian line source model was mainly designed to predict atmospheric concentrations within a few hundreds of meters from open roadways (California Department of Transportation, version 1.31, 2005). Our decision was motivated by a first series of tests in which application of CALINE4 to street canyons lead to high underestimation (Wroblewski *et al.*, 2008).

TEST CASES

Streets

Six streets were studied: three street canyons of Berlin, Hanover and Copenhagen instrumented during the European TRAPOS program (1994-1995) and three streets located in the city of Nantes:

- a deep street canyon (height/width ~2)
- a classical street canyon (height/width ~1)
- a semi-open street.

In each of those last three sites, a monitoring campaign was carried out by AIR Pays-de-Loire for a period of several months to two years. The presentation of the results will be limited to those cases (Table 1 and Figure 1).

Table 1. Characteristics of the three stu	idied streets.
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Name	Height	Width	H/L	Annual average traffic	Measurement period	Measured pollutants
Rue de Crébillon	21.0	9.3	2.3	10 650 veh./day	1 May 2004 to 30 April 2005	NO _x , PM ₁₀ , CO
Rue de Strasbourg	18.0	14.5	1.2	27 090 veh./day	1 January 2004 to 30 April 2005	NO _x , CO
Quai de la Fosse (built side)	15.9	30.0	0.5	43 810 veh./day	1 October 2004 to 31 January 2005	NO _x , PM ₁₀ , CO
Quai de la Fosse (open side)		30.0	1	43 810 veh./day	16 December 2004 to 31 January 2005	NO _x , PM ₁₀ , CO

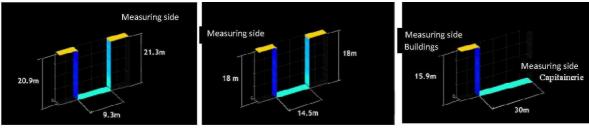


Figure 3. Cross sections of the streets.

Input data

Since no information about CO background levels was available, only NO_x , NO_2 and PM_{10} concentrations were modelled. The following data were used as input:

- Hourly NO_x and PM_{10} background measurement data. They were respectively taken from two urban background monitoring stations located in the surroundings of the streets and selected by AIR Pays-de-Loire. O_3 background measurements were also introduced into ADMS-Urban and SIRANE (for modelling chemistry).
- Hourly meteorological recordings of wind, cloud cover (for computing stability in ADMS-Urban and SIRANE) and global solar radiation (needed by OSPM simplified chemistry module) (Meteo-France, Nantes airport).
- Information about traffic and fleet composition. Data were provided by AIR Pays-de-Loire and used to compute NO_x and PM₁₀ hourly emissions in the three streets. COPERT IV emission factors (EEA, 2007) were applied.

SENSITIVITY TESTS

Preliminary sensitivity tests were first performed with ADMS-Urban, OSPM and SIRANE to better characterize the response of those models as a function of the input data. Crébillon street and all related input variables and parameters were taken as the reference case. In all the tests, a 12 month long modelling period (1 May 2004/30 April 2005) was considered. Given a dispersion model and a pollutant (NO_x or NO_2), the model sensitivity to each variation of an input (all other parameters being fixed) was quantified by the coefficient:

$$Q_i = \frac{\Delta \overline{C} [\%]}{\Delta p [\%]} = \frac{(\overline{C}_i - \overline{C}_{ref}) / \overline{C}_{ref}}{(p_i - p_{ref}) / p_{ref}} \text{ i=1, 2...,N=total number of variations for parameter p}$$

 $\Delta \overline{C}[\%]$ is the relative variation of NO_x or NO₂ mean concentration (average over the period) due to a relative change $\Delta p[\%]$ in the parameter value. Q_i=1 means that a 100% variation of the parameter entails a 100% variation of the average concentration.

All models appear to be most sensitive to: NO_x traffic emission rates, with more pronounced effect on NO_x concentrations; background concentrations, with more pronounced influence on NO_2 concentrations; the street geometry (Table 2).

However, the three models do not behave identically and reveal specificities:

- ADMS-Urban is highly sensitive to background levels, especially as regards NO₂.
- SIRANE is particularly sensitive to the street width and to the height of the meteorological measurements. Model
 results regarding NO₂ are much more sensitive to background concentrations than those related to NO_x.
- Though representation of canyon effects in ADMS-Urban is based on OSPM formulation, both models have different responses. In particular, OSPM is less sensitive to a variation in background concentrations whereas it is more sensitive to a variation in NO_x traffic emissions. This result could be attributed to the coupling made by ADMS-Urban between a street model like OSPM and an advanced Gaussian dispersion model.

	NOx				NO_2	
	ADMS-Urb.	OSPM	SIRANE	ADMS-Urb.	OSPM	SIRANE
Background	0.443 / 0.443	0.164 / 0;314	0.100 / 0.100	0.877 / 0.879	0.316 / 0.610	0.586 / 0.596
concentrations						
NO _x annual mean	0.505 / 0.551	0.572 / 0.758	0.900 / 0.900	0.299 / 0.375	0.252 / 0.509	0.576 / 0.779
emission rate						
% of primary NO ₂	No effect	No effect	No effect	0,082 / 0,082	On-going tests	0,384 / 0,386
in NO _x emissions						
Canyon height	0.221 / 0.324	0.402 / 0.627	0.237 / 0.484	0.278 / 0.318	0.297 / 0.523	0.131 / 0.261
Canyon width	0.360 / 0.687	0.441 / 0.539	1.009 / 2.412	0.211 / 0.369	0.121 / 1.155	0.568 / 0.778
Height of wind	0.088 / 0.109	-	0.747 / 1.086	0.069 / 0.088	-	0.444 / 0.656
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Table 2 Mean/maximum sensitivity coefficients for the most influent parameters.

MODEL EVALUATION RESULTS

Except for SIRANE and STREET, which calculate a unique value for the whole street, concentrations have been simulated on the same side as the measurements. With ADMS-Urban, it was possible to define two simulation points respectively located on the edge of the pavement (point 1) and slightly more inside the street (point 2). For each street and each model, simulated and measured concentrations were compared by computing and plotting a wide range of statistical scores and graphs. Former simulations (TRAPOS cases, Wroblewski *et al.*, 2009) highlighted how a good control of the input data, especially a precise knowledge of the hourly emissions and of the wind and stability conditions, determines the quality of the results. The recent simulations (Nantes cases, Létinois *et al.*, 2009), which benefitted from a better field expertise and more detailed input data, confirm that conclusion.

On average over one year, the relative differences between model outputs and observations are generally less than 30% for NO_2 and 50% for PM_{10} (Table 3), in compliance with the regulatory quality objectives (Directive 2008/50/EC, Annex I). From a temporal point of view, scatter plots and time series show a rather large dispersion between hourly simulated and measured concentrations (Figure 2). Correlation is higher for Strasbourg street, namely the most academic street according to the canyon geometry. Furthermore, the models do not respond the same way to an hourly variation of the input data (background concentrations, emissions, meteorology), each of those variables having a different contribution depending on the model. It should be noted that results are more scattered for NO_x than for NO_2 . As for PM_{10} , model performance is highly variable: unexpectedly, OSPM shows poor agreement with the measured values whereas ADMS-Urban and SIRANE almost systematically underestimate them; those results could be partly due to a lack of knowledge about PM_{10} emissions.

	ADMS-Urban (pt 1/pt 2)	OSPM	SIRANE	STREET	
NO _x – Strasbourg	FB = -0.52 / -0.07	FB = 0.45	FB = 0.03	Δ= 48% / 62%	
-	Cor = 0.84 / 0.77	Cor = 0.44	Cor = 0.72		
	$\Delta =$ -44% / -10%	$\Delta = 55\%$	$\Delta = 2.6\%$		
NO ₂ – Strasbourg	FB = -0.36 / -0.04	FB = 0.28	FB = 0.20	$\Delta = 1.5\% / 1.3\%$	
	Cor = 0.83 / 0.77	Cor = 0.41	Cor = 0.67		
	$\Delta = -31\% / -5.0\%$	$\Delta = 26\%$	$\Delta = 20\%$		
NO _x -Fosse	FB = 0.07 / 0.00	FB = 0.73	FB = 0.11	Type of street not included	
open side	Cor = 0.81 / 0.77	Cor = 0.75	Cor = 0.76	in STREET library	
NO ₂ – Fosse	FB = -0.11 / -0.13	FB = 0.22	FB = 0.14	Type of street not included	
open side	Cor = 0.82 / 0.82	Cor = 0.75	Cor = 0.74	in STREET library	
PM ₁₀ – Fosse	FB = -0.26 / -0.29	FB = 0.51	FB = -0.25	Type of street not included	
open side	Cor = 0.78 / 0.77	Cor = 0.28	Cor = 0.77	in STREET library	

Table 3. Examples of statistical comparison between models and measurements.

FB: fractional bias= $\frac{2}{N}$. $\sum_{i=1}^{N} \frac{P_i - O_i}{P_i + O_i}$ with P_i : hourly predictions, O_i : hourly observations; **Cor:** coefficient of correlation

 Δ : relative difference between modelled and measured annual average concentrations.

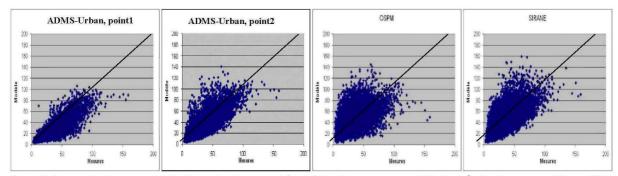


Figure 2. Scatter plots between modelled (y-axis) and measured (x-axis) hourly concentrations. $NO_2 [\mu g/m^3]$. Strasbourg street, Nantes. With ADMS-Urban, lower concentrations are calculated at point 1, i.e. the most exterior point compared to the centre of the street.

WEB SITE

With a view to transparency and better exchange of experience, all results and relevant information have been made accessible to French local actors through an Internet information bank (http://www.lcsqa.org/pollution-de-proximite) organized in the following way:

- technical sheets of commonly used models;
- detailed descriptive list of monitoring campaigns, with possible uploading of the corresponding input data files whenever available;
- output modelling data;
- statistical tools for comparing models and measurements (Excel calculation sheet);
- technical reports.

Those online resources are intended to be regularly updated with information coming from recent monitoring surveys, modelling studies and bibliographical reviews.

CONCLUSION

Modelling roadside concentrations for regulatory purposes or exposure assessment requires that the user be well aware of the model reliability and application domain. Measurement surveys conducted in street canyons or near roadways by local air quality monitoring agencies make a large and interesting renewable source of data sets to support modelling activities.

The aim of our study was to take advantage of this information and put technical and numerical data at the user's disposal through Internet. To enrich the website with simulation results and furnish examples of comparison between models and measurements, several common modelling tools were applied to some selected cases (five street canyons and one semi-open street).

On average over long periods, providing that favourable conditions are gathered: good knowledge of the sites, precise and temporally consistent input data (hourly variations of traffic emissions, background pollution, meteorology), rigorous definition of the parameters required by each model, the models yield satisfactory results with respect to regulatory quality objectives. The precision of the results is all the better as the models are used in situations for which they have been specially designed (classical street canyons for all models, open streets for ADMS-Urban and SIRANE). At short time steps, because of the parametric nature of the models, differences between simulated and observed concentrations can still be high. Note that the hourly variations of concentrations tend to be better reproduced when the hourly variations of the stability conditions are taken into account and background pollution weighs heavier on the results. Additional tests could be performed to see whether a finer adjustment of some parameters, such as the percentage of primary NO_2 in NO_x emissions (EMEP/EEA, 2009; INRETS, 2007), may improve the agreement between model outputs and measurements.

Further simulations will be carried out for two situations representing borderline cases for most models (open ways with intersections). Those tests will end off the practical part of the study which will then focus on experience sharing (enrichment of the website, meetings with the French local agencies in charge of air quality monitoring).

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