Towards a model evaluation protocol for urban scale flow and dispersion models

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Abstract: This paper reports on the stages forming a model evaluation protocol for urban flow and dispersion models proposed within the COST Action 732 on "Quality Assurance and Improvement of Micro-Scale Meteorological Models". It discusses the different components forming model evaluation with emphasis on validation and implementation of the protocol for the test case Mock Urban Setting Test (MUST). The protocol was proposed with building-resolving models in mind, but integral models have also been included. The suggested approach can be used for further micro-scale model evaluation and for the standardisation of their applications.

Keywords: COST action 732; model evaluation protocol; MUST experiment; CFD; non-CFD models.

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1 Introduction

Very recently, there has been an increase in the development and use of models within Europe for urban air quality applications. These models have begun to play a crucial role in environmental assessment and urban climate studies and studies that are undertaken to investigate and to quantify the effects of human activity on air quality and on the local climate. Until now, only limited work has been done to check the performance of these kinds of models and currently there is no standardised modelling practice for atmospheric applications.

The role of the COST Action 732 (2005–2009) has been to overcome this lack of information by also considering outcome from the previous European project on heavy gas model evaluation called SMEDIS (Carissimo et al., 2001). Particular attention has been given to producing a methodology for assuring the quality (fitness-for-purpose) of micro-scale meteorological models and providing the basis for a standardisation of modelling practice for flow and dispersion applications within urban areas. In this context, the Action has interpreted "micro-scale meteorological models" as models for the prediction of the flow or the dispersion of pollutants within and near the urban canopy or industrial landscape.

The impact of the COST Action 732 depends on whether the evaluation procedures suggested by the Action become widely accepted by the community of model developers and model users. In May 2007, the first version of the evaluation procedure was released in three official documents that are publicly available online at http://www.mi.uni-hamburg.de/Official-Documents.5849.0.html. These documents are:

- Background and Justification Document to Support The Model Evaluation Guidance and Protocol, Version 1, May 2007 (Britter and Schatzmann, 2007a).
- Model Evaluation Guidance and Protocol Document, Version 1, May 2007 – a stand-alone document to assist the setting up and executing of a model evaluation exercise (Britter and Schatzmann, 2007b).
- Best Practice Guideline for the CFD simulation of flows in the urban environment, Version 1, May 2007 – based on published guidelines and recommendations, which mainly deal with prediction of the statistically steady mean flow and turbulence in urban areas under conditions of neutral density stratification (Franke et al., 2007).

The Model Evaluation Guidance and Protocol Document is a condensed version of the background document. It gives specific guidance to model developers and users on how to evaluate and assure the quality of the model in an objective and defendable manner.

The evaluation process includes various components and, particularly, a scientific assessment, model verification and a model validation. To conduct a validation (comparison of model predictions with experimental observations), one will have to decide for which purpose the model results should later be used and thus to decide the variable(s) whose prediction is the most important. In other words, the validation objectives have to be explicitly specified. Briefly, a possible (very simple) baseline approach to a model validation (Britter and Schatzmann, 2007b) is to:

- Decide to allow those running the models to either have access to the experimental results or not (i.e., non-blind or blind simulations).
- Select the mean velocity and mean concentration (based on certain temporal and spatial scales) for comparison.
- Look at the streamline pattern and the concentration pattern to provide a qualitative view of the model quality.
- Produce a quantitative validation of the model quality by comparing the experimental and model data 'paired in space and time' and as 'arc maxima'. The complexity of the flow may make the latter choice less feasible where local maxima could be distributed widely; to use the metrics of FAC2 (for its transparency) and FB/NMSE (for information on bias and variance). The FB/NMSE weights the higher magnitudes at the expense of the smaller.

The documents have been updated with recommendations for data sets used in the validation work. The recommendations given in the documents listed earlier have been tested by the COST 732 Action itself. Many European academic and research groups have participated in this action with the objective of building a consensus within the scientific community on evaluation of micro-scale meteorological models. Currently, participants of the Action are continuing to analyse the results for the MUST case (Yee and Biltoft, 2004), which comprises both field and wind tunnel data from flow and dispersion experiments carried out within and above a simulated urban setting made up from 120 standard size shipping containers.

The wind tunnel measurements with a scaled model (1 : 75) of that configuration were carried out at the University of Hamburg (Bezpalcova, 2007). So far, several European groups of numerical modellers (using both CFD and non-CFD models) have simulated the wind tunnel MUST experiments following the model evaluation guideline. The experiments used were those with two main wind directions, 0° and –45° (and these correspond to 270° and 315°, respectively, in meteorological terminology) of the approaching flow. This study was launched in Athens in October 2006. Some of the results achieved are discussed in Franke et al. (2008) and Olesen et al. (2008).

The next phase was the launch of an exercise based on field experiments in a real city. This exercise was devoted to the simulation of dispersion experiments over Oklahoma City, USA. Several groups were involved in preparing simulation grids; simulation results were provided by about five teams. Initially, the simulations were done in the form of a blind test, i.e., only the geometry and the input data was given to the participants. Results from this are not included in this paper.

2 Protocol implementation and methodology

Computational Fluid Dynamics (CFD) models are an appropriate tool for this application and their evaluation is central to COST 732. However, the application of simpler models to these problems is of direct interest to many participants in COST 732. Our approach has been to develop a methodology that can be used for CFD models and can also be modified to accept simpler models.

Several CFD models have been used by different groups from many European countries to simulate the MUST experiment. They are: Miskam, Fluent, ADREA, Star-CD, Finflo, Cfx, Mitras, Tsu/M2UE, VADIS, Code_Saturne. Only recently, non-CFD models, such as Lasat, ADMS-Urban, RAMS, OML, ESCAPE and CALPUFF, have received increasing attention within COST 732 and results for them are available at the Cost Action website.

For the comparison of numerical results with experimental data, both qualitative and quantitative approaches have been chosen. There is a common understanding that exploratory qualitative data analysis using graphical comparison between model and data and an inter-comparison among models gives a simple, useful and transparent way of showing the strengths and weaknesses of models. For the evaluation of a model, both qualitative (through profiles and contours) and quantitative (through statistical analysis) approaches are needed; otherwise statistical parameters alone could obscure deficiencies of the model. This particular aspect is being investigated in Olesen et al. (2008).

In particular, in our proposed methodology model results need to be analysed in a combined way by means of:

- contours of velocity components, Turbulent Kinetic Energy (TKE) and Reynolds stress components
- vertical and horizontal profiles of velocity components and TKE
- profiles of dimensionless concentration. In the example provided, we only use the –45° approach flow case as concentration measurements were not available for the 0° case
- statistical analysis.

The first three are essentially a qualitative analysis, in which model results are evaluated using direct point-by-point comparisons with wind tunnel data. The fourth point is indeed quantitative and is used by employing several statistical measures, such as the Fractional Bias (FB), the Normalised Mean Square Error (NMSE), the fraction of predictions within a factor of two of observations (FAC2), the Geometric Mean bias (MG) and the Geometric Variance (VG). Typical magnitudes of the above-mentioned performance measures and estimates of model acceptance criteria have been summarised by Chang and Hanna (2004) based on extensive experience with evaluating many models with many field data sets. In terms of metrics, their criteria can be formulated as follows for good performing models: $-0.3 < FB < 0.3$; $NMSE < 4$; $FAC2 > 0.5$; $MG < 1$; $VG < 1.6$. These criteria can be used as guidance, although it should be noted that the values of Chang and Hanna refer to comparisons of concentrations from research-grade experiments in terms of maximum concentrations on arcs, i.e., unpaired in space. If used in other contexts (e.g., data paired in space and time, or for other parameters than concentration) less strict criteria might be applied. Performance can also be evaluated in terms of 'hit rate', as defined in VDI guideline 3783 Part 9, (2005–2011). In this guideline, a fractional deviation $D = 0.25$ is allowed in conjunction with specific absolute deviations W for the different variables analysed (the hit rate must not fall below 66% for the comparison with wind tunnel data).

The set of models involved in COST 732 is a representative sample of the micro-scale meteorological models currently available and widely used in Europe, and with the MUST exercise the Action's intention ha been to suggest criteria for the 'state-of-the-art' of the modelling process. The state-of-the-art is a dynamical concept; models constantly improve and the state of the art consequently changes. So the methodology, which the Action has followed, contains a procedure to update the criteria, so that if, in the future, new models are run using the COST 732-MUST case or other data, the value of the metrics reflecting the state of the art can be modified.

A somewhat different question concerns the 'fitness for purpose' criteria as this changes with the intended purpose of the model. An important point to be addressed by a model user is whether the 'state of the art' will satisfy the 'fitness for purpose' criteria for the particular purpose of the modeller. When determining model quality, it is obviously essential to consider and specify what the purpose of the model is. For example, models with a similar scientific basis may be required for quite different purposes such as:

- a model for planning or regulatory purposes may need to be run several thousands of times
- a model for emergency response may need real-time predictions or access to pre-calculated real-time output
- a model for post-accident investigation or air quality hot spot analysis could be very complex with less concern for computational cost or resource requirement.

And, an assessment of the 'fitness for purpose' of the same model could be very different for each of the above-mentioned purposes.

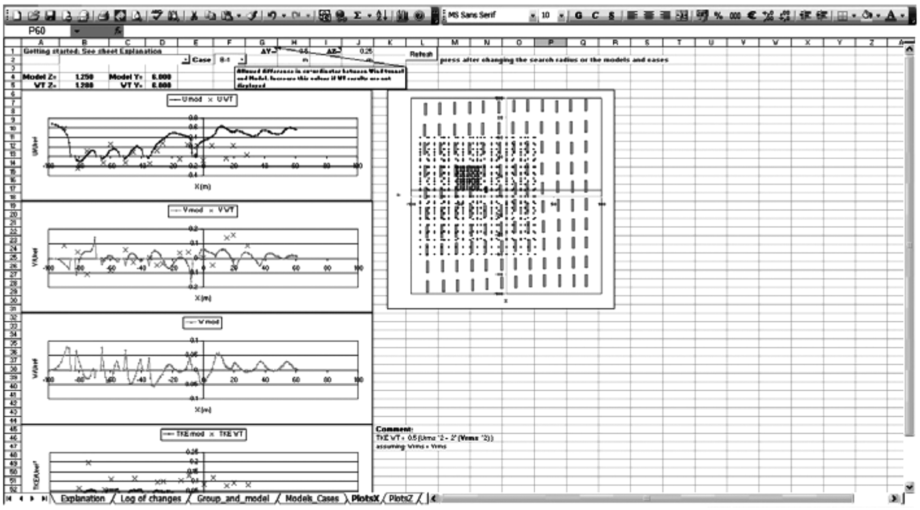
3 Evaluation exercise

3.1 *The MUST experiment*

Vertical and horizontal profiles of wind tunnel data and the results from the various model simulations have been collected in Excel spreadsheets that include a macro tool, which allows easy graphical comparisons. The tool was developed within this Action by Berkowicz et al. (http://www.dmu.dk/en/air/models/background/exceltools/). This tool was found to be extremely useful for exploratory data analysis to highlight both large errors and subtle differences among the models.

In particular, there is a group of Excel files that allows easy graphical inspection of the details of every case for all of the models. Another group of Excel workbooks contains essential information extracted from the above-mentioned Excel files with summary plots and metrics. As an example, one of the sheets with detailed information (PlotsX) is shown in Figure 1.

Figure 1 Example of the Excel spreadsheet with a macro tool for easy graphical comparisons



For the 0° approaching flow case (not shown here), the developed macro allows us to note that the qualitative behaviour of the models is different. Some of them seem to underestimate the wind velocity in the layer occupied by the buildings, while others overestimate the velocity. No model represents the *z*-velocity (vertical velocity) well at positions behind buildings.

As an example of the qualitative evaluation, some profiles of the dimensionless concentrations for the −45° case are shown in Figure 2, where concentration results along cross-sections at, respectively, the beginning, middle and end of the building array are plotted for the height $z = 0.5H$ (where H is the height of the building). The qualitative behaviour of the pollutant plume seems to be acceptable.

Results from this exercise has helped to formulate a Best Practice Guideline specifically for using the MUST data and to revise the Model Evaluation Guidance and Protocol Documents.

Figure 2 –45° case, samples of horizontal profiles of dimensionless concentrations from one CFD model at $z = 0.5H$ at the beginning, middle and end of the array (first/fourth, second/fifth and third/sixth picture, respectively). Please note that the building array is rotated so the *x*-axis points downwards and the source is on top

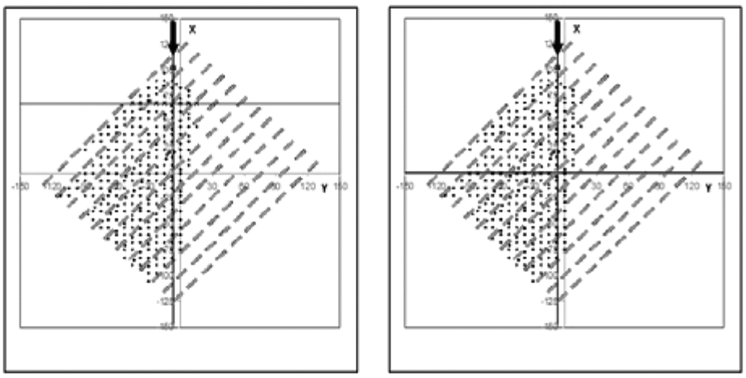
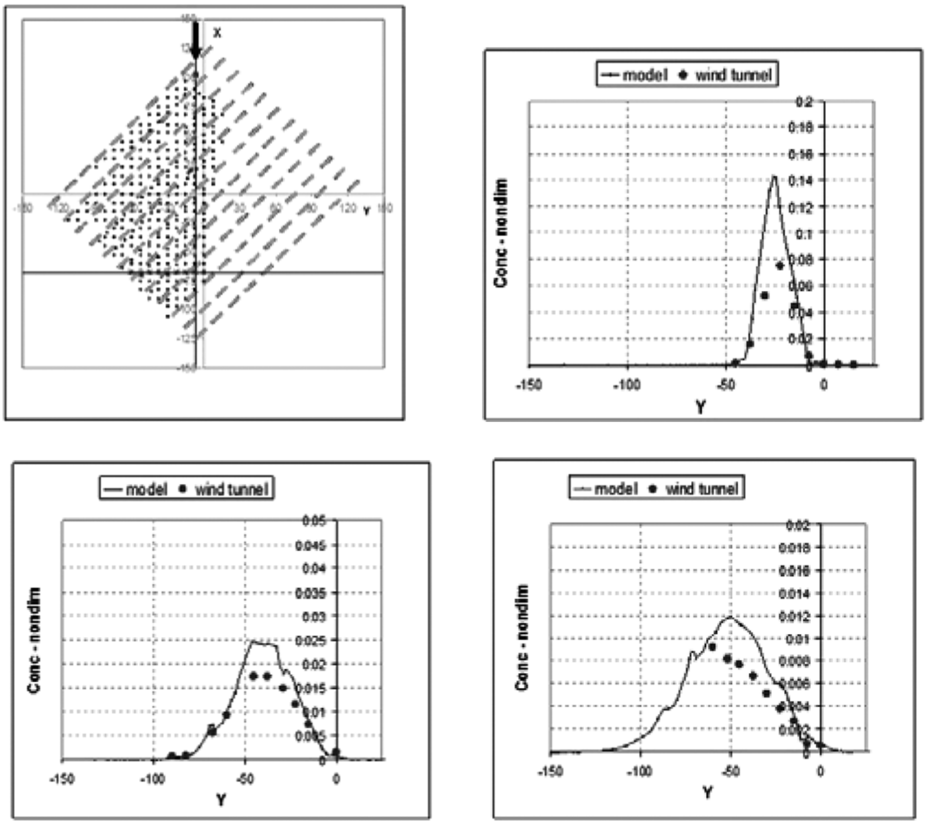


Figure 2 –45° case, samples of horizontal profiles of dimensionless concentrations from one CFD model at $z = 0.5H$ at the beginning, middle and end of the array (first/fourth, second/fifth and third/sixth picture, respectively). Please note that the building array is rotated so the x-axis points downwards and the source is on top (continued)



4 Conclusions and work in progress

The comparison carried out in the COST 732 action shows that flow and concentration model results compare relatively well with the measurements, although they share some common problems in predicting certain features of the flow. For example, all models have difficulty in predicting the vertical component of wind velocity, whereas prediction for the x-velocity component is much more successful. The Excel tool developed within the COST 732 has allowed us to make detailed studies of the differences in model results and has helped us to emphasise strength and weakness of synthetic statistical parameters. In some specific cases, the models show some weaknesses in predicting the complex flow especially the turbulent structure of flow. Correct specification of the inlet profiles and specific aspects of two-equation turbulence models were thought to require further investigation.

For the evaluation of the accuracy of a model, both qualitative and quantitative approaches are needed. Statistical measures alone could lead to wrong conclusions. This could be true especially when measurements are limited to few points/profiles or when raw data are used without special treatment of the values that are smaller than the allowed deviation considered in the statistical analysis.

The Action has finalised the MUST exercise and has suggested the best approach for further model evaluation for the standardisation of CFD modelling practice for micro-scale meteorological applications. This includes a critical review and refinement of the numerical results. To assist with this, several small working groups have been formed to investigate specific aspects including boundary conditions, statistical measures and non-CFD model evaluations.

The result of the protocol implementation through the large MUST experiment exercise have allowed us to:

- develop a coherent and structured quality assurance procedure for these types of models that gives clear guidance to developers and users of such models as to how to properly assure their quality and their proper application
- provide a systematically compiled set of appropriate and sufficiently detailed data for model validation work in a convenient and generally accessible form.

The Oklahoma City exercise has finally helped us to further strengthen our previous results and to finalise our original objectives that are:

- to build a consensus within the community of micro-scale meteorological model developers and users regarding the usefulness of the procedure
- to stimulate a widespread application of the procedure and the preparation of quality assurance protocols, which prove the 'fitness for purpose' of all micro-scale meteorological models participating in this activity
- to determine the current 'state of the art' of the modelling process and to give recommendations for the improvement of present models and, if necessary, for new model parameterisations or even new model developments.

The discussion of the quality assurance procedure, the use of specific data sets and the recommendations specified in the Best Practice Guideline should lead to a harmonised approach accepted at least at the European level. It is to be expected that the very existence of a widely accepted European standard for quality assurance in the field of micro-scale meteorological models in combination with the provision of suitable validation data will significantly improve 'the culture' within which such models are developed and applied.

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