12th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes

ctober 2008

732 Action
Quality Assurance and Improvement of Micro-Scale Meteorological Models

A MODEL EVALUATION PROTOCOL FOR URBAN SCALE FLOW AND DISPERSION MODELS

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INTRODUCTION

COST Action 732
Quality Assurance of Micro-Scale Meteorological Models

- METEOROLOGY
- ACTIVITIES INFLUENCED BY METEOROLOGY, PARTICULARLY DISPERSION IN URBAN AND BUILT UP ENVIRONMENTS
- MODELS AND THEIR FORMALISED EVALUATION BY ADOPTING THE "FIT-FOR PURPOSE" CRITERION
- FOCUS ON CFD MODELS WITH THE INCLUSION OF "NON-CFD" MODELS IN ORDER TO:
  - *BUILD A CONSENSUS WITHIN THE SCIENTIFIC AND USER COMMUNITY*
  - *STIMULATE A WIDESPREAD APPLICATION OF THE PROCEDURE AND THE PREPARATION OF QUALITY ASSURANCE PROTOCOLS*
  - *GIVE RECOMMENDATIONS FOR THE IMPROVEMENT OF PRESENT MODELS*

SO FAR...

- **Best Practice Guideline for the CFD simulation of flows in the urban environment** (Vers. 1 May 2007) **-** based on published guidelines and recommendations, which mainly deal with the prediction of the statistically steady mean flow and turbulence in the built environment for situations with neutral stratification
(J. Franke, A. Hellsten, H. Schlünzen and B. Carissimo, in press. The COST 732 best practice guideline for CFD simulation of flows in the urban enviroment - A summary. Int. J. of Environment and Pollution)

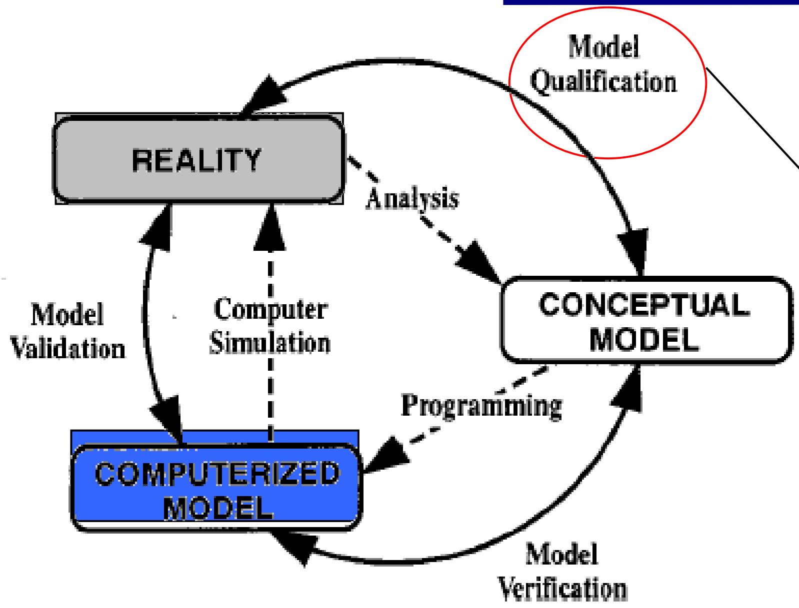
- **Model evaluation guidance and protocol document** (Vers. 1 May 2007) **-** a stand alone document to assist the setting up and executing of a model evaluation exercise

- **Background and justification document to support the model evaluation guidance and protocol** (Vers. 1 May 2007)
(M. Schatzmann and R. Britter, in press. Quality assurance and improvement of micro-scale meteorological models. Int. J. of Environment and Pollution)

Available on line at **http://www.mi.uni-hamburg.de/Official-Documents.5849.0.html**

- **The MUST wind tunnel exercise: Validation methods and results (in progress)** - guidance to interpretation of graphs and metrics. Protocol for the case of MUST experiment, as simulated in the Hamburg wind tunnel. Results from the various models in the form of graphs and metrics.

MODEL EVALUATION



Phases of modelling and simulation and the role of Verification and Validation (Schlesinger, 1979). Taken from Oberkampf et al. (2004).

Scientific Evaluation

•Schlesinger, S., 1979: Terminology for Model Credibility. Simulation, 32(3): 103-104.

•Oberkampf, W.L., Trucano, T.G., and Hirsch, C., 2004: Verification, validation, and predictive capability in computational engineering and physics. Appl Mech Rev., 57(5):345 - 384.

MODEL EVALUATION PROTOCOL

- Scientific Evaluation Process

- Verification Process

- Provision of “evaluated” (appropriate and quality assured) Data Sets (this includes statements on the nature of the data – from controlled laboratory experiments or/and from field measurements (routinely available or “controlled” measurement campaigns)

- Model Validation Process

- Operational Evaluation Process

SCIENTIFIC EVALUATION

Based on a questionnaire

- Specify clearly the model purpose(s)
- Produce a consensus of what “science” is required for this model and its applications
- Determine whether the “science” is present adequately
- Give proof and clear evidence on the above

MODEL VALIDATION

- Processing of the experimental data
- What variables to compare?
- How should the variables be compared?
- How should the model be run and the results interpreted? (modelling inputs, set-up, post-treatment of outputs ...)
- Exploratory data analysis (Olesen et al.)
- Metrics for a Model Validation (Franke et al.)
- Quality acceptance criteria
- Baseline approach to model validation

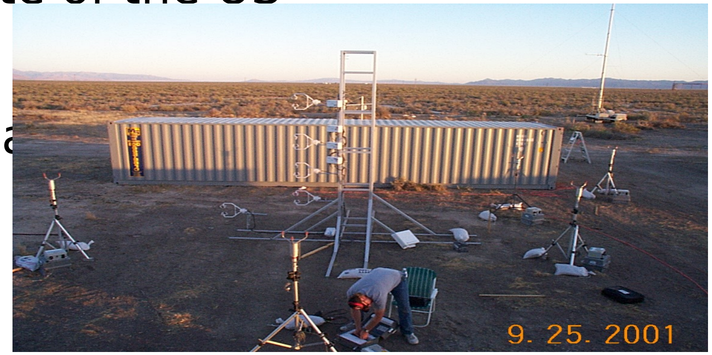
PROTOCOL FOR THE CASE OF THE MUST EXPERIMENT

LABORATORY OR FIELD EXPERIMENTAL DATA

Wind tunnel measurements at the Environmental Wind Tunnel Laboratory at Hamburg University

- scaled model of the MUST configuration (1:75)
- approaching flow cases: 0°, -30°, -45°, -60°, -90°
- flow and dispersion measurements: vertical and horiz profiles

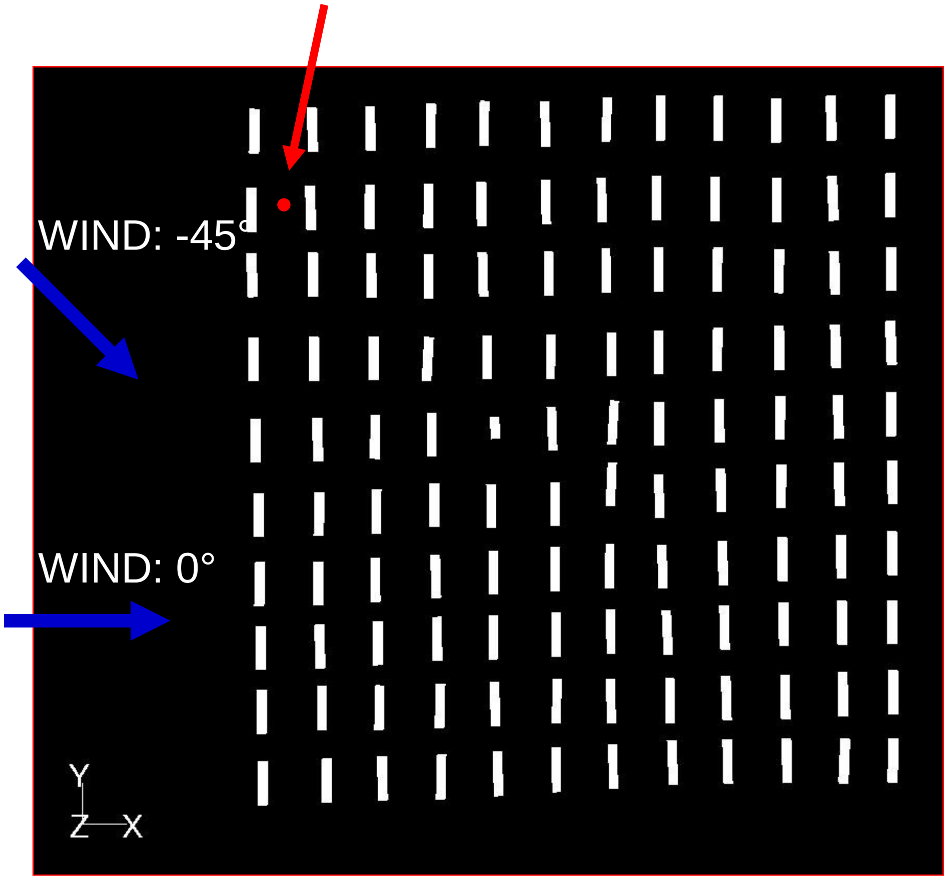
- extensive field test carried out on a test site of the US Army in the Great Basin Desert in 2001
- flow and dispersion data measured within a idealized urban roughness
- 120 standard size shipping containers (regular array of 10 by 12 obstacles)



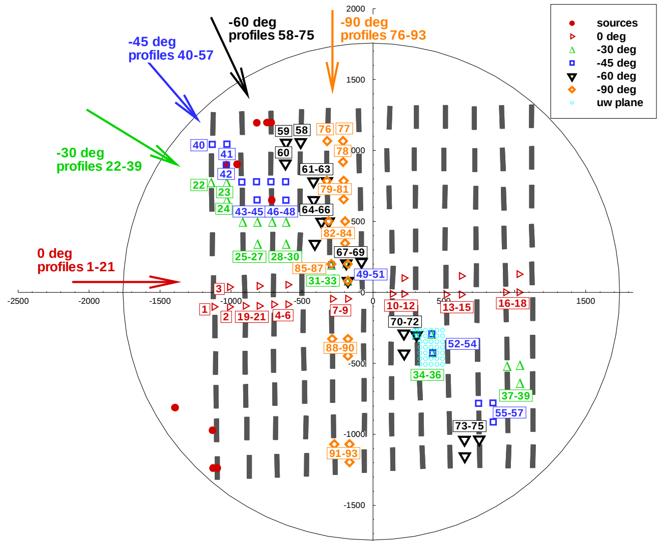
www.eng.utah.edu/~pardyjak/must.html

MUST - MEASUREMENTS

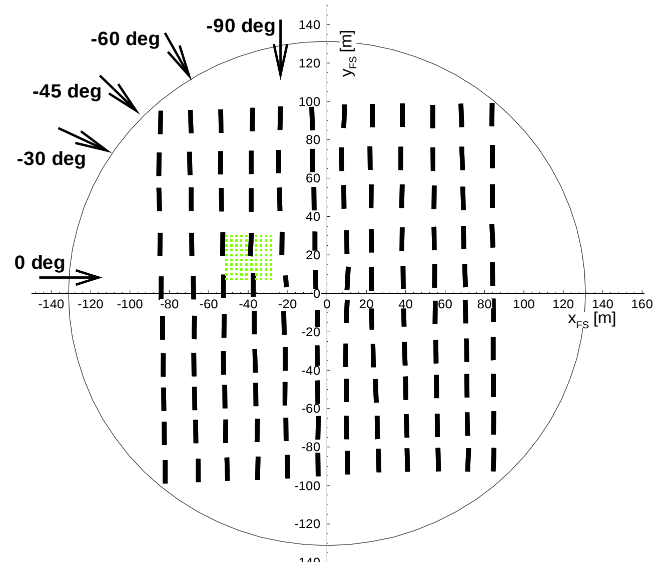
Source (Height: ground level)



Schematic view of the MUST building array and cases considered. The point source is positioned along the axis of the first street canyons line



Wind tunnel measurements: vertical profiles



Wind tunnel measurements: horizontal profiles

MUST - MODELS INVOLVED

Models can be thought for general OR SPECIFIC applications, it is important to check their fitness for purpose when we use them for solving a problem or for a new application…

Computational Flui Dynamics (CFD) models

- MISKAM
- FLUENT
- ADREA
- STAR-CD
- FINFLO
- CFX
- MITRAS
- TSU/M2UE
- VADIS
- CODE_SATUR NE

15 GROUPS INVOLVED

- ***0° case***: *about 40 model flow results*
- ***-45° case***: *about 30 model flow results*
- ***-45° case:*** *about 20 model dispersion results*

7 GROUPS INVOLVED

- ***-45° case***: *about 10 model dispersion re...*

Non-CFD models

- LASAT
- ADMS-URBAN
- RAMS
- OML
- ESCAPE
- CALPUFF

QUESTIONNAIRES - EXAMPLES

Physical parameters of simulations

Please give all required information if available. In case of non-CFD model, many questions may be irrelevant. Answer those questions that you find meaningful.

If different codes were used or one code with different turbulence models, then use a separate questionnaire for each computation.

1. Contact person

- Name SILVANA DI SABATINO
  RICCARDO BUCCOLIERI
- Institution: DIPARTIMENTO DI SCIENZA DEI MATERIALI, UNIVERSITY OF SALENTO, LECCE (IT)

2. Computer Code

- Name, version and precision: FLUENT 6.2.16, single precision
- CFD or non CFD: CFD
- If non CFD, describe the model briefly (obstacle resolving or not, etc.)
- Primary variables (i.e. variables solved from differential equations): u,v,w, p, TKE, epsilon, concentration

3. Reynolds number

- Value? 10 x 10^5
- What length scale is used in the above given Reynolds number (for instance container height)? Container height H=2.54m
- What velocity scale is used in the above given Reynolds number (for instance inflow reference velocity at z=7.29m)? inflow reference velocity u=5.5m/s

4. Turbulence model

- Model class (linear 2-equation model, nonlinear 2-equation model, RSM, other)? Linear 2-equation model

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- Wall treatment (wall-functions or solution up to the wall)? Standard wall function
- The velocity-scale-determining variable if not turbulent kinetic energy?
- The length-scale-determining variable (epsilon, omega other)?
- Model version name or developers' names (for instance: std. k-epsilon, Launder-Sharma k-epsilon, Launder-Reece-Rodi RSM, give also a literature reference if the model is not widely known)? Std k-epsilon
- Nonstandard coefficient values if used?
- Nonstandard correction terms if used?
- Nonstandard damping, mixing or other functions if used?
- Other nonstandard features if used?
- Other information? gradient diffusion model, Sct=0.7

- **Physical parameters** of simulations of the MUST wind tunnel case with -45° approach flow direction
- MUST Wind Tunnel Test Case -45° approach flow direction numerical modelling exercise - **Geometrical parameters questionnaire**
- **Boundary conditions** for dispersion of the MUST wind tunnel case with -45° approach flow direction
- **Numerical parameters** of simulations of the MUST wind tunnel case with -45° approach flow direction

MUST – VALIDATION

WHAT VARIABLES? AND EXPLORATORY DATA ANALYSIS

- Contours of u/U_{ref} - TKE/U_{ref}^2 -Turbulent fluxes ($u'w'$) ***Qualitative***

- Profiles of u/U_{ref}
- Profiles of w/U_{ref}
- Profiles of dimensionless concentration K (or C*)

Quantitative → ***EXCEL MACRO***

Chang and Hanna, 2004

METRICS (some example of statistical parameters)

Hit Rate Test

(the fraction of model results which differs within an allowed range D from the

VDI, 2005

$$q = \frac{N}{n} = \frac{1}{n}\sum_{i=1}^{n} N_i$$

$$N_i = \begin{cases} 1 \ \text{if} \ \left|\frac{P_i - O_i}{O_i}\right| \le D \ \text{or} \ |P_i - O_i| \le W \\ 0 \ \text{else} \end{cases}$$

N: number of measurement positions
D: allowed relative difference, **D = 0.25**
W: allowed absolute difference (based on error due to interpolation and exp. uncertainty due to repeatability)

Normalised mean square error

(normalised discrepancies between computed and experimental values)

$$\mathrm{NMSE} = \frac{\overline{(C_o - C_p)^2}}{\overline{C_o}\;\overline{C_p}}$$

Fractional BIAS

(over- or under-estimation)

$$\mathrm{FB} = \frac{(\overline{C_o} - \overline{C_p})}{0.5\;(\overline{C_o} + \overline{C_p})}$$

Factor2

$$\mathrm{FAC2} = \text{fraction of data that satisfy}\;\; 0.5 \le \frac{C_p}{C_o} \le 2.0$$

MUST – VALIDATION

Hit Rate Test

$$q = \frac{N}{n} = \frac{1}{n}\sum_{i=1}^{n} N_i$$

$$N_i = \begin{cases} 1 \;\; if \;\; \left|\frac{P_i - O_i}{O_i}\right| \le D \;\; or \;\; |P_i - O_i| \le W \\ 0 \;\; else \end{cases}$$

Threshold values for Hit Rate and FAC2

	Allowed absolute deviation W, referring to Hit rate. The same value is used as threshold when FAC2 is determined.	Allowed fractional deviation D, referring to Hit rate
u/u_{ref} (velocity component)	0.008	0.25
v/u_{ref} (velocity component)	0.007	0.25
w/u_{ref} (velocity component)	0.007	0.25
TKE/u^2_{ref}	0.005	0.25
c* (concentration)	0.003	0.25

MUST – VALIDATION

- variables (what variable?)
- definition (some of the above mentioned statistical parameters do not make sense for some variables)
- implementation (interpolation or closest point?)
- treatment of zero values
- measurement errors

MUST – VALIDATION

Normalised mean square error

$$\mathrm{NMSE} = \frac{\overline{\left(C_o - C_p\right)^2}}{\overline{C_o}\ \overline{C_p}}$$

$$\mathrm{FB} = \frac{\left(\overline{C_o} - \overline{C_p}\right)}{0.5\ \left(\overline{C_o} + \overline{C_p}\right)}$$

Fractional BIAS

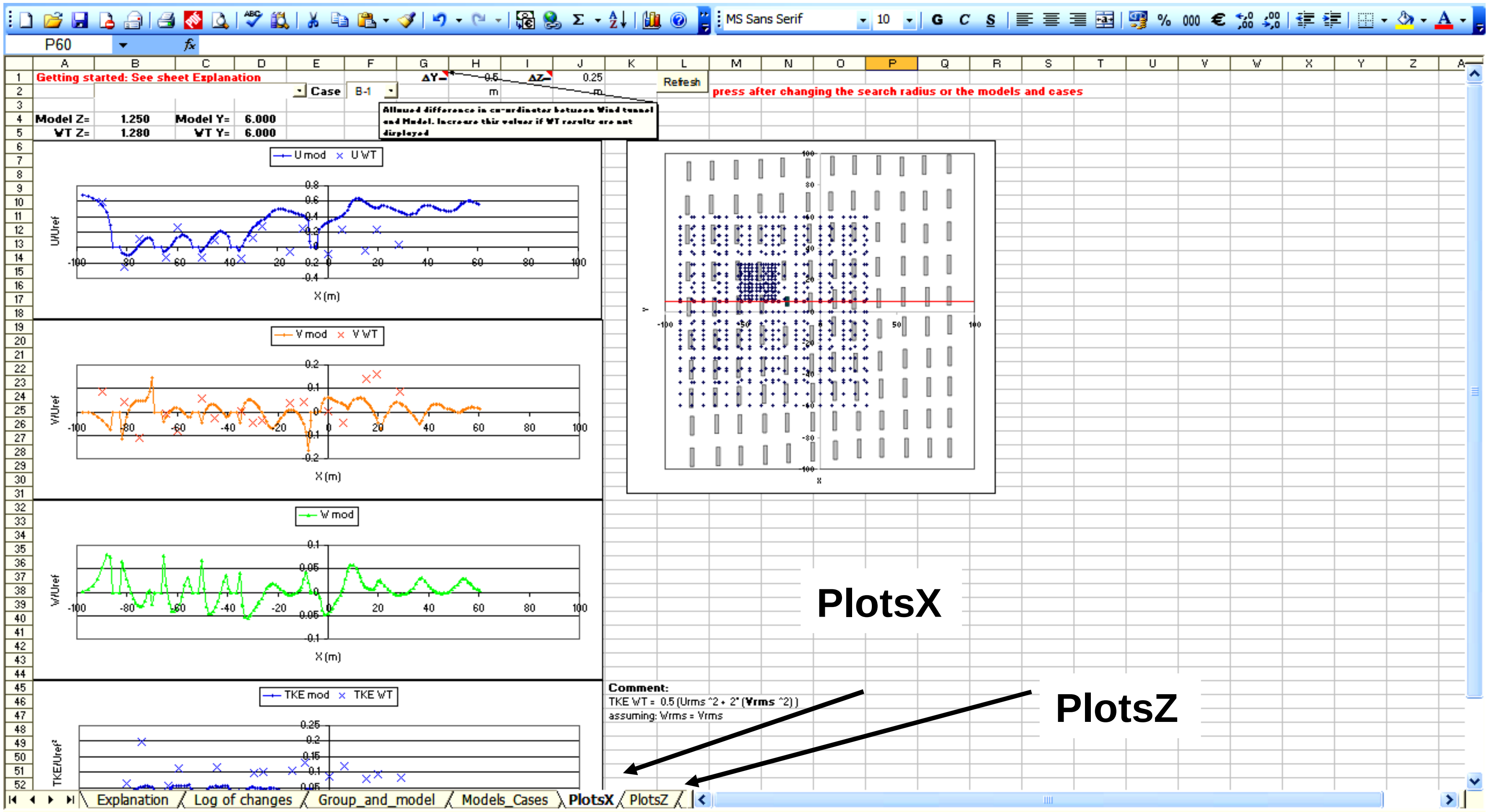
- Fractional bias (FB) and Normalised Mean Square Error (NMSE) make **no sense for parameters that can take both negative and positive values**, such as velocity components.

- FB is meant to be bounded within the range -2 to +2. It is -2 for extreme over-prediction, and +2 for extreme under-prediction. An over-prediction by a factor of two gives a value of FB = -0.67.

- In the MUST, for TKE, it is formally OK to compute FB and NMSE, but it should be kept in mind that the observed TKE is an artefact and cannot be directly compared to modelled values.

MUST - RESULTS

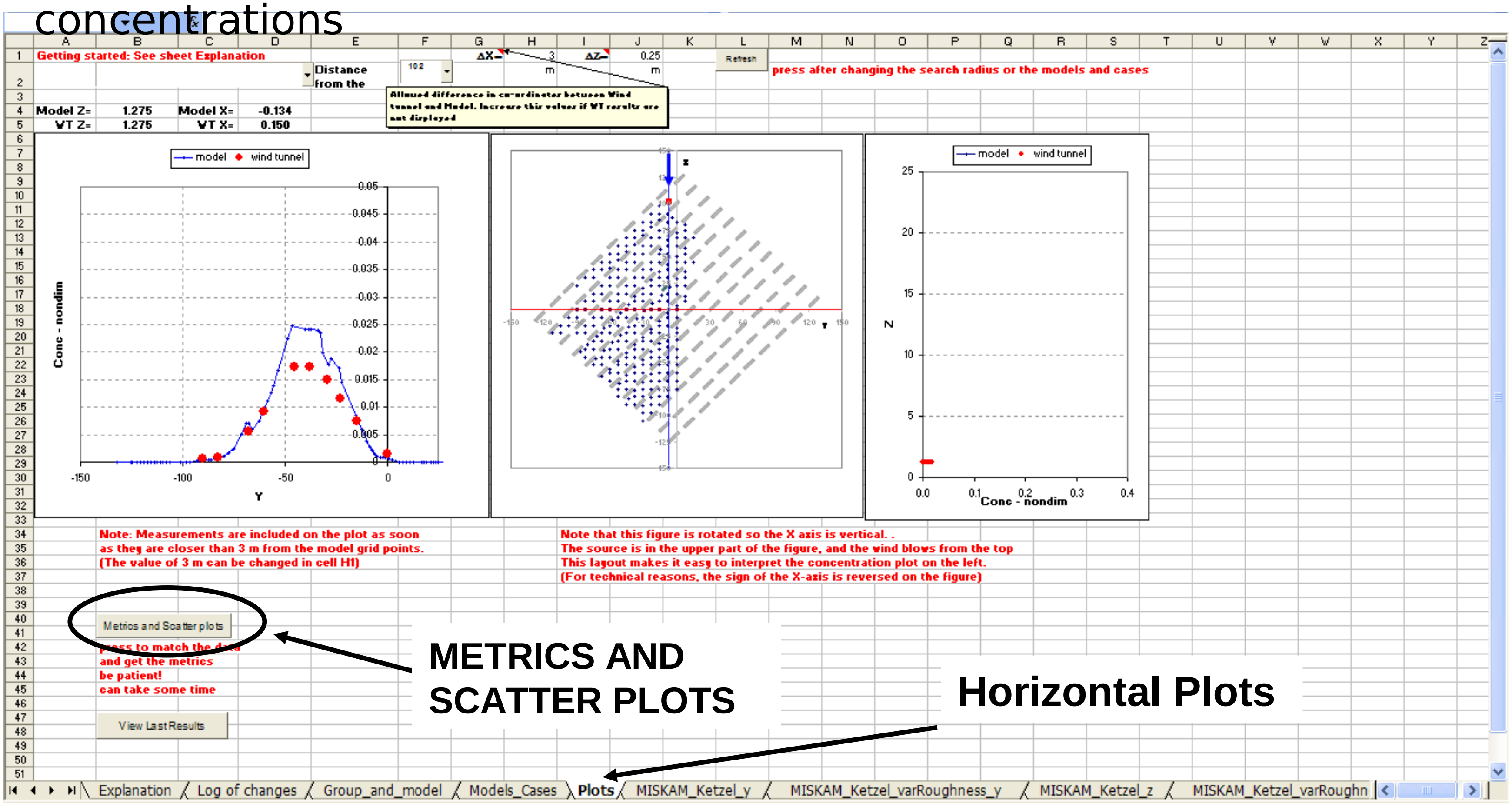
0° approach flow case - flow



Example of the Excel spreadsheet (Olesen et al.2008) including a macro tool which allows easy graphical inter-comparisons

MUST-RESULTS

-45° approach flow case - concentrations



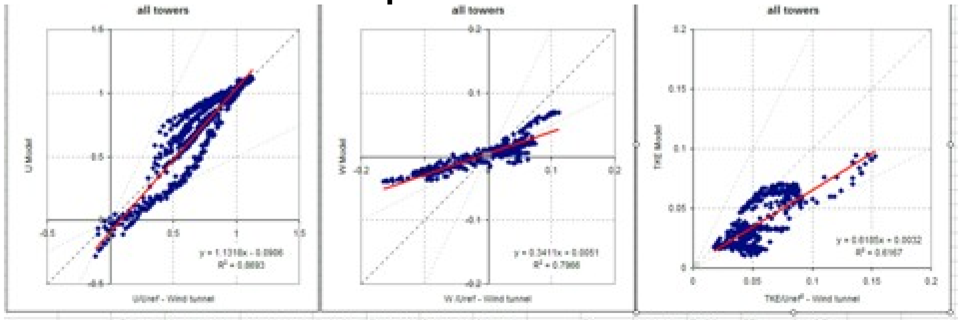
Example of the Excel spreadsheet including a macro tool which allows easy graphical inter-comparisons

EXPLORATORY DATA ANALYSIS

0°approach flow case - flow

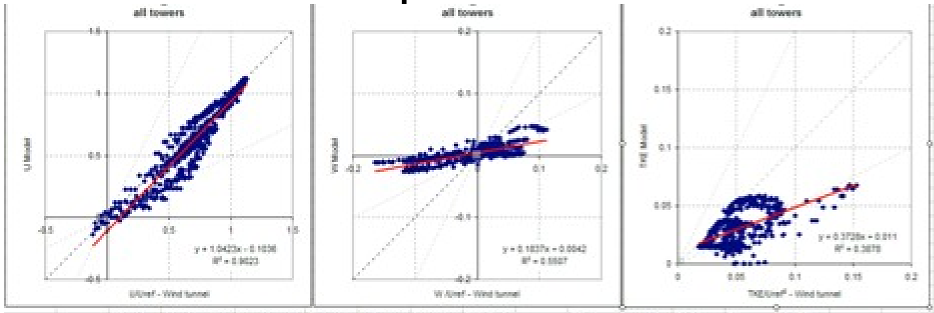
Examples

FLUENT_1



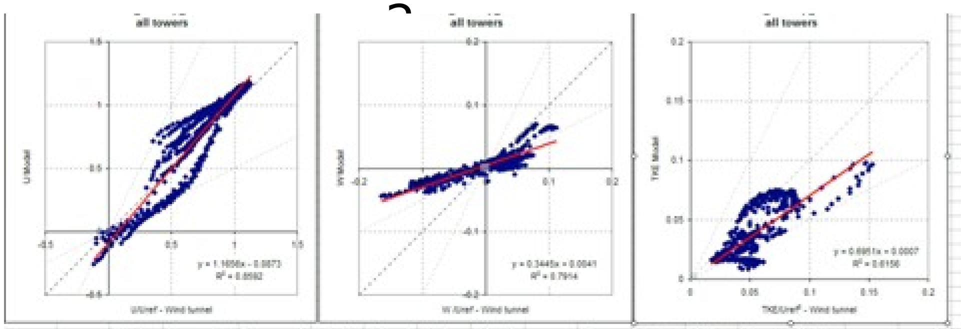
	#Points	Average obs.	Average mod.	Std. obs.	Std. mod.	CV obs.	CV mod.	R2	Hit rate	FAC2	FB	NMSE
U	566	0.684571822	0.68421242	0.283196	0.343764	0.413683	0.502423	0.8693	0.666078	0.863958	0.000525	0.03589
W	566	-0.00531686	0.003300552	0.054936	0.020995	-10.3325	6.361128	0.7966	0.243816	0.289753	8.547712	-83.862
TKE	566	0.051082543	0.034806696	0.024081	0.018965	0.471418	0.54487	0.6167	0.413428	0.787986	0.378996	0.273783

MISKAM 1



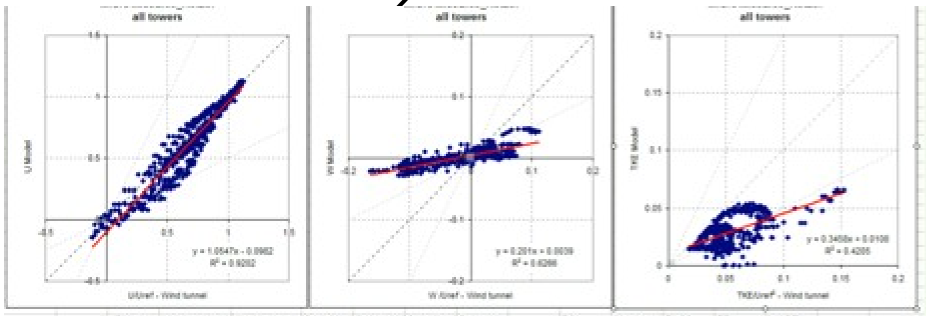
	#Points	Average obs.	Average mod.	Std. obs.	Std. mod.	CV obs.	CV mod.	R2	Hit rate	FAC2	FB	NMSE
U	566	0.684571822	0.609994092	0.283196	0.31076	0.413683	0.509448	0.9023	0.750883	0.897527	0.115217	0.036221
W	566	-0.00531686	0.003217093	0.054936	0.013599	-10.3325	4.226981	0.5507	0.213781	0.293286	8.128478	-126.472
TKE	566	0.051082543	0.030053474	0.024081	0.014417	0.471418	0.479728	0.3878	0.335689	0.671378	0.518366	0.519125

FLUENT_2



	#Points	Average obs.	Average mod.	Std. obs.	Std. mod.	CV obs.	CV mod.	R2	Hit rate	FAC2	FB	NMSE
U	566	0.684571822	0.710631323	0.283196	0.356098	0.413683	0.501101	0.8592	0.614841	0.874558	-0.03736	0.042537
W	566	-0.00531686	0.00226315	0.054936	0.021276	-10.3325	9.401007	0.7914	0.233216	0.293286	4.96446	-120.179
TKE	566	0.051082543	0.036240751	0.024081	0.021334	0.471418	0.588664	0.6156	0.439929	0.805654	0.339927	0.242396

MISKAM 2



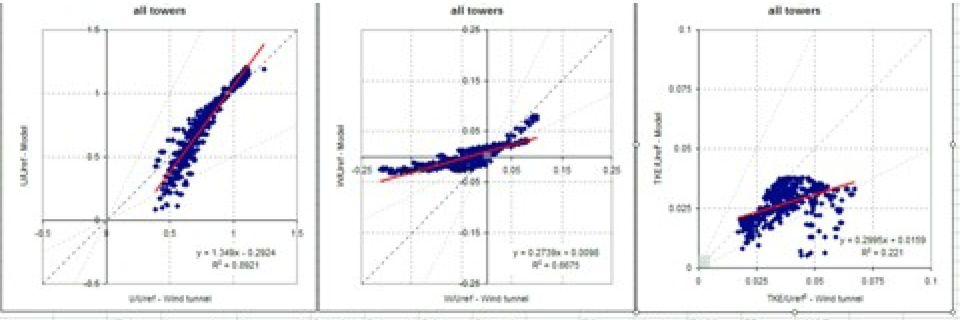
	#Points	Average obs.	Average mod.	Std. obs.	Std. mod.	CV obs.	CV mod.	R2	Hit rate	FAC2	FB	NMSE
U	566	0.684571822	0.623800765	0.283196	0.311377	0.413683	0.499161	0.9202	0.765018	0.916961	0.092896	0.027296
W	566	-0.00531686	0.002800839	0.054936	0.013945	-10.3325	4.967052	0.6266	0.208481	0.265018	6.478251	-138.086
TKE	566	0.051082543	0.028431092	0.024081	0.01284	0.471418	0.451633	0.4205	0.295053	0.644876	0.56975	0.589553

EXPLORATORY DATA ANALYSIS

-45°approach flow case - flow

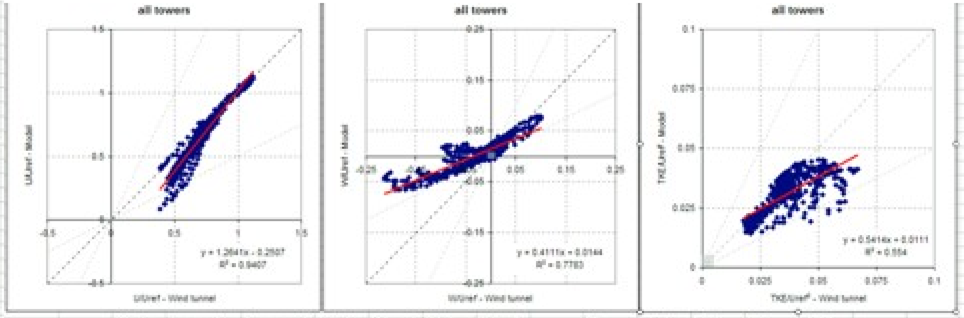
Examples

STAR-CD_1



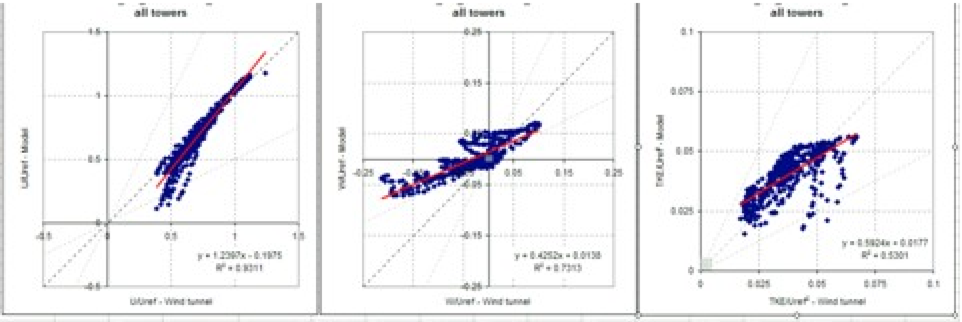
	#Points	Average obs.	Average mod.	Std. obs.	Std. mod.	CV obs.	CV mod.	R2	Hit rate	FAC2	FB	NMSE
U	498	0.739746313	0.706493243	0.183552	0.262159	0.248128	0.371096	0.8921	0.839357	0.961847	0.047401	0.024279
W	498	-0.033506719	0.000580937	0.064328	0.021569	-1.91987	37.12733	0.6675	0.228916	0.319277	2.070575	-179.474
TKE	498	0.036350438	0.026781712	0.011115	0.007081	0.305778	0.264394	0.221	0.594378	0.923695	0.303133	0.196246

FLUENT_1



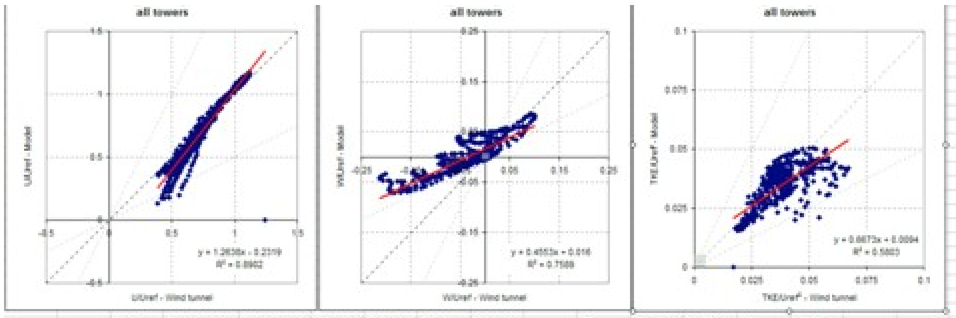
	#Points	Average obs.	Average mod.	Std. obs.	Std. mod.	CV obs.	CV mod.	R2	Hit rate	FAC2	FB	NMSE
U	497	0.738733125	0.683120794	0.182337	0.237651	0.246824	0.34789	0.9407	0.881288	0.973843	0.078225	0.017336
W	497	-0.03352127	0.000585317	0.064392	0.030009	-1.92094	51.26986	0.7783	0.2334	0.301811	2.071085	-142.572
TKE	497	0.036389378	0.030782113	0.011092	0.008068	0.304823	0.262116	0.554	0.792757	0.983903	0.166954	0.076995

STAR-CD_2



	#Points	Average obs.	Average mod.	Std. obs.	Std. mod.	CV obs.	CV mod.	R2	Hit rate	FAC2	FB	NMSE
U	498	0.739746313	0.71956712	0.183552	0.235822	0.248128	0.327728	0.9311	0.925703	0.96988	0.027656	0.011578
W	498	-0.033506719	-0.000408474	0.064328	0.031988	-1.91987	-78.3121	0.7313	0.15261	0.271084	1.951824	199.7725
TKE	498	0.036350438	0.039267954	0.011115	0.009044	0.305778	0.230322	0.5301	0.664659	0.987952	-0.07716	0.04719

FLUENT_2



	#Points	Average obs.	Average mod.	Std. obs.	Std. mod.	CV obs.	CV mod.	R2	Hit rate	FAC2	FB	NMSE
U	498	0.739746313	0.703040848	0.183552	0.245865	0.248128	0.349717	0.8902	0.903614	0.975904	0.050881	0.019822
W	498	-0.033506719	0.000708733	0.064328	0.03362	-1.91987	47.43665	0.7589	0.184739	0.267068	2.086436	-112.355
TKE	498	0.036350438	0.033636139	0.011115	0.009737	0.305778	0.289473	0.5803	0.901606	0.991968	0.077566	0.049668

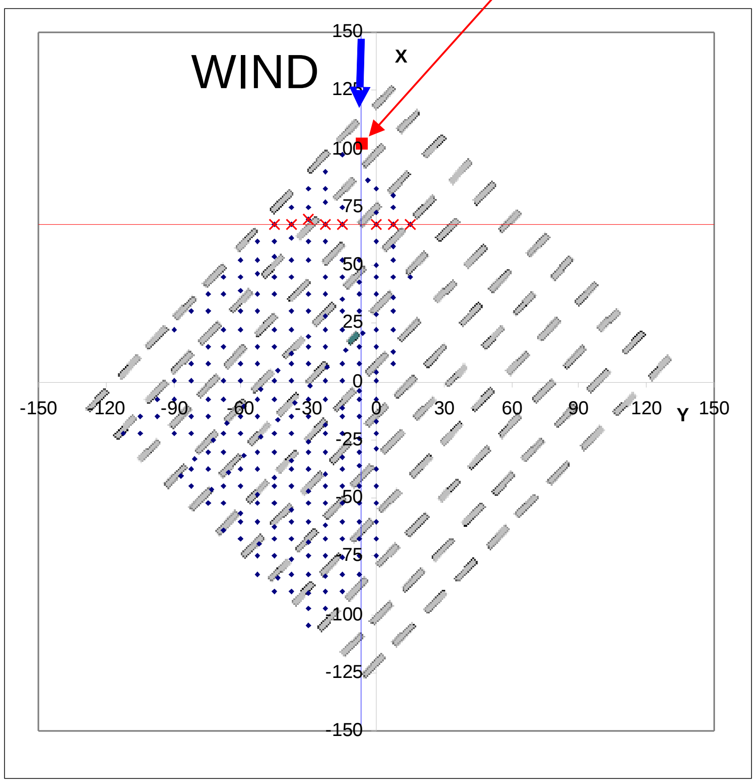
EXPLORATORY DATA ANALYSIS

-45° approach flow case concentrations

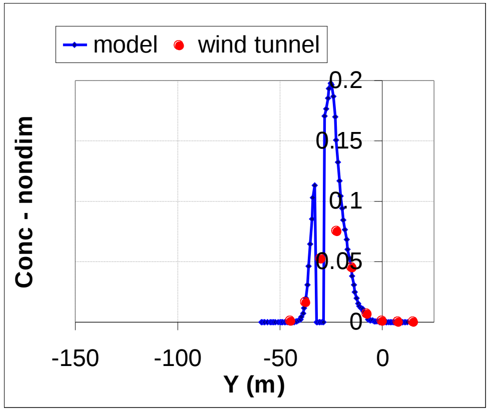
$$K = \frac{C U_{ref} H_{ref}^{2}}{Q}$$

C	measured or calculated concentration
U_{ref}	reference wind speed (undisturbed flow)
H_{ref}	building height
Q	emission rate

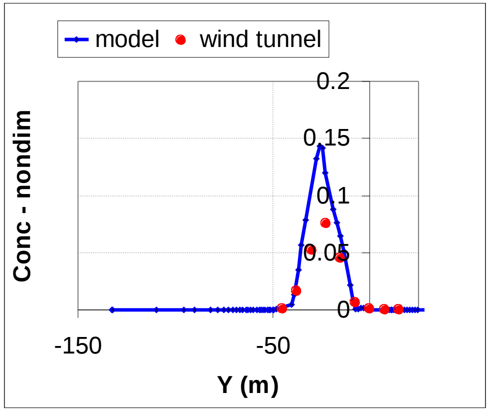
Source (ground level)



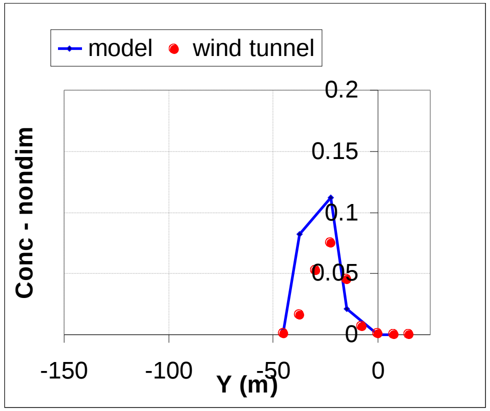
MISKAM_3



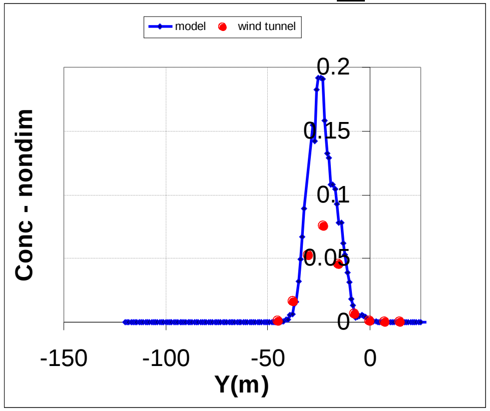
FLUENT_3



FINFLO



STAR-CD_2



Distance from the source: 35m

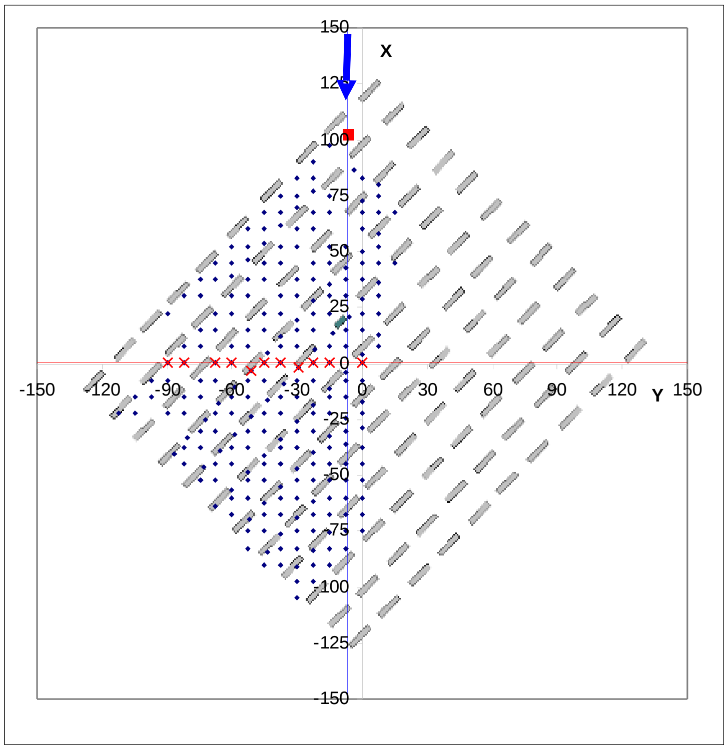
Profiles at z=0.5H

EXPLORATORY DATA ANALYSIS

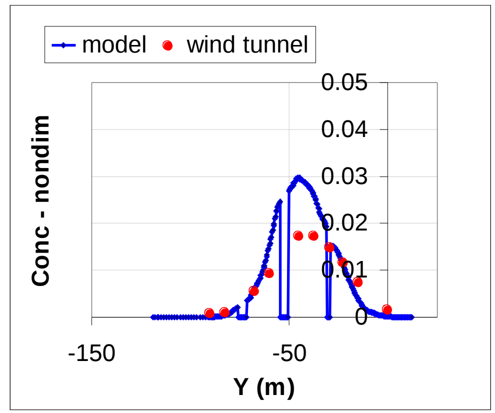
-45° approach flow case concentrations

$$K = \frac{C U_{ref} H_{ref}^{2}}{Q}$$

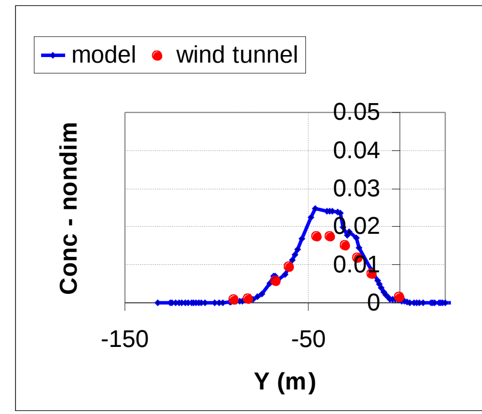
C	measured or calculated concentration
U_{ref}	reference wind speed (undisturbed flow)
H_{ref}	building height
Q	emission rate



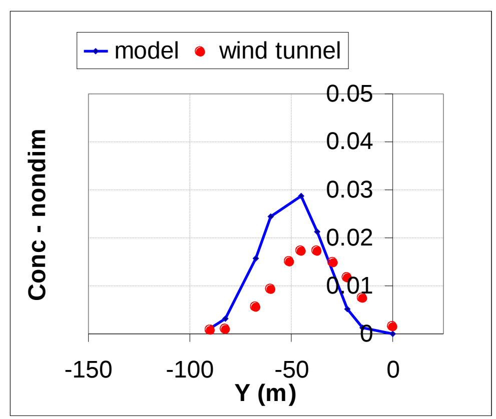
MISKAM_3



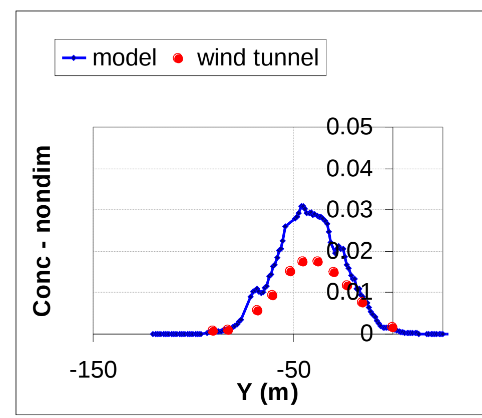
FLUENT_3



FINFLO



STAR-CD_2



Distance from the source: 102m

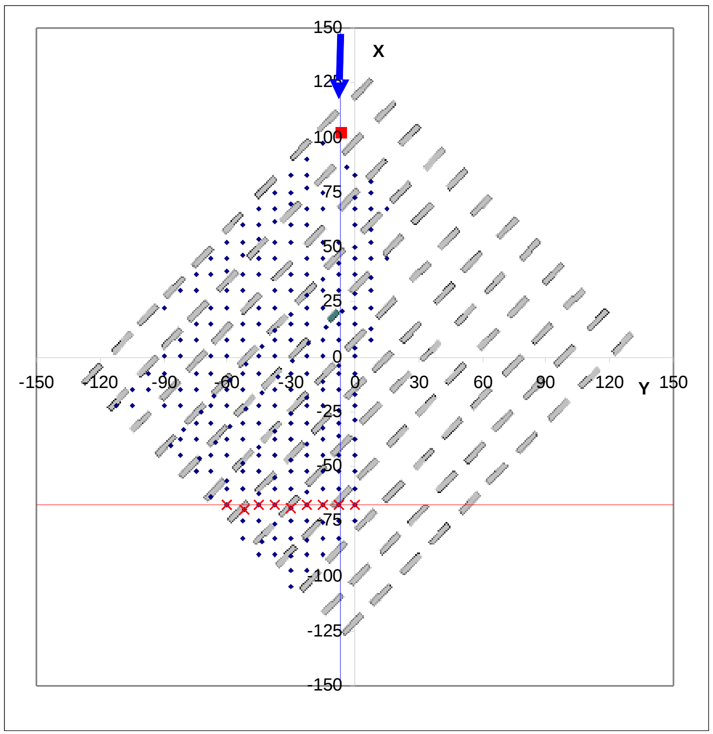
Profiles at z=0.5H

EXPLORATORY DATA ANALYSIS

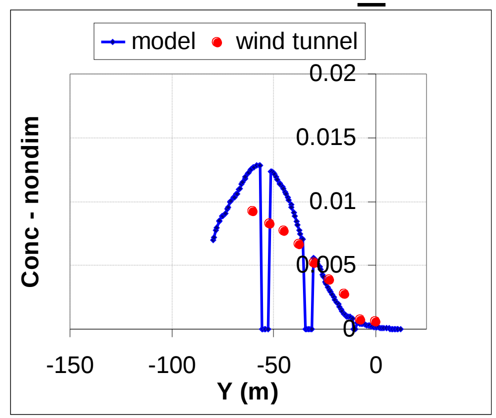
-45° approach flow case concentrations

$$K = \frac{C U_{ref} H_{ref}^{2}}{Q}$$

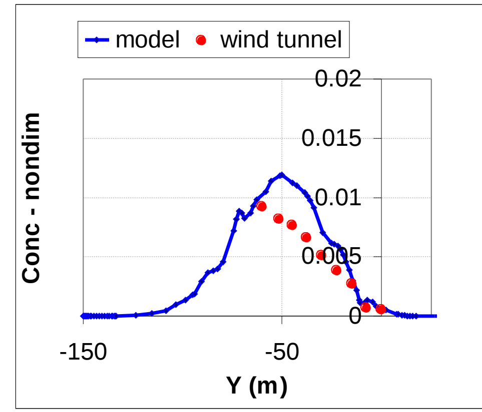
- ***C*** measured or calculated concentration
- ***U_{ref}*** reference wind speed (undisturbed flow)
- ***H_{ref}*** building height
- ***Q*** emission rate



MISKAM_3



FLUENT_3



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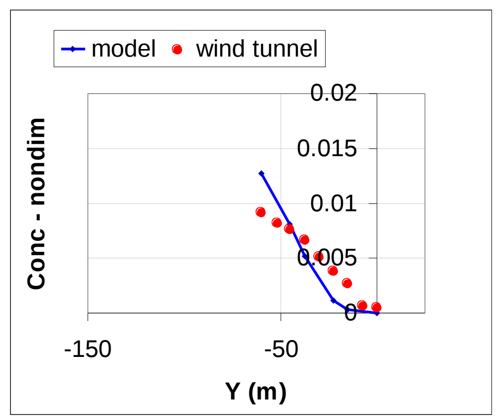

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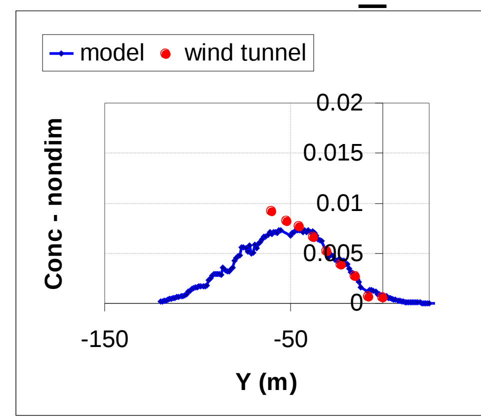
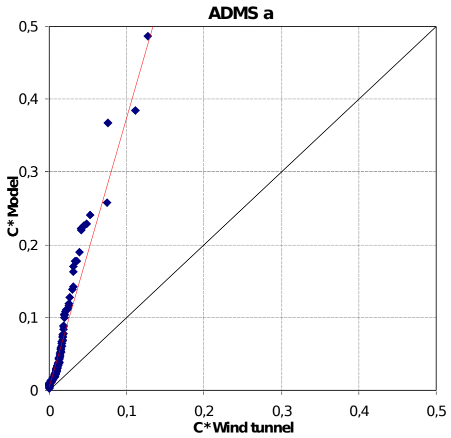
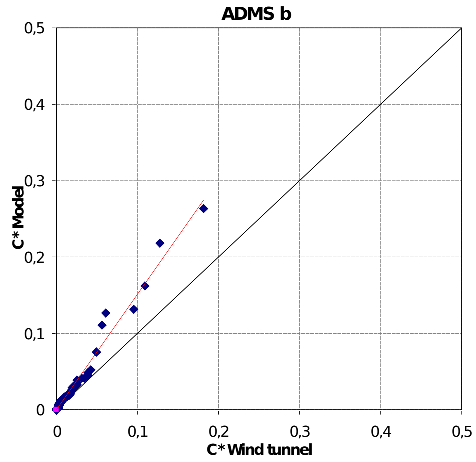


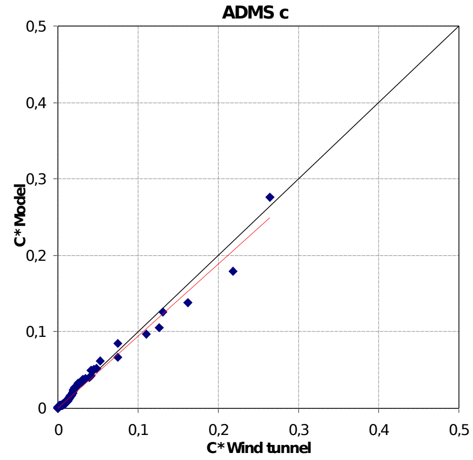
Distance from the source: 170m

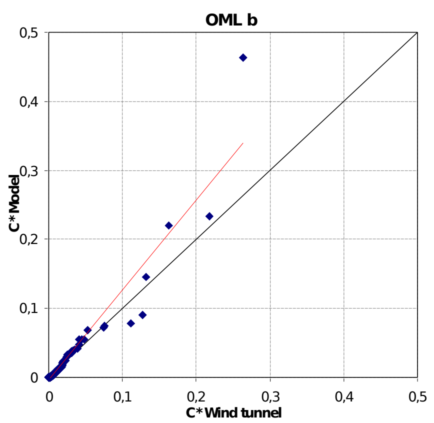
Profiles at z=0.5H

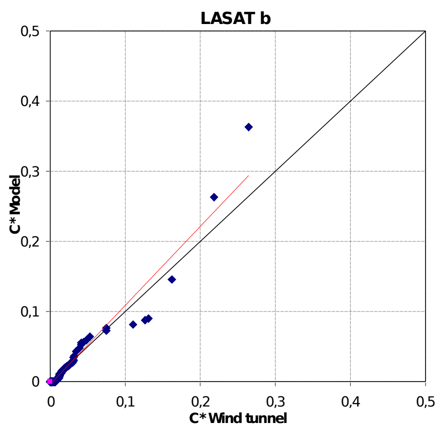
EXAMPLES FOR NON-CFD MODELS

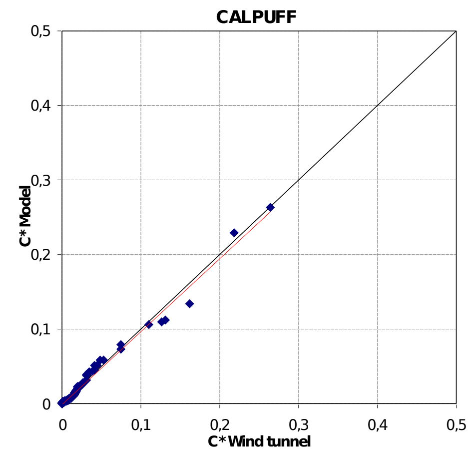












SUMMARY AND CONCLUSIONS

THE PROTOCOL IMPLEMENTATION TO THE MUST EXPERIMENTS HAS ALLOWED US TO FIND OUT WHAT CAN BE EXPECTED BY STATE OF ART MODELS (AS MANY MODELS ARE INVOLVED WHICH ARE WIDELY APPLIED IN EUROPE)

THE DEVELOPMENT OF A GRAPHICAL TOOL (MADE AVAILABLE TO ALL PARTICIPANTS) ALLOWS IN DEPTH ANALYSES OF MODEL PERFORMANCE IN AN ENVIRONMENT WHERE THE DIFFERENCES ARE NOT OBSCURED BY DIFFERENCES IN PRESENTATIONS

THIS IS A UNIQUE OPPORTUNITY OF SHARING EXPERIENCE NECESSARY TO FORM A GENERAL VIEW ABOUT MODEL EVALUATION (THIS MAY DIFFER ACCORDING TO EXPERIENCE AND APPLICATION INTERESTS)

SUMMARY AND CONCLUSIONS

THE IMPLEMENTATION OF THE PROTOCOL 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

THOSE STEPS ARE BELIEVED TO BE CRUCIAL TO BUILD A CONSENSUS (AT LEAST AT EUROPEAN LEVEL) ABOUT MODEL EVALUATION

THANK YOU !