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The FAIRMODE CT4: Intercomparison Exercise of Urban Microscale Models and Methodologies for deriving annual pollutant concentrations distribution with very high spatial resolution

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FAIRMODE
Forum for air quality modelling in Europe

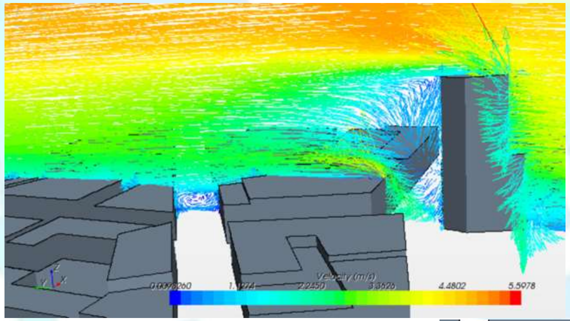
Introduction

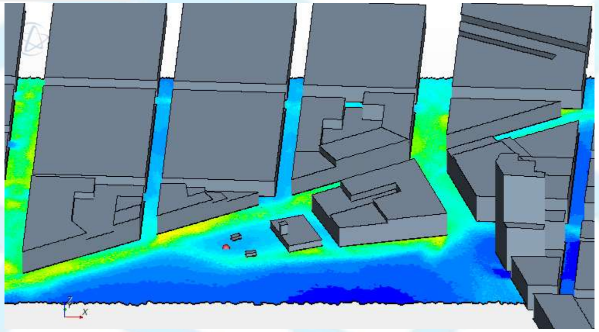
- FAIRMODE is the Forum for Air Quality Modelling in Europe created in 2007 for:
  - exchanging experience and results from air quality modelling in the context of the Air Quality Directives (AQD) and
  - for promoting the use of modelling for air quality assessment and management in a harmonized manner between Member States.
- Several working groups or cross-cutting tasks (CT) have been created to tackle several aspects of the air quality modelling in Europe.
- CT4 on Microscale Modelling is focused on air quality modelling at very high spatial resolution in urban environments, where local hot-spots occur, but restricted to applications in the context of the air quality directives (AQD)

Introduction

- Atmosphere – Urban Surfaces Interactions → Complex flow circulation in city
- Reduced Ventilation in Streets
- Traffic Emission heterogeneities

High pollutant concentration and **strong gradient of concentration** (spatial and temporal)





Street Scale

↓

High Spatial Resolution Needed

Introduction

- Results of microscale models are only useful if they can be aggregated to the temporal and spatial scales of interest for the AAQD
- Some types of microscale models such as CFD require large computational resources to perform simulations over a period of one year, which makes this type of models difficult to use.
- One of the main aims of FAIRMODE CT4 is to determine how to derive annual averaged concentrations (and other AQD statistics such as percentiles) with a micro-scale model as a first step to discuss how to use micro-scale models for air quality assessment or planning in the framework of AQ Directives.
- First activity: **Intercomparison exercise to compare methodologies for deriving annual statistics (using microscale modelling) to identify best practices.**

CT4 Intercomparison exercise

9 groups particpating:

ENEA, VITO, NILU, RICARDO, CERC, University of West Macedonia (UOWM), Széchenyi István University (SZE), UPM and CIEMAT

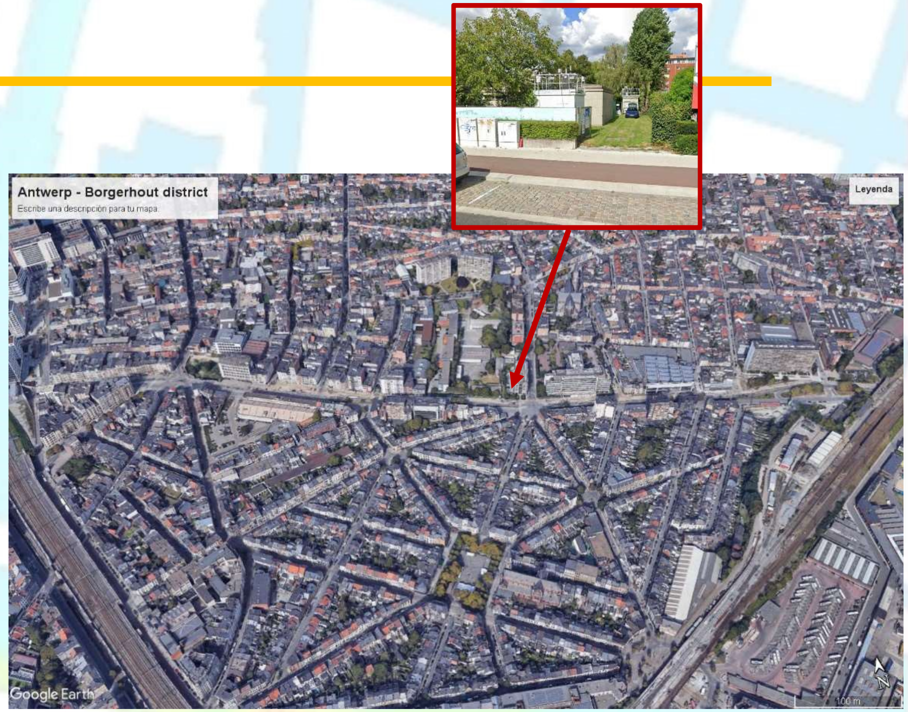
Models and methodologies:

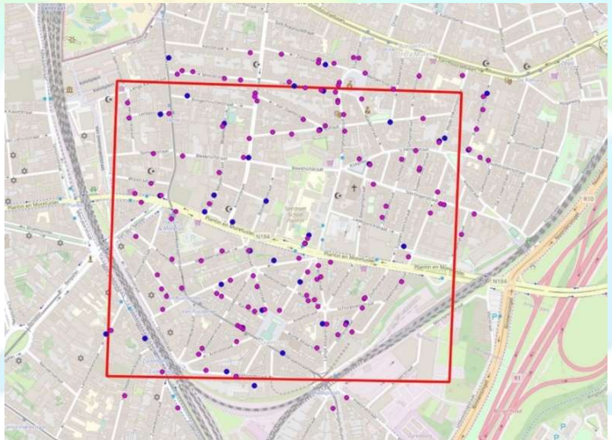
- Many are using CFD models (RANS mostly) but there are also other type of models (parametric, Gaussian, Lagrangian, etc).
- Different methods for computing annual indicators of pollutant concentrations.
  - **Methods based on simulating a set of selected scenarios** (wind scenarios and/or emission scenarios) **and then a postprocessing** (PDF of scenarios, rebuilding a entire year, etc) of model results for retrieving annual indicators.
  - **Methods based on simulating the complete year**, which is mostly for the case of no CFD models but some of them run CFD models a complete year.

CT4 Intercomparison exercise

Exercise details:

- Focused on a district of **Antwerp (Belgium). NO_2**
  - Area around two air quality stations.
  - Used in a FAIRMODE spatial representativeness intercomparison exercise in 2016.
  - Data of urban morphology, emissions from traffic, meteorological and air quality (two stations and passive NO_2 samplers (VITO).
  - Campaign of 2016 (April 30 – May 28) selected.
  - Precomputed NO_2 CFD simulations for 16 scenarios corresponding to 16 wind sectors (CIEMAT).

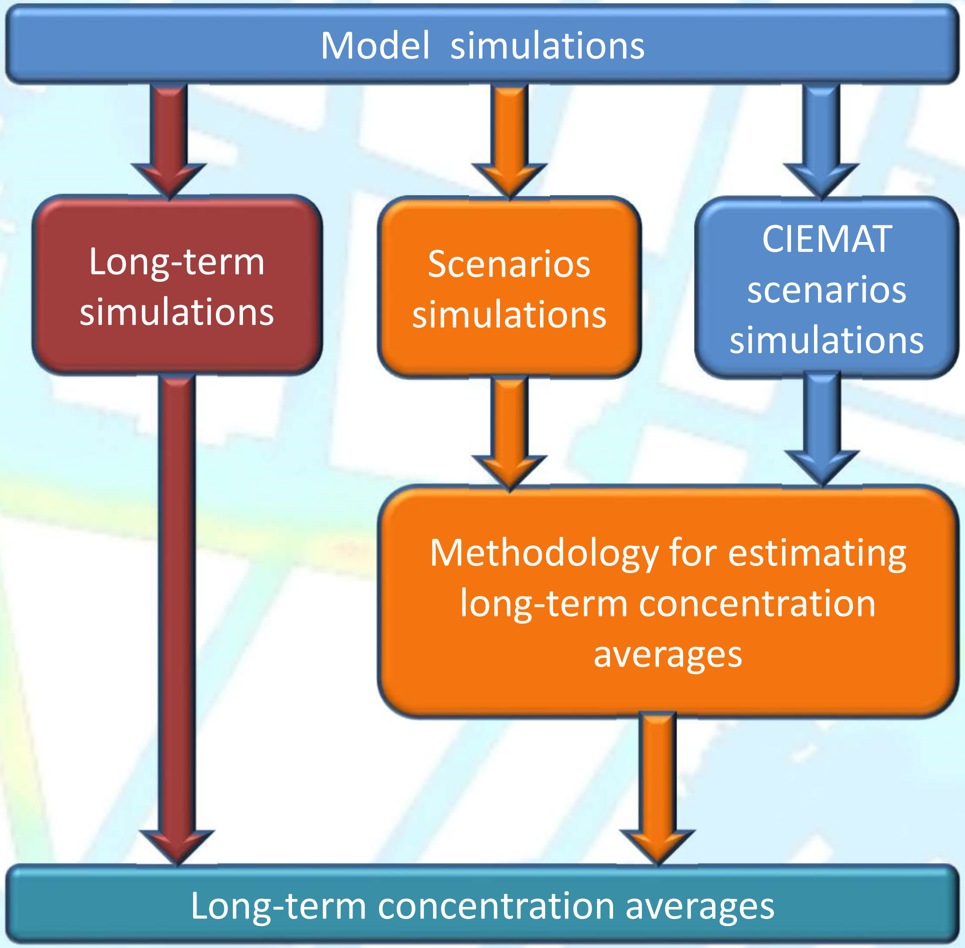




CT4 Intercomparison exercise

Ways of participating in the exercise:

- Running your own model for the complete period.
- Running your own model for representative scenarios and then applying your own methodology for computing long term concentration indicators.
- Using the precomputed simulations of CIEMAT as starting point for applying a methodology for estimating long-term averages of pollutant concentration.



CT4 Intercomparison exercise

3 steps:

1. ***To simulate <u>one day</u> from the one-month passive sampler campaigns.***
   - ***May 6th, 2016 selected to simulate.***
   - ***The model results would be compared with AQ stations data***
   - ***Models results would be intercompared.***

2. ***To compute averages (concentration maps) for the <u>campaign period</u> (April 30 – May 28).***
   1. ***Comparison with passive samplers' data and AQ station data***
   2. ***Intercomparison among models results (2D maps).***

3. ***To compute averages (concentration maps) for <u>2016 year</u> applying the methodologies of each group.***
   - ***Intercompare results from every methodology (2D maps).***

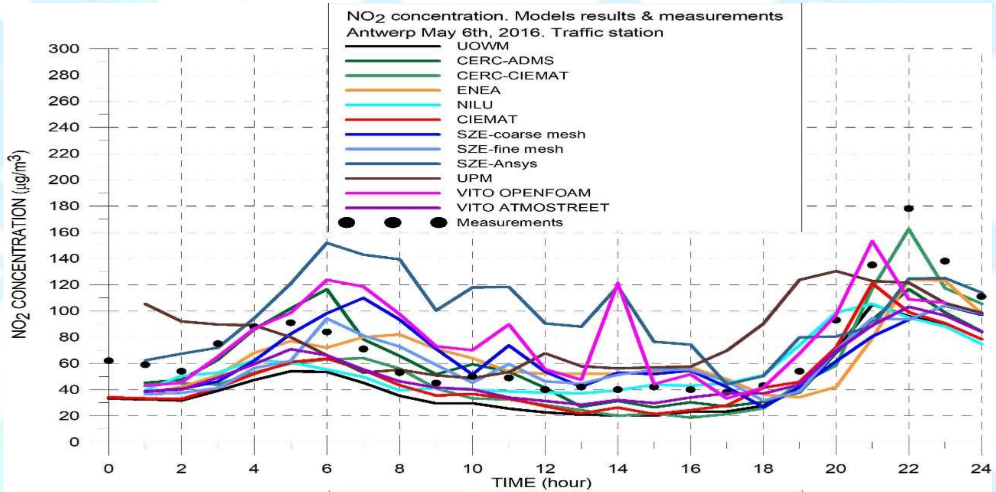
Modelling results sent by the participants

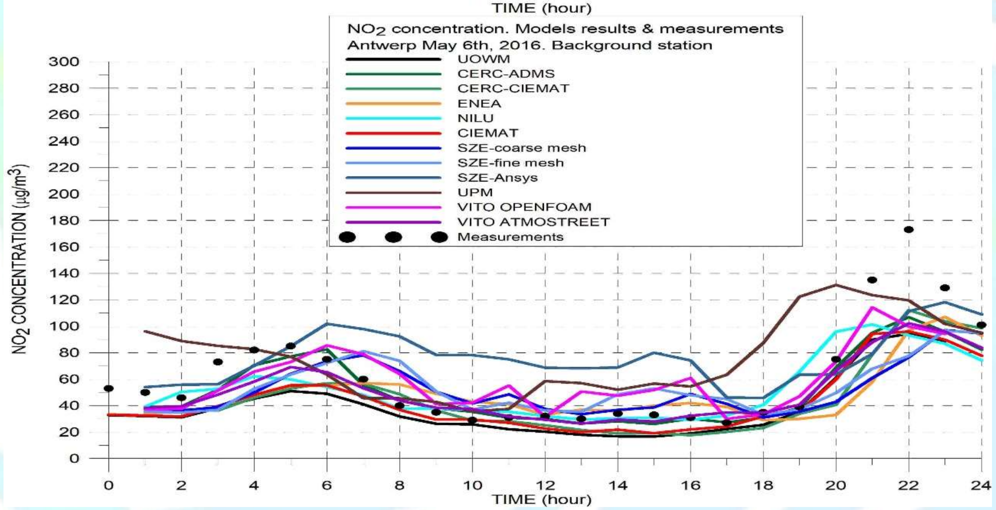
GROUP	STEP1	STEP2.1	STEP2.2	STEP3	Model / Type	Methods for averaging
CIEMAT	X	XXX	XXX	XXX	STAR CCM+ / CFD RANS	3 techniques (16 wind direction/wind dir and speed / hourly maps)
CERC	X X	X X	X X	X X	ADMS-URBAN / Gaussian urban CIEMAT simulations / CFD RANS	Running model (all period) Processing CIEMAT CFD data (wind and emission cases + correction factors)
UOWM	X	X	X	X	ADREA HF / CFD RANS	Running model (32 wind direction + hourly maps)
ENEA	X	X	X	X	PMSS / CFD+Lagrangian urban	Running model (all period)
NILU	X	X	X	X	EPISODE / Gaussian	Running model + interpolation (all period)
SZE	XX X	X	X	X	OPENFOAM / CFD RANS ANSYS / CFD RANS	Running models (2 OPEN FOAM / 1 ANSYS) (all period)
UPM	X	X	X	X	PALM-4U / CFD-LES	Representative days
VITO	X X	X X	X X	 X	OPENFOAM / CFD RANS ATMO-Street model / Gaussian urban	Wind statistics + Averaging hourly maps Running model (all period)
RICARDO				X	RapidAir / Gaussian urban	Running model (all Antwerp)

Analysis of data (all methodologies vs observations)

Step 1. Hourly data (May 6th, 2016)

- **Most of the models simulate quite well time evolution** of NO_2 concentration specially the background station. (0.60<R<0.97)
- **Problems**:
  - slight **underprediction (evening peak)**
  - **timing** of the **concentration peaks** (several models)

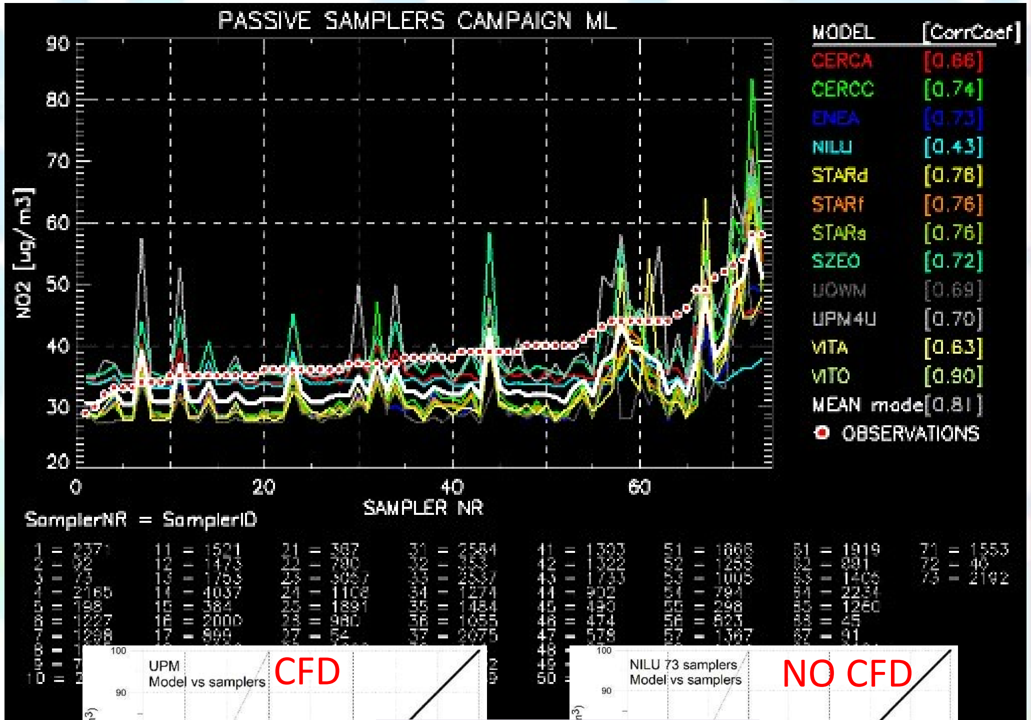


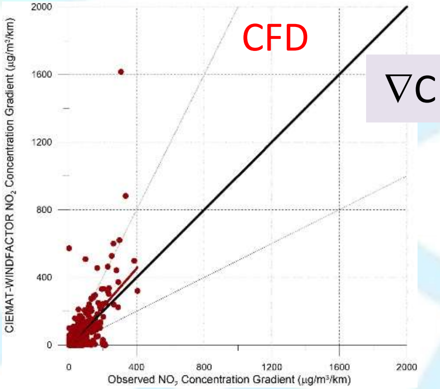


Analysis of data (all methodologies vs observations)

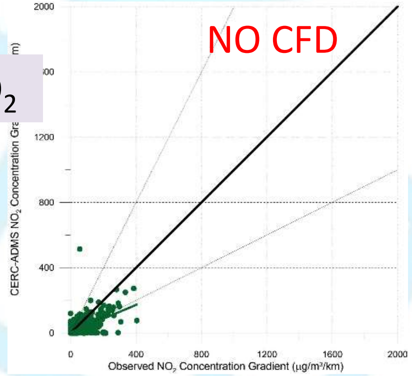
Step 2.1. Monthly data from samplers (May, 2016)

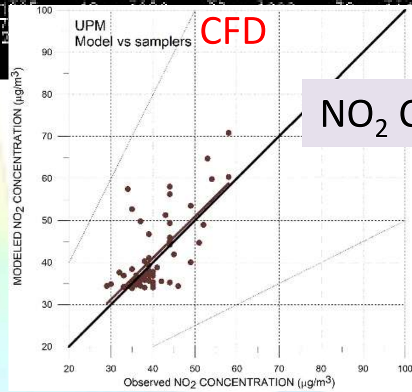
- **Most of the models (mainly CFD) seem to predict fairly good NO2 average concentration (mostly R>0.60).**
- **CFD models seem to simulate better the spatial distribution of the monthly averaged concentrations** than simpler approaches.

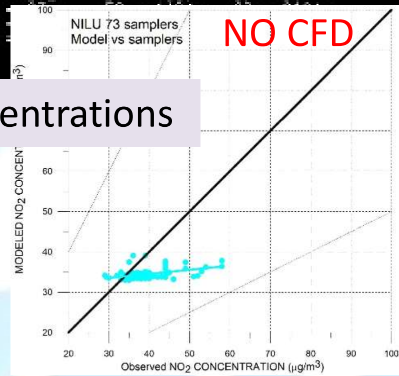




∇C of NO_2







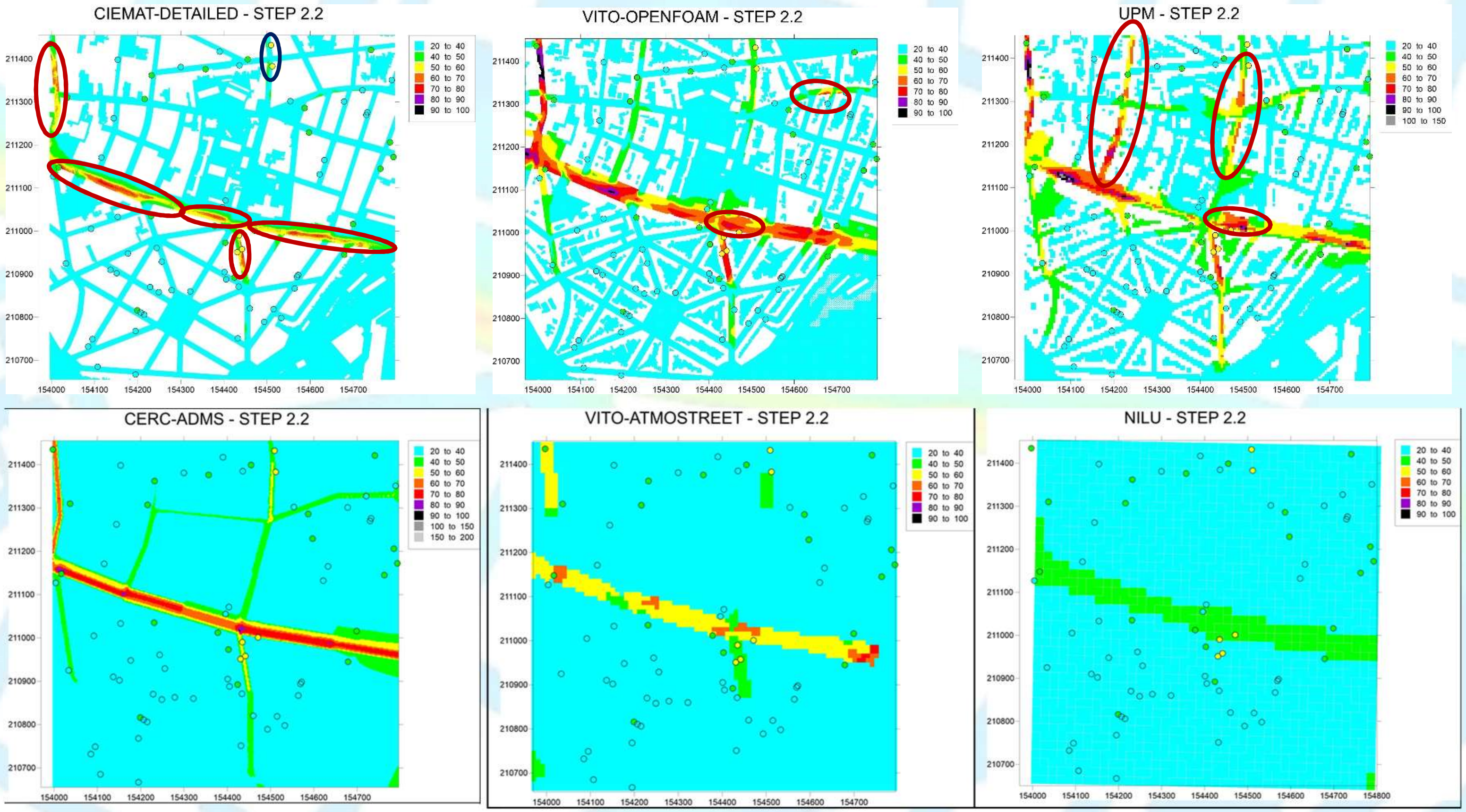
NO_2 Concentrations

Analysis of data (all methodologies vs observations)

Step 2.2. Maximum monthly concentration areas (May, 2016)

CFD models

NO-CFD models

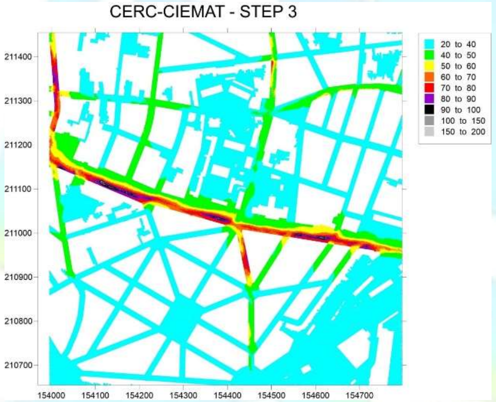


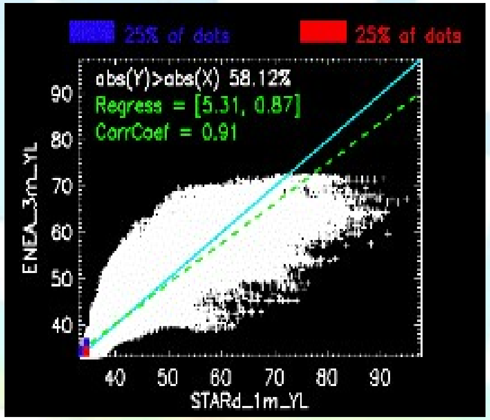
Analysis of data (all methodologies)

Step 3. Intercomparison of yearly averaged maps (2016)

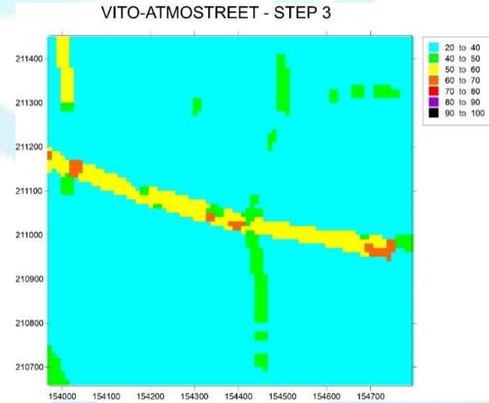
CFD models

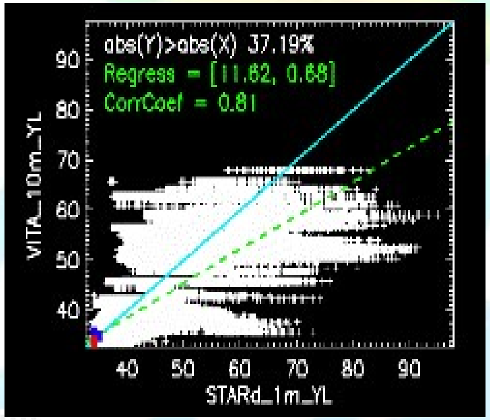
Maximum annual concentration areas similar to Maximum Monthly average concentration areas



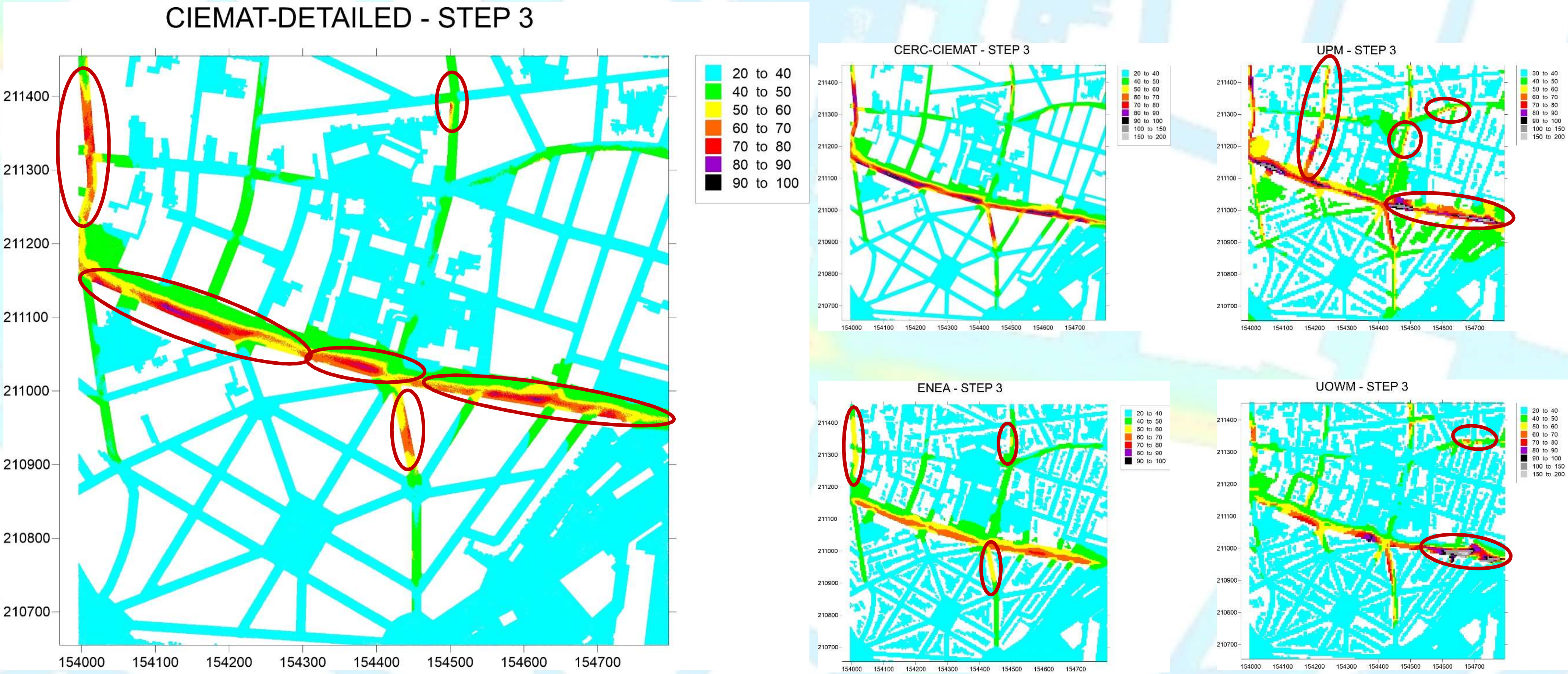


NO-CFD models





Maximum annual concentration areas. STEP 3



Analysis of data (all methodologies vs observations)

Step 2.2. Monthly data from samplers (May, 2016) and

Step 3. Intercomparison of yearly averaged maps (2016)

- **CFD results:**
  - **Significant differences in the magnitude of the maxima in the CFD results**.
  - **Most of the areas with maxima concentration are common to the CFD models, but another maxima areas do not**.
  - Reasons: CFD model configurations, input data as emissions, post-processing methodology?
- **Gaussian models (except CERC-ADMS) predict lower maxima and smooth concentration fields than CFD models**

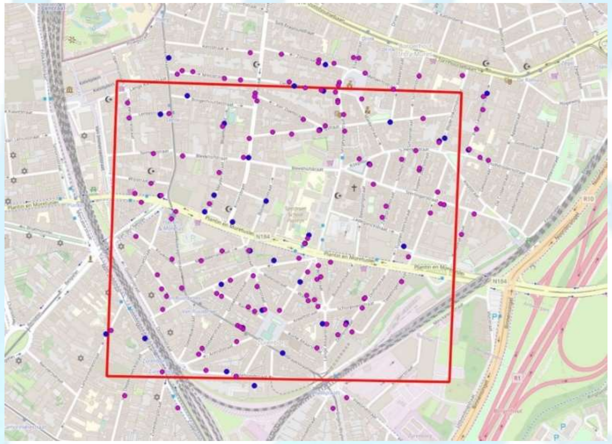
Additional analysis

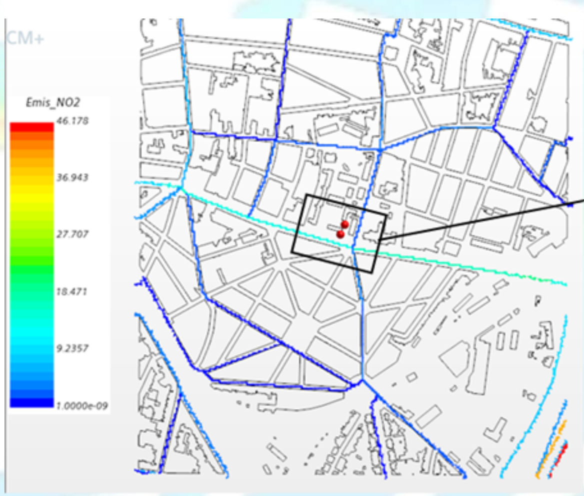
Some questions to answer:

- **What is the impact of the emissions data?**
- **What type of models are more suitable?**
- **Long term simulations versus methodologies based on limited scenarios?**
- **How many simulations (scenarios) could be needed to provide good results?**

What is the impact of the emissions data?

- Emission data are only in major streets.
- Many samplers were located (>60%) in streets without emissions data.
- **Step 2.1. Lack of emission data in some streets strongly influences on the CFD model performance but no in NOCFD model one**





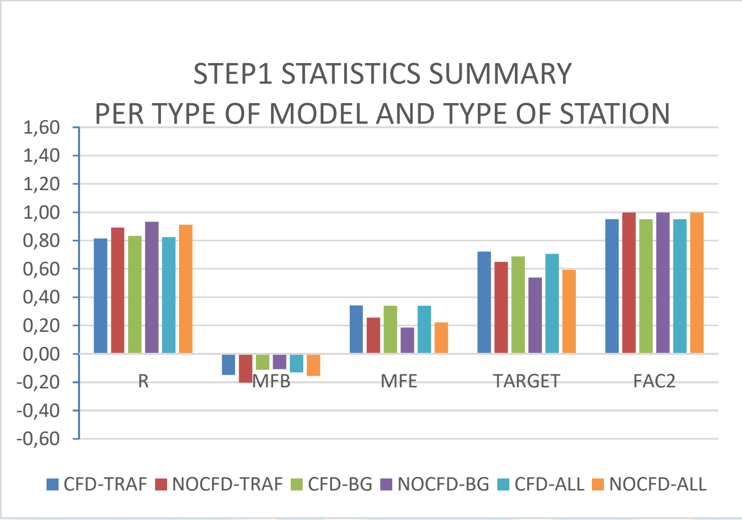
MODEL TYPE	CFD	CFD-EMIS	CFD-NOEMIS	NOCFD	NOCFD-EMIS	NOCFD-NOEMIS
R	0,73	0,76	0,54	0,57	0,54	0,56
MFB	-0,15	-0,09	-0,17	-0,13	-0,12	-0,16
MFE	0,18	0,17	0,18	0,16	0,17	0,17
TARGET	1,31	1,06	1,75	1,19	1,09	1,65
FAC2	1,00	1,00	1,00	1,00	1,00	1,00

What type of models are more suitable?

Step 1. Hourly NO2 concentrations at traffic and background stations (May 6th, 2016)

- **NOCFD models seem to provide better results** but showing better results for the BG station and no so good for the traffic one.
- CFD models seems to perform in similar way for both type of stations.

MODEL TYPE	CFD-TRAF	NOCFD-TRAF	CFD-BG	NOCFD-BG	CFD-ALL	NOCFD-ALL
R	0,82	0,89	0,83	0,93	0,82	0,91
MFB	-0,15	-0,20	-0,11	-0,11	-0,13	-0,15
MFE	0,34	0,26	0,34	0,19	0,34	0,22
TARGET	0,72	0,65	0,69	0,54	0,71	0,59
FAC2	0,95	1,00	0,95	1,00	0,95	1,00



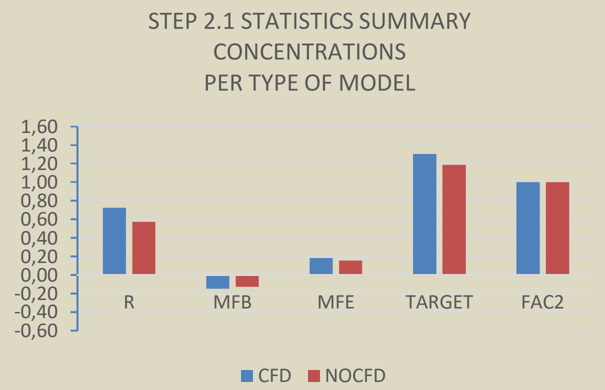
What type of models are more suitable?

Step 2.1. Monthly NO_2 concentrations of samplers(May 6th, 2016)

- **CFD models seems to simulate better** the spatial distribution of **monthly averaged concentrations**.
- **CFD models are able to reproduce better the differences/gradients** of the monthly averaged concentrations.

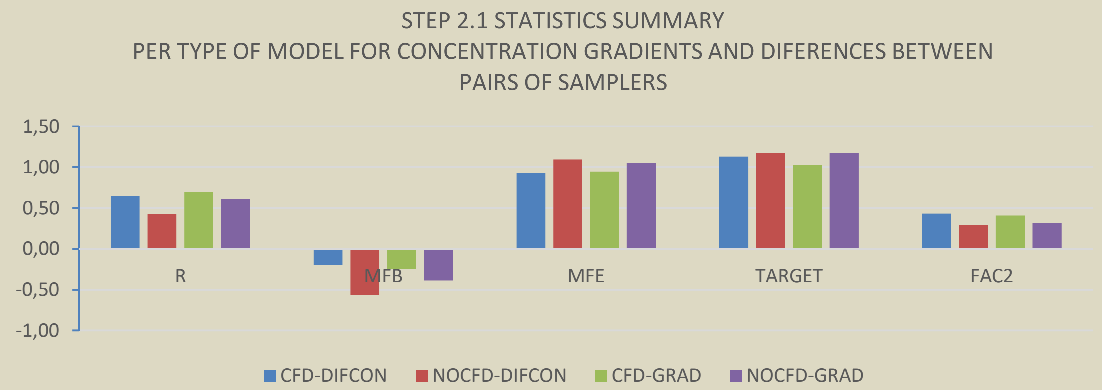
Monthly averaged concentrations

MODEL TYPE	CFD	NOCFD
R	0,73	0,57
MFB	-0,15	-0,13
MFE	0,18	0,16
TARGET	1,31	1,19
FAC2	1,00	1,00



Differences between pair of samplers and concentration gradients

MODEL TYPE	CFD-DIFCON	NOCFD-DIFCON	CFD-GRAD	NOCFD-GRAD
R	0,65	0,43	0,69	0,61
MFB	-0,20	-0,56	-0,25	-0,39
MFE	0,92	1,10	0,94	1,05
TARGET	1,13	1,17	1,03	1,18
FAC2	0,43	0,29	0,41	0,32



Long term simulations vs methodologies based on limited scenarios?

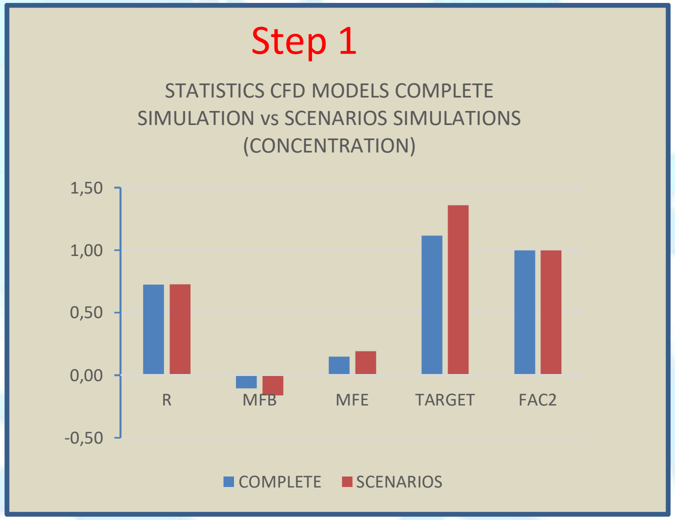
- 2 long-term simulation (SZE, ENEA) and the 5 methodologies based on simulating a set of scenarios with CFD models
- **Results do not seem to be conclusive**:

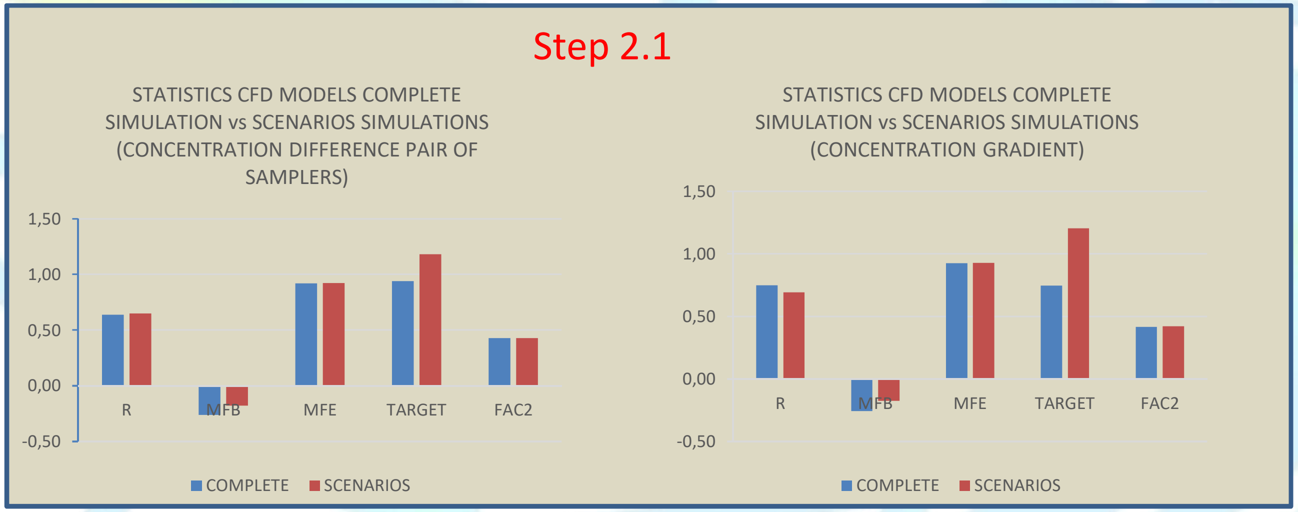
Concentrations

- little differences between the results of R from complete period model simulations and scenarios based methodologies
- Long-term simulations seem to give slight better values of MFB, MFE and TARGET (1.12, 1.36)

Gradients and Concentration differences between pair of stations:

- Similar R (long-term simulation slight better for gradients), MFE and FAC2
- Less MFB with scenarios, best TARGET with long-term simulation





How many scenarios could be needed to provide good results?

MODEL	TYPE-STATION	Correl	MFB	MFE	TARGET	FAC2
CIEMAT_4S	TRAFFIC	0,968	-0,373	0,373	0,770	1,000
CIEMAT_8S	TRAFFIC	0,935	-0,359	0,359	0,726	1,000
CIEMAT_16S	TRAFFIC	0,930	-0,383	0,383	0,739	1,000
CIEMAT_4S	BACKGROUND	0,970	-0,292	0,298	0,647	1,000
CIEMAT_8S	BACKGROUND	0,966	-0,291	0,297	0,632	1,000
CIEMAT_16S	BACKGROUND	0,963	-0,315	0,316	0,639	1,000

Step 1. Hourly NO2 concentración time series at stations:

Predictions obtained with more scenarios 16S (16 sectors) do not seem to provide better results, they are even slightly worse than the predictions with 4 or 8 sectors. **Why?**

model	Correl	MFB	MFE	TARGET	FAC2
CIEMAT-DETAILED-4S	0,783	-0,140	0,174	1,077	1,000
CIEMAT-DETAILED-8S	0,812	-0,146	0,170	1,000	1,000
CIEMAT-DETAILED-16S	0,829	-0,145	0,165	0,942	1,000

Step 2.1. Monthly averaged NO2 concentrations (samplers)

16-S predictions seem to simulate better respect the spatial distribution of monthly averaged concentrations. The results for 4S predictions are the worse. It seems to there be a more significant improvement in the statistics when passing from 4S predictions to 8S predictions.

model	Correl	MFB	MFE	TARGET	FAC2
CIEMAT-DETAILED-4S	0,628	0,047	0,777	1,343	0,489
CIEMAT-DETAILED-8S	0,661	0,029	0,749	1,129	0,529
CIEMAT-DETAILED-16S	0,683	0,019	0,764	0,958	0,532

Step 2.1. Concentration differences/gradients between pairs of samplers

16-S Predictions seem to simulate better monthly averaged concentration differences/gradients. The results for 4S predictions are the worse. It seems to there be a more significant improvement in the statistics when passing from 4S predictions to 8S predictions.

Preliminary conclusions / remarks

- **Most of the models (CFD and non-CFD) simulate quite well the hourly time evolution of the NO_2 concentrations** but underpredicting mainly in traffic station.
- **CFD models seem to simulate better the spatial distribution** (more realistic and detailed)of the monthly averaged concentrations than simpler non-CFD approaches. In most cases, the concentration gradient is slightly overpredicted by the CFD models.
- **Good emission data are of crucial importance** for the microscale modelling in urban areas
- **The steady state CFD RANS approach seems to be a good choice** for retrieving long-term concentrations by using selected wind sectors simulations.
- **The required number of wind sectors to compute reliable long-term average concentrations seems to be higher than or equal to 8.**
- **Simulated wind sectors with only one reference wind speed could be sufficient for computing long-term average concentrations.**
- To compute long term averaged concentrations, **the preferred methodologies could be those reconstructing the time series by hourly concentration maps based on the precomputed wind sectors**.
- The results are **very sensitive to the Sct number**.

Pending questions

- Is an unsteady simulation for a complete year much better than the wind sector approaches?
- Does the number of simulated wind sectors required for computing good long-term average concentrations depend on urban morphology?
- Are the data recorded at a limited number of AQ monitoring stations sufficient to evaluate the methodology performance at microscale?
- Are the investigated models/methodologies good enough to compute other indicators besides average concentrations, that is: maxima/peak concentrations or high percentiles?

Challenges

- How relevant could be the chemical reactions at microscale? How to deal with atmospheric chemistry for the estimation of annual averaged concentrations? Observed NO_2/NOx ratio vs chemical schemes at microscale?
- Are there good microscale emission data?
- How important could be the atmospheric stability for the estimation of annual averaged concentrations?

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Thank you for your attention
Questions?

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