CT4 MICROSCALE MODELING

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FAIRMODE Technical Meeting.

October 18-20, 2022

CT4 activities: Context and aims

1. CT4 is focused on microscale modelling but restricted to applications in the context of the air quality directives (AAQD)
2. In this context, results of these models are only useful if they can be aggregated to the temporal and spatial scales of interest for the AAQD
3. An intercomparison exercise carried out to compare methodologies for deriving annual statistics (using microscale modelling) to identify best practices.
4. 9 participant groups:

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

2020 - 2022 activities

- CT4 Microscale Modeling was endorsed in FAIRMODE Plenary Meeting, Berlin, Feb 2020.
- During 2020, meetings (FAIRMODE Technical Meeting and hackathon in December) for design and preparation of an Intercomparison Exercise.
- **Intercomparison exercise started in March 2021 / modelling results by September 2021**
- **Discussions about how to proceed to process and analyze the results provided for the participants during HARMO20 Special Session (June) and 2021 FAIRMODE Technical Meeting (October).**
- **Processing/analysis of results by CIEMAT team during November 2021/February 2022.**
- **Hackathon showing the first results in February 2022**
- **Additional analysis and some new simulations during February-April 2022.**
- **Hackathon for discussion of results and defining remarks, recommendations and challenges in June 2022**
- **Some new simulations by SZE and reanalysis of results August-October 2022**

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CT4 agenda

1. Last results of the intercomparison exercise
2. Is an unsteady simulation for a complete year better than the wind sector approaches? (results from SZE)
3. Presentation of Felicita Russo (ENEA) about their modelling approach
4. Presentation of John Bartzis (UOWM) about their experiences.
5. Other related works beyond the CT4 exercise (presentation of Xavier Jurado, Strasbourg)
6. Are the draft recommendations written in summer good enough (feedback from participants)?
7. Discussion on next CT4 activitives (road map 2023-2025)

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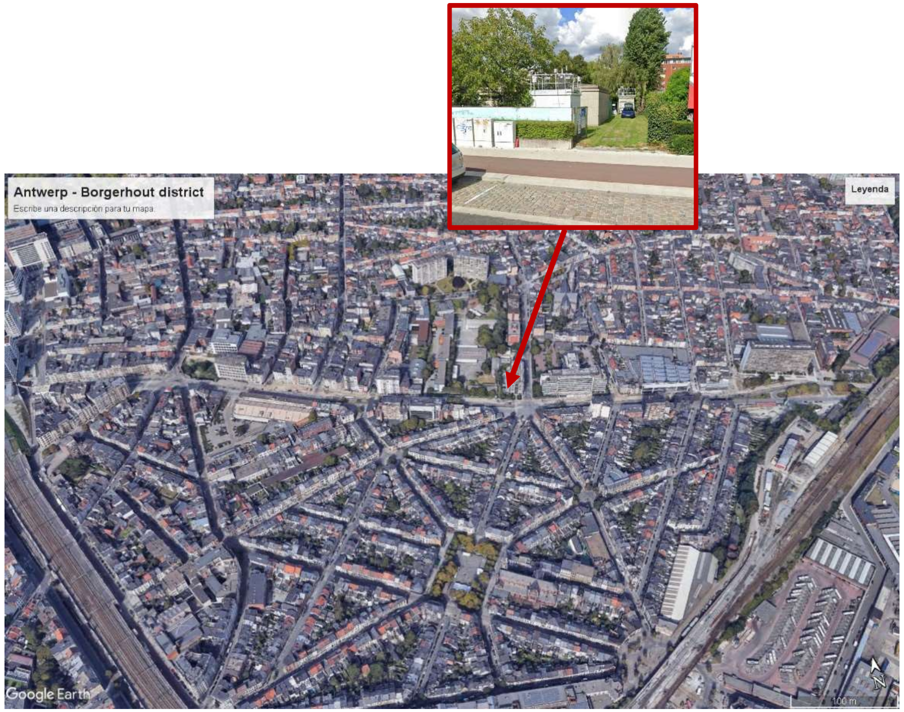
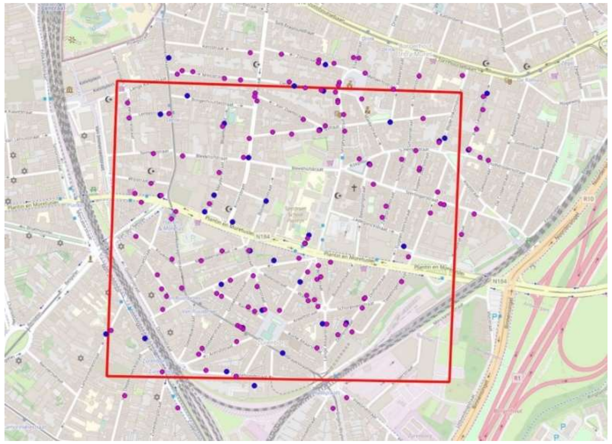
CT4 Intercomparison exercise

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).



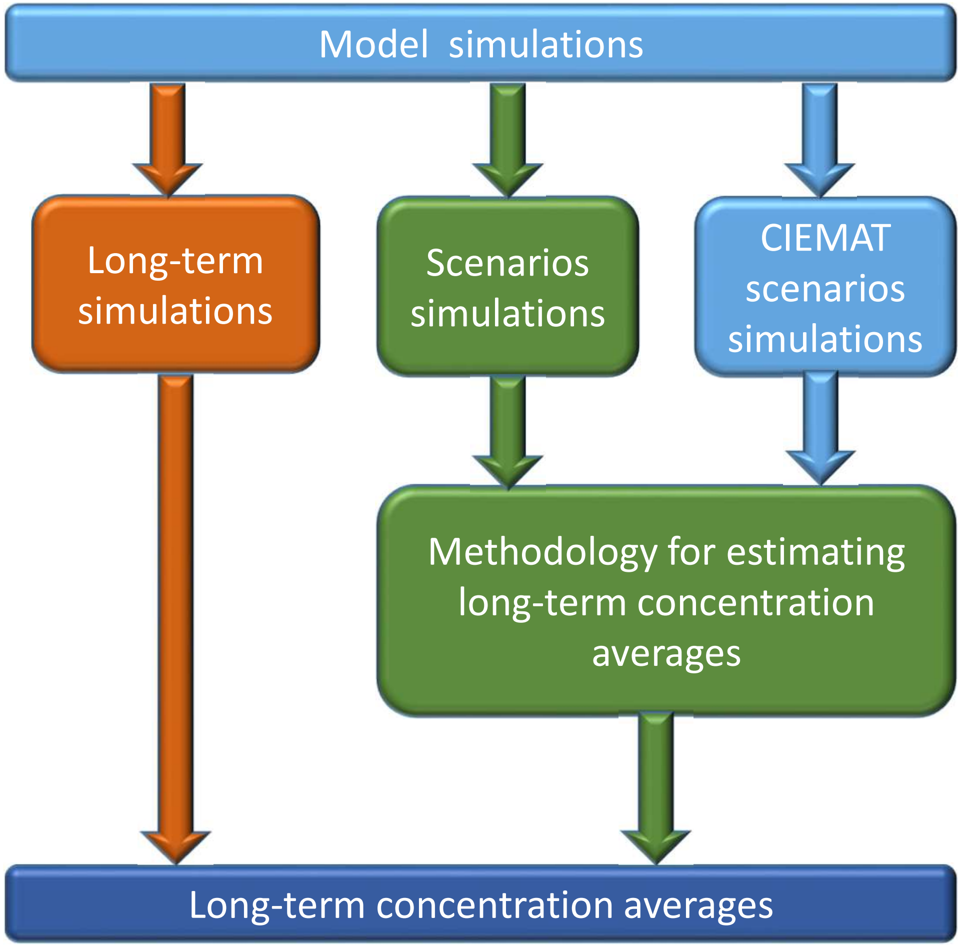


CT4 Intercomparison exercise

Models and methodologies:

- Focused on the **Antwerp (Belgium). NO_2**
- Many are using CFD models (RANS mostly) but there are also other type of models (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.

Ways of participating in the exercise:



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).*

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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)

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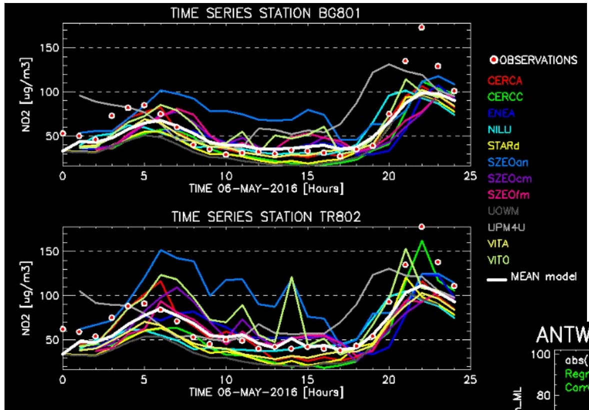
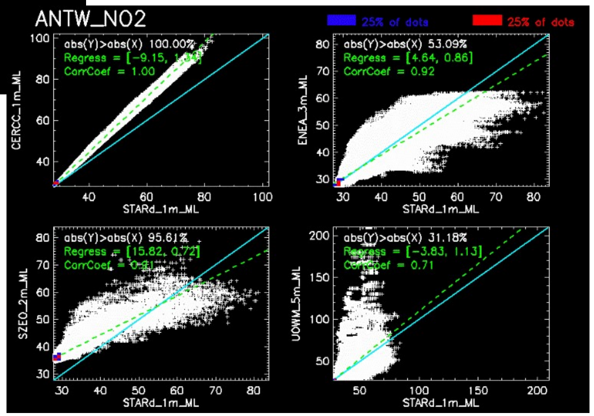
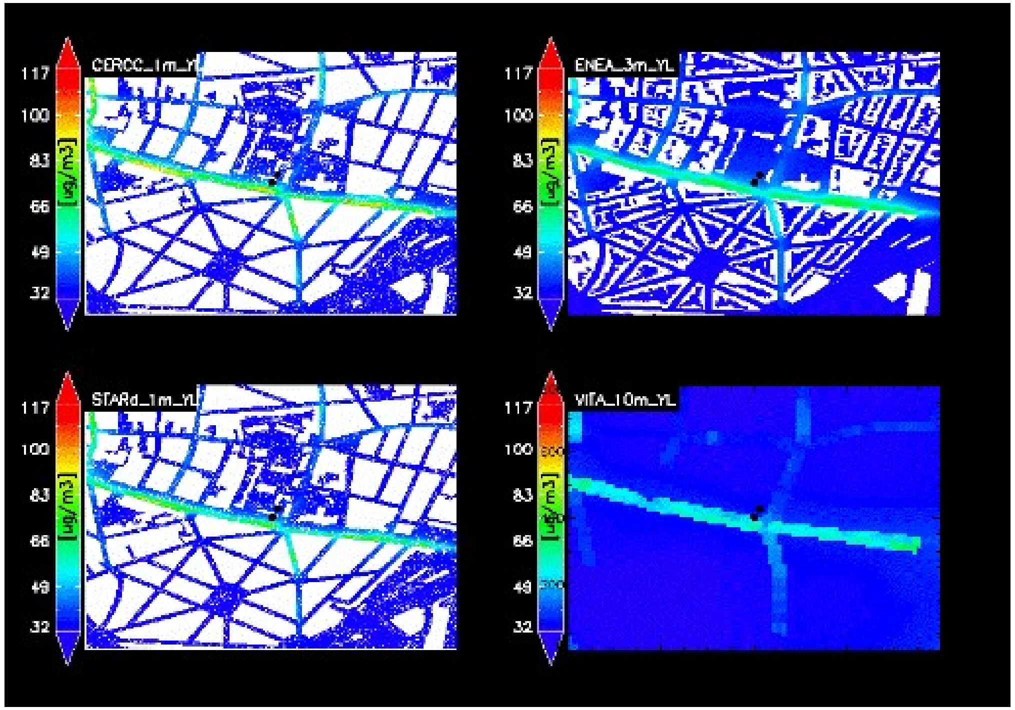
CT4 tool

- Kees Cuvelier has developed a software to help to the processing and analysis of the results provided by the participants and comparison with observations







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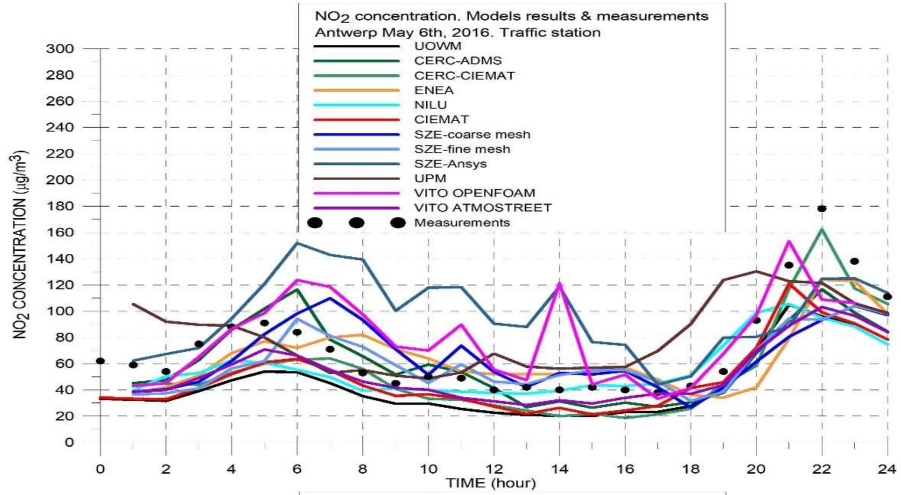
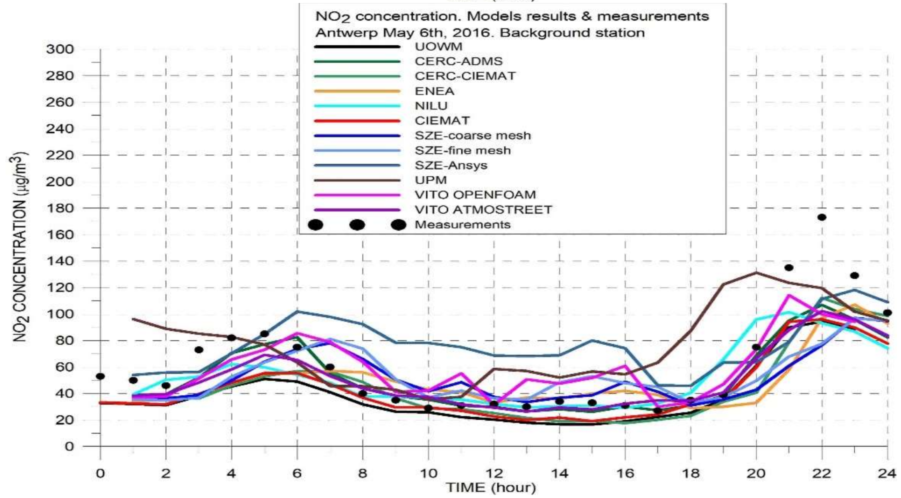
Analysis of data (for AQ stations)

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

- **Most of the models simulate quite well time evolution** of NO2 concentration.
- Best statistics for Gaussian models but worse for traffic station
- CFD and Lagrangian models perform very similar for background and traffic station
- **Problems**:
  - slight **underprediction (evening peak)**
  - **timing** of the **concentration peaks** (several models)





MODEL TYPE	CFD-TRAF	GAUSS-TRAF	LAGR-TRAF	CFD-BG	GAUSS-BG	LAGR-BG	CFD-ALL	GAUSS-ALL	LAGR-ALL
R	0,82	0,89	0,78	0,84	0,93	0,79	0,83	0,91	0,79
MFB	-0,16	-0,20	-0,05	-0,11	-0,11	0,12	-0,13	-0,15	-0,09
MFE	0,35	0,26	0,29	0,34	0,19	0,33	0,35	0,22	0,31
TARGET	0,74	0,65	0,65	0,68	0,54	0,72	0,71	0,59	0,68
FAC2	0,95	1,00	0,96	0,96	1,00	0,92	0,95	1,00	0,94

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Analysis of data (for passive sampler data)

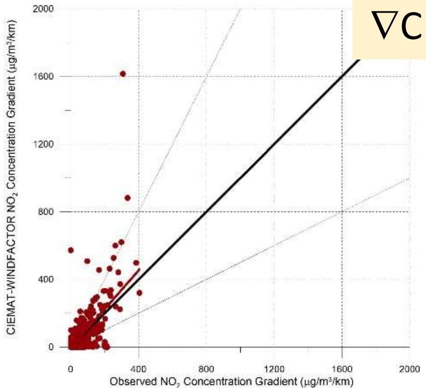
Step 2.1. Monthly data from samplers (May, 2016)

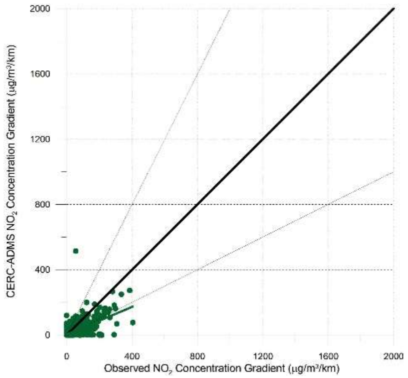
- **CFD and Lagrangian models seem to predict fairly good NO2 average concentration.**
- **CFD and Lagrangian models seem to simulate better the spatial distribution (gradients and spatial differences) of the monthly averaged concentrations** than simpler approaches.

MODEL TYPE	**CFD-DIFCON**	**GAUSS-DIFCON**	**LAGR-DIFCON**	**CFD-GRAD**	**GAUSS-GRAD**	**LAGR-GRAD**
R	0,65	0,43	0,66	0,69	0,61	0,75
MFB	-0,18	-0,56	-0,30	-0,24	-0,39	-0,30
MFE	0,93	1,10	0,91	0,95	1,05	0,91
TARGET	1,17	1,17	0,84	1,07	1,18	0,68
FAC2	0,43	0,29	0,43	0,41	0,32	0,42

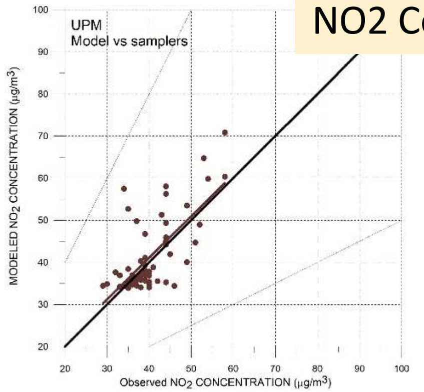
MODEL TYPE	**CFD**	**GAUSS**	**LAGR**
R	0,73	0,57	0,73
MFB	-0,14	-0,13	-0,21
MFE	0,18	0,16	0,22
TARGET	1,29	1,19	1,42
FAC2	1,00	1,00	1,00

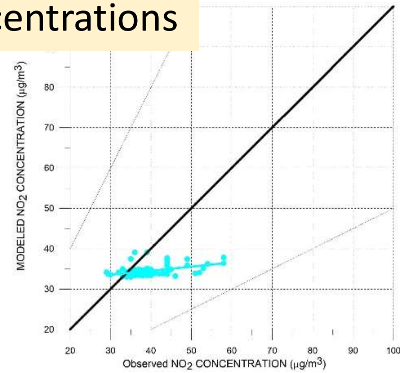
∇C of NO2





NO2 Concentrations





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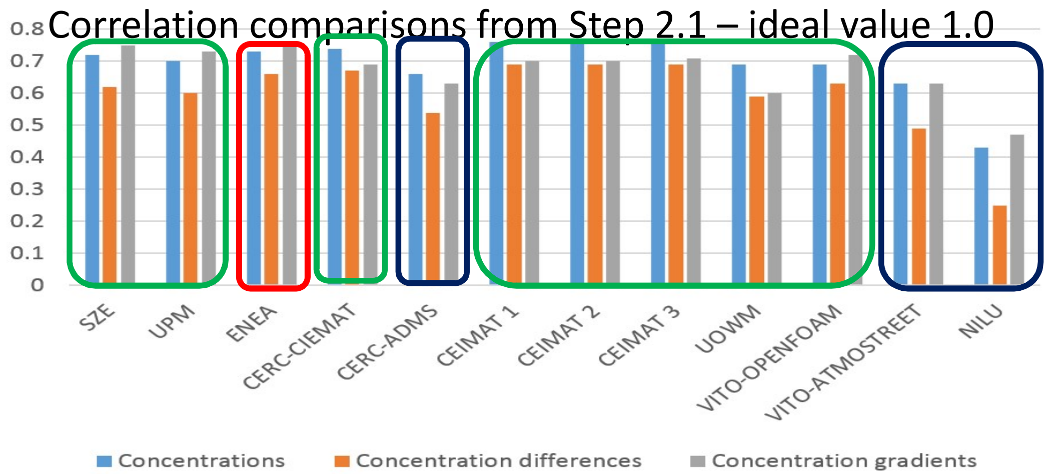
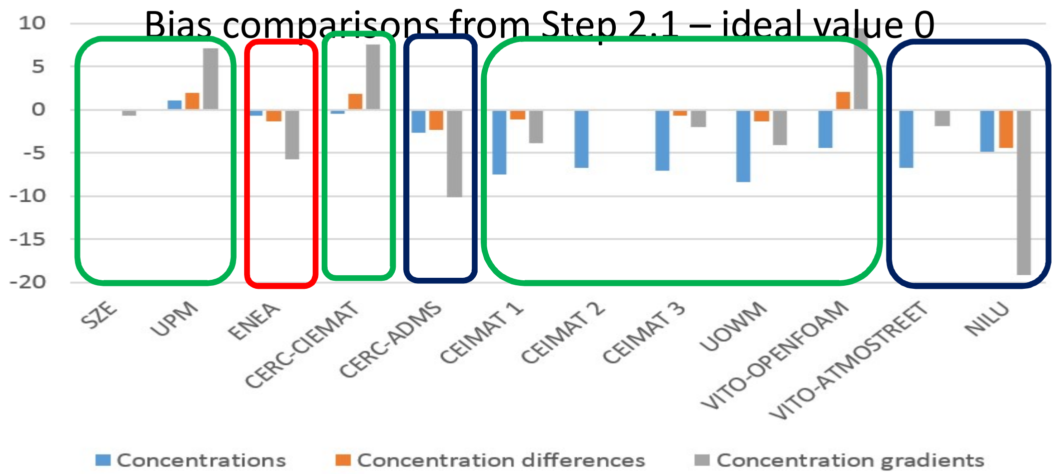
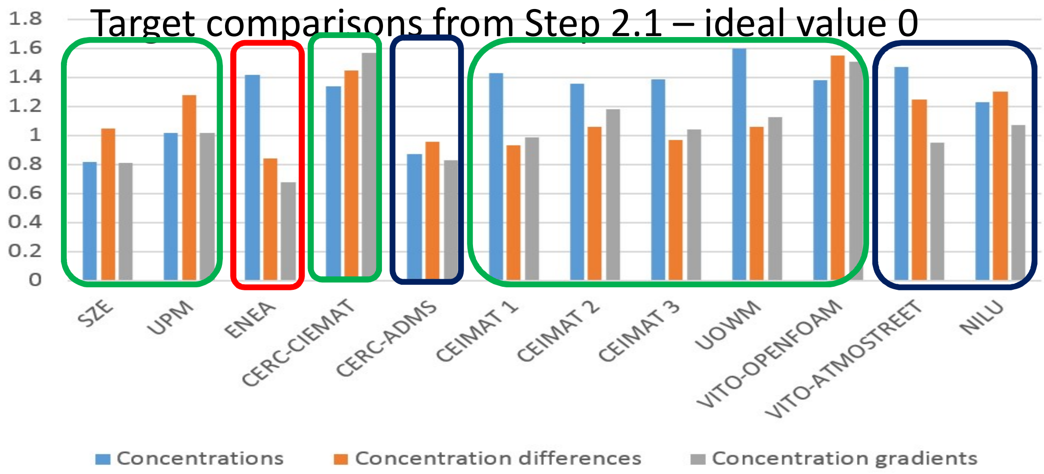
Results of each model (Step 2.1)

(plots from Jenny Stocker, CERC)





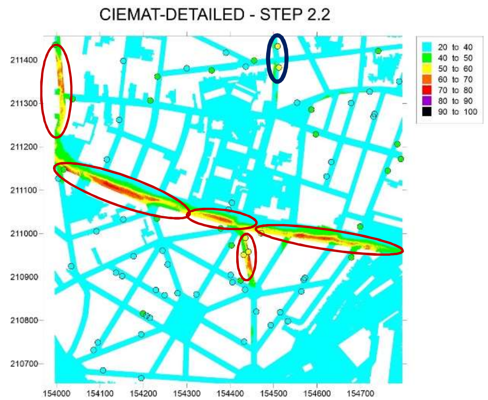


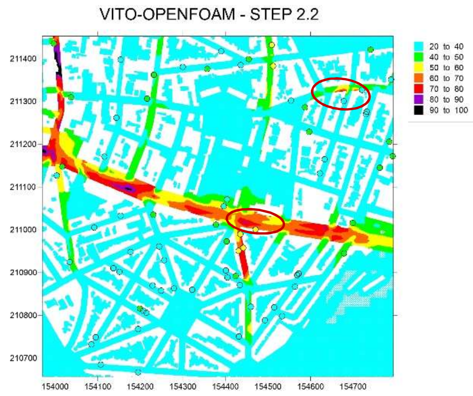
Green: CFD
Blue: Gaussian
Red: Lagrangian

Analysis of data (all methodologies vs observations)

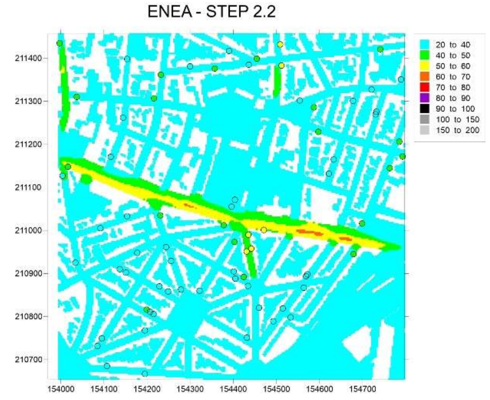
Step 2.2. Maximum monthly concentration areas

CFD models

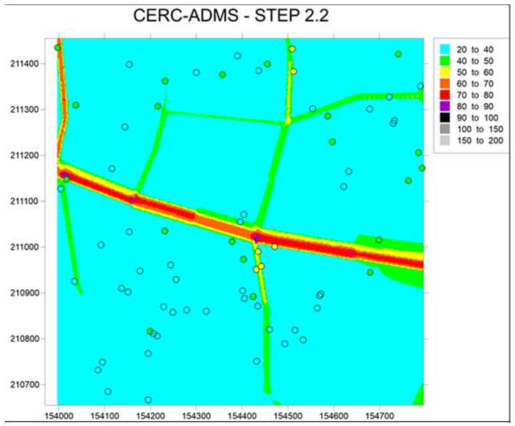


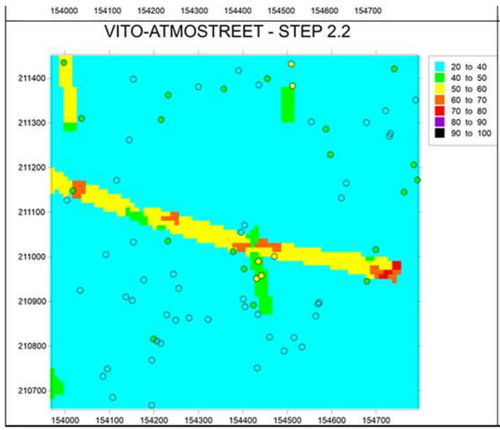


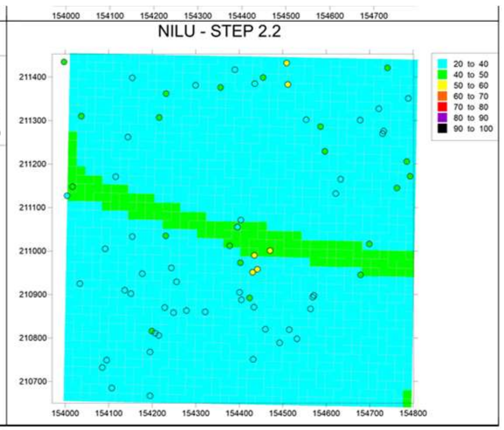
Lagrangian model



Gaussian models







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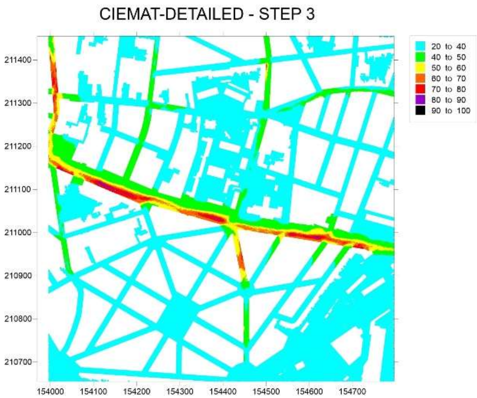
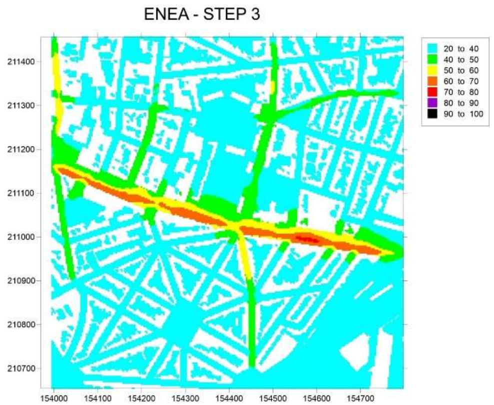
Analysis of data (all methodologies)

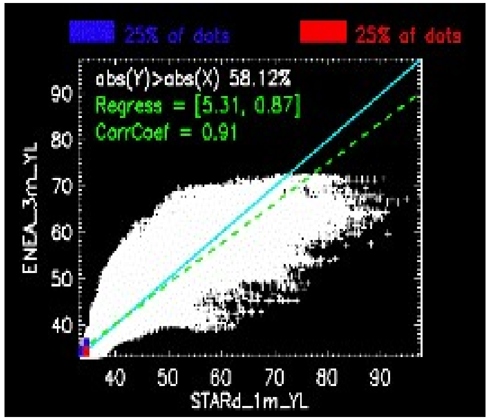
Step 3. Intercomparison of yearly averaged maps (2016)

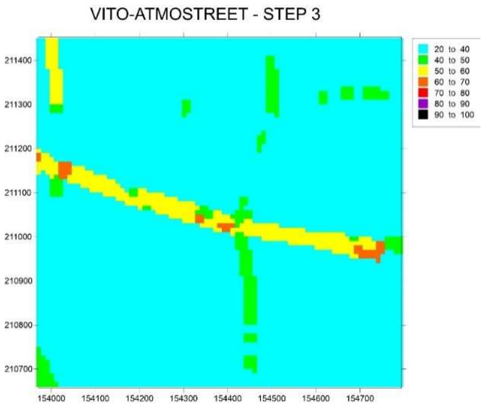
CFD and Lagrangian models

Maximum annual concentration areas similar to Maximum Monthly average concentration areas

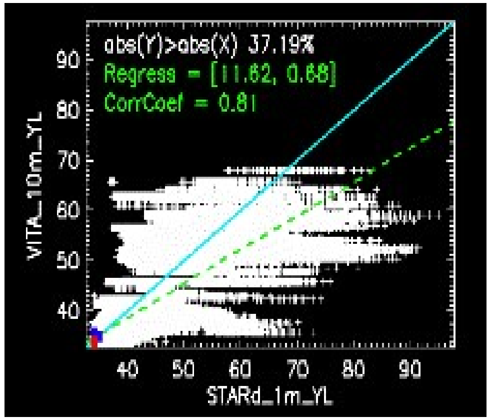








Gaussian models



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)

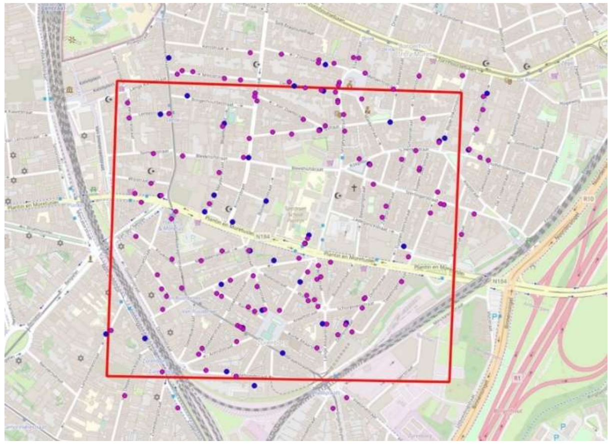
- **CFD/Lagrangian results:**
  - Significant differences in the magnitude of the maxima.
  - Most of the areas with maxima concentration are common to the CFD/Lagrangian models, but another maxima areas do not.
- **Gaussian models (except CERC-ADMS)** predict lower maxima and smooth concentration fields than CFD models

Other analysis

Need to deep into the results to answer to some questions:

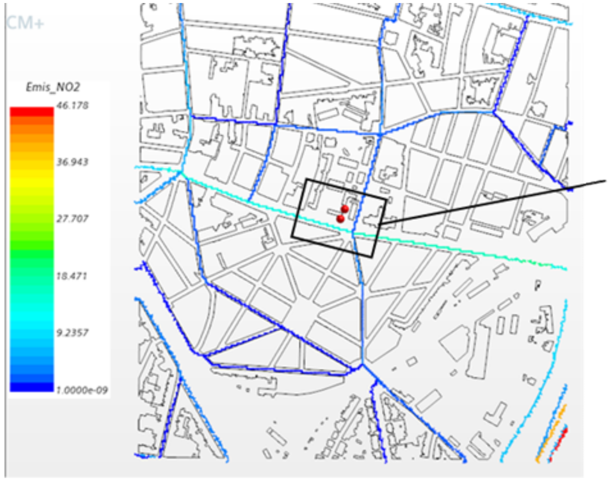
- **What is the impact of the emissions data?**
- **How many simulations (scenarios) could be needed to provide good results?**
- **Long term simulations versus methodologies based on limited use of simulations (scenarios)?**

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/Lagrangian model performances but no in NOCFD model one**

MODEL TYPE	CFD	CFD-EMIS	CFD-NOEMIS	GAUSS	GAUSS-EMIS	GAUSS-NOEMIS	LAGR	LAGR-EMIS	LAGR-NOEMIS
R	0,73	0,76	0,53	0,57	0,54	0,56	0,73	0,77	0,57
MFB	-0,14	-0,08	-0,16	-0,13	-0,12	-0,16	-0,21	-0,17	-0,23
MFE	0,18	0,17	0,17	0,16	0,17	0,17	0,22	0,18	0,23
TARGET	1,29	1,06	1,71	1,19	1,09	1,65	1,42	1,05	2,11
FAC2	1,00	1,00	1,00	1,00	1,00	1,00	1,00	1,00	1,00



How many simulations (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

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

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 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?**

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.

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.

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Long term simulations versus methodologies based on limited use of simulations (scenarios)?

Comparing results based on CFD long-term simulation (SZE) and Lagrangian (ENEA) and the methodologies based on simulating a set of scenarios with CFD models (UPM, CERC-CIEMAT, CIEMAT, UPWM, VITO-OPENFOAM). **Results do not seem to be conclusive**:

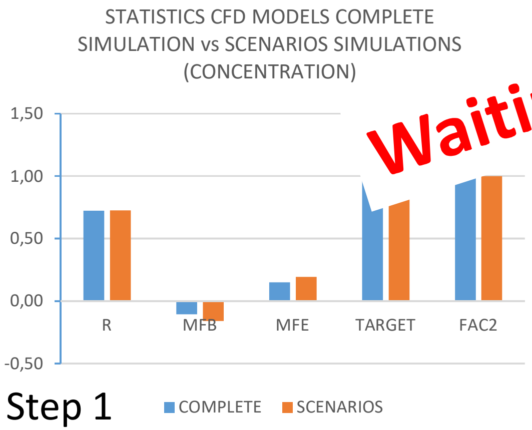
Concentrations

- little differences between the results of R from complete period model simulations and scenarios based methodologies
- Long-term simulations seem to give somewhat better values of MFB, MFE and TARGET (1

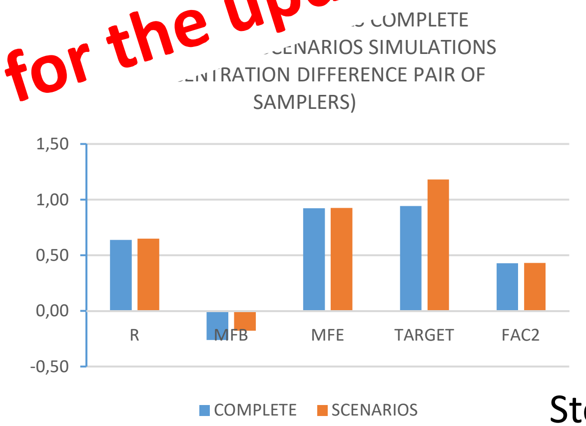
Gradients and Concentration differences between pair of stations:

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

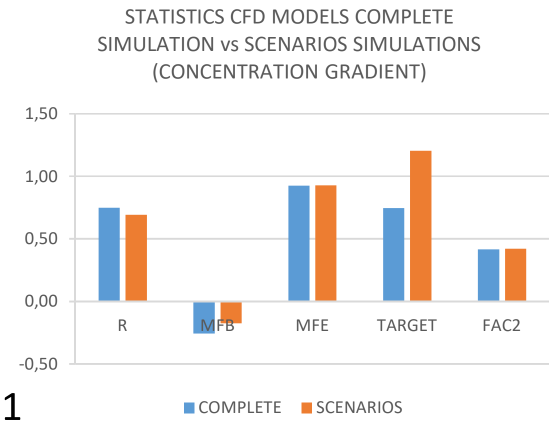
Waiting for the updated SZE simulations



Step 1



Step 2.1



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