

# CT4 MICROSCALE MODELING

*Status of activity and next steps*

***F. Martin, J.L. Santiago (CIEMAT) & S. Janssen (VITO)***

FAIRMODE Plenary Meeting.

April 28, 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 is ongoing 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

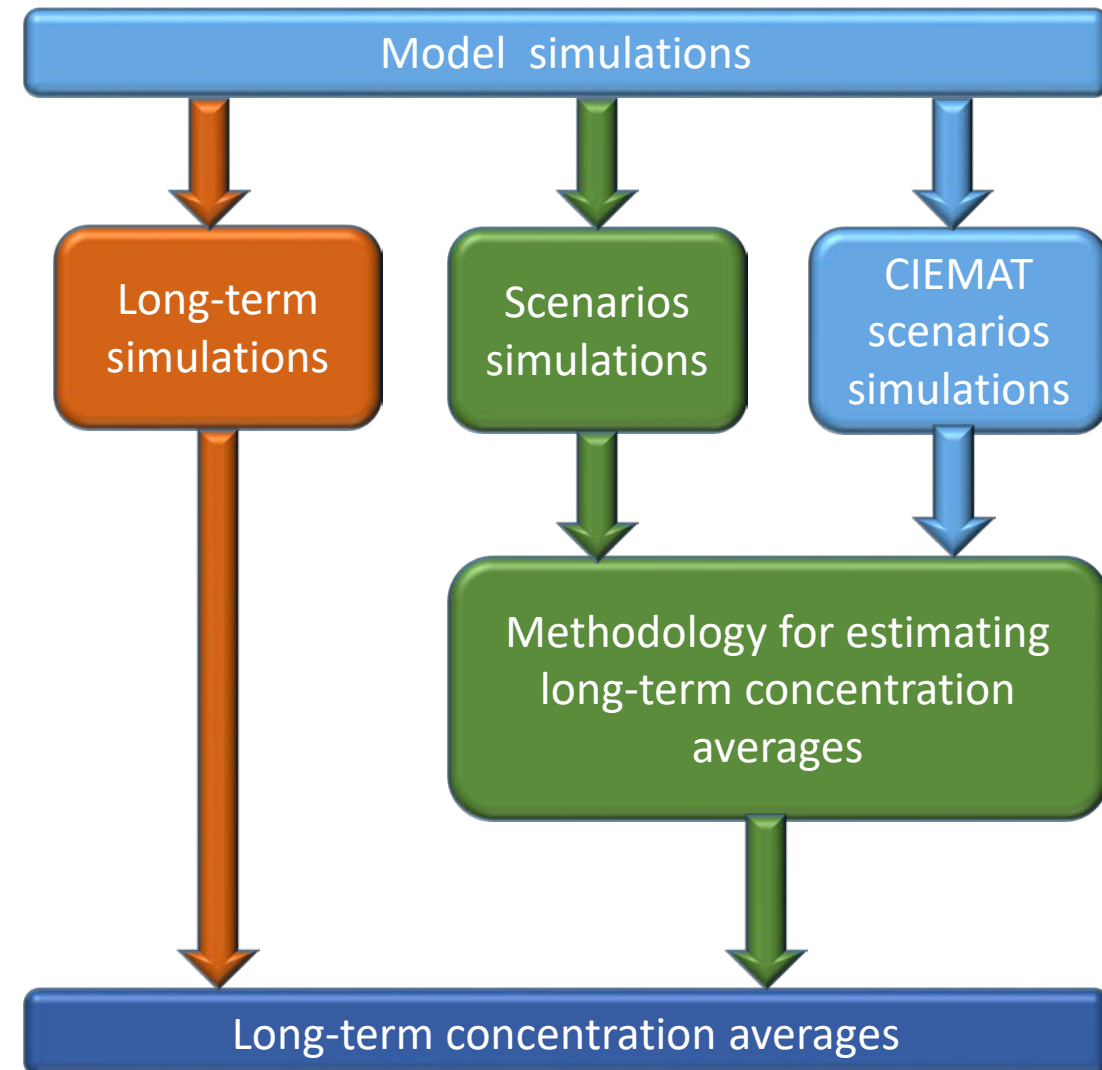
- CT4 Microscale Modeling was endorsed in FAIRMODE Plenary Meeting, Berlin, Feb 2020.
- During 2020, meetings (FAIRMODE Technical Meeting and hackathon in December) for design and preparation of an Intercomparison Exercise.
- **Intercomparison exercise started in March 2021**
- **Reception of modelling 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.**

# CT4 Intercomparison exercise

## Models and methodologies:

- Focused on the **Antwerp (Belgium). NO<sub>2</sub>**
- 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.

## Ways of participating in the exercise:



# CT4 Intercomparison exercise

## 3 steps:

**1. To simulate one day from the one-month passive sampler campaigns.**

- *May 6<sup>th</sup>, 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 campaign period (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 2016 year applying the methodologies of each group.**

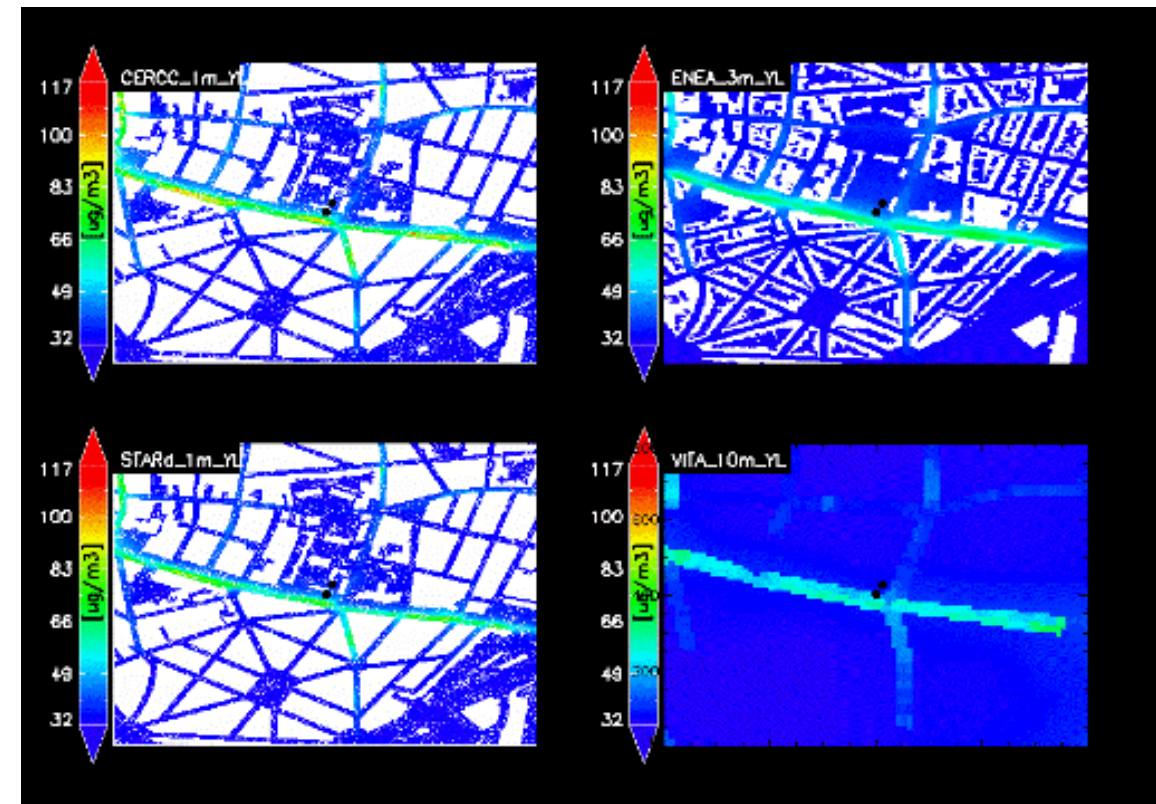
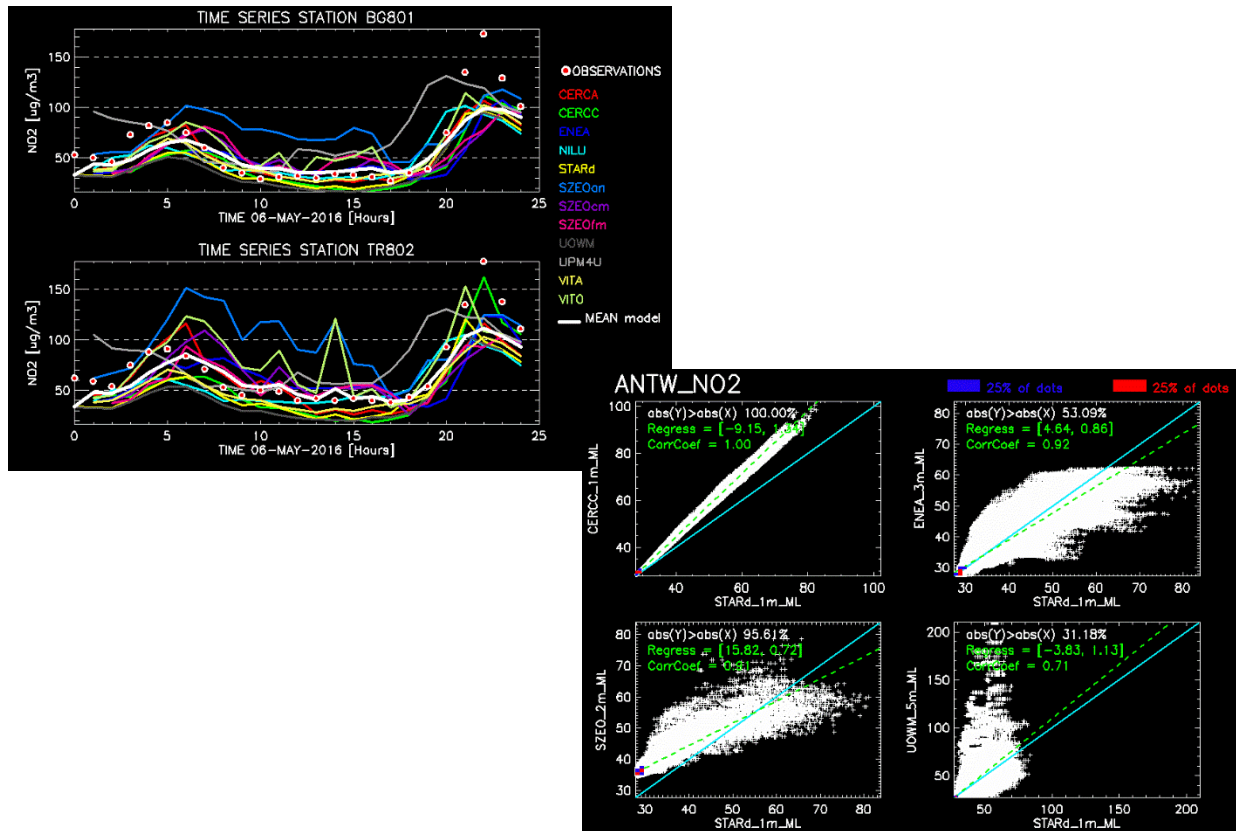
- *Intercompare results from every methodology (2D maps).*

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

# CT4 tool

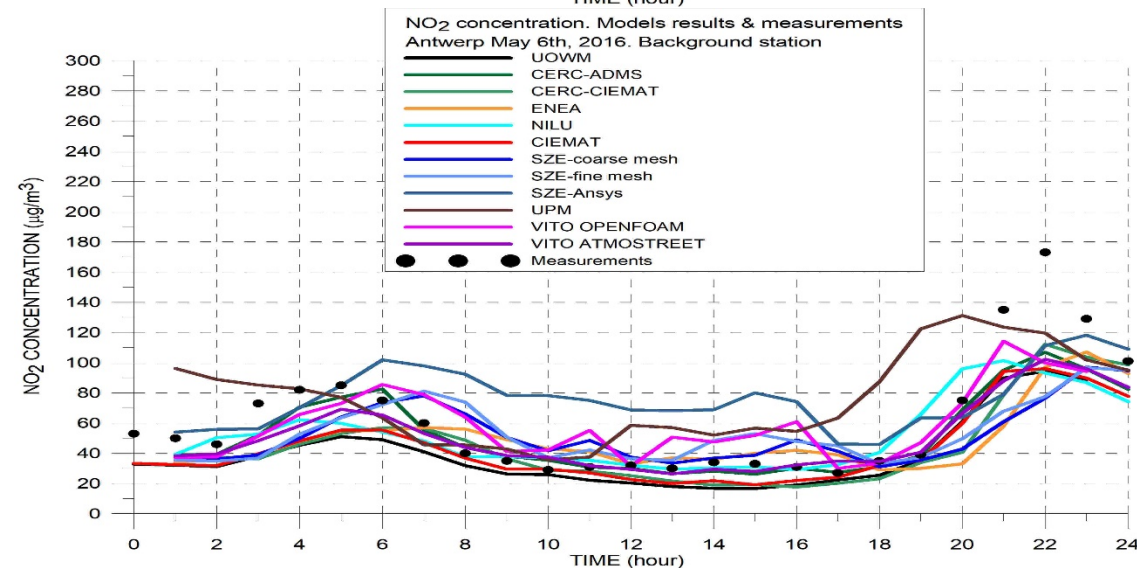
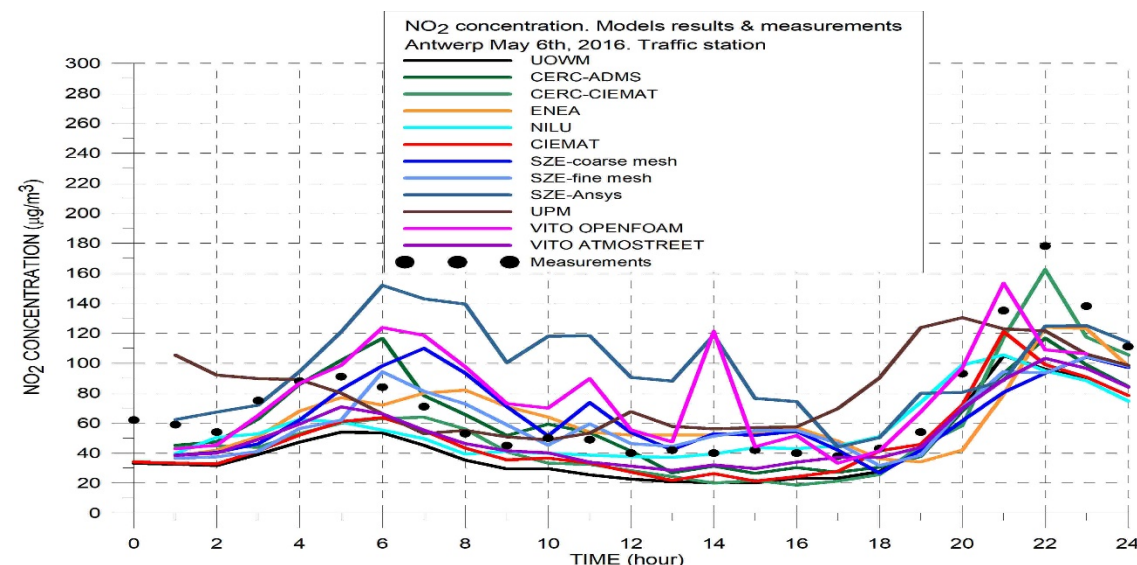
- Kees Cuvelier has developed a software to help to the processing and analysis of the results provided by the participants and comparison with observations



# 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<sub>2</sub> concentration.
- Problems:
  - slight underprediction (evening peak)
  - timing of the concentration peaks (several models)

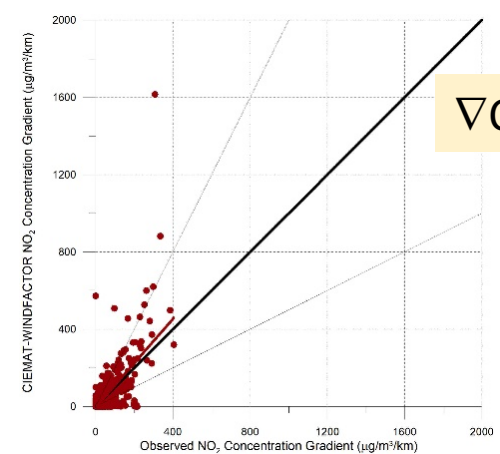
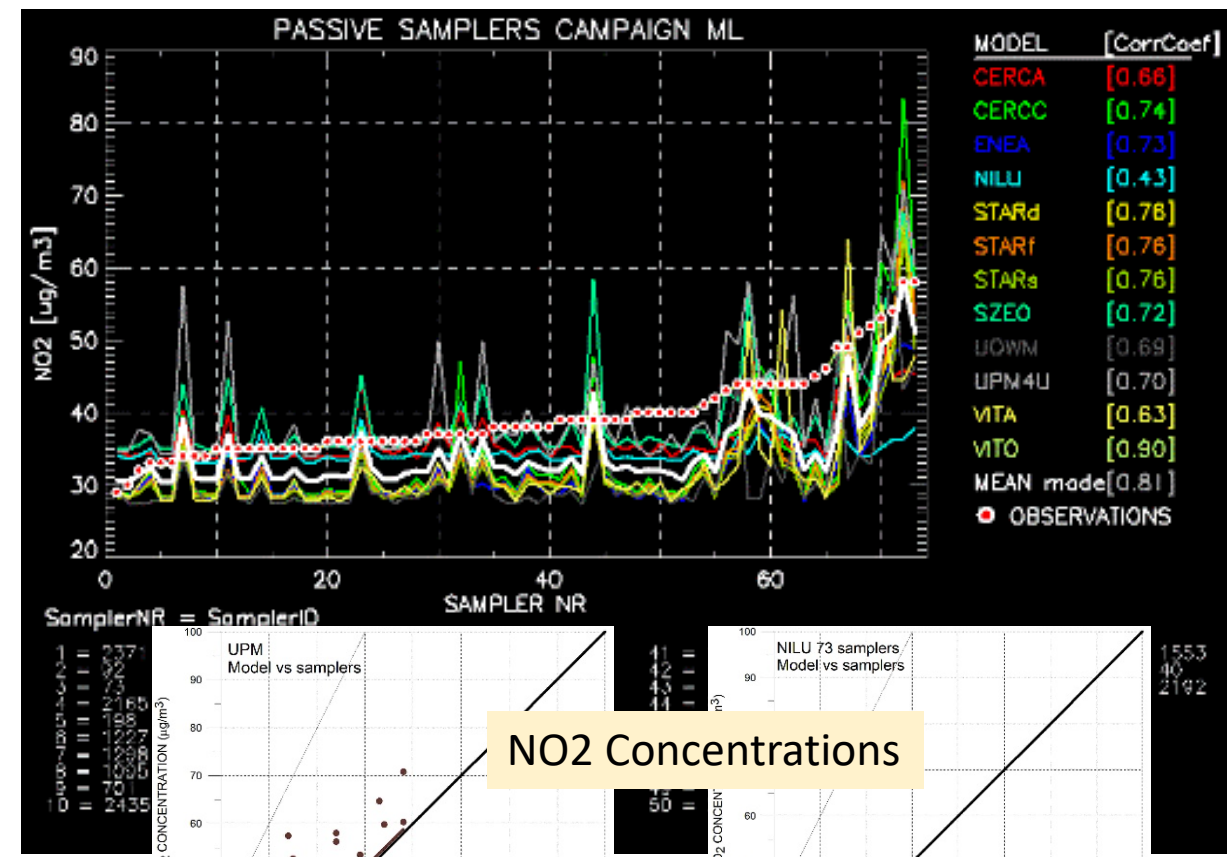




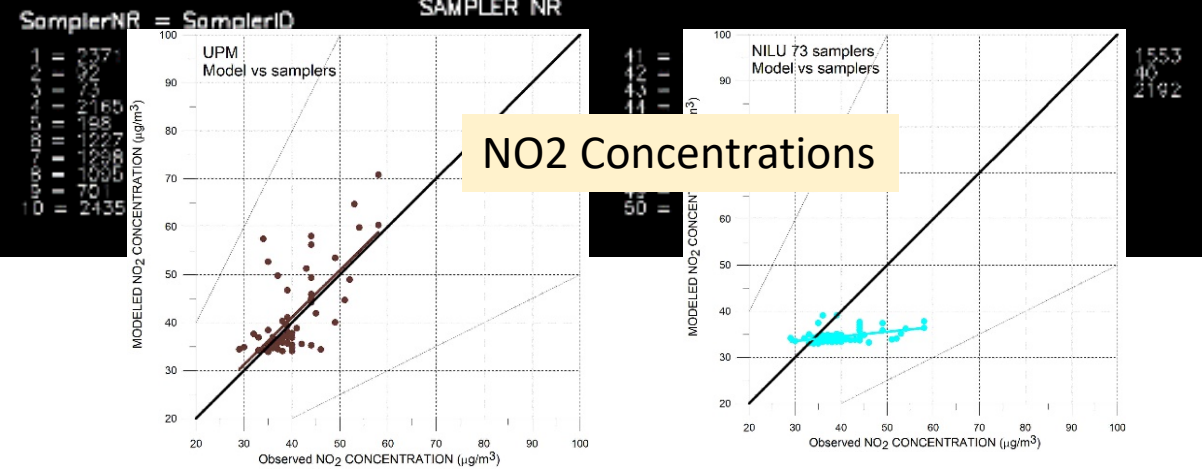
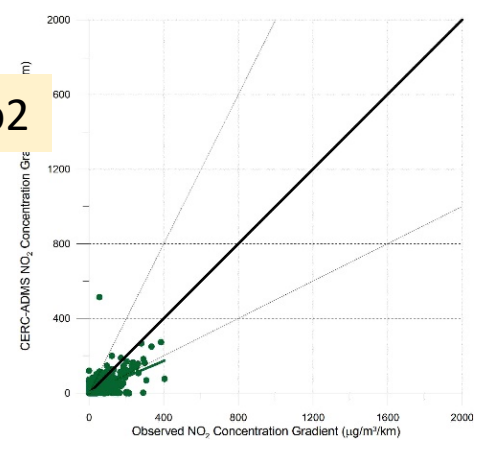
# Analysis of data (all methodologies vs observations)

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

- Most of the models (mainly CFD) seem to predict fairly good NO<sub>2</sub> average concentration.
- CFD models seem to simulate better the spatial distribution of the monthly averaged concentrations than simpler approaches.



∇C of No<sub>2</sub>

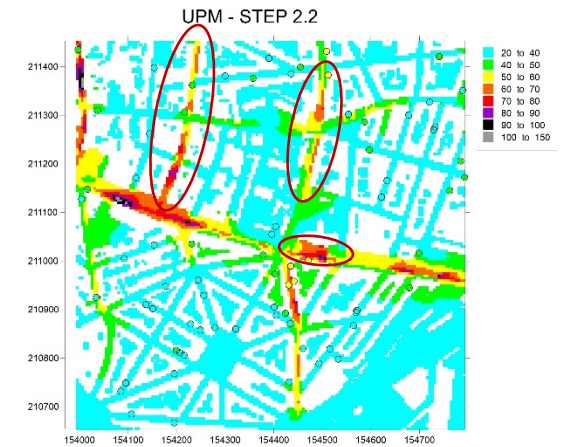
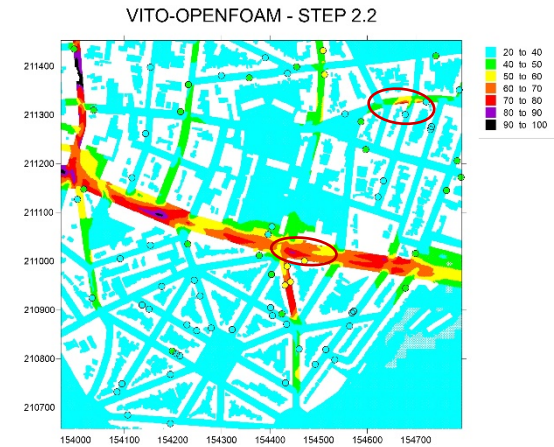
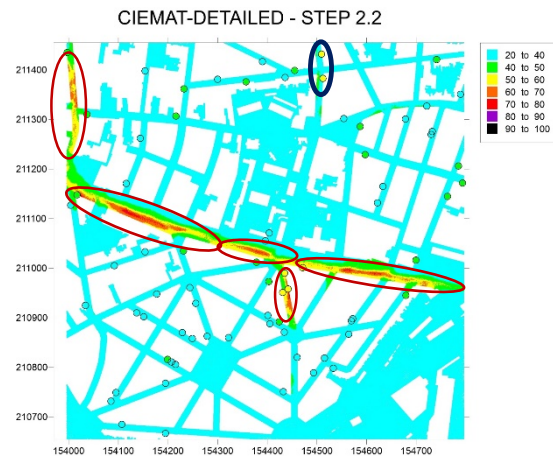


NO<sub>2</sub> Concentrations

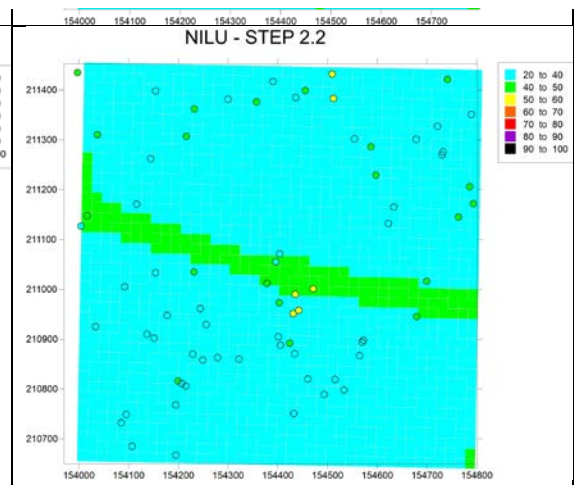
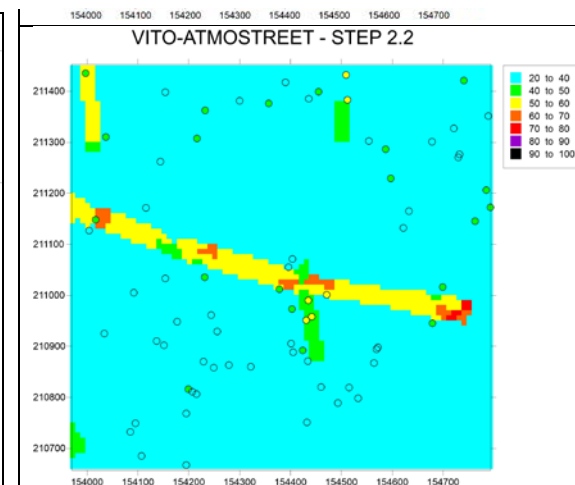
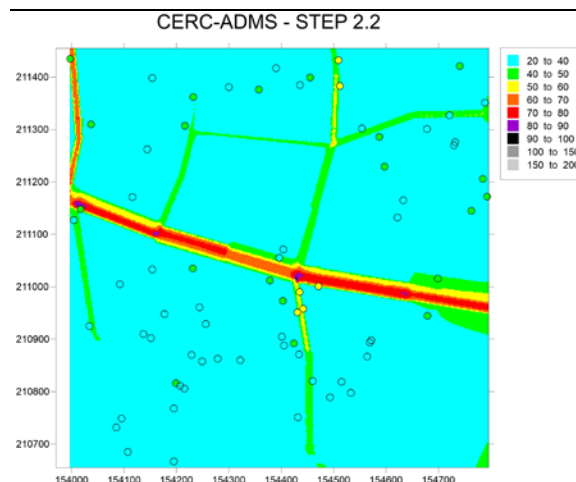
# Analysis of data (all methodologies vs observations)

## Step 2.2. Maximum monthly concentration areas

**CFD models**



**NO-CFD models**

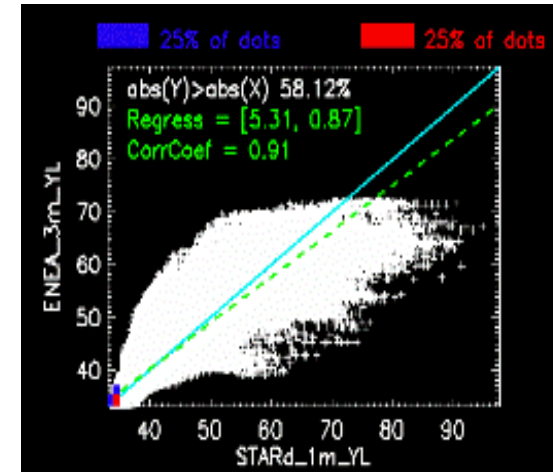
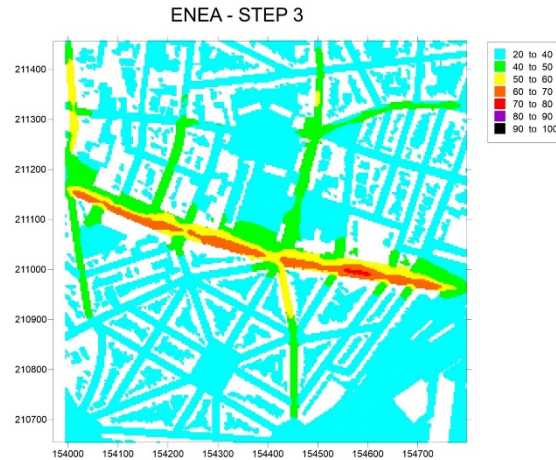


# Analysis of data (all methodologies)

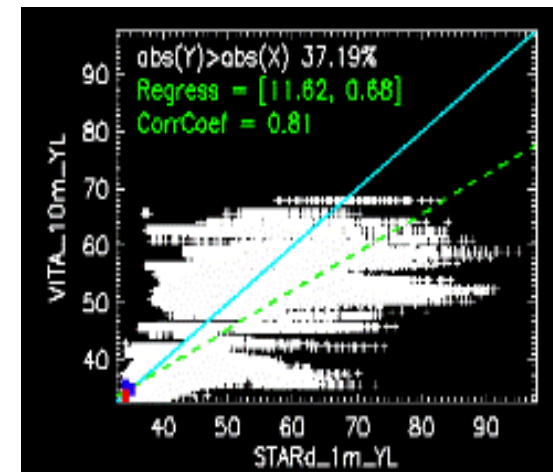
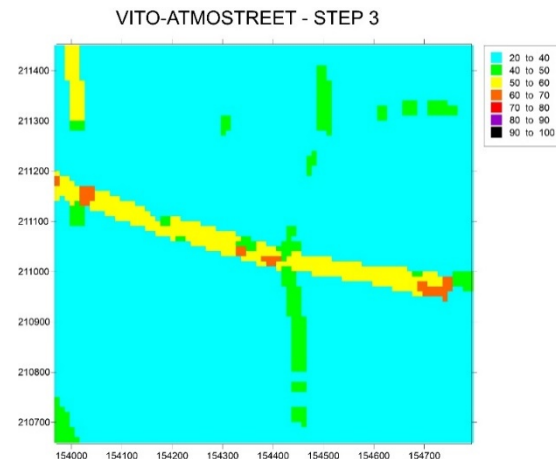
## Step 3. Intercomparison of yearly averaged maps (2016)

### CFD models

Maximum annual concentration areas similar to Maximum Monthly average concentration areas



### NO-CFD models



# 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**

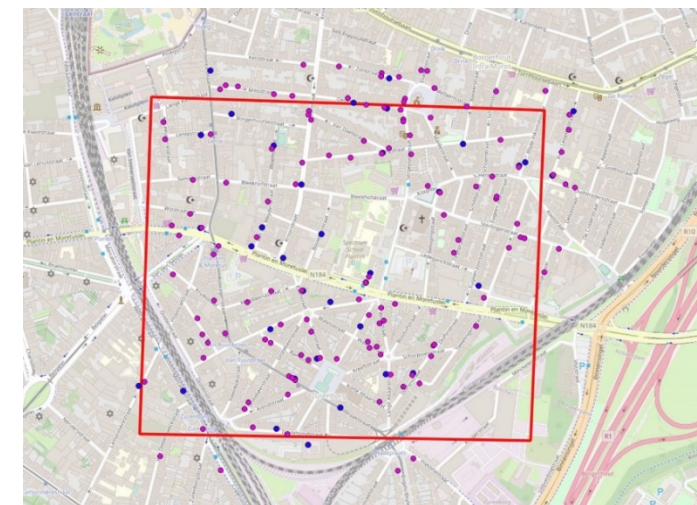
# Additional analysis done

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

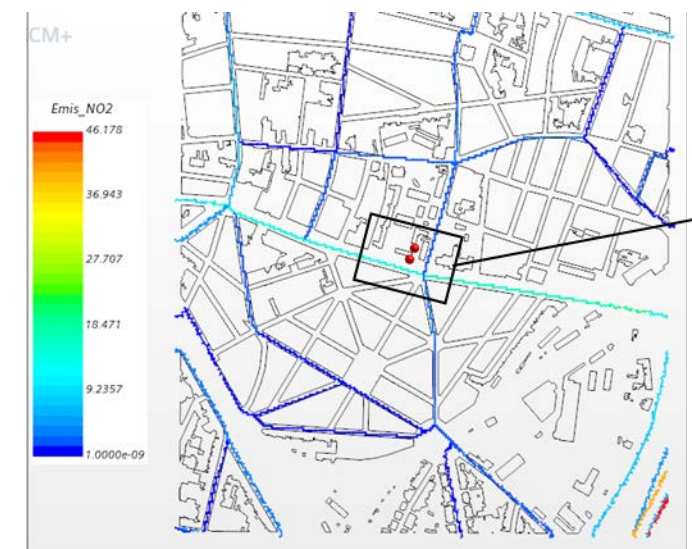
- **What is the impact of the emissions data?**
- **What type of models are more suitable?**
- **Long term simulations versus methodologies based on limited use of simulations (scenarios)?**
- **How many simulations (scenarios) could be needed to provide good results?**

# 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 NO2 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 versus methodologies based on limited use of simulations (scenarios)?

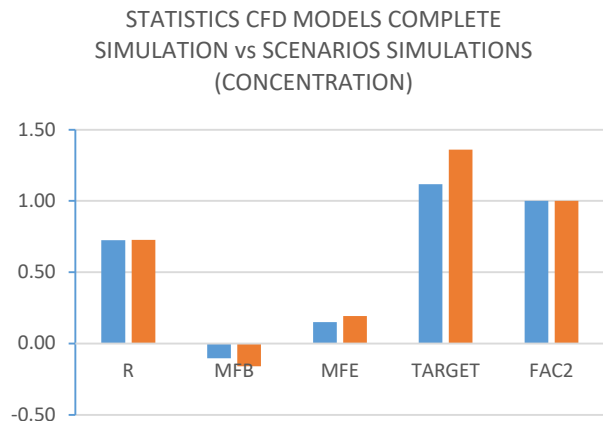
Comparing results based on CFD long-term simulation (SZE, ENEA) and the methodologies based on simulating a set of scenarios with CFD models (UPM, CERC-CIEMAT, CIEMAT, UPWM, VITO-OPENFOAM). **Results do not seem to be conclusive:**

## Concentrations

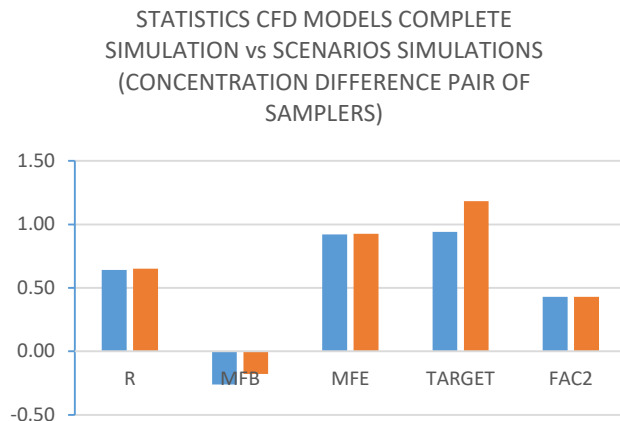
- little differences between the results of R from complete period model simulations and scenarios based methodologies
- Long-term simulations seem to give somewhat better values of MFB, MFE and TARGET (1.12, 1.36)

## Gradients and Concentration differences between pair of stations:

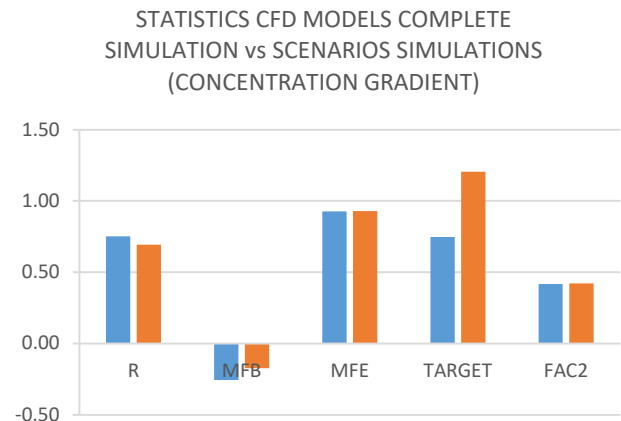
- Similar R (long-term simulation slight better for gradients), MFE and FAC2
- Less MFB with scenarios, best TARGET with long-term simulation



Step 1 ■ COMPLETE ■ SCENARIOS



■ COMPLETE ■ SCENARIOS



Step 2.1 ■ COMPLETE ■ SCENARIOS

# 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.

# Another analysis and pending questions (discussion)

1. Can results showed before be considered conclusive? I think no yet.
2. Can we derive some solid recommendations right now? I think no yet
3. Need more work? I think yes

## **Some questions are pending:**

1. Comparison of complete year simulation from SZE with results from methodologies based on scenarios but with the same model.
  - Should it be good SZE compute also annual concentration using scenarios?
2. How many simulations (scenarios) are recommended to use?
  - Extending the work of checking to other groups such UOWM, VITO, SZE, ....?
  - Revising a work presented as part of a PhD Thesis (University of Strasburg) tackling this question?
3. What methodologies for retrieving long-term concentration averages could be good enough? Wind sectors scenarios? Emission scenarios? Both? Representative cases?
4. Another questions?

# Next steps (discussion)

- Another hackathon for discussing last results and aforementioned additional work (May 2022)
- Harmo21 presentation (September 2022)
- **Additional work?:**
  - More analysis tackling aforementioned questions?
  - More intercomparison exercises? Győr (Hungary)?
- **Elaboration of recommendations ...**
- **Report and paper preparation...**