# FAIRMODE WG4 Hackathon

22nd of November 2023

# Agenda

- 9:30 – 11:00 Paper A
- 11:00 – 11:15 Coffee-break
- 11:15 – 13:00 Paper B

# Paper A. Key points

- Models or methodologies or applications terminology, harmonize? (maybe models are more appropriate – Stijn Janssen). Models versus methodologies based on scenarios' simulations (explain it clearly in introduction or methodology section saying: Several ways of computing annual averages are intercompared. Models running the whole year and methodologies based on scenario simulation. In order to be more concise, we are referring all the time to models…(something like that?)?
- Improve Quality of some figures: Figure 2, Figure 17 and Figures of concentration maps (we will do it)
- NOx chemistry is enough referred in Discussion section or Conclusions? Only ATMOSTREET, ADMS, NILU and PALM4U include some chemical module. Suggestion for Conclusions : "For future works, we have to highlight the need of investigate how the models can improve their results if NOx chemistry is accounted for…"
- Are all needed references?

# Paper A. Key points

- Check if the Schmidt number of each CFD simulation was the same? It is not said in paper. Only referred in page 20 for hourly time series : *"…This behavior of the model applications could be related to their limited capability of reproducing the formation of night thermal inversion as most of them are assuming neutral atmospheric stability, to the different Schmidt numbers used in the case of the CFD models, or to ….."*
- *To be included* in the tables describing the model setup…
- CIEMAT – Sct = 0.3
- AIR&D – Sct = 0.7

# 3.1. Hourly data from two air quality stations…

**Hourly time series analysis (May 6th) highlights a particular pattern at 10 p.m. (CET). What part is due to the RIO model, which may also underestimate background concentrations??**

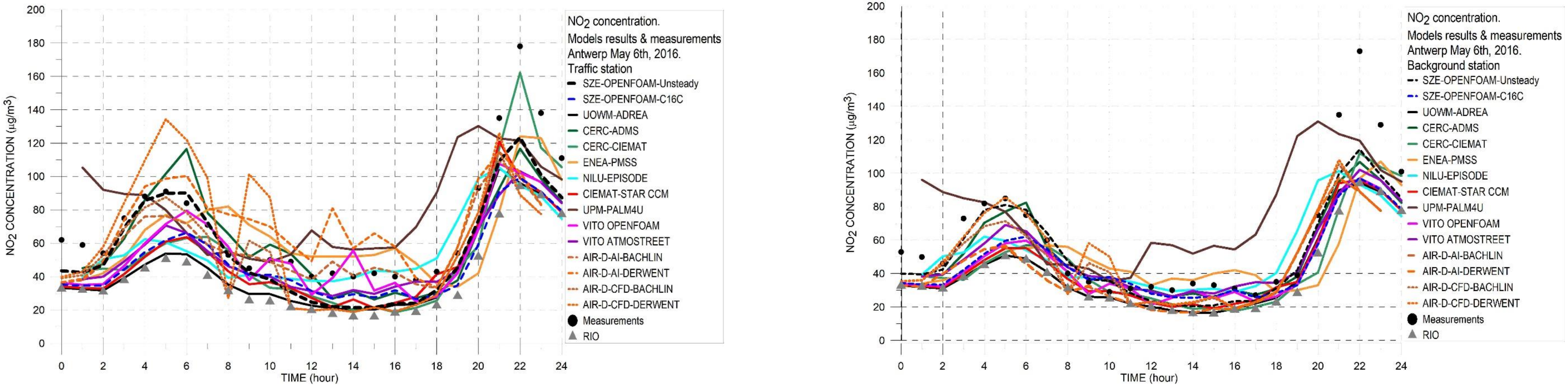



Figure 3. Time series of model predictions of hourly $NO_2$ concentrations and observations for the traffic station (left) and background station (right)

# 3.1. Hourly data from two air quality stations…

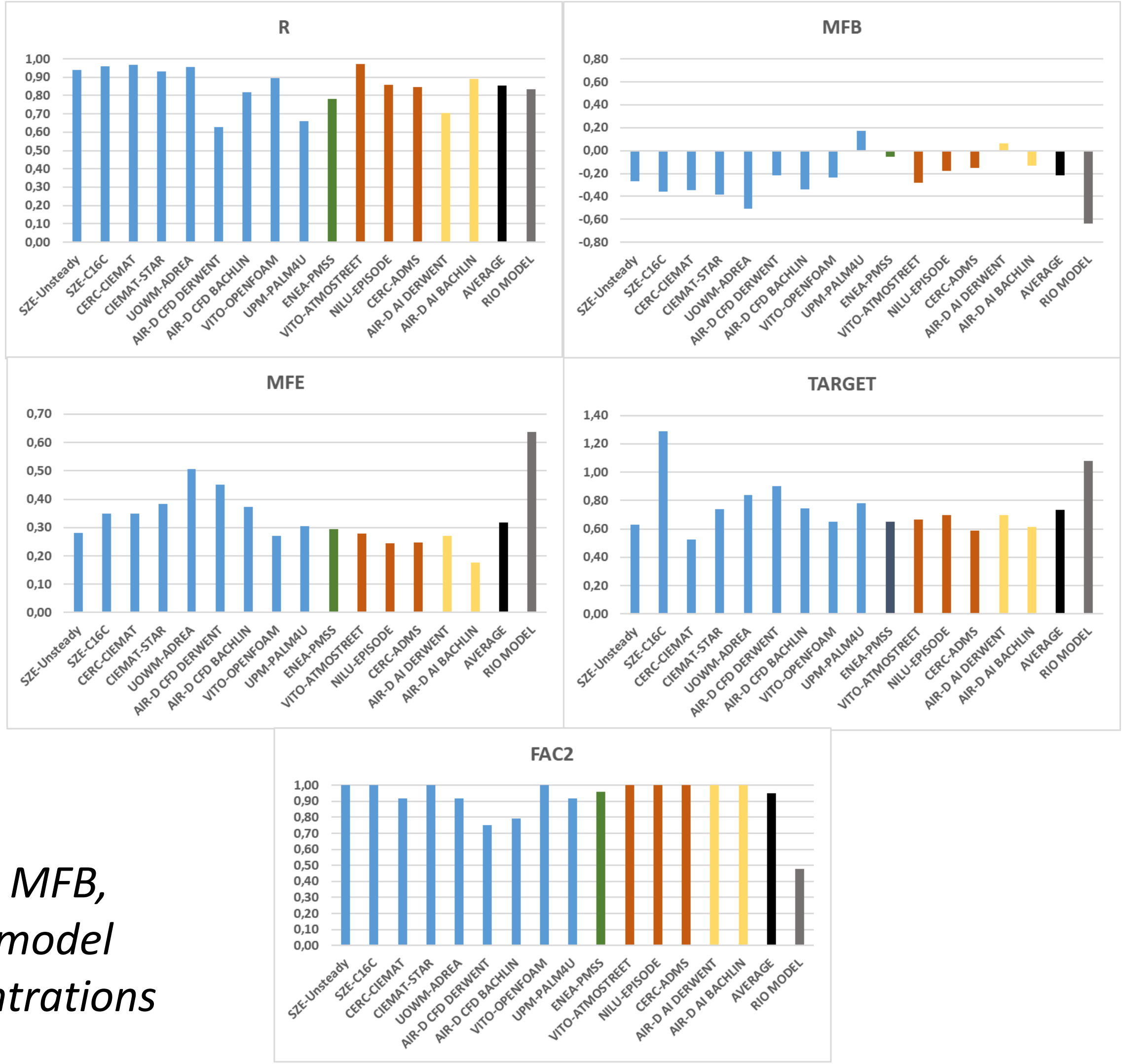



*Figure 4. Statistical results of R, MFB, MFE, TARGET and FAC2 for the model prediction of hourly $NO_2$ concentrations for the traffic station*

# 3.1. Hourly data from two air quality stations…

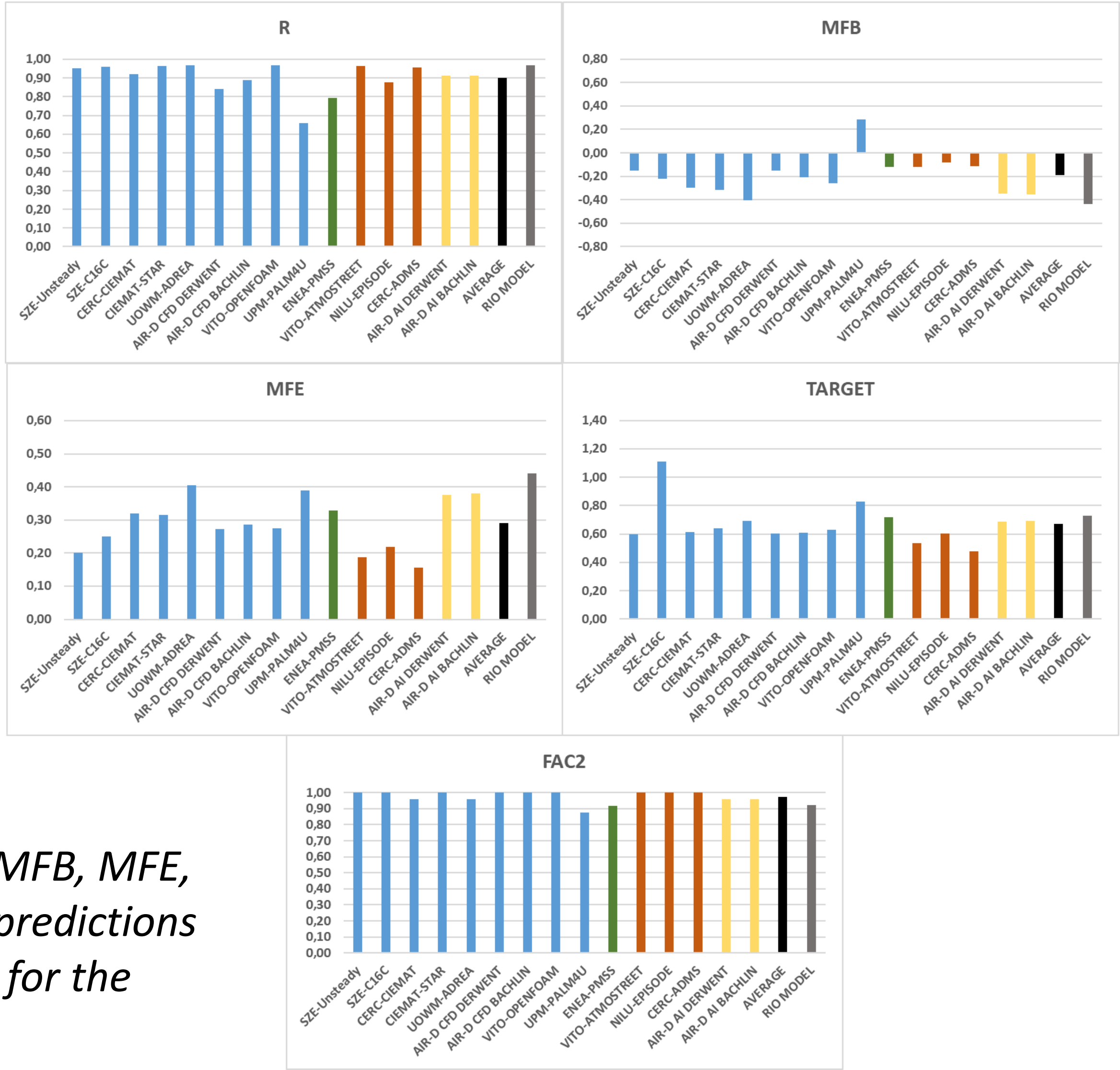



*Figure 5. Statistical results of R, MFB, MFE, TARGET and FAC2 for the model predictions of hourly $NO_2$ concentrations for the background station.*

# 3.2. Monthly average data of NO2 concentrations recorded by passive samplers

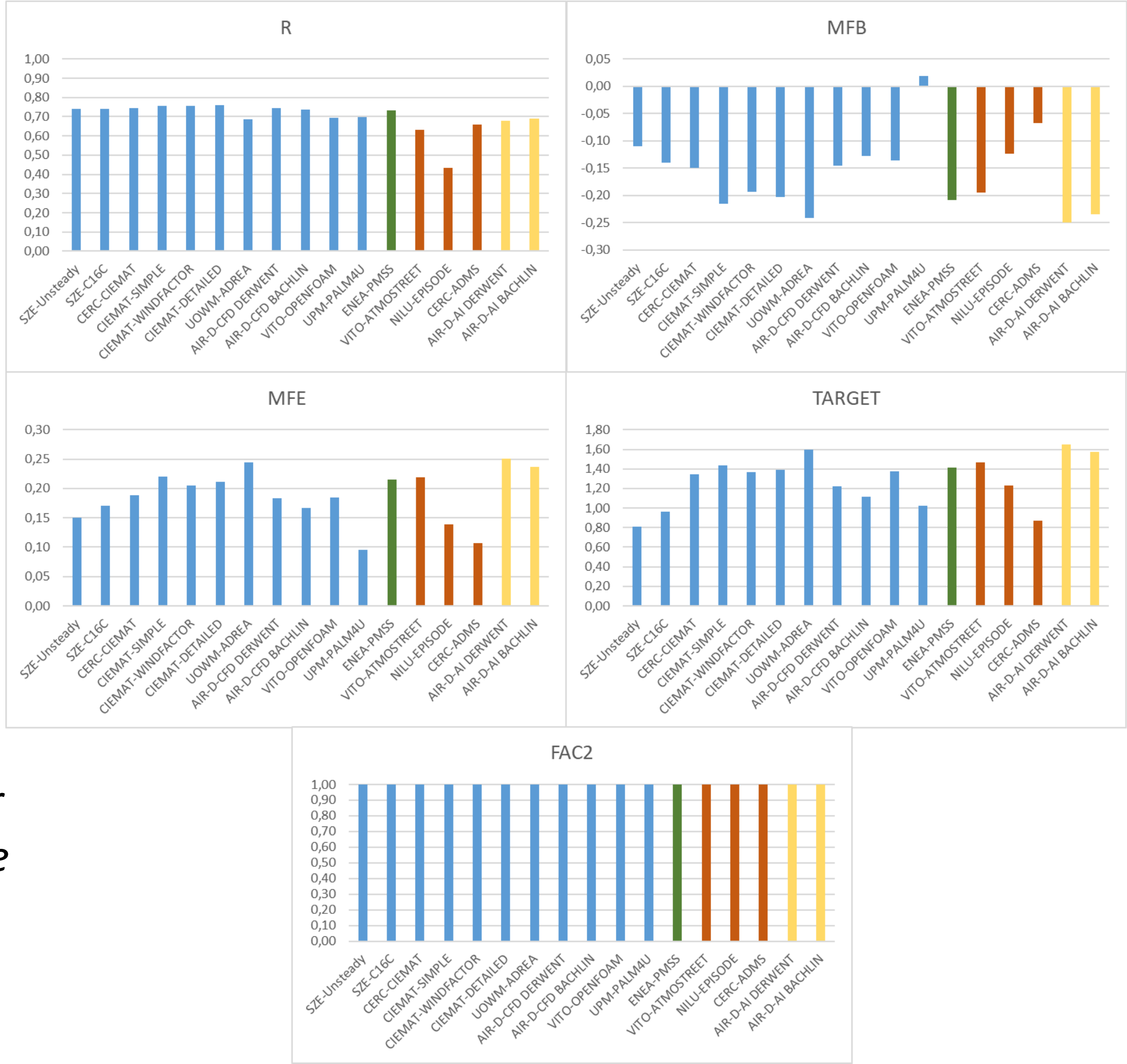
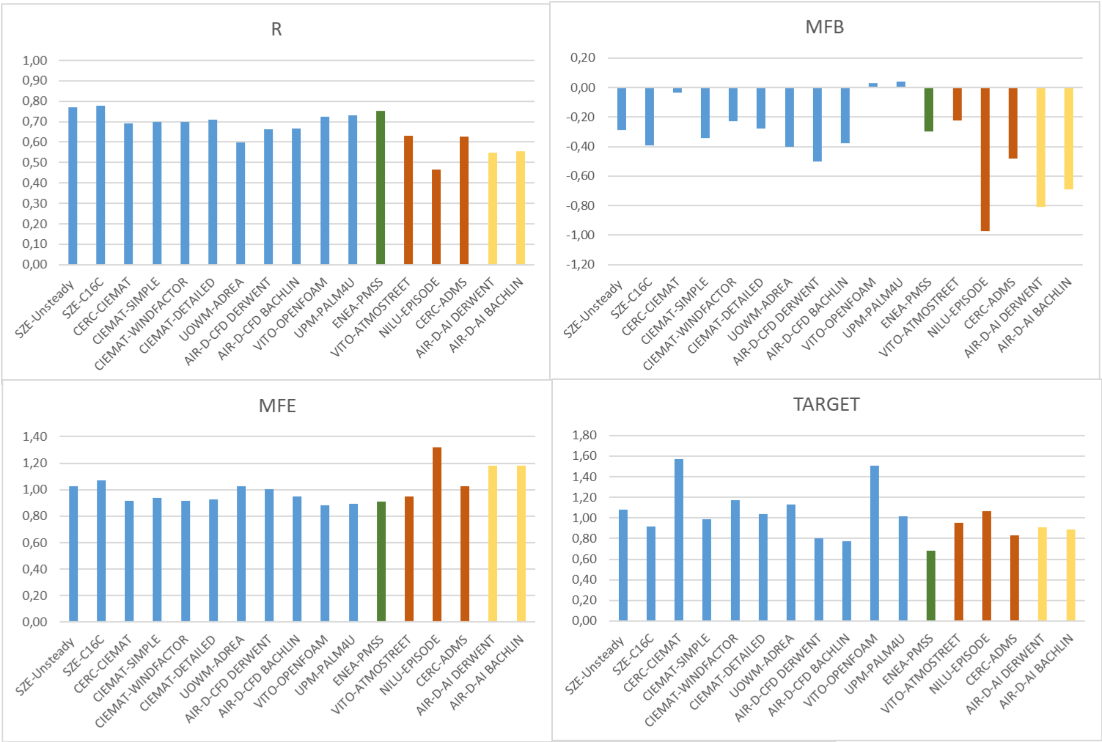



*Figure 6. Statistical results of R, MFB, MFE, TARGET and FAC2 for the model predictions of average $NO_2$ concentrations at sampler points for the campaign period (April 30$^{th}$ to May 28$^{th}$, 2016).*

# 3.2. Monthly average data of NO2 concentrations recorded by passive samplers




$$\nabla C_{i,j} = \frac{C_i - C_j}{d_{i,j}}$$

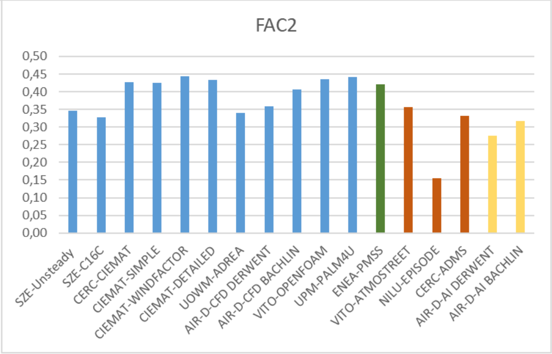



*Figure 7. Statistical results of R, MFB, MFE, TARGET and FAC2 for the methodology predictions of $NO_2$ concentration **gradients** between every pairs of sampler points for the campaign period (April 30$^{th}$ to May 28$^{th}$, 2016).*

# 3.3. Monthly average NO2 concentration maps

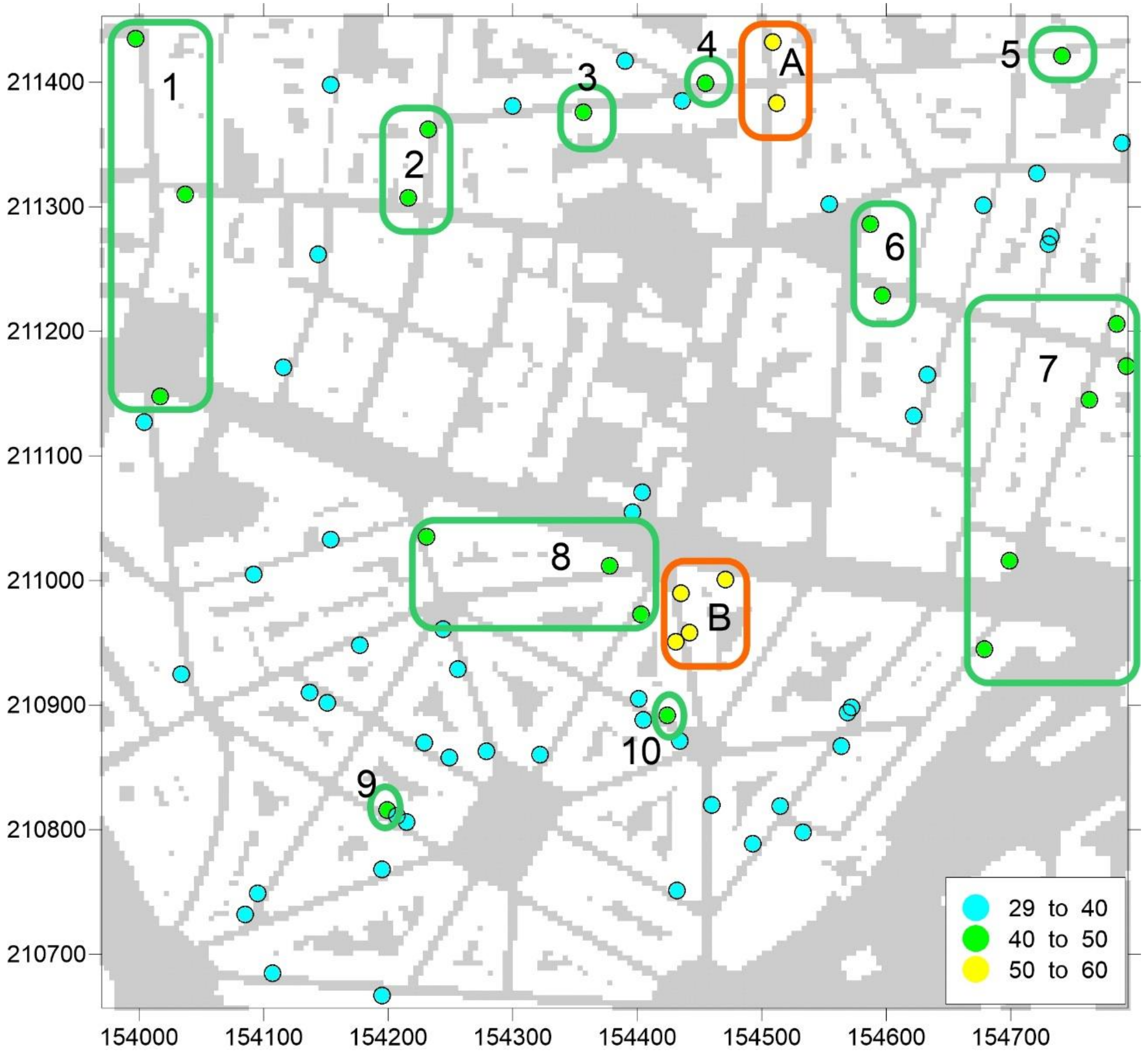



*Figure 8. Map showing the monthly $NO_2$ concentrations at each sampler point.* The *green rectangles and circles show the samplers with concentrations between 40 and 50* µg/m$^3$and the orange ones grouped the samplers about 50 µg/m$^3$.

# 3.3. Monthly average NO2 concentration maps

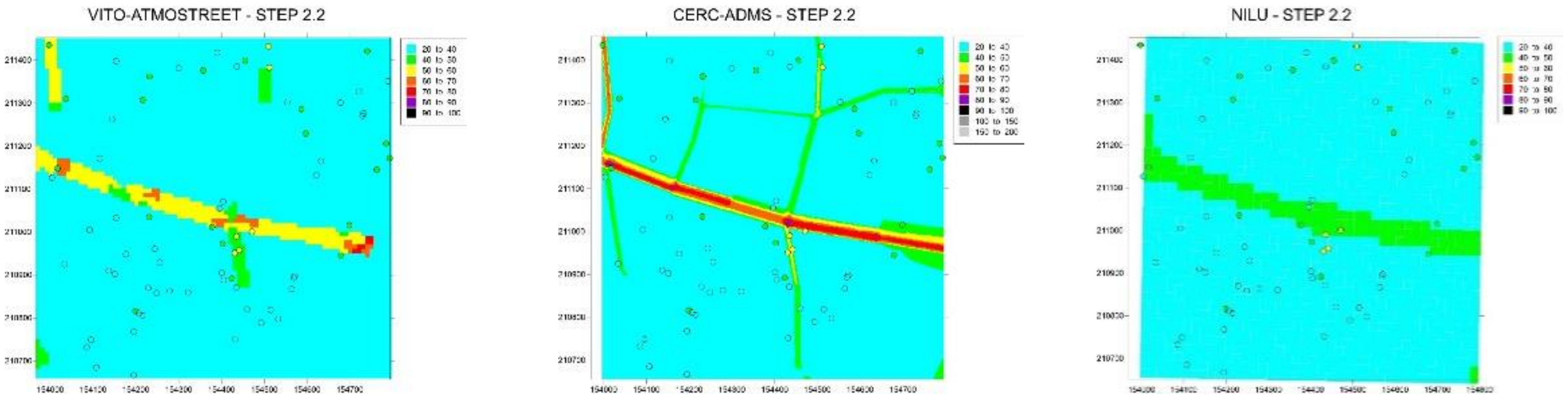



*Figure 9. Maps of the monthly average $NO_2$ concentrations for the 3 Gaussian models and concentrations measured by passive samplers (colored dots).*

# 3.3. Monthly average NO2 concentration maps

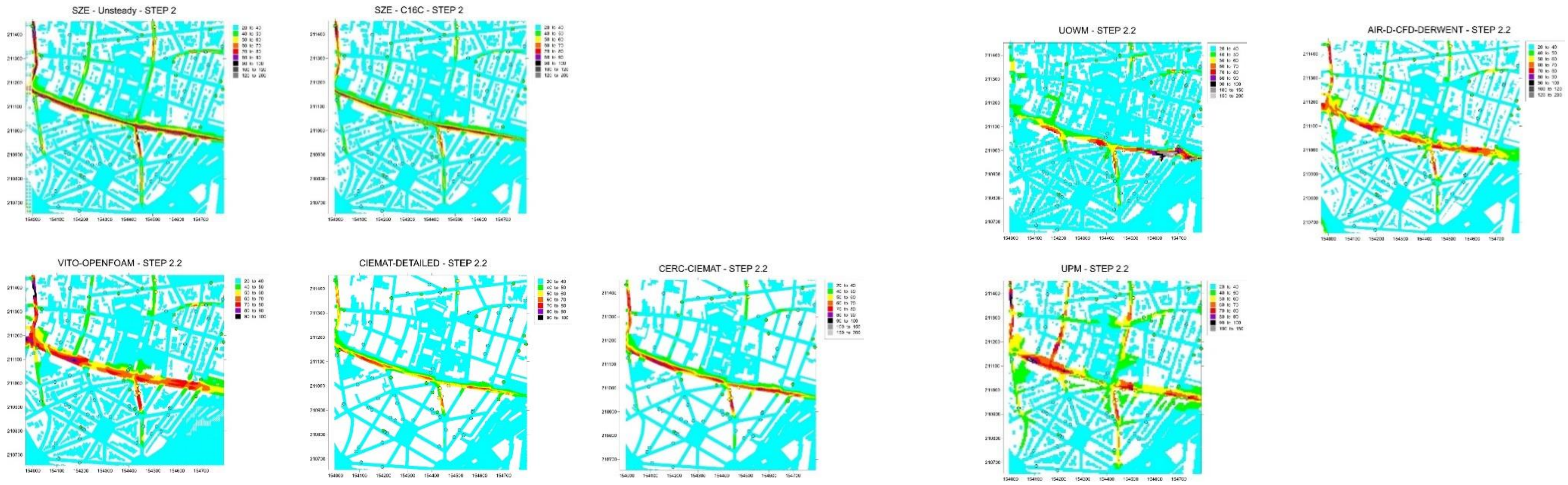



*Figure 10. Maps of the monthly average $NO_2$ concentration for the long-term CFD unsteady simulation (upper left) and for 8 methodologies based on scenario CFD simulations and concentration measured by passive samplers (colored dots).*

# 3.3. Monthly average NO2 concentration maps

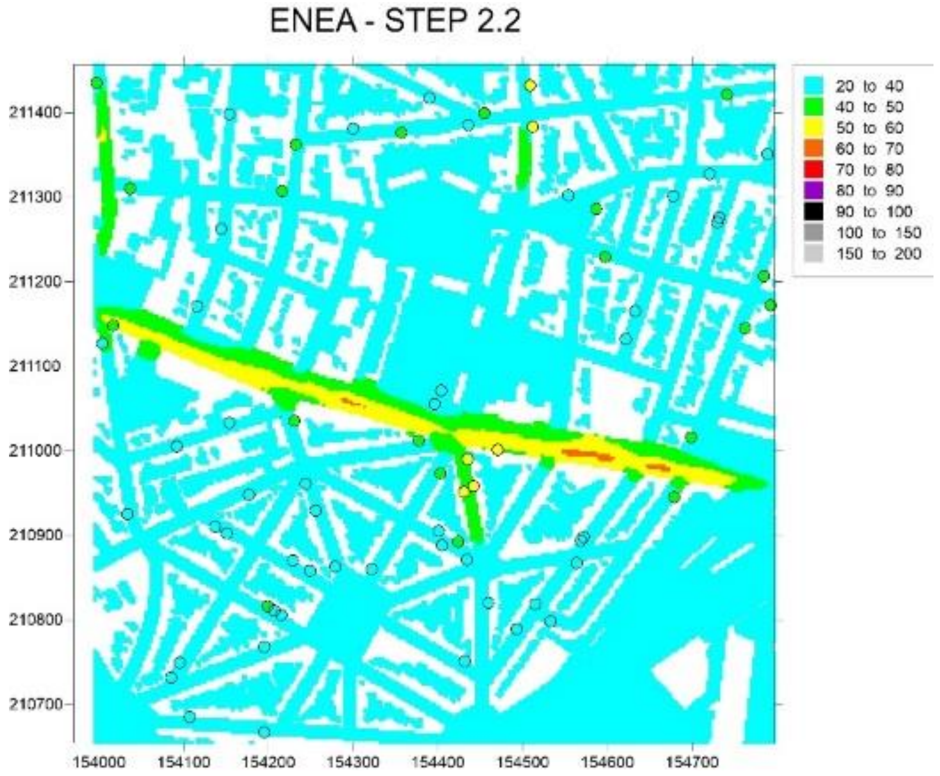



*Figure 11. Map of the monthly average $NO_2$ concentration for the ENEA-PMSS model and concentration measured by passive samplers (colored dots).*

# 3.3. Monthly average NO2 concentration maps

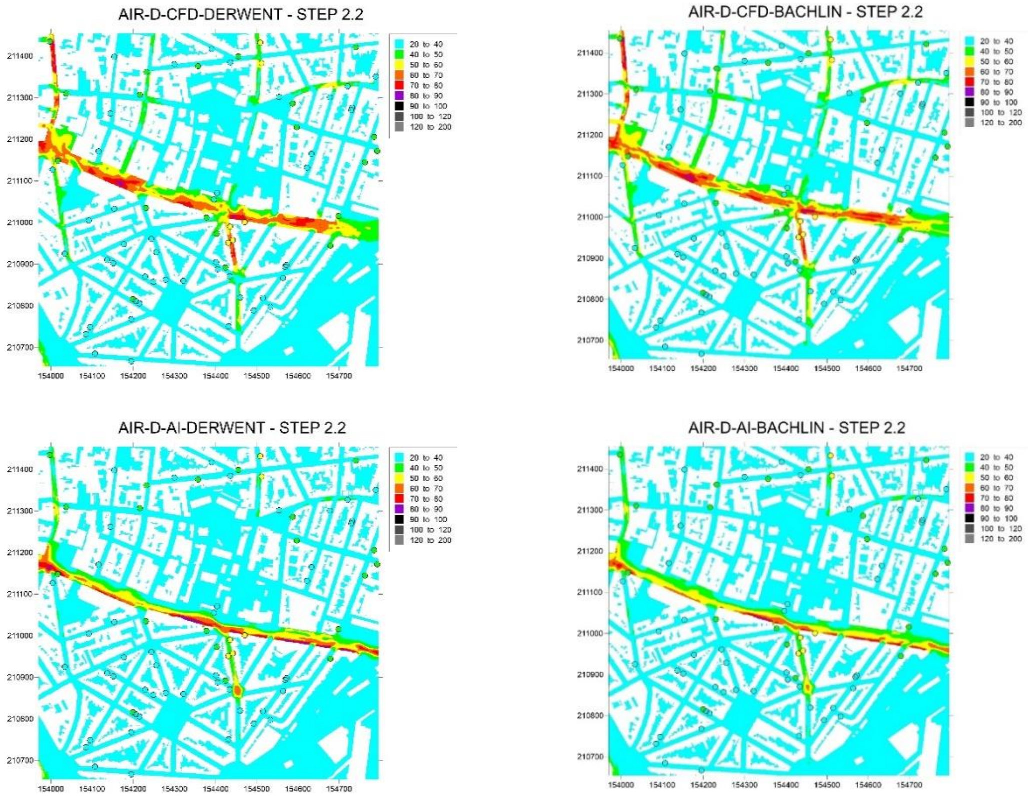



*Figure 12. Maps of the monthly average $NO_2$ concentration for the AIR-D-CFD (upper) and AIR-D-AI (lower) for the Derwent (left) and Bachlin (right) parametrizations accounting for the $NO_2$/NOx ratios and concentration measured by passive samplers (colored dots).*

# 4.1. What is the impact of the emissions data?

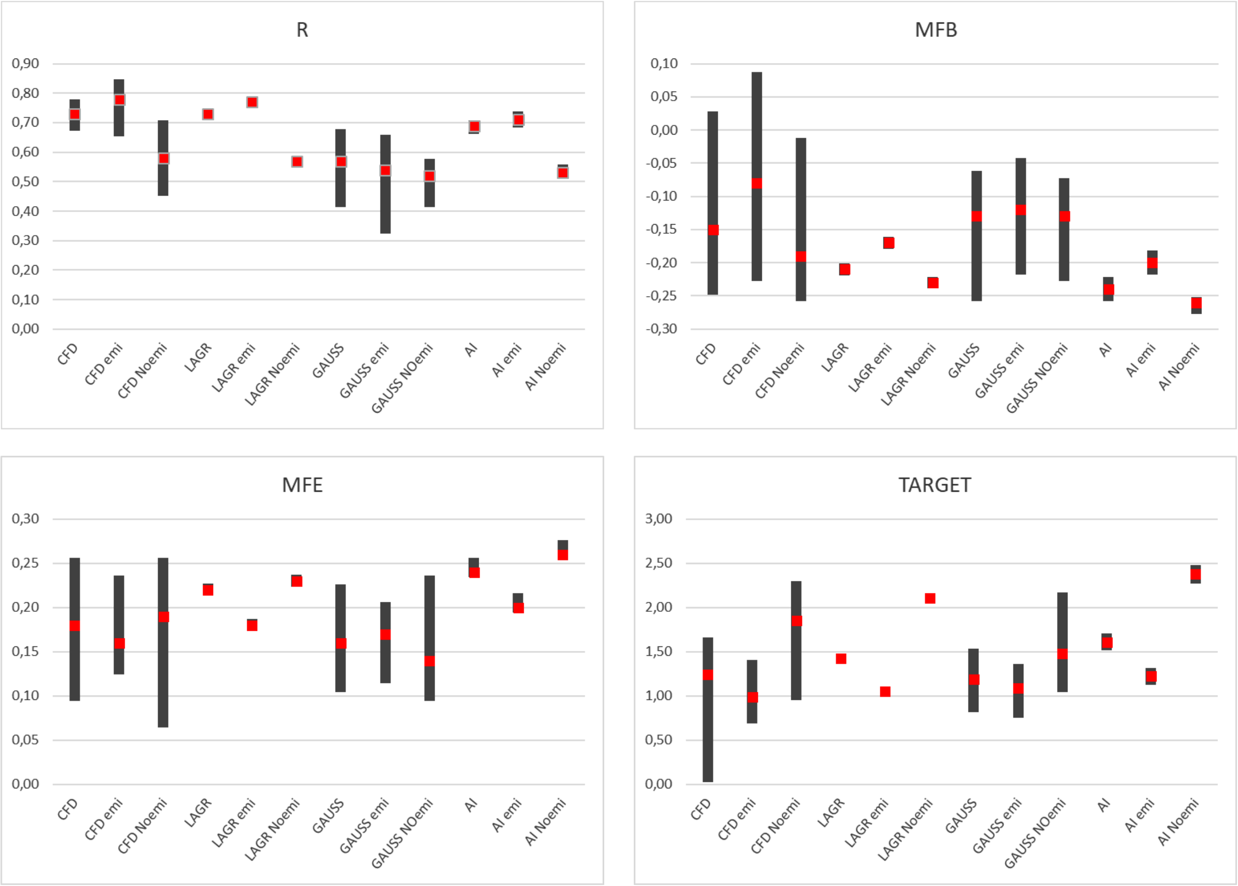



*Figure 13. Statistical results of R, MFB, MFE, TARGET and FAC2 for the methodology predictions of average $NO_2$ concentrations at sampler points for the campaign period (April 30$^{th}$ to May 28$^{th}$, 2016) for the different type of models/methodologies using data from all the samplers, only from samplers located in streets with emission data (labeled EMIS) and without emission data (labeled NOEMIS). CFD = Computational Fluid Dynamics, GAUSS= Gaussian models, LAGR= Lagrangian models, and AI=Artificial Intelligence models).*

# 4.2. What type of methodologies are more suitable to reproduce spatial distribution of long-term averaged NO2 concentrations?

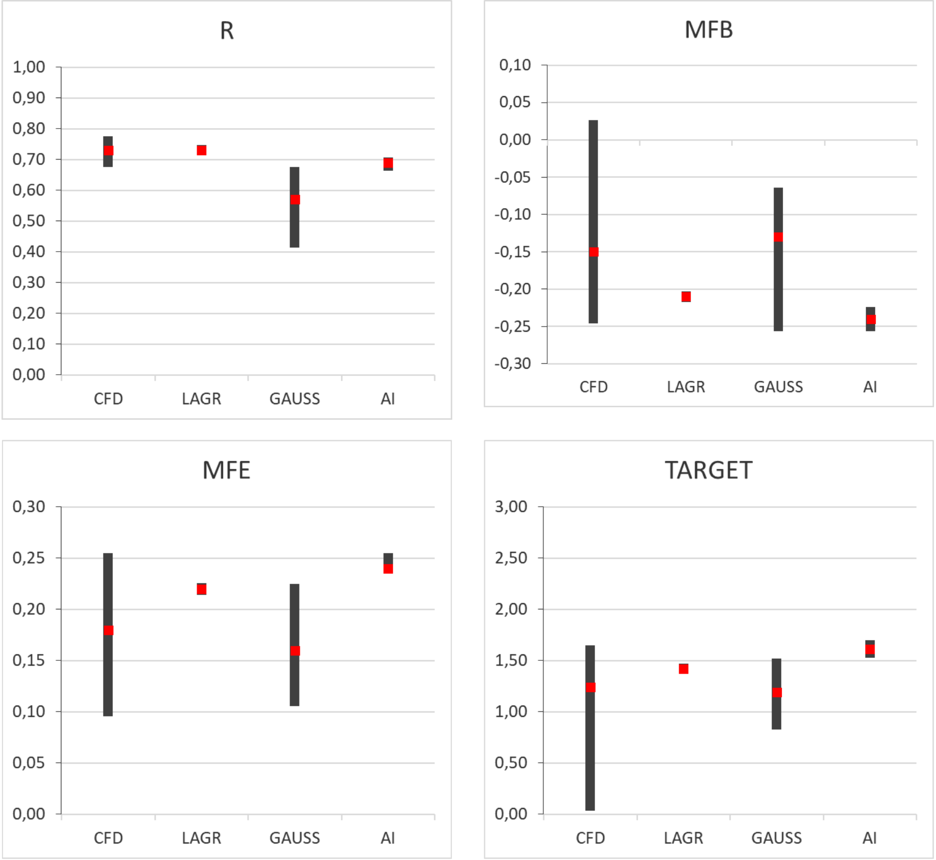



*Figure 14. Statistical results of R, MFB, MFE, TARGET and FAC2 for the methodology predictions of average $NO_2$ concentrations at sampler points for the campaign period (April $30^{th}$ to May $28^{th}$, 2016) for each type of models (CFD, Computational Fluid Dynamics, Gaussian models, Lagrangian models, and AI, Artificial Intelligence models).*

# 4.2. What type of methodologies are more suitable to reproduce spatial distribution of long-term averaged NO2 concentrations?

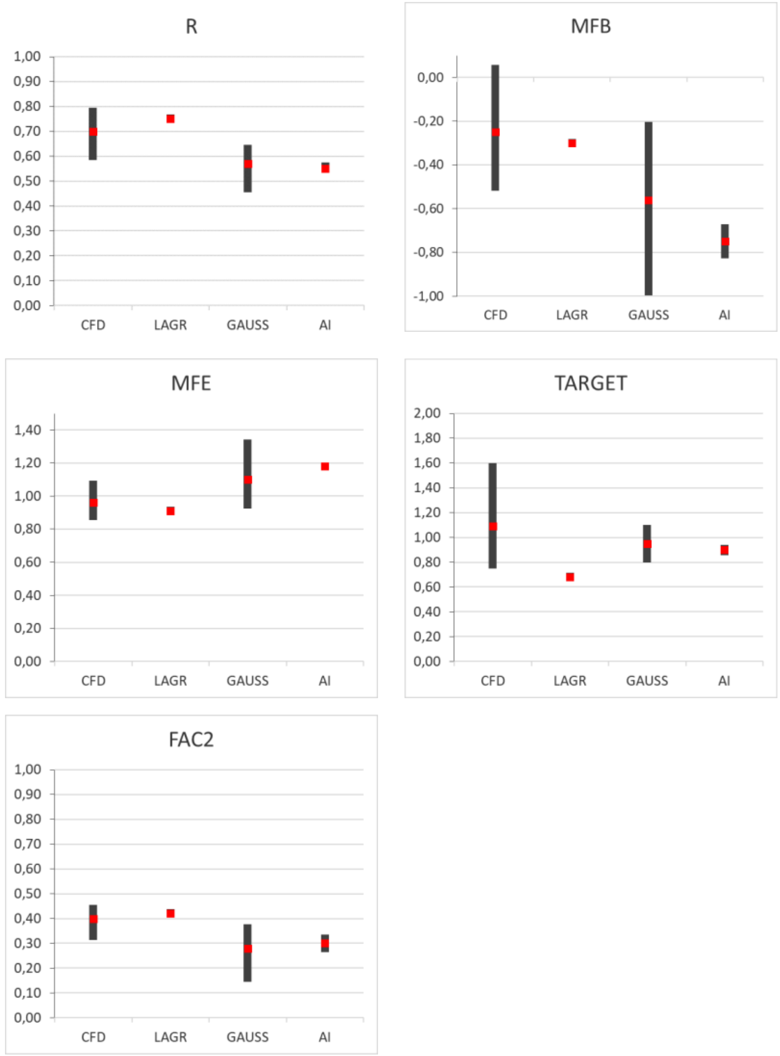



*Figure 15. Statistical results of R, MFB, MFE, TARGET and FAC2 for the methodology predictions of $NO_2$ concentration gradients between every pairs of sampler points for the campaign period (April $30^{th}$ to May $28^{th}$, 2016) for each type of models (CFD, Computational Fluid Dynamics, Gaussian models, Lagrangian models, and AI, Artificial Intelligence models).*

# 4.3. Long term simulations versus methodologies based on a limited number of scenarios

| Group/Model | Number of wind direction sector scenarios |
|---|---|
| SZE OpenFOAM | 4, 8, 16, 32 |
| UOWM ADREA | 8, 16, 32 |
| VITO OpenFOAM | 4, 8, 16, 32, 36 |
| CIEMAT STAR CCM+ | 4, 8, 16 |

*Table 3. Group, model and number of wind direction sectors used for computing average $NO_2$ concentrations for the campaign period (April 30th to May 28th, 2016).*

# 4.3. Long term simulations versus methodologies based on a limited number of scenarios

With respect to the first question, in general methodologies based on wind direction sector scenarios provide results at least as good as the SZE unsteady simulation

Need some explanation/discussion

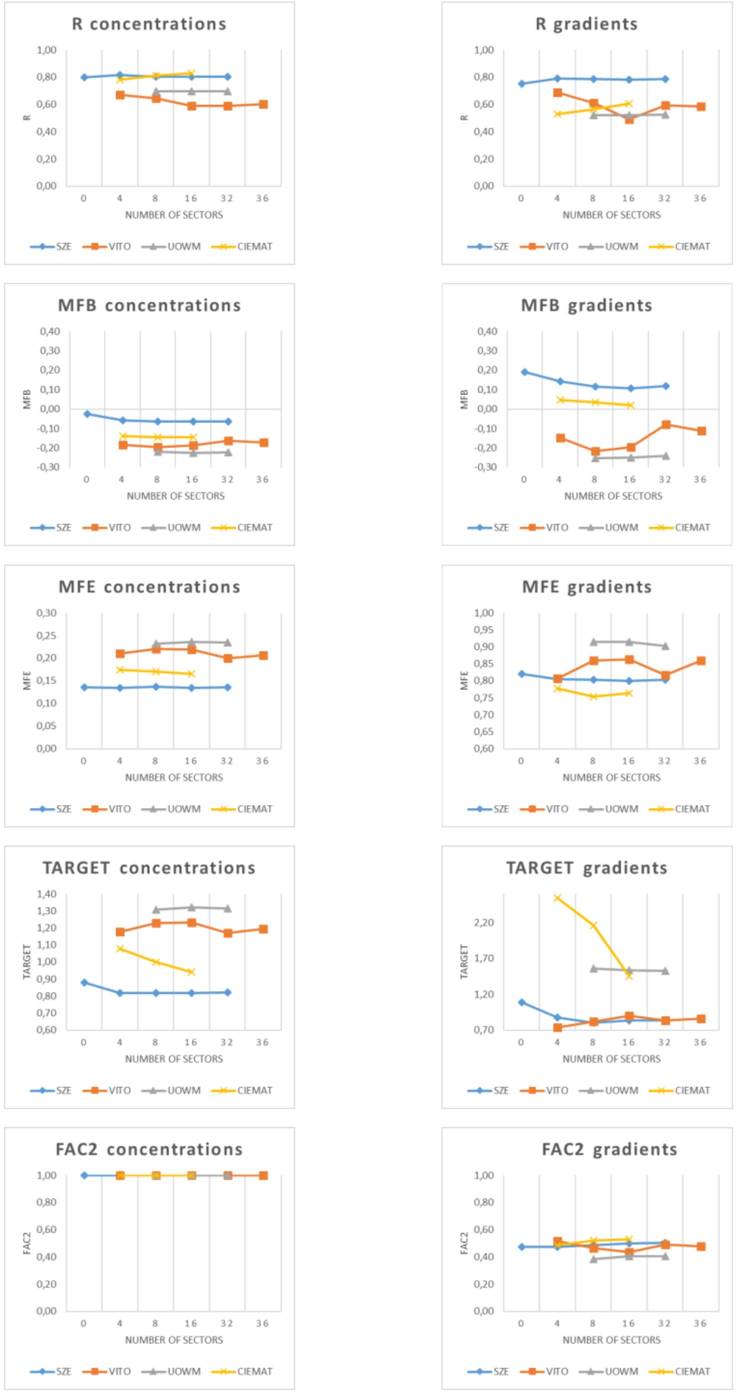
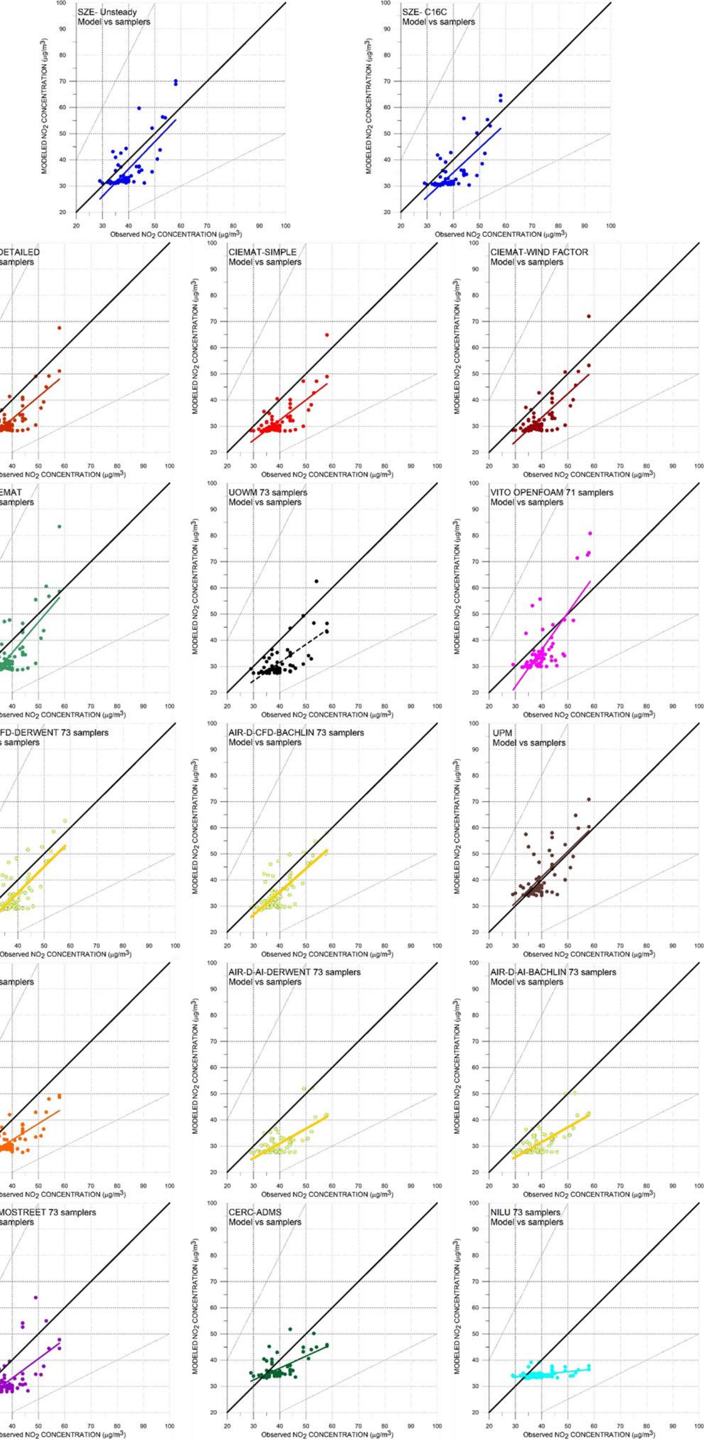
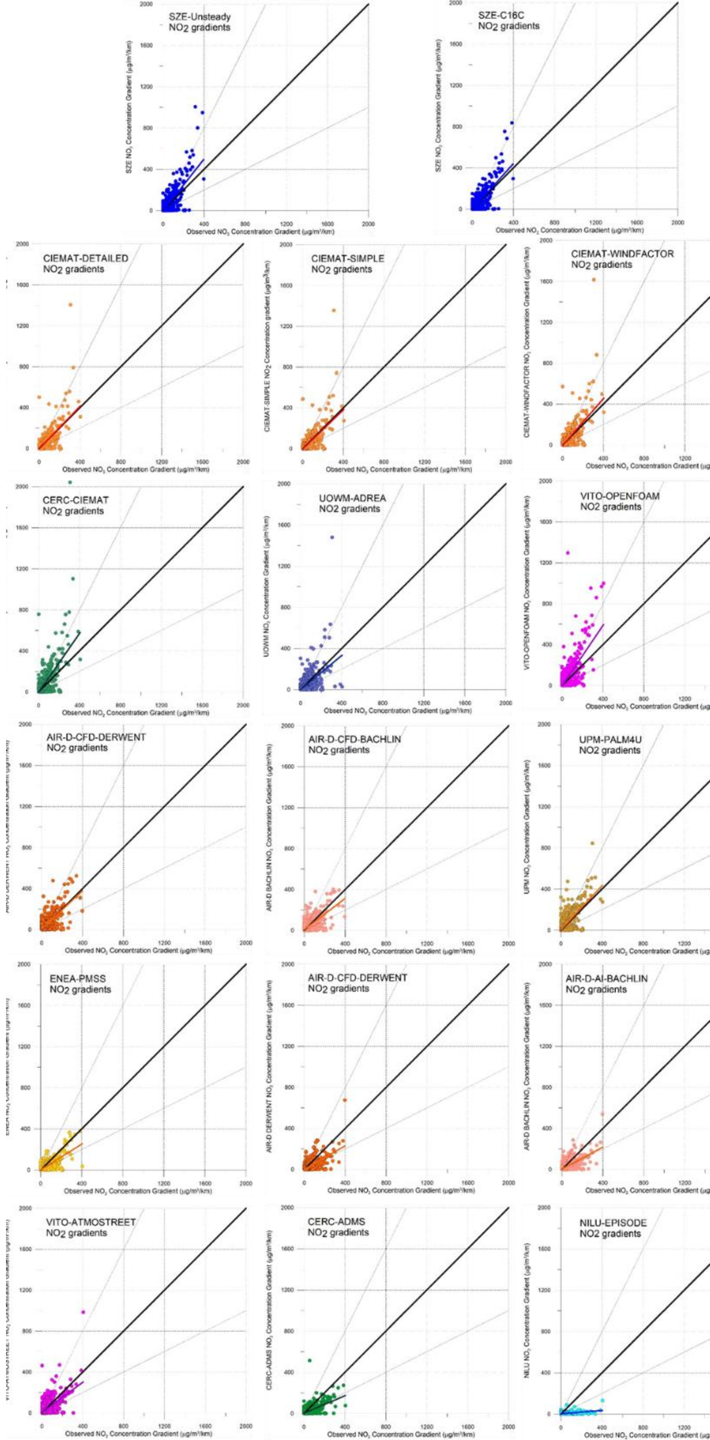



*Figure 16. Statistical results of R, MFB, MFE, TARGET and FAC2 for the model predictions of average $NO_2$ concentrations (left) and gradients (right) at the passive sampler locations for the experimental campaign (April 30th-May 28th, 2016) for the SZE, VITO, UOWM and CIEMAT simulations for different number of wind direction sector scenarios and for the long-term unsteady simulations (labelled as 0 scenarios).*




# Which figures can be moved to supplementary material section: scatter plots…?



# Conclusions

- The CFD models, and to some extent the Lagrangian and AI models, are able to simulate the spatial variation of pollutant concentrations both along and across street canyons. Where the Gaussian models, which account for street canyons, strong across road variations are modelled, but along-road variability associated with changes in building density **are not well simulated/** accounted for at a relatively coarse resolution.
- The consequence of including more detailed NO2/NOx chemistry is that the background concentrations are better estimated, e.g., CERC-ADMS and UPM have low MFB, MFE and TARGET for NO2 magnitude (as opposed to gradient) because they have a better approach to modelling chemistry. **Additionally, the AI model results seem to have little sensitivity to the NO2/NOx parameterizations used in this study.**

# Title

| TITLE | CIEMAT | UA | VITO | JRC | SZE | CERC | ENEA | AIR-D | UPM | NILU | Kees | Total |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | | | | | | | | | | X | | 1 |
| 2 | | | | | | | | | | X | | 1 |
| 3 | | | | | | | | | | X | | 1 |
| 4 | X | | | | x | | x | | | | | 3 |
| 5 | X | | x | | x | | x | | X | X | | 6 |
| **6** | **X** | **X** | **x** | | **x** | **x** | **x** | | **X** | | | **7** |

1. How to compute long-term average air pollutant concentration map in urban hot spots using dispersion models?
2. How good are the modelling applications for computing long-term average air concentration pollutant map in urban hot spots?
3. Intercomparison exercise of modelling applications for computing long-term average air pollutant concentration map in urban hot spots.
4. The FAIRMODE WG4: An intercomparison Exercise of Urban Microscale Models and Methodologies for deriving long-term average pollutant concentrations distribution with very high spatial resolution
5. How to compute long-term average air pollutant concentration map in urban hot spots using dispersion models? An intercomparison exercise for a case study in Antwerp
6. **Using microscale models to assess long-term air pollution and air quality standards in urban hot spots: A FAIRMODE joint Intercomparison exercise for a case study in Antwerp**

# Journal

| TITLE | CIEMAT | UA | VITO | JRC | SZE | CERC | ENEA | AIR-D | UPM | NILU | Kees | Total |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| STOTEN | | X | | | X | | | | X | | | 3 |
| APR | | | | | | | | | | | | |
| ATMOSPHERE | | | | | | | | | | | | |
| ACP | | X | | | X | | | | | | | 2 |
| Atmospheric Environment | | X | | | X | | | | | | | 2 |
| AIRQ | | | | | | | | | | | | |
| OTHER (please, add a row) | | | | | | | | | | | | |
| ALL GOOD | | | | | | x | X | | | | | 2 |