WG4 MICROSCALE MODELING

Vera Rodrigues (UA), Fernando Martin (CIEMAT)

FAIRMODE Technical Meeting.

Athens, October 4th, 2023

WG4 activities: Context and aims

1. WG4 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. 10 groups:

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

2020 - 2023 activities

1. CT4 Microscale Modeling was endorsed in FAIRMODE Plenary Meeting, Berlin, Feb 2020.
2. Design and preparation of an Intercomparison Exercise, second half 2020,
3. Modelling simulations during 2021
4. Processing of results mainly during 2022
5. **New contributions and new participants 2023**
6. **New evaluation for other air quality indicators 2023**

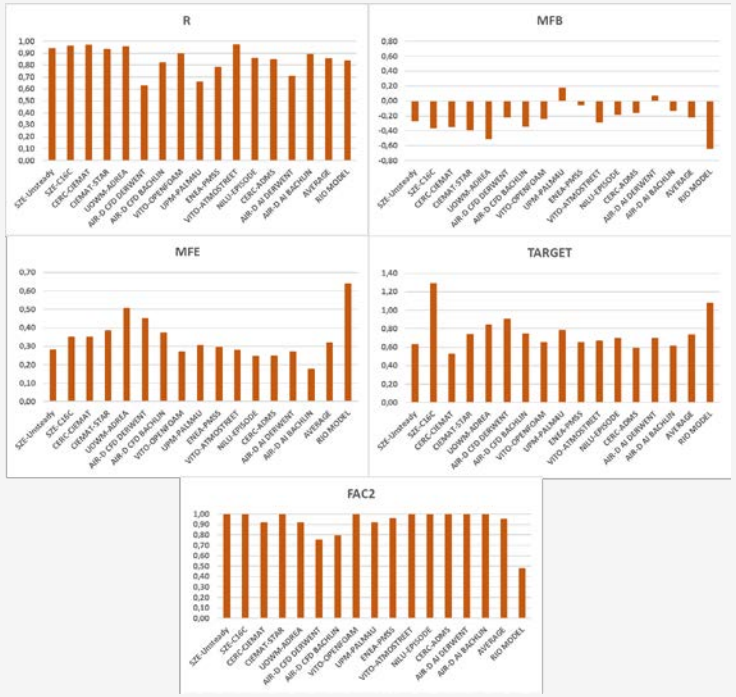
WG4 session – agenda

INERIS/LCSQA urban modeling intercomparison exercise.	F. Tognet (INERIS)	10’
Last findings of Intercomparison Exercise - Antwerp Case - First paper	V. Rodrigues (U. Aveiro)	45’
Intercomparison of spatial representativeness/ exceedances areas - Antwerp Case	F. Martín (CIEMAT)	20’
Future Recommendations/Guidance Document	F. Martín (CIEMAT)	15’
Chemistry impact – how important is this topic at microscale?	V. Rodrigues (U. Aveiro)	15’
Setup a new intercomparison exercise at a new location (e.g., Gyor)	F. Martín (CIEMAT)	15’

Last findings of Intercomparison Exercise - Antwerp Case - First paper

Last findings of Intercomparison Exercise - Antwerp Case

- **Traffic station**
- *Statistical results of R, MFB, MFE, TARGET and FAC2 for the model predictions of hourly NO_2 concentrations for the traffic station.*
- **Use these bar plots grouping results by model types including range of data instead of the individual results plots with all models?**



Last findings of Intercomparison Exercise - Antwerp Case

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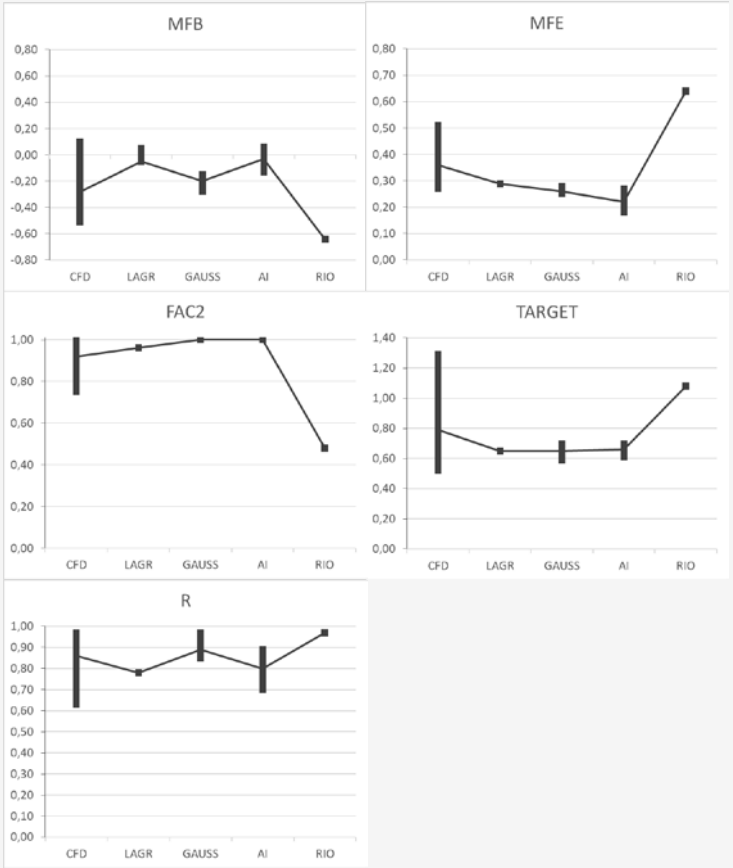

Last findings of Intercomparison Exercise - Antwerp Case

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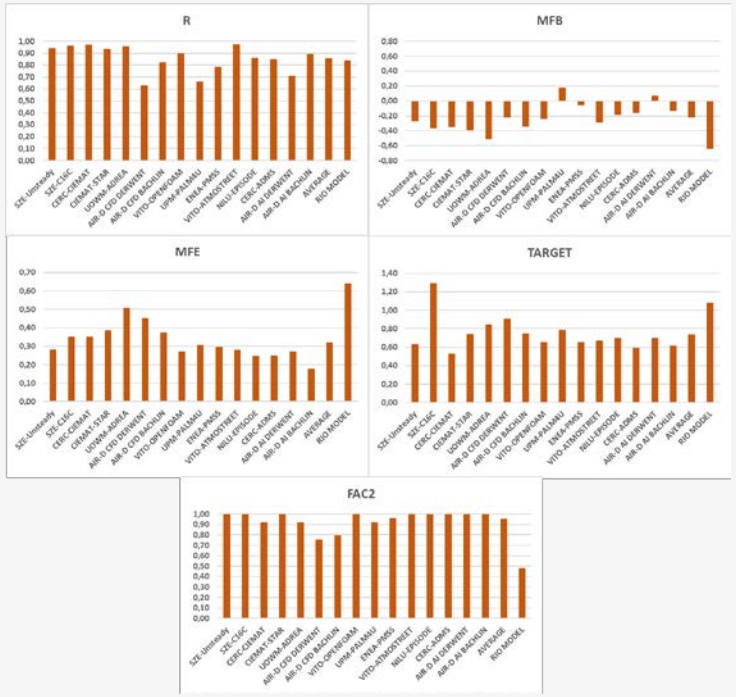

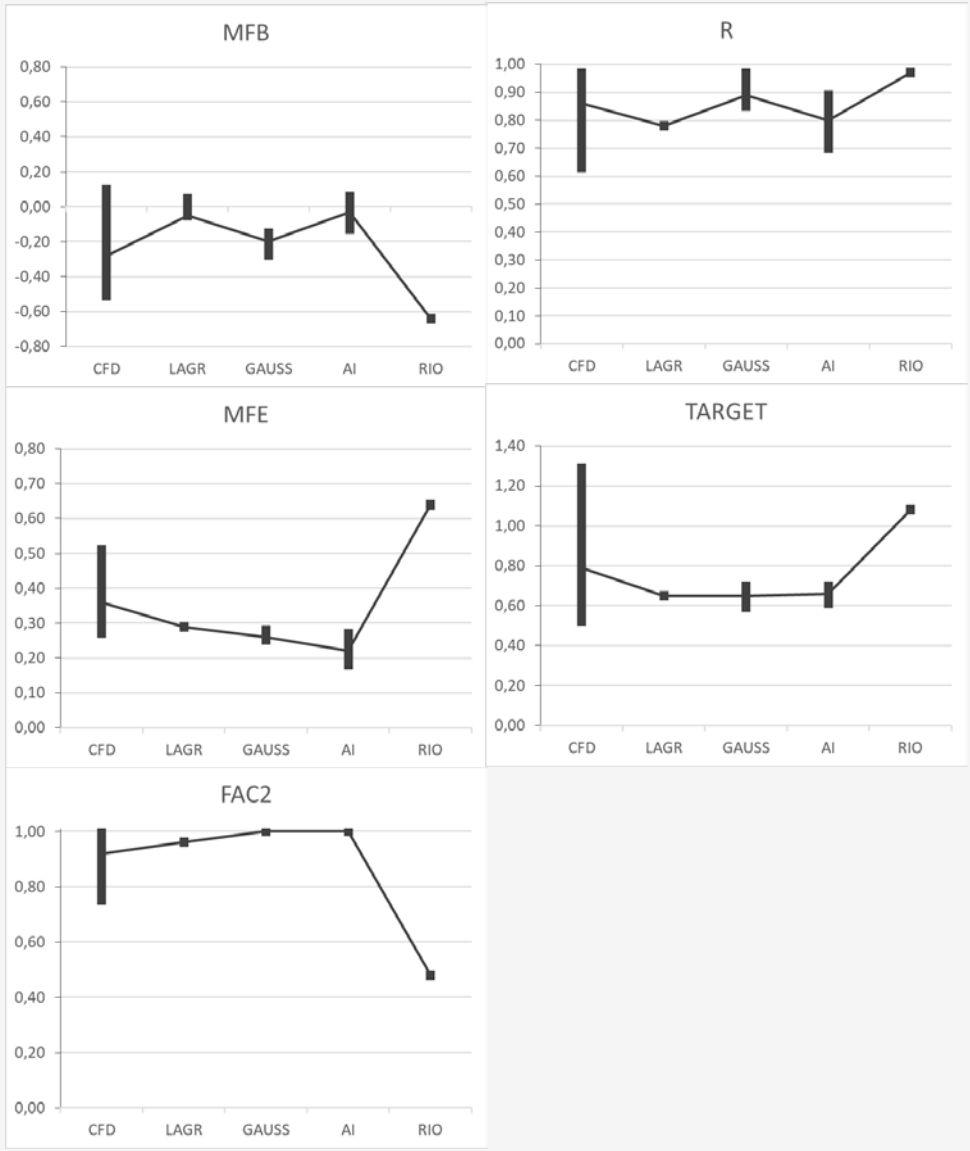

Last findings of Intercomparison Exercise - Antwerp Case

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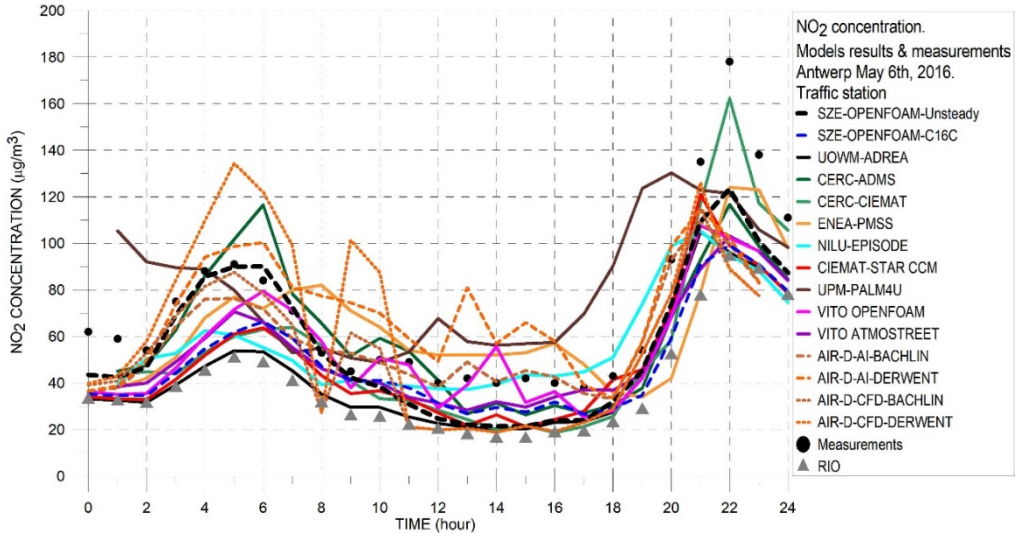
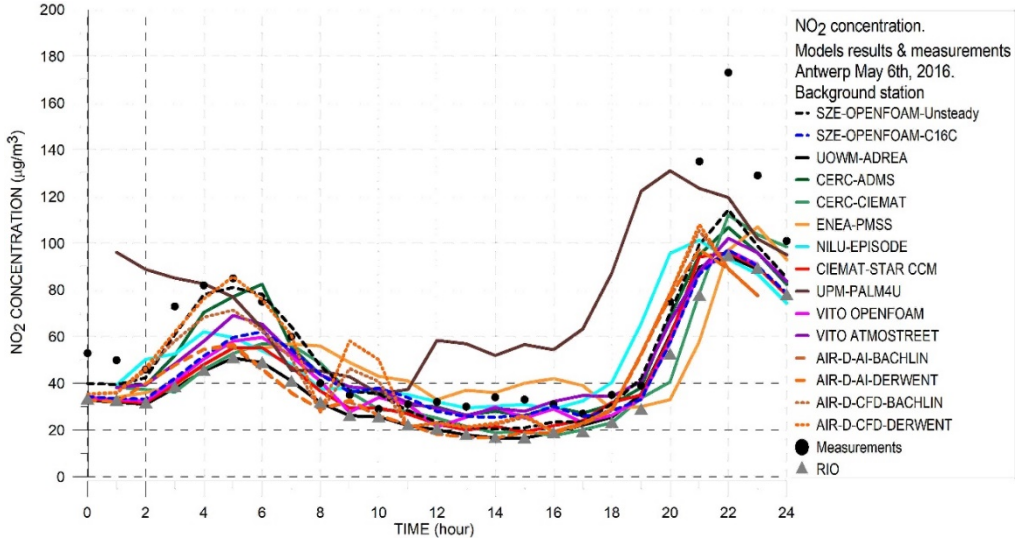
- **Main conclusions: RIO model is able to simulate the time series of the background station in a good agreement**

Last findings of Intercomparison Exercise - Antwerp Case

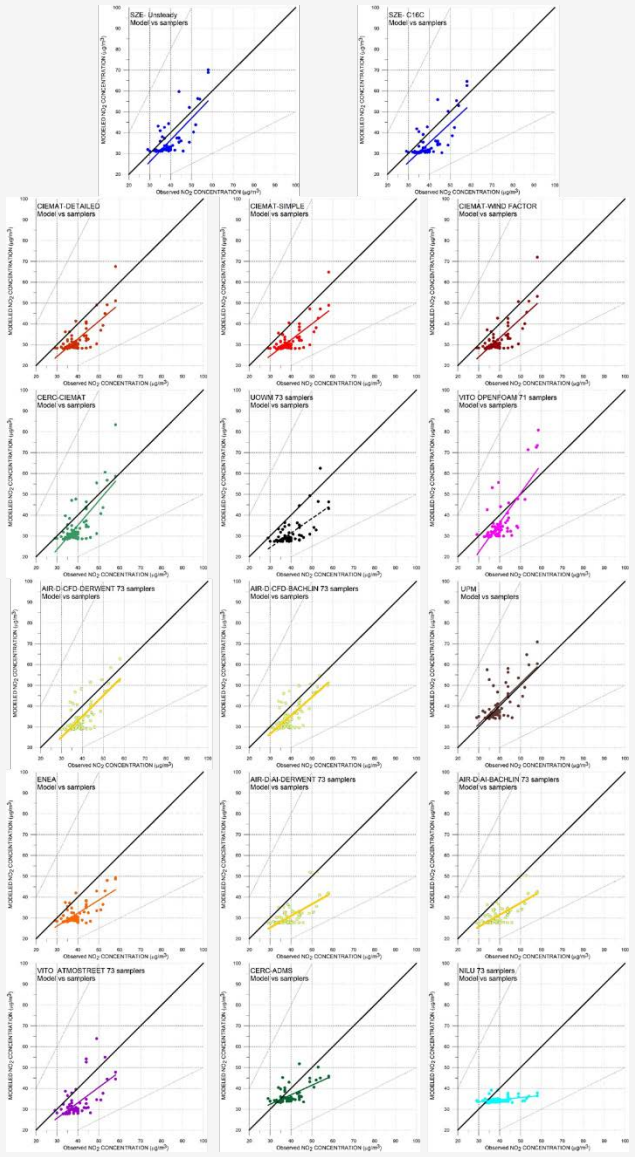
- Time series of model predictions of hourly NO_2 concentrations and observations for the traffic station
- Does the night-time peak directly correspond to traffic peak, or its more stagnation conditions / boundary layer collapsing that is causing the peak?



Traffic station

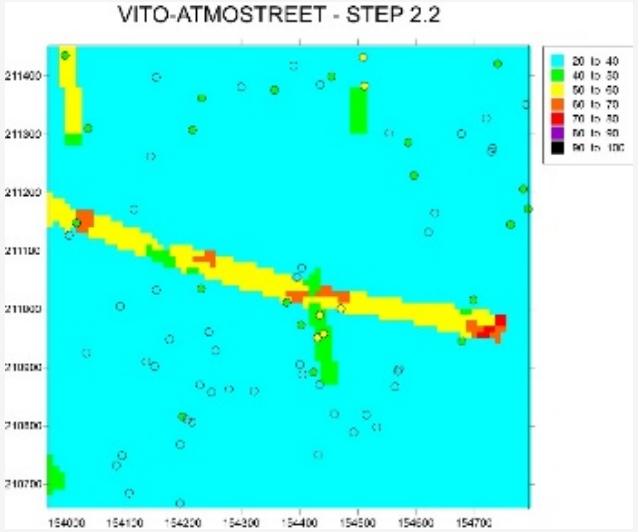


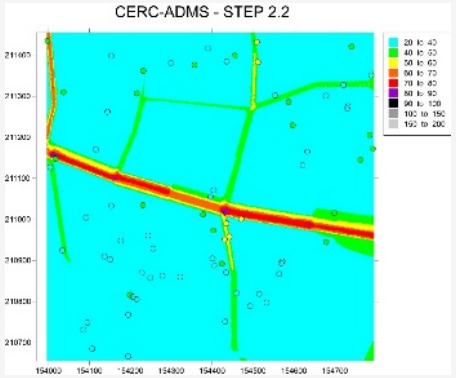
Background station

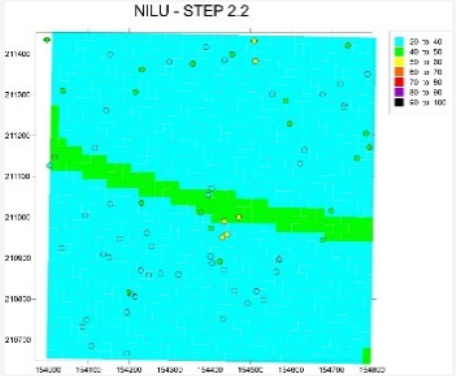


Last findings of Intercomparison Exercise - Antwerp Case

- **Monthly average data of NO_2 concentrations recorded by passive samplers**
- *Scatter plots of methodology predictions versus measurements of averaged NO_2 concentration for the 73 passive samplers deployed in the domain and for all the models/methodologies*





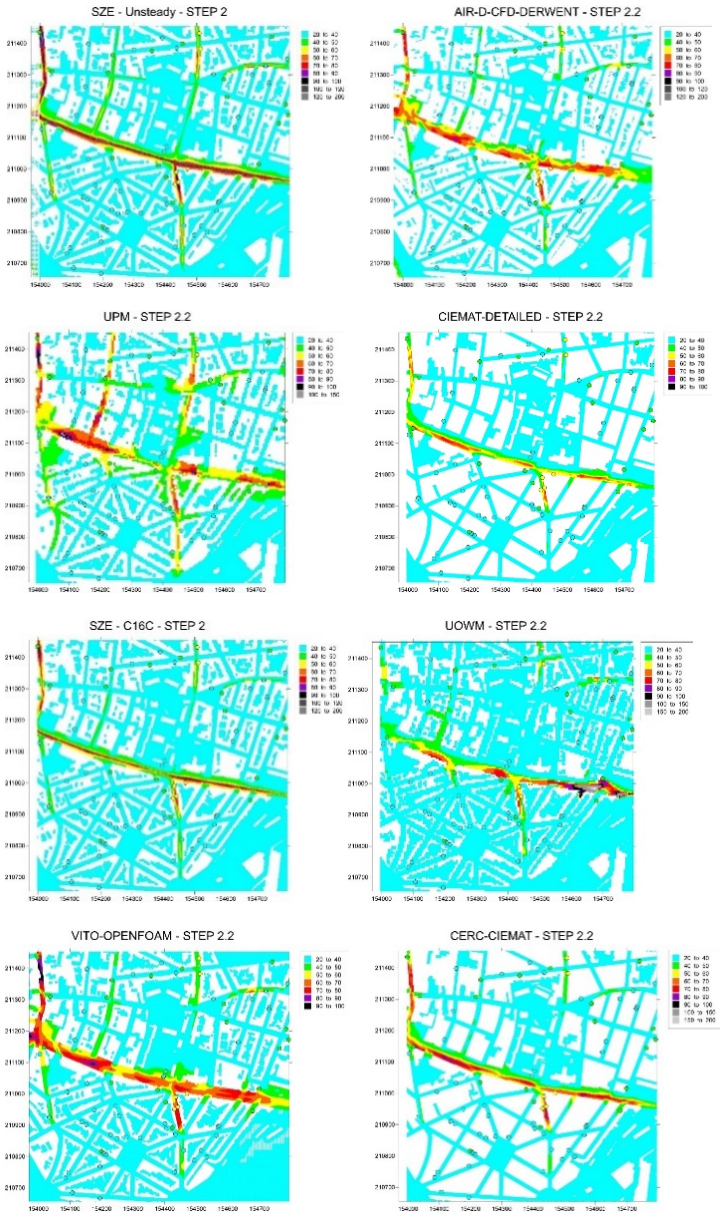


Last findings of Intercomparison Exercise - Antwerp Case

- *Maps of the monthly average NO_2 concentration for the Gaussian models and concentration measured by passive samplers (colored dots)*

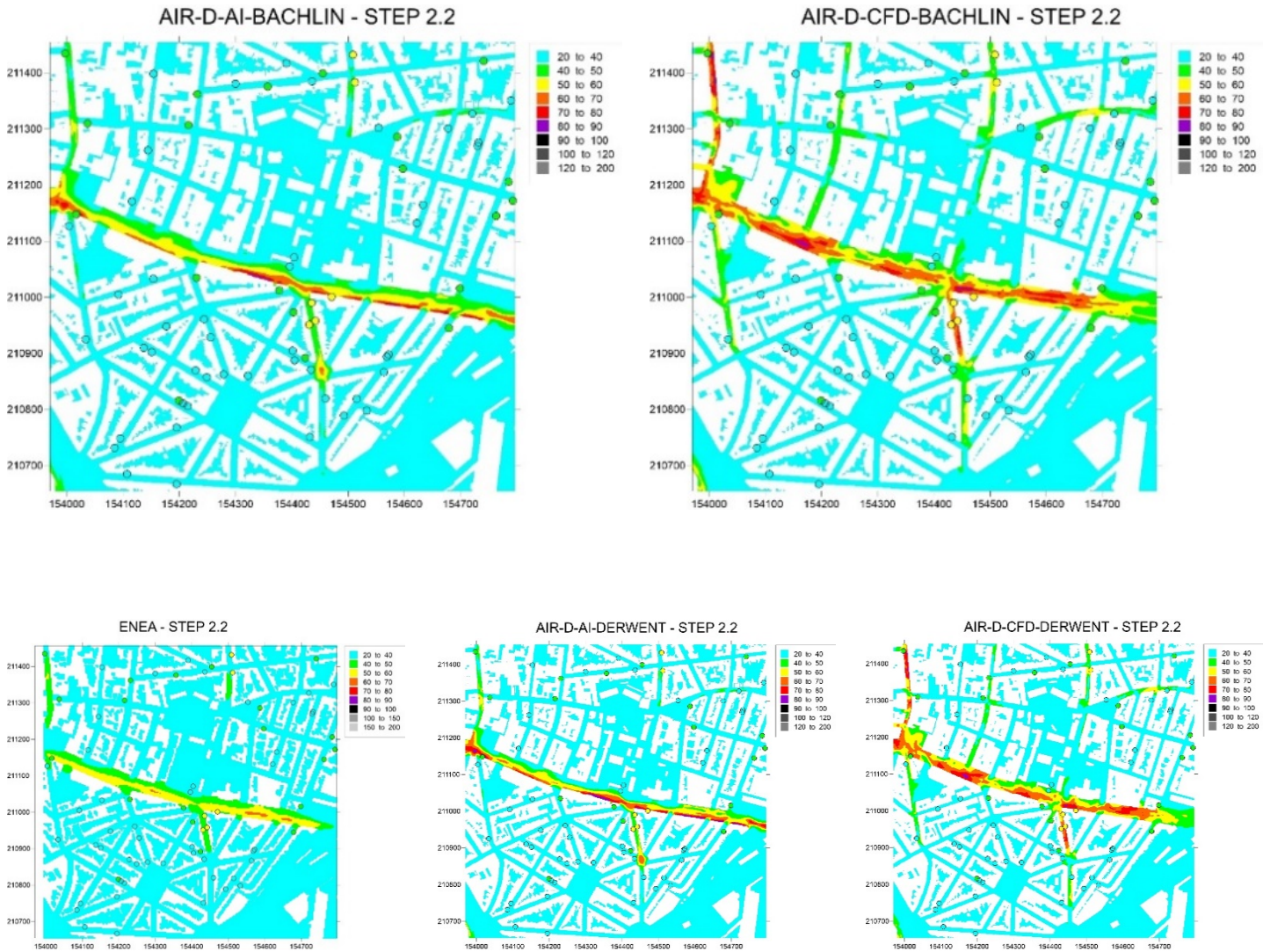
Last findings of Intercomparison Exercise - Antwerp Case

•*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)*



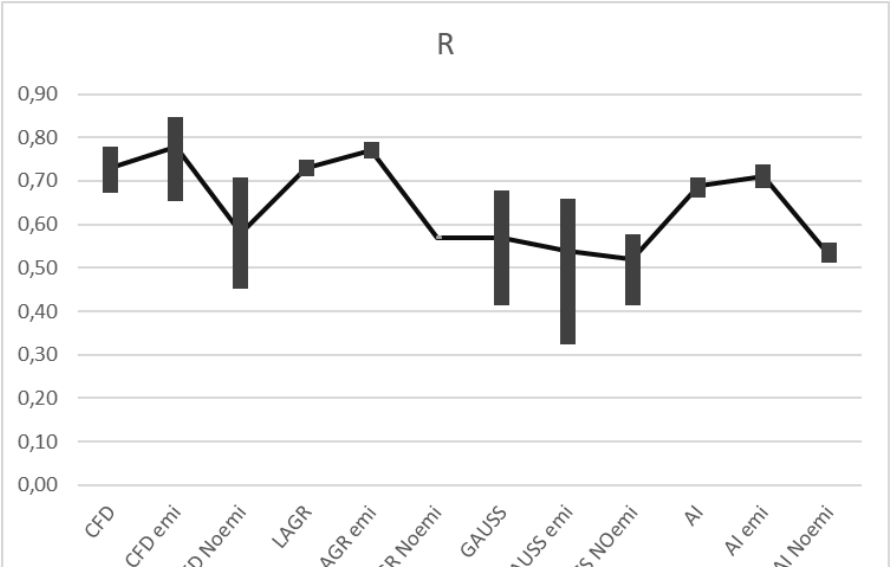
Last findings of Intercomparison Exercise - Antwerp Case

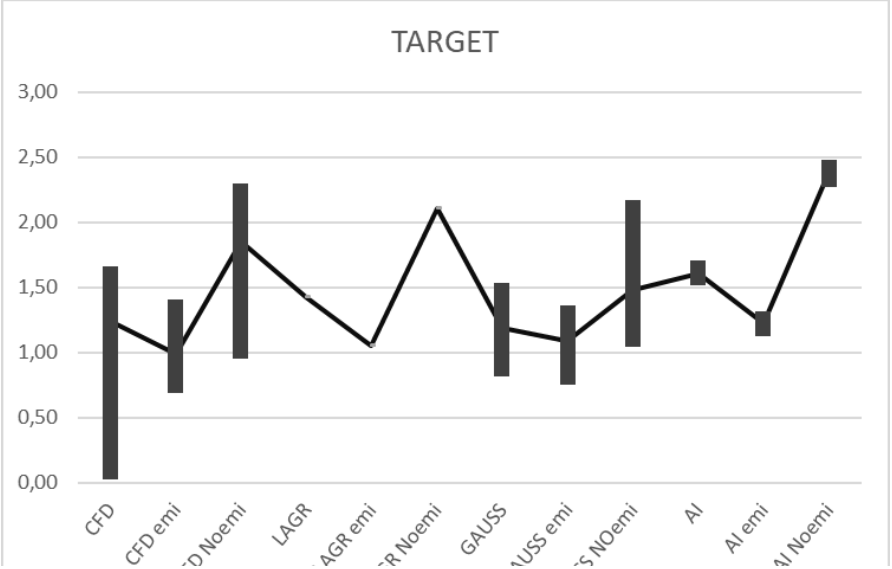
- Map of the monthly average NO_2 concentration for the ENEA-PMSS + AIR-D-CFD (upper) and AIR-D-AI (lower) for the Derwent (left) and Bachlin (right) parametrizations accounting for the NO_2/NOx ratios and concentration measured by passive samplers (colored dots)



Last findings of Intercomparison Exercise - Antwerp Case

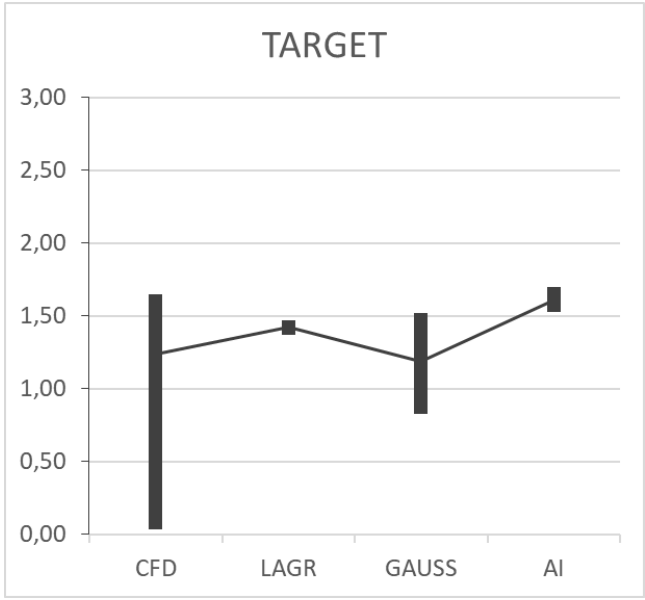
- **Discussion**
- **What is the impact of the emissions data?**

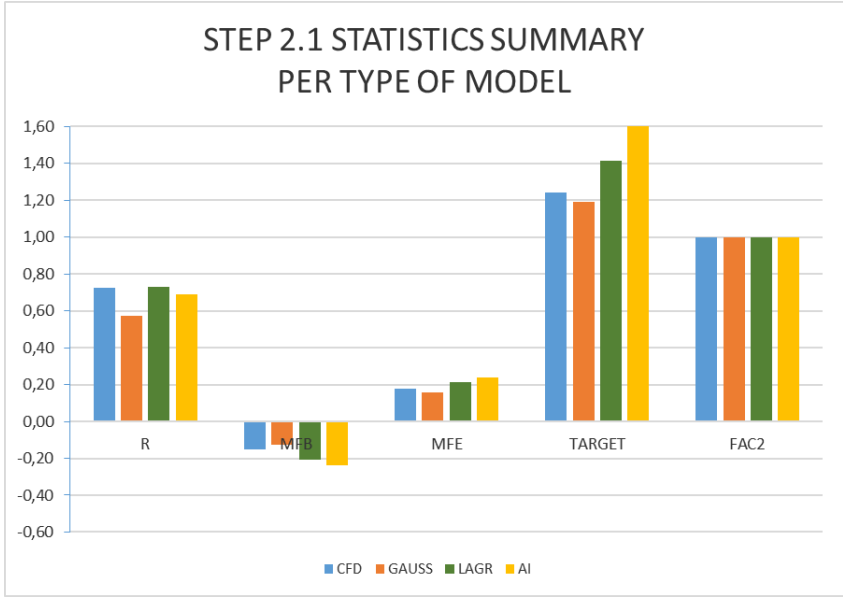




Last findings of Intercomparison Exercise - Antwerp Case

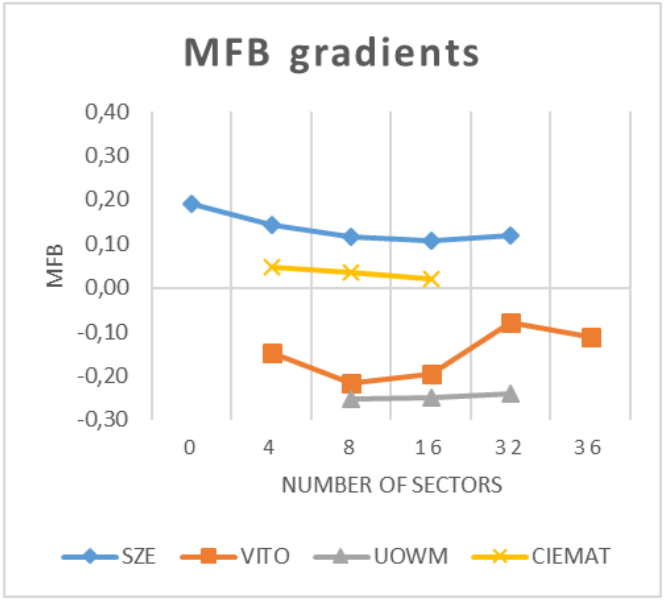
- **Discussion**
- **What type of methodologies are more suitable to reproduce spatial distribution of long-term averaged NO_2 concentrations?**

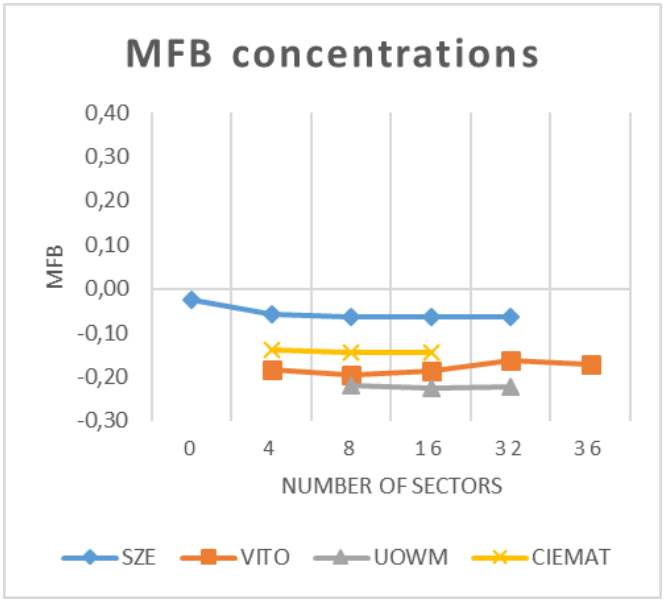




Last findings of Intercomparison Exercise - Antwerp Case

- **Discussion**
- **Long term simulations versus methodologies based on a limited number of scenarios**





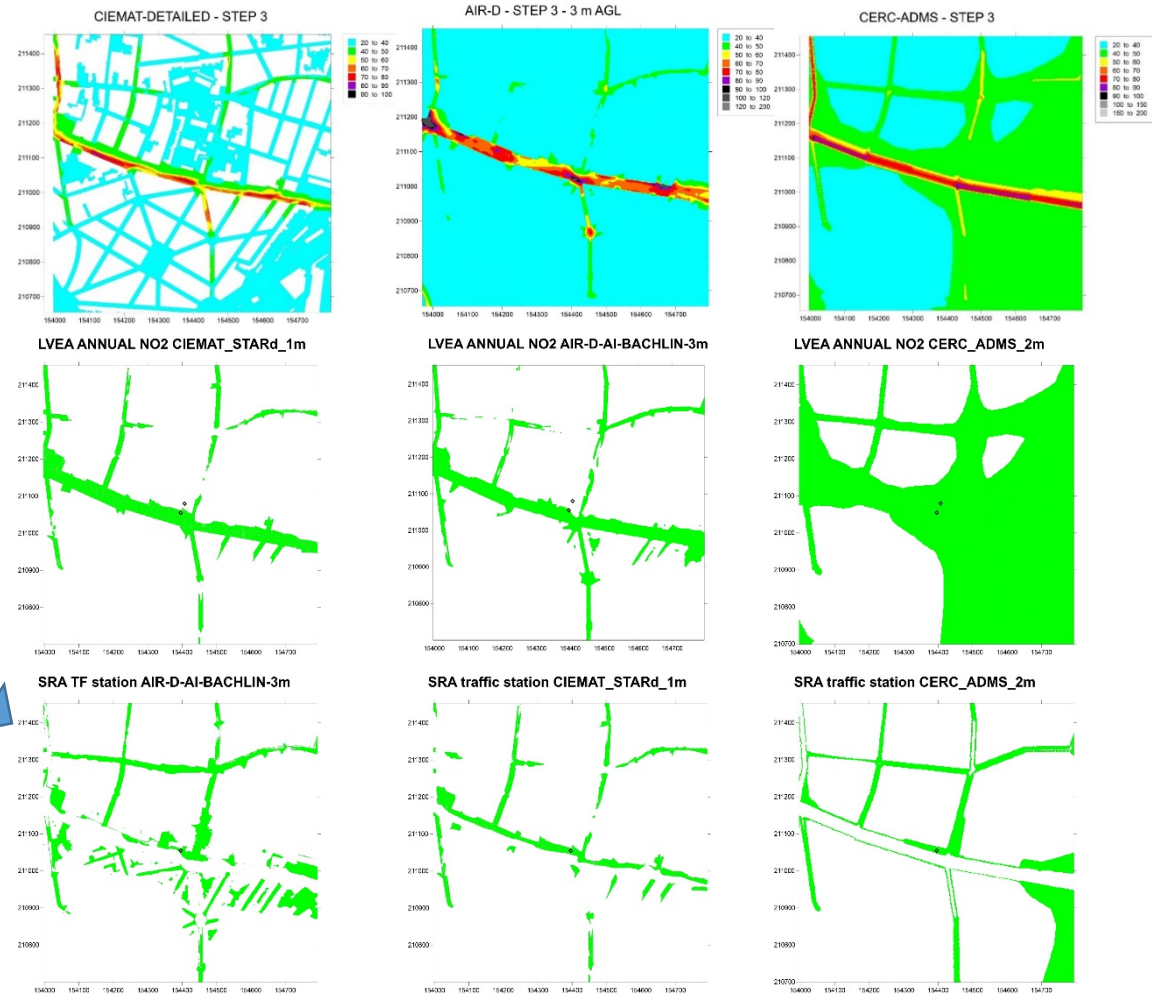
Last findings of Intercomparison Exercise - Antwerp Case

- **Timeline**
  - **Hackathon (paper) – last week October/ 1st week November**
  - **Attempt submission date: late-November 2023**

Intercomparison of spatial representativeness/ exceedances areas - Antwerp Case

Intercomparison of spatial representativeness/exceedances areas

- Using the results of annual average of NO_2 computed by the different models/methodologies for Antwerp domain.
- Intercomparison of:
  - NO_2 anual limit value (40 µg/m^3) exceedance areas (LVEA) in the Antwerp district domain.
  - Spatial representativeness areas (SRA) of the two air quality stations
- Two key questions:
  - How different are the LV exceedance areas?
  - How different are the spatial representativeness areas?
- Discussion about areas computed leaving out the area covered by buildings



Intercomparison of exceedances areas (LVEA)

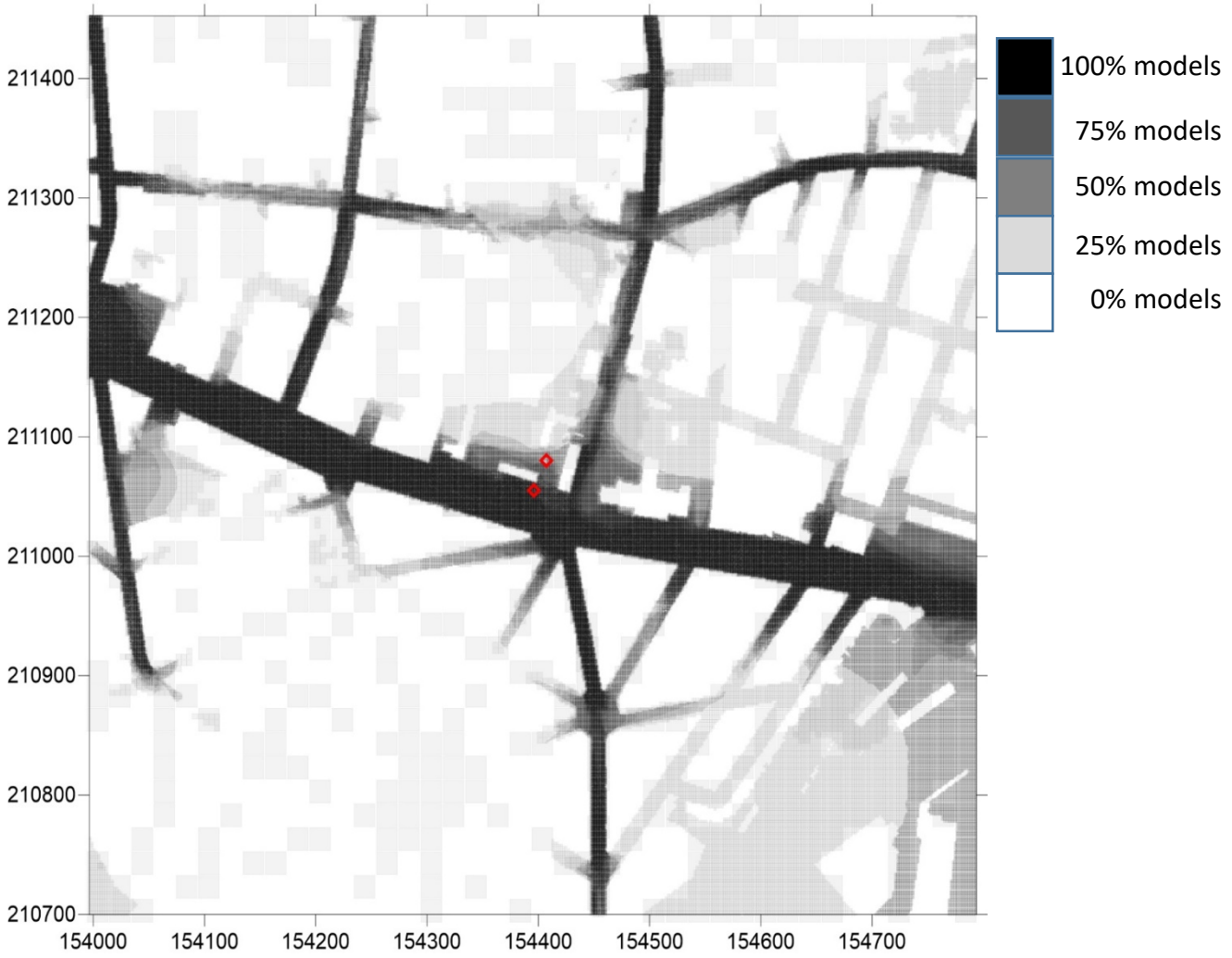
20 models/methodologies

5 Gaussian

12 CFD

1 Lagrangian

2 Artificial Intelligence



Intercomparison of exceedances areas (LVEA)

LVEA according to type of models

20 models/methodologies

5 Gaussian

12 CFD

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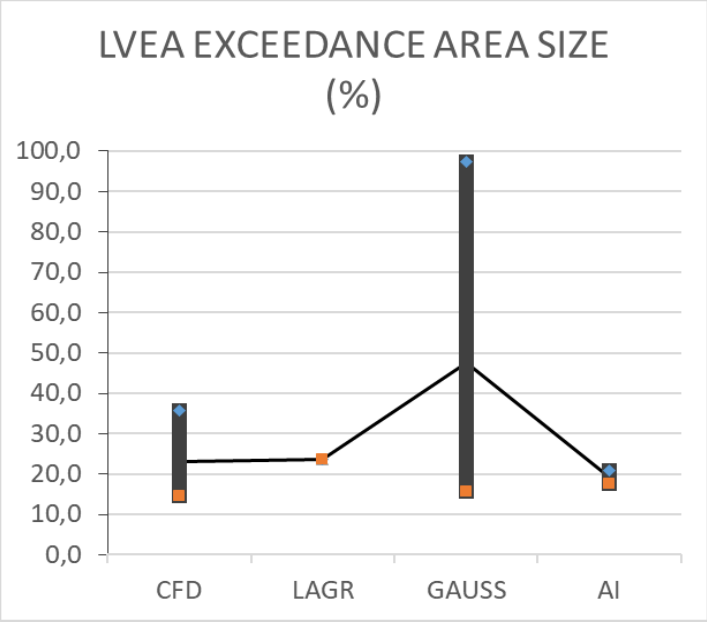
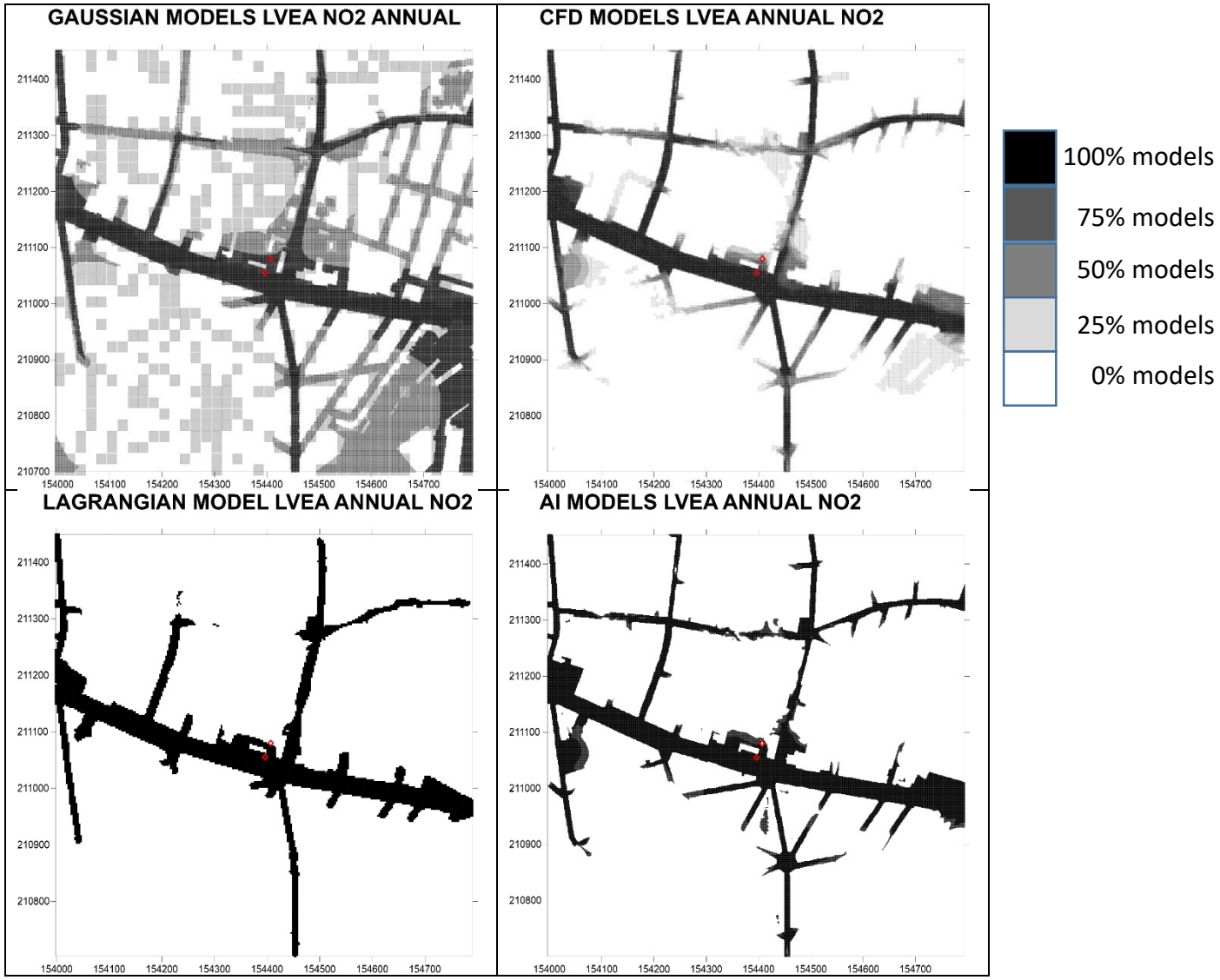




Intercomparison of exceedances areas (LVEA)

LVEA according to resolution

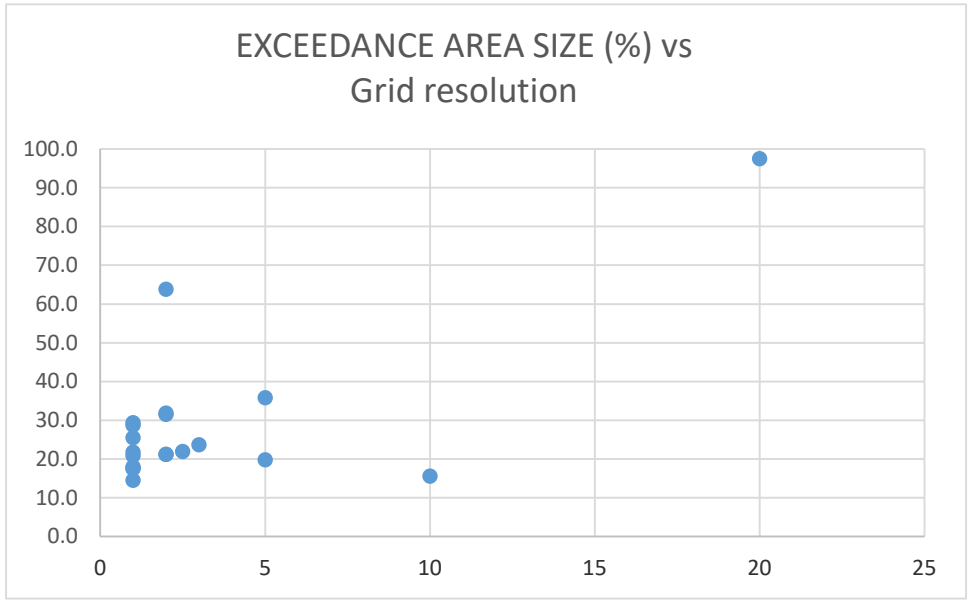
20 models/methodologies

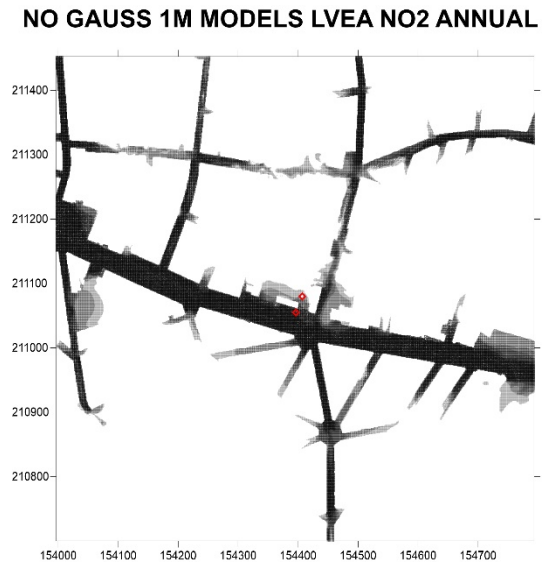
5 Gaussian

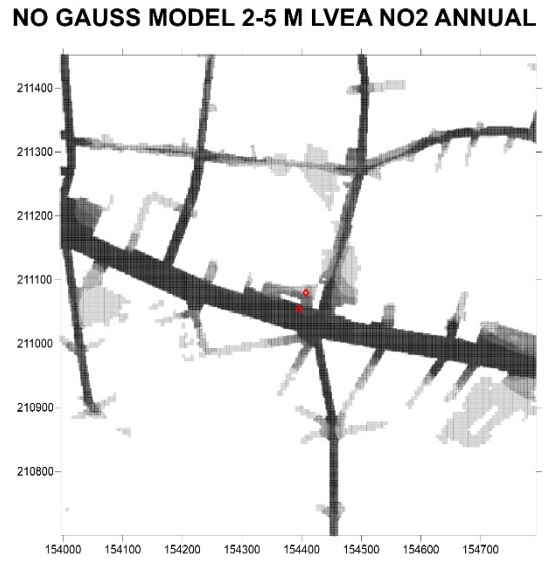
12 CFD

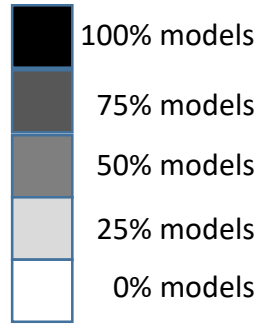
1 Lagrangian

2 Artificial Intelligence









Some comments about LV exceedance areas (LVEA)

- All models coincide, exceeding VL on main streets, but there are differences in shape and size of LVEA.
- Larger LVEA for most of Gaussian models, but strong variability (highest for EPISODE).
- Size and shape of LVEA for CFD, Lagrangian and AI models is rather similar, but some variability for CFD (highest for PALM4U and then for OPEN FOAM unsteady full-year simulation from SZE).
- LVEA size seems to not depend on grid resolution.
- Some “little” differences when using same CFD model but different methodologies for retrieving long-term average concentrations. Need for further analysis.
- Some “little” differences when using same CFD model & methodology but different number of scenarios. Need for further analysis.
- Could be good to compute LVEA using normalized concentrations maps (using data from AQ station)?

Intercomparison of spatial representativeness areas (SRA)

20 models/methodologies

5 Gaussian

12 CFD

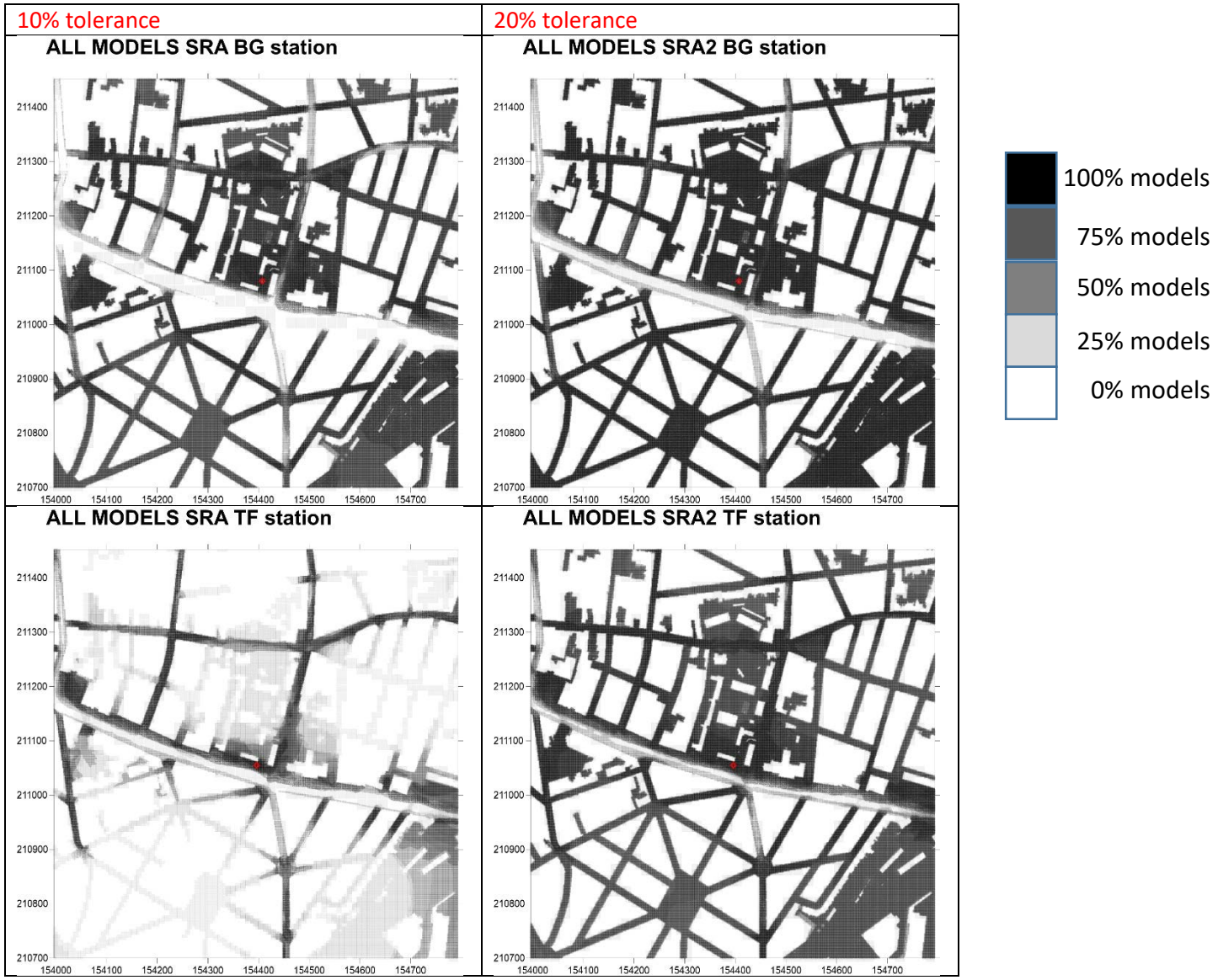
1 Lagrangian

2 Artificial Intelligence

Two tolerances:

10% SRA

20% SRA2



Intercomparison of spatial representativeness areas (SRA)

SRA according to type of models

20 models/methodologies

5 Gaussian

12 CFD

1 Lagrangian

2 Artificial Intelligence

Two tolerances:

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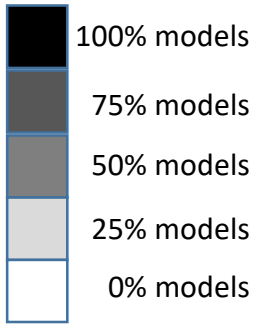
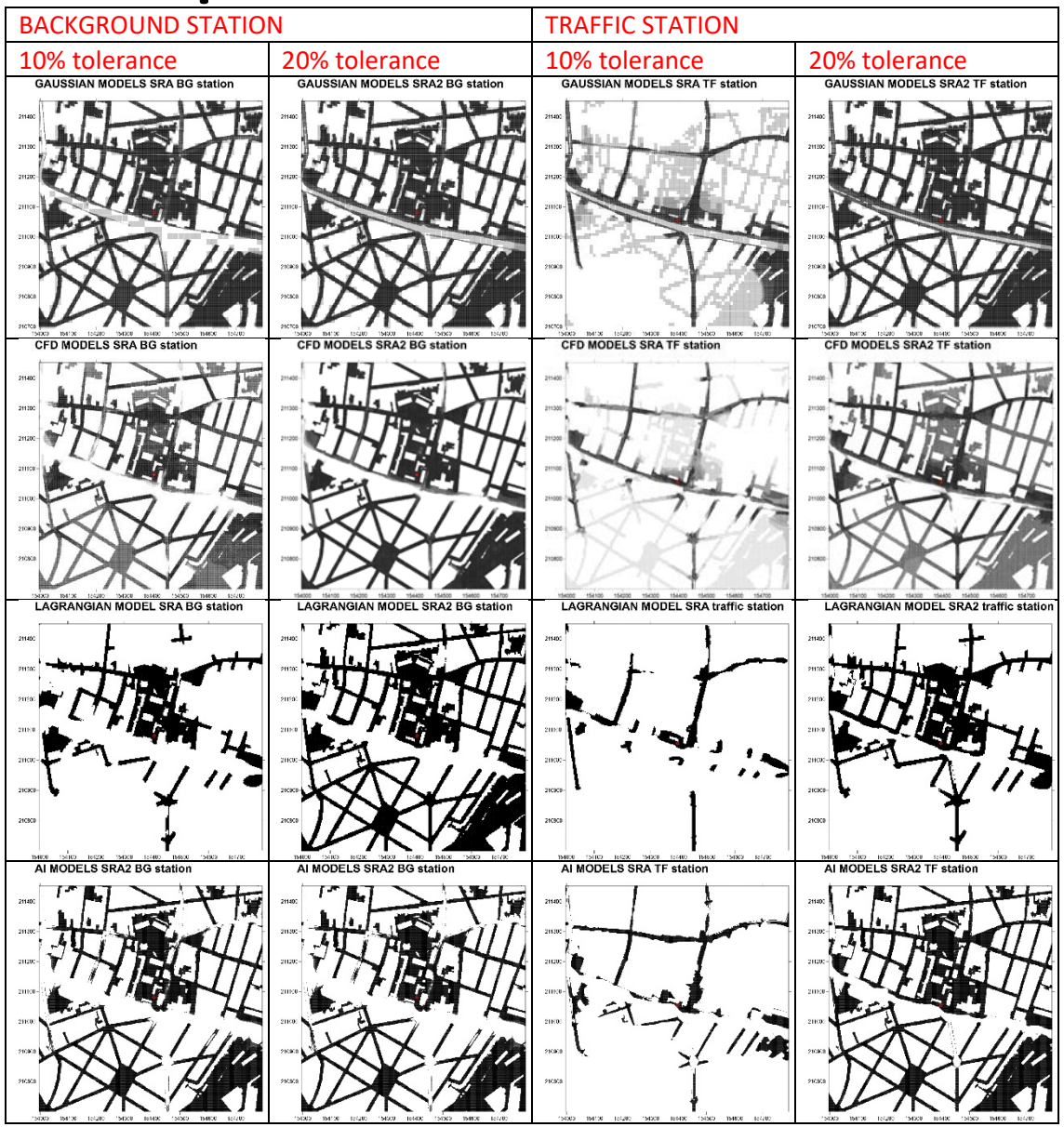
20% SRA2





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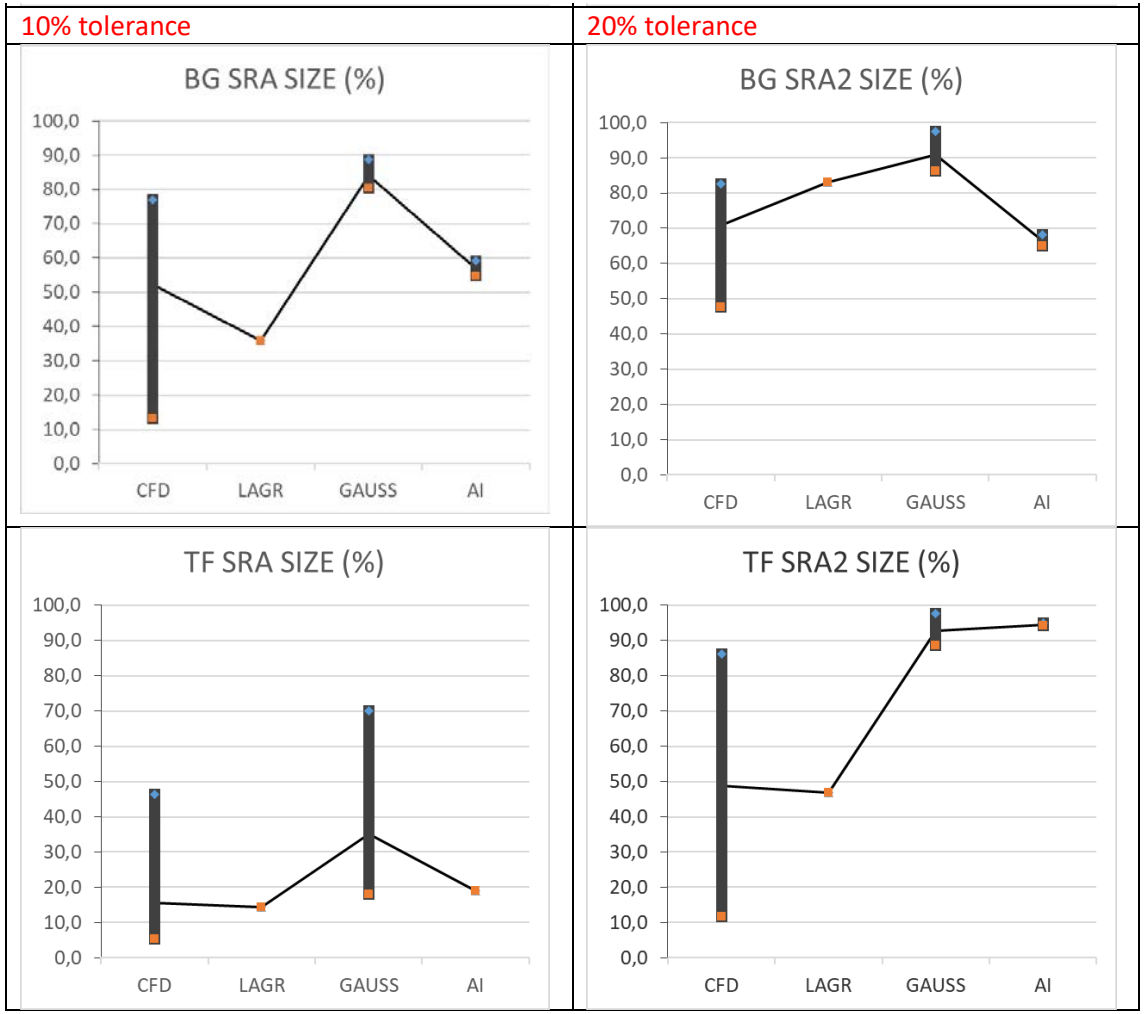

Intercomparison of spatial representativeness areas (SRA)

SRA according to resolution

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5 Gaussian

12 CFD

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2 Artificial Intelligence

Two tolerances:

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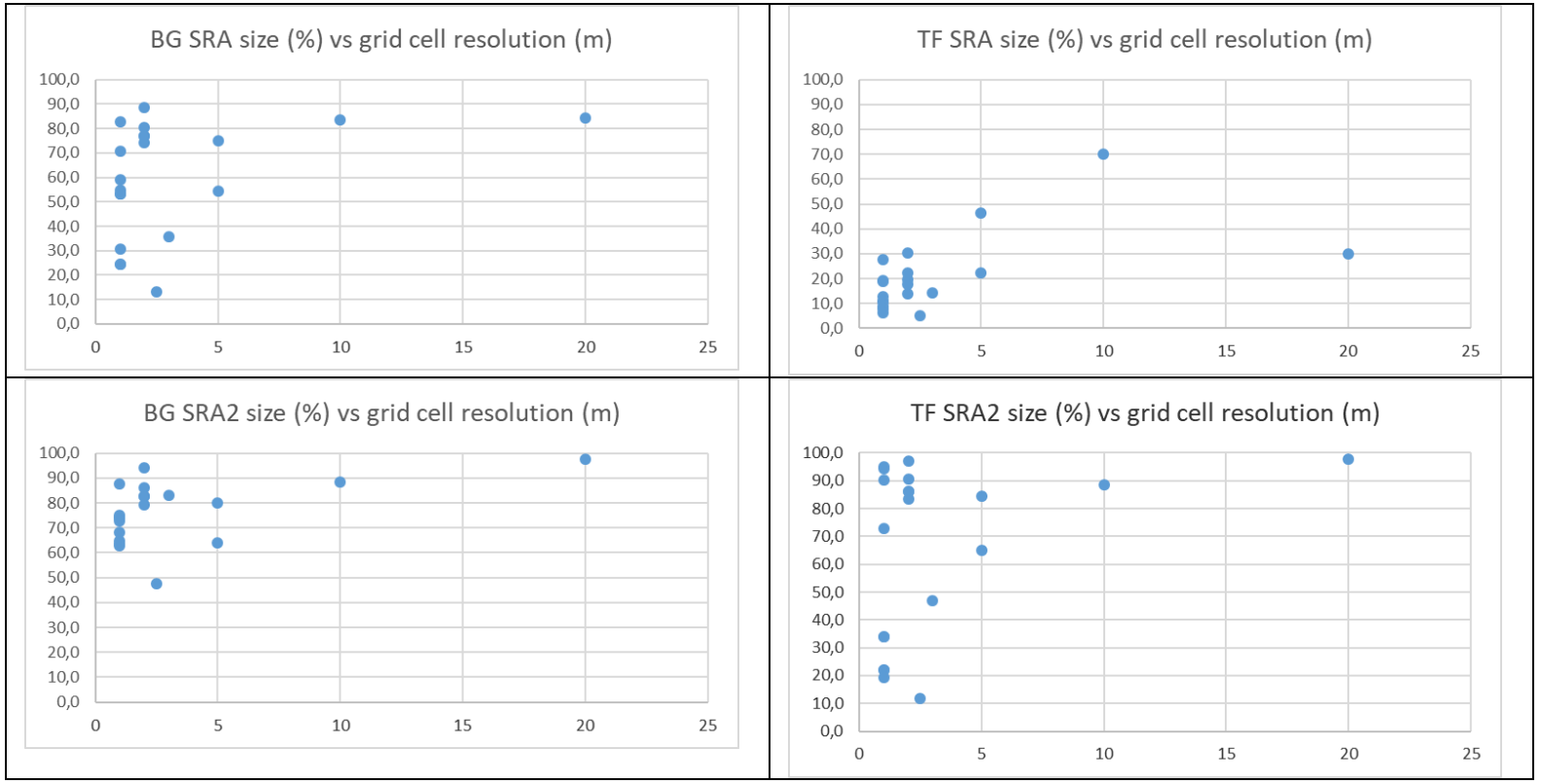
20% SRA2



Intercomparison of spatial representativeness areas (SRA)

SRA according to concentration at station grid cell

20 models/methodologies

5 Gaussian

12 CFD

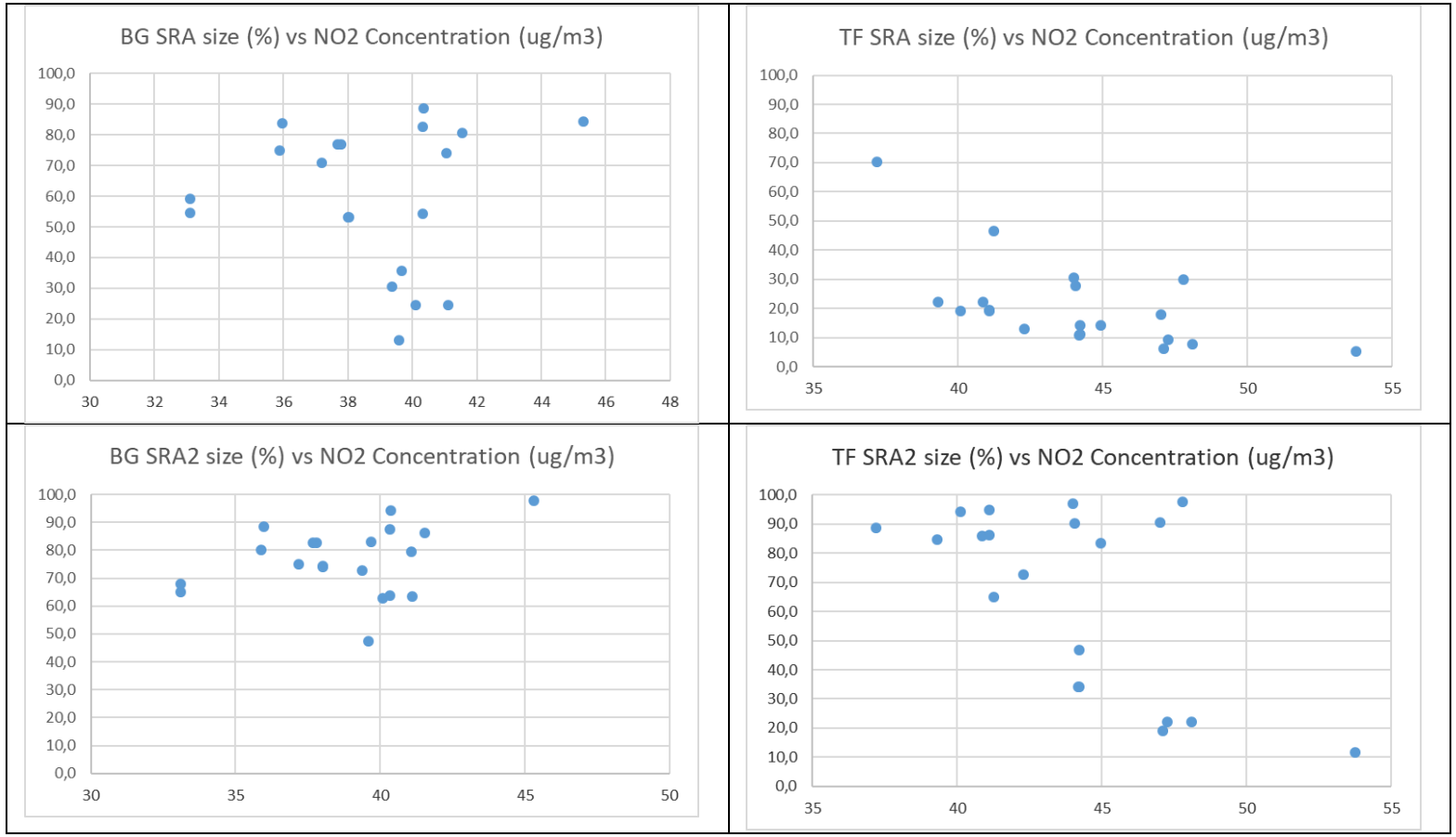
1 Lagrangian

2 Artificial Intelligence

Two tolerances:

10% SRA

20% SRA2



Some comments about SRA

- SRA are larger for the background station than for the traffic one.
- 20% tolerance provides much larger SRA (SRA2) than when using 10% tolerance (SRA). The highest increases for the traffic station. Is 20% tolerance too high for computing SRA for traffic stations?
- Larger SRA (10% tolerance) and SRA2 (20% tolerance) for most of Gaussian models, but strong variability (highest for EPISODE).
- Large variability of SRA and SRA2 computed with CFD models specially for the traffic station.
- Large variability of SRA computed with Gaussian models for the traffic station, not for background station or 20% tolerance.
- Except for one (EPISODE) of the Gaussian models, the estimated SRAs of both stations do not include most part of the main street (inside the LVEA).
- It seems low grid resolution used to provide larger SRA, but high grid resolution can give large and small SRA.
- Both SRA and SRA2 for the traffic station seem to depend on the concentration at station grid cell
- More analysis is needed for SRA and SRA2 depending on methodologies and the number of scenarios used with CFD models and comparison with OPEN FOAM unsteady full-year simulation from SZE). Now we have more results with different number of scenarios for different methodologies (CIEMAT, VITO, UOWM and SZE)!!

Intercomparison of spatial representativeness/exceedances areas

- Hints about the intercomparison of the estimated LV exceedance and spatial representativeness areas for an urban district.
  - How different are the LV exceedance areas?
  - Are there significant differences when using different types of models?
  - Dependency on model resolution?
  - Could be good to compute LVEA using normalized concentrations maps (using data from AQ station)?
- How different are the spatial representativeness areas?
  - Are there significant differences when using different types of models?
  - What tolerance should be suitable (10% or 20%)?
  - Dependency on model resolution?
  - Dependency on concentration at station grid cell?
- Very related to the WG8 activities.
- Need of a specific hackathon for discussing details (late October or early November?)

Future Recommendations/Guidance Document

Future Recommendations/Guidance Document

- There is a preliminar document elaborated last year.
- Most of **main conclusions** remain or have to be slight modified, but others are new:
  - Micro-scale models (taking into account buildings and street-canyon effects) are fit for AAQD-purpose
  - Spatial patterns and temporal profiles at micro scale can be simulated rather well
  - The RANS approach seems appropriate for CFD models in the context of the AAQD, but sensitive to Schmidt number (Sc)
  - Good emission data suited for the micro scale are crucial
  - Suitable validation data (high resolution in time and space!) is essential for proper model validation
    - Passive samplers are quite good spatial pattern (more dense network needed) but not for time profiles
  - Annual averages can be computed via a wind sector approach:
    - Some methodologies using a limited number of CFD simulated scenarios provide quite similar monthly NO_2 maps to those obtained with the long-term CFD unsteady simulation.
    - Simulation with only one reference wind speed could be sufficient to get good results (1/v scaling)
    - Little differences in the performance of scenario-based methodologies depending on the number of scenarios, but some methodologies give slightly better results when 8 or more wind direction sector scenarios are used. These results can strongly depend on the urban area under study, and hence, more studies in other type of urban areas are needed.
    - Annual means derived via the reconstruction of an hourly time series of concentration maps seems to give slightly better results.

Future Recommendations/Guidance Document

- Some **questions** were answered, by many **open questions/challenges** remain or new ones rise:
  - Do the needed number of wind sectors or the model/methodology results depend on urban morphology?
  - How to derive other AAQD indicators than the annual average (percentiles related with the limit values) in a wind sector approach?
  - Can the NO_X-O_3 chemistry be taken into account?
  - How many stations do we need for a proper validation at micro scale? Passive samplers? Sensors?
  - Is the atmospheric stability relevant or depends on the urban area? Not seems to be relevant based on studies of UOWM.
  - Are models/methodologies analysed suitable for computing LV exceedances areas and spatial representativeness? What models/methodologies are better?

Chemistry impact – how important is this topic at microscale?

Chemistry impact – how important is this topic at microscale?

What is the relevance of chemical reactions at this very local spatial scale?

What criteria should be considered when integrating time-scale with chemical reactions? How do we account for seasonal variability and its impact on the relevance of chemical reactions, as well as the application of scenario-driven methodologies?

We suggest organizing a hackathon to brainstorm the next steps for WG4's work. If we decide to shift to a different case study, it is important to remember the need to address this particular topic.

New intercomparison exercise at a new location

New intercomparison exercise at a new location

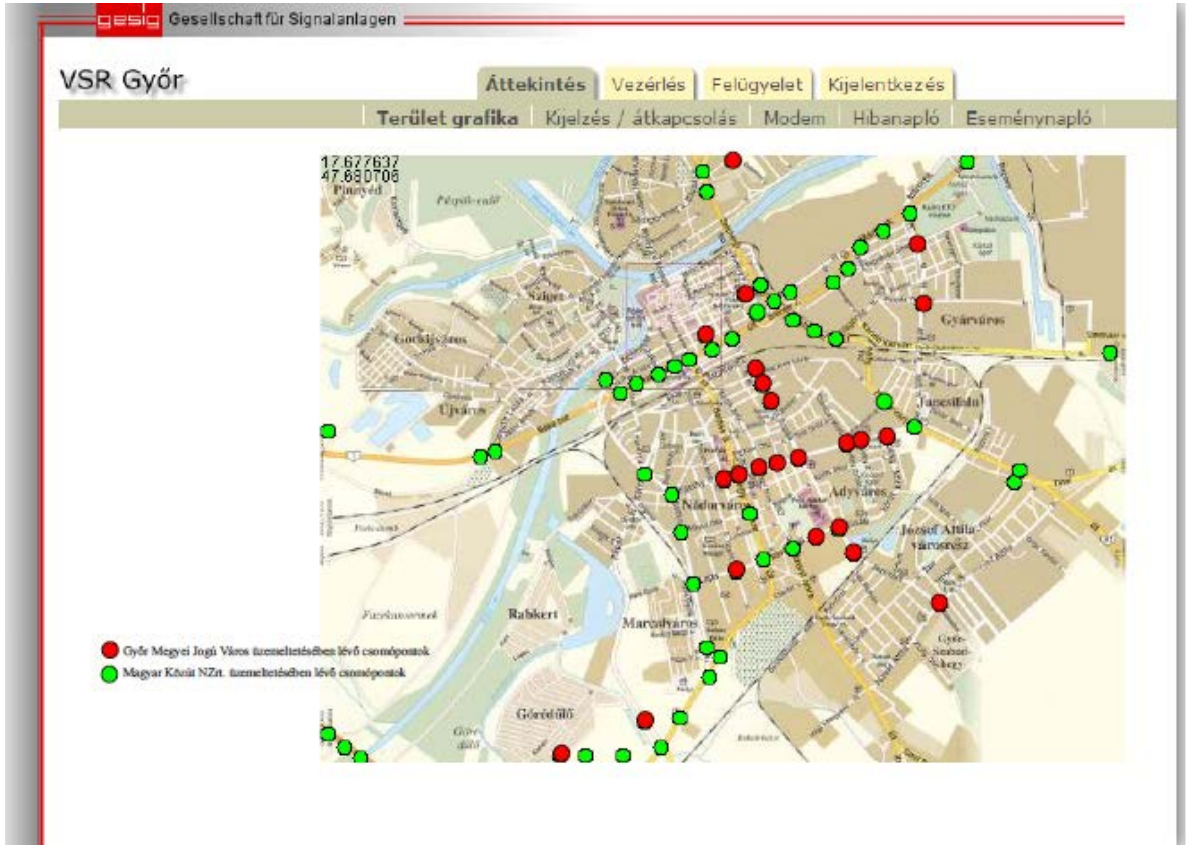
- From former conclusions ➔ suspicion of the results can depend on the type of urban area:
  - Little differences in the performance of scenario-based methodologies depending on the number of scenarios, …. These results can strongly depend on the urban area under study, and hence, more studies in other type of urban areas are needed.
  - Do the needed number of wind sectors or the model/methodology results depend on urban morphology?
- There is a feeling that a new intercomparison exercise should be needed.
- During, Technical meeting of 2022, many WG4 participants answered yes to participate in a new intercomperison.

New intercomparison exercise at a new location

Győr (Hungary)

- Proposed by Zoltán Horváth (SZE).
- Data from meteorological stations, AQ microsensors and AQ stations
- Real-time emission data for traffic.
- CFD model simulations for the entire year (but need several months of computing)

Do we start to prepare this new exercise during 2024?



FAIRMODE
WG4 – Microscale modelling

THANKS

Questions?