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Spatial Representativeness Evaluation by Point-Centred Variography

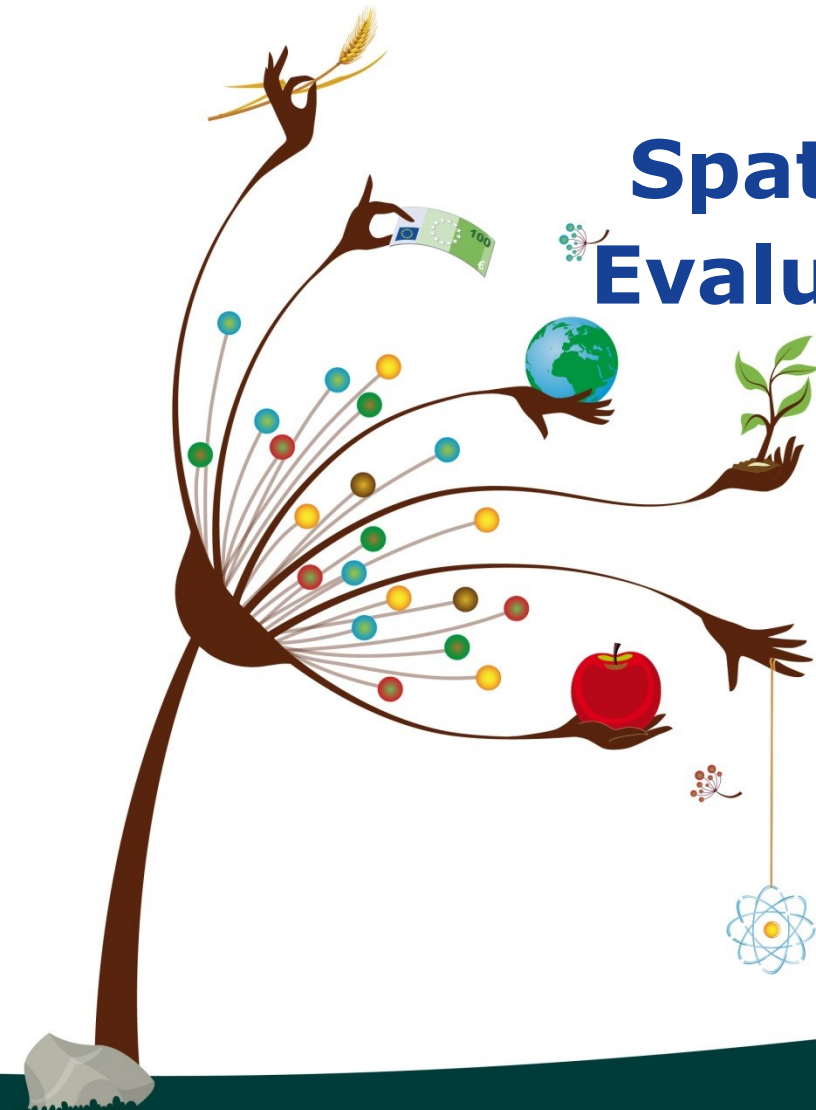
and links to the FAIRMODE /
AQUILA SR Intercomparison
Exercise

Oliver Kracht & Michel Gerboles

18th International Conference on Harmonisation within
Atmospheric Dispersion Modelling for Regulatory Purposes

HARMO

9th - 13th October 2017
Bologna - Italy



Outline & Context

Spatial Representativeness (SR)

Most basic definition:

- The **representativeness area** is described by the set of all locations where the concentration of a pollutant does not differ from the measurements at the central point (monitoring station) by more than a certain threshold.

A geostatistical approach:

- Classical geostatistical analysis would describe the **spatial correlation structure** of the whole concentration field in terms of the **variogram**.
- The **point-centred variogram** is based on the average of squared concentration **differences** observed in pairs formed between a **particular central point** and the set of **all other points** in the domain.

Context:

- FAIRMODE activities on spatial representativeness (SR).
- FAIRMODE / AQUILA **Intercomparison Exercise (IE)** of Spatial Representativeness Methods (SR-IE).

A geostatistical approach to SR:

Traditional versus Point-Centered Semivariance

Traditional semivariance

$$\gamma(h) = \frac{1}{2} \frac{1}{N_h} \sum_{i=1}^{N_h} [Z(s_i) - Z(s_i + h)]^2$$

Half the average of the squared deviations between **all paired observations** at distance h.

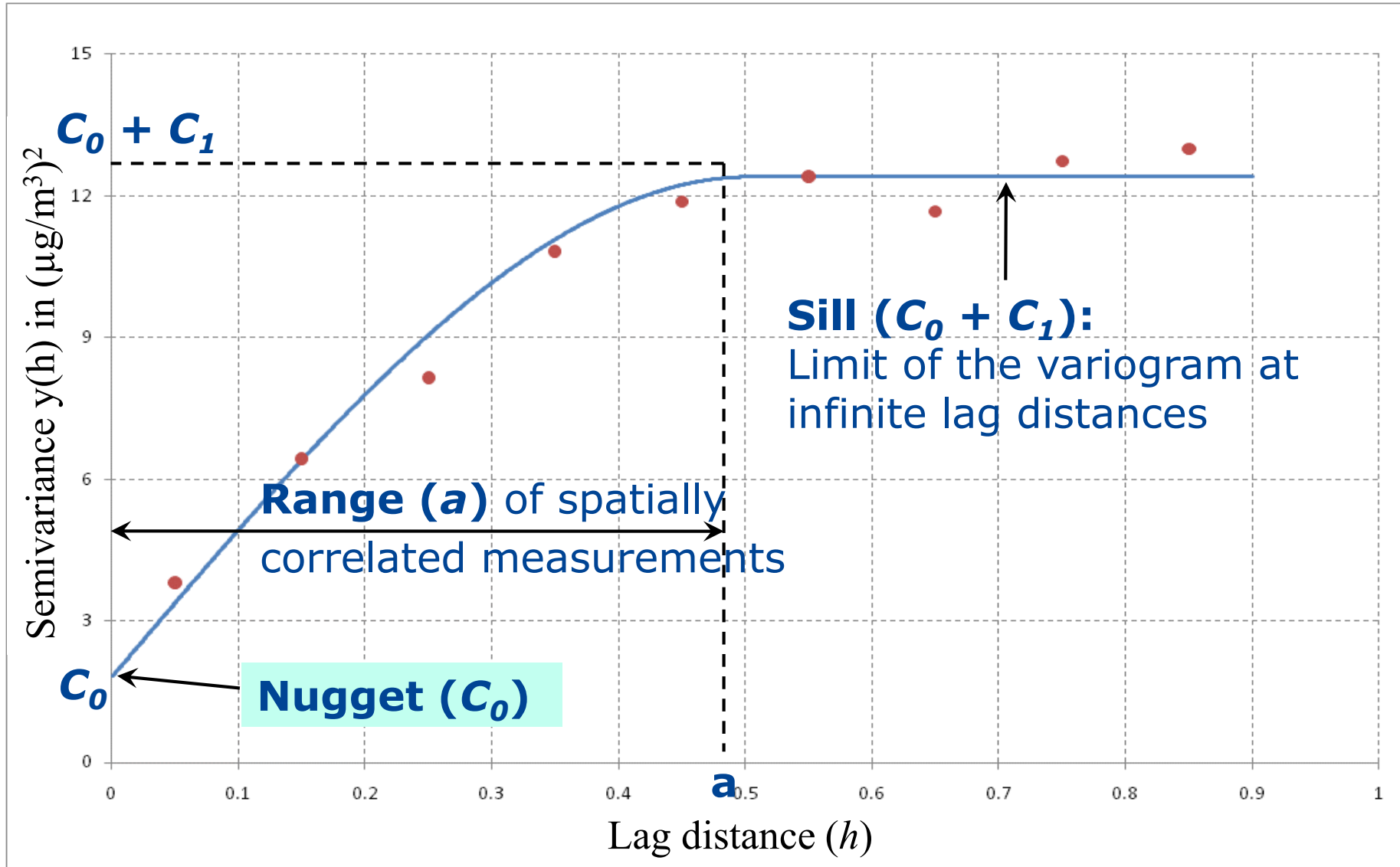
Point-centered semivariance

$$\gamma_{cp}(h) = \frac{1}{2} \frac{1}{N_{cp,h}} \sum_{i=1}^{N_{cp,h}} [Z(s_{cp}) - Z(s_{cp} + h)]^2$$

Half the average of the squared deviations within pairs formed by a **single central point (cp)** and all other observations at distance h from this cp.

Point-centered variography places a monitoring station in the **context of the local or regional air quality pattern**.

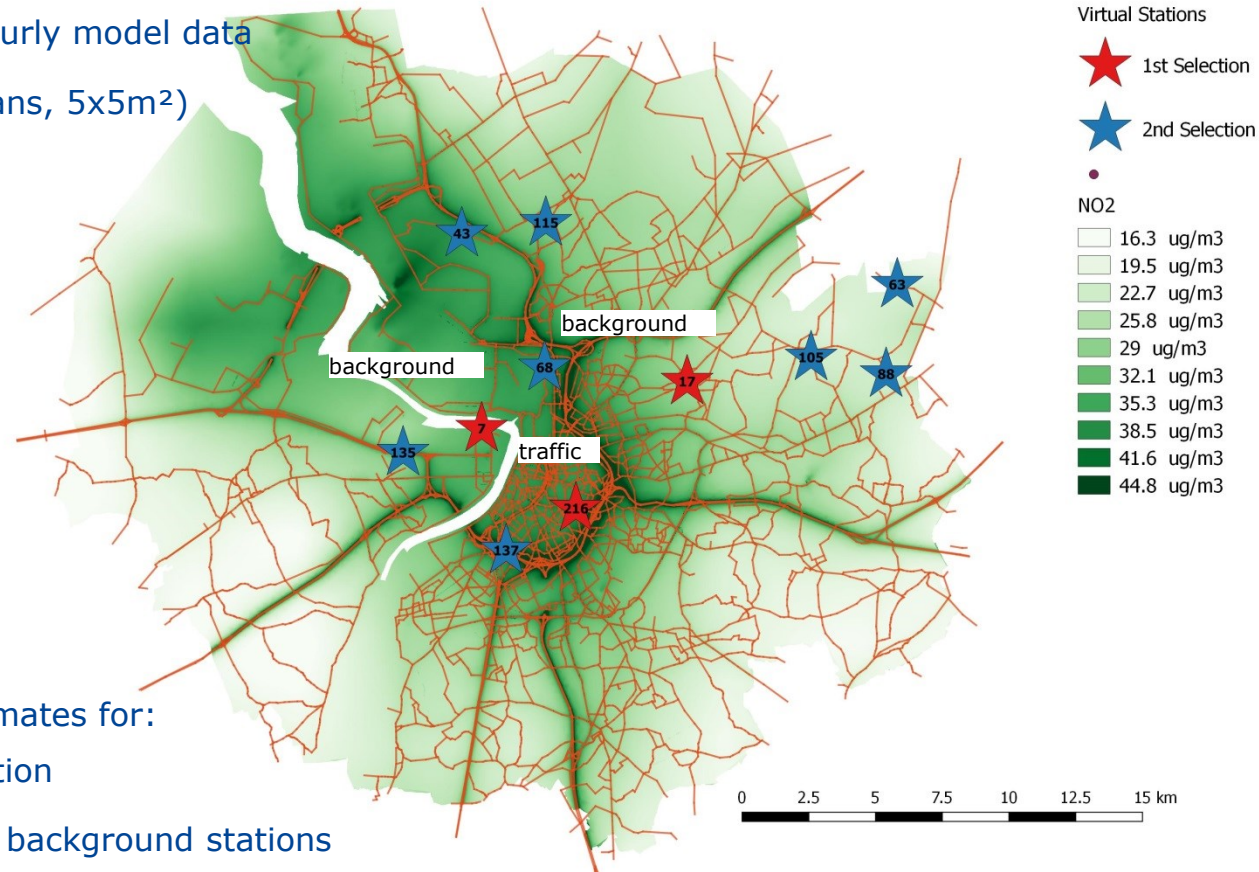
Besides that: same terminology



Context / Case study:

FAIRMODE / AQUILA Intercomparison Exercise of Spatial Representativeness Methods

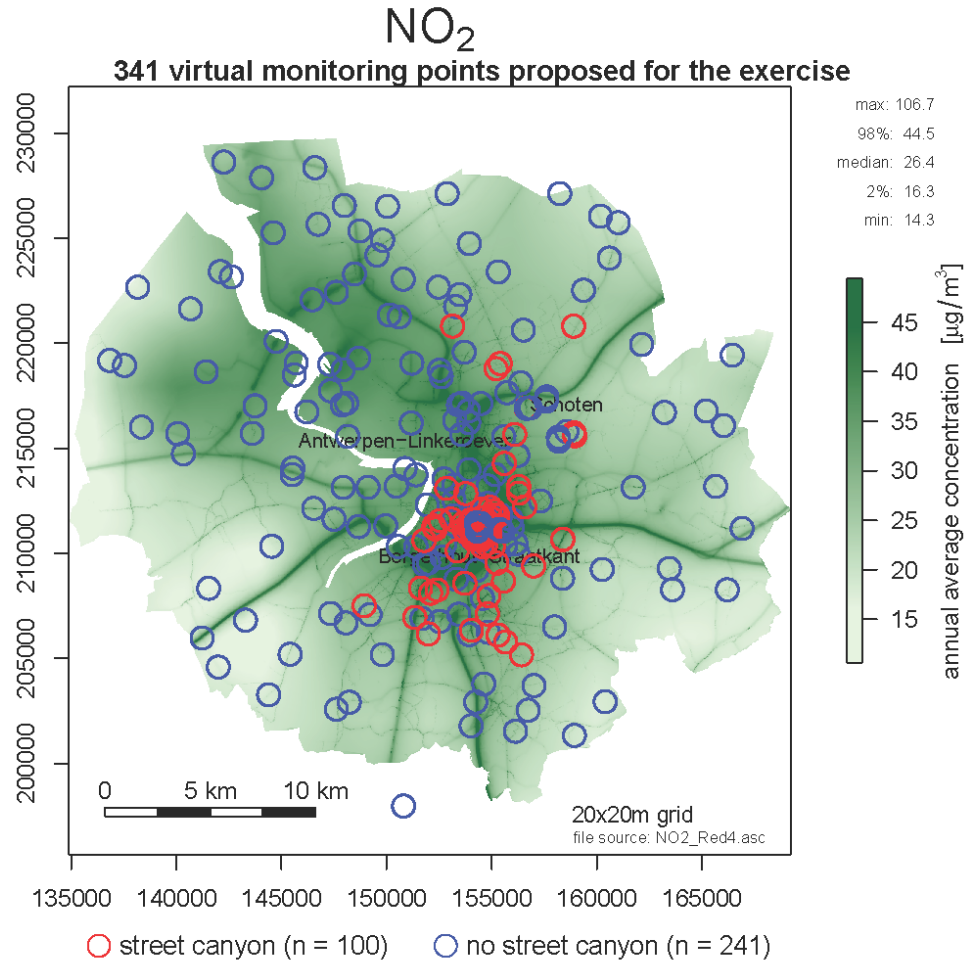
- Performed by **11 different groups**, but on the same **shared dataset** (prepared by VITO).
- Existing stations for PM₁₀ (n=15), NO₂ (n=18) and O₃ (n=3)
- Dataset based on outputs from the **RIO-IFDM-OSPM model chain** for the region of **Antwerp** (year 2012).
- **Virtual stations** (n=341) from hourly model data
- **Gridded model data** (annual means, 5x5m²)
- Emissions
- Population density
- Building heights
- CORINE land cover



- **Spatial representativeness** estimates for:
 - PM₁₀ and NO₂ at one traffic station
 - PM₁₀, NO₂ and O₃ at two urban background stations

Case study data:

- **n=341 receptor points** ("virtual stations") from hourly model data
- **aggregated to 14-day averages** (i.e. to emulate diffusive samplers)
- classified into **street canyon (SC)** and **non-street canyon (non-SC)** locations



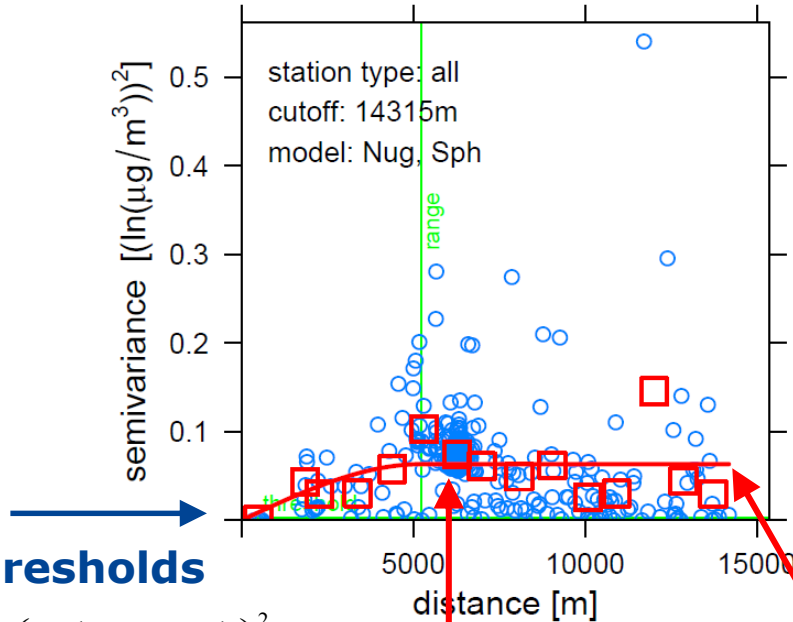
Workflow:

- Aggregate modelled time series of virtual receptors to different integration time scales (shown here: only 14-day averages).
- Log-transformation of concentration values.
- Calculate the point-centered variogram clouds.
 - all data pairs formed between the central point and the other virtual receptors
 - 15 equidistant lag classes
 - cutoff-distance of 14315 m corresponds to one third of the diagonal of the bounding box of the total Antwerp modelling domain.
- Three variations:
 - all receptors ("all")
 - street canyons only ("SC")
 - non-street canyons only ("non-SC")
- Fit point-centered variogram models to the clouds.
 - Using a spherical variogram model
 - Evaluate and filter out (remove) singular model fits (non-convergence)
- Define the semivariance at the limits of spatial representativeness.
 - Threshold values for the maximum relative deviation of concentrations permissible
 - 25% (PM₁₀), 15% (NO₂) , 15% (O₃) at the 2σ-level
 - To obtain these thresholds, used the DQO of European Directive 2008/50/EC as a proxy.
- Invert the variogram models to estimate the distance of spatial representativeness (dist.SR).

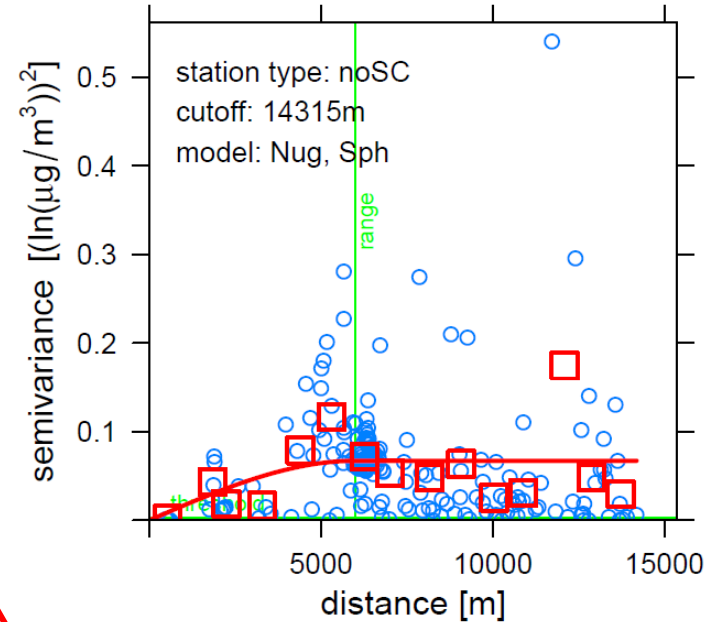
Fitting the Variogram Models (examples)

Omnidirectional variogram clouds

Central Point 17 – Ozone
timestamp: 05.02.2012 00:00



Central Point 17 – Ozone
timestamp: 05.02.2012 00:00



SR thresholds

$$\gamma(h_{SR}) = \frac{1}{2} \left(\ln \left(1 + \frac{DQO}{2} \right) \right)^2$$

PM ₁₀	NO ₂	Ozone
25 %	15 %	15 %

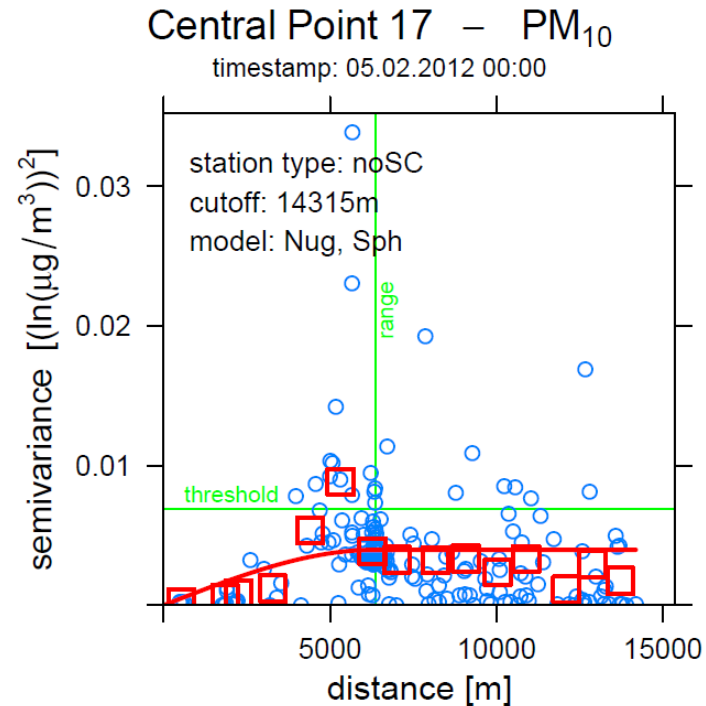
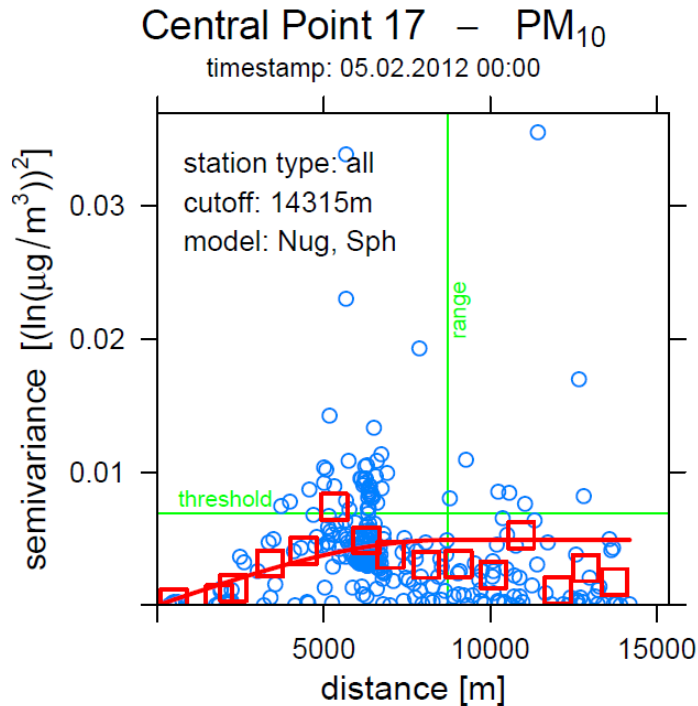
15 lag-classes

Spherical Variogram Model

$$\gamma_{cp}(h) = C_0 + C_1 \left[1.5 \frac{h}{a} - 0.5 \left(\frac{h}{a} \right)^3 \right] \quad \text{if } 0 \leq h \leq a$$

$$\gamma_{cp}(h) = C_0 + C_1 \quad \text{if } h > a$$

Fitting the Variogram Models (examples)

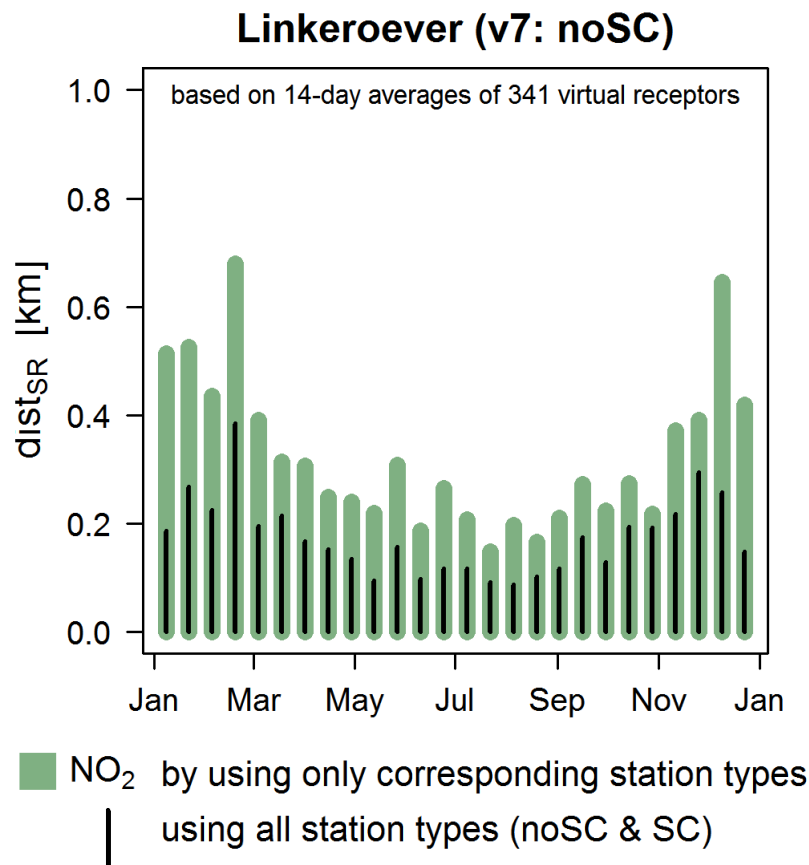


Exception handlings:

- Required semivariance threshold might not be reached within the range of the variogram.
- In such cases we chose the distance of spatial representativeness to equal the value of the range parameter.
- Other interpretations are conceivable ("infinite SR" ?)

Time Series of SR-distance estimates:

dist_{SR} in [km] for station Linkeroever (urban background site)

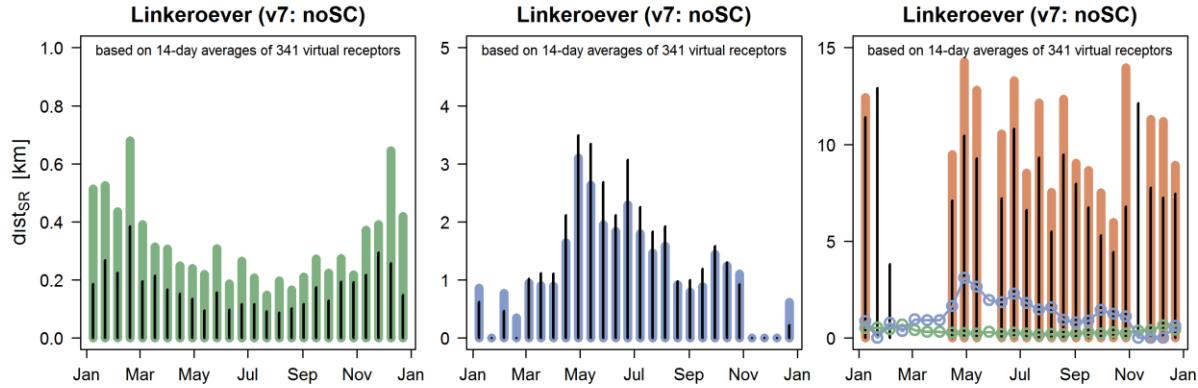


(year 2012)

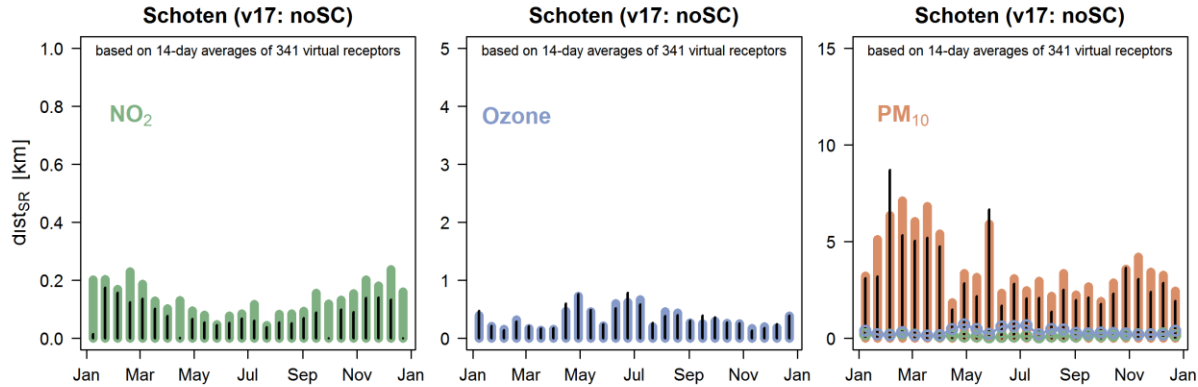
Estimated dist_{SR} tends to be larger when only receptor points of corresponding station types are considered for the analysis (as expected; more homogeneous).

Time Series of SR-distance estimates:

urban
background site

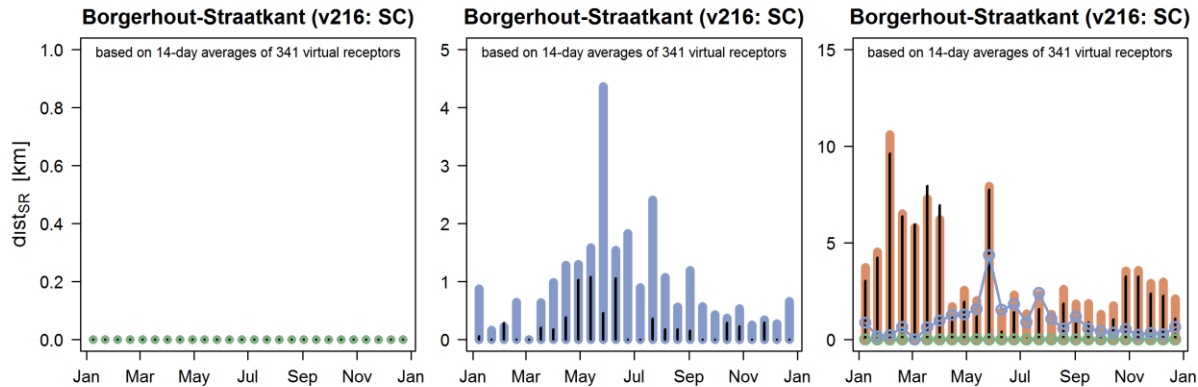


urban
background site



(year 2012)

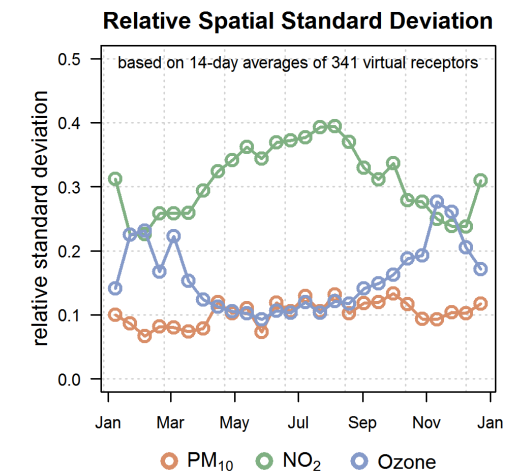
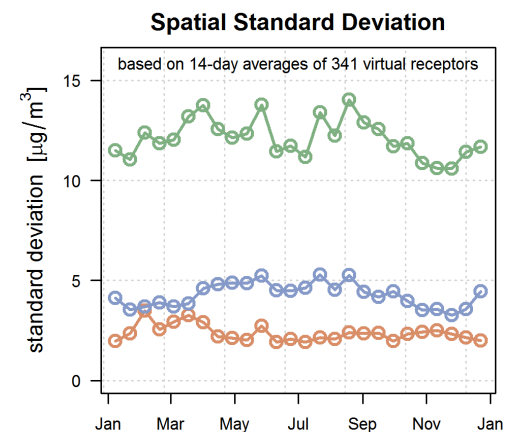
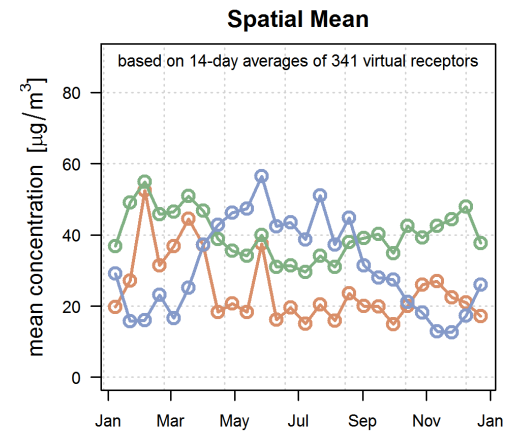
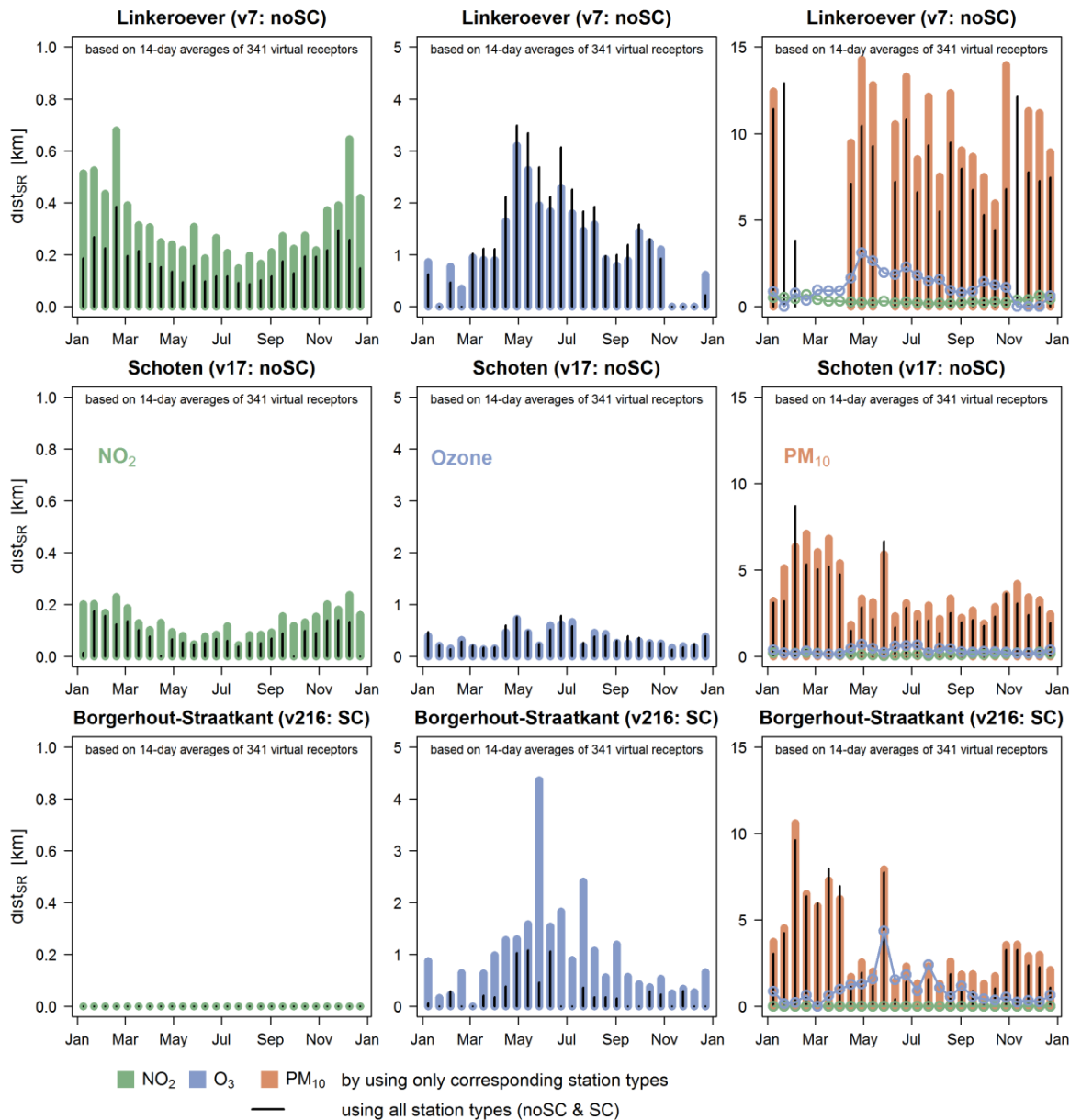
traffic site



■ NO₂ ■ O₃ ■ PM₁₀ by using only corresponding station types
 — using all station types (noSC & SC)

Note the different scales of the Y-axis: $dist_{SR}(PM_{10}) > dist_{SR}(O_3) > dist_{SR}(NO_2)$

Time Series of SR-distance estimates



from evaluating the full dataset

Might trigger questions like: Does one need more dense NO₂ observations in summertime?

relation to the FAIRMODE / AQUILA SR Intercomparison Exercise

How do the estimates from the **Point-Centered Variography** compare to the outcomes of the **SR Intercomparison Exercise**?

with contributions from:

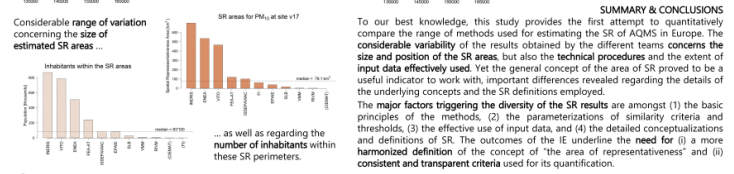
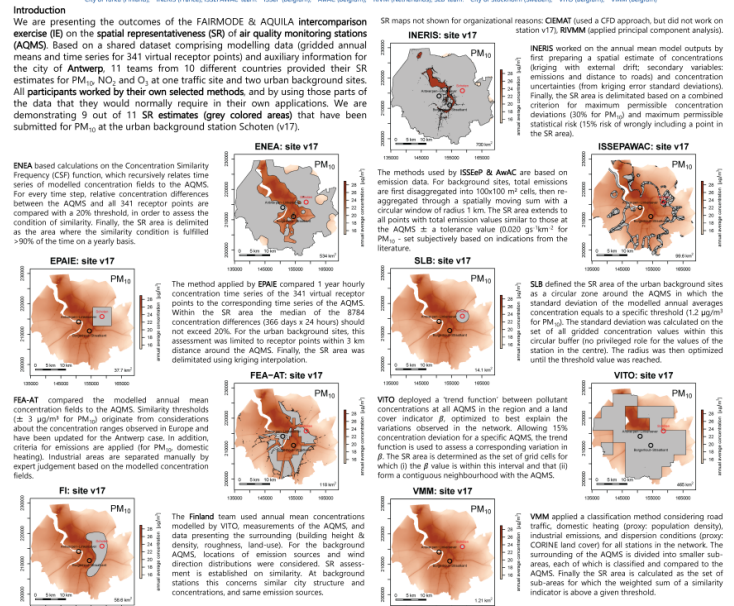
José Luis Santiago & Fernando Martin (CIEMAT), Antonio Piersanti, Giuseppe Cremona, Gaia Righini & Lina Vitali (ENEA), Kevin Delaney (EPA IE), Bidroha Basu & Bidisha Ghosh (TCD), Wolfgang Spangl & Christine Brendle (FEA-AT), Jenni Latikka (FMI), Anu Kousa (HSY), Erkki Pärjälä (City of Kuopio), Miika Meretoja (City of Turku), Laure Malherbe, Laurent Letinois & Maxime Beauchamp (INERIS), Fabian Lenartz (ISSeP), Virginie Hutsemekers (AWAC), Lan Nguyen & Ronald Hoogerbrugge (RIVM), Kristina Eneroth & Sanna Silvergren (City of Stockholm), Hans Hooyberghs, Peter Viaene, Bino Maiheu & Stijn Janssen (VITO), David Roet (VMM)



Intercomparison Exercise on Spatial Representativeness

Oliver Kracht¹, José Luis Santiago², Fernando Martin³, Antonio Piersanti⁴, Giuseppe Cremona⁵, Gaia Righini⁶, Lina Vitali⁷, Kevin Delaney⁸, Bidroha Basu⁹, Bidisha Ghosh¹⁰, Wolfgang Spangl¹¹, Christine Brendle¹², Jenni Latikka¹³, Anu Kousa¹⁴, Erkki Pärjälä¹⁵, Miika Meretoja¹⁶, Laure Malherbe¹⁷, Laurent Letinois¹⁸, Maxime Beauchamp¹⁹, Fabian Lenartz²⁰, Virginie Hutsemekers²¹, Lan Nguyen²², Ronald Hoogerbrugge²³, Kristina Eneroth²⁴, Sanna Silvergren²⁵, Hans Hooyberghs²⁶, Peter Viaene²⁷, Bino Maiheu²⁸, Stijn Janssen²⁹, David Roet³⁰ & Michel Gerboles³¹

¹AWAC, ²CIEMAT, ³CIEMAT, ⁴CIEMAT, ⁵ENEA, ⁶ENEA, ⁷ENEA, ⁸EPA, ⁹TCD, ¹⁰TCD, ¹¹FEA-AT, ¹²FEA-AT, ¹³FMI, ¹⁴HSY, ¹⁵City of Kuopio, ¹⁶City of Turku, ¹⁷AWAC, ¹⁸AWAC, ¹⁹AWAC, ²⁰INERIS, ²¹INERIS, ²²INERIS, ²³RIVM, ²⁴City of Stockholm, ²⁵City of Stockholm, ²⁶AWAC, ²⁷AWAC, ²⁸AWAC, ²⁹AWAC, ³⁰AWAC, ³¹AWAC

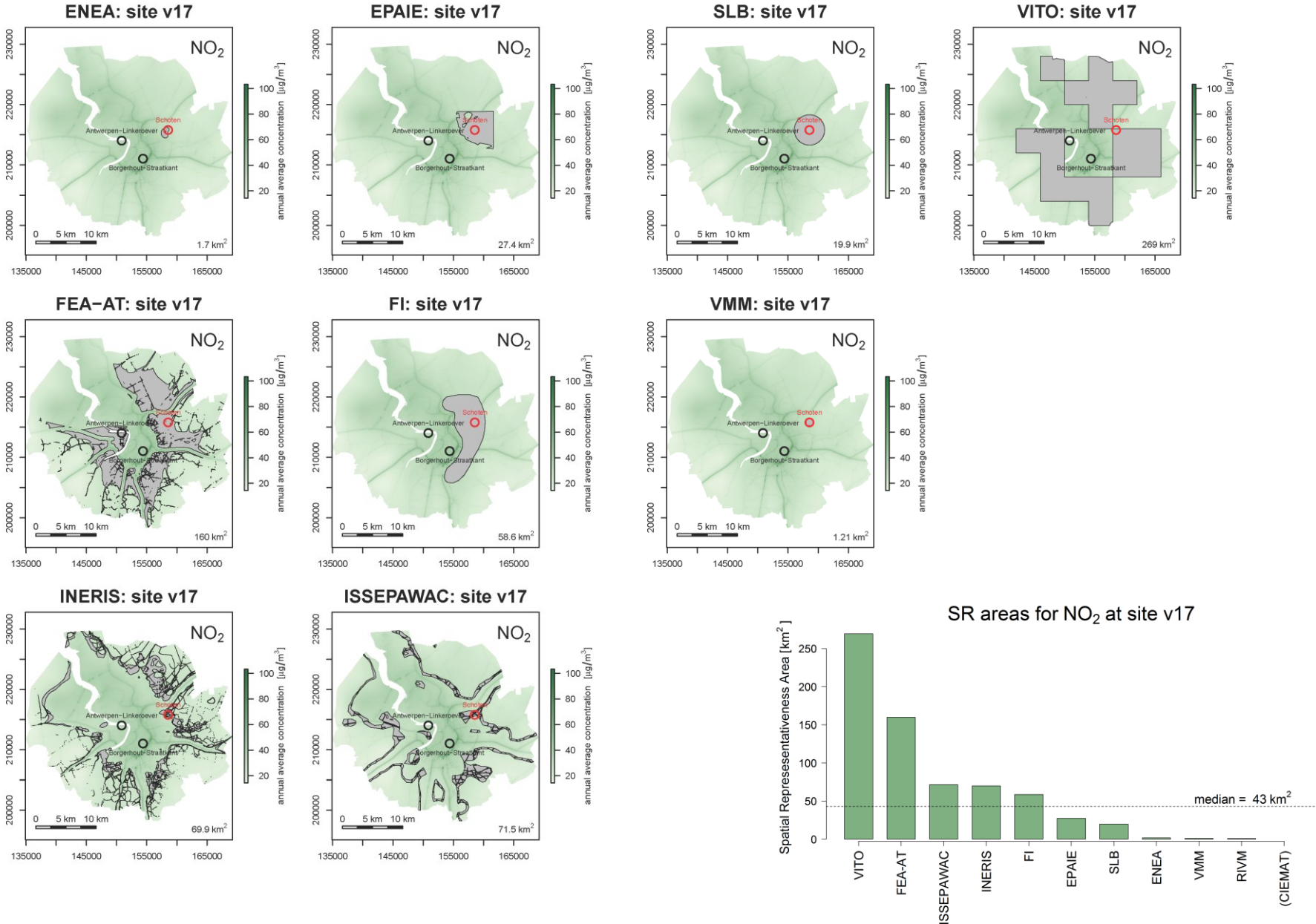


SUMMARY & CONCLUSIONS
To our best knowledge, this study provides the first attempt to quantitatively compare the range of methods used for estimating the SR of AQMS in Europe. The considerable variability of the results obtained by the different teams concerns the size and position of the SR areas, but also the technical procedures and the extent of input data effectively used. Yet the general concept of the area of SR proved to be a useful indicator to work with; important differences revealed regarding the details of the underlying concepts and the SR definitions employed. The major factors triggering the diversity of the SR results are amongst (1) the basic principles of the methods, (2) the parameterizations of similarity criteria and thresholds, (3) the effective use of input data, and (4) the detailed conceptualizations and definitions of SR. The outcomes of the E underlines the need for (i) a more harmonized definition of the concept of 'the area of representativeness' and (ii) consistent and transparent criteria used for its quantification.

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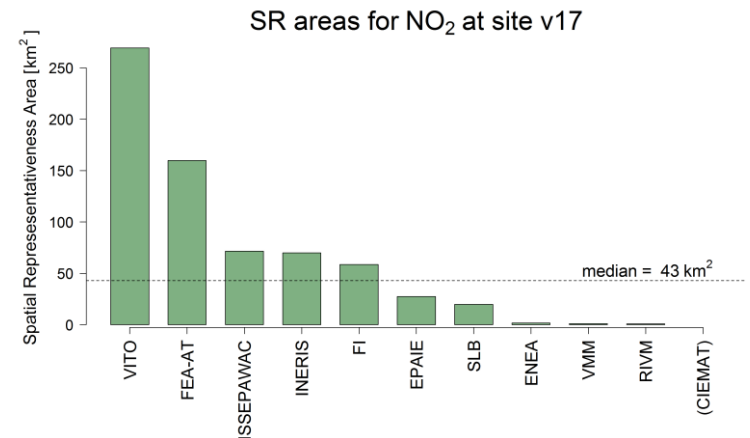
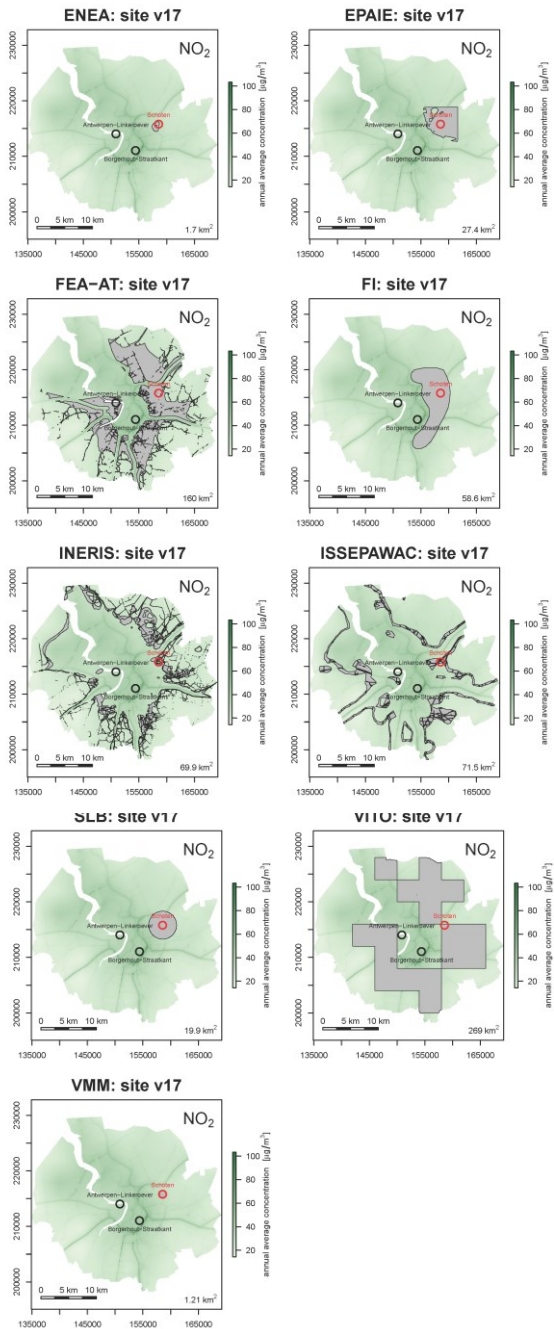
(refer to poster H18-112 for details)

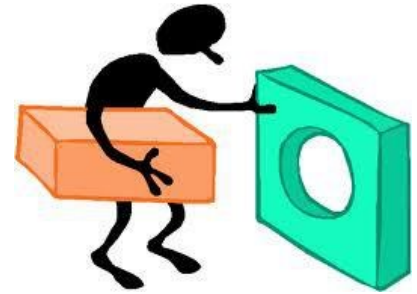
Size and Location of estimated SR areas (NO₂ at site v17)



Interim Conclusion from the IE have been:

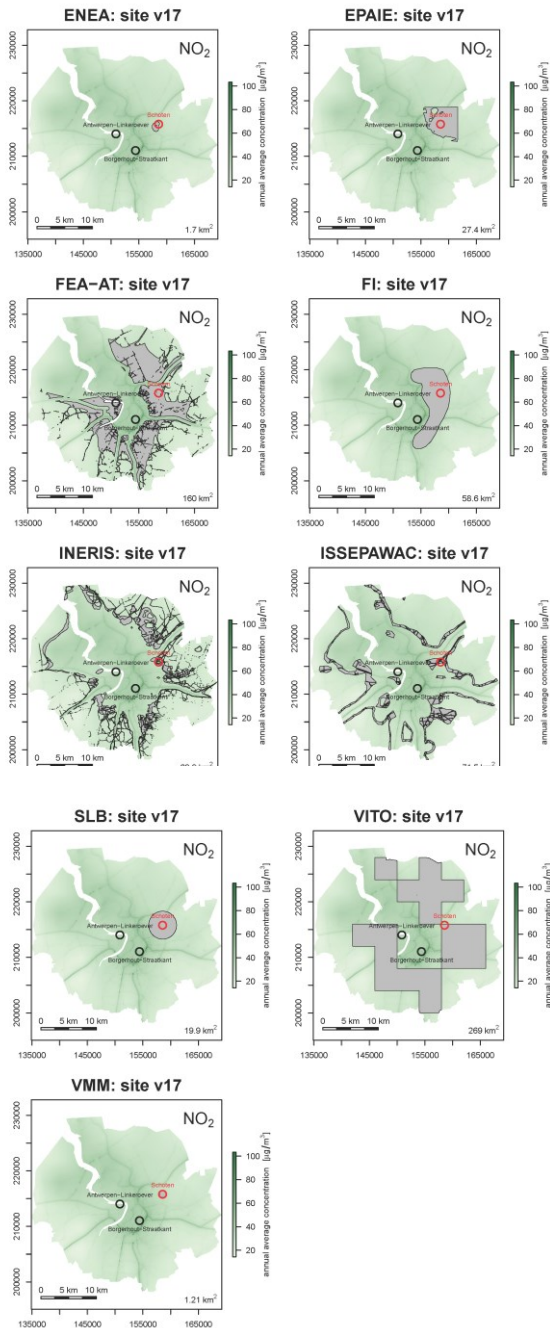
- The Spatial Representativeness Areas estimated by the different participants are **quite diverse**.
- The results in particular reveal an enormous **scattering of the extent and position** of the estimated polygons.
- This diversity of results deserved a closer look behind the scenes.

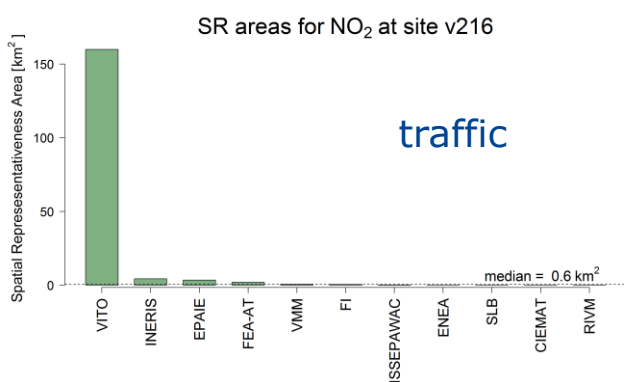
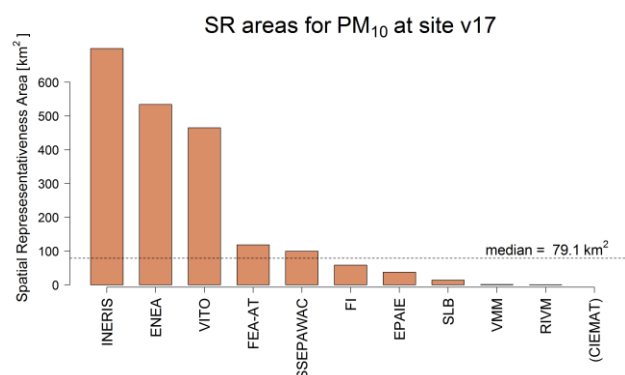
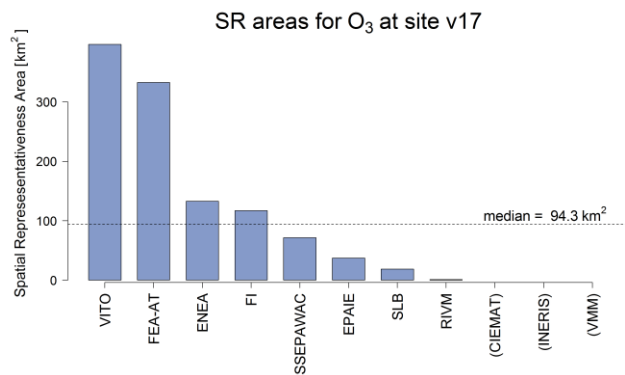
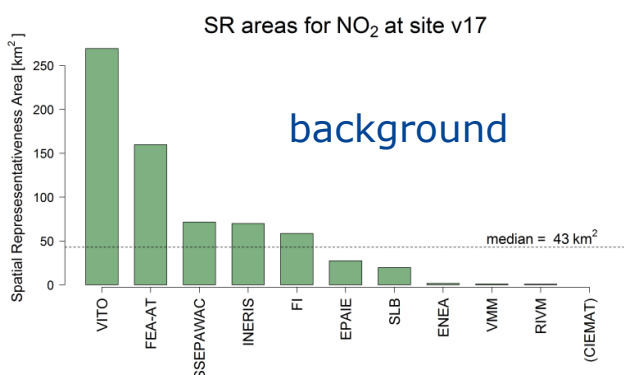
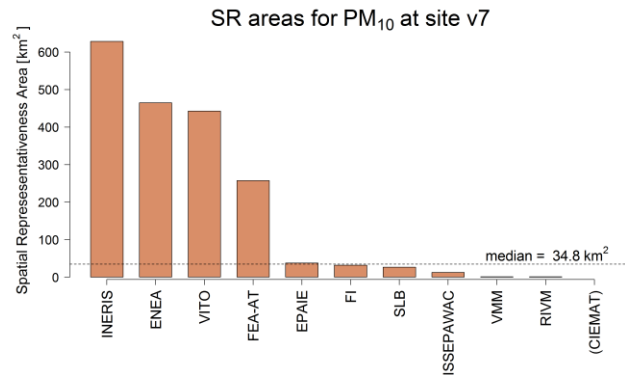
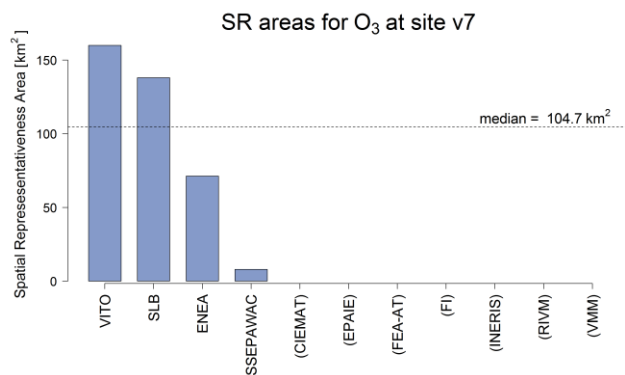
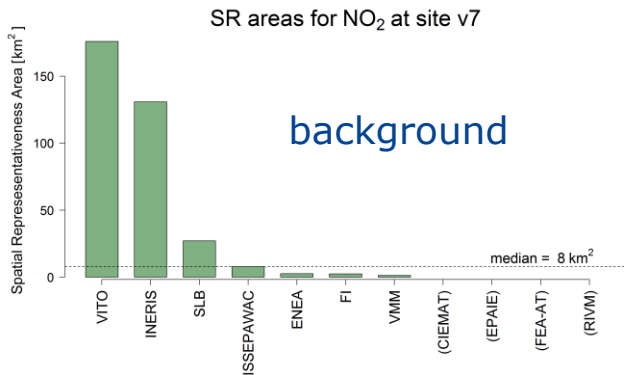




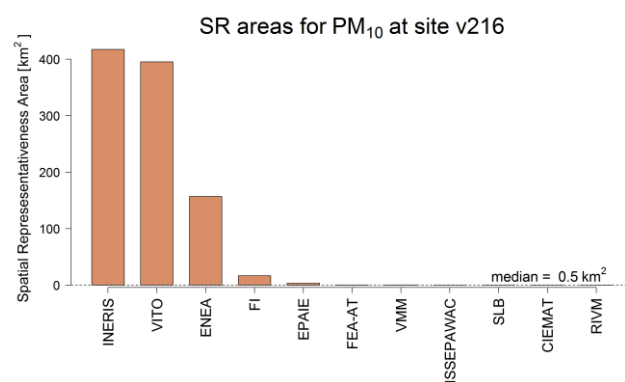
How to compare the PCV results with the IE ?

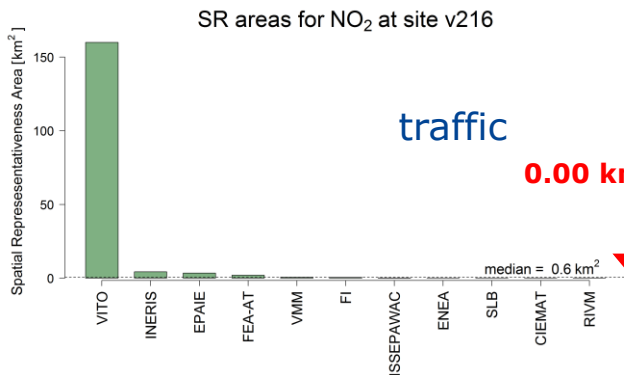
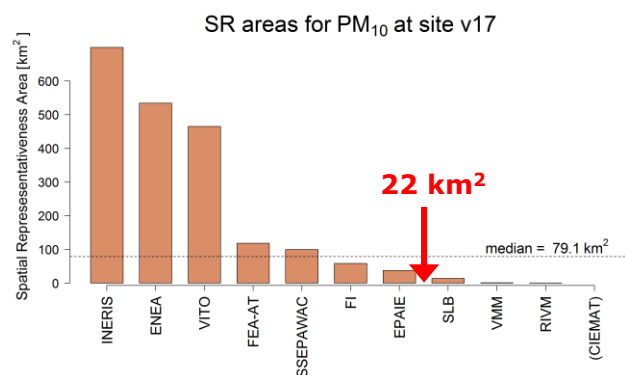
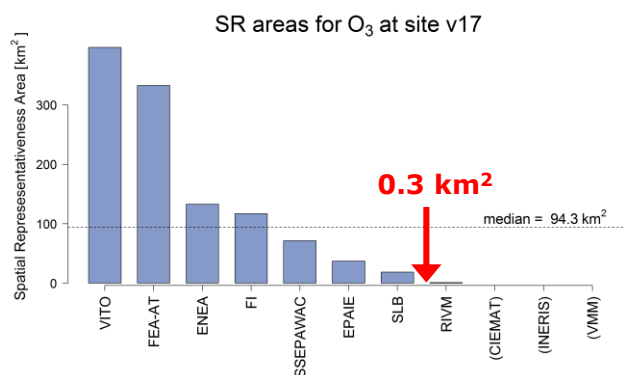
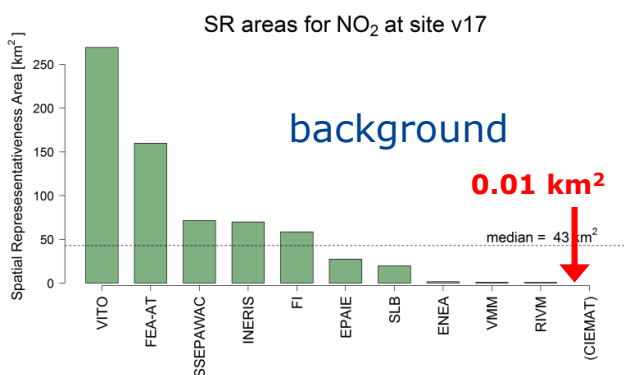
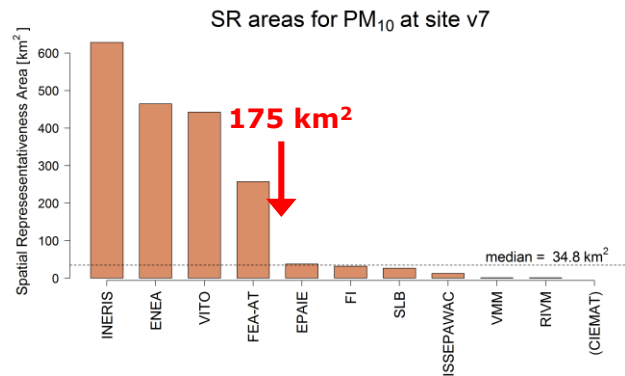
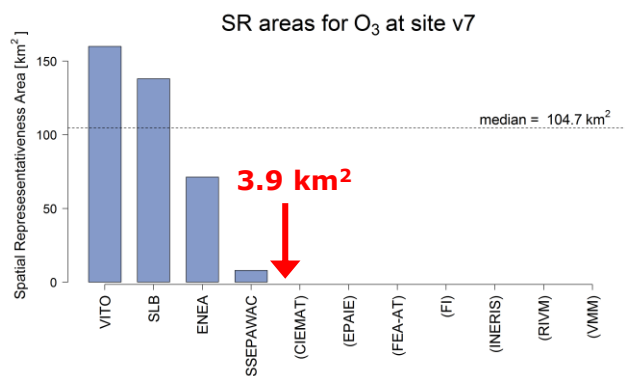
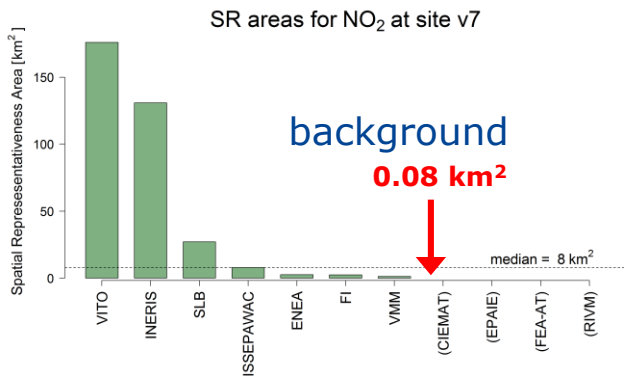
- Subject to site specific conditions and to different SR approaches, SR areas can have **quite complex, irregular** and even **discontinuous** shapes.
- In contrast, the point-centered variogram method (as presented here) **delivers on single value** (distance of spatial representativeness: $dist_{SR}$).
- From a conceptual point of view, the latter corresponds to the conception of a **simple circular shaped** area of representativeness.
- We need to accept, that this is likely **oversimplified**.
- In order to compare the results, we **recalculate** the PCV $dist_{SR}$ to the **surface area equivalent of a corresponding circle**.





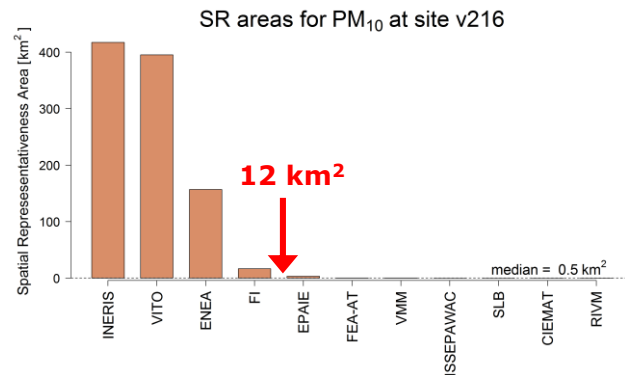
Overview:
results from the
Intercomparison





Results from PCV

- PCV results tend to be on the **lower end** of the conceivable SR scale
- PCV delivers **rather strict** SR estimates



Conclusions (1)

Depending on the spatial scale of the investigation, the **Point-centered Variogram** places a monitoring station in the **context of the local or regional air quality pattern**.

The Point-centred Variogram **does not**, however, serve as a **substitute** for **the traditional variogram** in the sense that geostatistical methods like kriging require a model fitted for the traditional variogram.

Point-centred Variography can on the other hand provide **valuable information** with regard to the **spatial representativeness** of air quality monitoring sites.

We may also obtain information about the **temporal variation of SR**.

However, a **comparison with** results obtained by **other spatial representativeness approaches** or based on different conceptualizations is **not necessarily simply one-to-one**.

Conclusions (2)

Way forward:

The concept of a **single spatial representativeness distance** (dist.SR) value implies the assumption of a **radially symmetric area** of spatial representativeness. This corresponds to the use of an **omni-directional variogram**.

The omni-directional approach is **probably overly simplified** and more detailed information (i.e. about the **anisotropy** of the variogram) could be extracted from the data.

In **future developments** it would be **recommendable** to extend the evaluation by applying **directional variograms**. Disadvantage could be the **limited number of data-pairs** available in the individual directional sectors.

Thank you for your attention!

Conclusions from the SR Workshop in Athens (June 2017)

Participants agreed that the discrepancies observed in this exercise **require further efforts** towards the **quantitative definition of the concept of “the area of representativeness”** and in **eliminating unnecessary differences** in the methodologies.

In the second part of the workshop it was therefore more intensively discussed, if for the aim of **harmonization** the concept of spatial representativeness would require a **paradigm shift in** its definition:

- 1) What are the future needs for **harmonization** and for establishing a **common frame of reference**?
- 2) Is there a future need for **standardization**, too?
- 3) Beyond standardization, should the regulators / political bodies make the use of standards **mandatory**?
- 4) Would it conversely be preferable to have at disposal a **set of transparent definitions** and **practical guidelines**, but maintaining the freedom of choosing the most appropriate procedures for the **different** particular **purposes** and **applications**?

It was found consensus amongst participants that currently it **would not (yet) be reasonable to start discussing about (2) or (3)**, but that for the **mid term** future the **efforts** of the experts community should be directed **towards (4)** first.