Application and intercomparison of three data assimilation methods for air quality evaluation on the Île-de-France area

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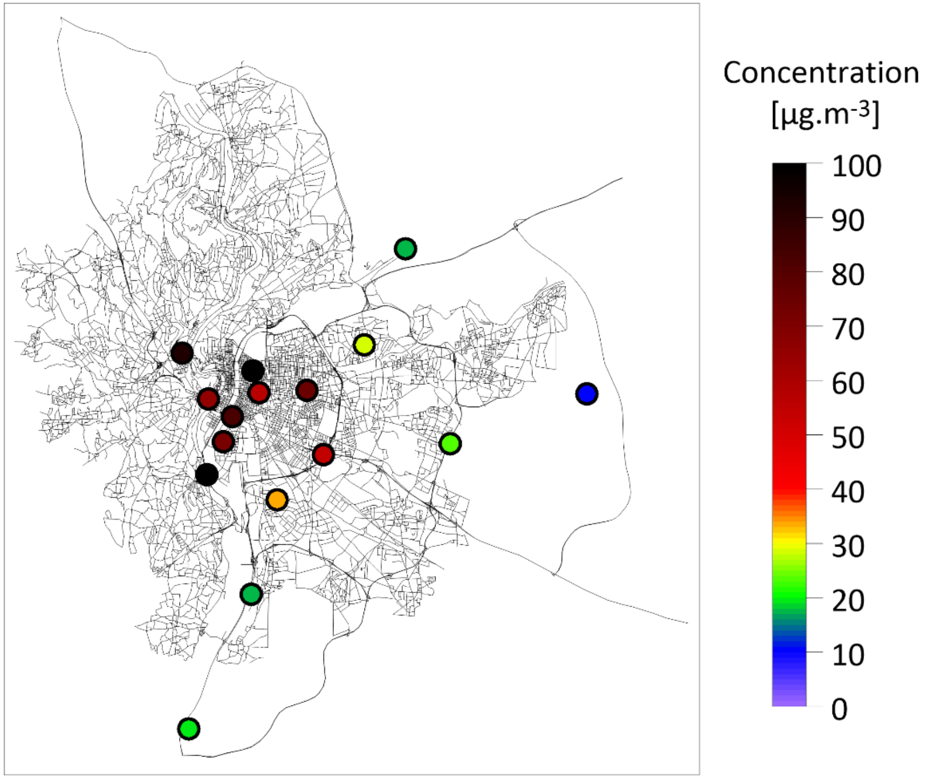
INTRODUCTION

Introduction

Evaluation of urban air quality: measurements

✓ Accurate data

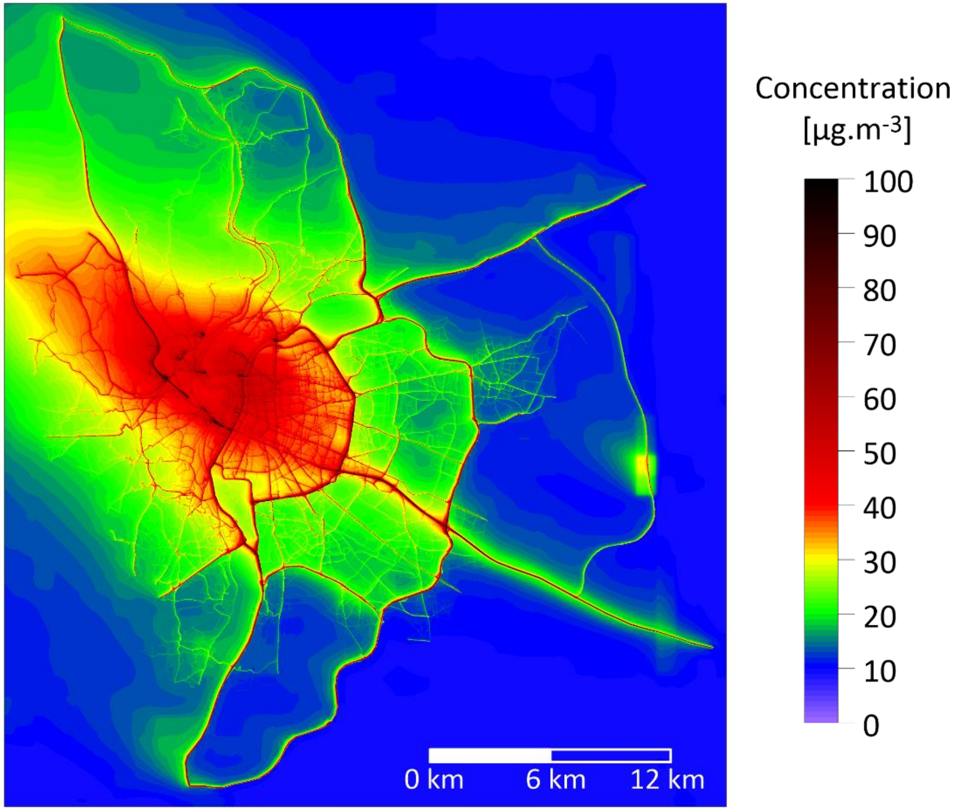
X Heterogeneous spatial distribution



Introduction

Evaluation of urban air quality: modelling

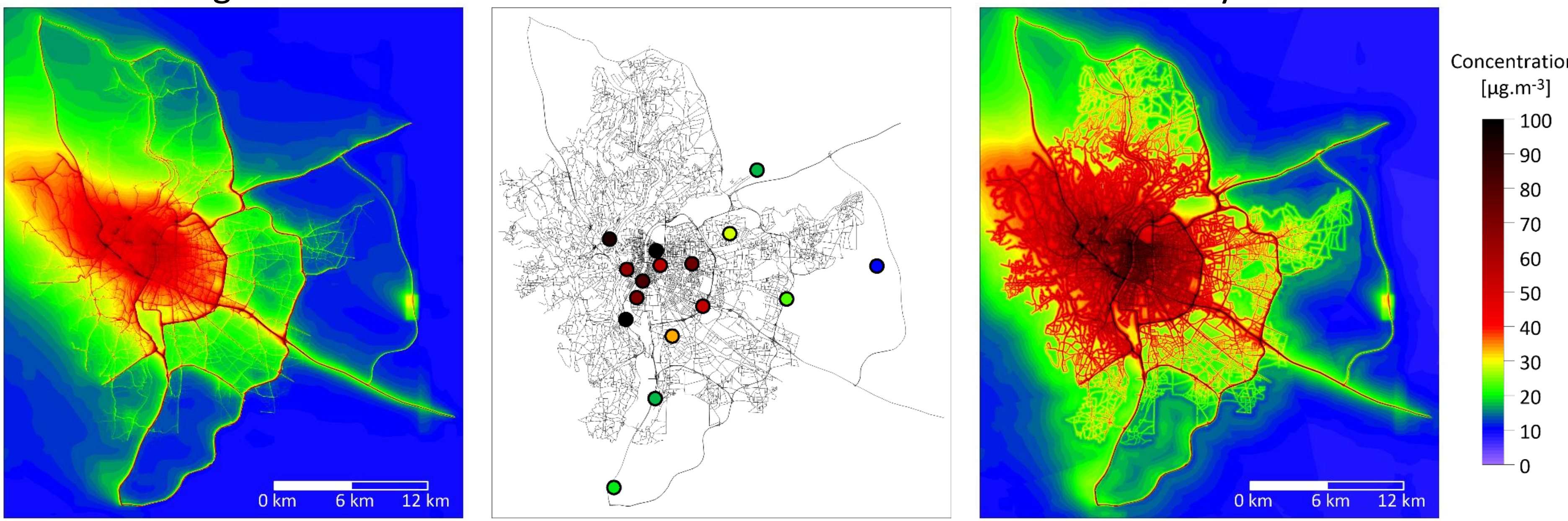
- ✓ Fine spatial resolution
- ✓ Forecast
- ✓ Scenario studies
- ✓ High number of species
- X High uncertainties



Introduction

Evaluation of urban air quality: data assimilation

Background | Measurements | Analysis



Data assimilation (DA): combination of measurements and modelled data to determine the best estimate of the system state

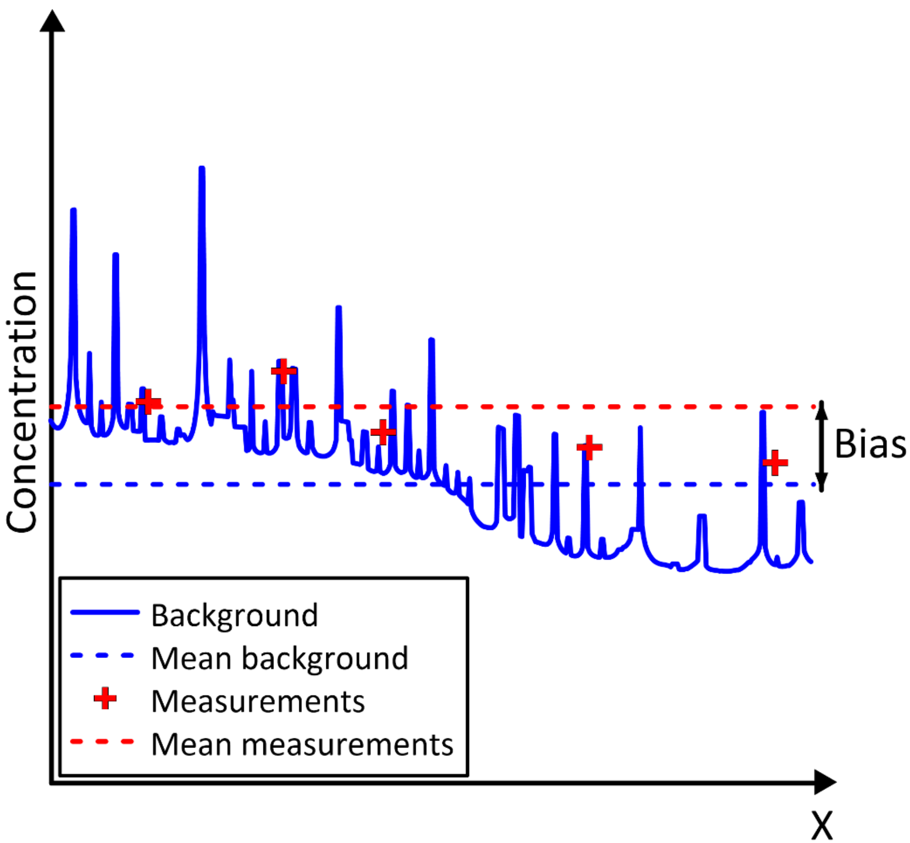
- $\mathbf{x}^{\mathbf{b}}$: background (n)
- $\mathbf{y}$: observations (m)
- $\mathbf{x}^{\mathbf{a}}$: analysis (n)
- $\mathbf{H}$: observation operator (m x n)

DATA ASSIMILATION

Data assimilation

Bias Adjustment Technique (BAT)

a) Before assimilation
b) After assimilation



- Analysis: $\mathbf{x^a} = \alpha \mathbf{x^b}$
- Correction coefficient: $\alpha = \dfrac{\sum_i^m y_i}{\sum_i^m x_i^b}$

with:

- x_i^b: background at point p_i
- y_i: measurement at point p_i
- m: number of observations

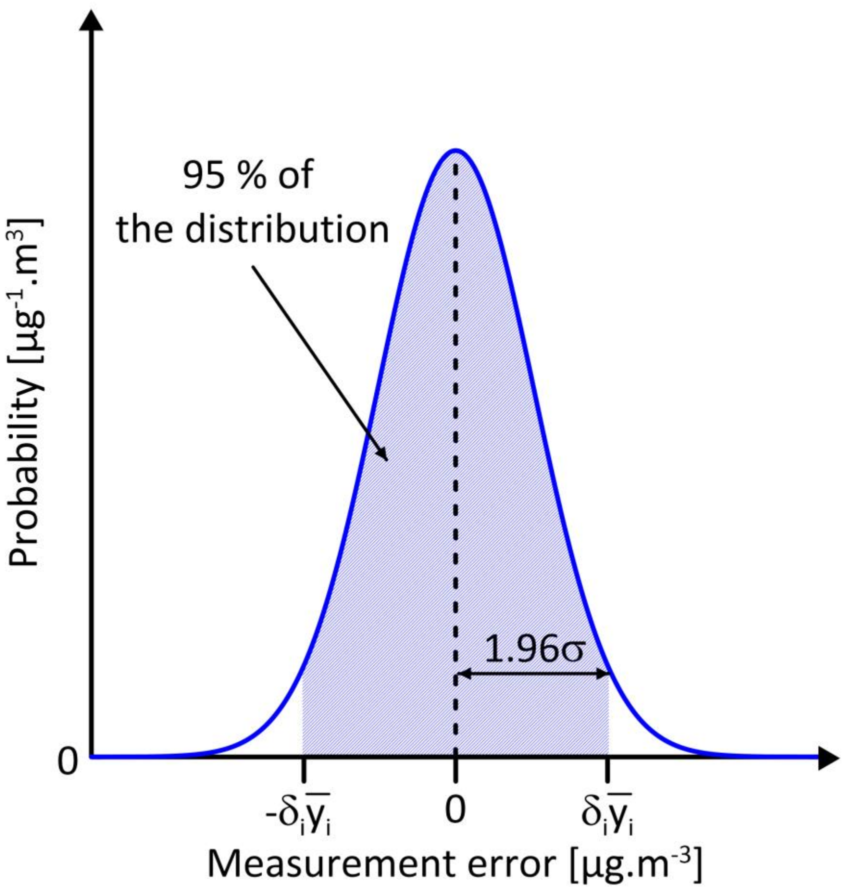
Data assimilation

Best Linear Unbiased Estimator (BLUE)

- Analysis: $\mathbf{x^a} = \mathbf{x^b} + \mathbf{K}\left(\mathbf{y} - \mathbf{H}\mathbf{x^b}\right)$
- Kalman gain: $\mathbf{K} = \mathbf{B}\mathbf{H}^{T}\left(\mathbf{H}\mathbf{B}\mathbf{H}^{T} + \mathbf{R}\right)^{-1}$

with:

- $\mathbf{K}$: Kalman gain
- $\mathbf{R}$: observation error covariance matrix
- $\mathbf{B}$: background error covariance matrix



- Modelling of matrix $\mathbf{R}$:
  - $\mathbf{R} = \mathrm{diag}(\sigma_1^2, \sigma_2^2, \dots, \sigma_m^2)$
  - $1{,}96\sigma_i = \delta_i \overline{y}_i$

  with:
  - $\overline{y}_i$: mean measurement at point p_i
  - δ_i: uncertainty at the point p_i

Data assimilation

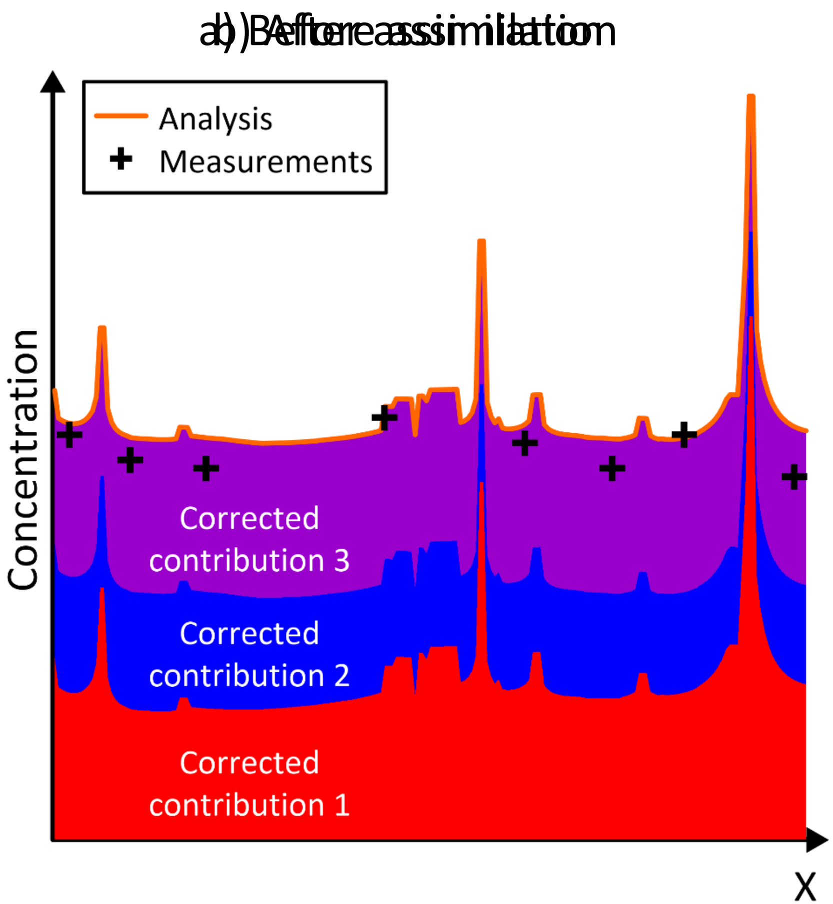
Best Linear Unbiased Estimator (BLUE)

- Modelling of matrix $\mathbf{B}$:
  - **Assumption**: background errors at points $\mathrm{p_i}$ and $\mathrm{p_j}$ are more correlated when these points are impacted by the same events
  - $\mathrm{B_{ij}} = \gamma\sqrt{\sigma_i^{2,b}\sigma_j^{2,b}}\rho_0 \exp\left(\frac{\rho_{ij}^b - 1}{L_\rho}\right)$

  with:
    - $\sigma_i^{2,b}$: background variance at point $\mathrm{p_i}$
    - ρ_{ij}^b: correlation coefficient of the background at points $\mathrm{p_i}$ and $\mathrm{p_j}$
    - γ: adjustment coefficient
    - ρ_0: characteristic correlation coefficient
    - L_ρ: characteristic correlation distance
  - γ, ρ_0 and L_ρ are estimated with the χ^2 diagnosis and by minimising the RMSE after cross-validation

Data assimilation

Source Apportionment Least Square (SALS)



- **Assumption**: modelling errors are mainly due to errors on emissions estimates

- Analysis: $\mathbf{x^a} = \sum_{\mathrm{g}}^{\mathrm{G}} \beta_g \, \mathbf{x_g^b}$

with:

  - $\mathbf{x_g^b}$: background of the source group g
  - β_g: modulation coefficient of the source group g
  - G: number of source groups

- The β_g coefficients are estimated by minimising the cost function J:

$$J(\beta_1, \beta_2, \dots, \beta_{\mathrm{G}}) = (\mathbf{y} - \mathbf{x^a})^T (\mathbf{y} - \mathbf{x^a})$$

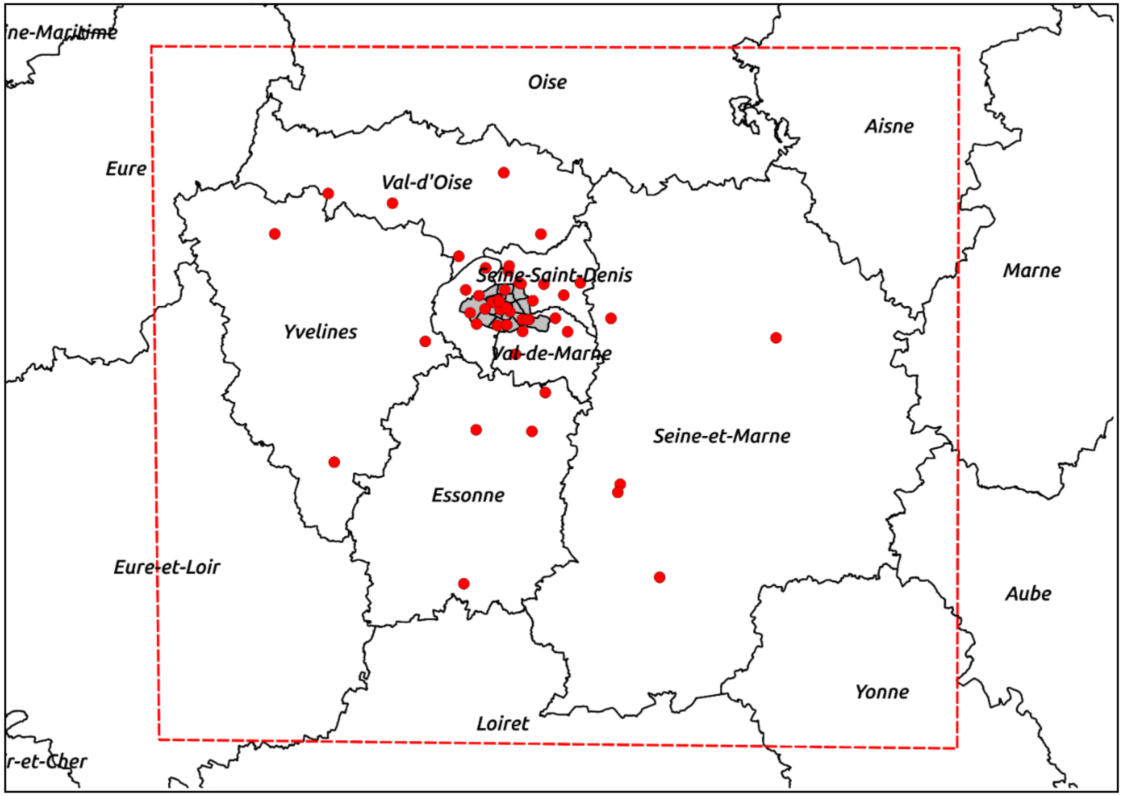
CASE STUDY

Case study
Description

- **Goal: air quality evaluation on the Île-de-France area**

- Scenario:
  - From 01/12/16 to 30/06/17
  - Pollutant: NO_2
  - 35 monitoring stations

- 3 groups for the SALS:
  - Traffic
  - Other emissions
  - Background concentration



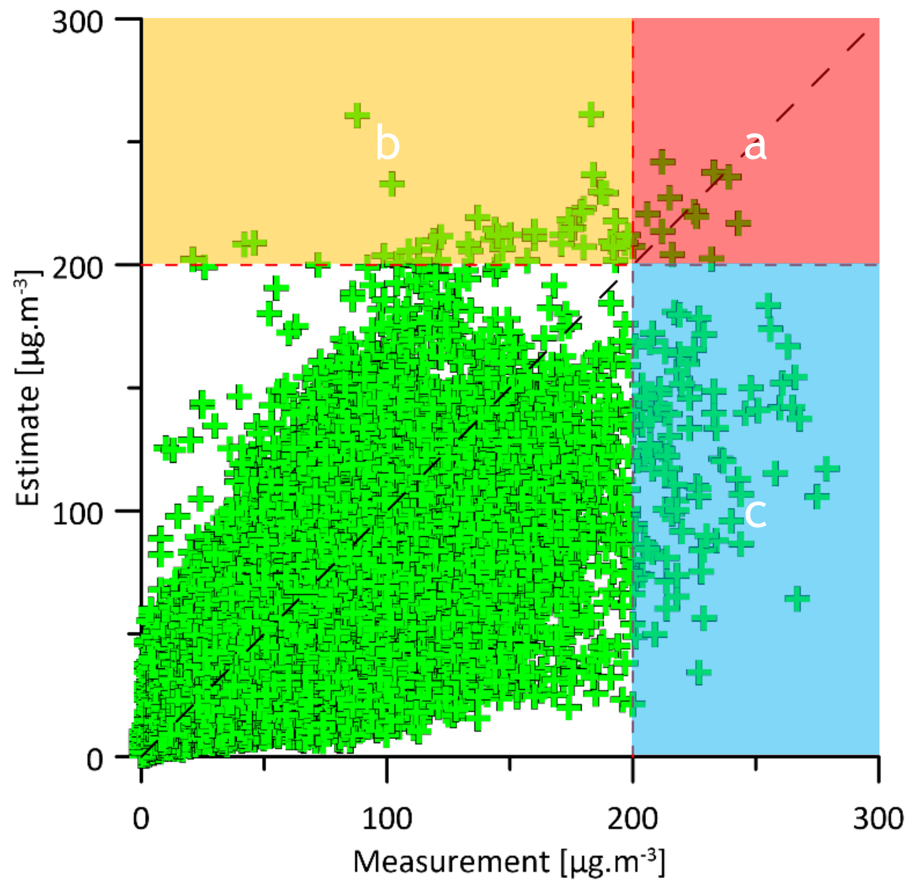
Domain of the case study

Case study

Statistical indices

Statistical indices	Expression	Optimal value
Bias	$\overline{\mathbf{x^m}} - \bar{\mathbf{y}}$	0
RMSE	$\sqrt{\overline{(\mathbf{x^m} - \mathbf{y})^2}}$	0
Corr	$\dfrac{\overline{(\mathbf{x^m} - \overline{\mathbf{x^m}})(\mathbf{y} - \bar{\mathbf{y}})}}{\sqrt{\overline{(\mathbf{x^m} - \overline{\mathbf{x^m}})^2}\ \overline{(\mathbf{y} - \bar{\mathbf{y}})^2}}}$	1
POD	$\dfrac{\mathrm{a}}{\mathrm{a + c}}$	1
FAR	$\dfrac{\mathrm{b}}{\mathrm{a + b}}$	0

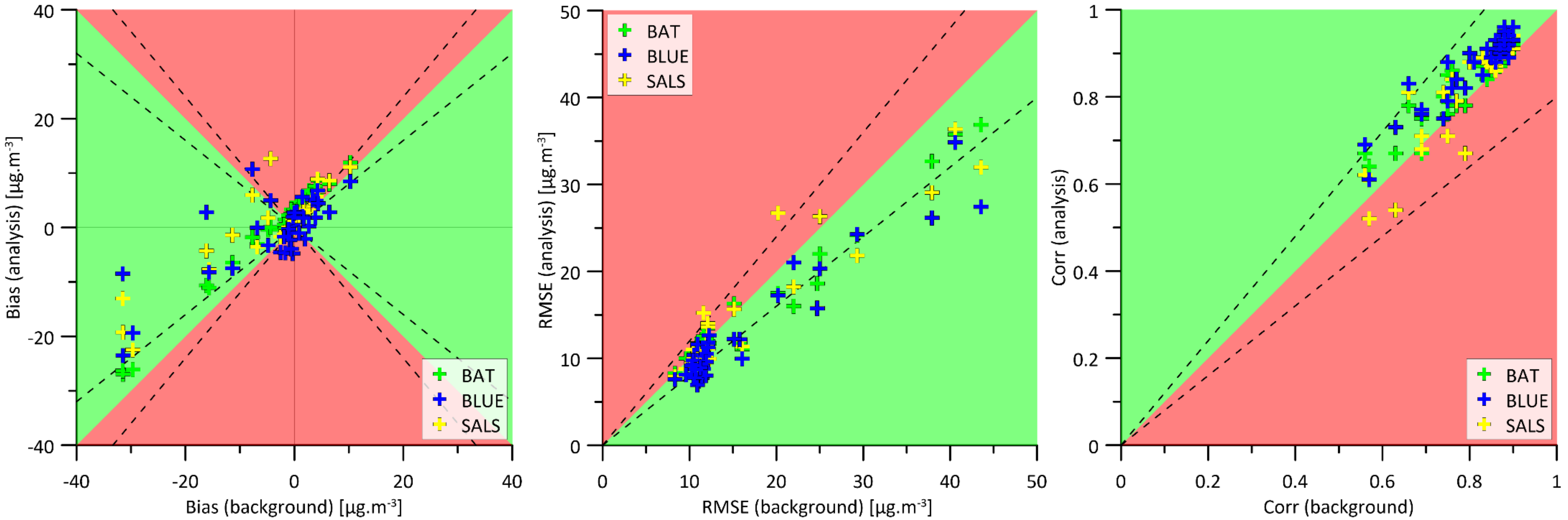
$\mathbf{x^m}$: estimates; $\mathbf{y}$: observations



The analysis is estimated with the leave-one-out cross-validation

Case study

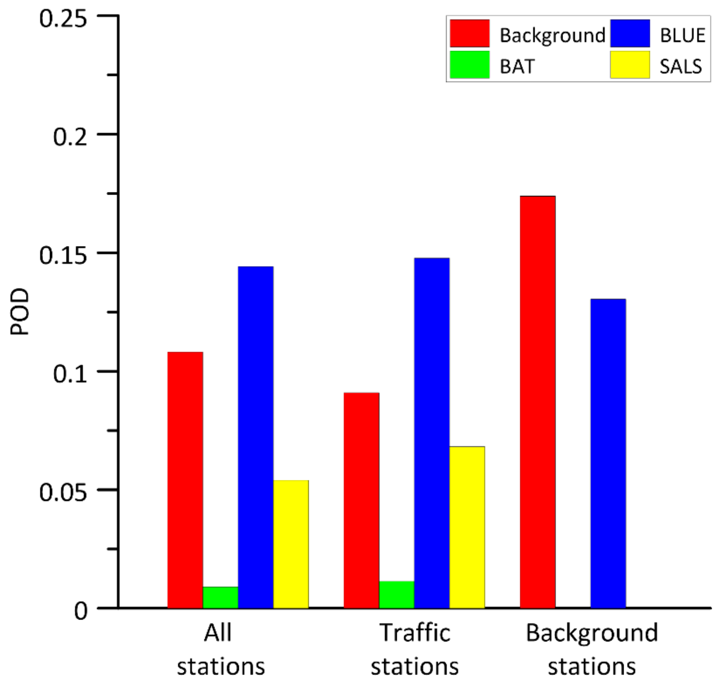
Results: Bias, RMSE and Corr

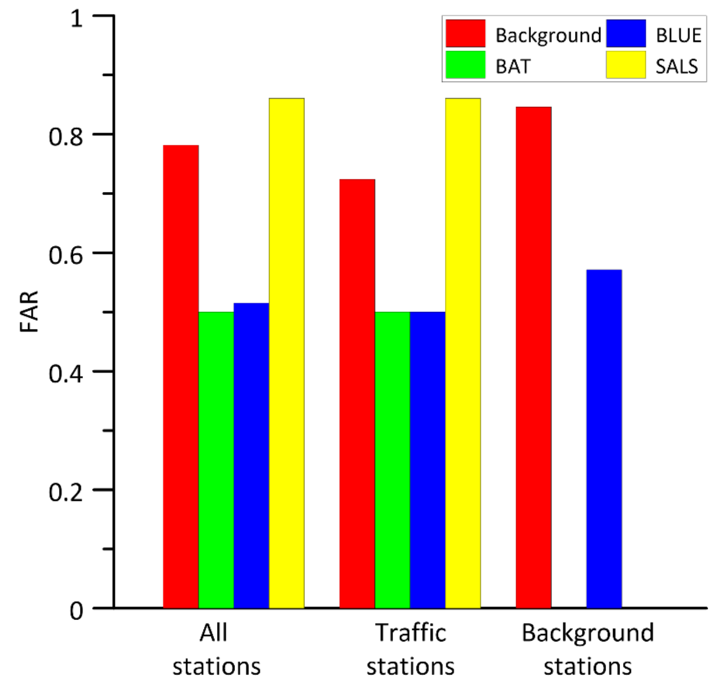


- Mixed results for the Bias
- Improvement of the RMSE (≈ 20 %) and Corr (≈ 10 %)
- The BLUE method leads to the best results

Case study

Results: POD and FAR

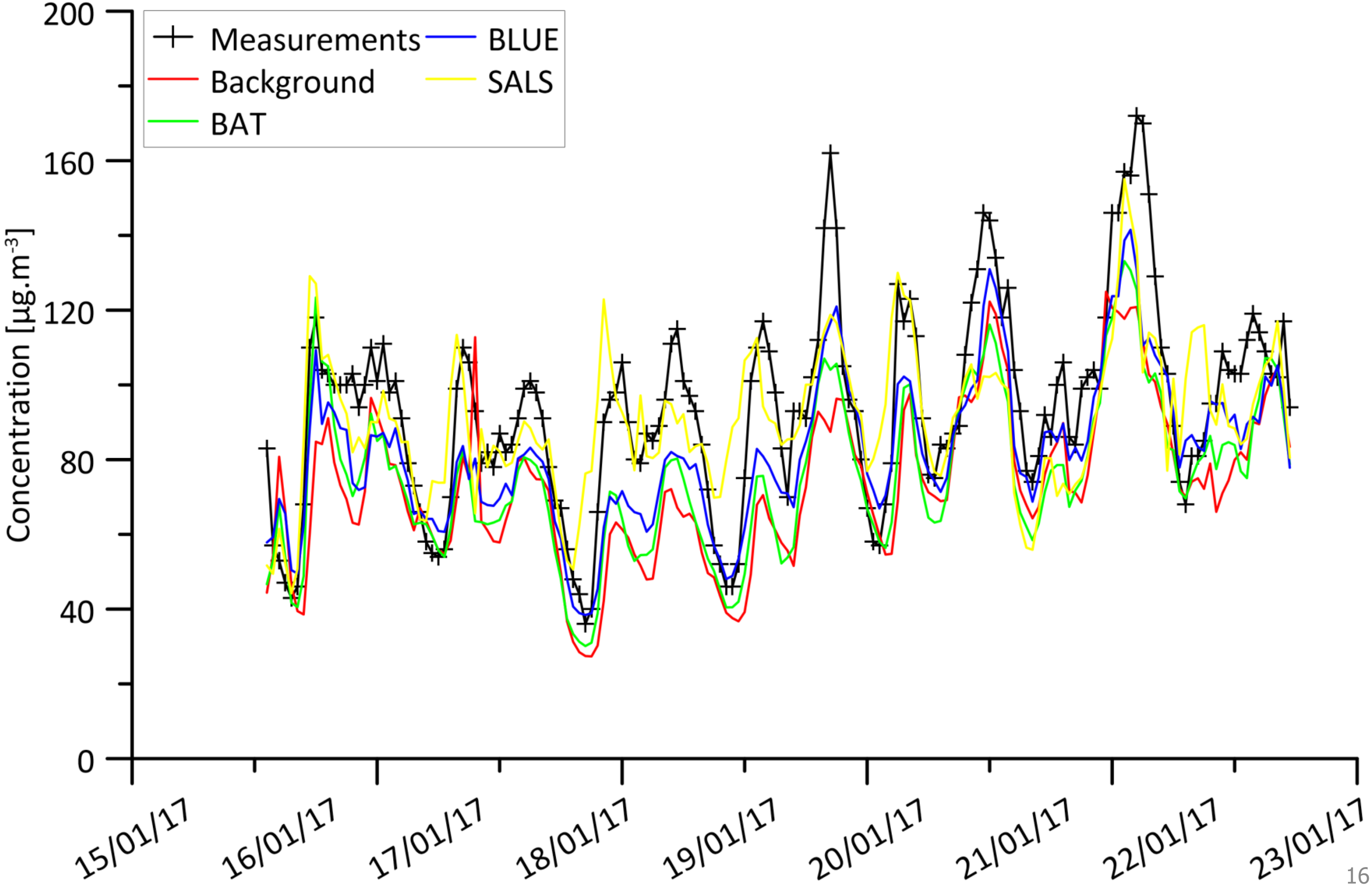




- Improvement of high concentration (> 200 µg.m^{-3}) detection with the BLUE method
  - Increase of the POD from 36 % to 67 % (except for the background stations)
  - Decrease of the FAR from 30 % to 36 %
- However, a significant number of high concentrations remain undetected

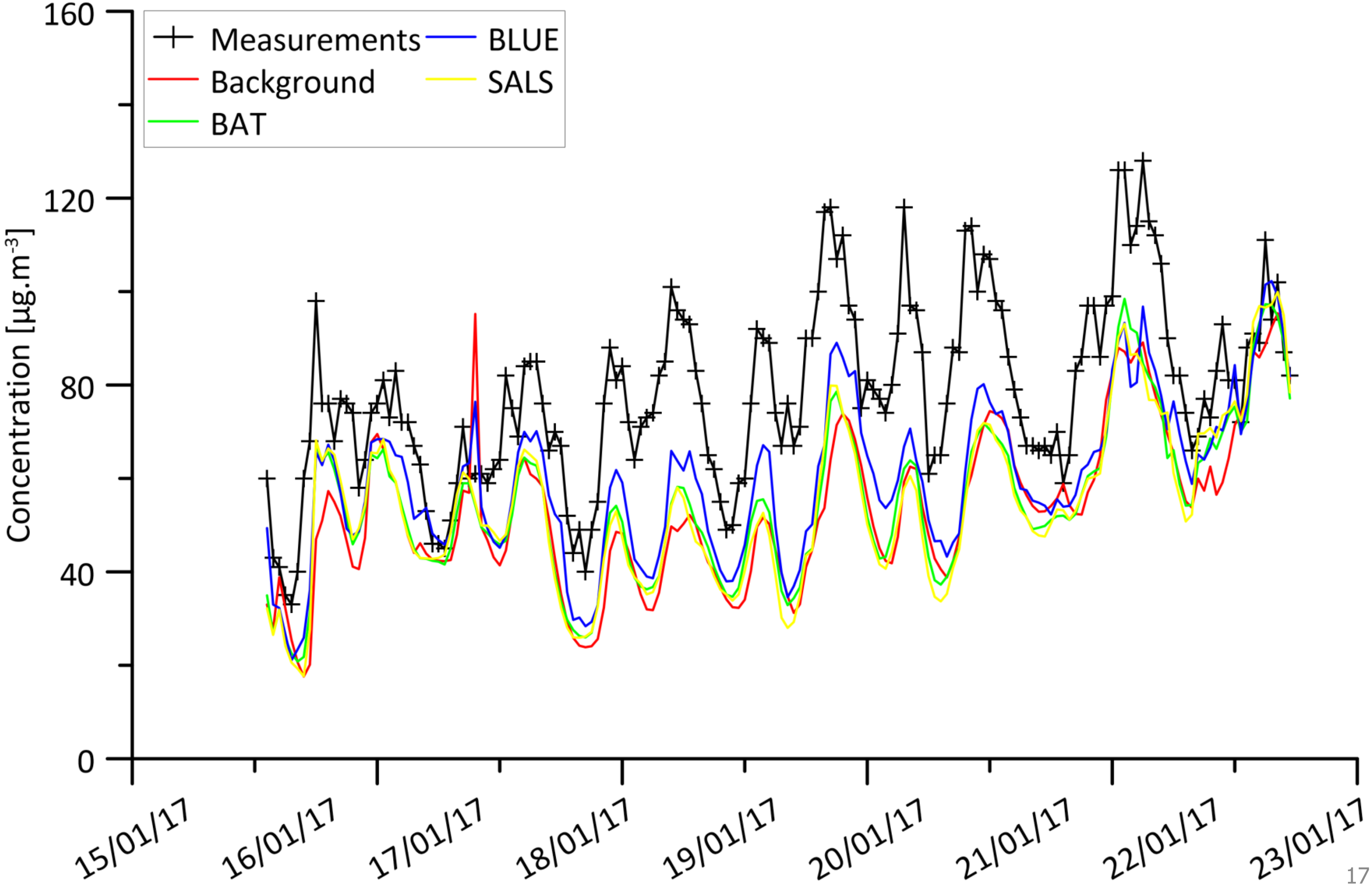
Case study

Results: hourly concentrations (A1)



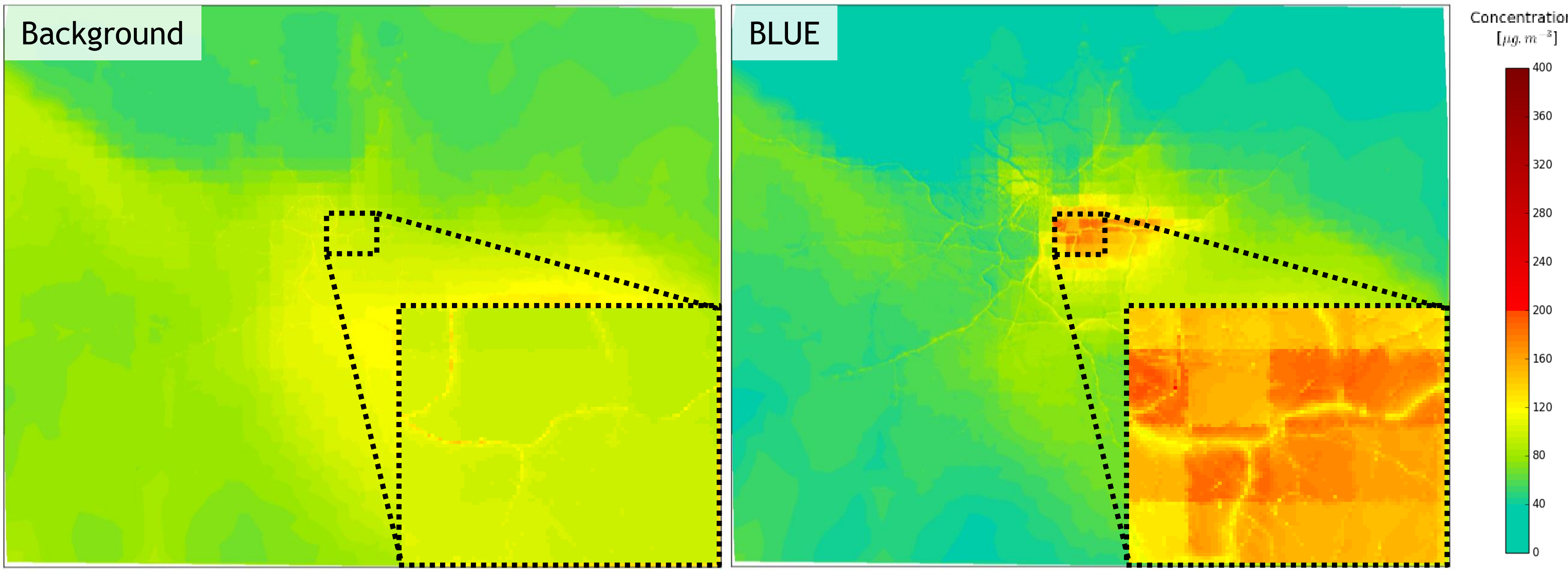
Case study

Results: hourly concentrations (RN2)



Case study

Results: concentration fields (0h 02/12/2016)



- **The BLUE method can lead to concentration fields which are not physically consistent because:**
  - This method is a statistical method which is not governed by physical laws
  - This method is an interpolation of the innovation
  - The matrix $\mathbf{B}$ has a *monotonous behavior* regardless of the innovation

CONCLUSION

Conclusions

- Data assimilation:
  - Global improvement of the statistical indices
  - Sometimes an improvement of the *high* concentration detection
  - Occasionally the estimates are worse after DA

- Performances of the 3 DA methods:
  - Globally the BLUE method leads to the best results
  - The best estimates are not always associated to the same method temporally and spatially

- The BLUE method can lead to concentration fields which are not physically consistent

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Acknowledgements

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Thank you for your attention ☺

Questions ?