Implementation and application of a source apportionment approach in the SIRANE urban air quality model

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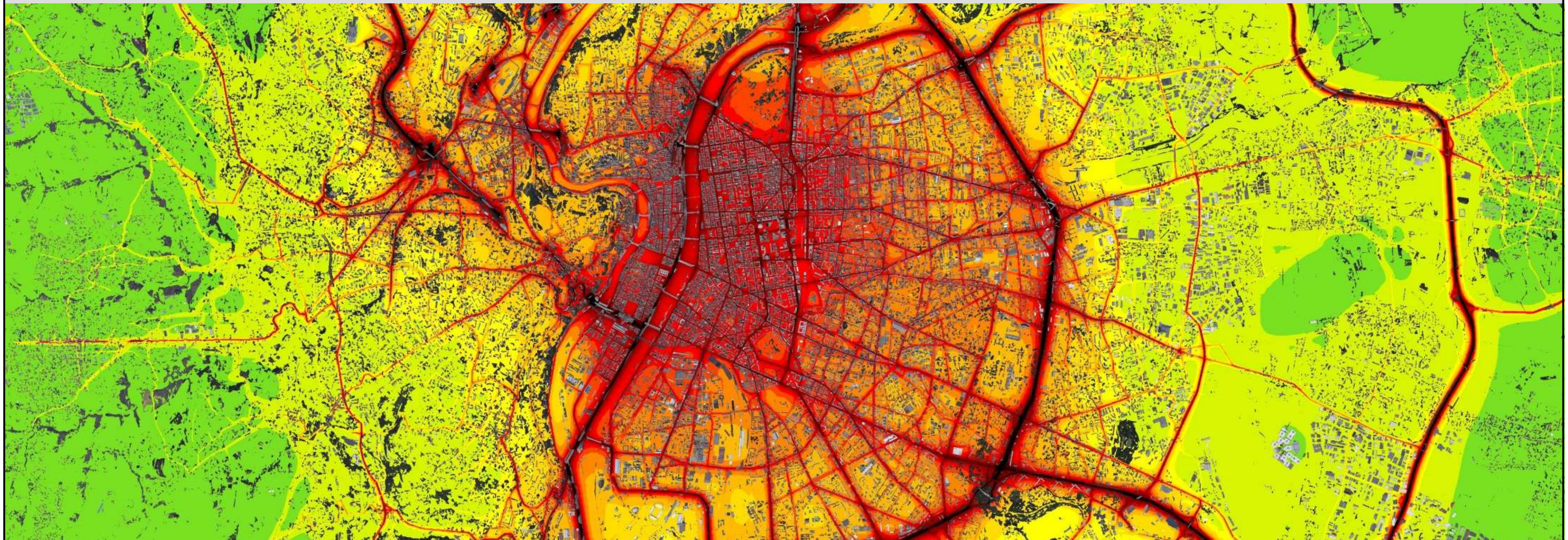
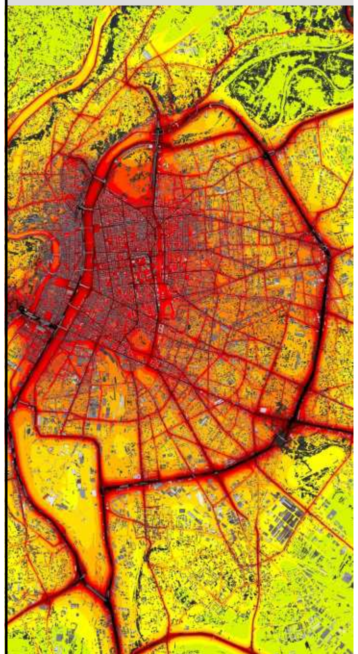


17th Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes Conference

Outline



1. Introduction and motivations
2. Brief description of the SIRANE model
3. Source apportionment (SA)
4. Application to “data assimilation”
5. Conclusions and perspectives

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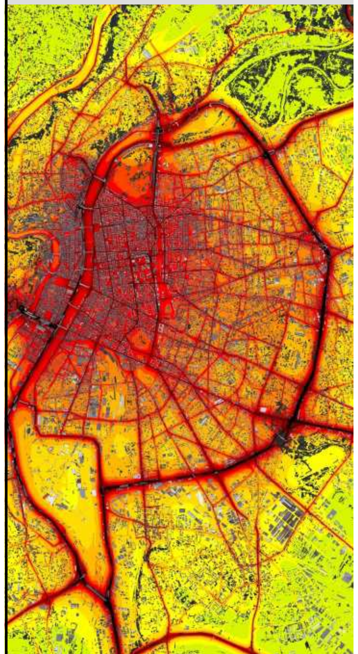

1 – Introduction and motivations

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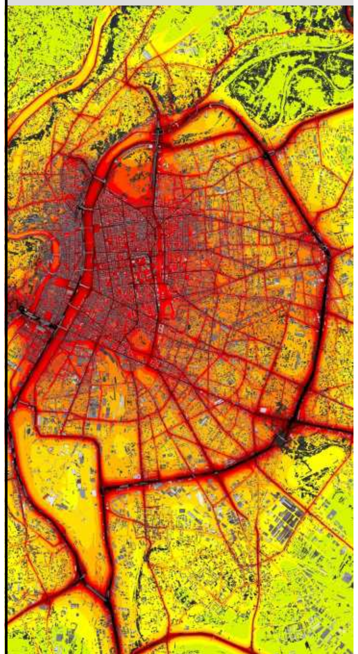
Practical problems motivating urban air quality modelling



- **Urban air quality statistics**
  - Annual statistics according to EU regulatory thresholds
  - Cartography of concentration
  - Population exposure
- **Prediction and operational control**
  - Tomorrow forecast of concentration values
  - Simulation of reduction scenario
- **Urban planning**
  - Impact of a new urban equipment
  - Impact of new traffic plan
  - Impact of new legislation for vehicles or fuel

1 – Introduction and motivations

Motivations for source apportionment

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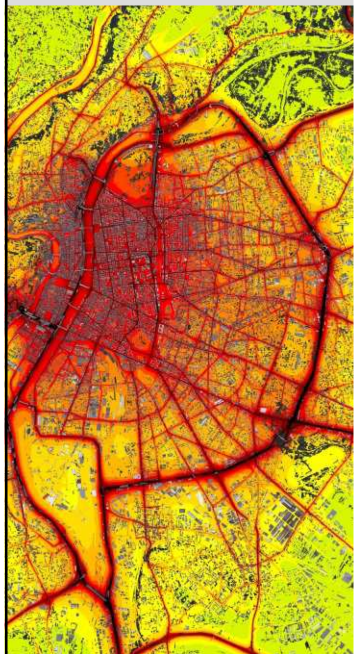
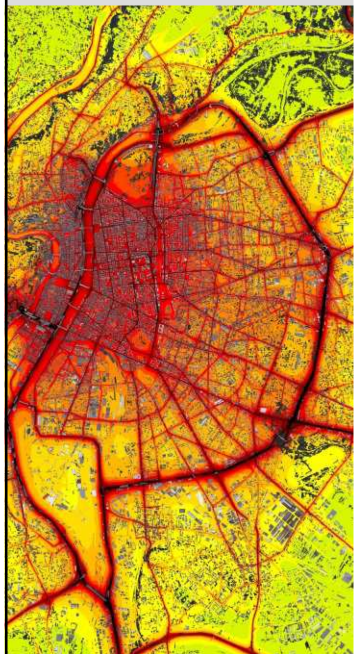


- **Source apportionment motivations**
  - To estimate the origin of concentration at a given location
  - To quantify a priori the effect of a source reduction
  - To adjust emissions in order to reduce model-measurements differences (data assimilation)

- **State of art on source apportionment**
  - Already used in transport & chemistry models at the regional scale
    - CAMx (Wagstrom et al. 2008)
    - CMAQ (Kwok et al., 2013)
  - As we are award, few applications at urban scale (street and district scale)



2 – Brief description of the SIRANE model

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Streets network approach

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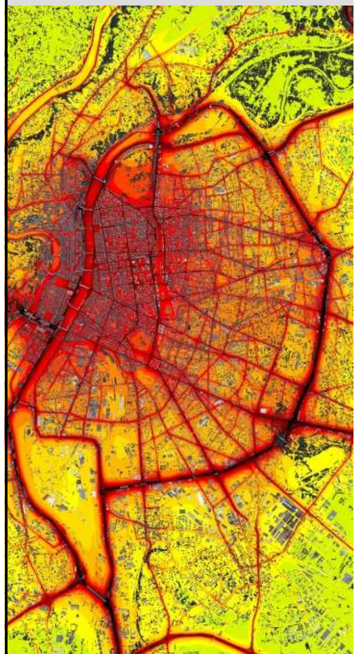
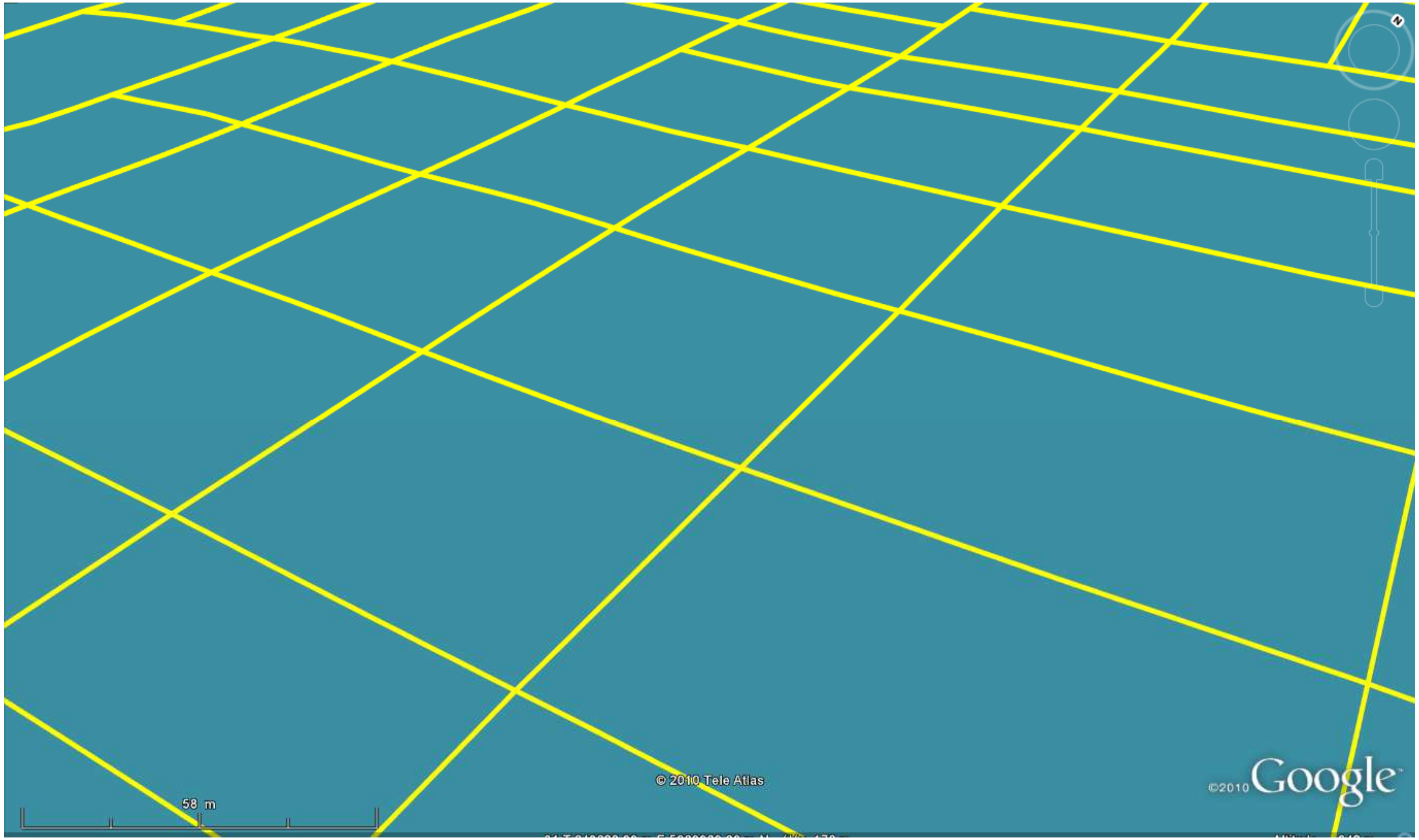
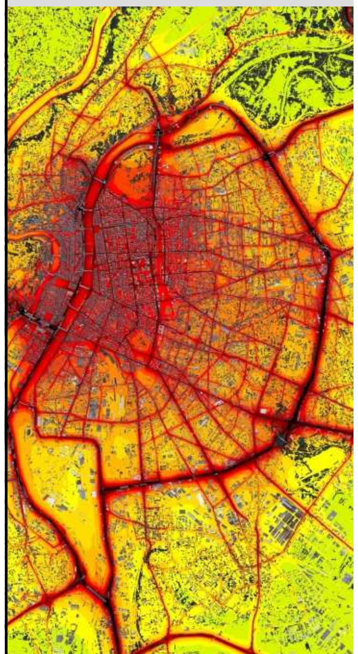
Real geometry → Street volumes → Street-canyons → Network of streets



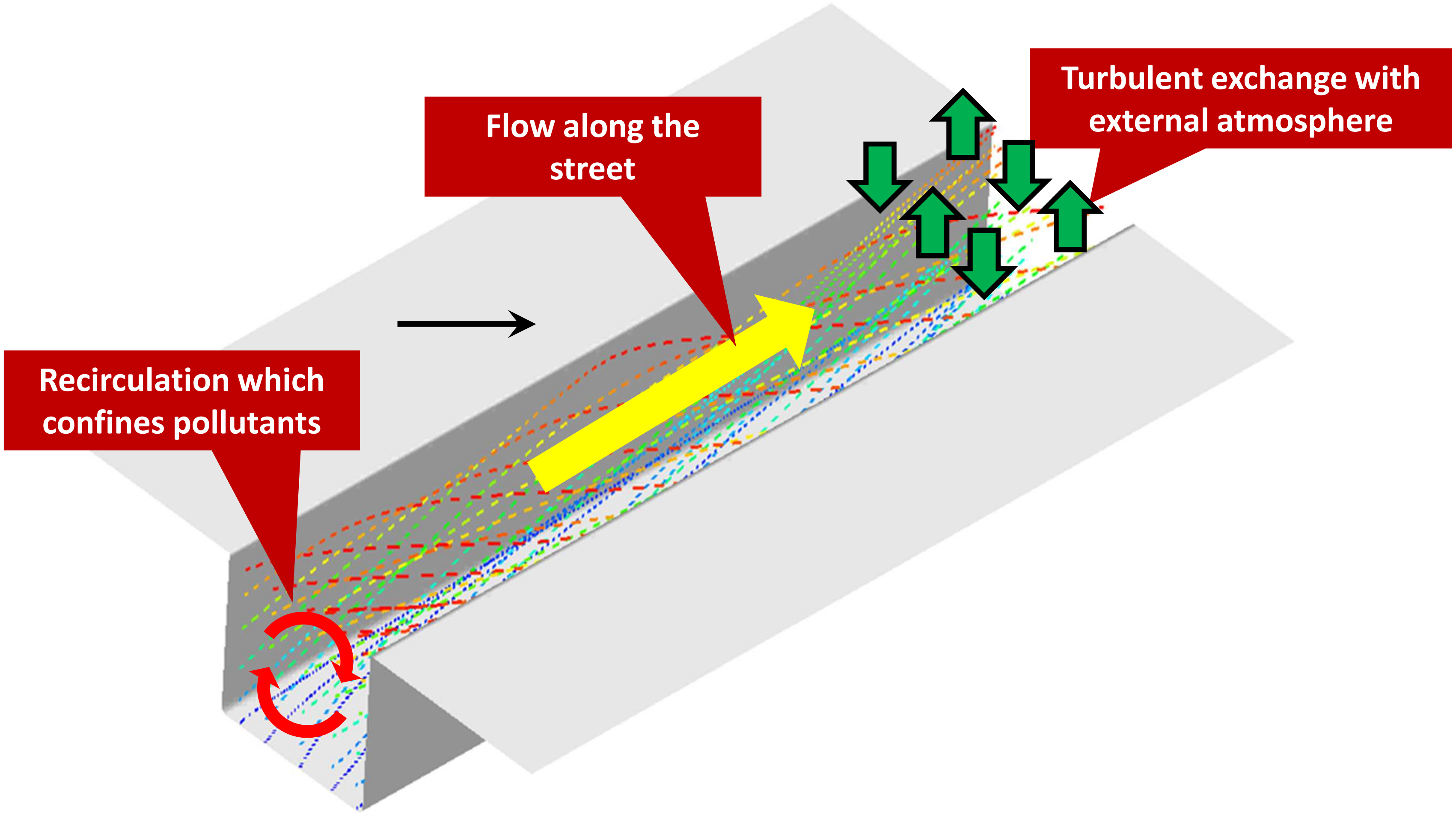


2 – Brief description of the SIRANE model

Phenomenology of the street canyon



- **Flow in a street canyon (Soulhac et al., 2008)**



Soulhac, L., Perkins, R. J. et Salizzoni, P., 2008. *Flow in a street canyon for any external wind direction*, Boundary Layer Meteorology, Volume 126, Issue 3, 365-388.

2 – Brief description of the SIRANE model

Street canyon model

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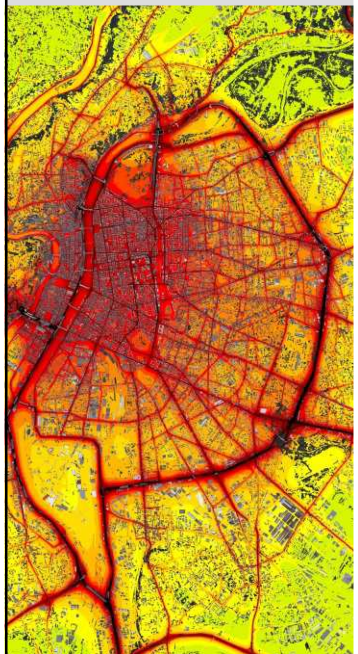
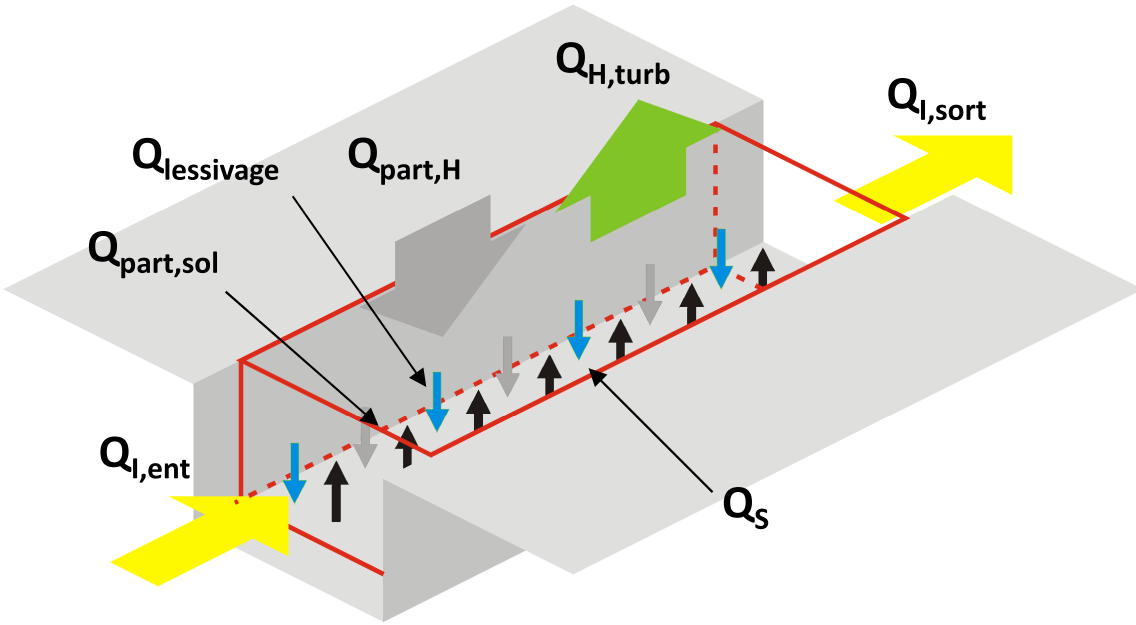


- **Budget of pollutant fluxes within the street**

$$\underbrace{Q_S + Q_{I,ent} + Q_{part,H}}_{\text{Fluxes in}} - \underbrace{Q_{H,turb} + Q_{I,sort} + Q_{part,sol} + Q_{lessivage}}_{\text{Fluxes out}} = 0$$



2 – Brief description of the SIRANE model

Other physical and numerical aspects

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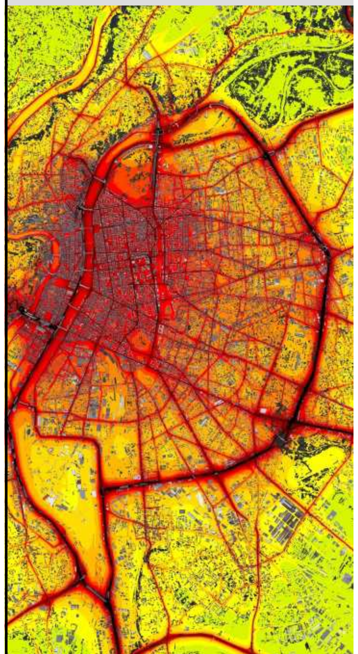
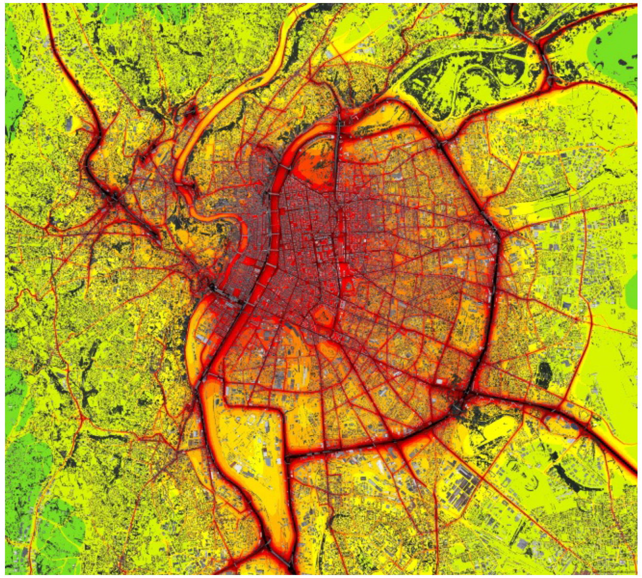


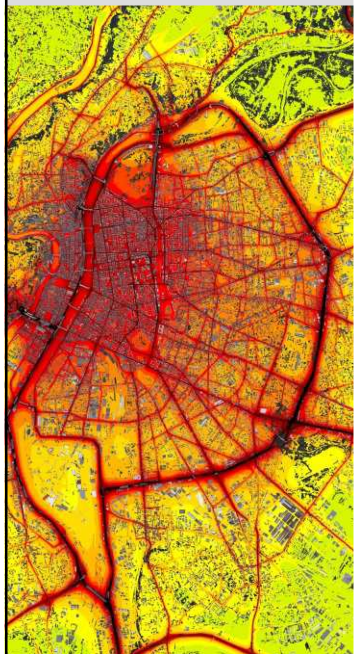
- **Physical processes**
  - Exchanges in intersections
  - Flow and dispersion above the roof level
  - Chapman NO_X chemical model
  - Plume rise model
  - Dry and wet deposition

- **Example of the Lyon city results**
  - Domain: 36 km x 40 km
  - Resolution: 10 m
  - 21922 streets/roads
  - 15 h for 1 year (144 threads)

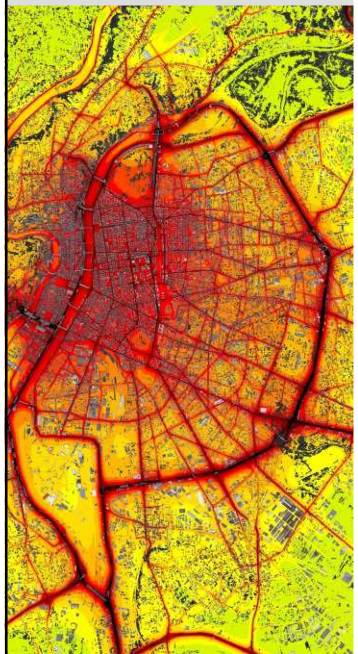


2 – Brief description of the SIRANE model

References and validation studies



- **Flow in the street canyon**
  - Soulhac et al., 2008
  - Soulhac and Salizzoni, 2010
- **Flow at the intersection**
  - Soulhac et al., 2009
- **Exchanges by turbulent diffusion at the street-atmosphere interface**
  - Salizzoni et al., 2011
  - Soulhac et al., 2013
- **Wind tunnel validation studies**
  - Carpentieri et al., 2012
  - Ben Salem et al., 2015
- **Real case validation study**
  - Soulhac et al., 2012



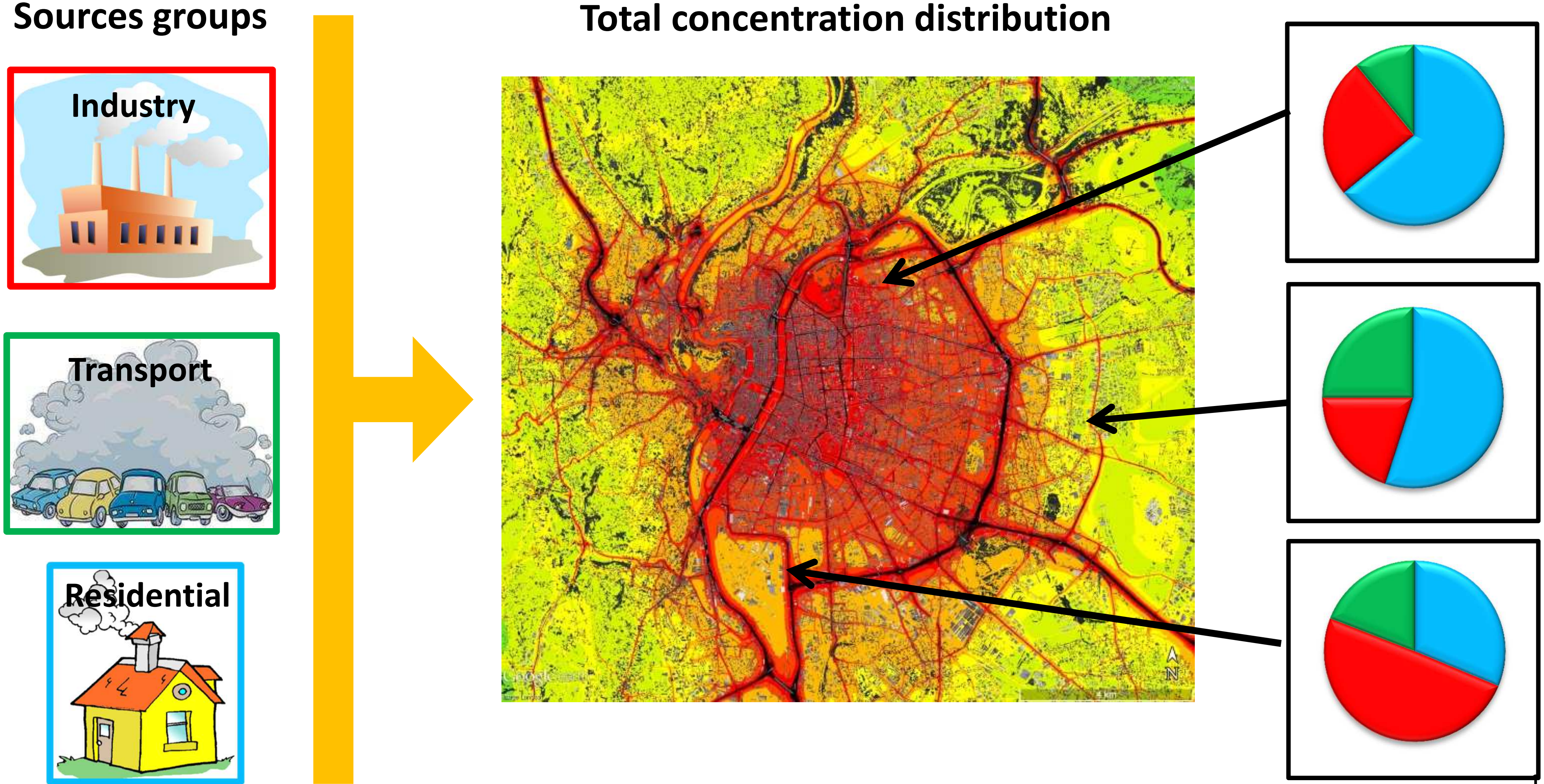
3 – Source apportionment (SA)

3 – Source apportionment
Issue

Sources groups

Total concentration distribution

Source apportionment in different locations



3 – Source apportionment

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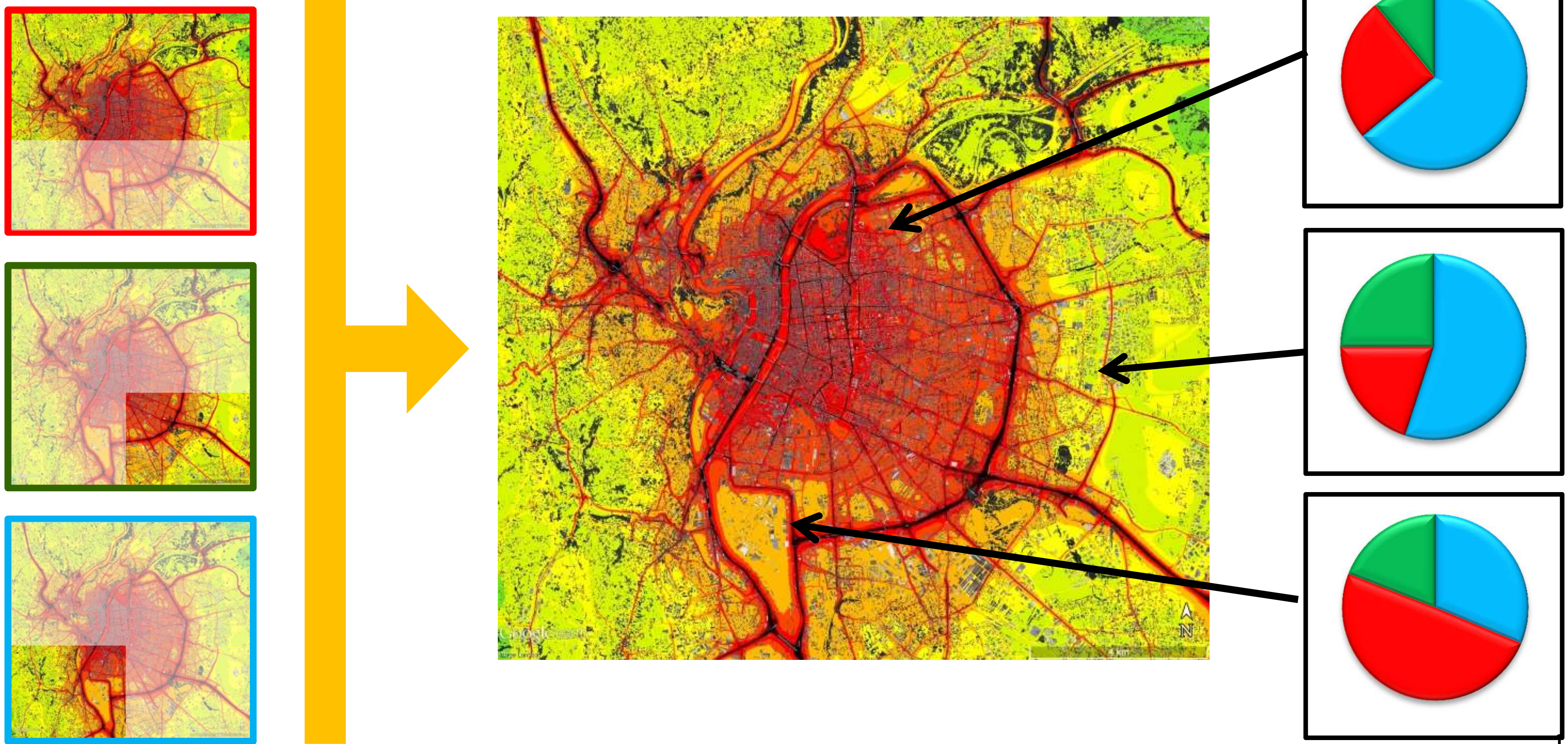
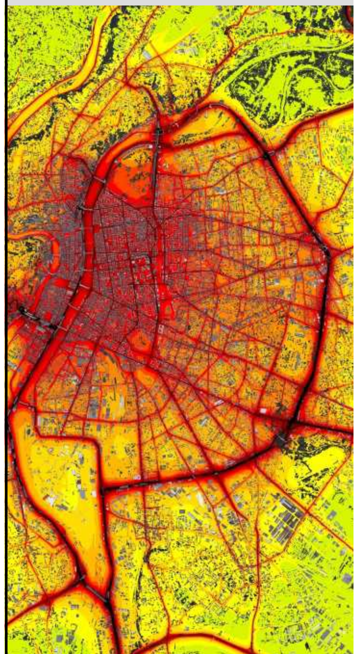


3 – Source apportionment

Implementation in the SIRANE model

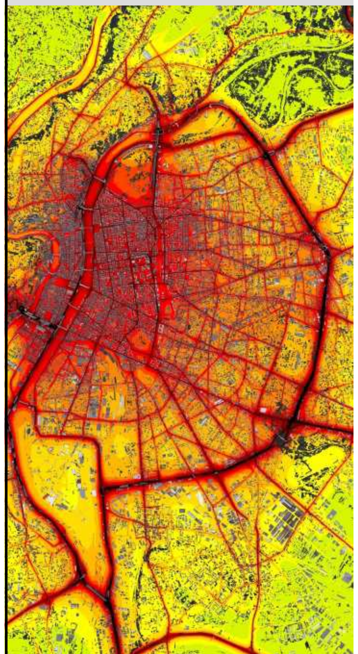


- **Passive species**
  - Linear phenomena
  - Tagged species approach

- **Reactive species**
  - Non-linear phenomena
  - Difficult problem
  - Koo et al. 2009 : “there is no true apportionment to which all methods can be compared”

3 – Source apportionment

Chemical reactions in the SIRANE model



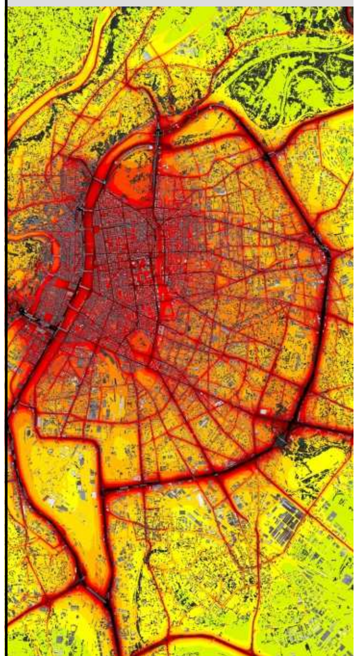
- **Chemical reactions**
  - Chapman cycle

$$\begin{cases} NO_2 + h\nu \xrightarrow{k_1} NO + O^\bullet \\ O^\bullet + O_2 \xrightarrow{k_2} O_3 \\ NO + O_3 \xrightarrow{k_3} NO_2 + O_2 \end{cases}$$

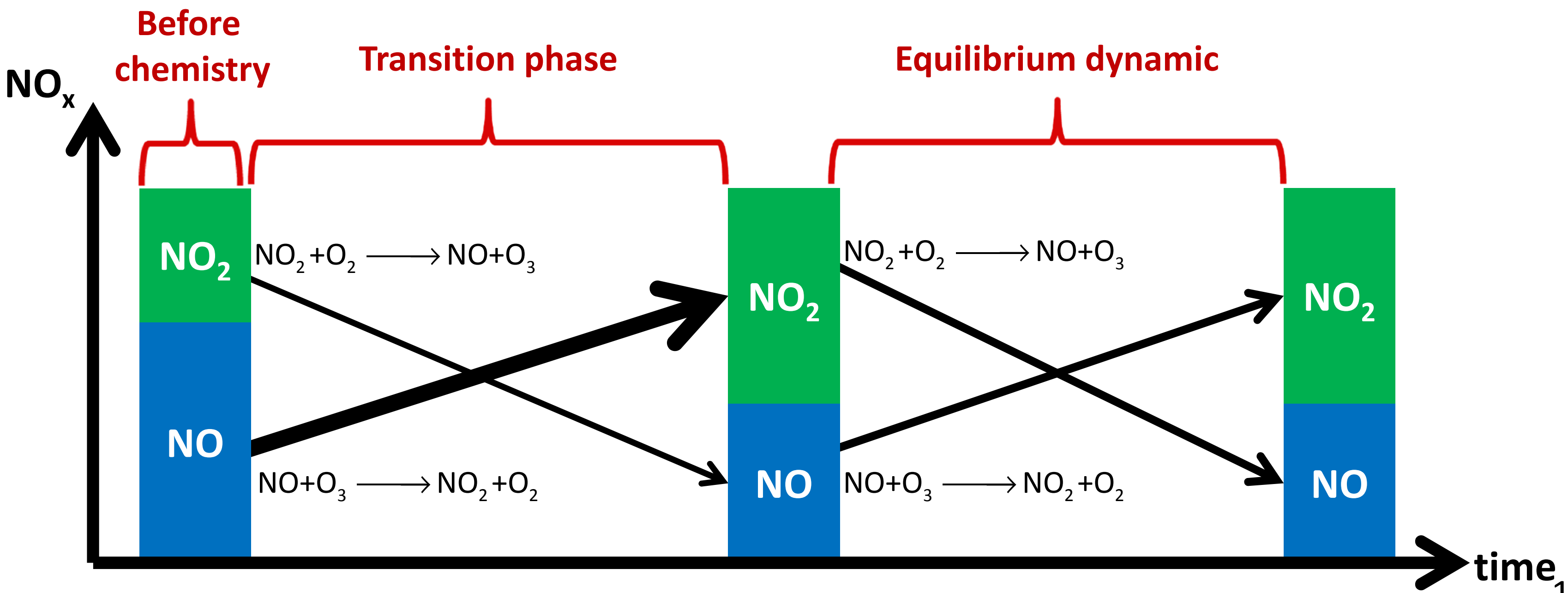
  - Assumption: Photo-stationary dynamic equilibrium

$$NO + O_3 \rightleftarrows NO_2 + O_2 \qquad \frac{k_1}{k_3[O_3]} = \frac{[NO]}{[NO_2]}$$

- **Remarks**
  - Chemical reactions are implemented after the dispersion step
  - $[E^d]$: molar concentration of the specie E before chemical reactions
  - $[E]$: molar concentration of the specie E after chemical reactions



- **Global approach**
  - <u>Assumption:</u> All the molecules of a specie have the same probability of reacting regardless of their source
  - <u>First step:</u> chemical reactions are applied without distinction of the different source groups
  - <u>Second step:</u> the source contributions are estimated as a fraction of the total concentration



3 – Source apportionment

Treatment of the chemical reactions

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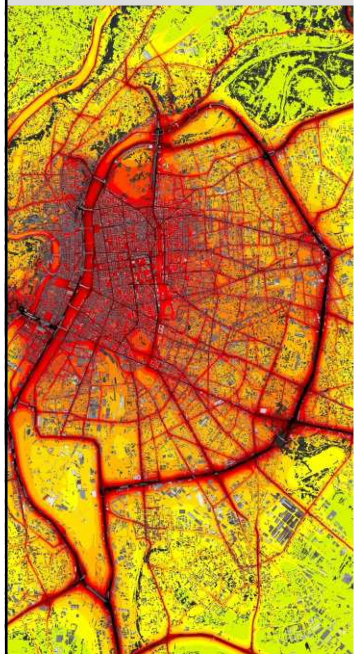


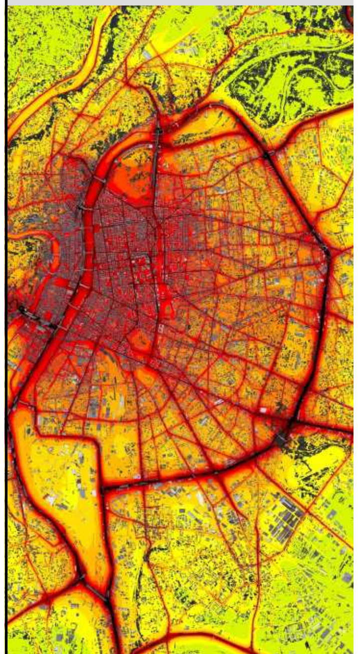
- **Method 1 (M1)**
  - Assumption: $$\left(\frac{\left[NO^d\right]}{\left[NO_2^d\right]}\right) > \left(\frac{[NO]}{[NO_2]}\right)$$
  - The chemical reactions can be simplified as: $NO + O_3 \rightleftharpoons NO_2 + O_2$
  - The production of NO_2 and the consumption of NO and O_3 for the source g is function of $[NO^d]_g$:

$$[E]_g = \left[E^d\right]_g + \left([E] - \left[E^d\right]\right)\frac{\left[NO^d\right]_g}{\left[NO^d\right]}$$

- **Remarks on M1**
  - The contribution can negative
  - A source must emit NO to contribute to [NO]

3 – Source apportionment

Treatment of the chemical reactions



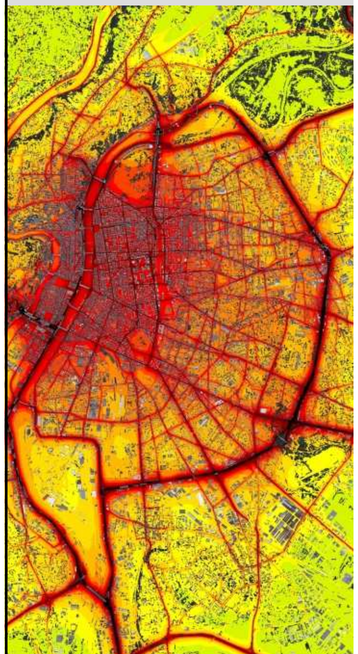
- **Method 2 (M2)**
  - Considering: $NO + O_3 \longleftrightarrow NO_2 + O_2$
  - Assumption: The total source contribution for the NO_x (NO and NO_2), species is equal before and after the chemical reactions and the contribution is similar (proportionally) for each specie after the chemical reactions

$$[E]_g = [E]\frac{\left[NO^d\right]_g + \left[NO_2^d\right]_g}{\left[NO^d\right] + \left[NO_2^d\right]}$$

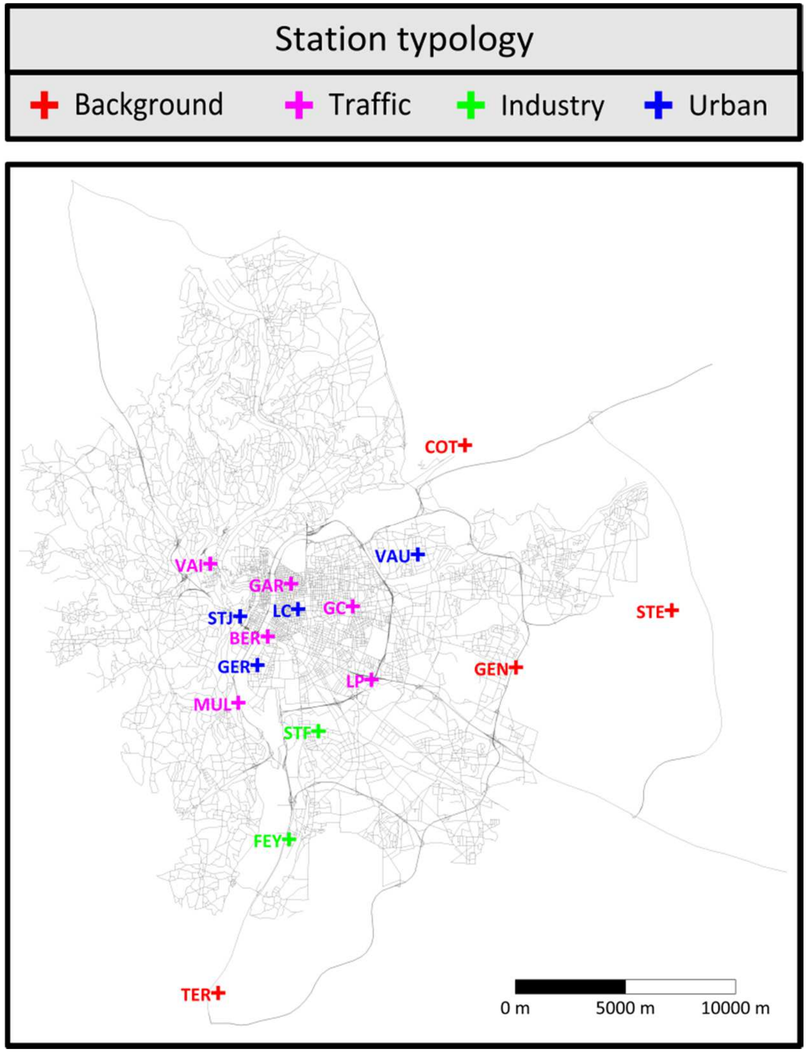
- **Remarks on M2**
  - The contribution are only positive
  - Regardless the emitted species, a source contribute to [NO], $[NO_2]$, and $[O_3]$

3 – Source apportionment

Application: estimate the source contribution

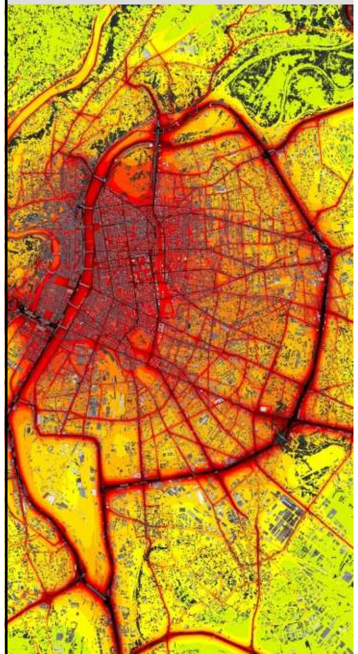


- **Scenario:**
  - Place: Lyon city (France)
  - Period: 2008
  - Pollutant: NO_2
  - 16 measurement stations
  - Sources groups:
    - Traffic
    - Residential
    - Industry
    - Background

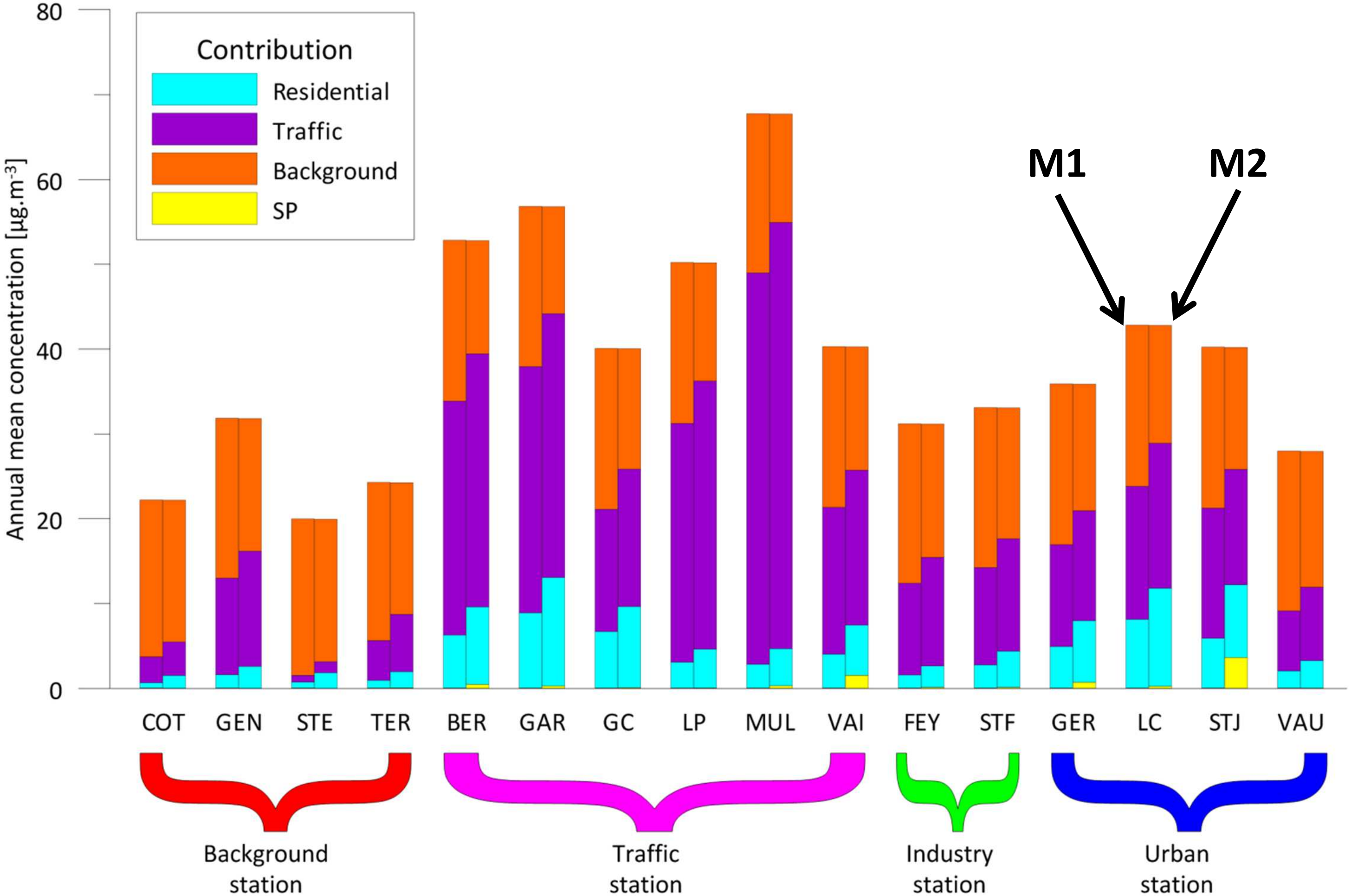


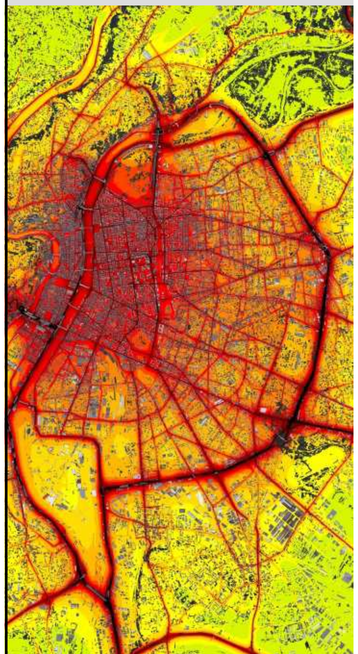
3 – Source apportionment

Application: estimate the source contribution



Contribution to the NO_2 annual mean concentration at the measurement station (left and right column refer respectively to the method 1 and 2)





4 – Application for “data assimilation”

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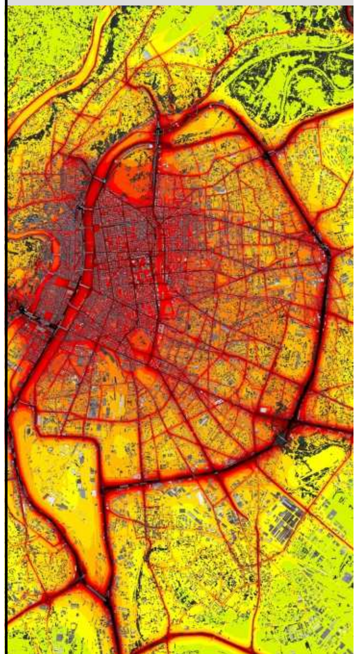
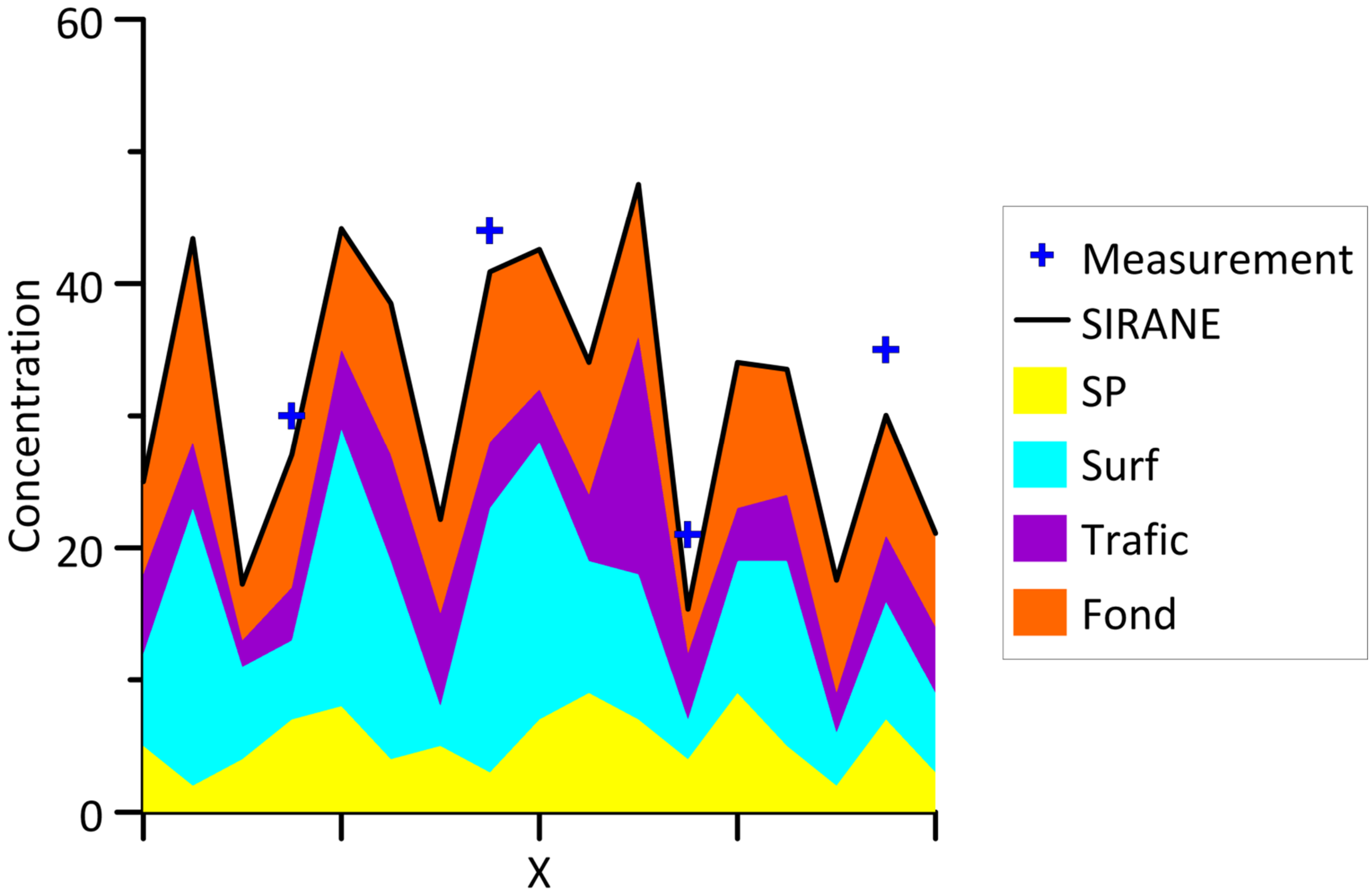
Principle

- **Aim: Correct the emissions to improve the model estimation**

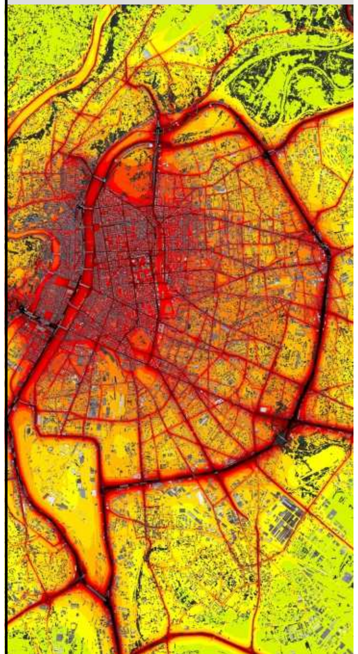


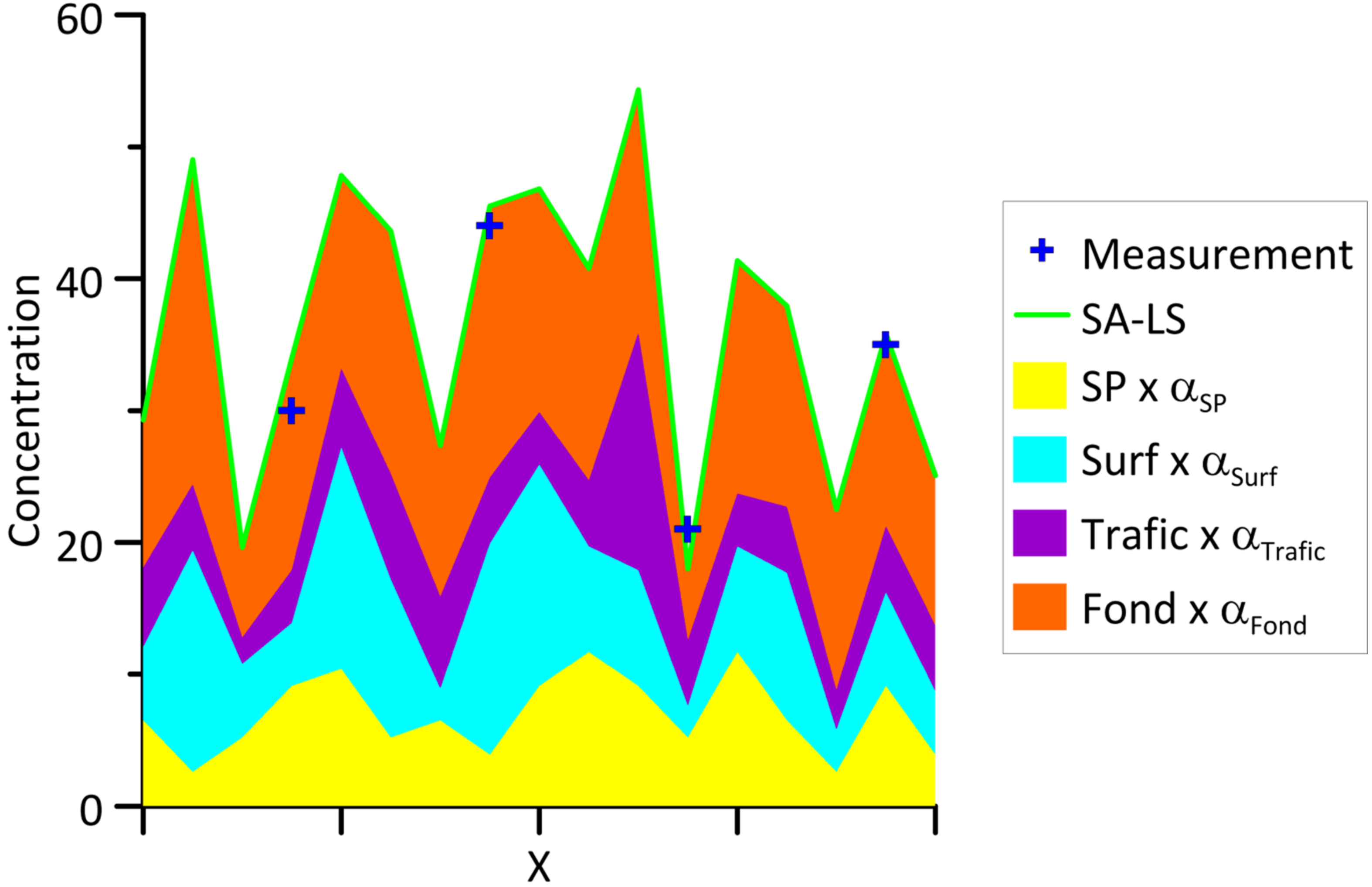


4 – Application for “data assimilation”

Principle

- **Aim: Correct the emissions to improve the model estimation by multiplying the contribution with a coefficient**





4 – Application for "data assimilation"

Algorithm (SA-LS)

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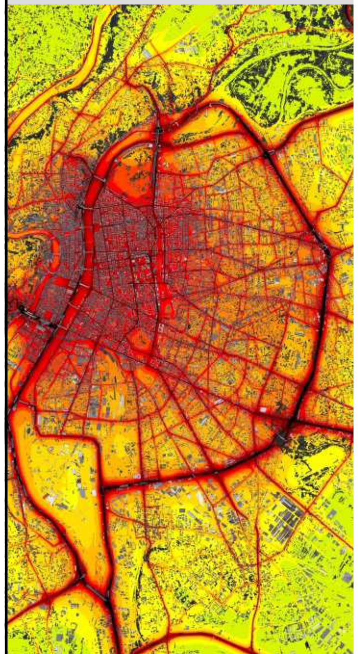


- **The total concentration is the sum of the source contributions**

$$C = \sum_{g}^{G} C_g$$

- **Determination of the optimal concentration**

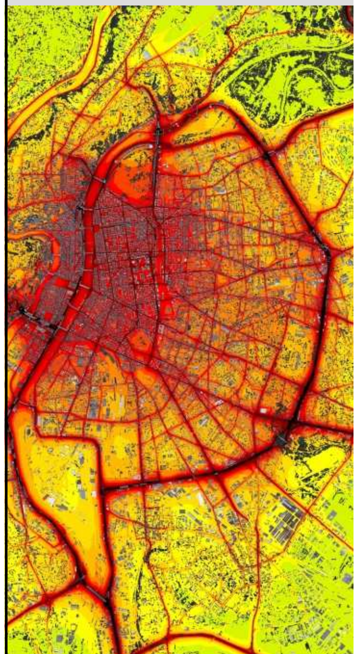
$$\hat{C}(s_i, t_n) = \sum_{g}^{G} \alpha_g(t_n) C_g(s_i, t_n)$$

- **The $\alpha_g(t_n)$ coefficients are calculated at each time step minimizing the J_n quantity**

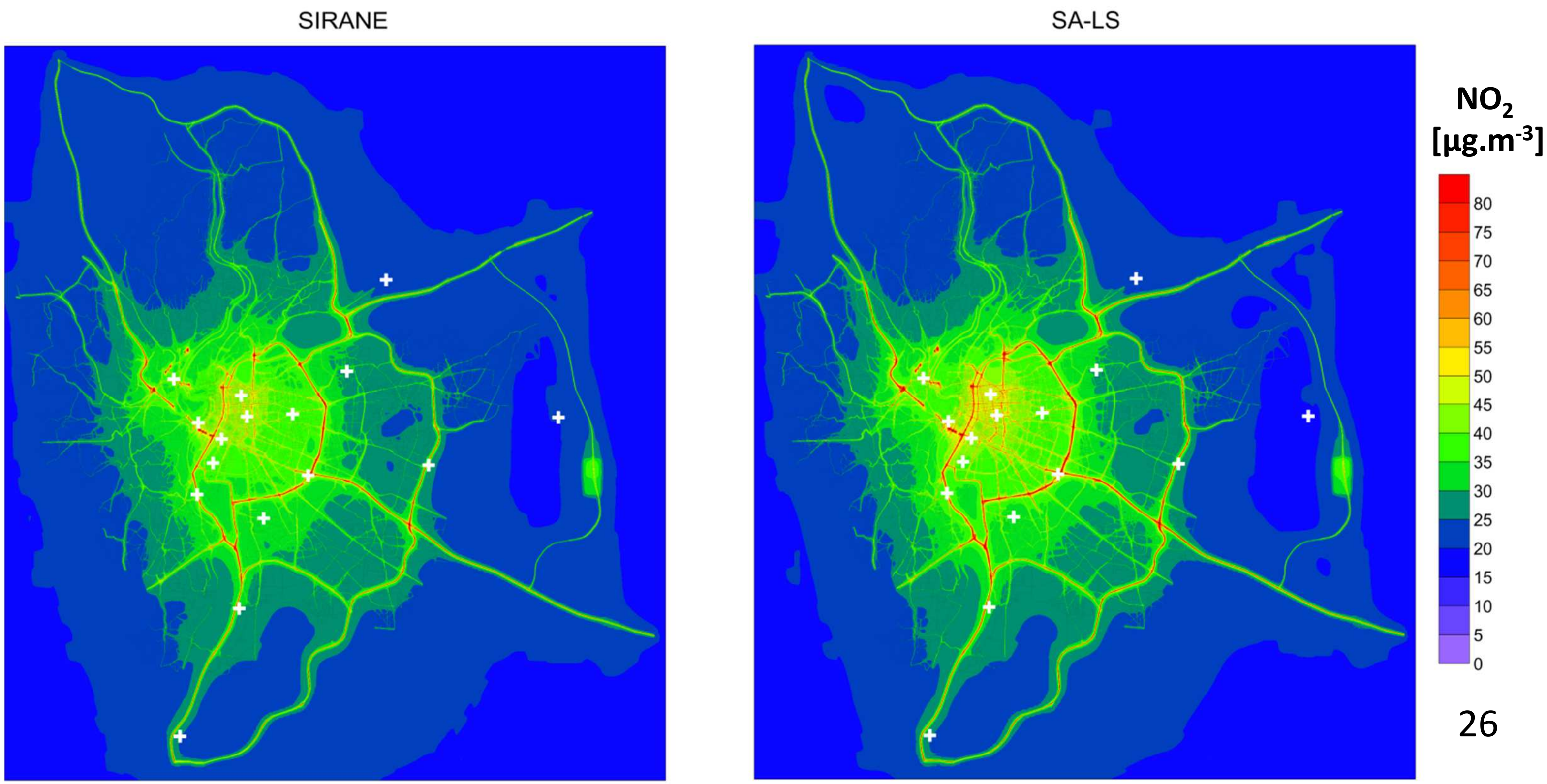
$$J_n = \frac{1}{m} \sum_{i}^{m} \left(C_{mes}(s_i, t_n) - \sum_{g}^{G} \alpha_g(t_n) C_g(s_i, t_n) \right)^2$$

4 – Application for "data assimilation"

Application

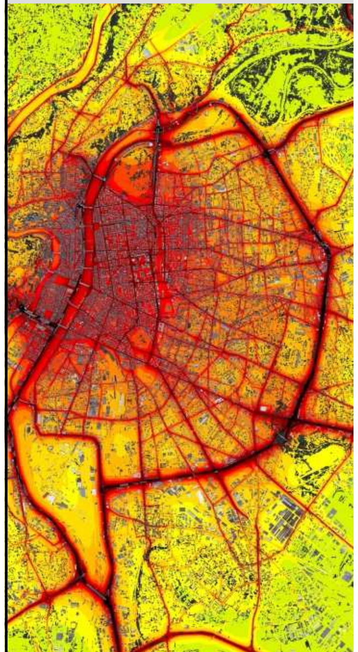


	Bias [µg.m^{-3}]	RE	RMSE [µg.m^{-3}]	Corr
Expression	$\overline{C_m - C_p}$	$\overline{\left(\frac{\lvert C_m - C_p \rvert}{C_m}\right)}$	$\sqrt{\overline{(C_m - C_p)^2}}$	$\frac{\overline{(C_m - \overline{C_m})(C_p - \overline{C_p})}}{\sigma_m \sigma_p}$
SIRANE	3.51	0.48	20.68	0.69
SA-LS	**0.30**	**0.43**	**18.15**	**0.80**



4 – Application for “data assimilation”

Application



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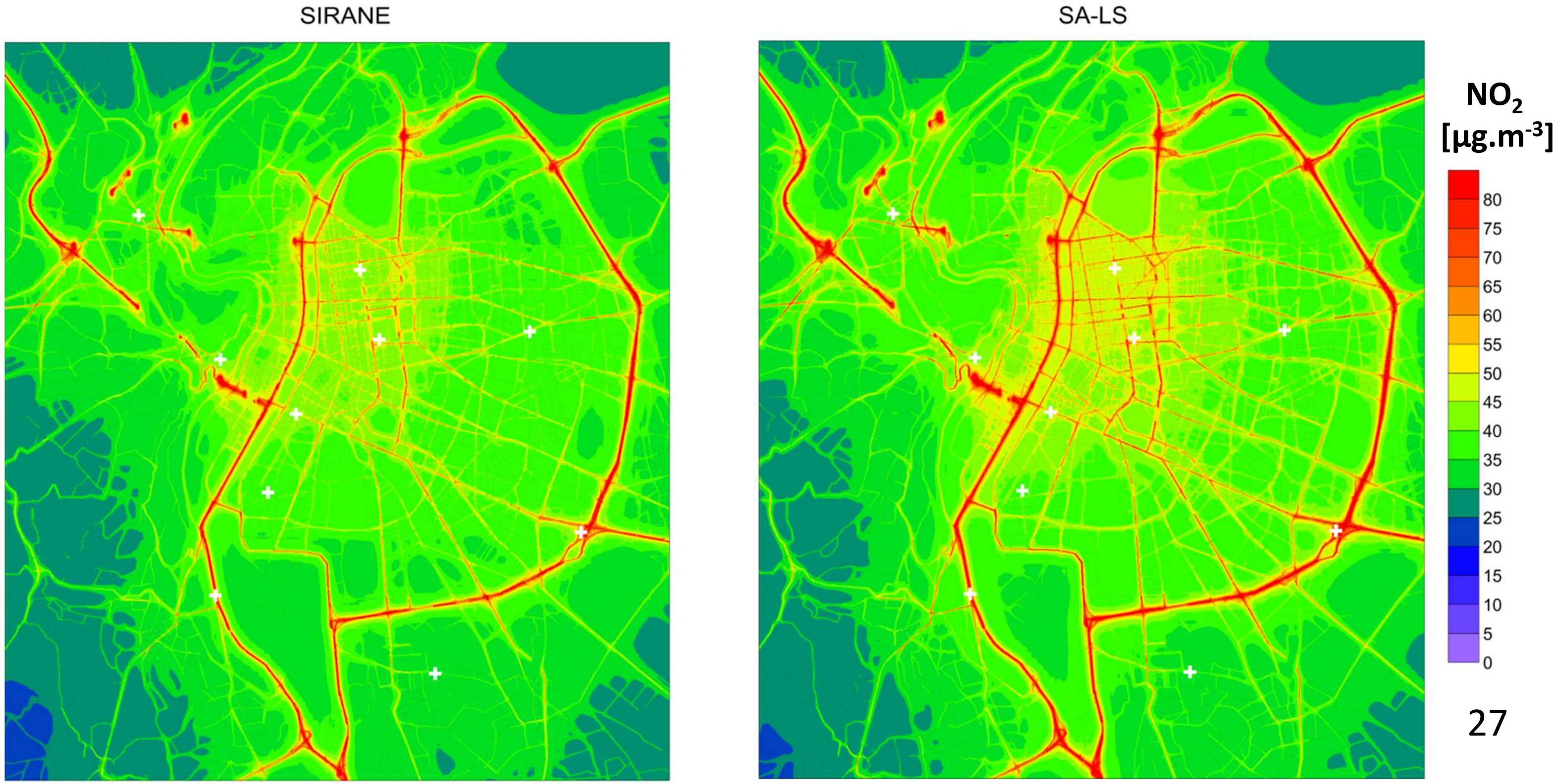

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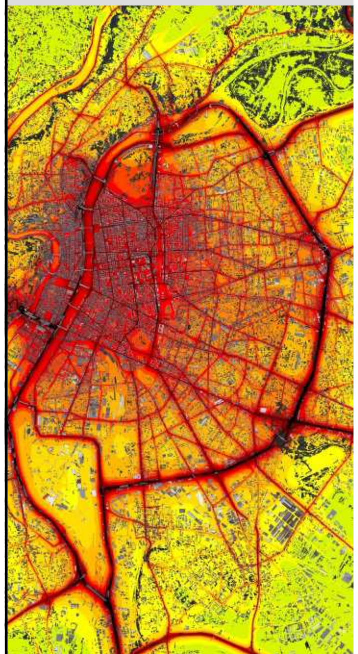

5 – Conclusions and perspectives

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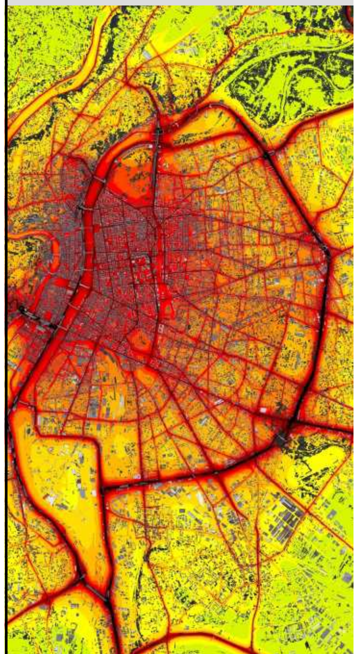
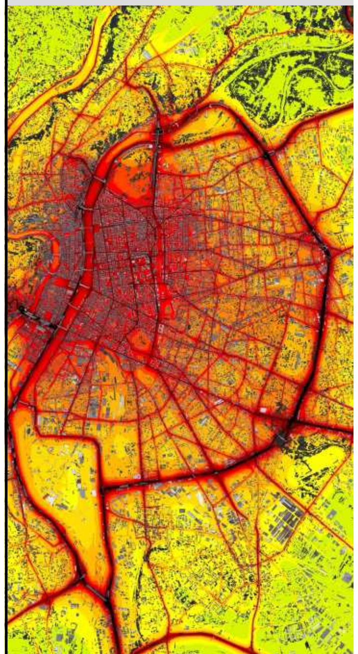


- **Source apportionment**
  - Development of source apportionment module in the SIRANE urban air quality model
  - Two different approaches to handle the chemical reactions

- **Application for “data assimilation”**
  - Least square problem
  - Can improve the global estimation of the SIRANE model

- **Perspectives**
  - Comparison of the application for “data assimilation” with other assimilation techniques (see the poster H17-178)



Thank you for your attention ☺

Questions ?