

# WG1 - Source apportionment

Exercise SA

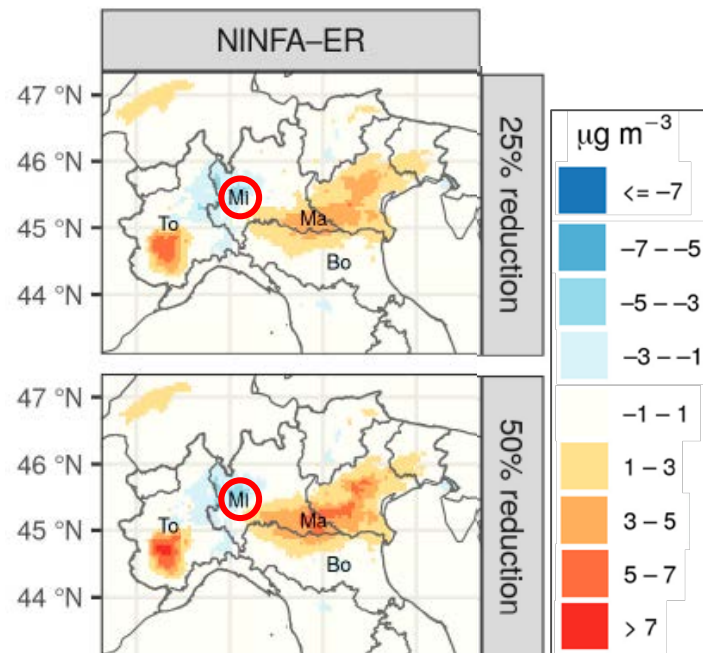


# Exercise 1



# Chemical Regime NO<sub>x</sub> vs. NH<sub>3</sub>

Atmosphere 2023, 14, 762. <https://doi.org/10.3390/atmos14050762>



Article

## Impact of NO<sub>x</sub> and NH<sub>3</sub> Emission Reduction on Particulate Matter across Po Valley: A LIFE-IP-PREPAIR Study

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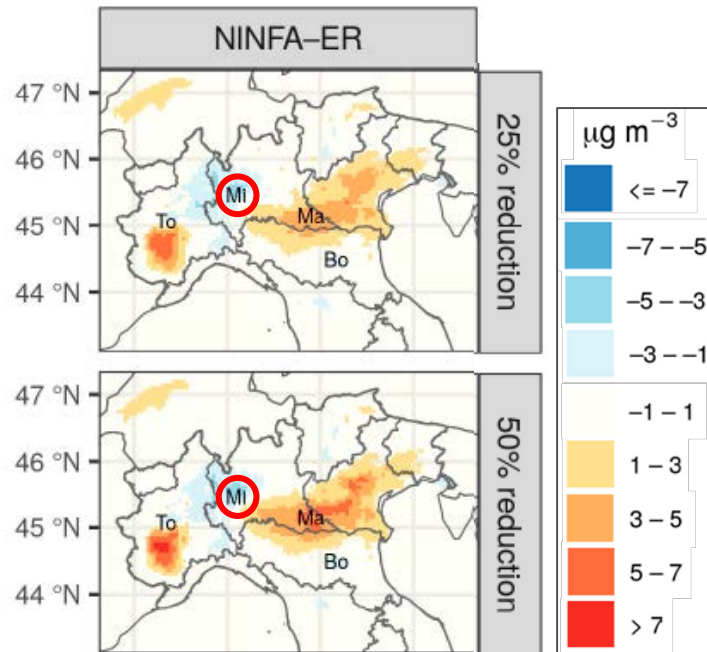
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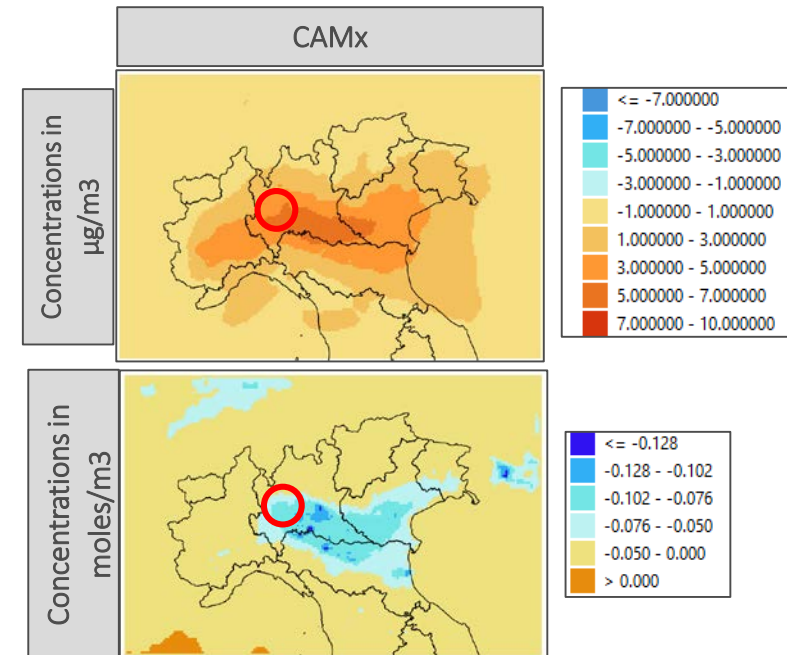


# Chemical Regime NOx vs. NH3

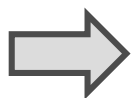
Difference  $P_{NOx}^\alpha - P_{NH3}^\alpha$  based on NINFA/Brut Force for  $\alpha=25\%$  and  $\alpha=50\%$



Difference  $\text{Cnt}_{NOx}(\text{NO}_3^-) - \text{Cnt}_{NH3}(\text{NH}_4^+)$  based on CAMx/PSAT



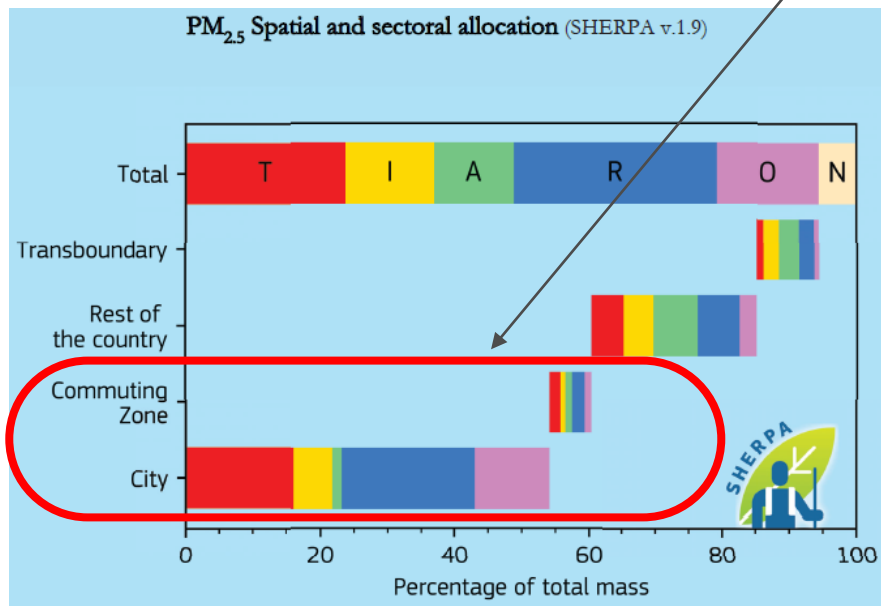
Which precursor would you recommend to reduce in priority in the Milan area to abate PM2.5 concentration?



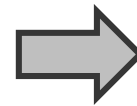
*NH3 because its reduction impacts more the PM concentrations than the reduction of NOx*

# Spatial Scale and Sectorial Impacts

The decision maker, who mandates you, can only take decision in the area of Milan

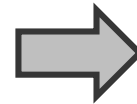


Which activity sectors should be reduced to produce the largest impact on PM abatement (in the city and commuting zone)?



*Residential and transport have the highest impact  
Other sources and Industry have a lower impact  
Agriculture have the lowest impact*

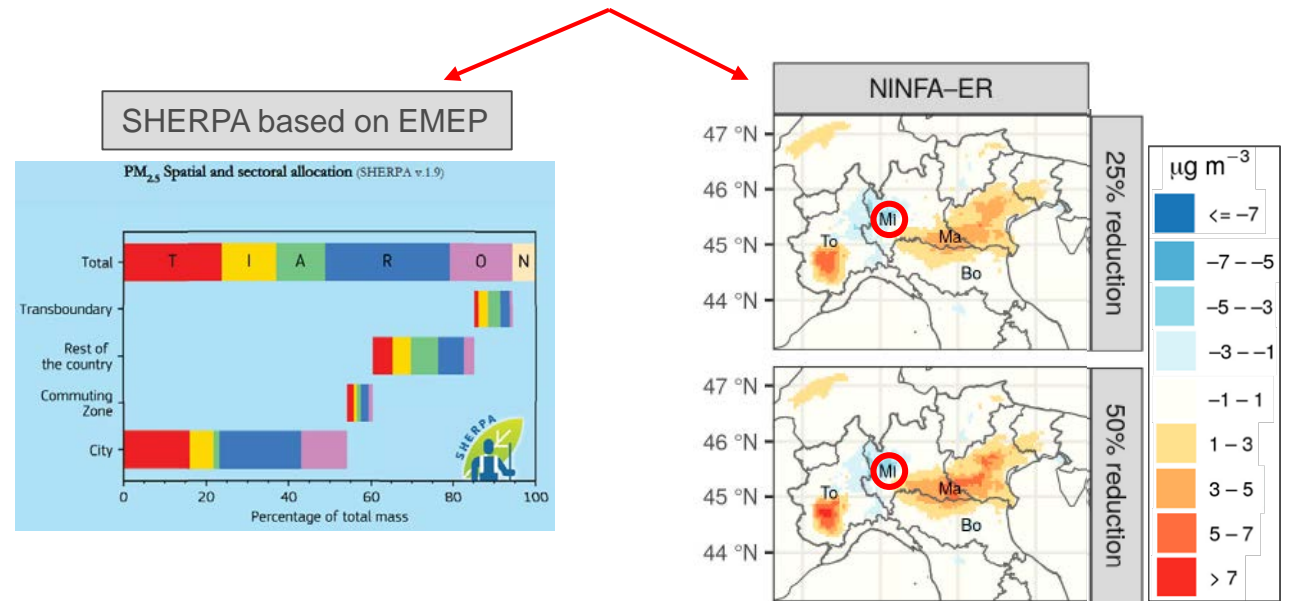
Could this recommendation be in contradiction with the previous one?



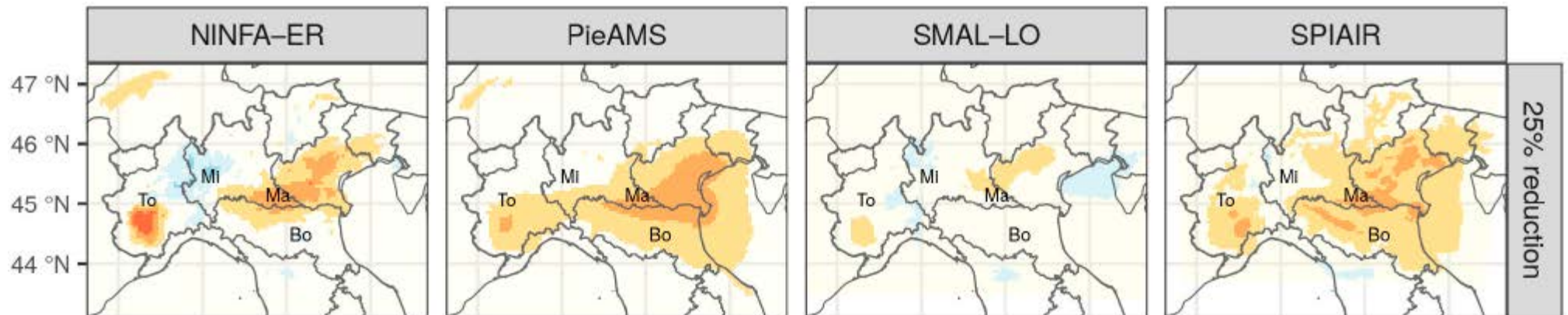
*NH3 is mainly emitted by Agriculture, while NOx is mainly emitted by Transport and Industry. A reduction of NOx should lead to a higher reduction of PM than a reduction of NH3 which seems to be in contraction with the previous conclusion.*

# Why?

« Model systems » are different

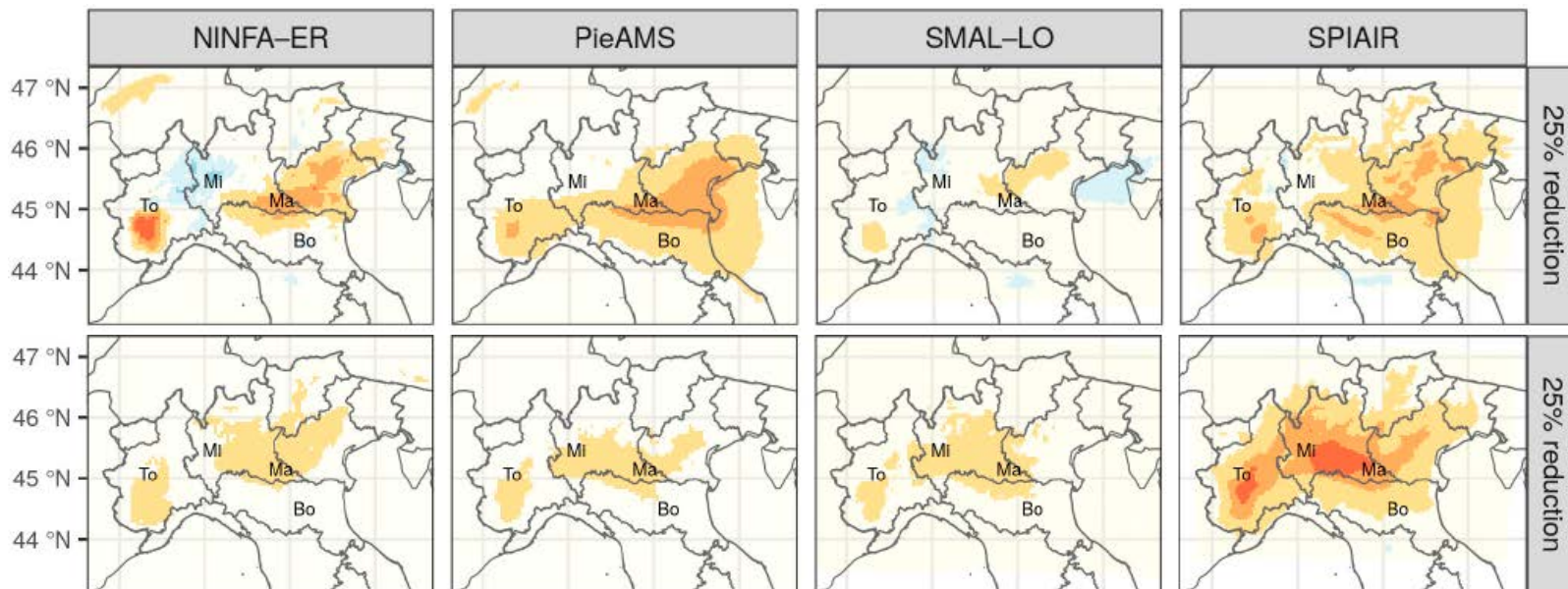
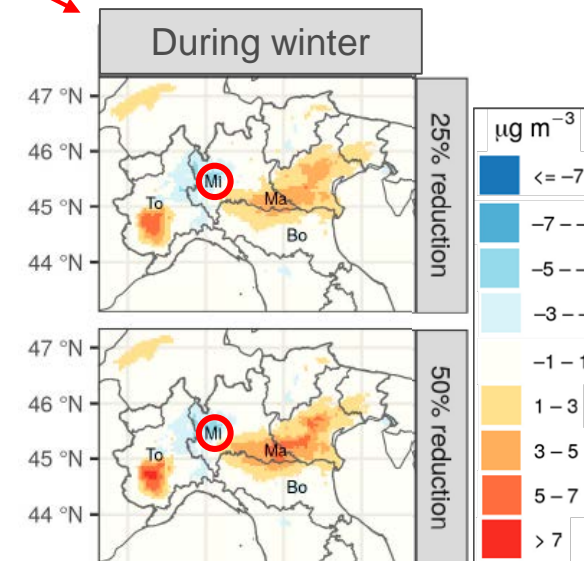
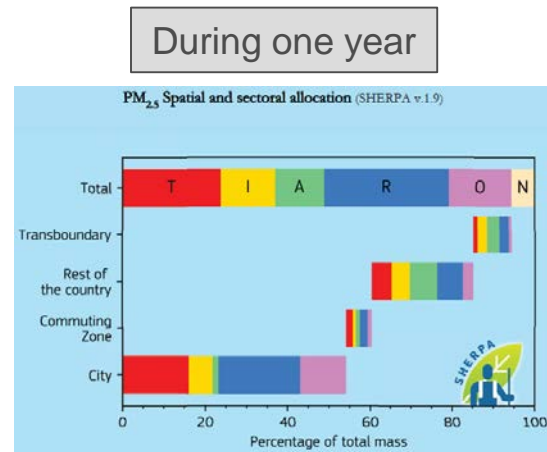


## Comparison between different models



# Why?

- « Model systems » are different
- Time scale are different  
(was not indicated in the exercise)

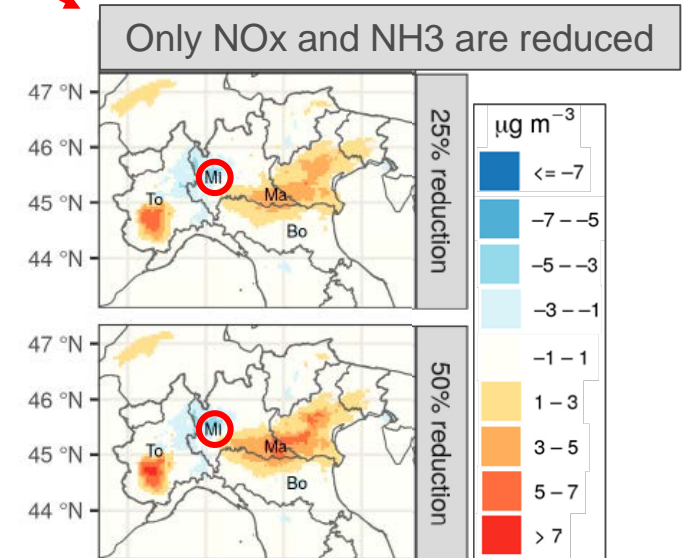
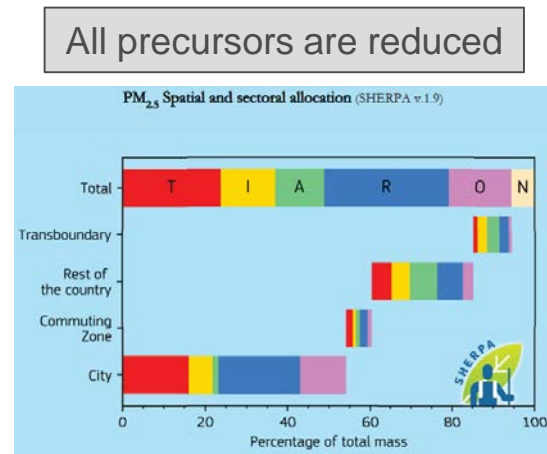


← WINTER

← SUMMER

# Why?

- ❑ « Model systems » are different
- ❑ Time scale are different  
(was not indicated in the exercise)
- ❑ Reductions affect different precursors



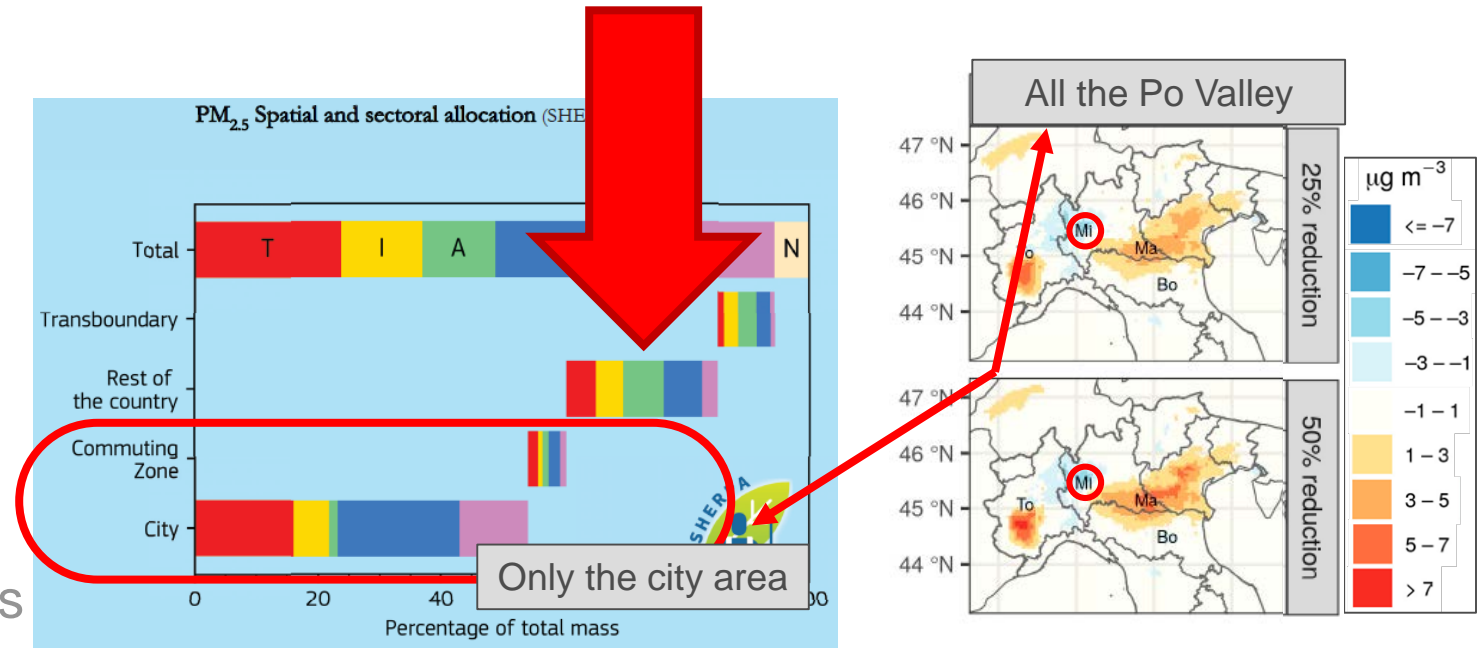
We could imagine that the PM in Milan are composed by a large amount of PPM emitted in their majority by the Residential and Transport sectors and not by Agriculture.

Then, the reductions are mainly driven by PPM and not by NO<sub>x</sub> or NH<sub>3</sub>.



# Why?

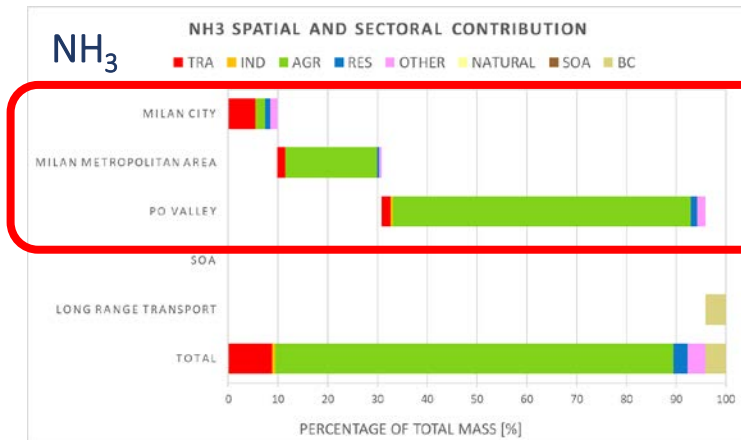
- ❑ « Model systems » are different
- ❑ Time scale are different  
(was not indicated in the exercise)
- ❑ Reductions affect different precursors
- ❑ Spatial scales of the reductions are different



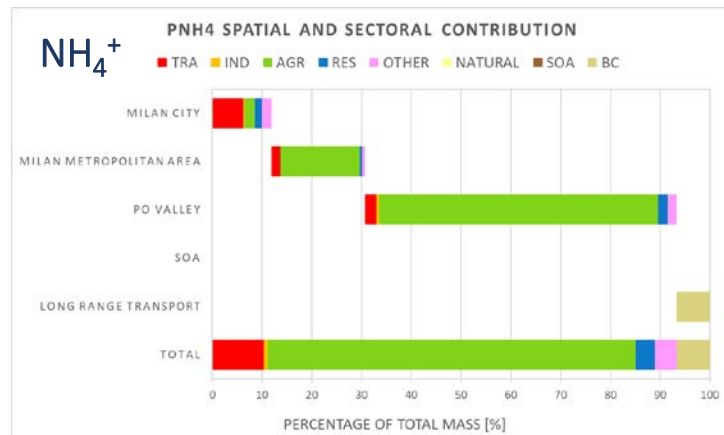
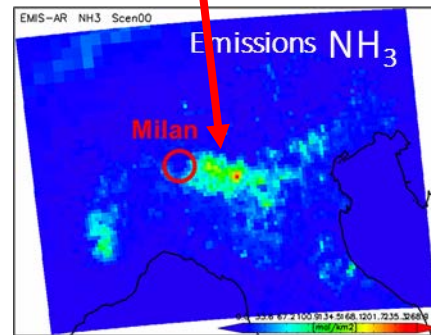
In SHERPA's results, the most significant impacts of agriculture come from reductions on a national scale.

# Spatial Scales and Tagging

MILAN receptor: Sectoral and spatial contributions based on CAMx/PSAT

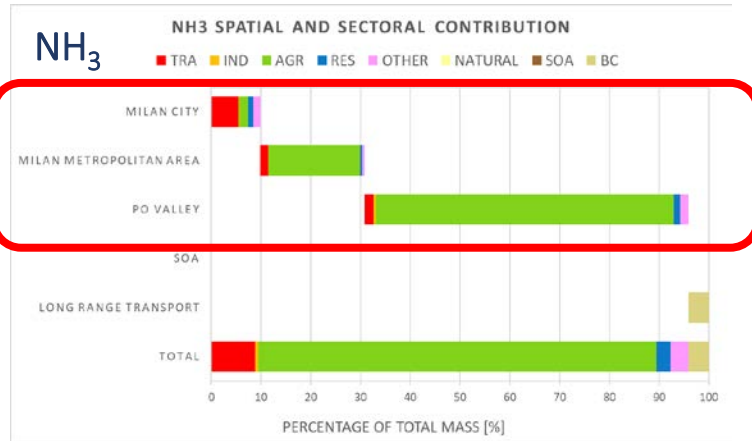


NH<sub>3</sub> is emitted mainly by the agriculture at the scale of the Po Valley outside the city

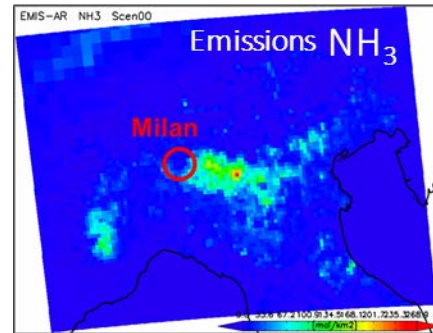
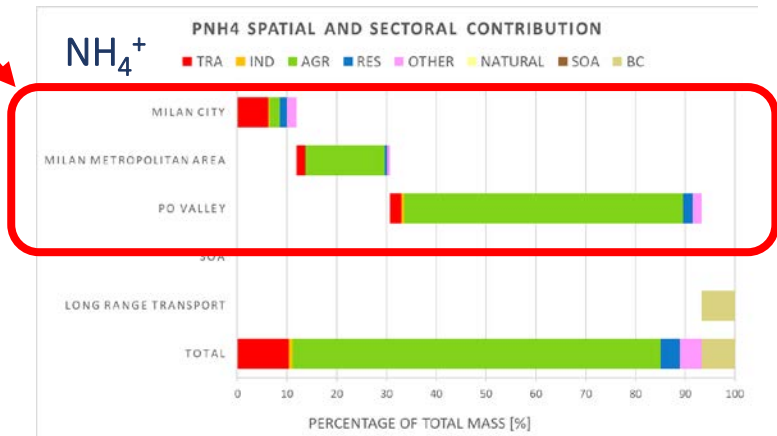


# Spatial Scales and Tagging

MILAN receptor: Sectoral and spatial contributions based on CAMx/PSAT

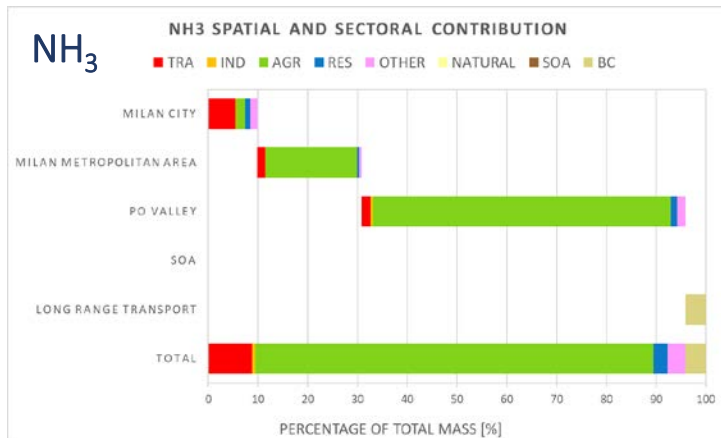


NH<sub>4</sub> is produced from NH<sub>3</sub>, it comes, like NH<sub>3</sub>, mainly from the scale of the Po Valley.

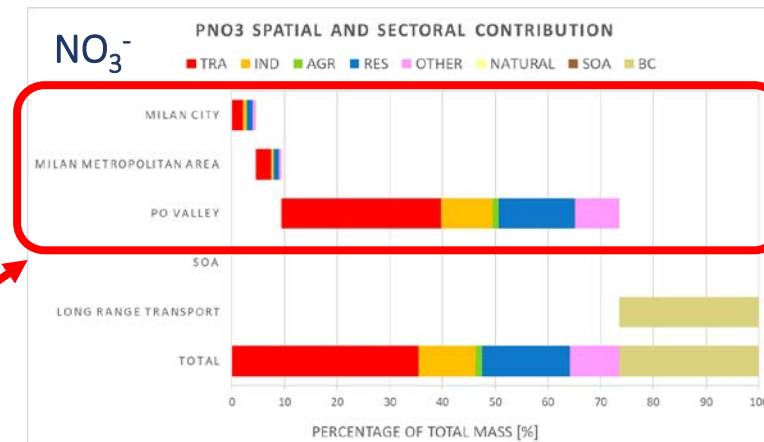
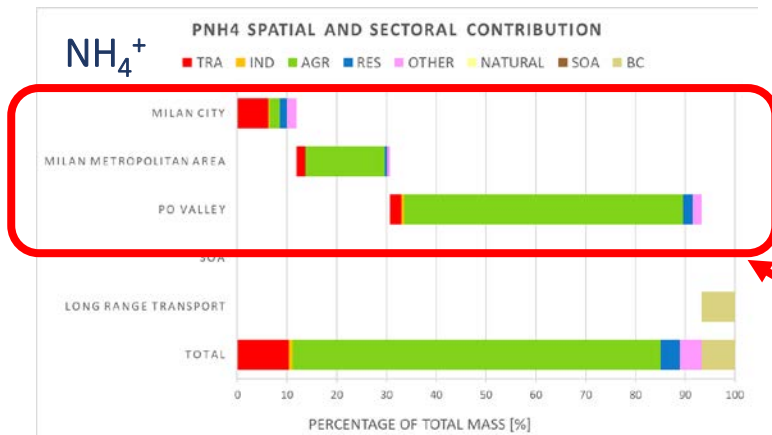
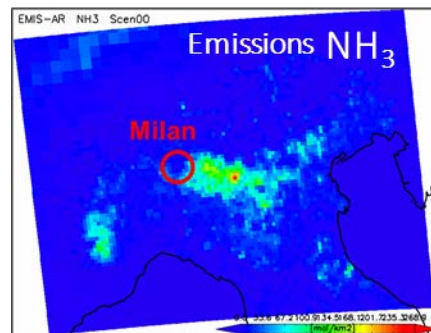


# Spatial Scales and Tagging

MILAN receptor: Sectoral and spatial contributions based on CAMx/PSAT

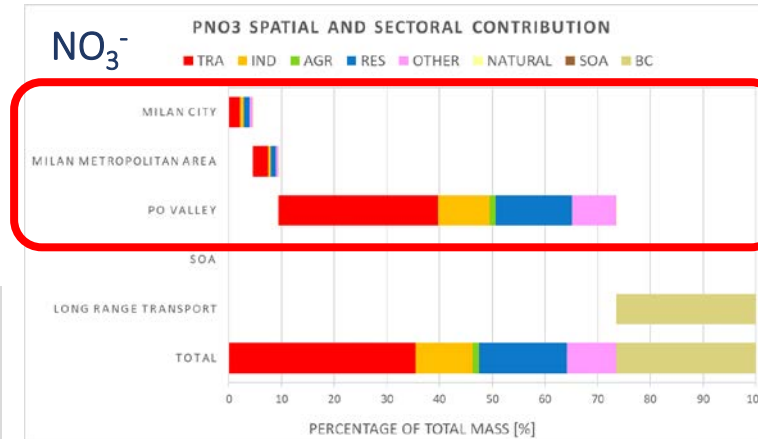
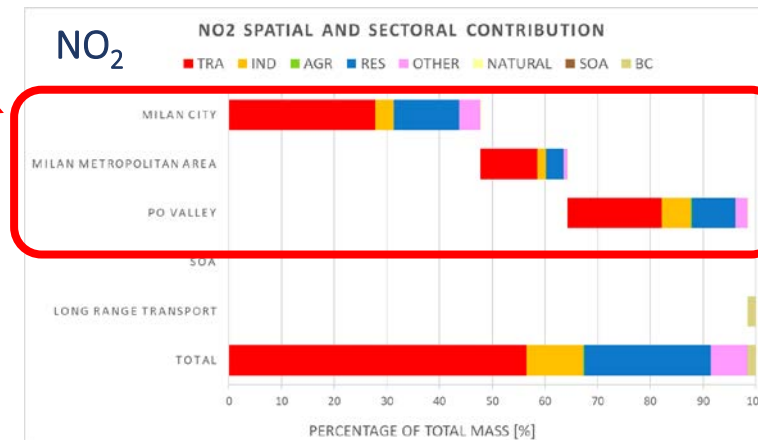
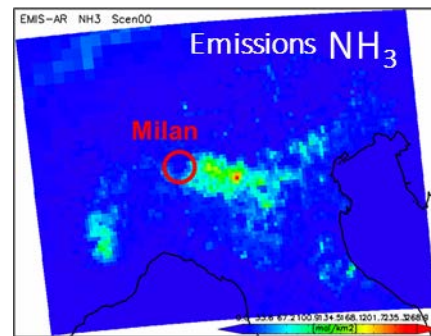
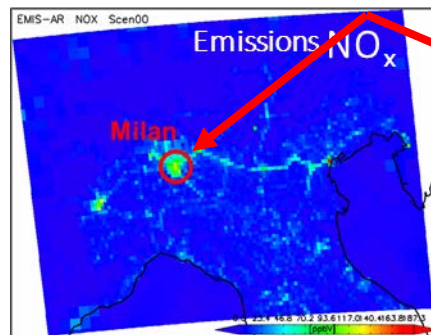
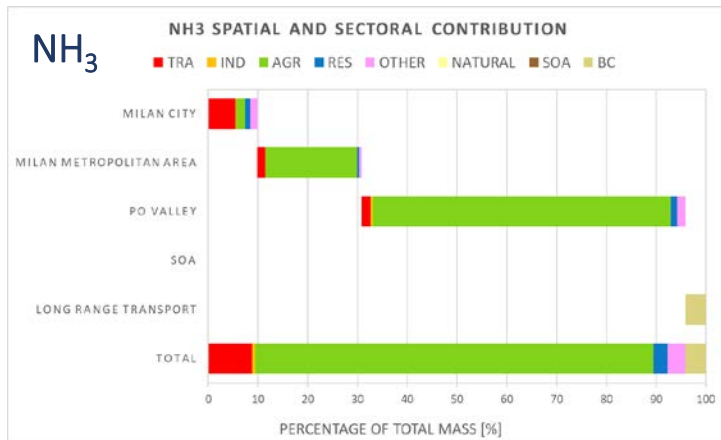


The formation of NH<sub>4</sub> from NH<sub>3</sub> required the presence of NO<sub>3</sub> and vice versa.  
NO<sub>3</sub> comes, like NH<sub>4</sub>, mainly from the scale of the Po Valley.



# Spatial Scales and Tagging

MILAN receptor: Sectoral and spatial contributions based on CAMx/PSAT

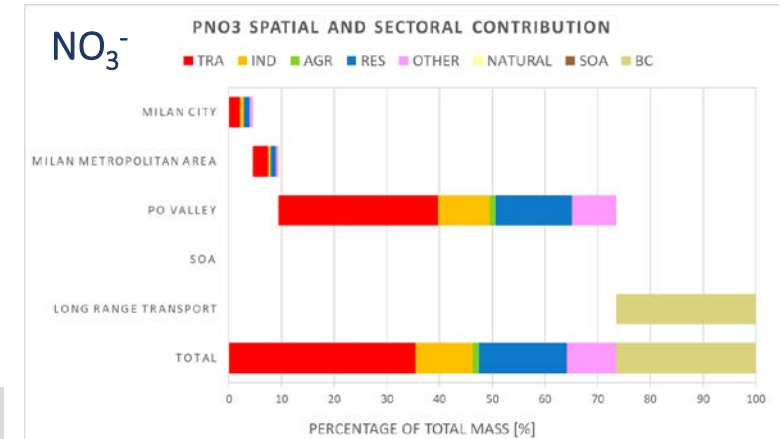
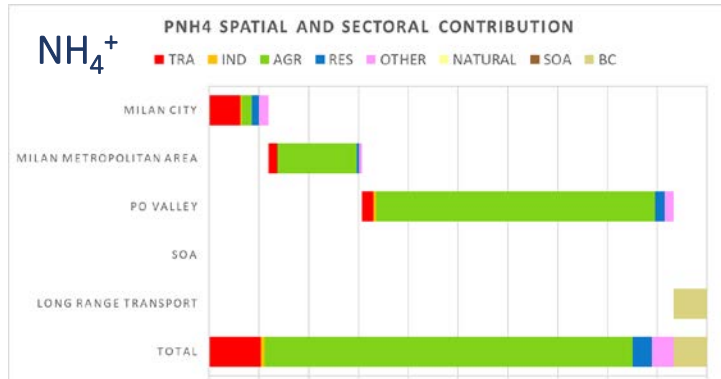
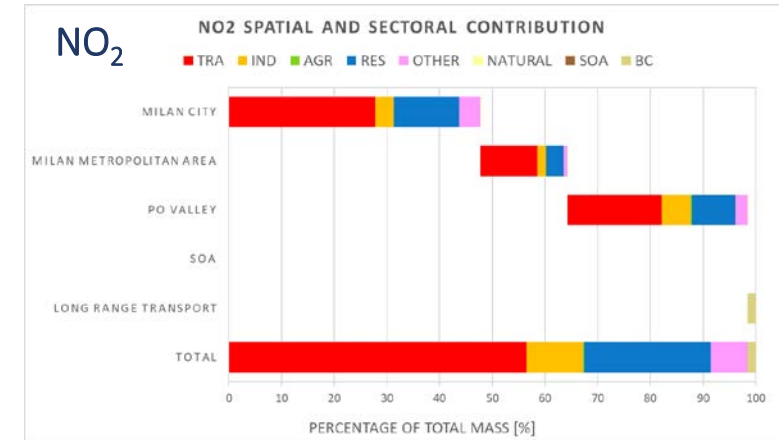
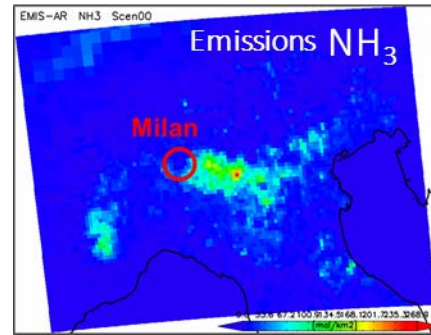
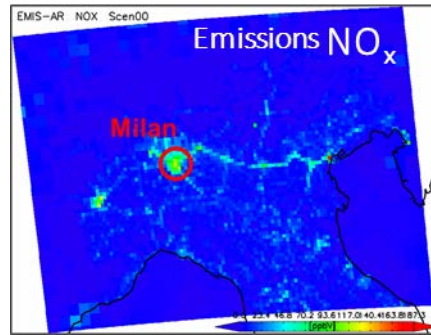
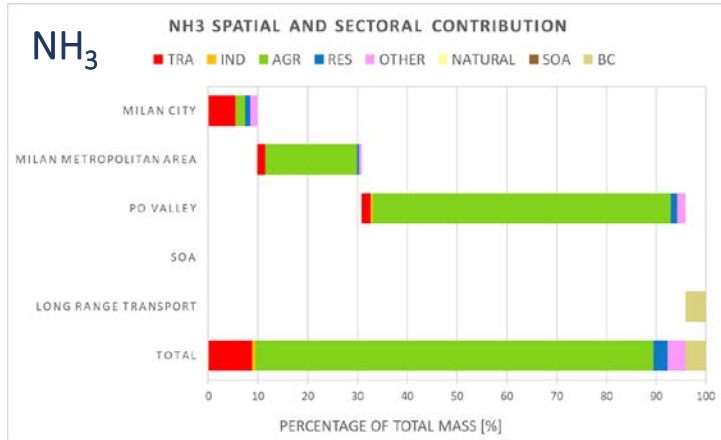


NO<sub>3</sub> is produced from NO<sub>2</sub> in presence of NH<sub>4</sub>.

The PSAT results show that main part of NO<sub>3</sub> is chemically formed at the scale of the Po Valley while a large part of the NO<sub>2</sub> comes the emissions at the scale of the city..

# Spatial Scales and Tagging

MILAN receptor: Sectoral and spatial contributions based on CAMx/PSAT



Milan's atmosphere is saturated with NO<sub>2</sub> emitted mainly inside the city, so NO<sub>2</sub> reductions have less impact than NH<sub>3</sub> reductions, but NH<sub>3</sub> comes from outside the city, so NH<sub>3</sub> reductions confined to the city can be important.

# Exercise 2



# Two Different Goals

- ❑ Reduce concentrations on average over the year,
- ❑ Reduce concentrations when an excessively high daily threshold is reached.

Each of these goals can lead to choosing completely different strategies.

How to use models to design strategies able to reach these two goals?



# Time Scale

Reducing peaks of exceedance requires the implementation of immediate reduction measures during (or before) the period of exceedance, while reducing annual averages requires implementing strategies over the entire year.

Models should to simulate these two situations which correspond to the two green square

BUT...

		Emission reduction	
		Short term (3 to 4 days)	Long term (over one year)
Concentration analysis	Short term (3 to 4 days)		
	Long term (over one year)		

# Time Scale

## Analyzing the efficiency of short-term air quality plans in European cities, using the CHIMERE air quality model

P. Thunis<sup>1</sup> · B. Degraeuwe<sup>1</sup> · E. Pisoni<sup>1</sup> · F. Meleux<sup>2</sup> · A. Clappier<sup>3</sup>

... reducing emissions over a long period always has an impact over a limited period, depending on the « residence time of the reductions ».

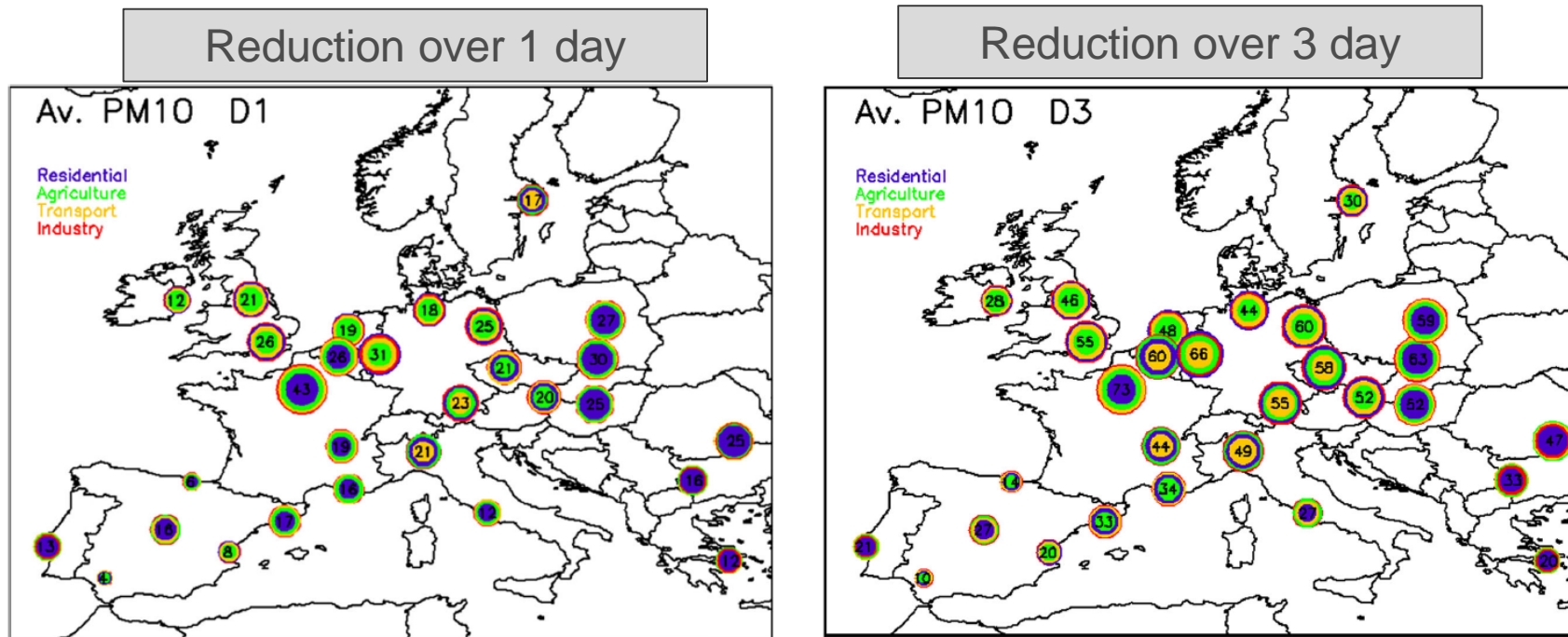


Fig. 1 Map of relative potentials (i.e.,  $\Delta C/\alpha C$ ) at  $D_{AQP} = 1$  for  $PM_{10}$ . The circled area is proportional to the potential with the most important contributors placed from center to outwards. The four activity sectors are represented by different colors. The number in each circle is the overall potential (i.e., corresponding to all sectors reduced simultaneously)

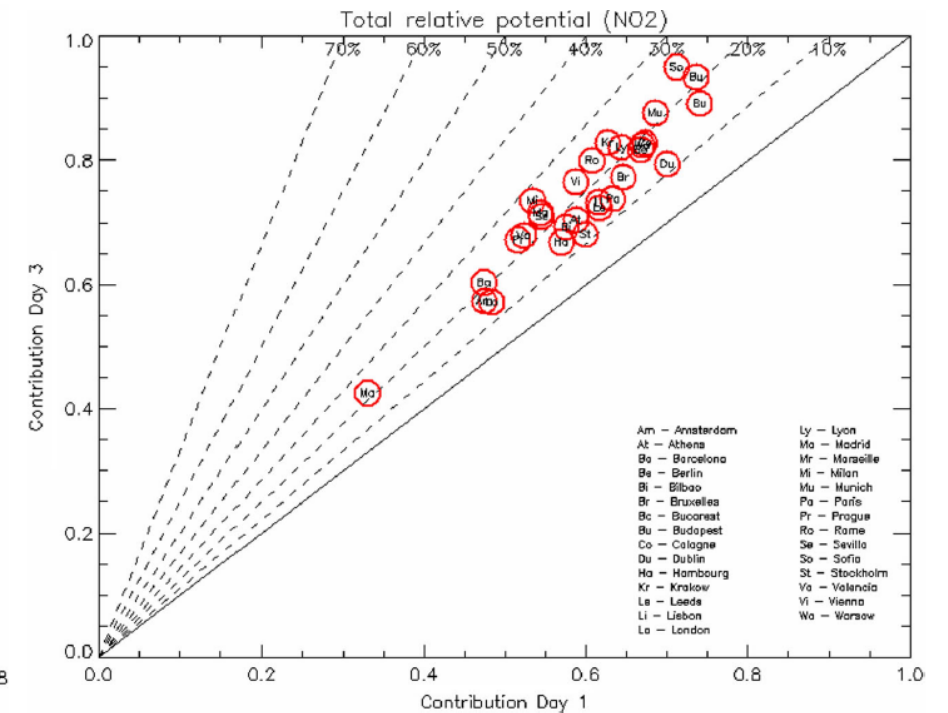
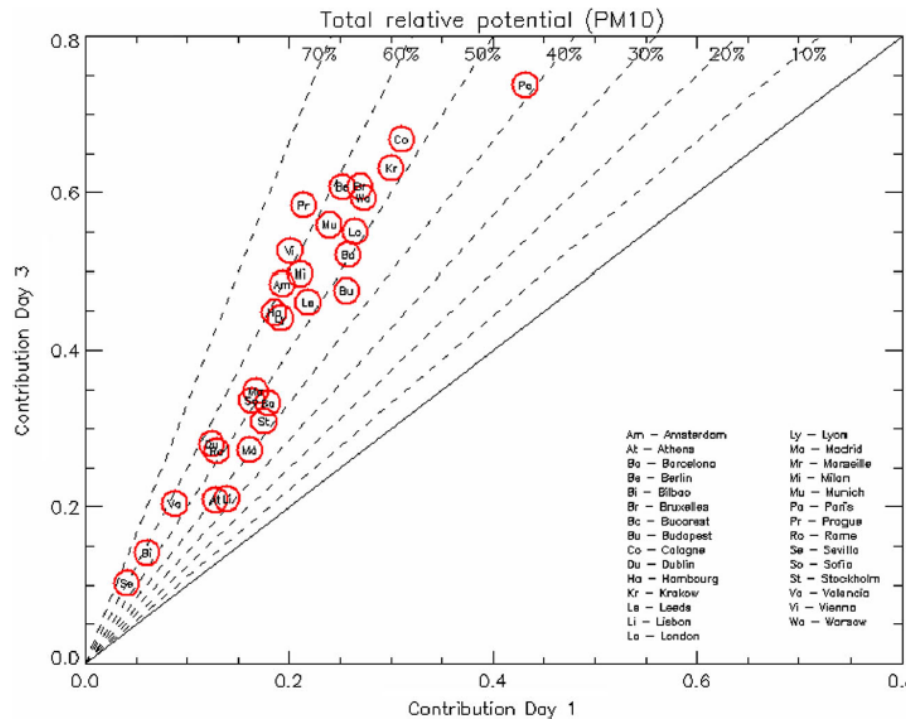
# Time Scale

## Analyzing the efficiency of short-term air quality plans in European cities, using the CHIMERE air quality model

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The residence time of reduction depends from the pollutants concern...

Day3 vs. Day1 for different European cities



... but also from the area which is reduced.

# Time Scale

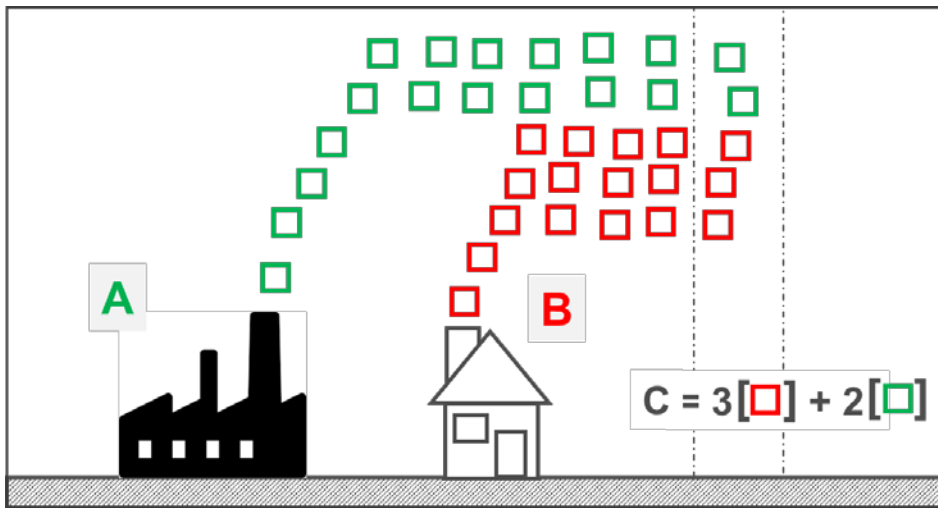
Long-term emission reductions could be used to assess the impact of shorter-term strategies, **provided that the « residence time of reductions » is verified.**

		Emission reduction	
		Short term (3 to 4 days)	Long term (over one year)
Concentration analysis	Short term (3 to 4 days)		
	Long term (over one year)		

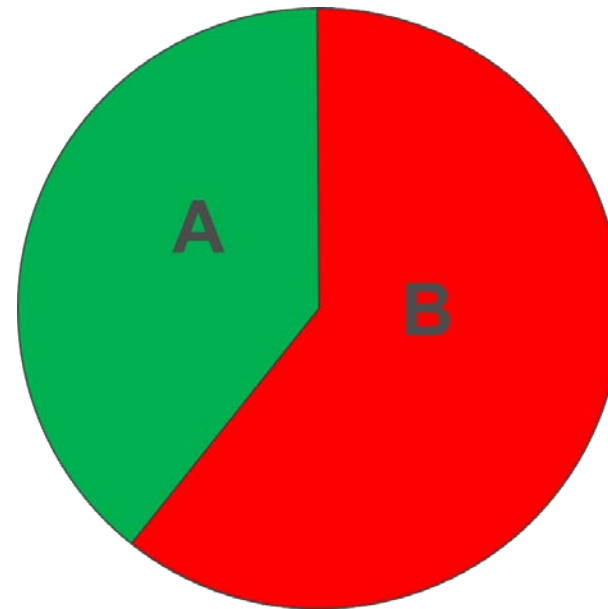
# Exercise 3



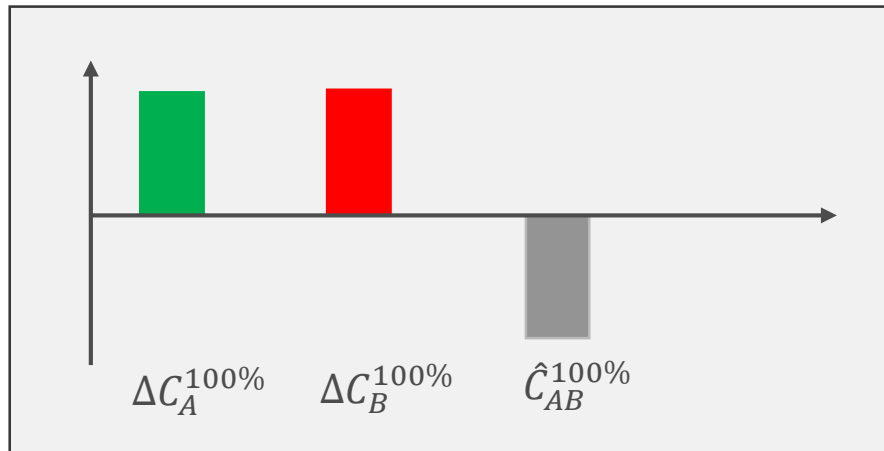
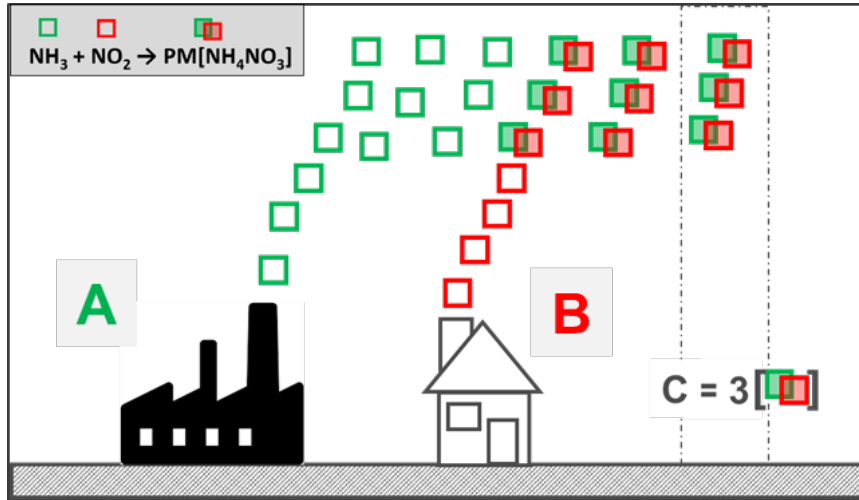
# Ideal Situation



Easy to explain and to understand, ideal for the communication



# Real Situation



Concentration changes resulting from an emission reduction:

$$\Delta C_A^{100\%} = 3 \quad \longrightarrow \quad \Delta C_A^{100\%} + \Delta C_B^{100\%} = 6$$

$$\Delta C_B^{100\%} = 3$$

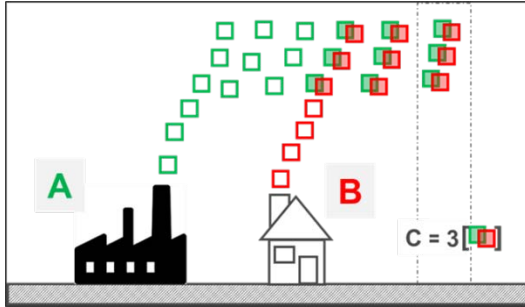
$$\Delta C_{AB}^{100\%} = 3 \quad \longrightarrow \quad \Delta C_{AB}^{100\%} \neq \Delta C_A^{100\%} + \Delta C_B^{100\%}$$

$$\Delta C_{AB}^{100\%} = \Delta C_A^{100\%} + \Delta C_B^{100\%} + \hat{C}_{AB}^{100\%}$$

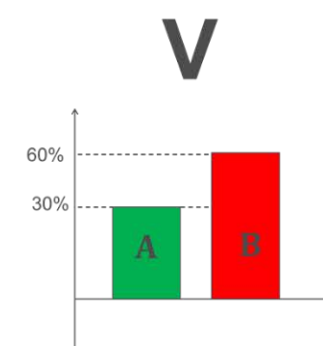
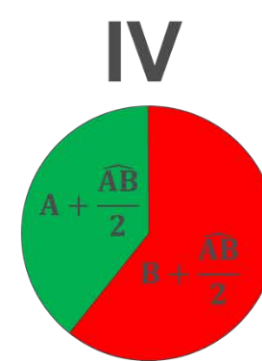
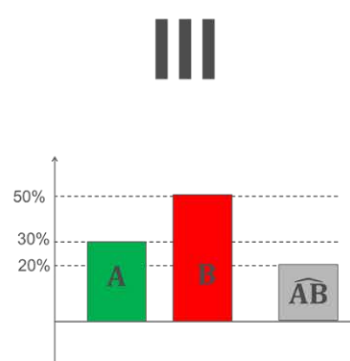
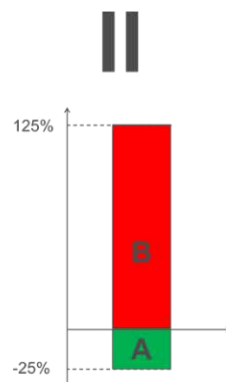
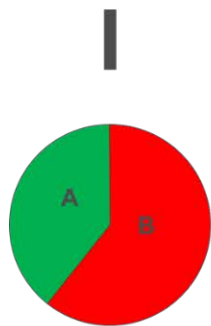
$$\hat{C}_{AB}^{100\%} = \Delta C_{AB}^{100\%} - \Delta C_A^{100\%} - \Delta C_B^{100\%} = 3 - 6 = -3$$

Interactions between sources and precursors can lead to negative terms and terms which can not attributed to only one unique source

# Real Situation

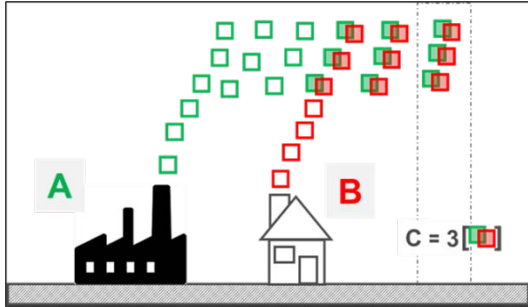


- ❑ Should the sum of the terms calculated by a SA method always be equal to 100%?
- ❑ Should an SA method produce only positive terms?
- ❑ Should an SA method only produce terms that can be attributed to a single source?





# Favor simplicity



If we favor simplicity, we would answer YES to all the 3 questions

- Should the sum of the terms calculated by a SA method always be equal to 100%?
- Should an SA method produce only positive terms?
- Should an SA method only produce terms that can be attributed to a single source?

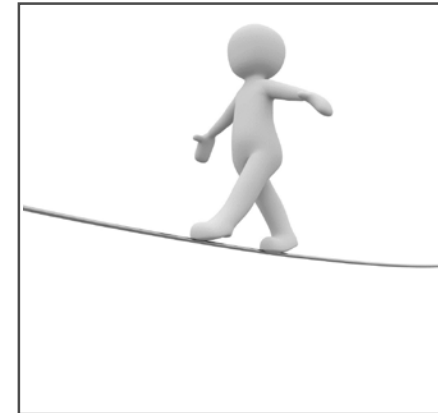
The most suitable representation is then the pie chart



It is a simple representation but we lose the possibility of communicating on the negative impacts (e.g. increases in O3 linked to reductions in NOx) and different terms could be different than the impacts resulting emission reductions (impacts  $\neq$  contributions).

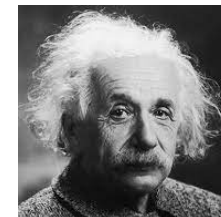
# A matter of compromise?

Your answers reflect a willingness to compromise between a complete representation and a simplified representation.



		Yes	No	?	Why
I			✗		no need to add up to 100%
II			✗		too confusing
III		✗			
IV			✗		no need to add up to 100%
V		✗			

« Everything should be made as simple as possible, but no simpler »  
A. Einstein





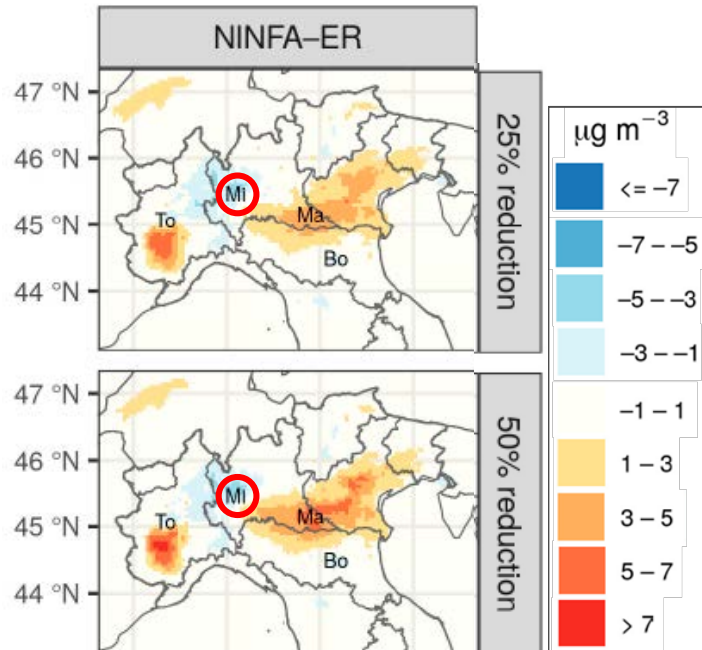
# Thank you for your attention

Which precursor would recommend to reduce in priority, why?

# First question: chemical regimes $\text{NH}_3$ vs. $\text{NO}_x$

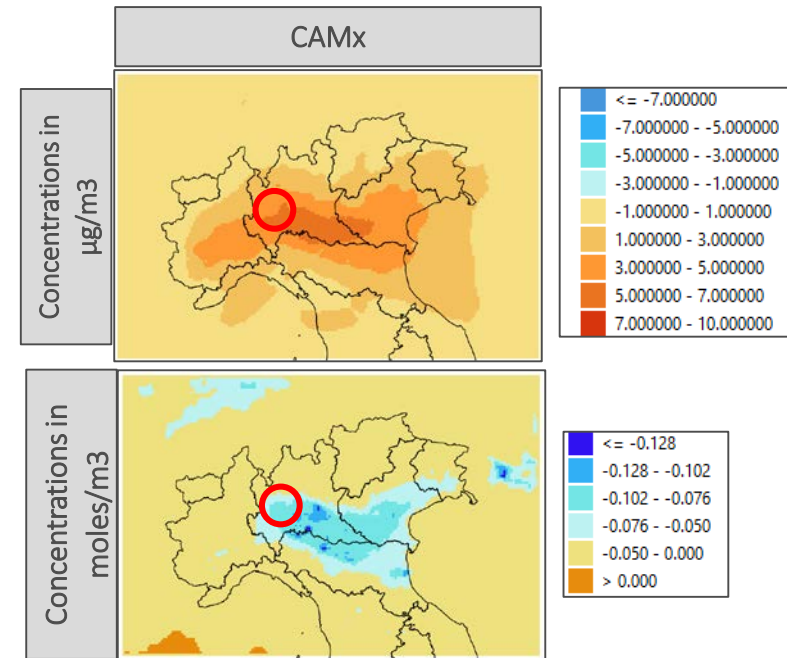
You have access to the following maps which give information about the sensitivity to  $\text{NO}_x$  and  $\text{NH}_3$

Difference  $P_{\text{NO}_x}^\alpha - P_{\text{NH}_3}^\alpha$  based on NINFA/Brut Force for  $\alpha=25\%$  and  $\alpha=50\%$



These maps show simulated results obtained reducing independently  $\text{NO}_x$  and  $\text{NH}_3$  of 25% (map above) and 50% (map below) over the all Po Valley with the NINFA-ER model. Blue color shows areas where the impact of  $\text{NH}_3$  over the PM concentrations is higher than the impact of  $\text{NO}_x$  reduction. Orange and red color show the opposite.

Difference  $\text{Cnt}_{\text{NO}_3} - \text{Cnt}_{\text{NH}_4}$  based on CAMx/PSAT



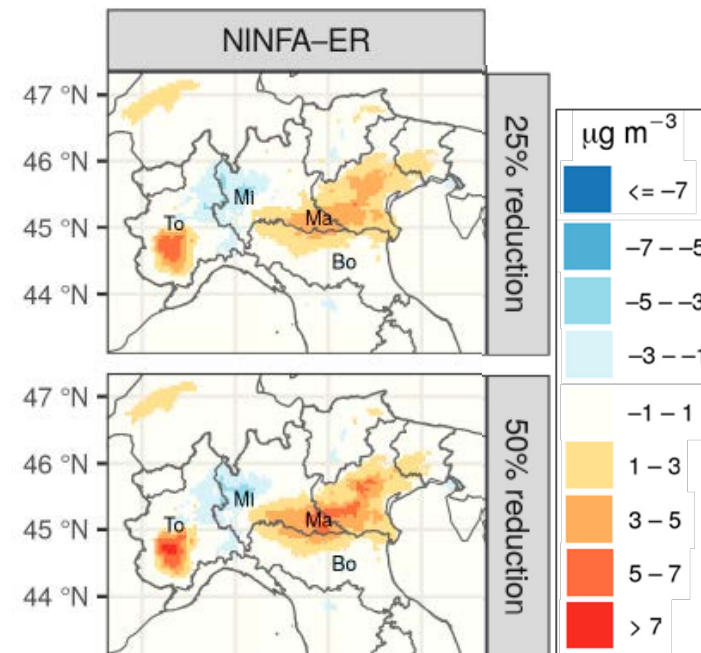
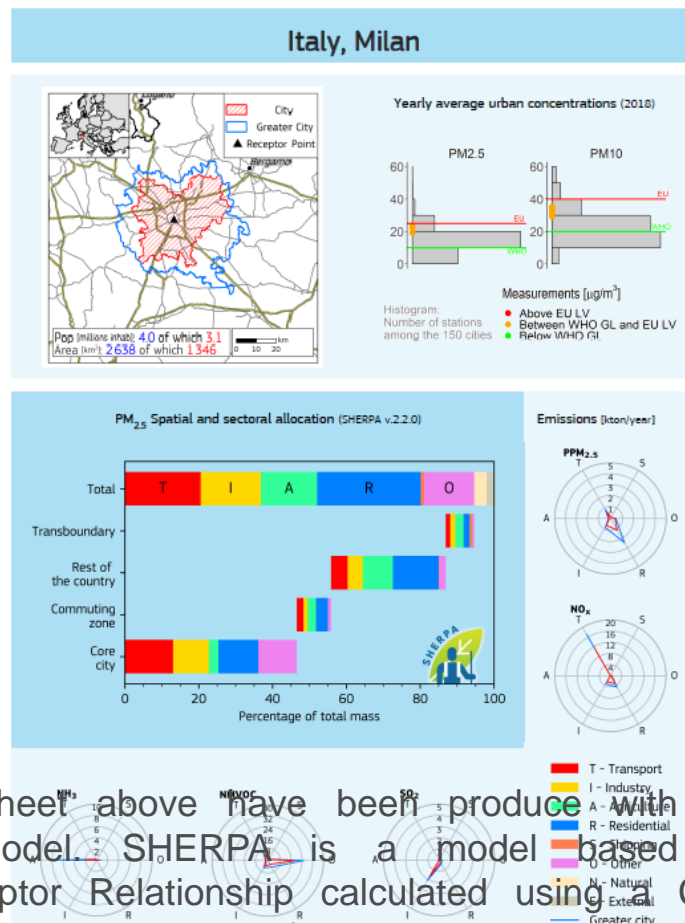
These maps show the fraction of  $\text{NH}_4$  and  $\text{NO}_3$  composing the Ammonium Nitrate PM obtained with the CAMx model and SA module PSAT. The map above shows mass fraction while the map below shows moles fraction. Blue color shows areas where the fraction of  $\text{NH}_3$  is higher than the fraction of  $\text{NO}_x$  reduction. Orange and red color show the opposite.

The decision makers who mandate you can only take decision in the area of Milan. Please use the SHERPA results concerning Milan core city and Commuting zone to recommend which activity sector could be reduced to produce the highest impact on PM abatement ?

Could this recommendation be in contradiction with the following one? Why?

## Second question: Spatial Scale

Additionally to the previews maps you have access to the following graphics:



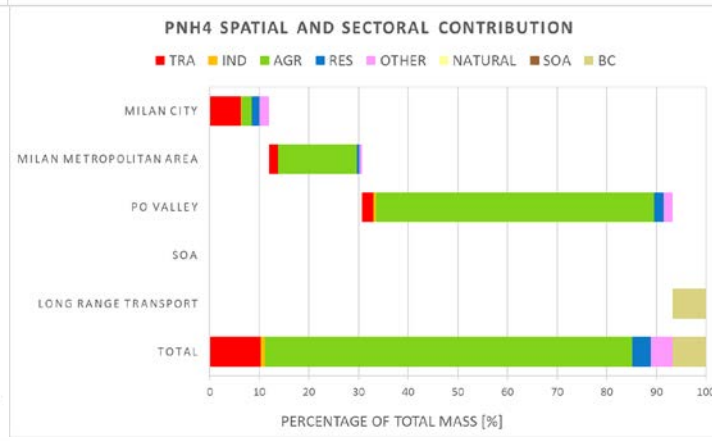
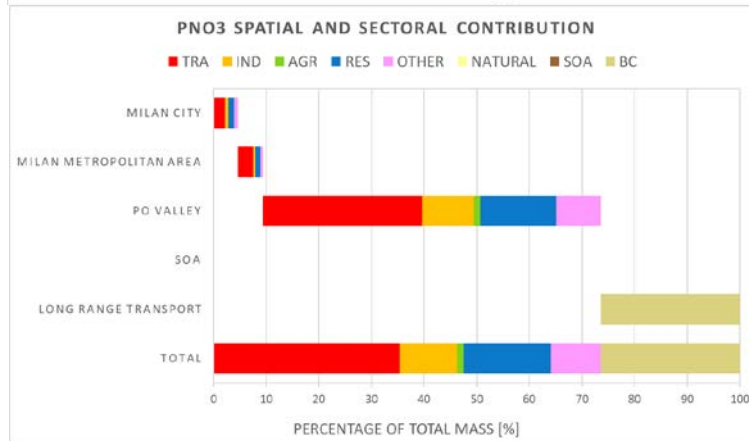
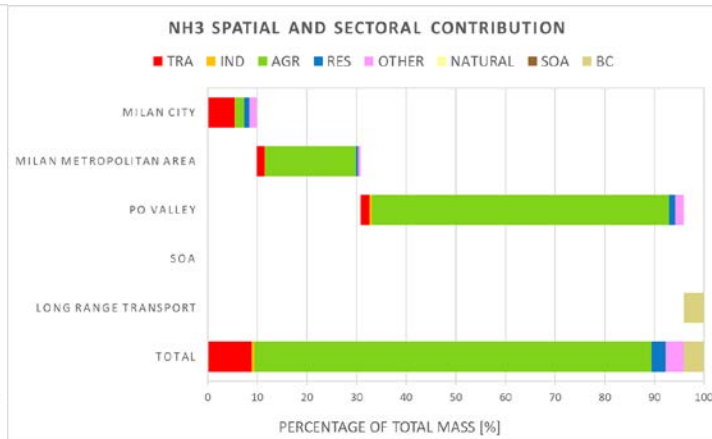
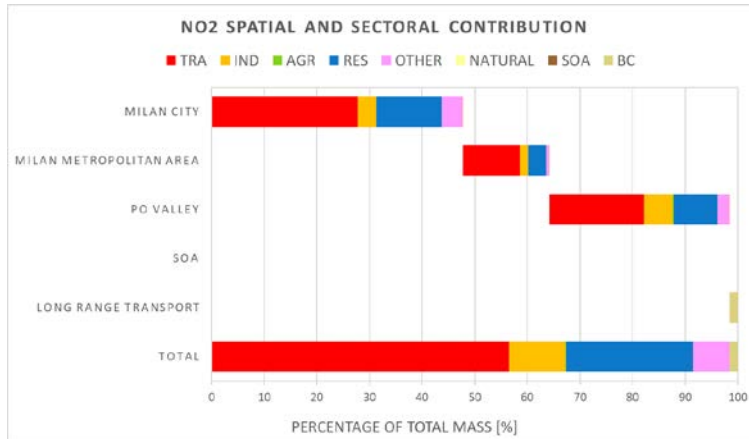
The data sheet above have been produce with the SHERPA model. SHERPA is a model based on Source/Receptor Relationship calculated using a CTM model (here the EMEP model). It is used to evaluate the impact of emission reductions

# Third question: Spatial Scales

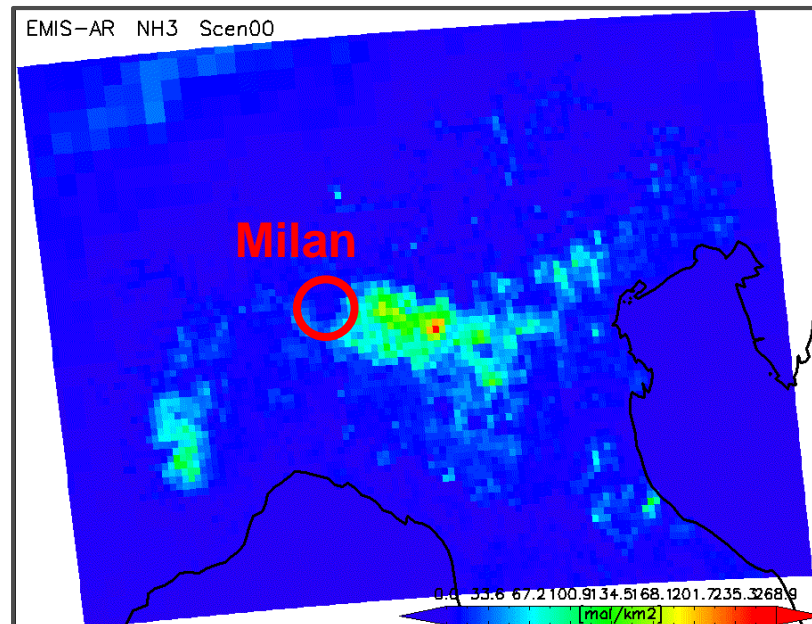
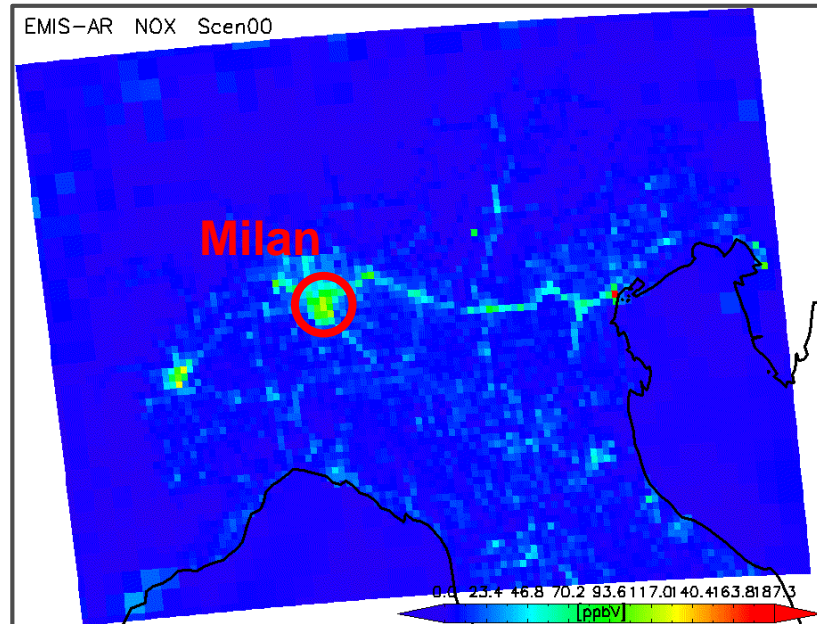
These graphics show the mass fraction of NO<sub>2</sub> and NO<sub>3</sub> coming from different spatial scales.

NO<sub>2</sub> and NO<sub>3</sub><sup>-</sup> MILAN receptor: Sectoral and spatial contributions based on CAMx/PSAT

NH<sub>3</sub> and NH<sub>4</sub><sup>+</sup>



# Third question:

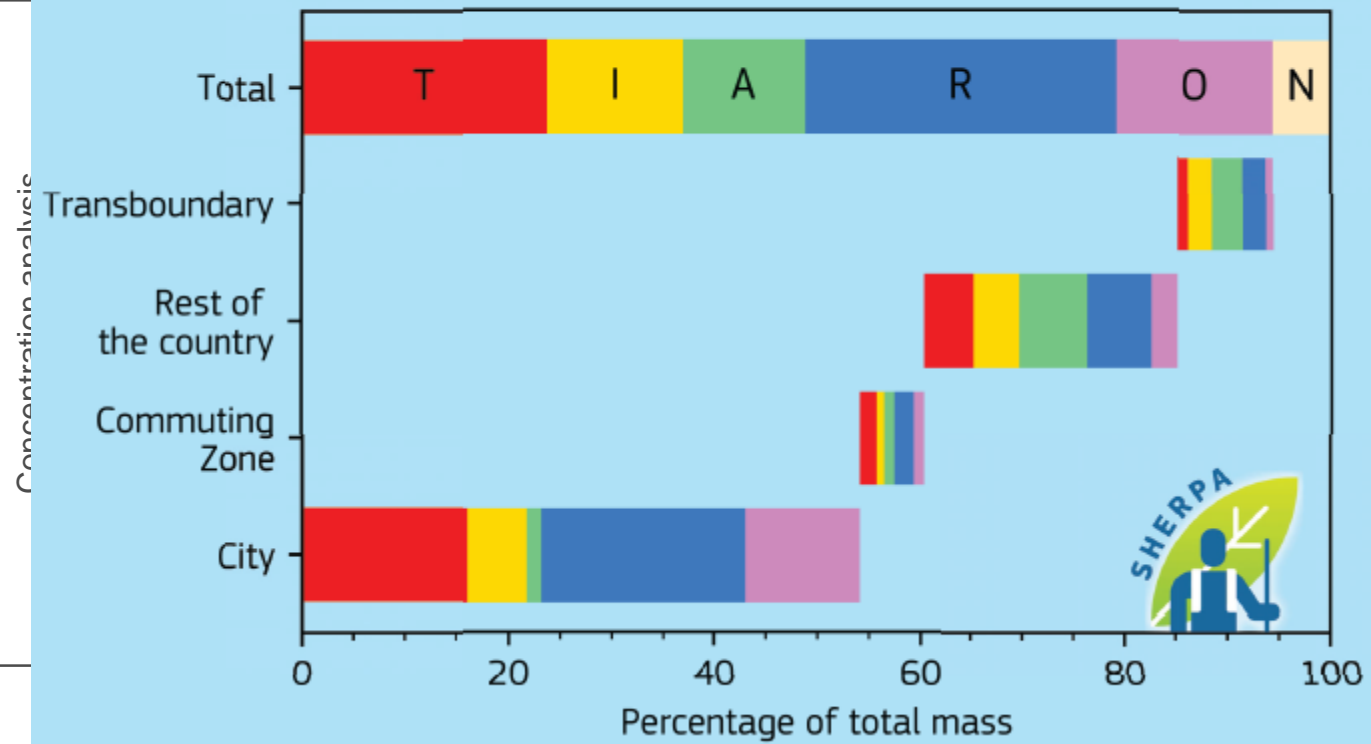


# Exercise 2





### PM<sub>2.5</sub> Spatial and sectoral allocation (SHERPA v.1.9)



		Emission reduction	
		Short term (3 to 4 days)	Long term (over one year)
Concentration analysis	Short term (3 to 4 days)		
	Long term (over one year)		

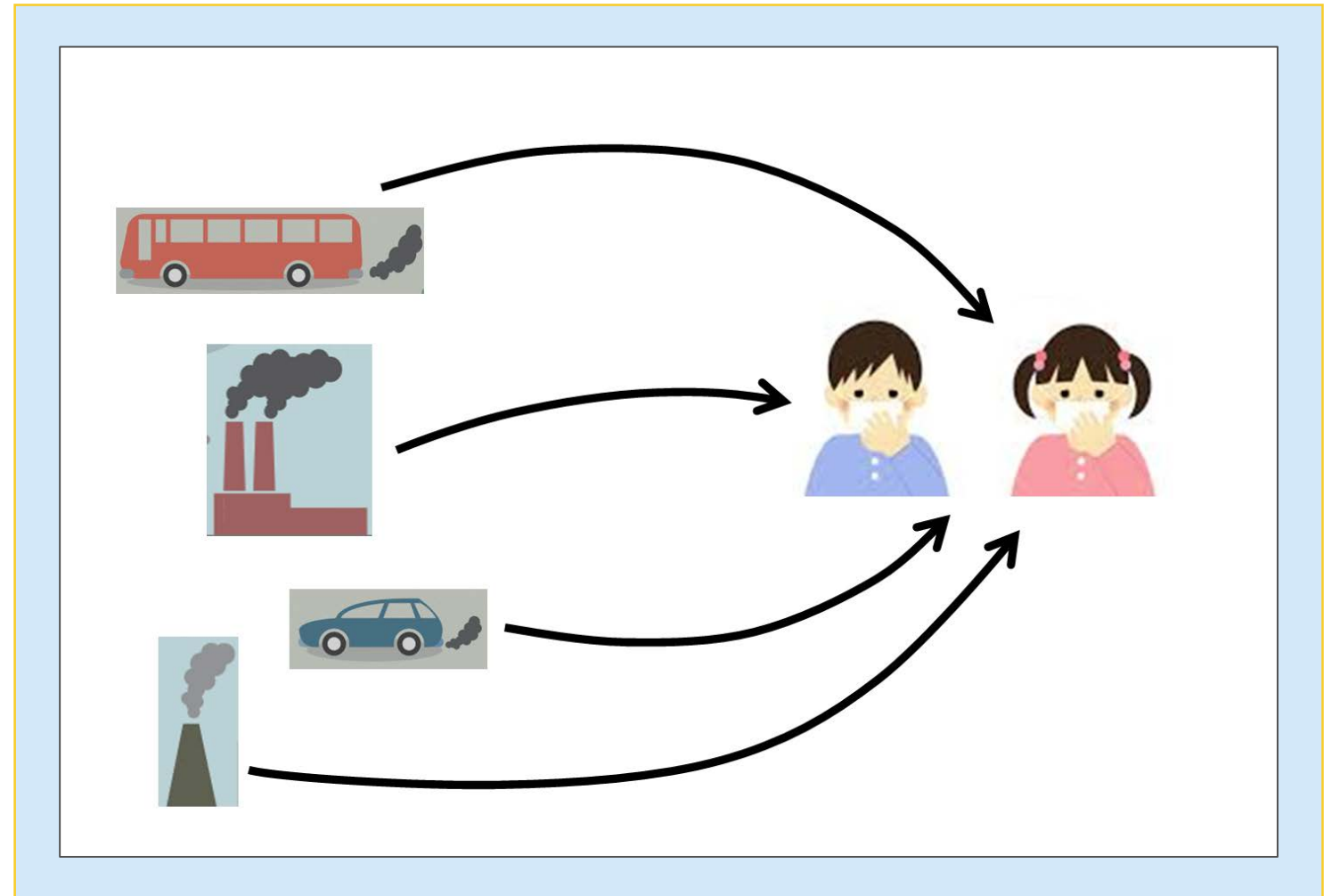
# Exercise 3



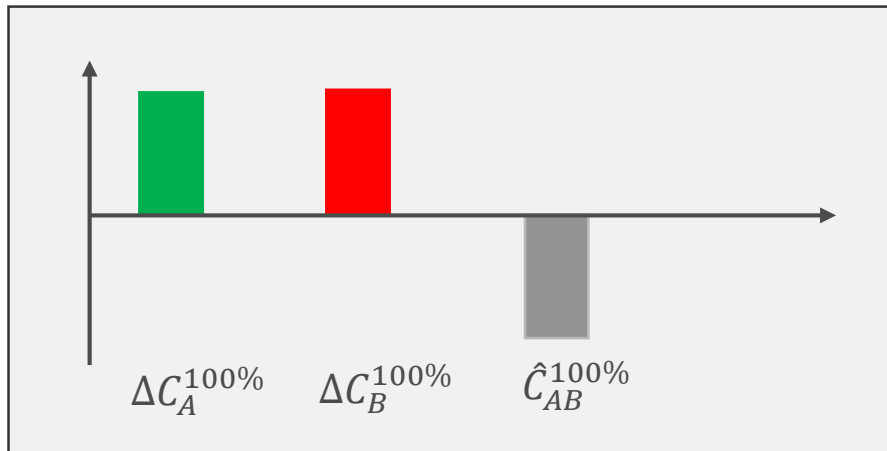
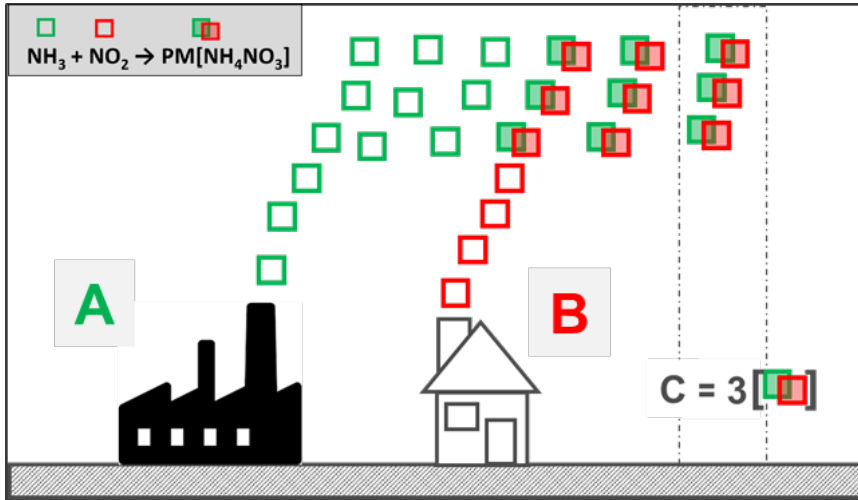
# SA Method: Definition

Source apportionment is a technique used to **relate emissions from various pollution sources to air pollution concentrations** at a given location and for a given time period.

**but what does « relate » means?**



# Impacts of Emission Reductions



Concentration changes resulting from an emission reduction:

$$\Delta C_A^{100\%} = 3$$



$$\Delta C_A^{100\%} + \Delta C_B^{100\%} = 6$$

$$\Delta C_B^{100\%} = 3$$

$$\Delta C_{AB}^{100\%} = 3$$



$$\Delta C_{AB}^{100\%} \neq \Delta C_A^{100\%} + \Delta C_B^{100\%}$$

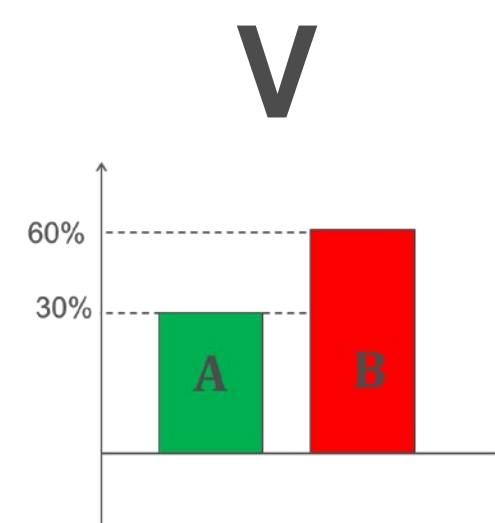
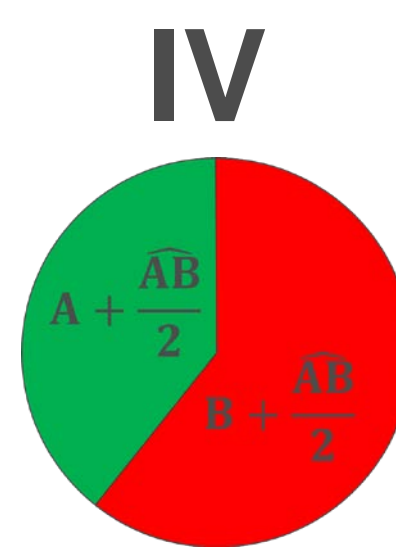
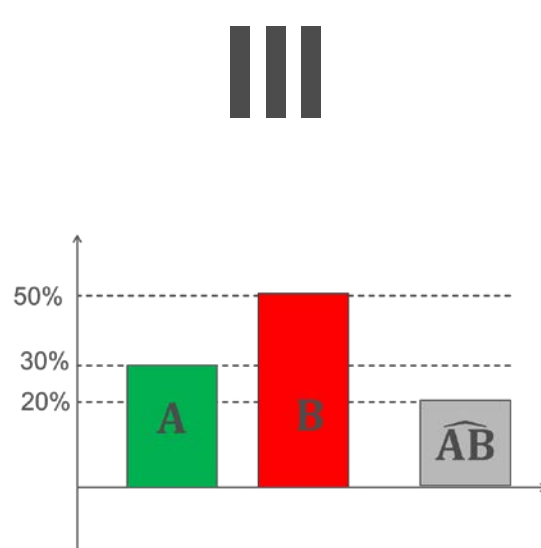
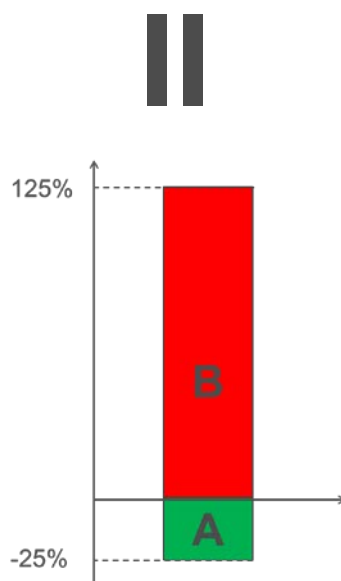
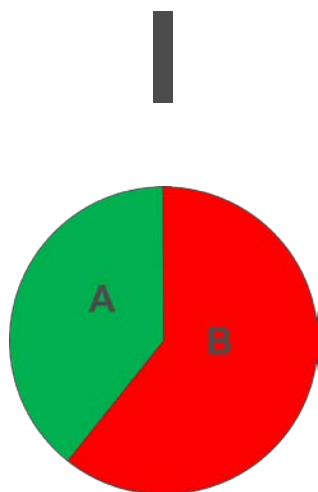
$$\Delta C_{AB}^{100\%} = \Delta C_A^{100\%} + \Delta C_B^{100\%} + \hat{C}_{AB}^{100\%}$$

$$\hat{C}_{AB}^{100\%} = \Delta C_{AB}^{100\%} - \Delta C_A^{100\%} - \Delta C_B^{100\%} = 3 - 6 = -3$$

# to be SA or not to be SA ?



5 methods produced the following results for two sources A and B?



which of these methods can be considered as a SA method?

# to be SA or not to be SA ?



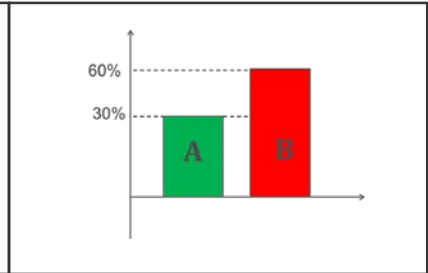
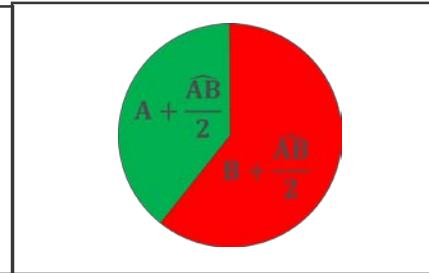
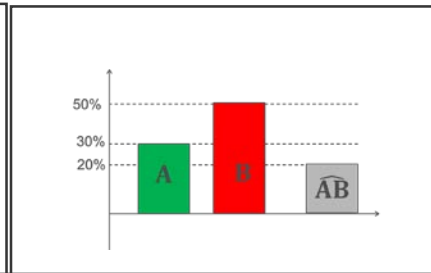
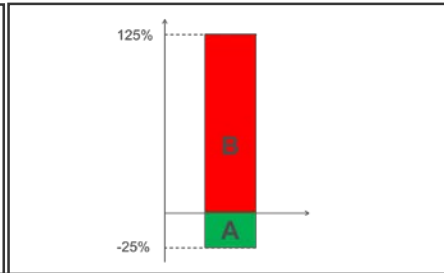
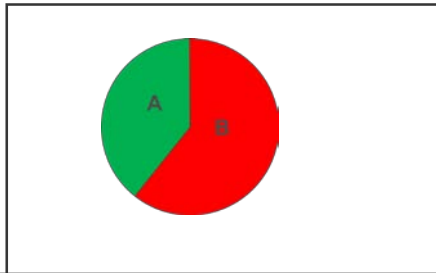
I

II

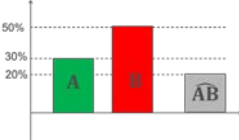
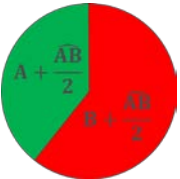
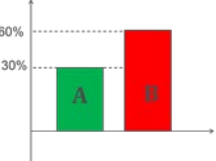
III

IV

V



Yes					
No					
?					

		Yes	No	?	Why
I					
II					
III					
IV					
V					



clappier@unistra.fr



Thank you for your attention



The aim of this exercise is to analyze how to use SA results to design specific and efficient reduction scenarios.

In Milan, PM concentrations quite regularly exceed the thresholds specified by the European directive. Decision-makers want to reduce exceedances, but only have the authority to act on the city's emissions and don't know which are the best measures to take. They mandate you to help them to use SA results to design specific and efficient reduction scenarios.

you answer to the two following questions:

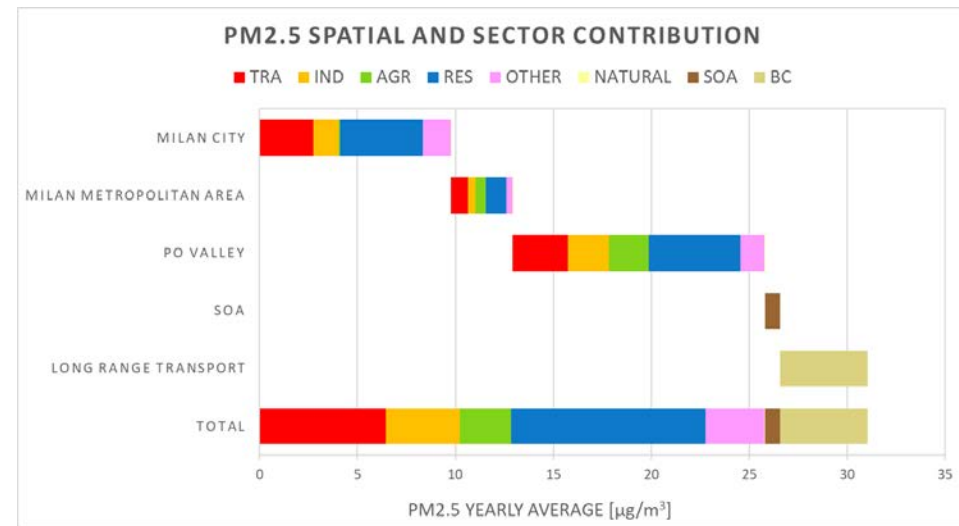
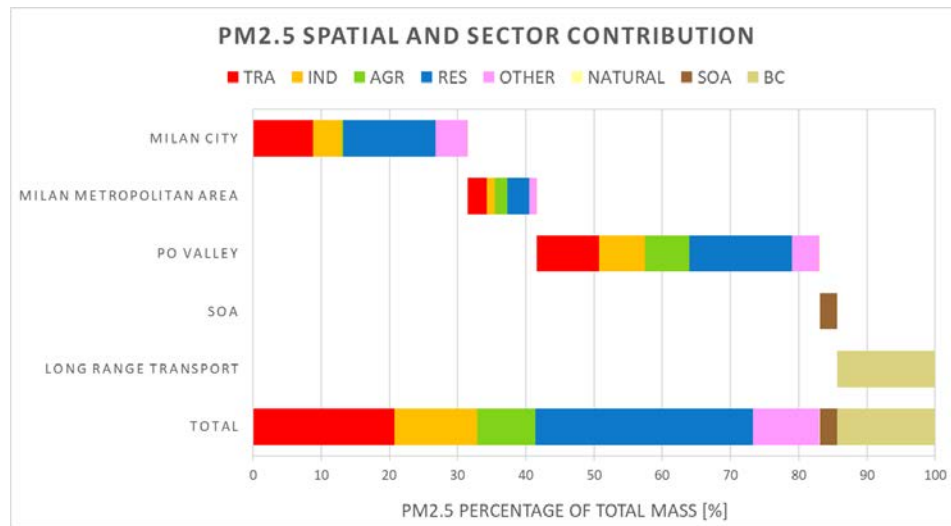
- 1) which precursor should be target in priority
- 2) at which activity sector should be targeted in priority



# Second question: target an activity sector

MILAN receptor

PM2.5 - Sectoral and spatial contributions based on CAMx/PSAT

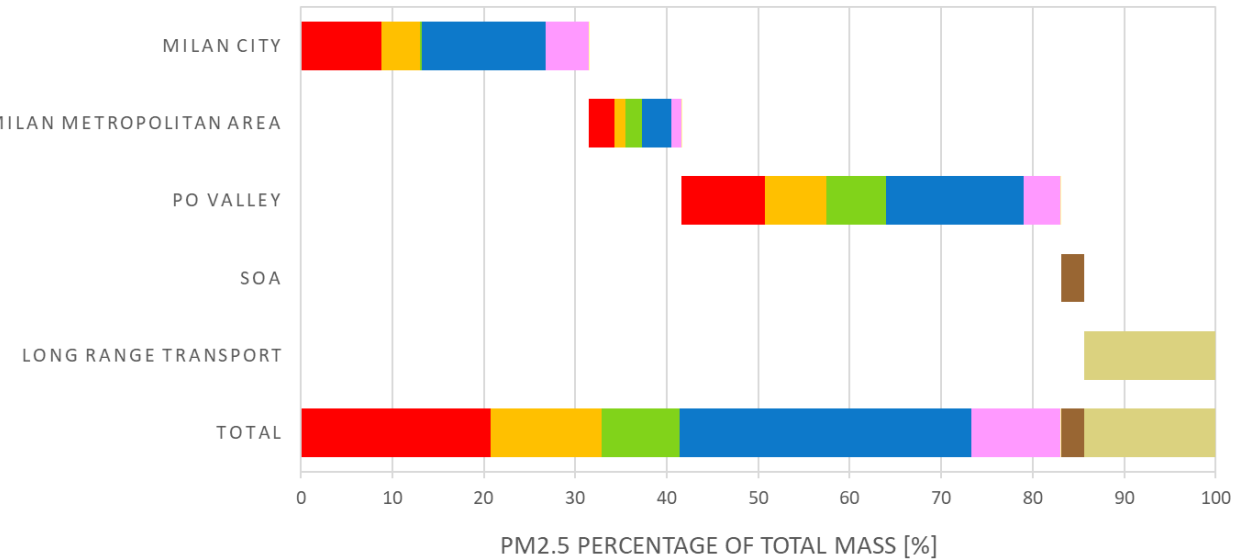


# MILAN receptor

## PM2.5 - Sectoral and spatial contributions based on CAMx/PSAT

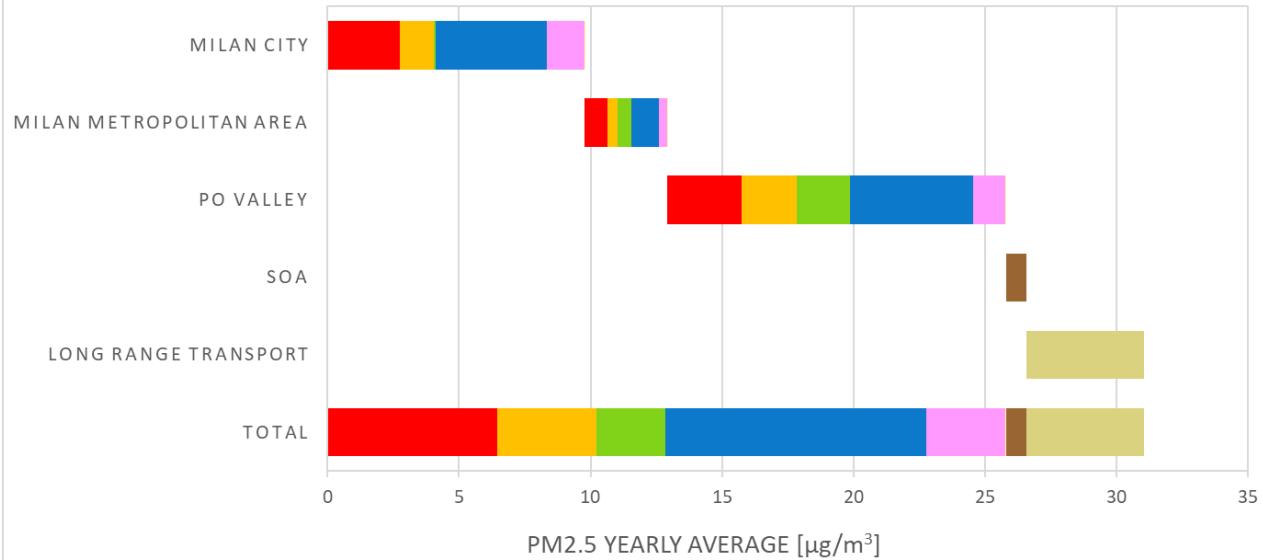
PM2.5 SPATIAL AND SECTOR CONTRIBUTION

TRA IND AGR RES OTHER NATURAL SOA BC



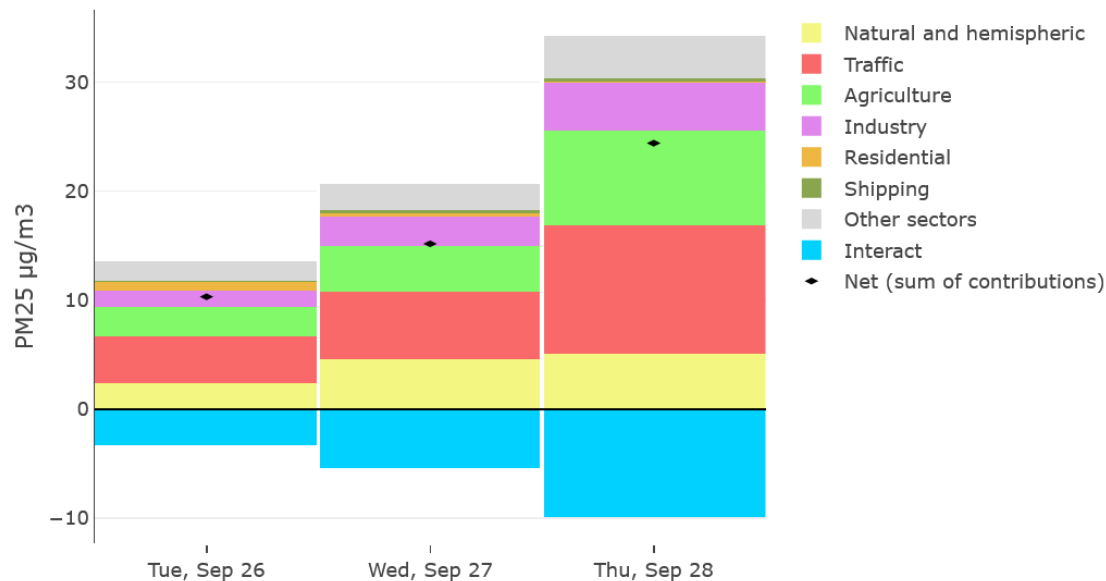
PM2.5 SPATIAL AND SECTOR CONTRIBUTION

TRA IND AGR RES OTHER NATURAL SOA BC



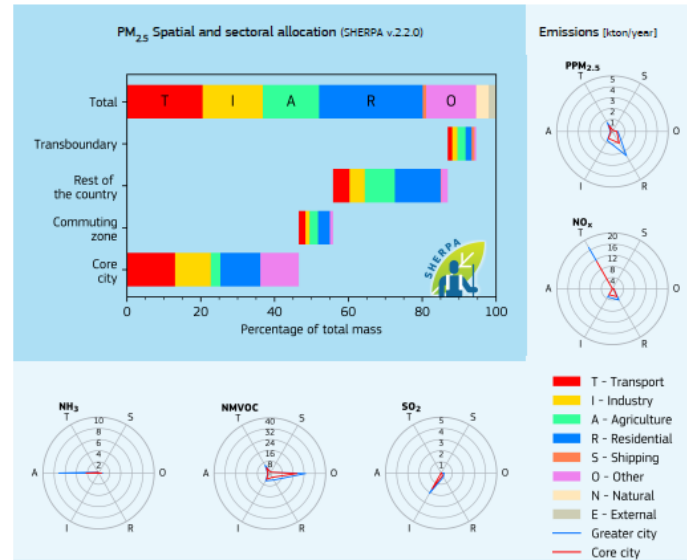
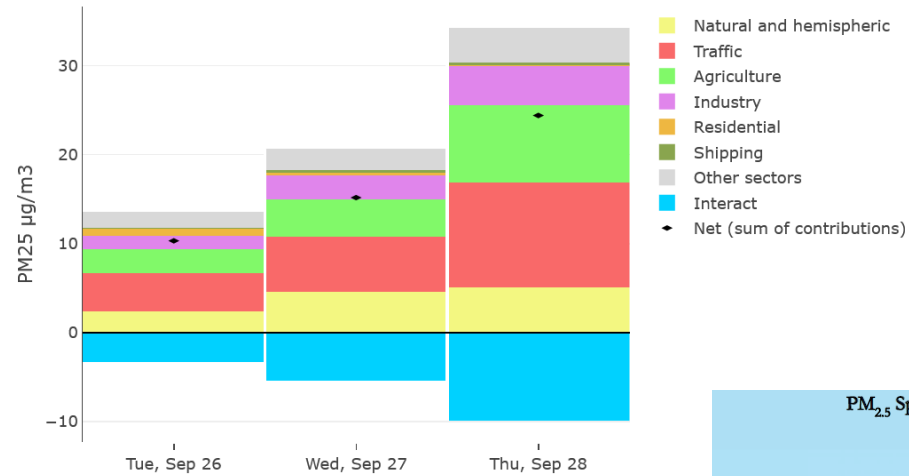
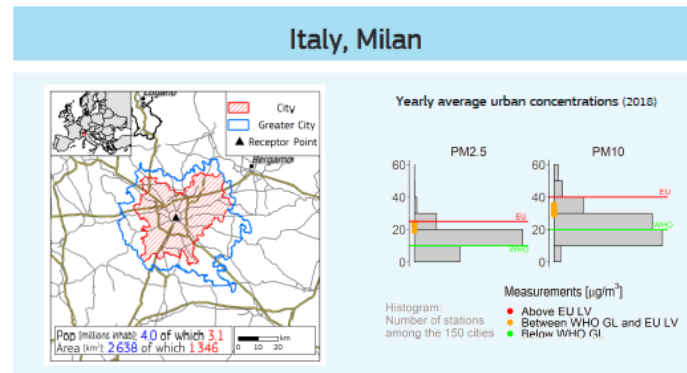
## B. In a second step,

1. Reduction scenarios to be implemented throughout the year.
2. Reduction scenarios to be implemented for a limited period on days when concentrations exceed limits

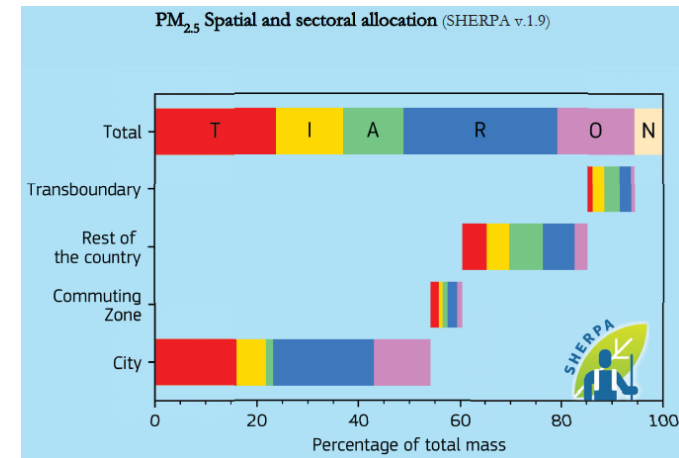
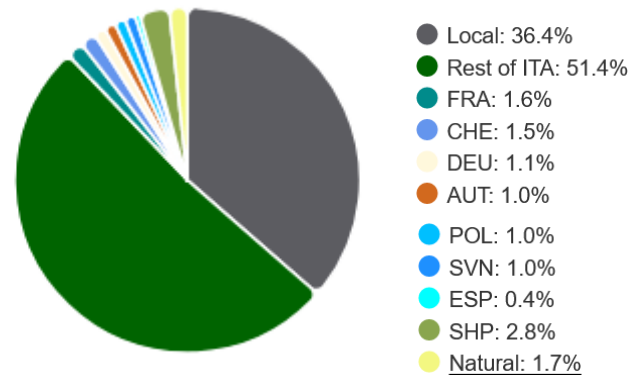


# Second question: target an activity sector

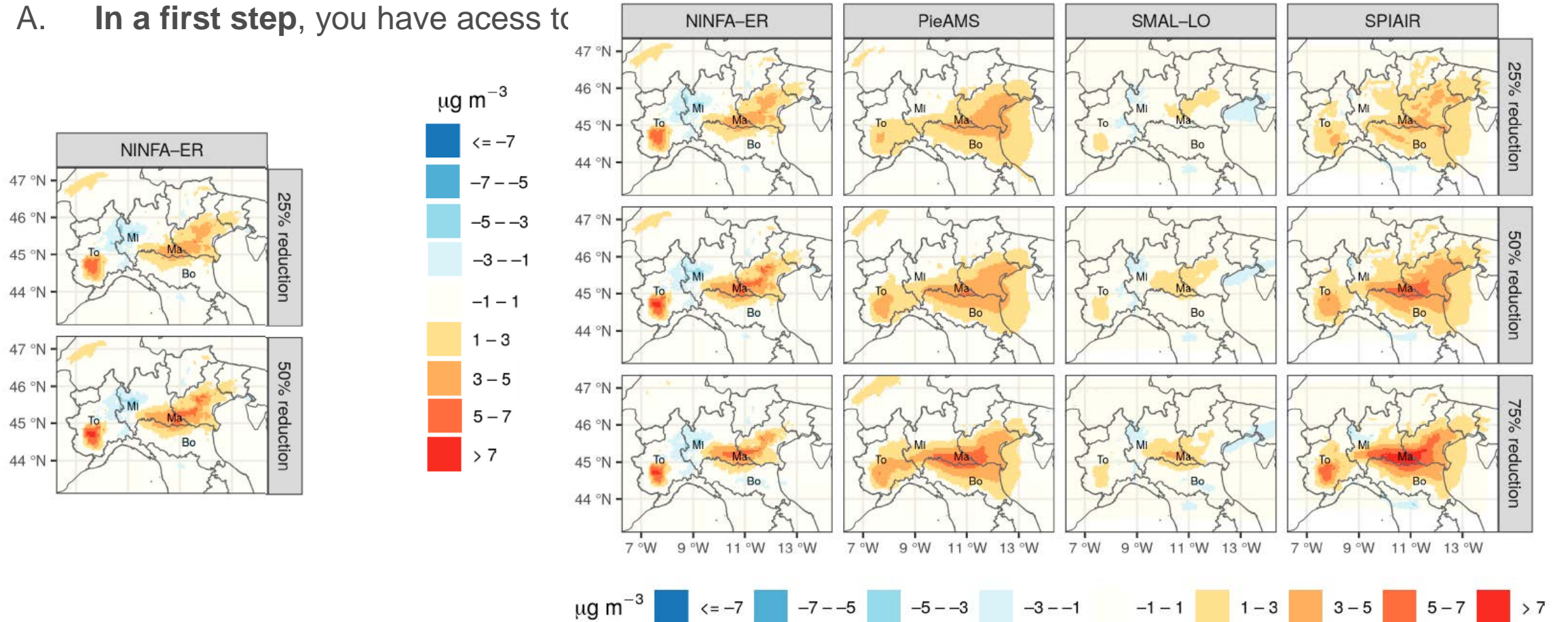
you have access to the following maps:



Sun Jan 01 2023 - Sun Dec 31 2023



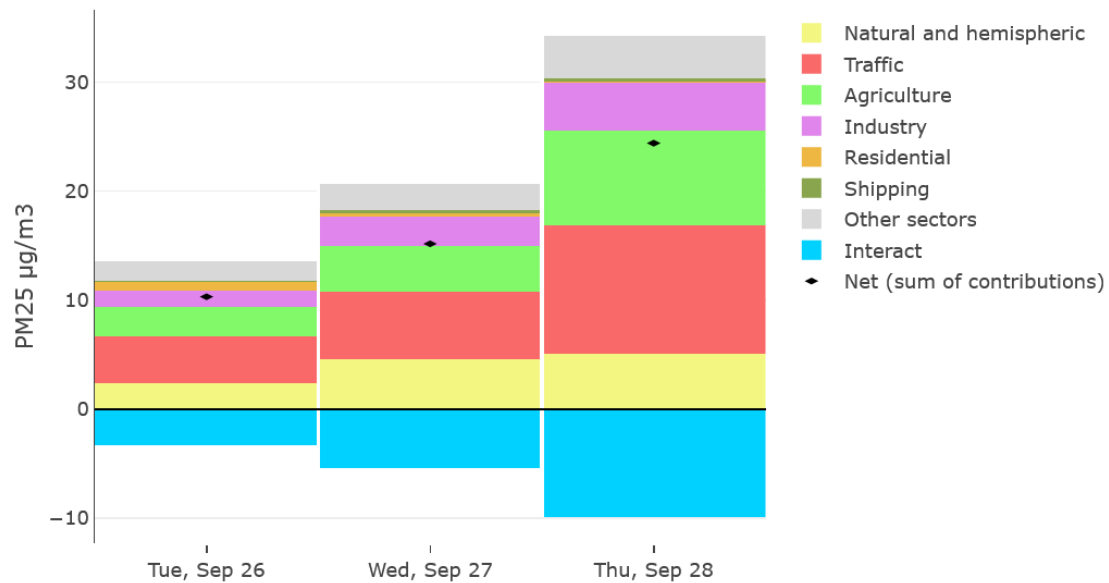
A. In a first step, you have access to

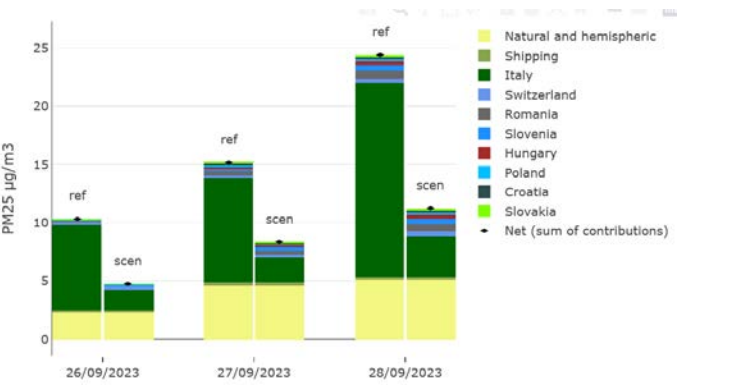
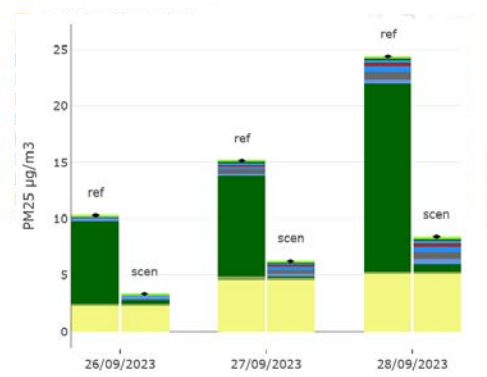
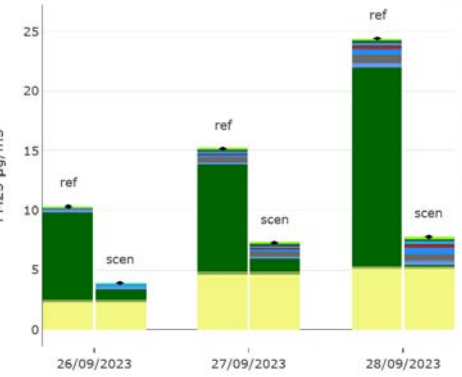
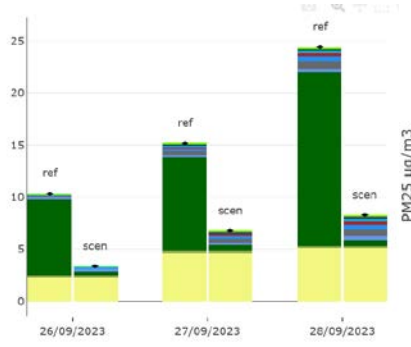
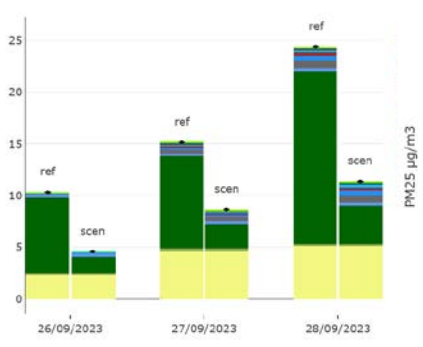
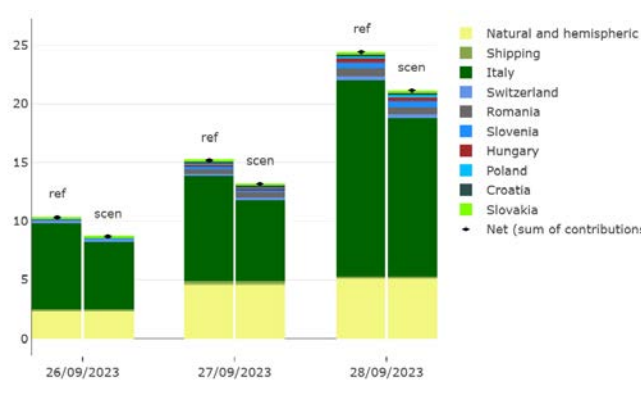
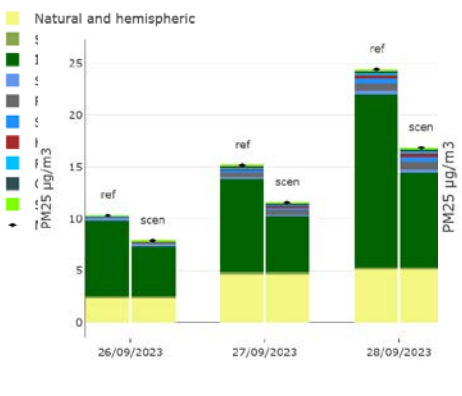
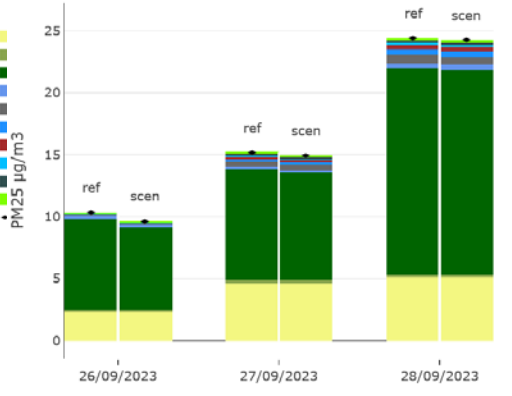
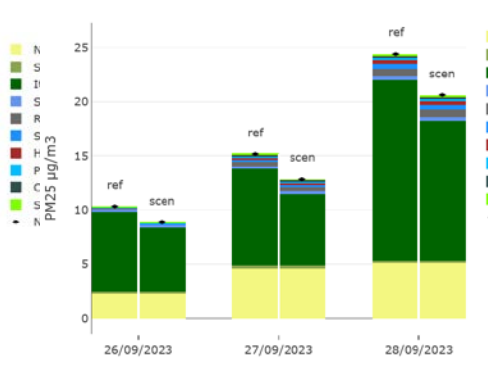
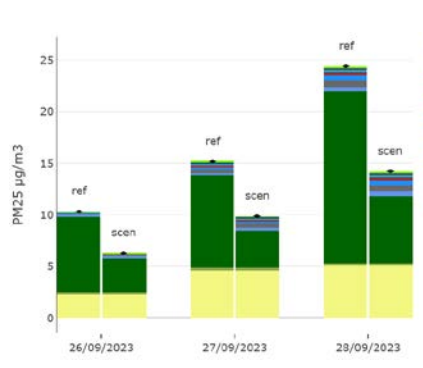




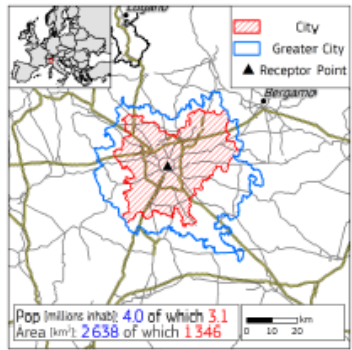
## B. In a second step,

1. Reduction scenarios to be implemented for a limited period on days when concentrations exceed limits

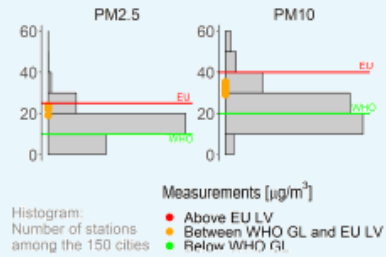




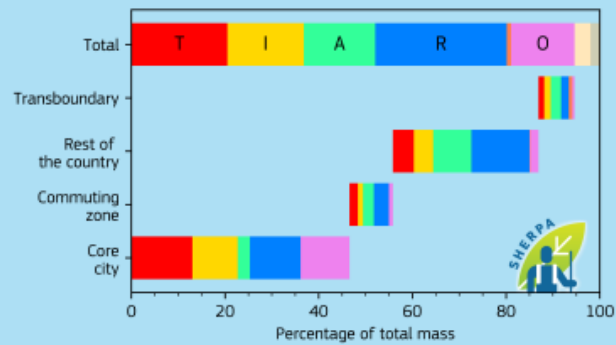
# Italy, Milan



Yearly average urban concentrations (2018)



PM<sub>2.5</sub> Spatial and sectoral allocation (SHERPA v.2.2.0)

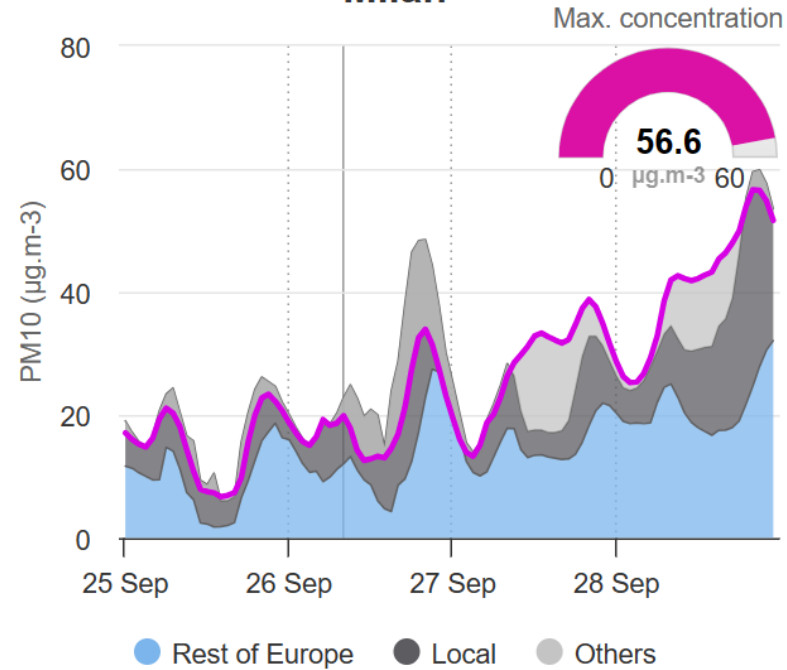


Emissions (kton/year)

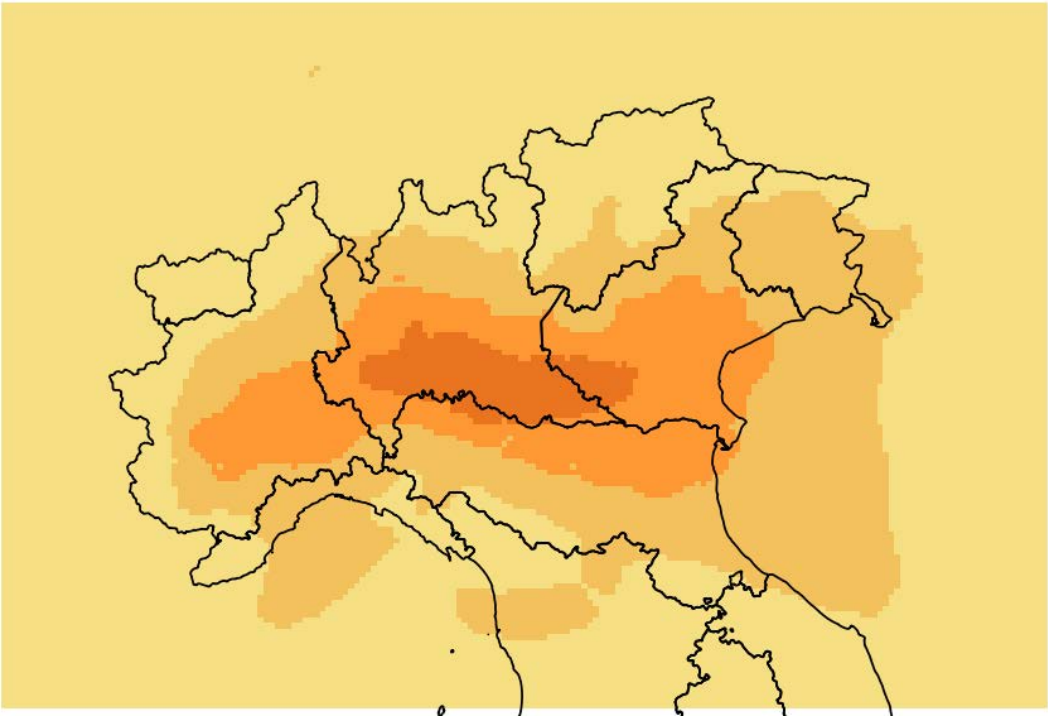


- T - Transport
- I - Industry
- A - Agriculture
- R - Residential
- S - Shipping
- O - Other
- N - Natural
- E - External
- Greater city
- Core city

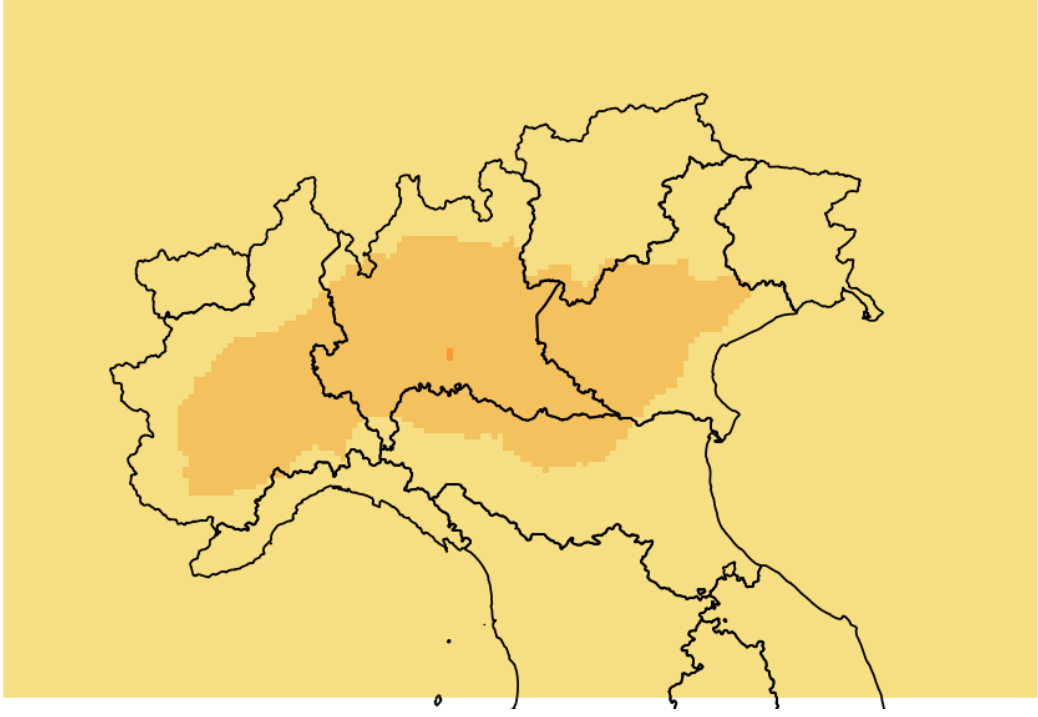
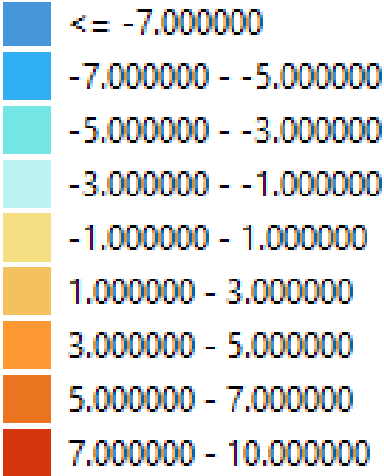
## Milan



Difference  $P^{\alpha}_{NOX} (NO_3^-) - P^{\alpha}_{NH3} (NH_4^+)$  based on CAMx/PSAT



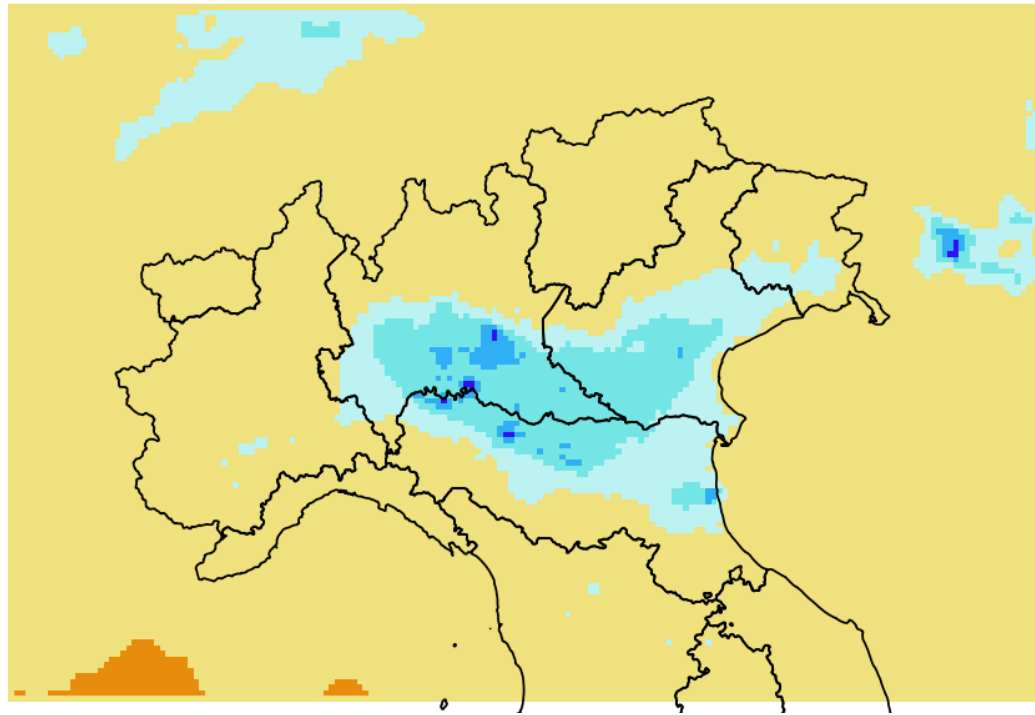
WINTER



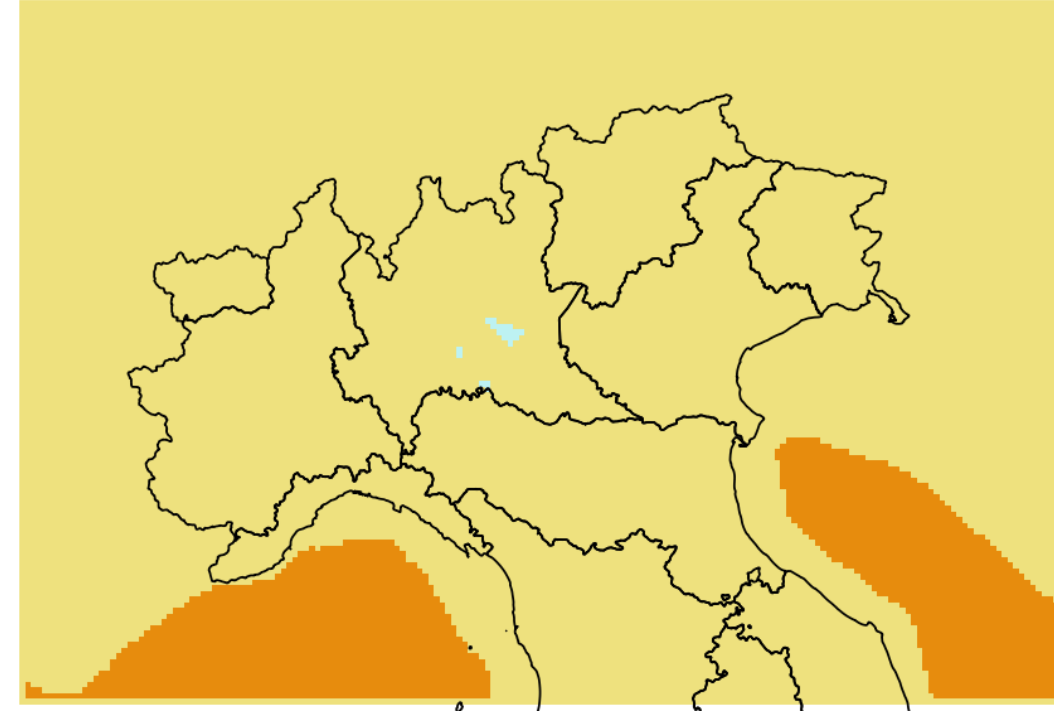
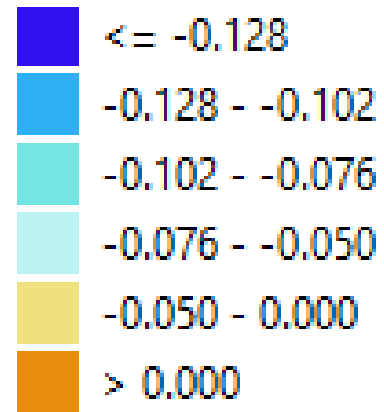
SUMMER

Concentrations in  $\mu\text{g}/\text{m}^3$

Difference  $P^{\alpha}_{\text{NOX}} (\text{NO}_3^-) - P^{\alpha}_{\text{NH}_3} (\text{NH}_4^+)$  based on CAMx/PSAT



WINTER

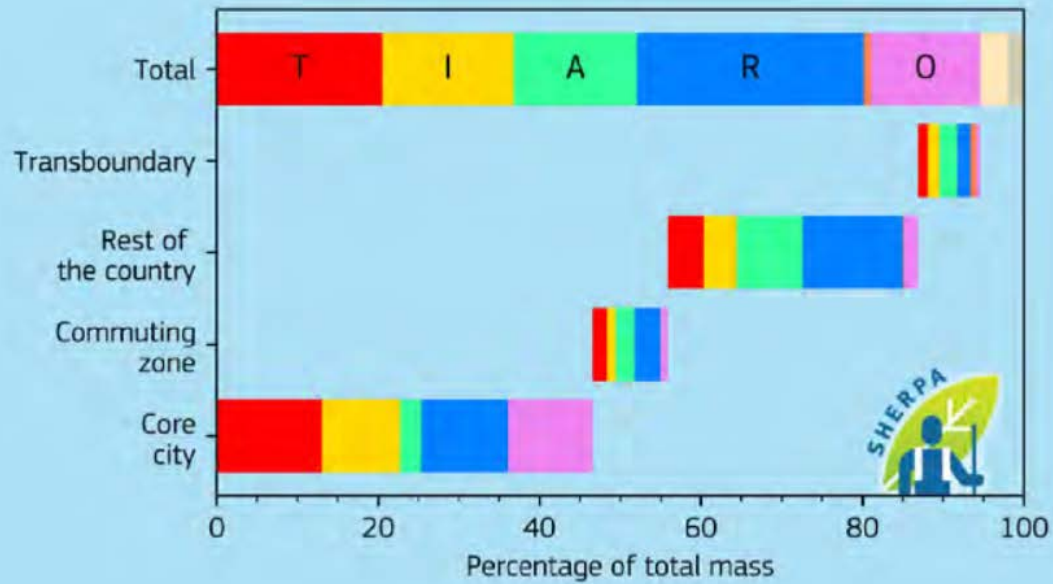


SUMMER

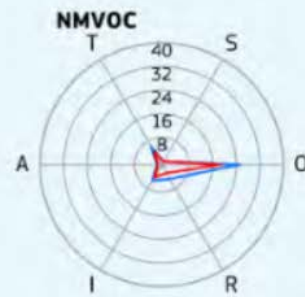
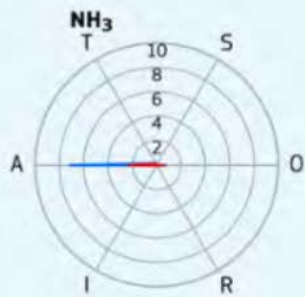
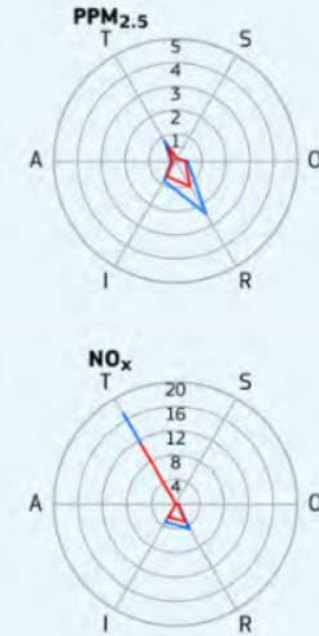
Concentrations in moles/m<sup>3</sup>

# MILAN receptor

PM<sub>2.5</sub> Spatial and sectoral allocation (SHERPA v.2.2.0)



Emissions [kton/year]



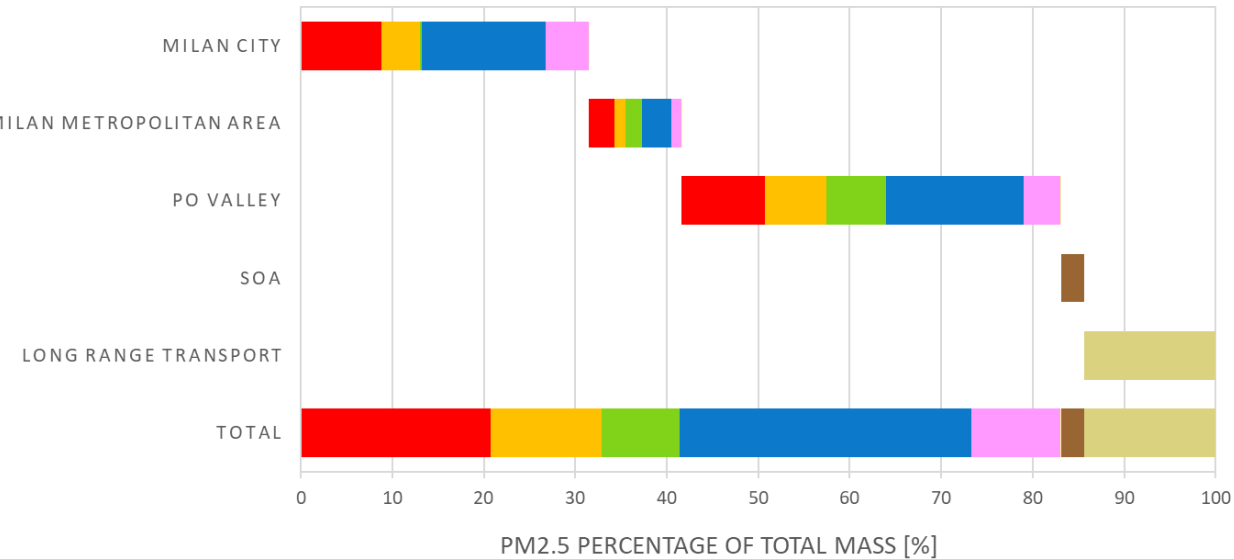
- T - Transport
- I - Industry
- A - Agriculture
- R - Residential
- S - Shipping
- O - Other
- N - Natural
- E - External
- Greater city
- Core city

# MILAN receptor

## PM2.5 - Sectoral and spatial contributions based on CAMx/PSAT

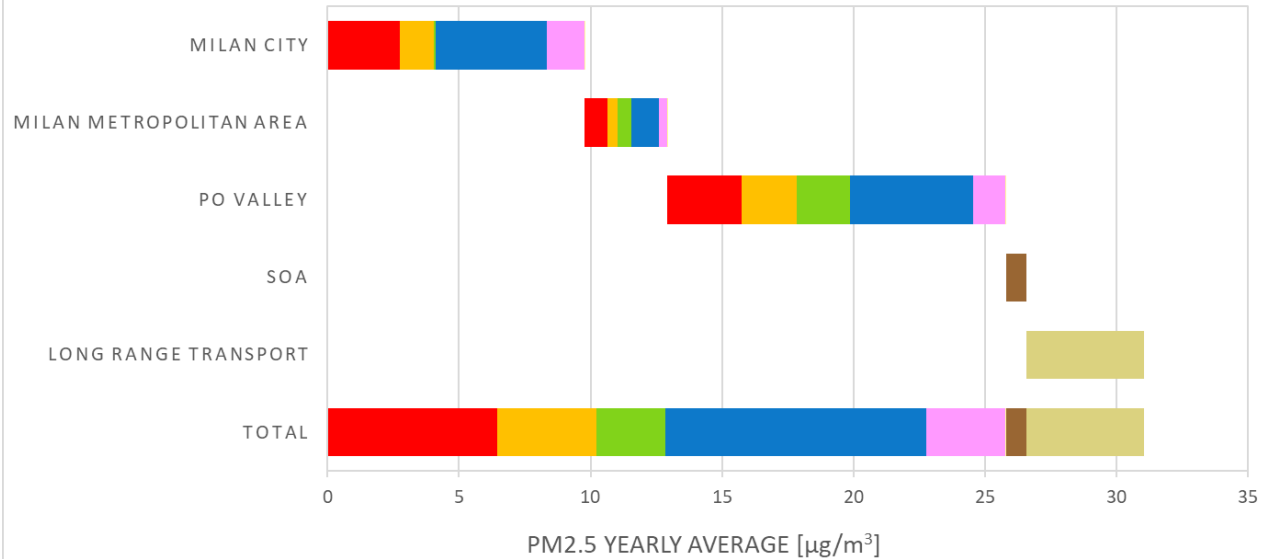
PM2.5 SPATIAL AND SECTOR CONTRIBUTION

TRA IND AGR RES OTHER NATURAL SOA BC



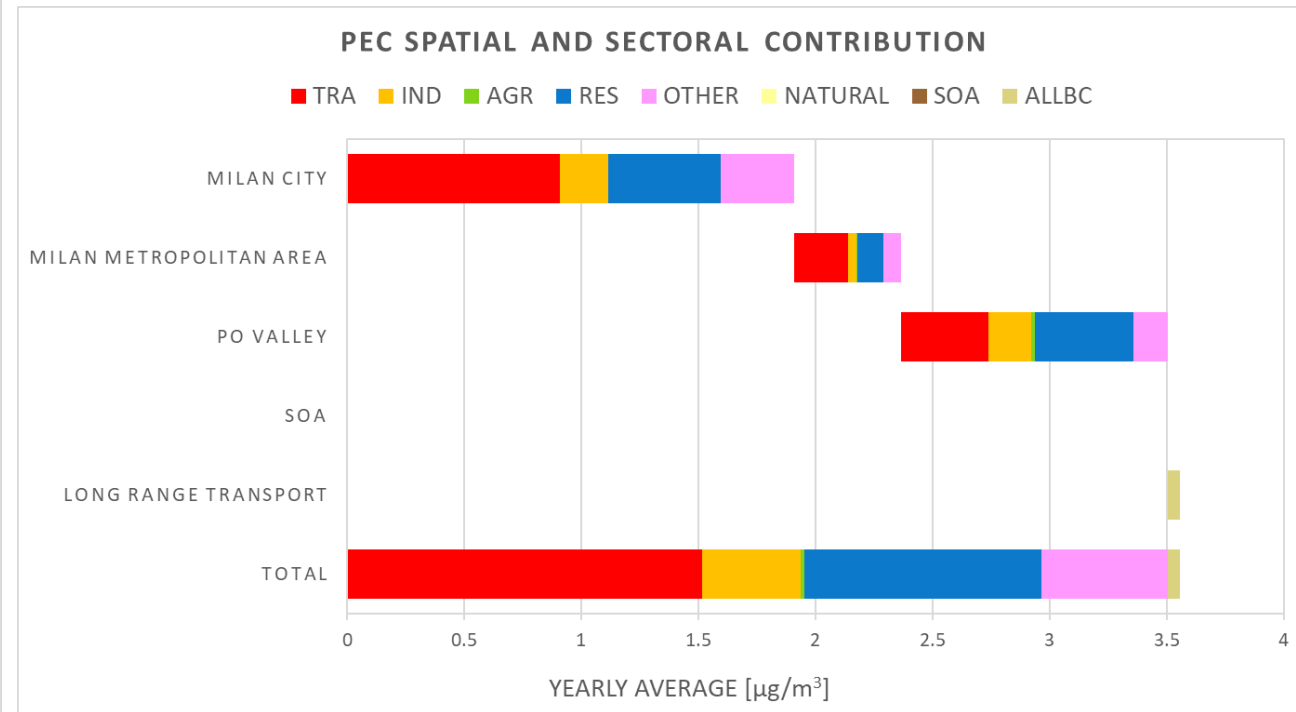
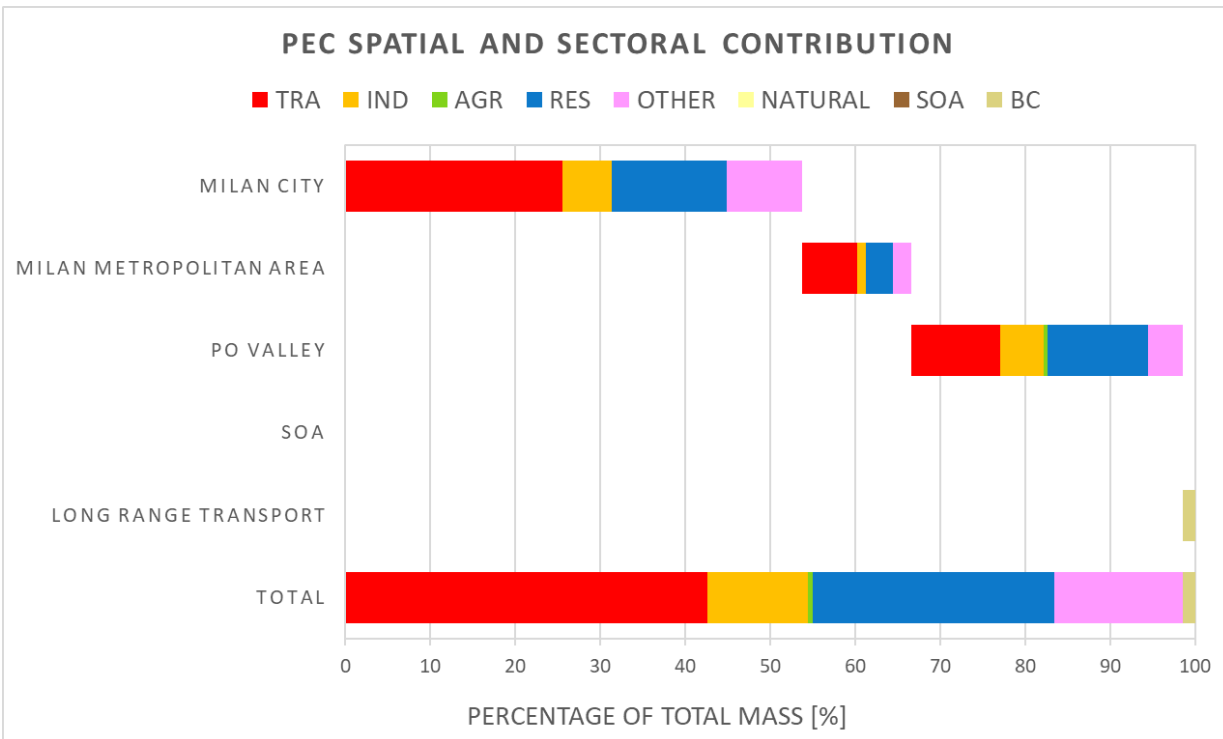
PM2.5 SPATIAL AND SECTOR CONTRIBUTION

TRA IND AGR RES OTHER NATURAL SOA BC



# MILAN receptor

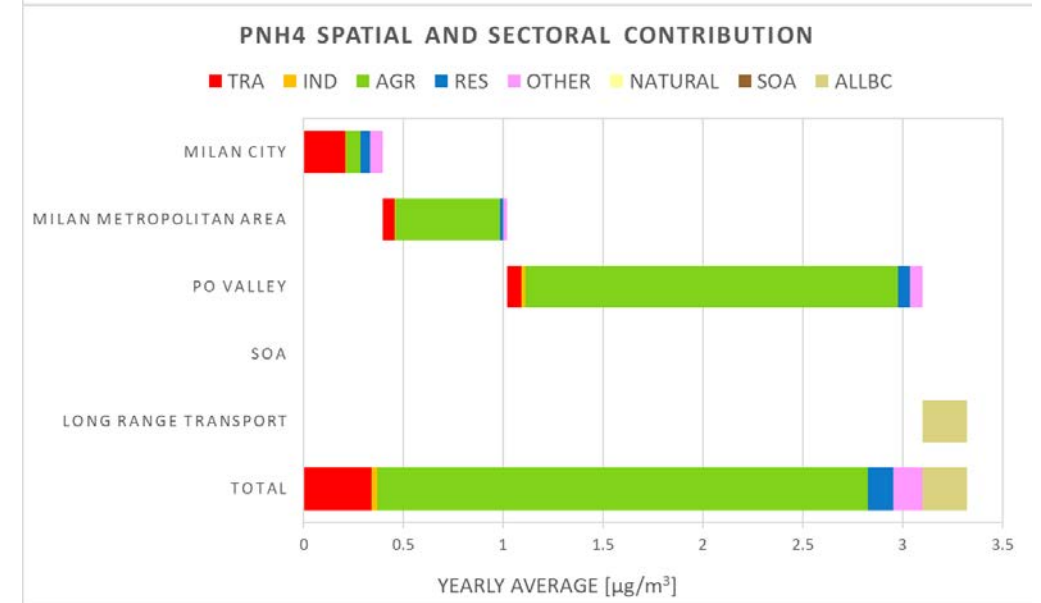
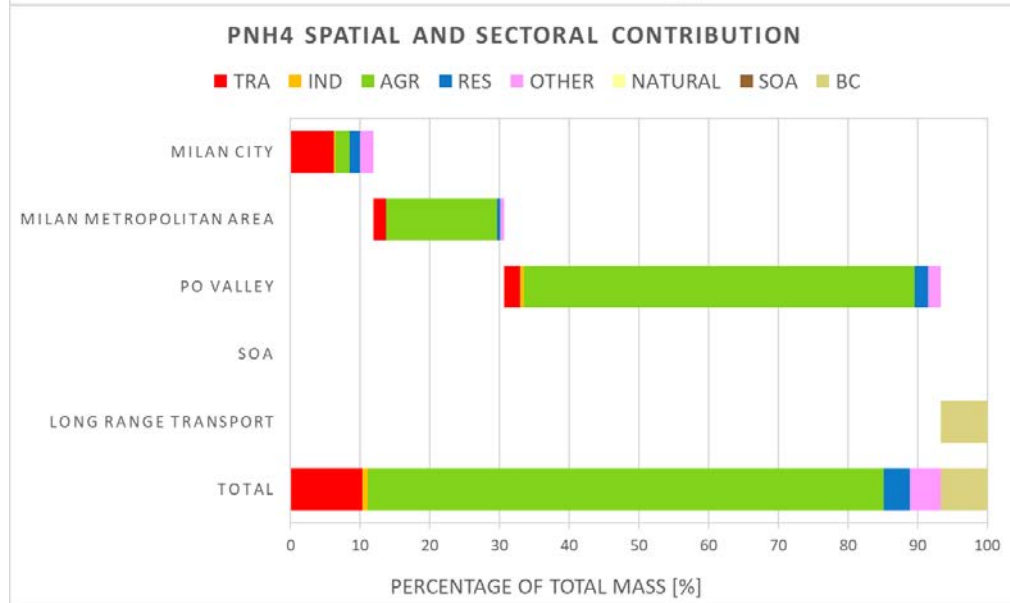
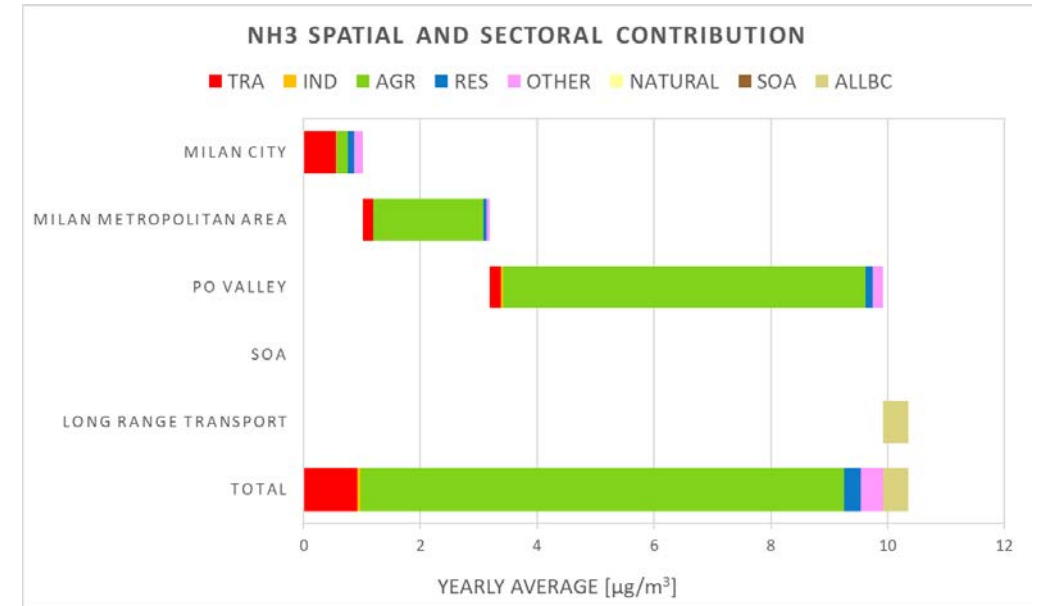
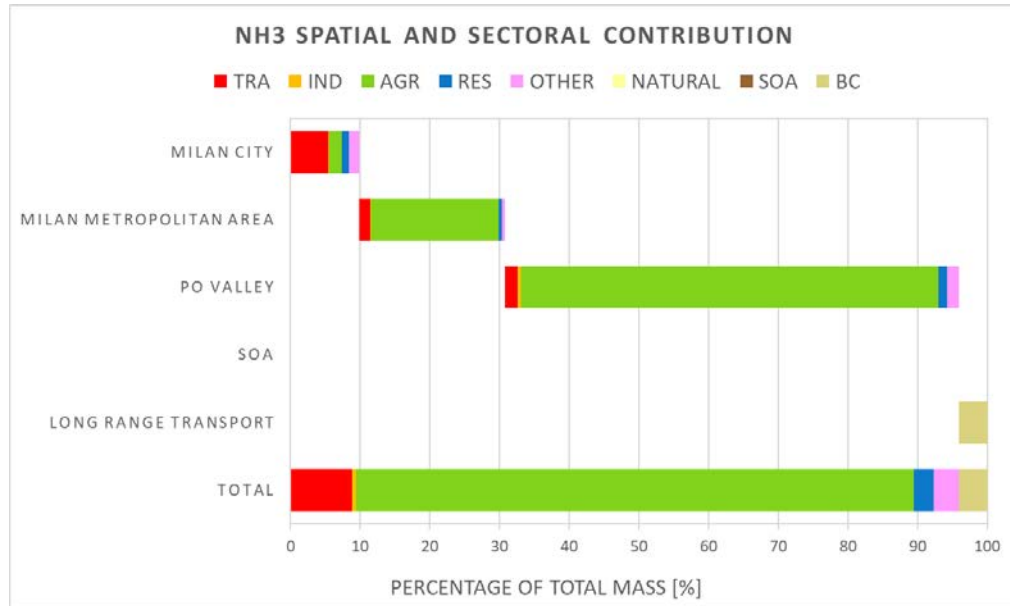
## EC - Sectoral and spatial contributions based on CAMx/PSAT





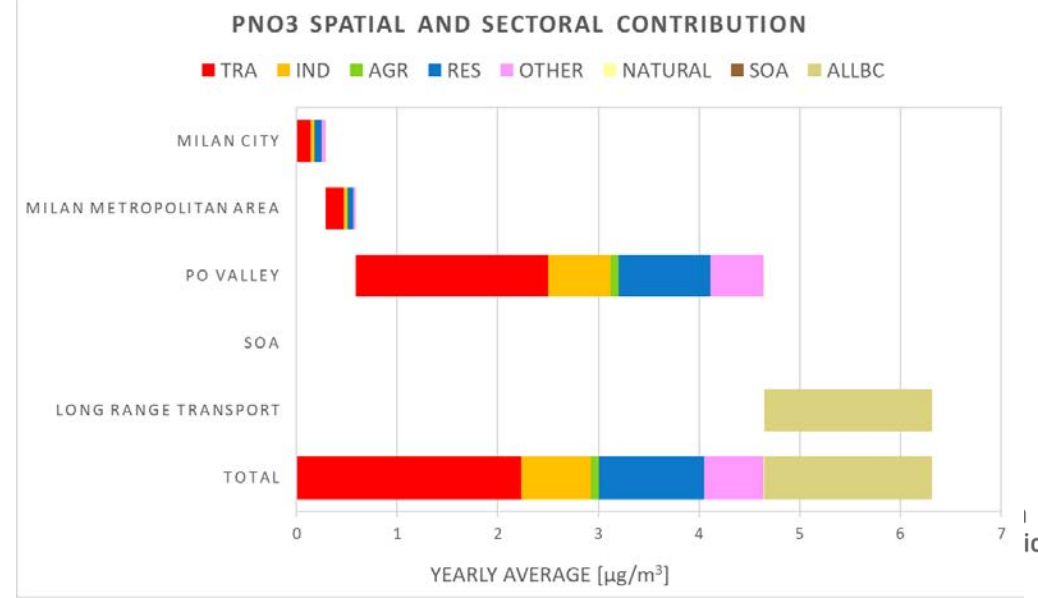
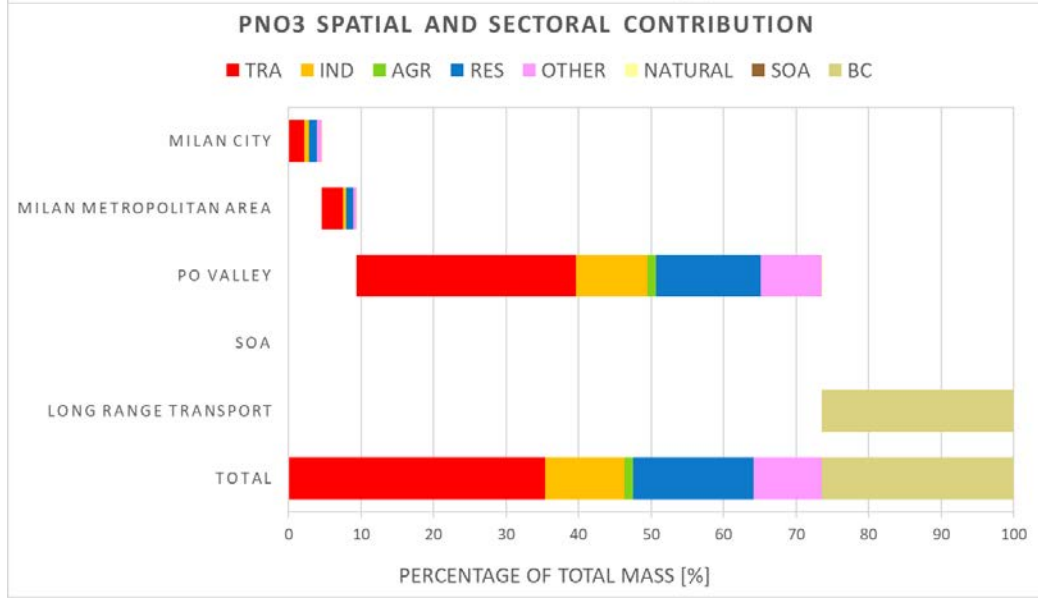
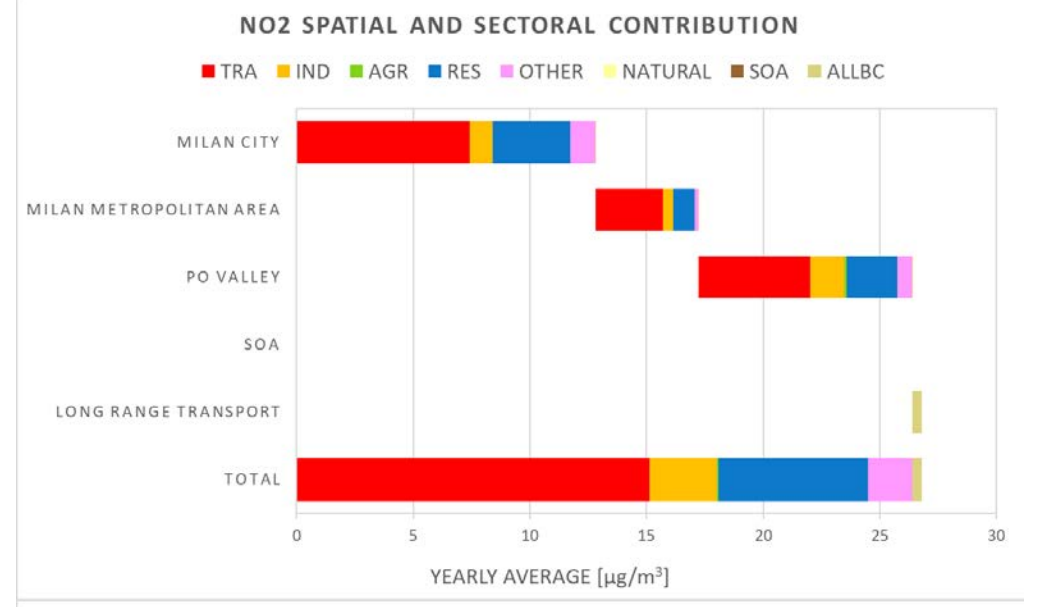
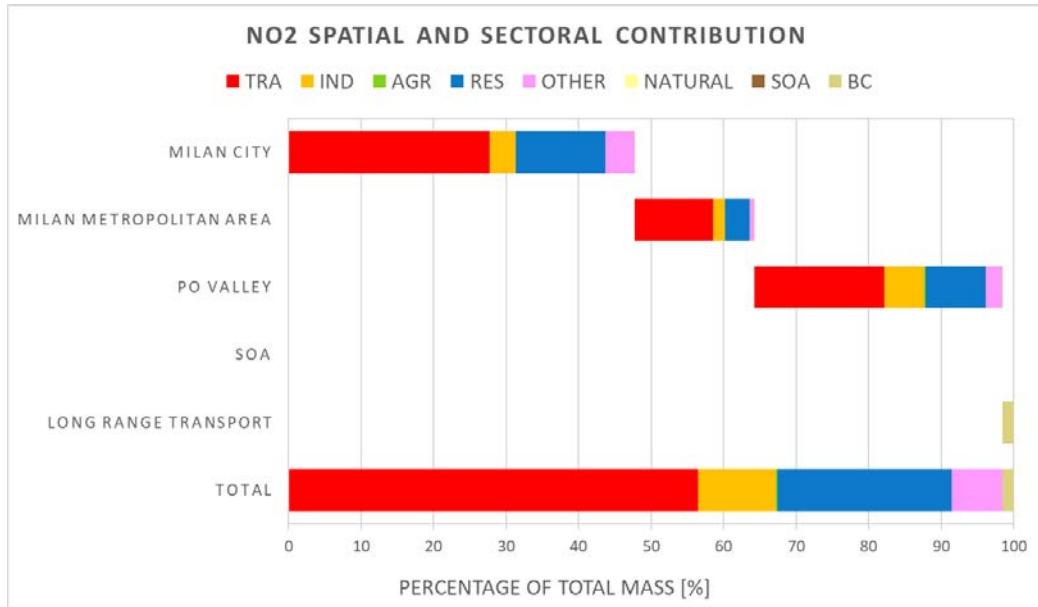
# MILAN receptor

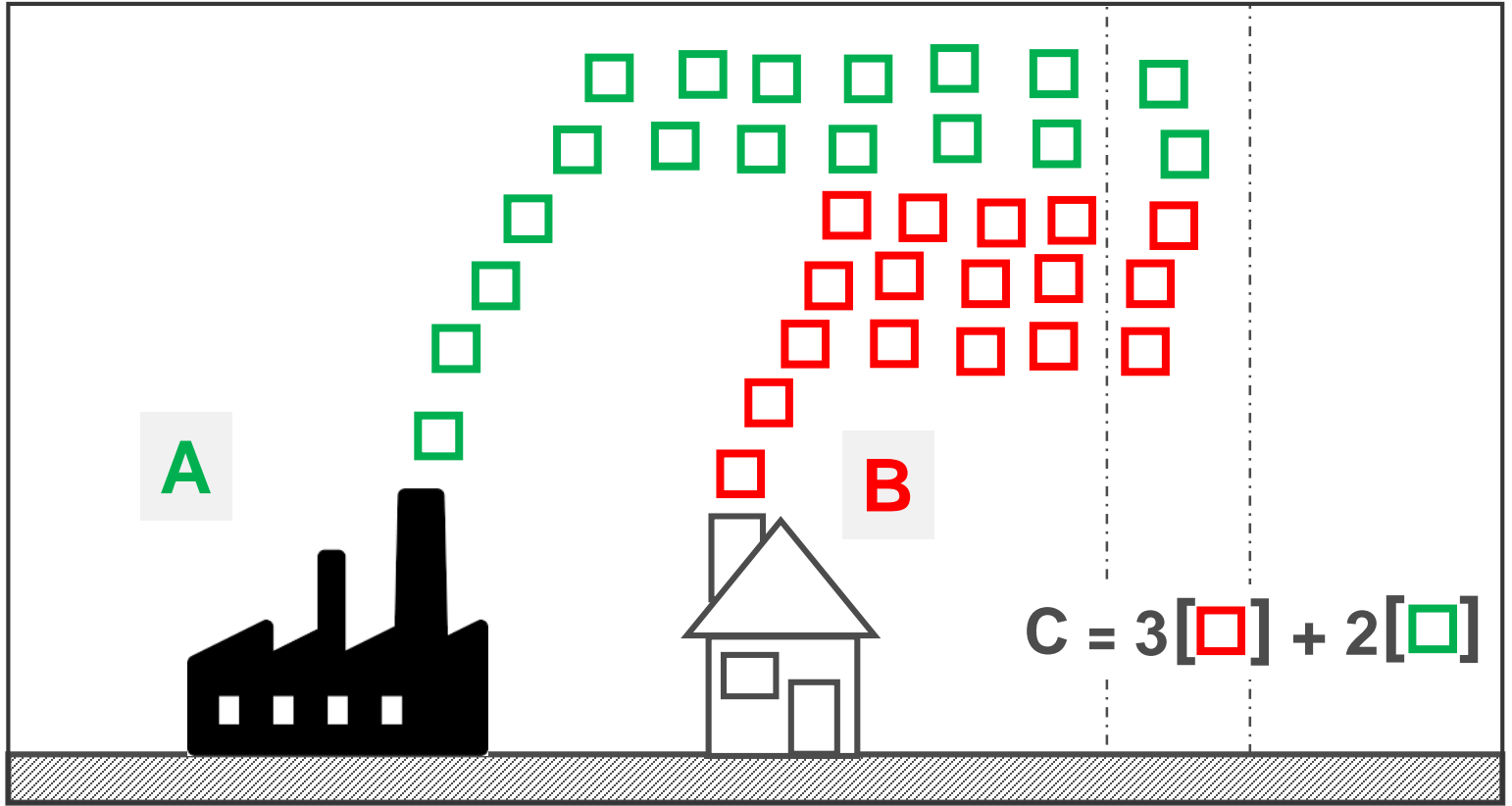
## NH<sub>3</sub> and NH<sub>4</sub><sup>+</sup> - Sectoral and spatial contributions based on CAMx/PSAT



# MILAN receptor

## NO<sub>2</sub> and NO<sub>3</sub><sup>-</sup> - Sectoral and spatial contributions based on CAMx/PSAT





for the temporal analysis, exercise 2, we discussed as follows:

1) at first, one should think about the domain under study, in this case, Milan...the knowledge of the domain under study is very important as a starting point

2) then we discussed PM. For PM:

- in general, for Milan, winter period is the focus, as PM is high in winter. But the analysis on the temporal scale cannot be considered separately from the geographical dimensions (that means, it is important to know if pollution depends on local or background sources. The same for sources). It means, to perform a temporal analysis and take decisions on this, one needs also to take into account geographical and sectoral dimensions, to have the full picture

- to reduce PM yearly averages, an annual approach to source apportionment is sufficient

- to reduce PM exceedances, one could also use source apportionment techniques, but a similar information can be derived through simpler approaches, as i.e. correlation analysis, etc...

3) for NO<sub>2</sub>

- this pollutant is much more local and much more short term, so in principle source apportionment can be done in an easier way

- in this case, an annual approach to source apportionment is already sufficient, both to control averages and exceedances

4) in any case, all the tools available are useful to support decision makers, but then final decisions will be taken by policy makers, also considering other factors

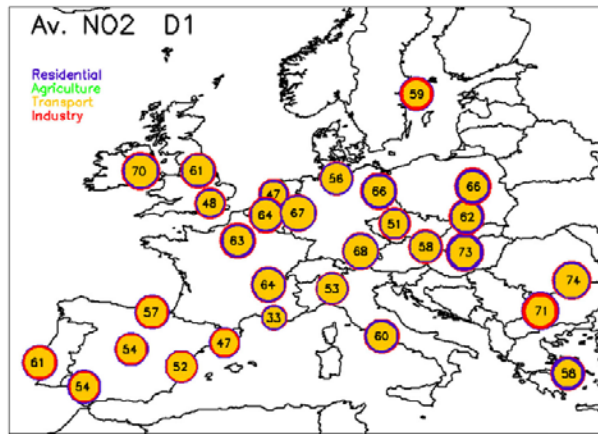
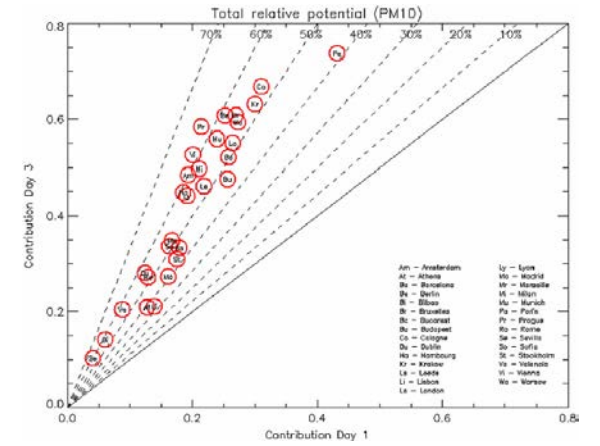
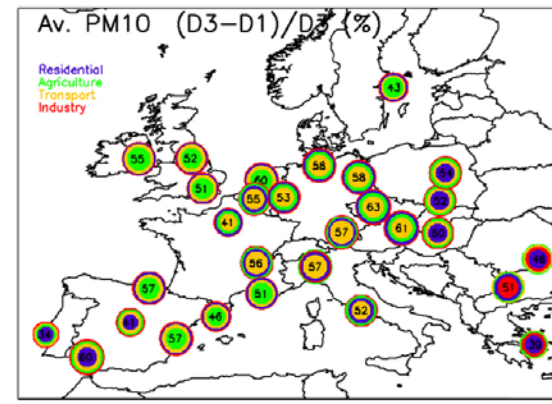
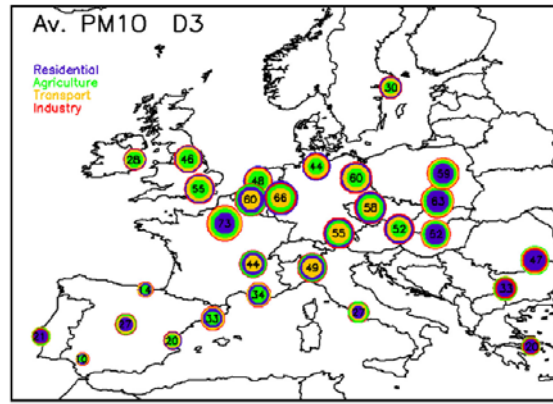
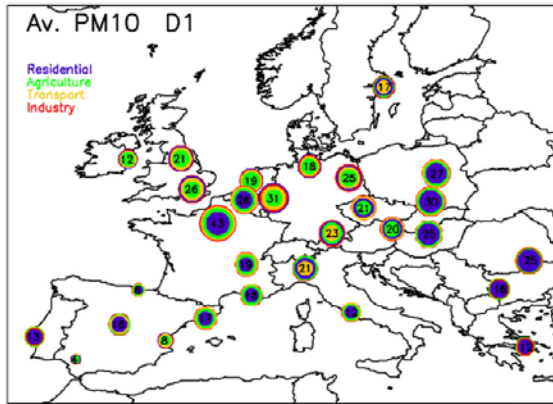


Fig. 1 Map of relative potentials (i.e.,  $\Delta C/\alpha C$ ) at  $D_{AQP} = 1$  for  $PM_{10}$ . The circled area is proportional to the potential with the most important contributors placed from center to outwards. The four activity sectors are represented by different colors. The number in each circle is the overall potential (i.e., corresponding to all sectors reduced simultaneously)

