Preliminary analysis of FAIRMODE CT9 results

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with inputs from CT9 participants modelling teams

JRC (EC/EU)
ZAMG (AT)
Met Norway (NO)
CyI (CY)
NKUA (GR)
DHMZ (HR)
LMD/IPSL (FR)
UH-CACP (UK)
CIEMAT (ES)
ENEA (IT)
UNIBS (IT)
IRCELINE (BE)

JRC, Ispra, IT

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Joint Research Centre

FAIRMODE CT9

- Models provide different absolute results C_{scen}^{M}
- **BUT HOW DO THEY BEHAVE ON DELTAS?**

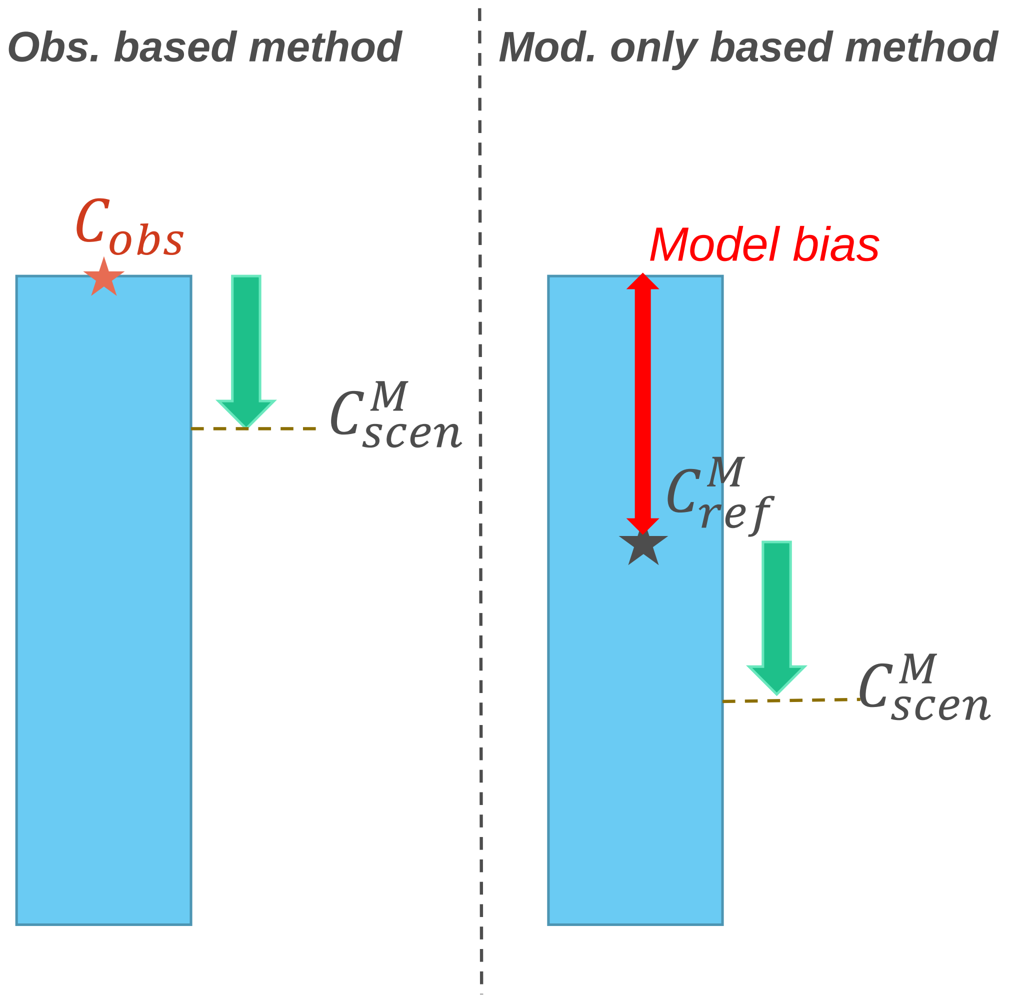
$$\Delta = C_{scen}^{M} - C_{bc}^{M}$$

- What is the order of magnitude of differences? How to evaluate these differences? Which indicators?
- Can we explain the differences, what are the main drivers?

FAIRMODE CT9

- Many intercomparison exercises of air quality models
- Willing to have a long term intercomparison plateform to continually assess the response of model
- No recent exercises to assess the capacity of models to simulate “delta” (Formerly CityDelta, EURODELTA)

- A Concentration Delta for model M can be applied to an observation C_{obs} to evaluate a scenarios based on ‘*bc*’ reference and ‘*scen*’ simulations:
  - Absolute (for O3?): $C_{scen} = C_{obs} + (C^M_{scen} - C^M_{bc})$
  - Relative (for NO2 or PM?): $C_{scen} = C_{obs} \times (C^M_{scen} - C^M_{bc})/C^M_{bc}$
  - ***Techniques often used but rarely assessed***



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FAIRMODE CT9

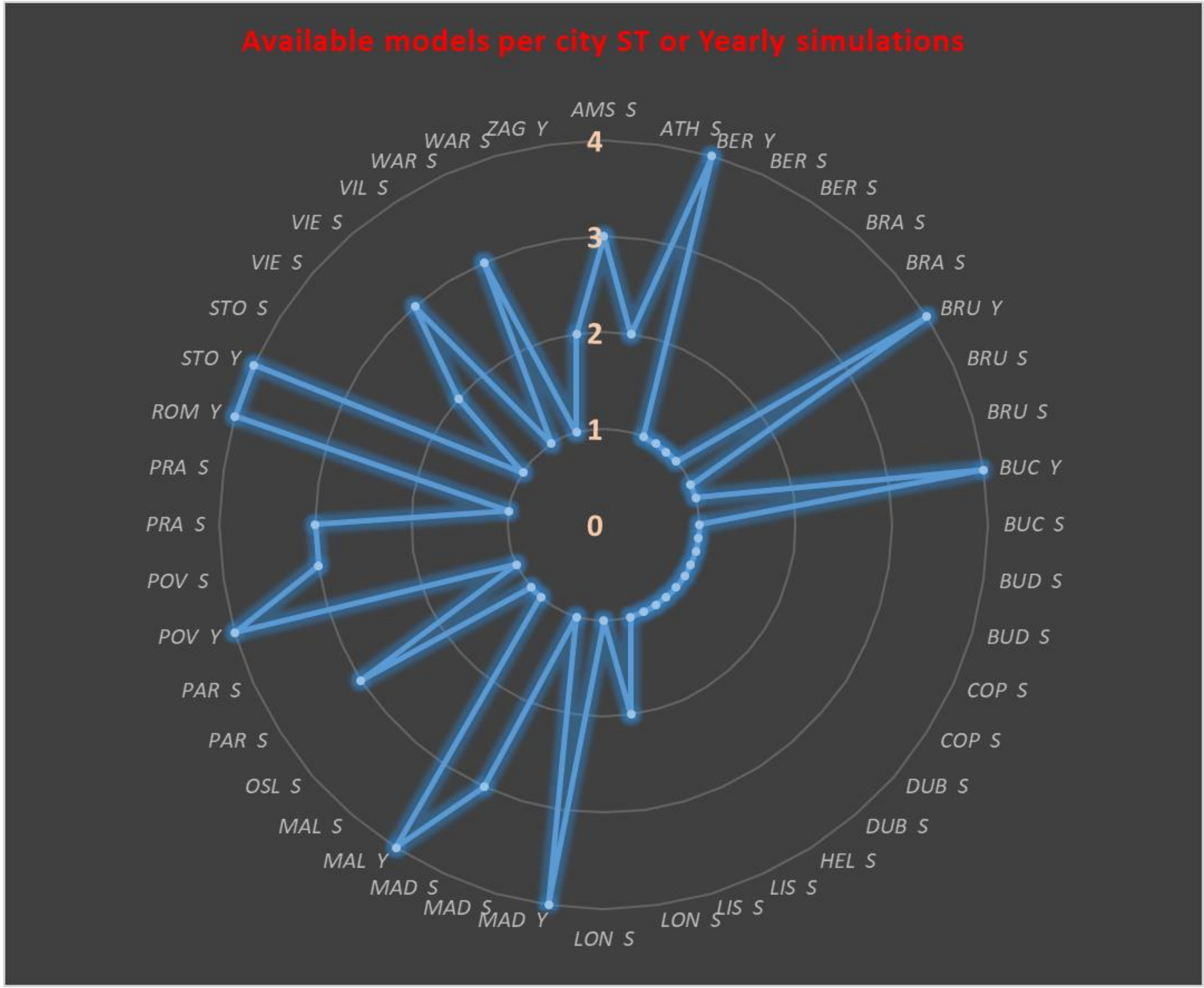
- Models have different behaviours between each other because:
  - Different processes (chemistry and physics) … magic parameters ☺
  - Different settings like resolutions (vertical, horizontal)
  - Different input data
    - Emissions
    - Meteorology
    - Boundary conditions
- Even if sharing the “same” inputs, models remain differents…
  - Remaining meteorological diagnosed data (diffusion, PBL)
  - Emission pre-processing (spatial/temporal redistribution, VOC split, PM split)
  - Management of interpolations, grids
  - Others like : user dependency, compilers…

CT9 Database

- JRC box
  - 10 Participants
  - 15 Models

  - Many cities and regions are covered by one or more models
  - Number of DBMC (Concentration) files > 5000, Resol: HL, DL, YL
  - Number of DBME (Emissions) files = 170, Resol: YL, ML

- Box will be moved to an other place this month
- <u>Access</u>: Contact coordinators



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IDL Vizualisation tool

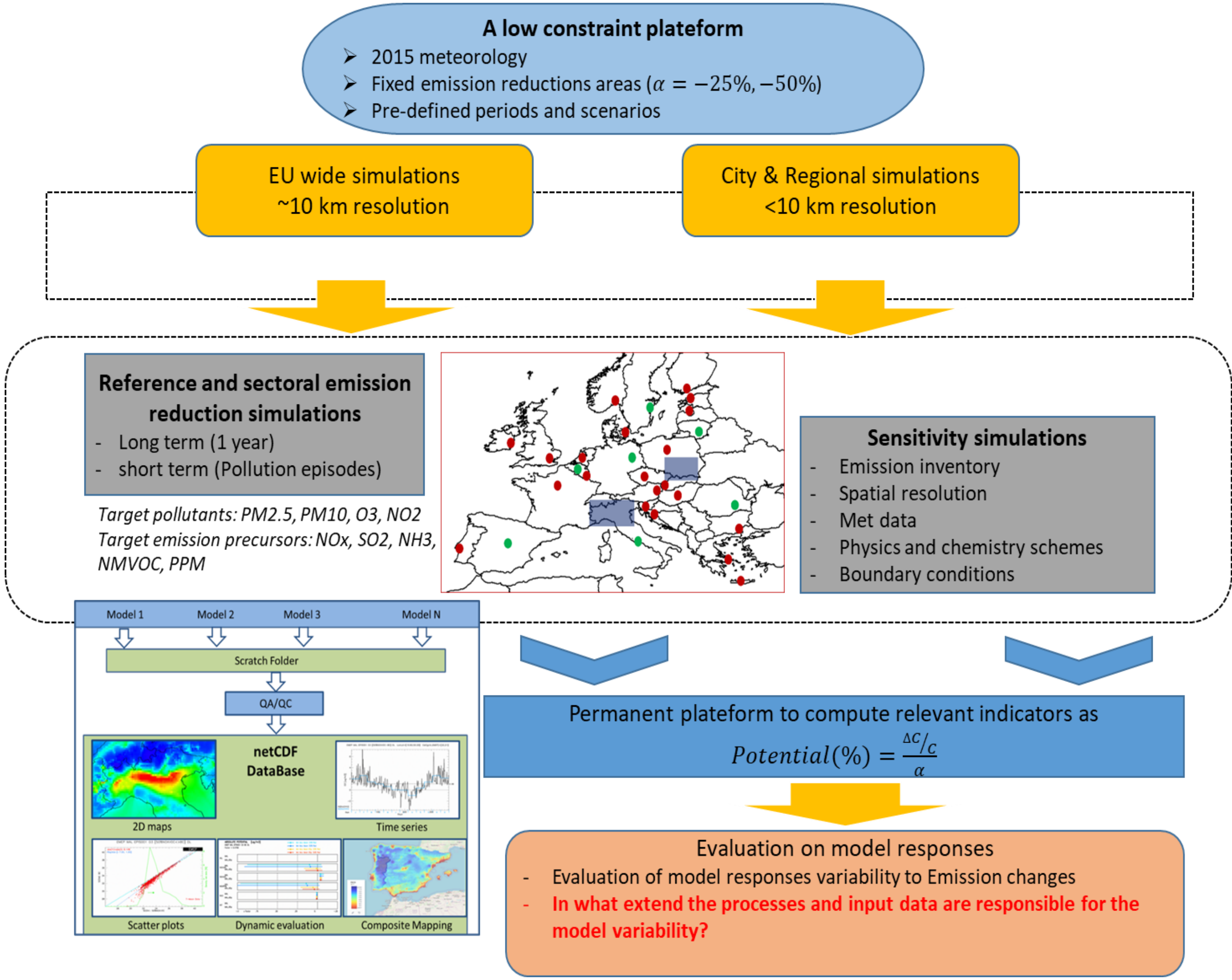
- 2D maps
- Scatter Plots
- Dynamic Evaluation diagrams
- Tests for compliance with the CT9 standards
- Link to Composite Mapping
- Freely downloadable
- Easy installation
- Easy to use
- No license

Models and teams involved

Team name - Country		Model Name	Emission Inventory, resolution, date
JRC	(EU)	EMEP	EDGAR V5.0, 2015
JRC	(EU)	EMEP	CAMS V2.2.1, 2015
JRC	(EU)	EMEP	EMEP - GNFR, 2015
JRC	(EU)	EMEP	CAMS REG V4.2 + Condensables 2015
JRC	(EU)	WRF-Chem	EDGAR V5.0, 2015
ZAMG	(AT)	WRF-Chem	CAMS-REG 2015
Met Norway	(NO)	EMEP	EMEP, 0.1x0.1, 2015
Met Norway	(NO)	EMEP + uEMEP	EMEP, 0.1x0.1, 2015
CyI	(CY)	WRF-Chem	EDGAR V5.0, 0.1° x 0.1°, 2015
NKUA	(GR)	WRF-Chem	EDGAR HTAP, 2010
DHMZ	(HR)	ADMS-Urban	Croatian National Emission Inventory for Zagreb
DHMZ	(HR)	LOTOS-EUROS	CAMS-AP-v2.2.1 2015
LMD/IPSL	(FR)	WRF-CHIMEREv2020r1	CAMS REG V4.2 2015
UH-CACP	(UK)	WRF-CMAQ	EDGAR V5.0, 2015
CIEMAT	(ES)	IFS-CHIMEREv2017r4	EMEP + NEI, 2015
ENEA	(IT)	WRF-MINNI	ISPRA Italian national inventory 2015
UNIBS	(IT)	WRF-CAMx	INEMAR 2015+EMEP
IRCELINE	(BE)	CHIMERE + RIO + ATMOSTREET	Local inventories

The overall framework

- Short term (ST) on episodes (PM10, NO2, O3)
  - Emissions reduced only during the episodes from 00:00 to 23:00
- Long term (LT) simulations (PM10, NO2, O3)
  - Emissions reduced the whole year
- Two reductions so far:
  - 25% and 50% from a base case (BC)
- Reduced species depends on target pollutants
  - **PM10**: PPM, NOx, VOC, NH3, SO2, ALL
  - **Ozone**: NOx, VOC, ALL
  - All together or separately
- Notation:
  - **POL#PRE**: Pollutant concentrations POL for an emission reduction of precursor PRE
  - Ex. **PAR014** : Paris episode 014



Indicators I/II

- Indicators defined for a single pollutant reductions
- The **Absolute Potential** is defined as the reduction in µg/m^3 scaled by the reduction $\boldsymbol{\alpha}$ of the scenario (25 or 50%) of a precursor from base case BC
    - $\boldsymbol{APl = \left(C \quad - C^{BC}\right) / (\alpha \quad)}$ ($\boldsymbol{APl \times \alpha}$ is the delta of concentrations)
- The **Relative Potential** is defined as the reduction in % scaled by the reduction $\boldsymbol{\alpha}$ of the scenario (25 or 50%) of precursor ***n*** from base case BC and by the BC concentrations.
    - $\boldsymbol{RPl = \left(C \quad - C^{BC}\right) / (\alpha \quad \times C^{BC})}$
- The **Absolute Potency** in µg/m^3/(ton/day) is defined as the derivative of the concentration with respect to the emissions density E of a precursor or in other words the rate with which the concentrations (***C***) will change as a result of an emission density E)
    - $\boldsymbol{APy = \left(C \quad - C^{BC}\right) / (\alpha \quad \times E^{BC})}$

Clappier et al. 2016

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Indicators II/II

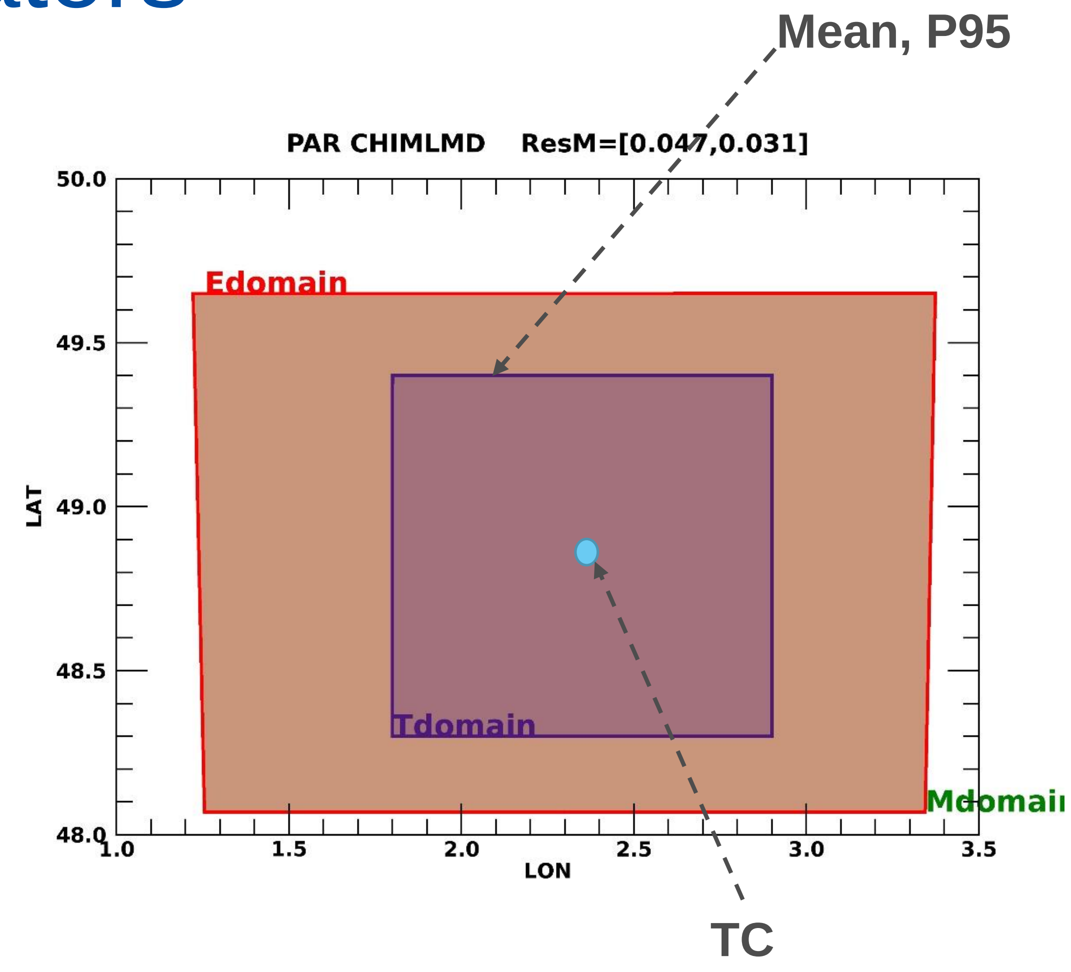
- Absolute Potential **APl** or **AbsPotential** directly linked to concentration delta

- Relative Potential **RPl** or **RelPotential** allows to indirectly scale the concentration delta to model peculiarities, input, settings

- Absolute Potency **APy** or **AbsPotency** is a direct scaling with absolute emissions reductions, then excluding model settings and other inputs

Where to calculate indicators

- Reminder
  - Edomain: model emission reporting
  - Mdomain: model concentration reporting
  - Tdomain: target domain where emissions are reduced
- Three target locations in **Tdomain** for the concentrations common to all teams so far:
  - Averaged over the Target domain Tdomain : **Mean**
  - Take the values above P95th: **P95**
  - Take central point of Tdomain: **TC**



Assessing the variability of indicators

- The Normalized Standard Deviation (NSD) is adapted
  - IND can be calculated for:
    - Concentration value (Mean, Tcenter, P95) over the Target area:
      - **Mean** : average over time and Target domain of all concentrations
      - Tcenter (**TC**): center of the domain
      - **P95**: averaged values over percentile 95th
  - For a given indicator : $NSD_{IND} = \sqrt{\frac{\sum_M (IND_M - \overline{IND})^2}{(\overline{IND})^2}}$
    - For the list of models M in a given city/region
    - $\overline{IND}$ the average value for all models $\overline{IND} = \frac{1}{N}\sum_M IND_M$

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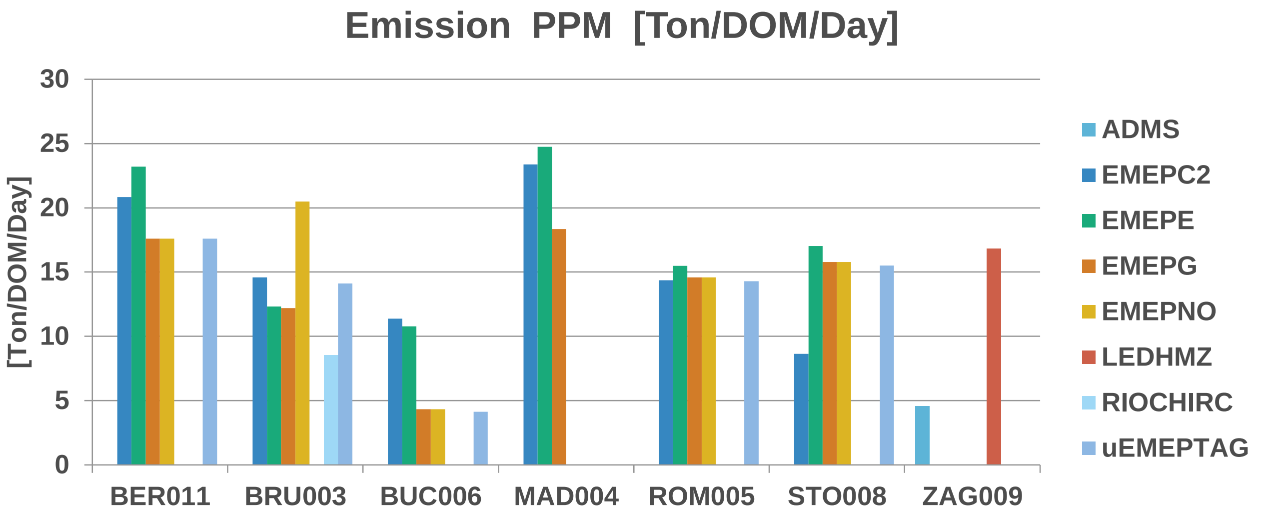
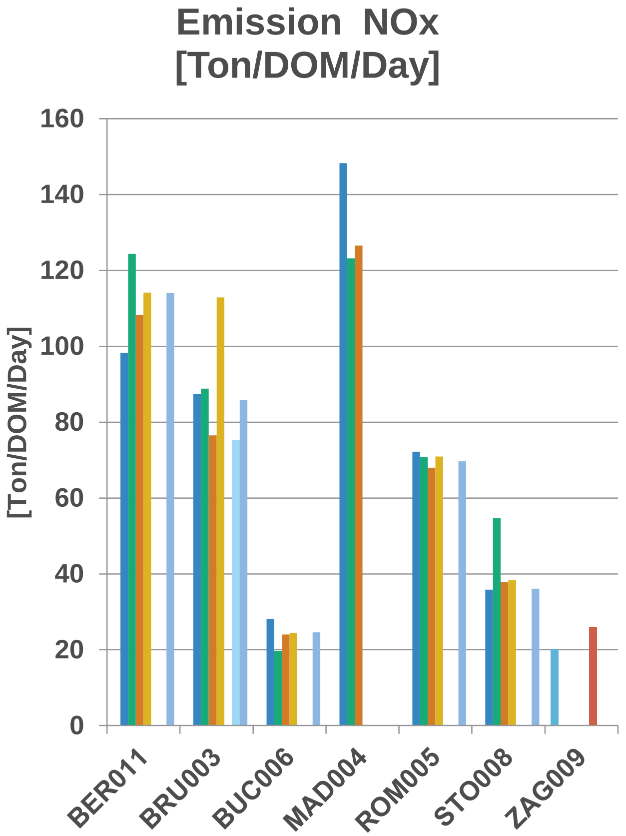
Outline

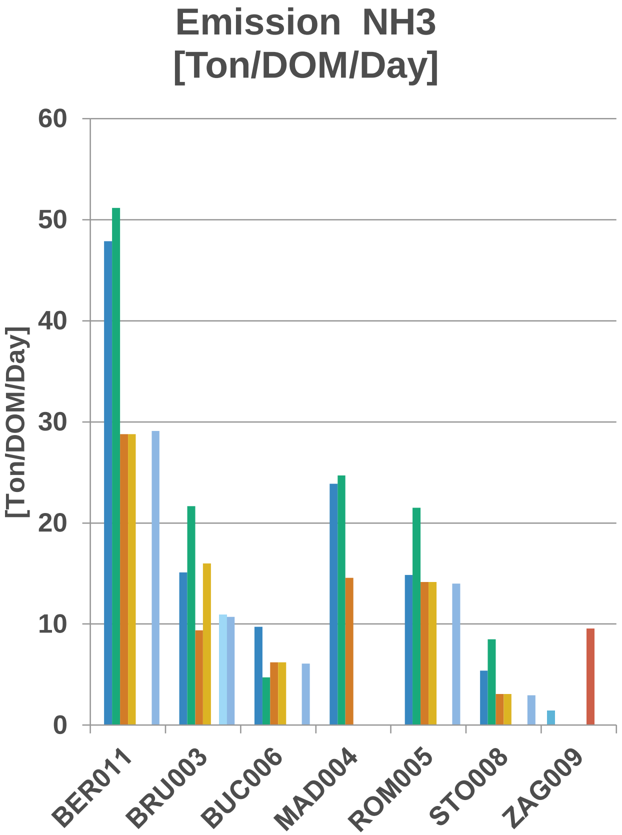
- **Results mainly based on EMEP simulations with different settings, we wait for more runs on episodes and long term simulations**
- Focus on PM10 and O3 for the indicators mainly the RPI
- Parameter of variability based on NSD
- Linearity assessment
- Different type of concentrations:
  - **Mean** : average over time and Target domain of all concentrations
  - Tcenter (**TC**): center of the domain
  - **P95**: averaged values over percentile 95^{th}
- Some results on Short Term simulations
- Concluding remarks and next steps

Yearly Emissions

- Large differences observed for the BC
- Less differences for NOx emissions
- Keep in mind that NH3 has a low molar mass compared to NOx related species
  - Crucial for ammonium nitrate formation

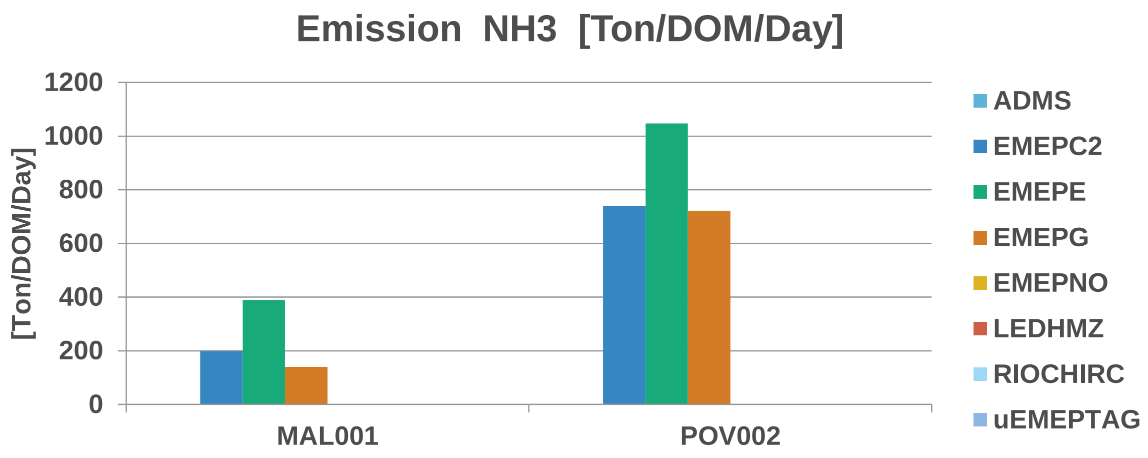


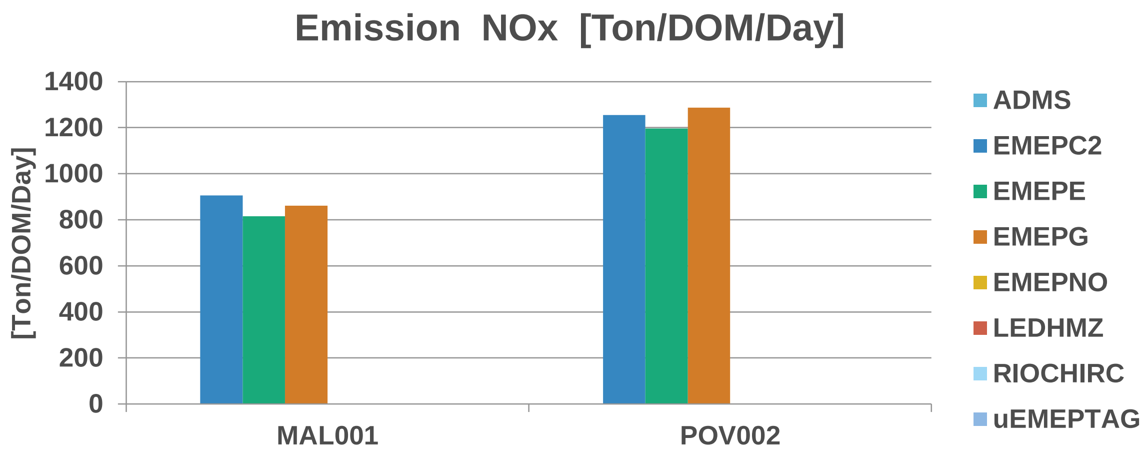




Yearly Emissions

- For MAL and POV regions, some significant differences for NH3 even for similar inventories





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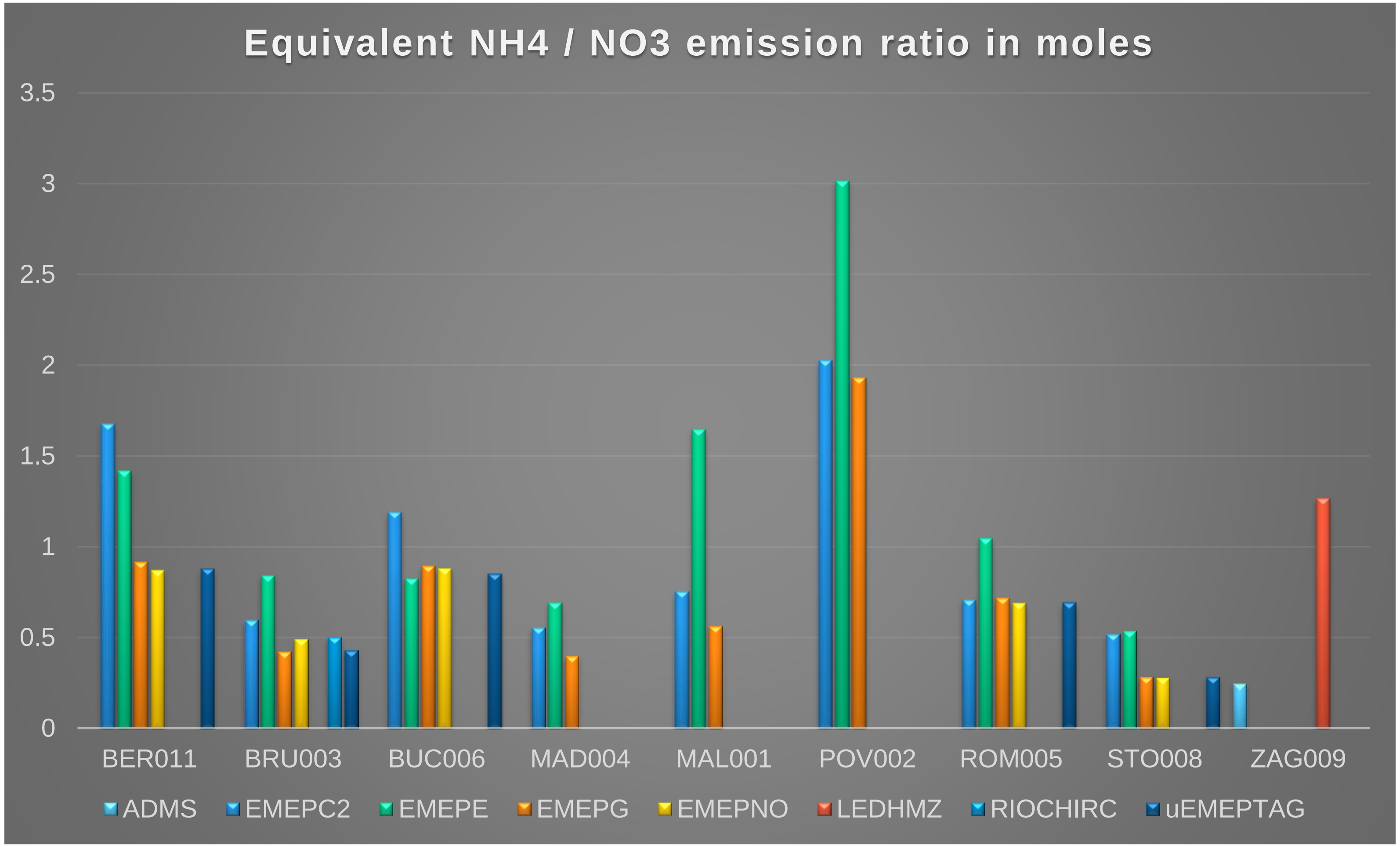
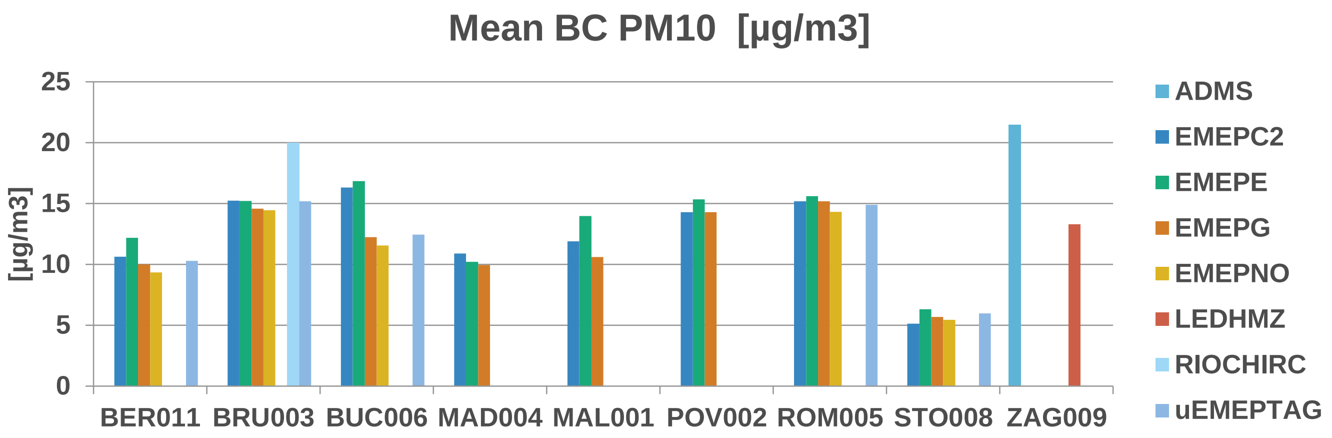
Emission ratio NH_3 vs NO_x

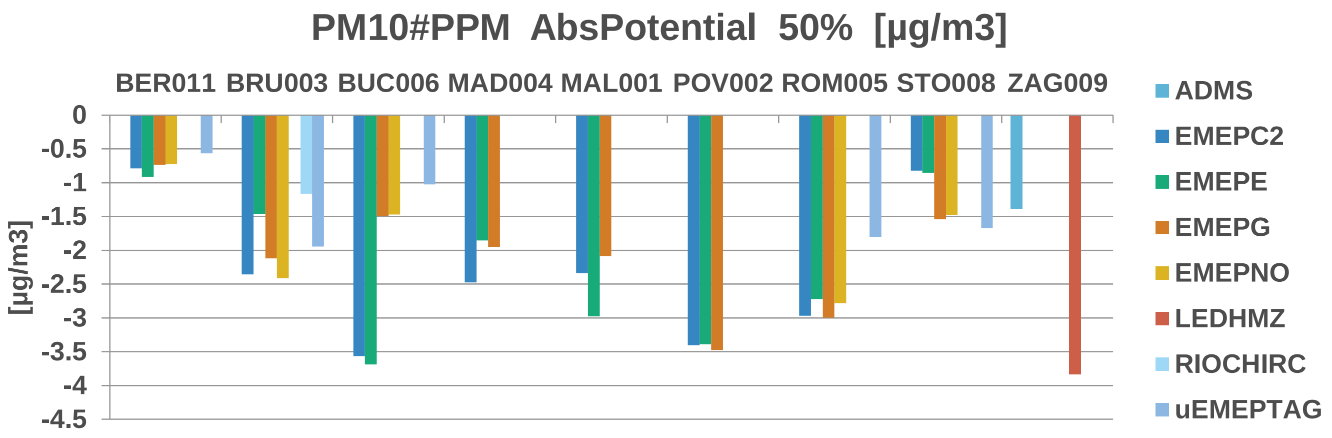
- $NH_3 + NO_3 >> NH_4NO_3$
  - Emission ratio $= \frac{63}{18} \times \frac{E_{NH3}}{E_{NOx}}$
- An indicator of chemical regime for the BC
- But large spatial variability



Yearly mean API – PM10

- API is the delta divided by the reduction (%)
- Negative every where (Fortunately…)





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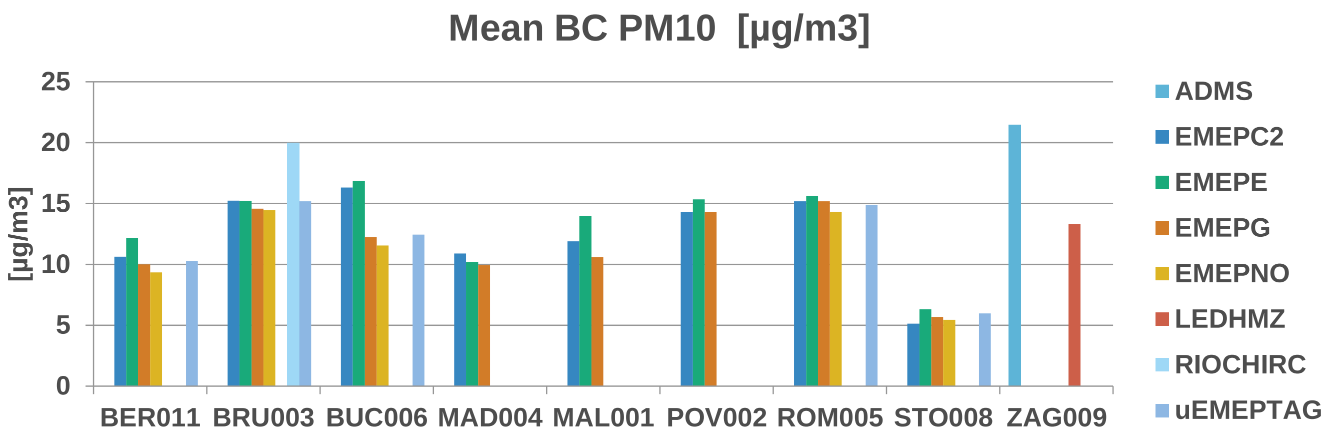
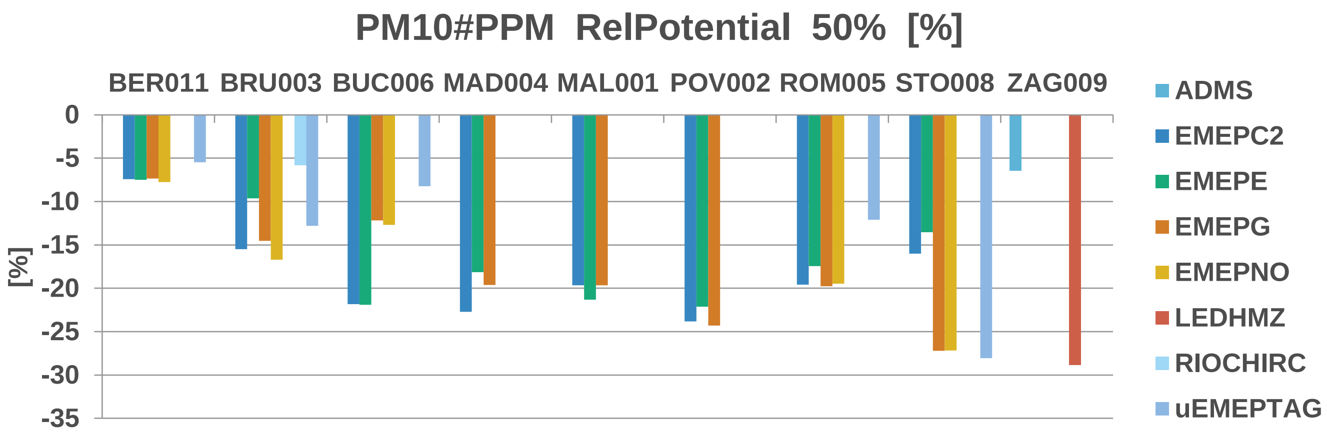
Yearly mean RPI – PM10

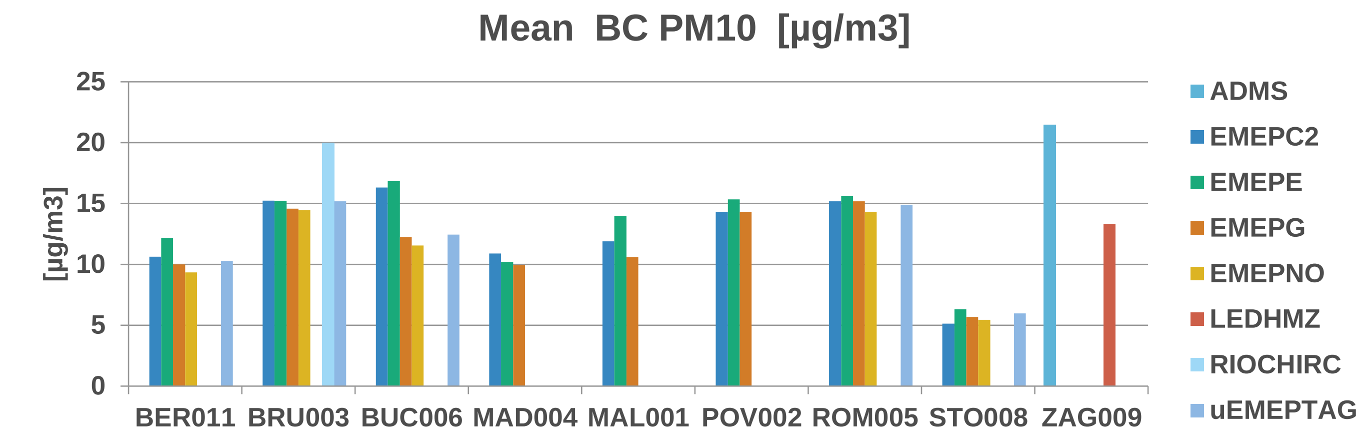
- Reduction of variability
- But still important in STO, a factor of 2

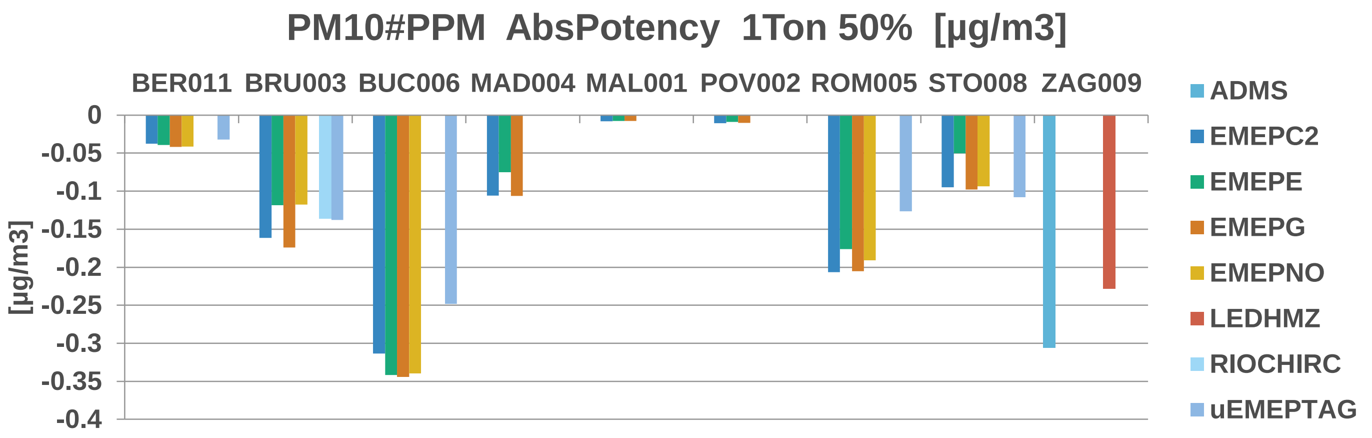




Yearly mean APy – PM10

- Delta per ton of emission reduced over the target domain





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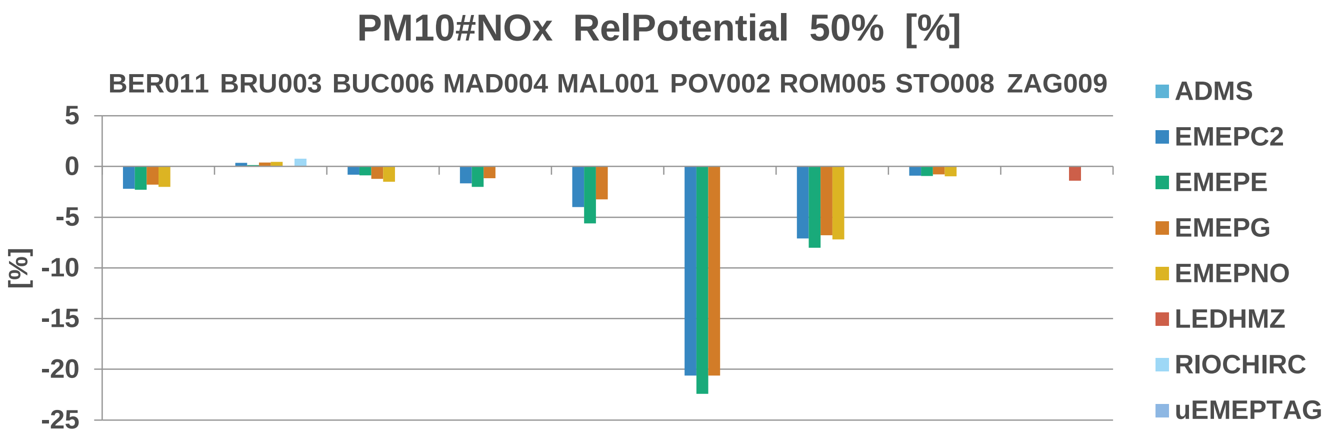
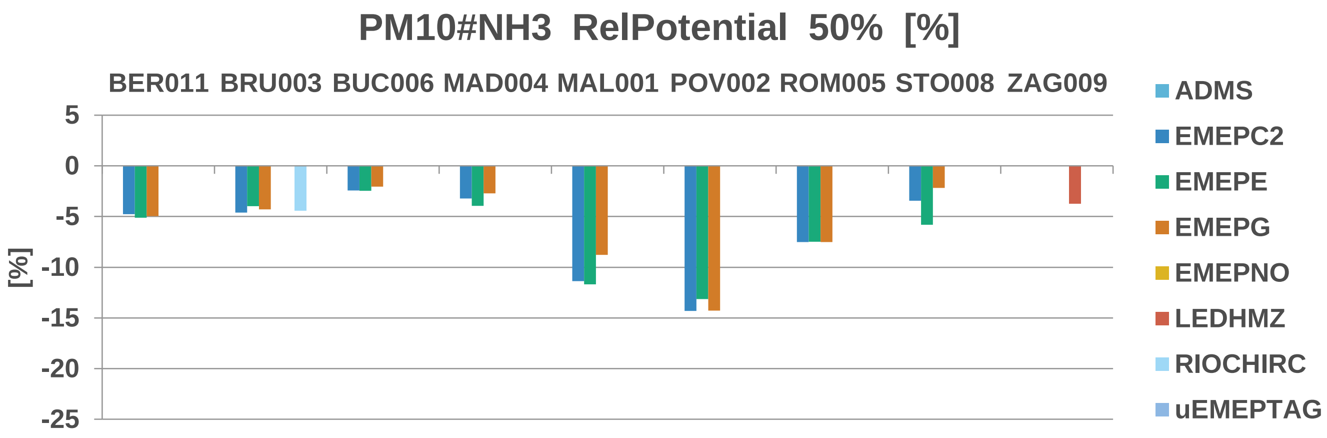
Yearly mean RPI – PM10 (NOx versus NH3 emissions)

- Slight increase of PM10 over Brussel for NOx emissions reductions
- Large reduction over POV
- In general low variability
- Large variability over STO for NH3 emission reductions





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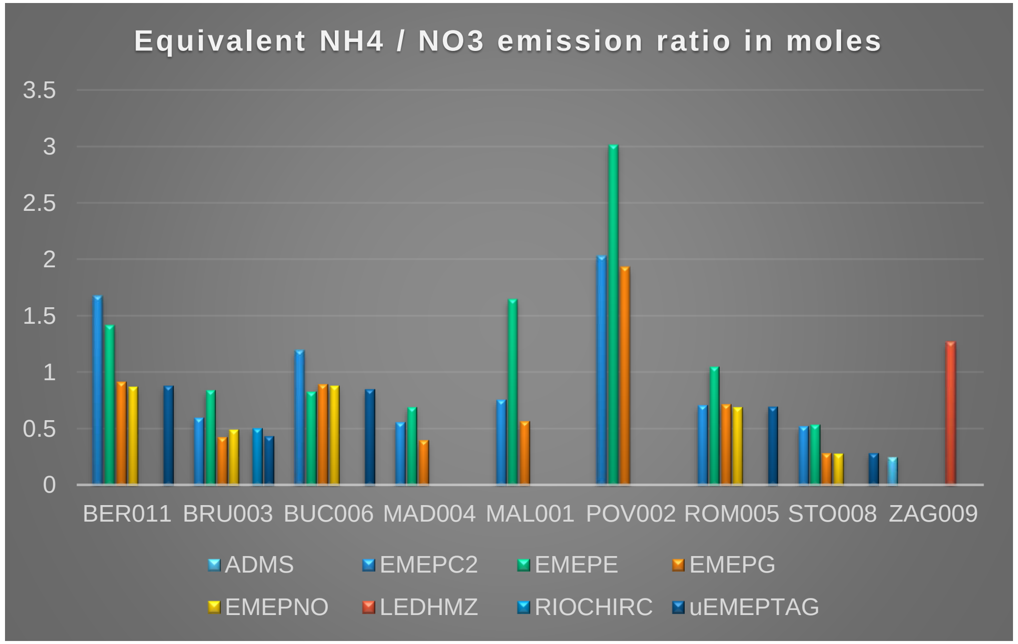
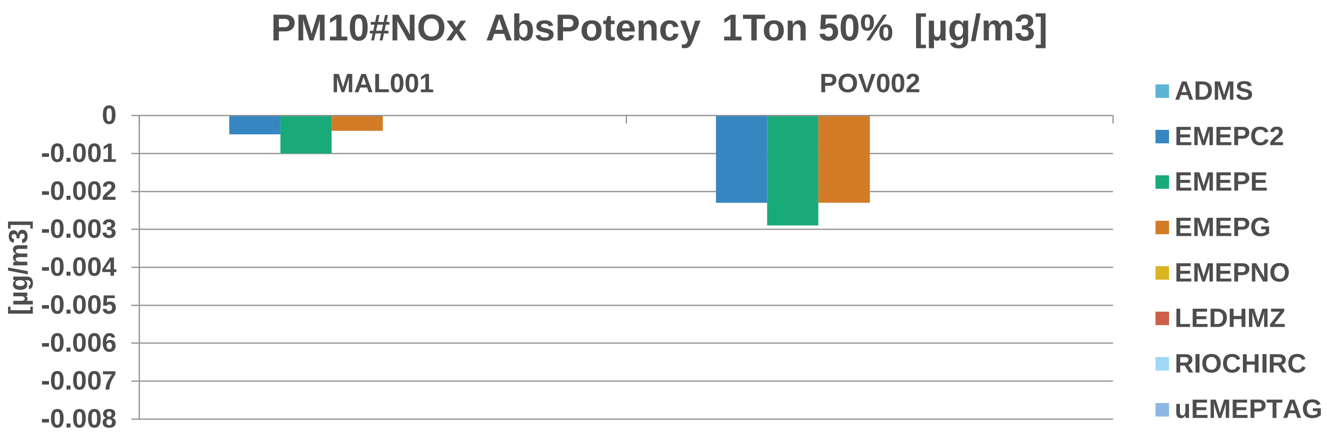
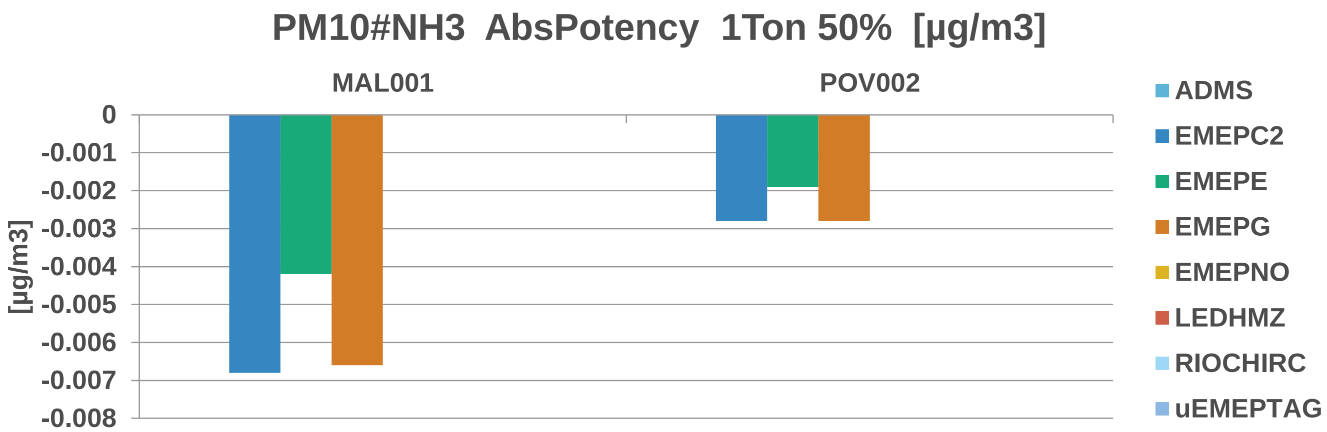
Yearly mean APy – PM10 (NOx versus NH3 emissions)

- Much more effective to reduce PM in MAL region by reducing Ammonia per ton (excess of NOy species)







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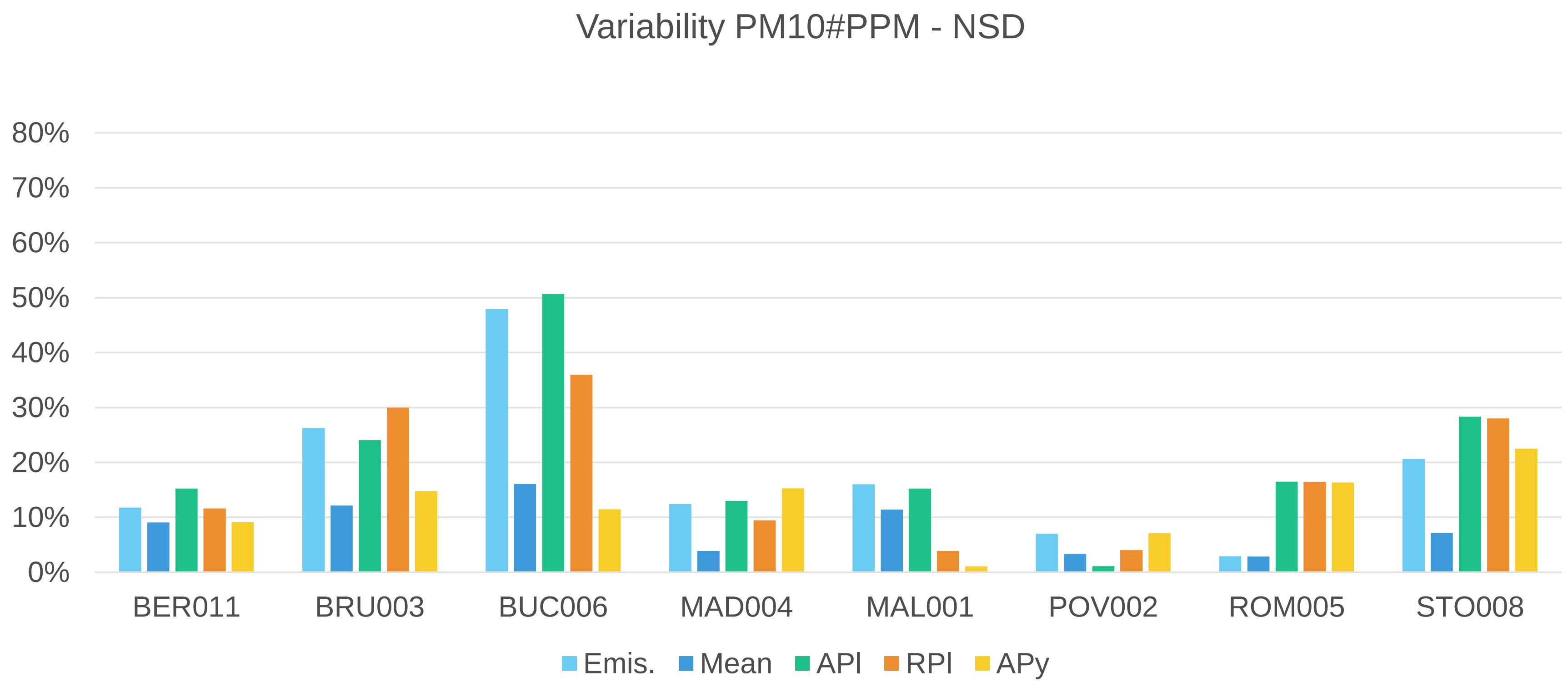
Variability on PM10 LT scenarios – PM10

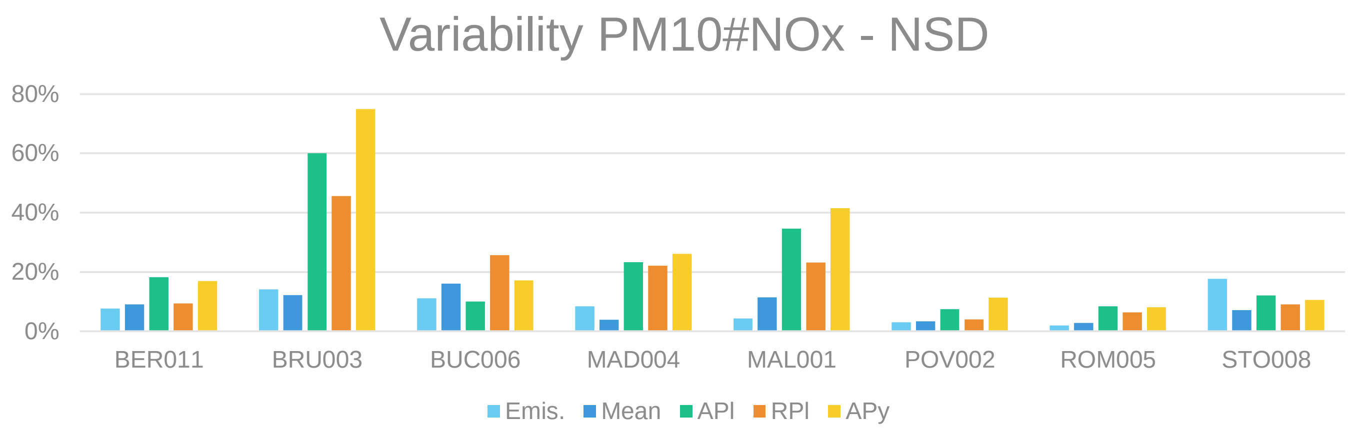
- Reminder: $NSD_{IND} = \sqrt{\frac{\sum_{m=1}^{M}(IND-\overline{IND})^2}{(\overline{IND})^2}}$

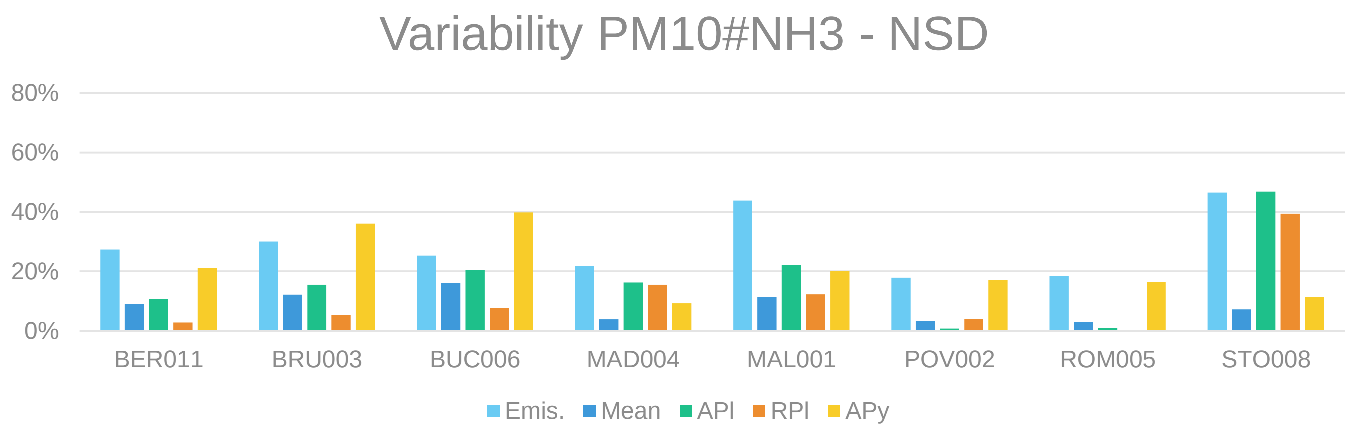


Variability on PM10 LT scenarios – PM10

- Variability of RPI looks more important when the influence of the emission is high

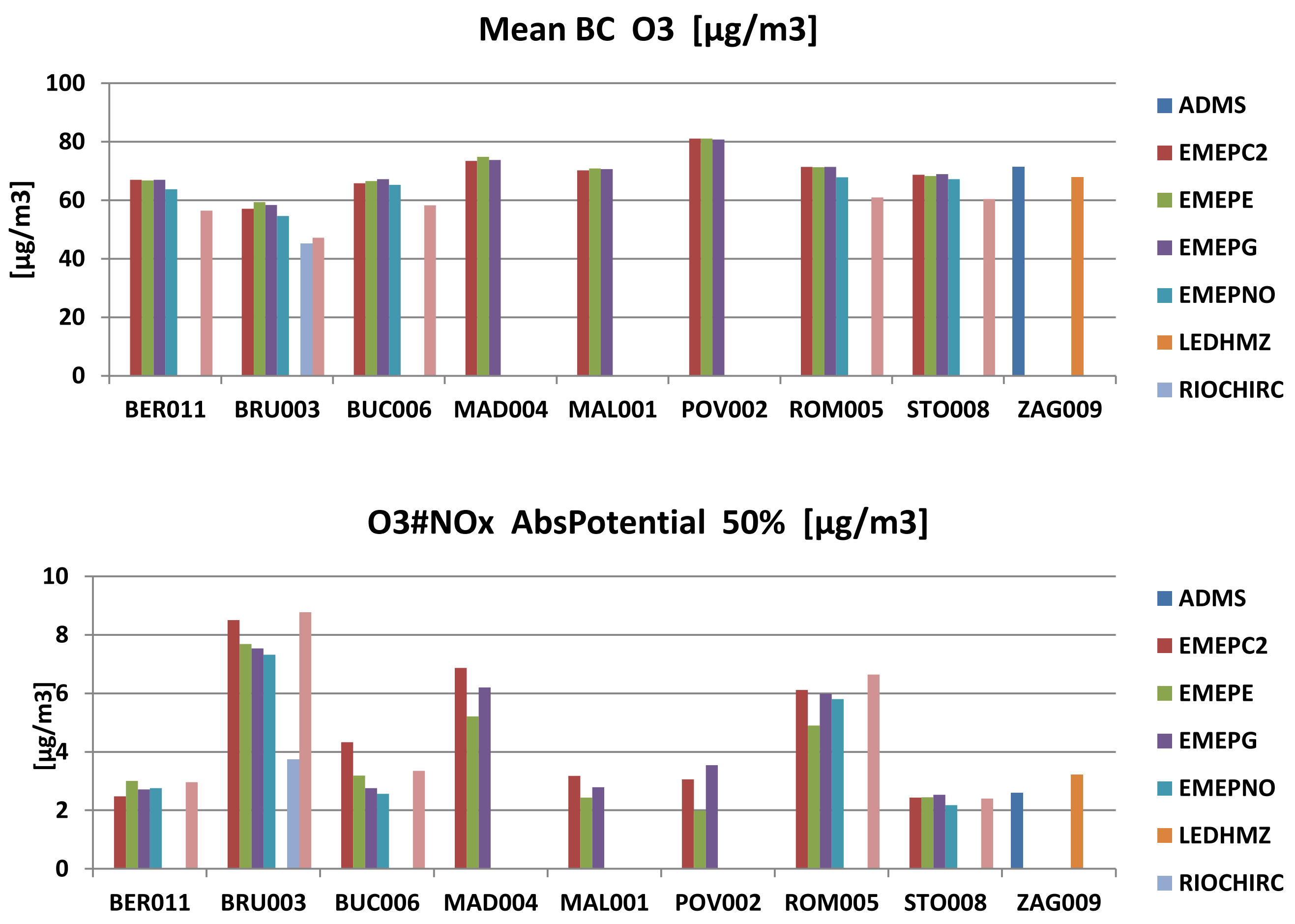
$$NSD_{IND} = \sqrt{\frac{\sum_{m=1}^{M}(IND - \overline{IND})^2}{(\overline{IND})^2}}$$





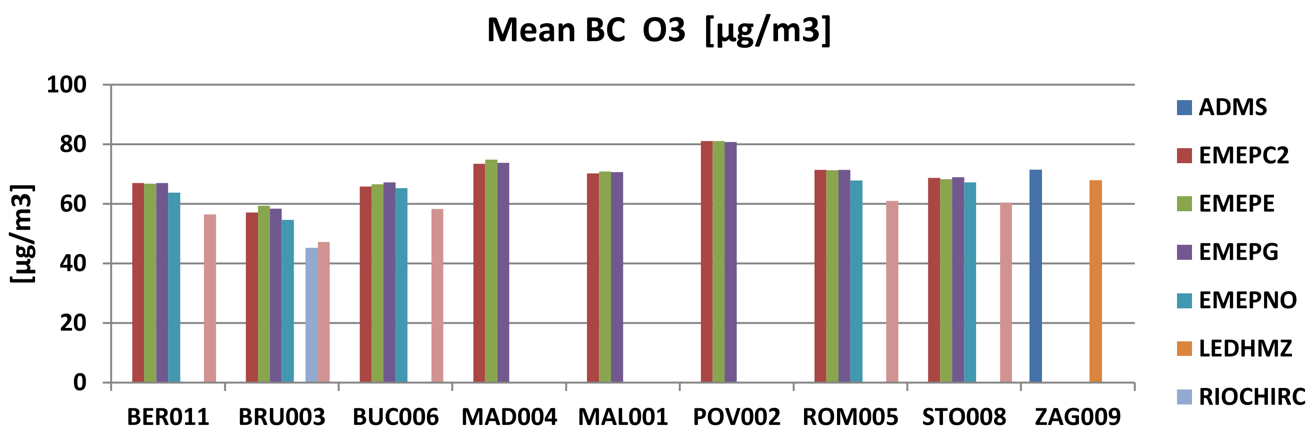
Yearly mean API – O3

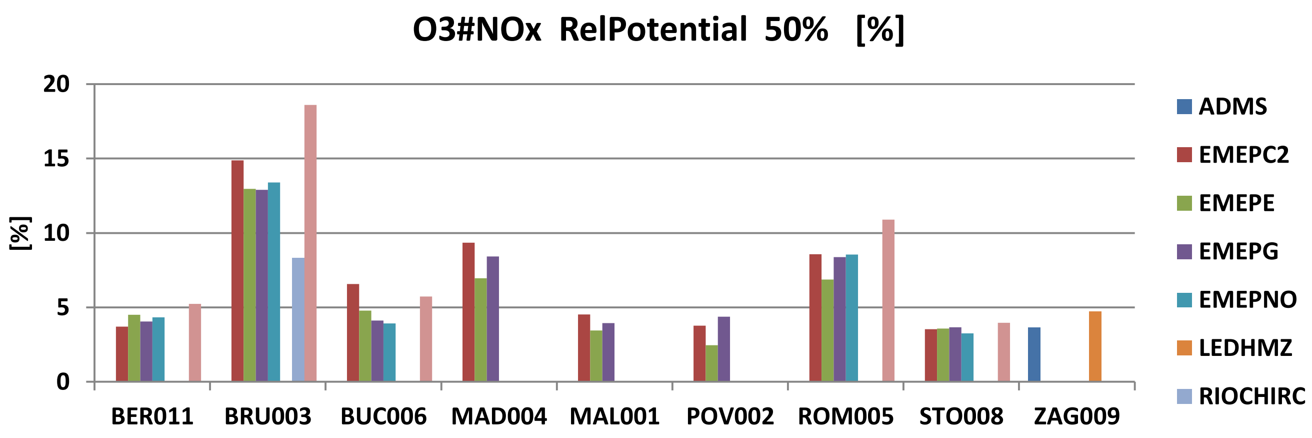
- Low variability on mean concentrations
- API is the delta divided by the reduction (%)
- Positive every where due to the titration effect
- Lower over large domains like MAL and POV
- Slightly lower values for LOTOS and RIO over Brussels



Yearly mean RPI – O3

- Low variability on mean concentrations





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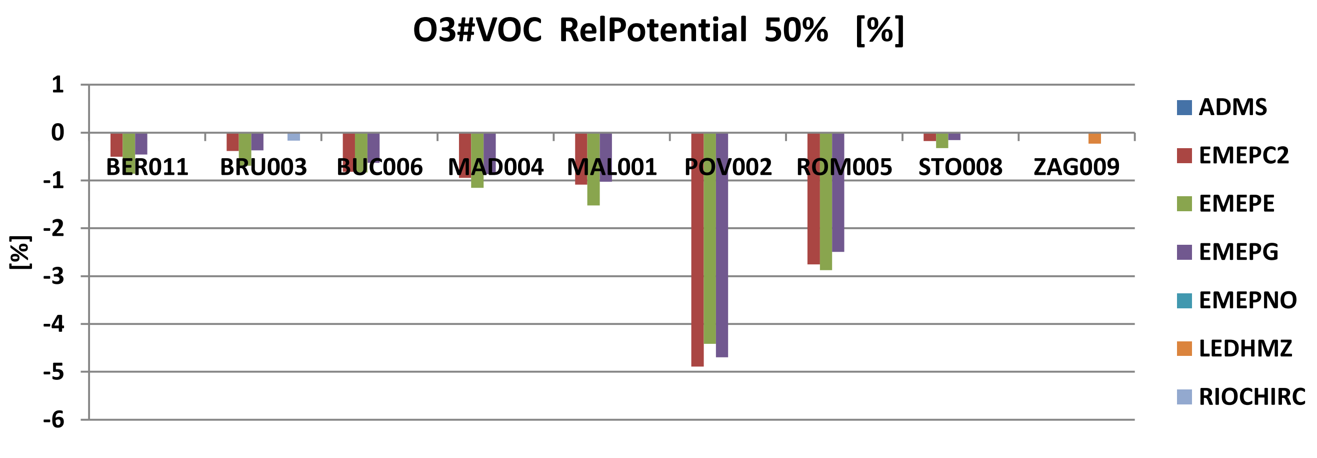
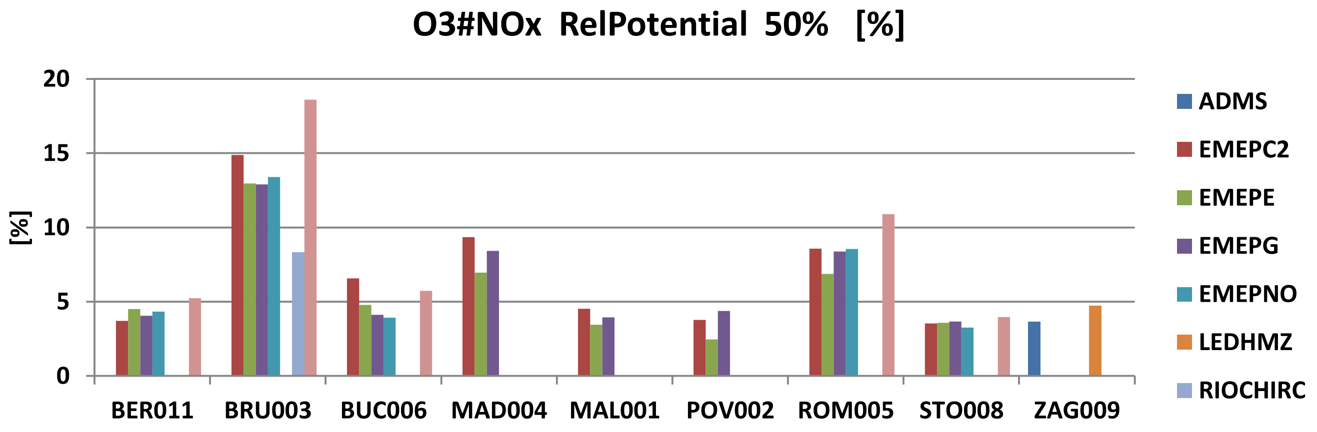
Yearly mean RPI – O3 (NOx versus VOC)

- Negative impact od VOC reduction (normal)
- Very slight increase in Zagreb for ADMS
- On absolute values lower impact of VOC emissions





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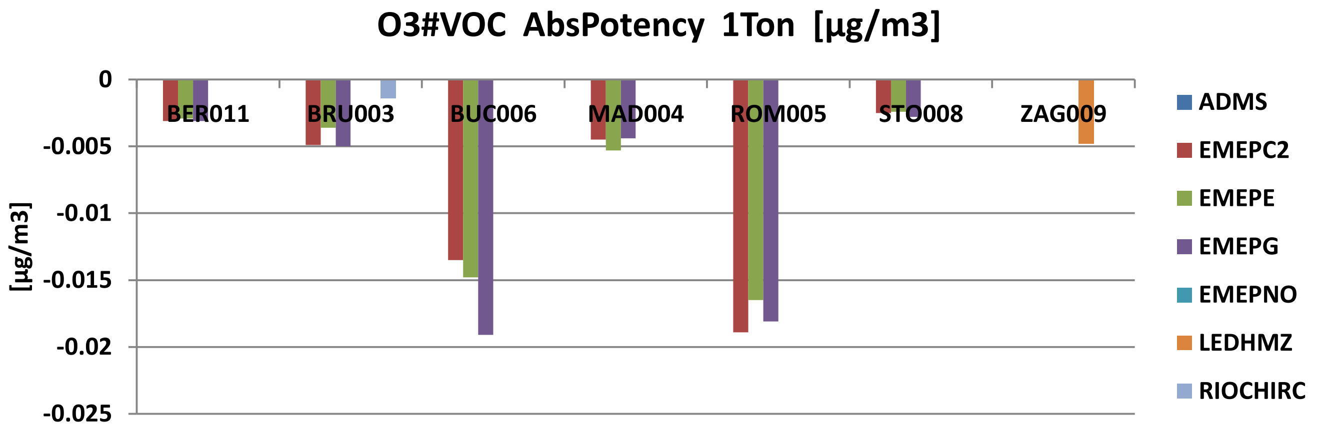
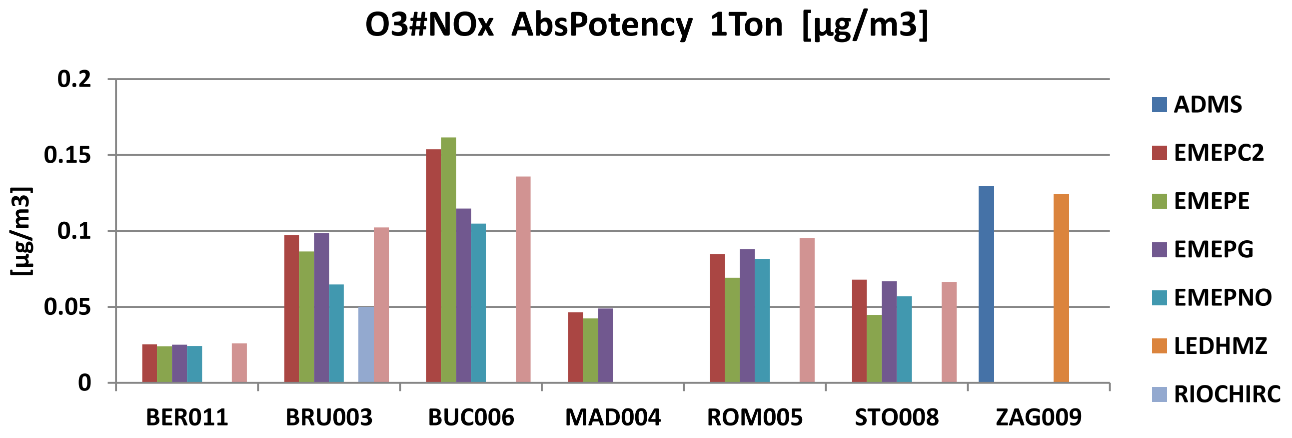
Yearly mean APy – O3 (NOx versus VOC)

- Focus on cities (POV and MAL removed)
- Still larger values for NOx impact
- Very low variability in Berlin and low values
  - Other processes and input than emissions





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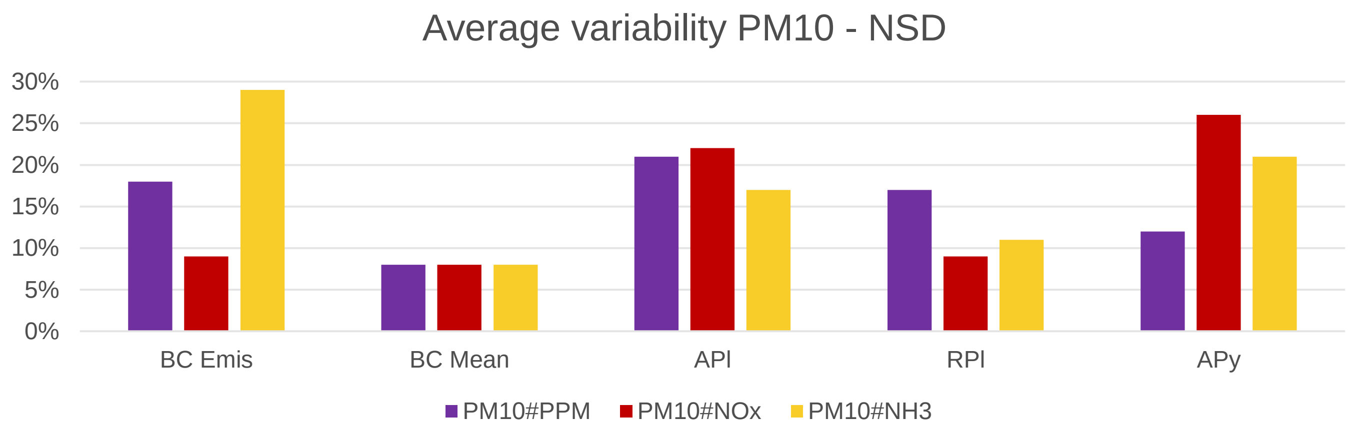
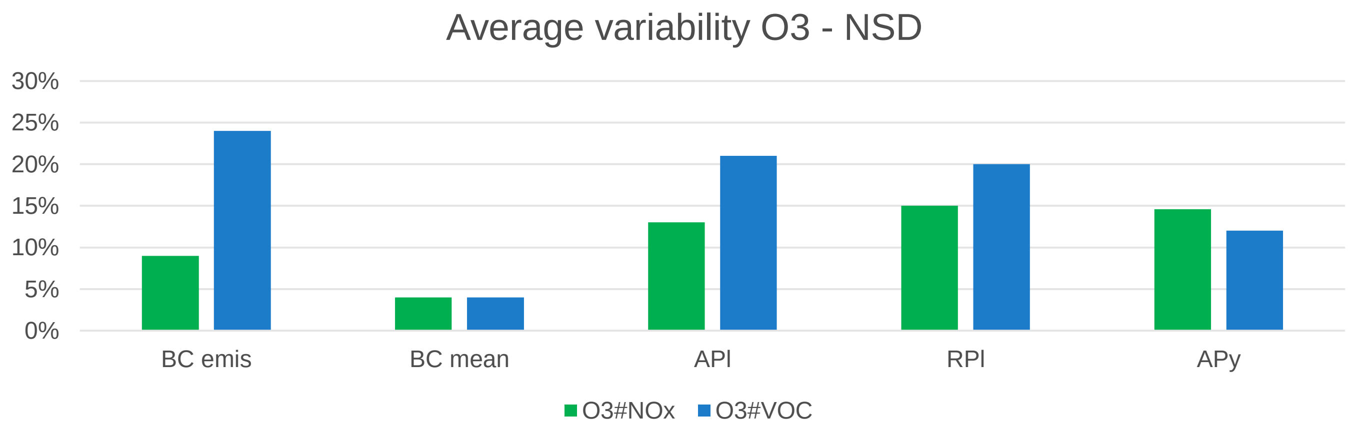
Summary of variability

- Less variability on O3 BC Mean than PM10 BC Mean
  - 4 versus 8 %
- Variability of RPI << API (less clear for O3)
  - 10 to 25% depending on the indicator

$$NSD_{IND} = \sqrt{\frac{\sum_{m=1}^{M}(IND - \overline{IND})^2}{(\overline{IND})^2}}$$





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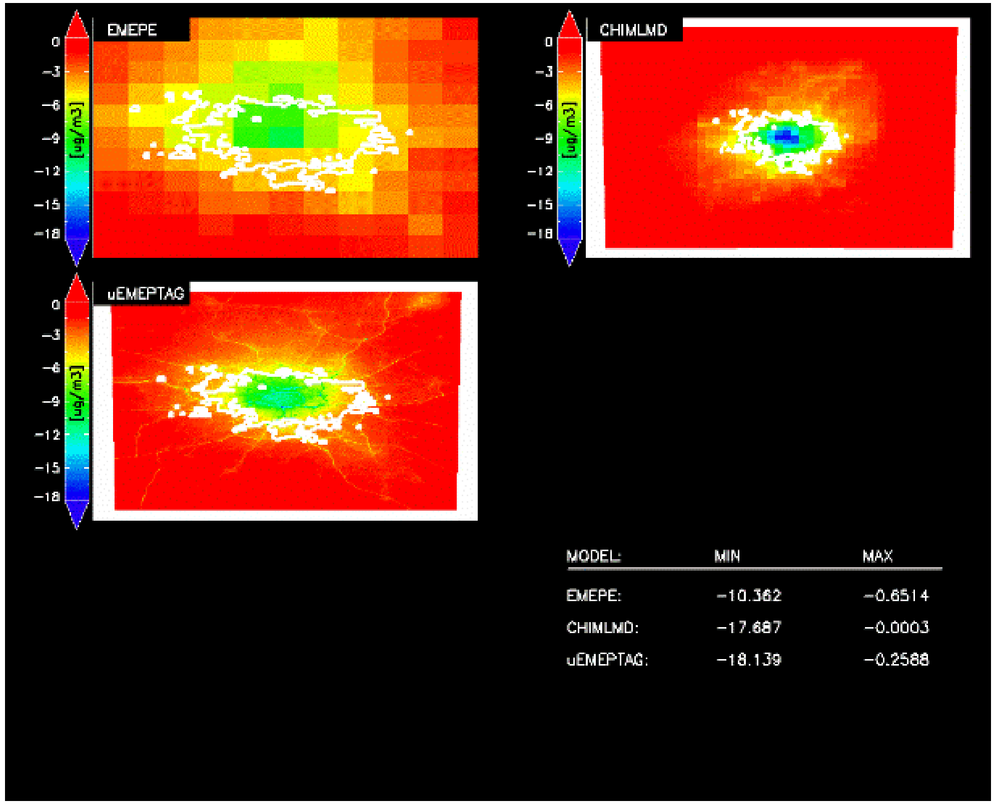
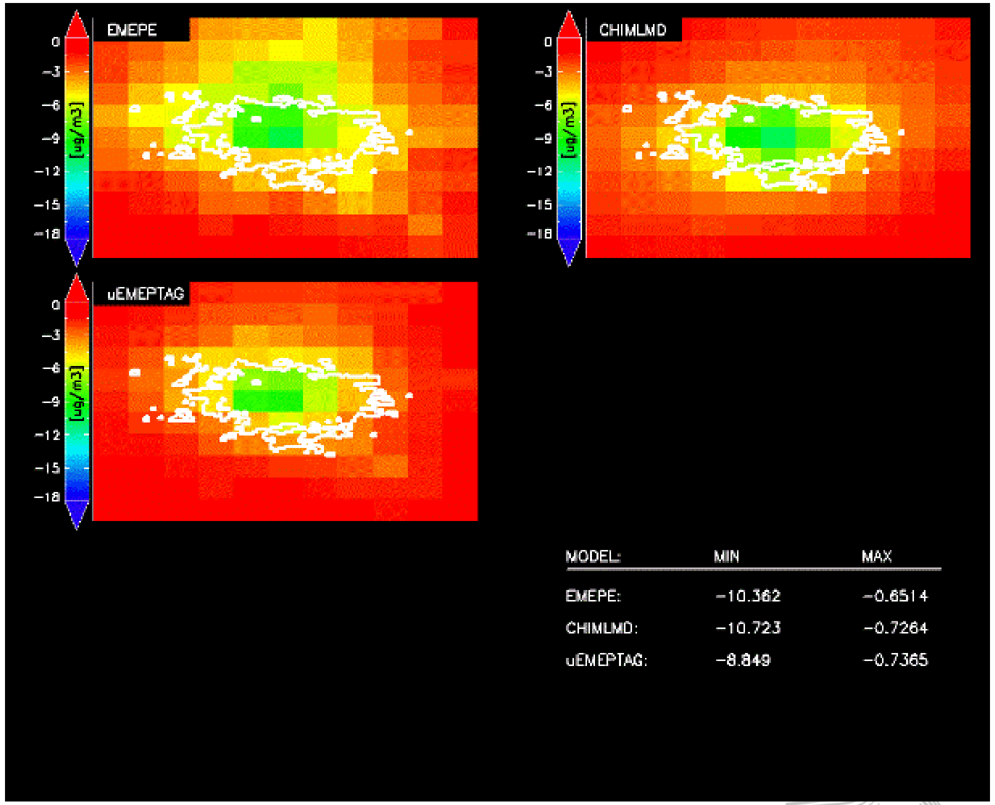
Spatial variability with 2D plots

Absolute Potential (API) 25% PM10#PPM over Berlin

Model grid



Common grid



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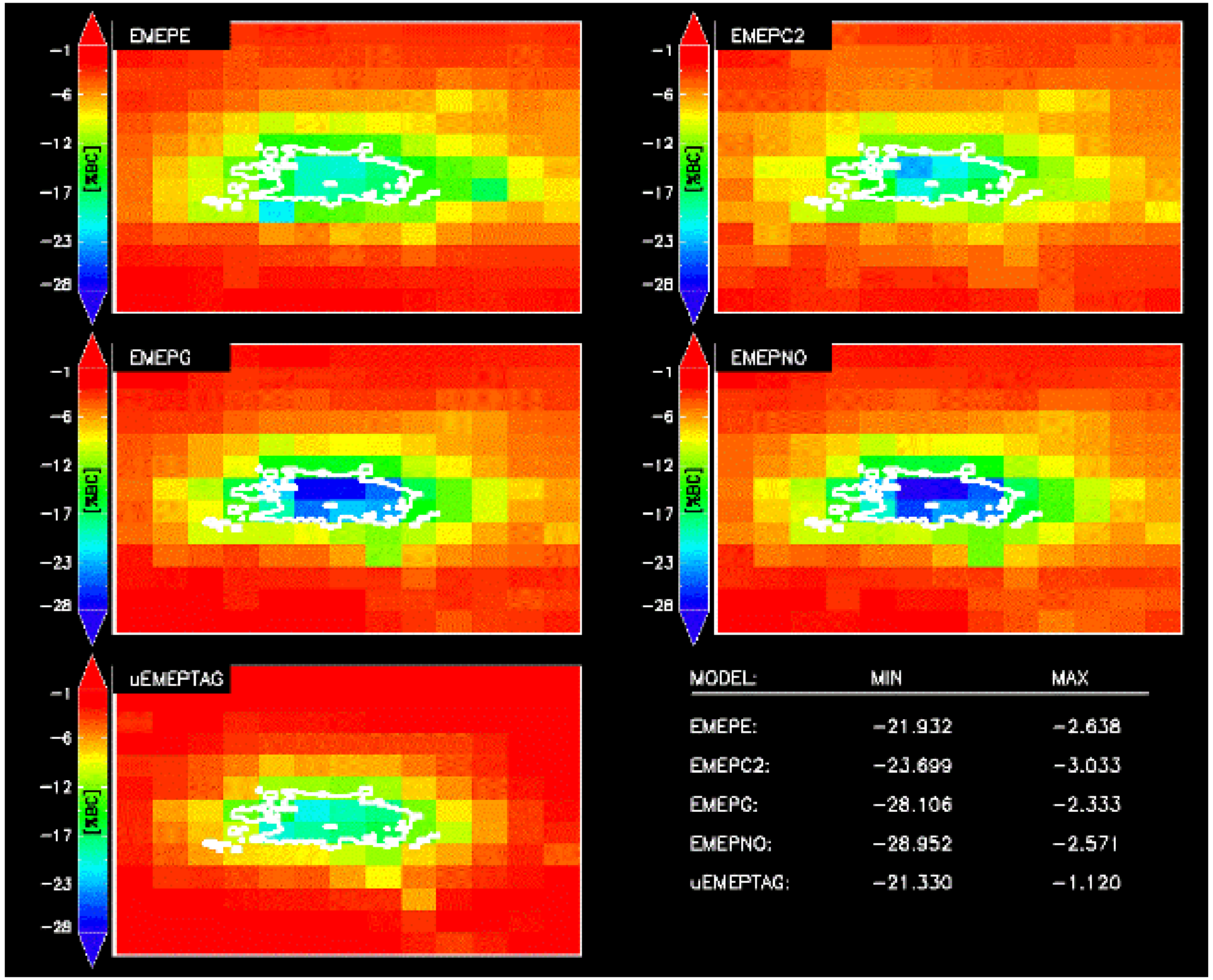
Spatial variability with 2D plots

PICT_2D_PM10_BER011_RPI_50%PPM



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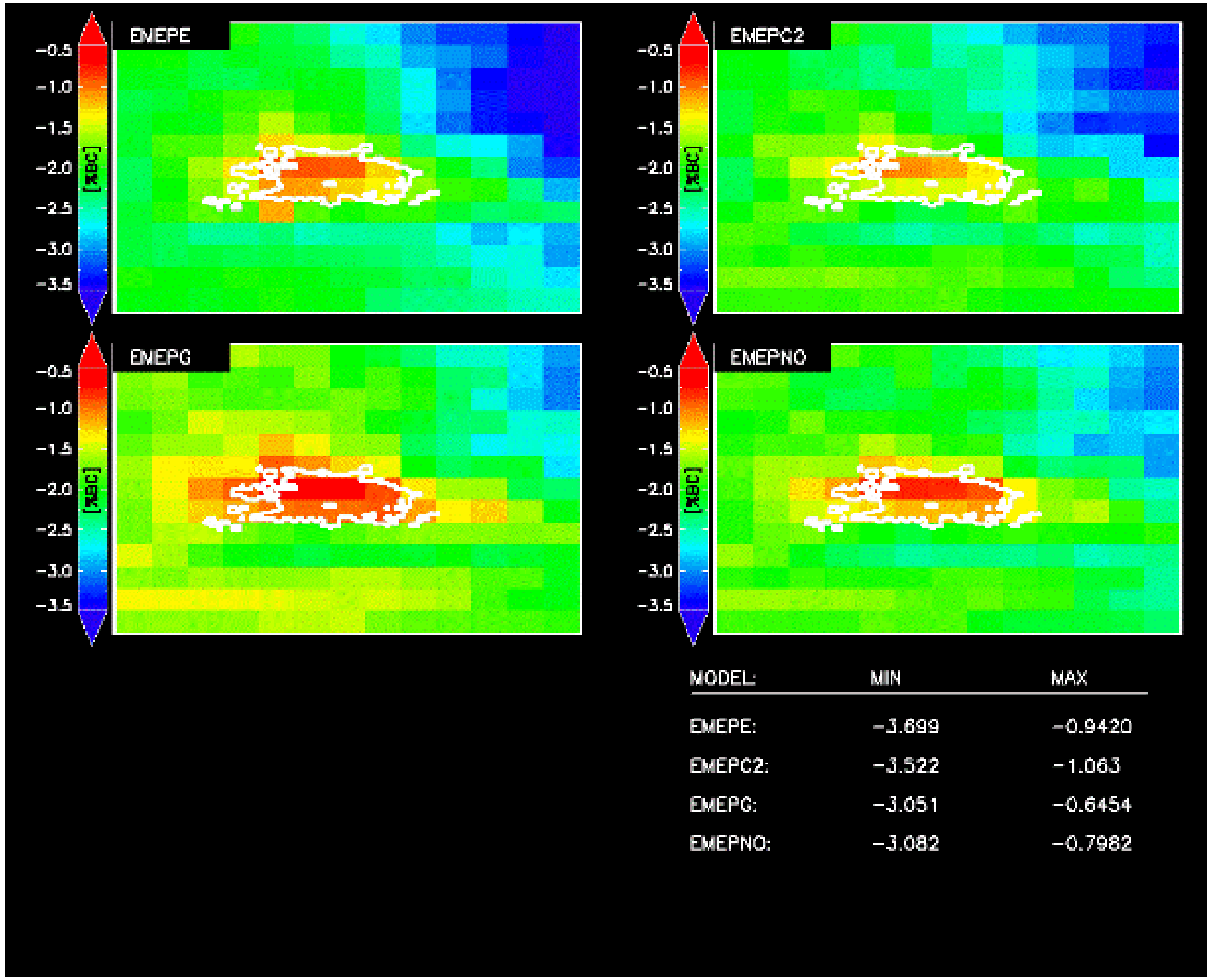
Spatial variability with 2D plots

PICT_2D_PM10_BER011_RPI_50%NOx



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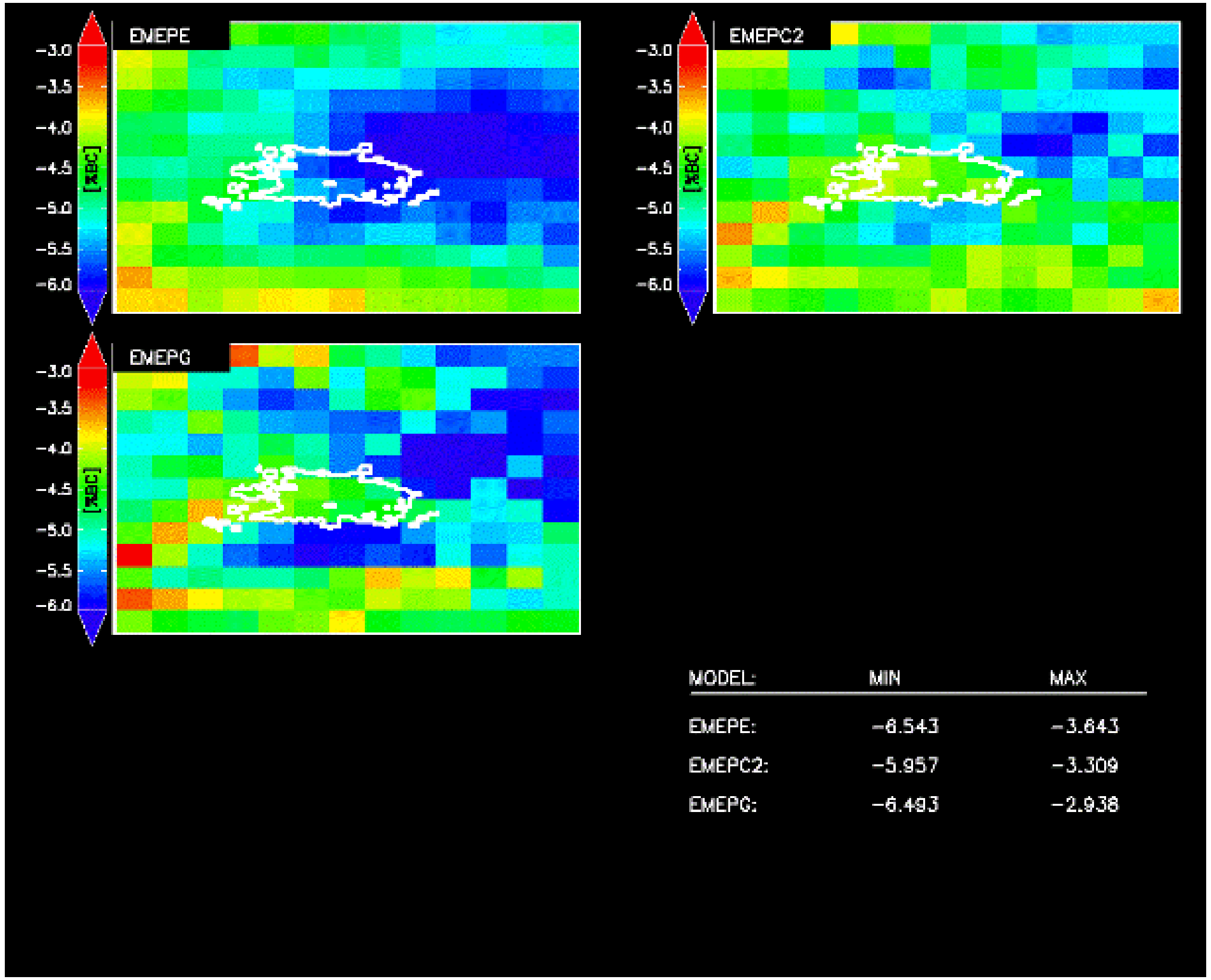
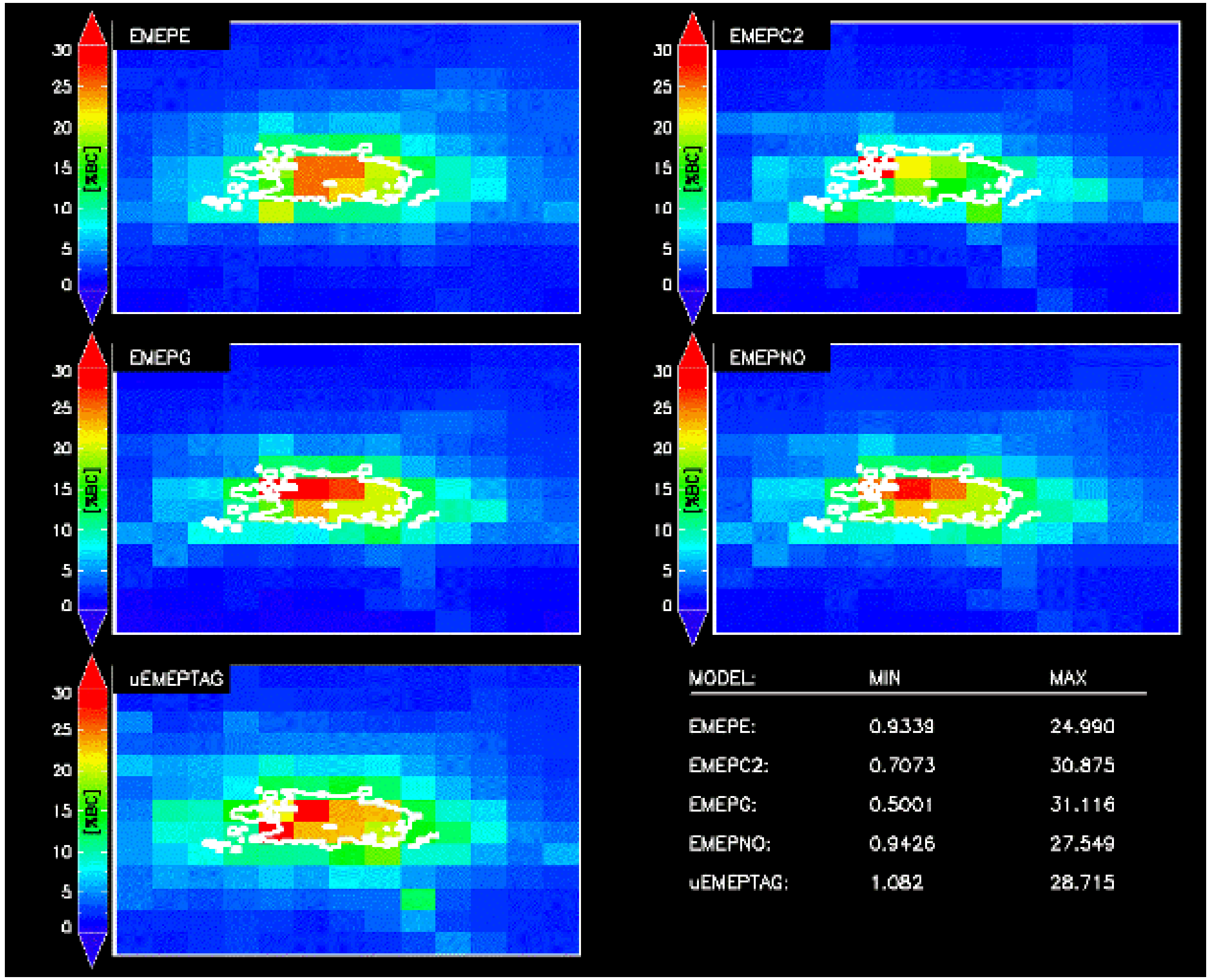
Spatial variability with 2D plots

PICT_2D_PM10_BER011_RPI_50%NOx



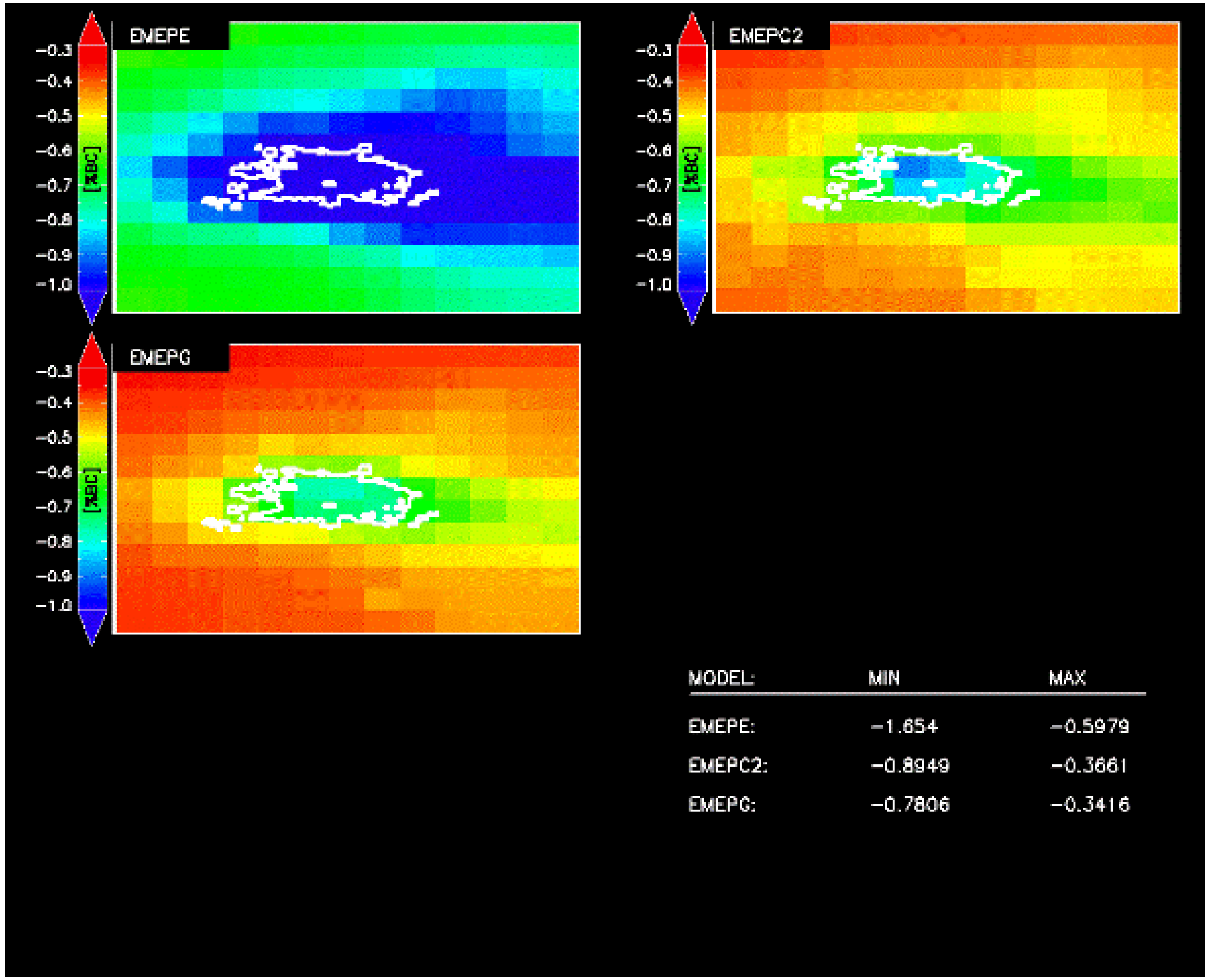
Spatial variability with 2D plots

PICT_2D_O3_BER011_RPI_50%NOx



Spatial variability with 2D plots

PICT 2D O3 BER011 RPI 50%VOC



Chemical features

- Possible interactions of PPM emission reduction on O_3 through heterogeneous reactions (still in debate in the scientific community)
- NO_x emission reactions usually lead to PM reduction through the reduction of Ammonium nitrate by atmospheric reactions
  - But increasing O_3 due to titration effects lead to an enhancement of the atmospheric oxidizing capacity
  - …then lead to more SOA formation and then a PM increase
    - (S, I)VOCs(g) + oxidants → (S, I)OVOCs(g) ↔SOA(s)
  - SO_4 can increase also due to complex effects in aqueous chemistry with O_3 increase

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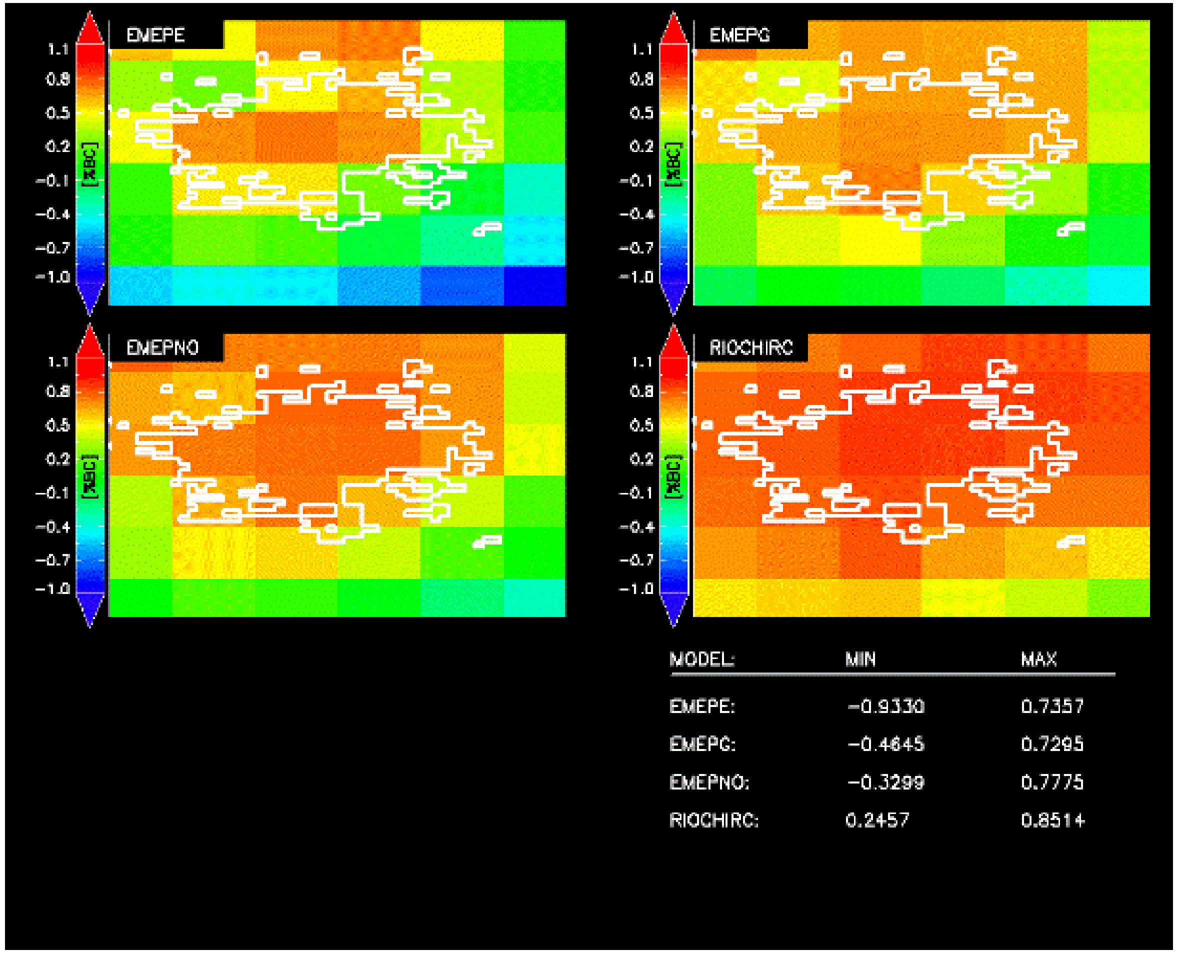
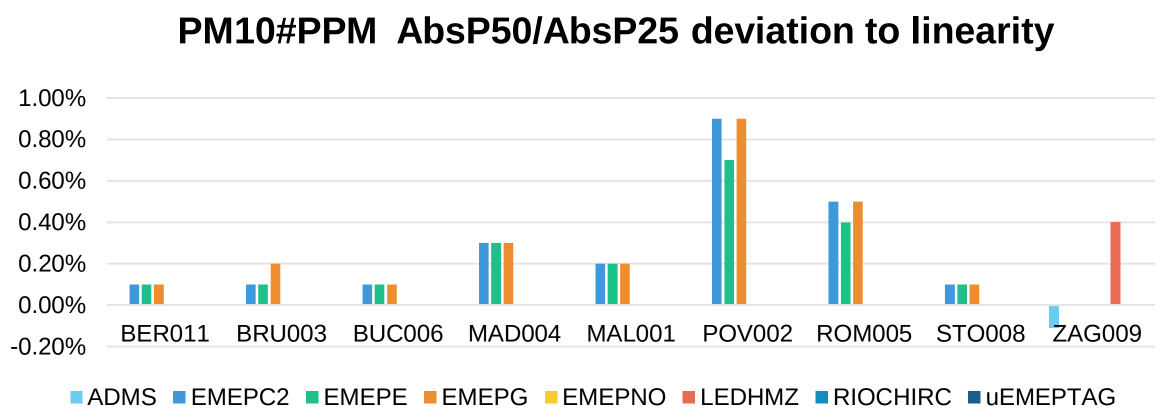
Non linearities in models?

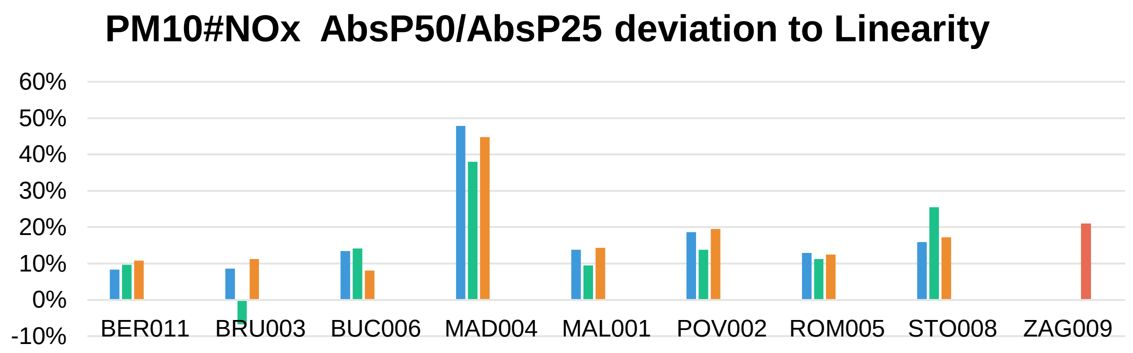
PICT_2D_PM10_BRU003_RPI_50%NOx

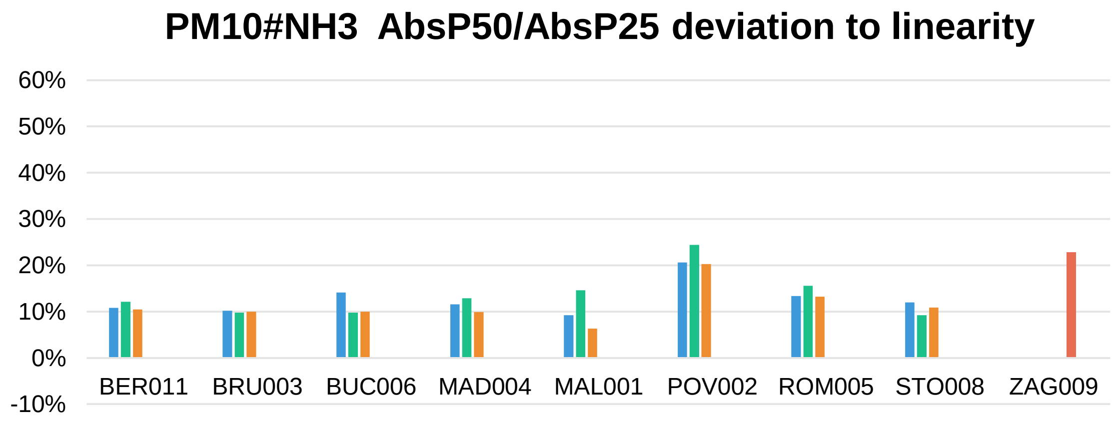


Linearities (PM10)

- Deviation % to linearity:
  - *as (AbsP50/AbsP25 - 1)x100*
  - *"0%" means perfect linearity*
- Perfect linearity for PPM, as it is considered as chemically inert (deviation < 1%)
- Usually higher efficiency when NOx or NH3 are reduced by 50% compared to 25%
  - *NH3 or NOx becoming no longer on average in excess and then being limiting in nitrate formation*







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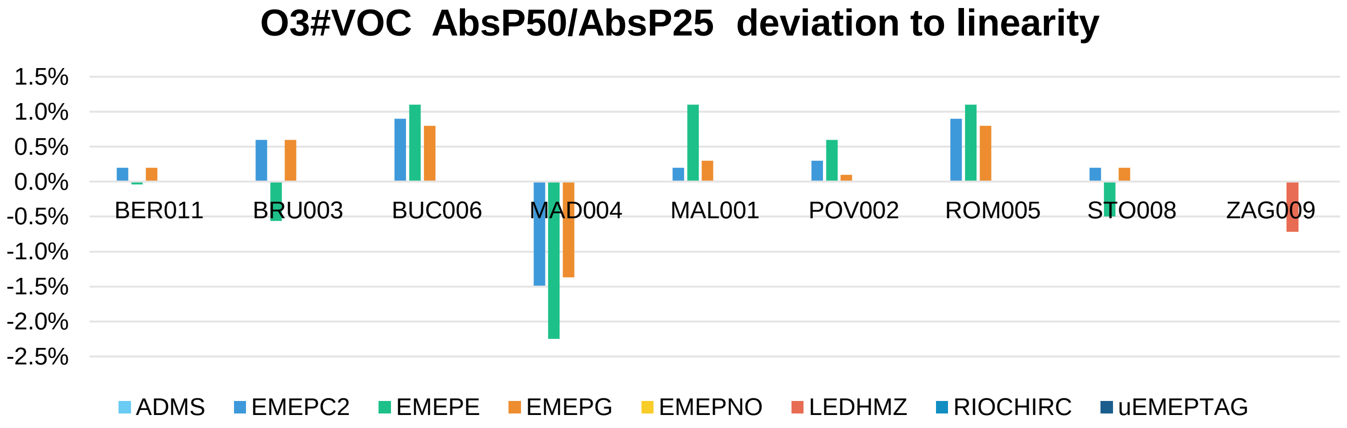
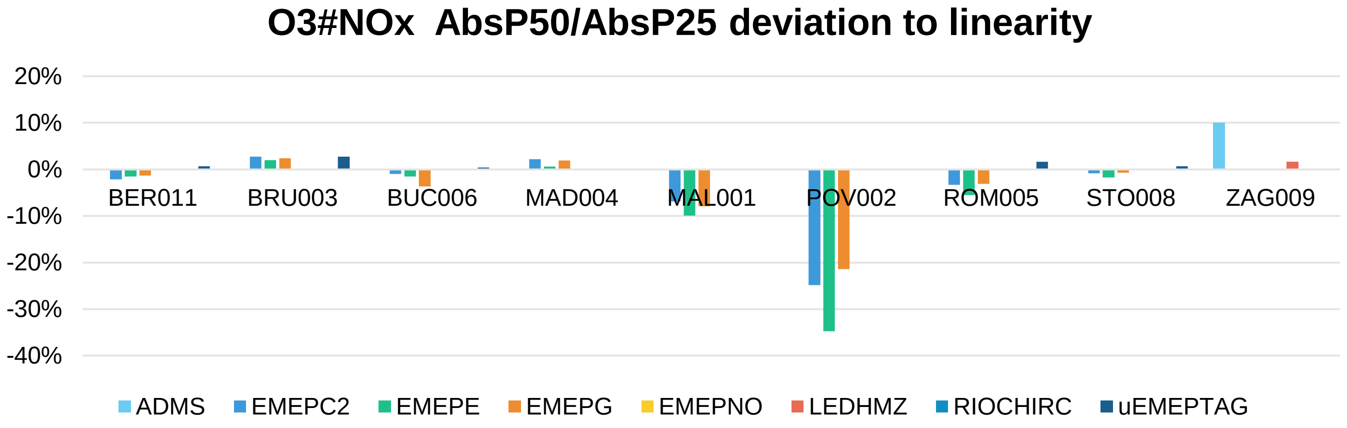
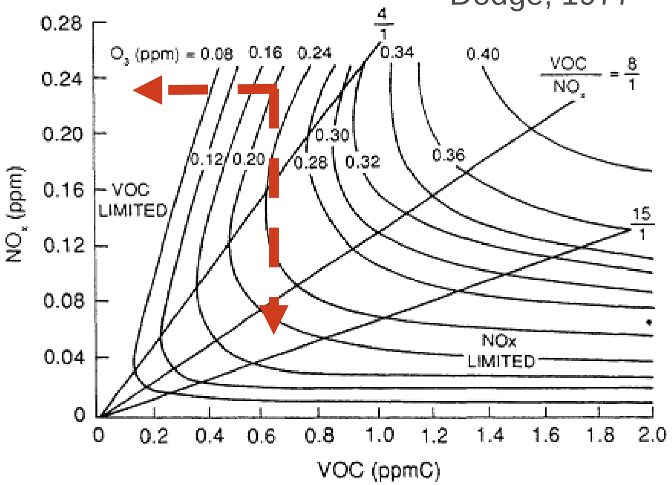
Linearities (O3)

- Linearity for VOC emission reduction
- More or less linear in urban areas (VOC limited)
- Non linear for large regions (POV and MAL)



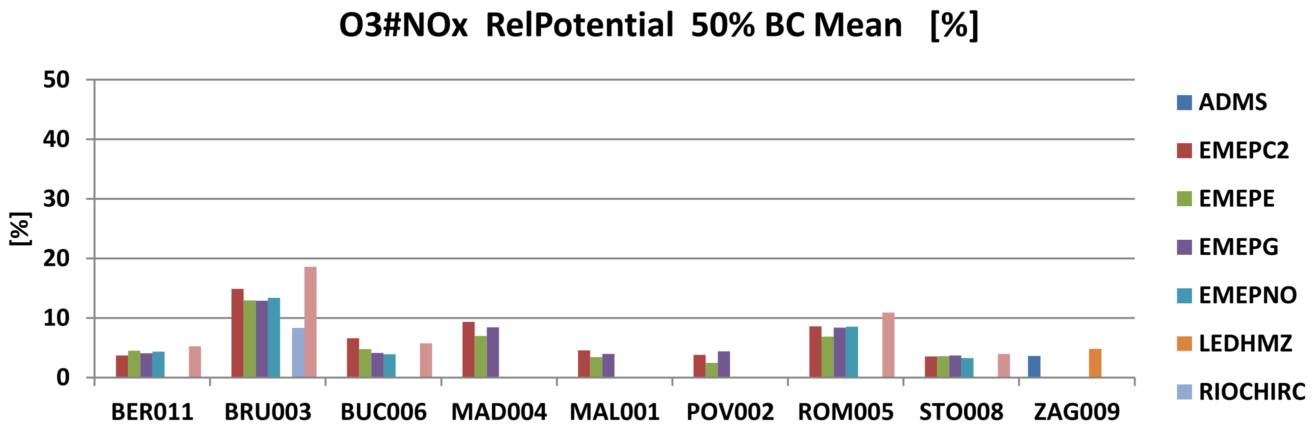


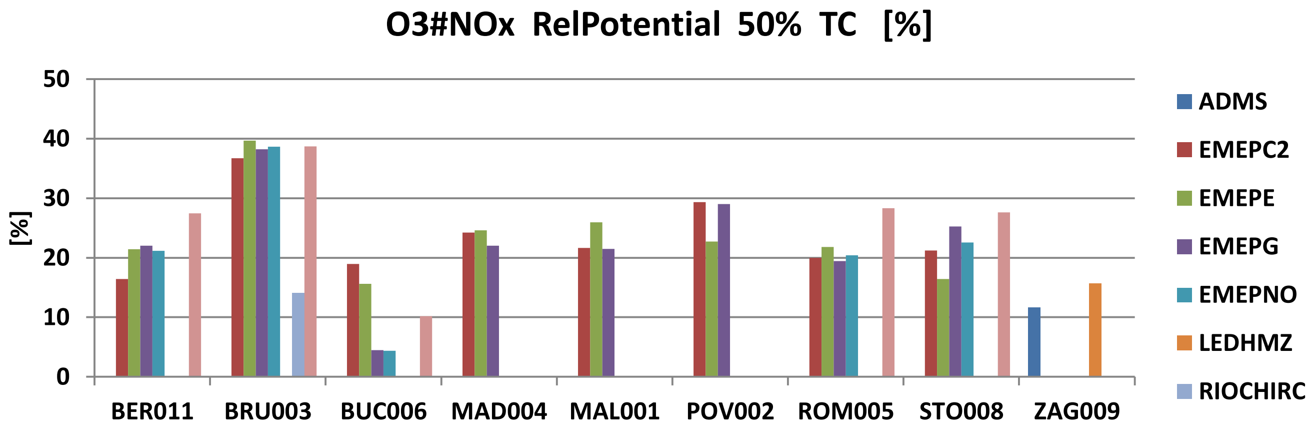
Dodge, 1977



Tcentre versus Mean on O3

- Big jump on relative potential from Mean to Tcentre





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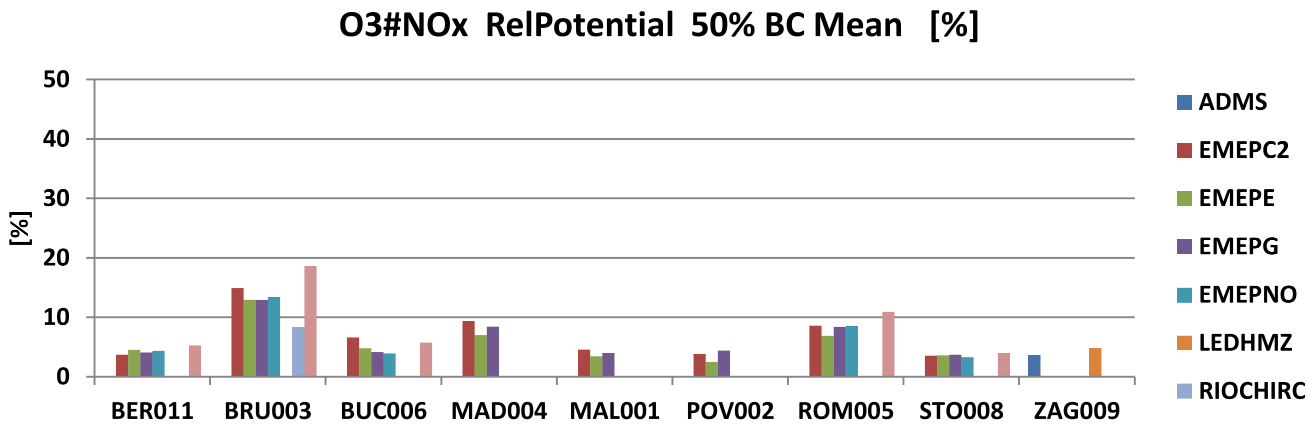
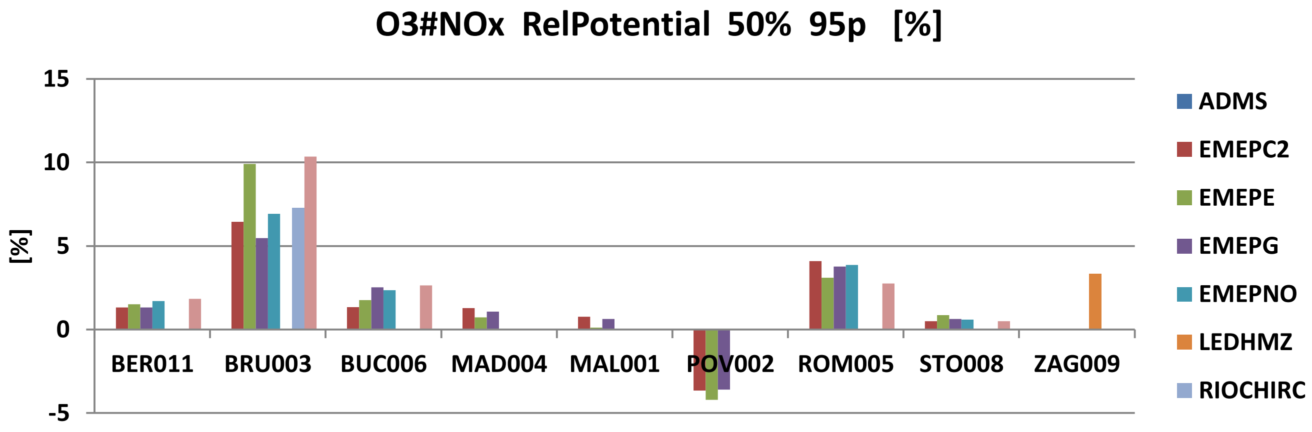
Tcentre versus Mean on O3

- The sign can change for P95 of course for Ozone when including large zones (Po Valley)





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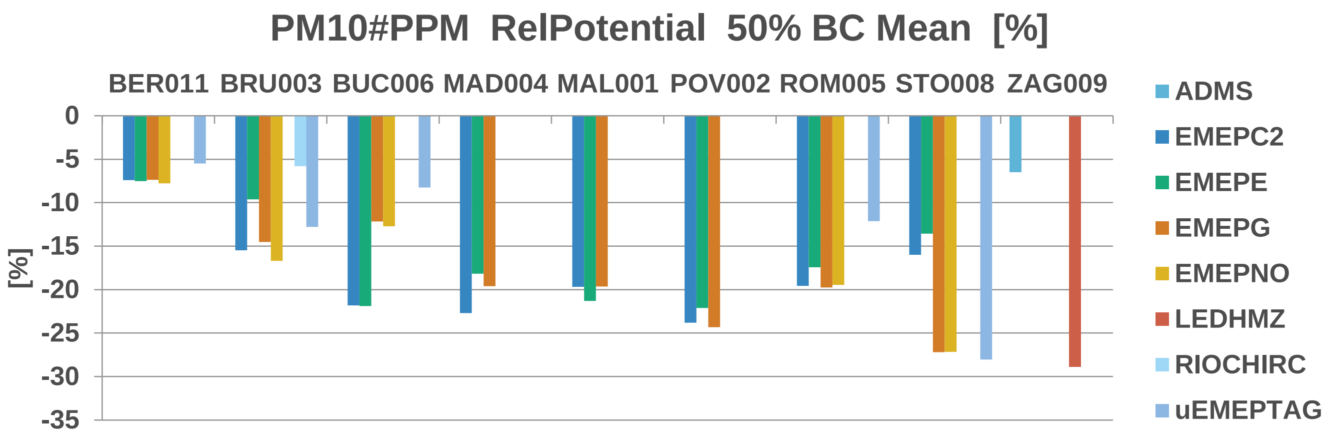
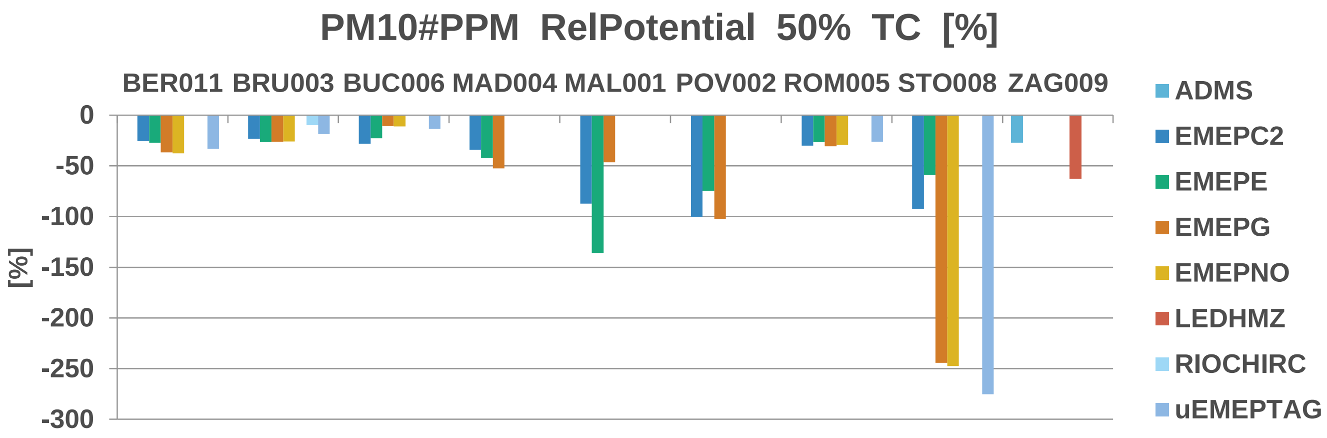
Tcentre versus Mean on PM10

- A clear increase of the relative potential





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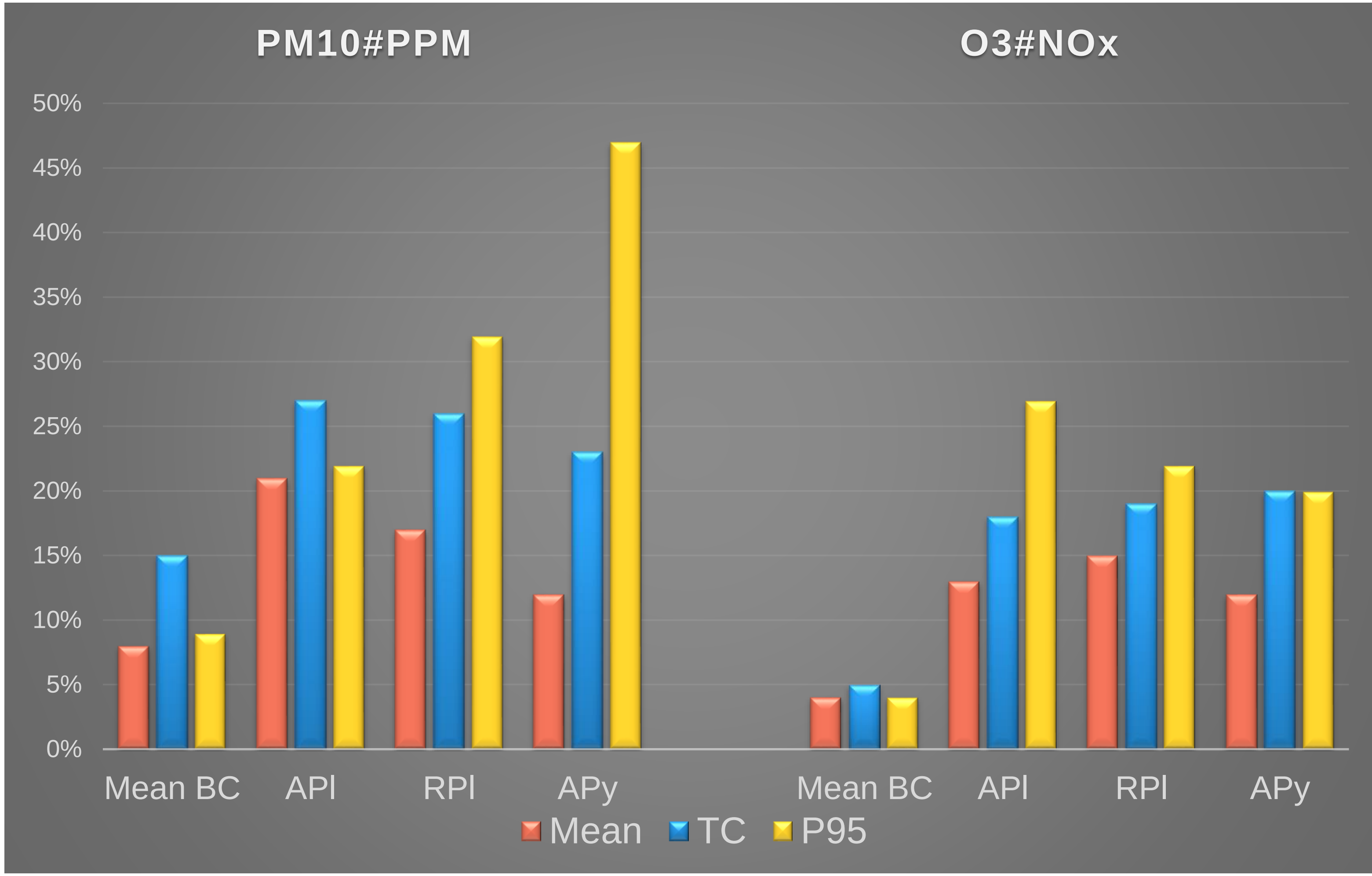
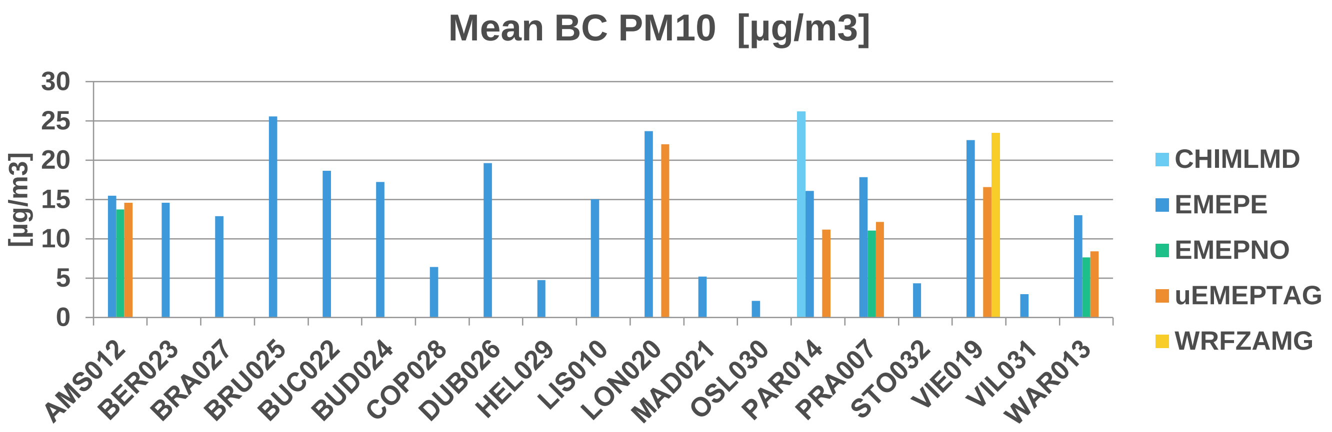
Variability change **Mean** *versus* **TC** *versus* **P95**

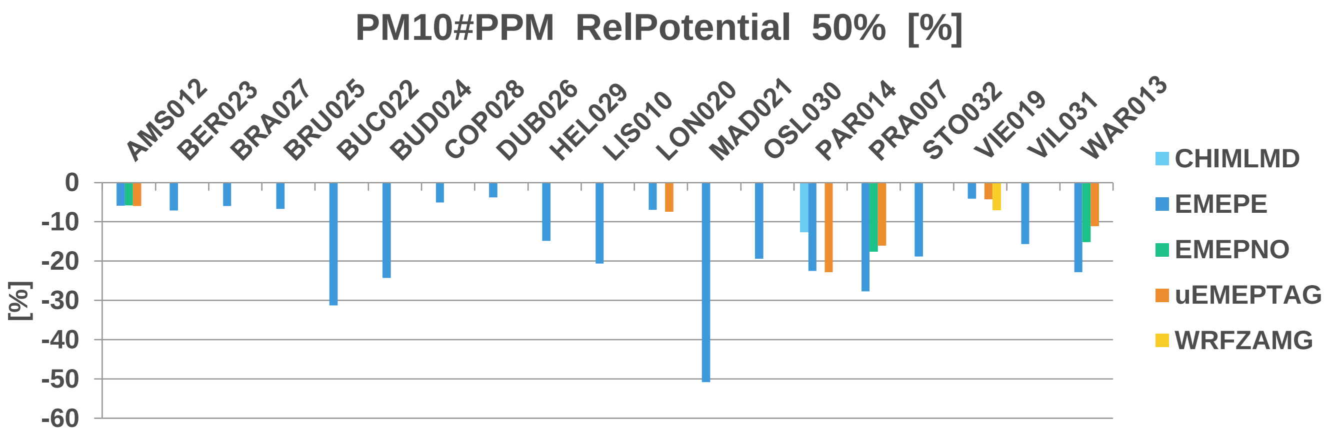
- Clear increase of variability of indicator scaled by concentrations or emissions



A look at short term

- So far 5 cities with at least 3 different model settings for a PPM emission reductions





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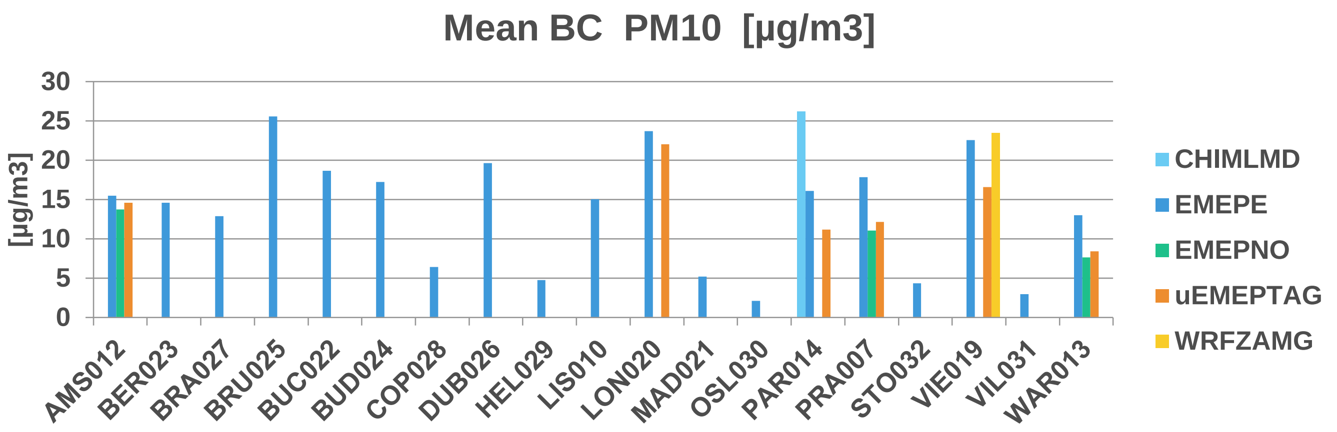
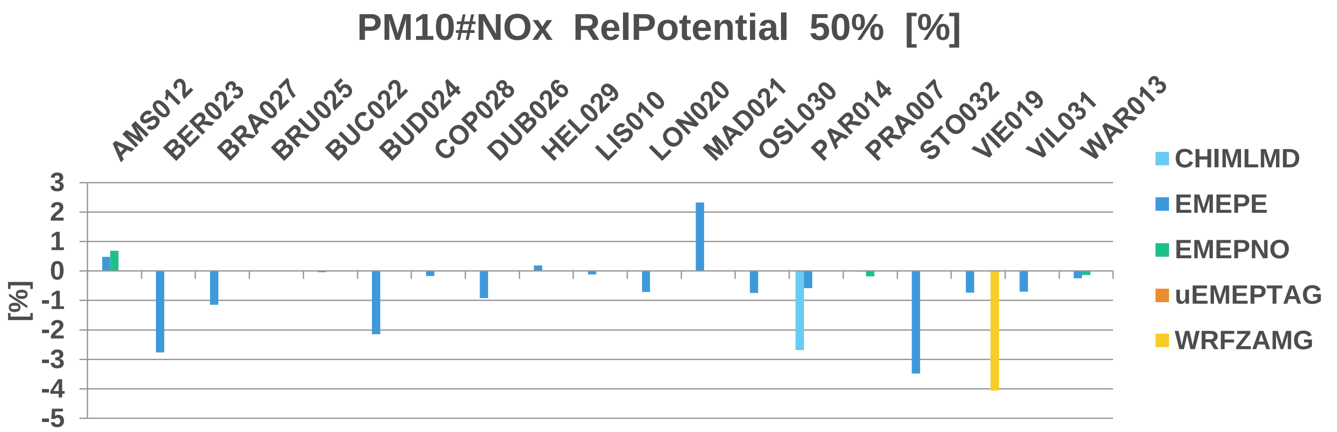
A look at short term

- So far 0 city with at least 3 different model settings for a PPM emission reductions





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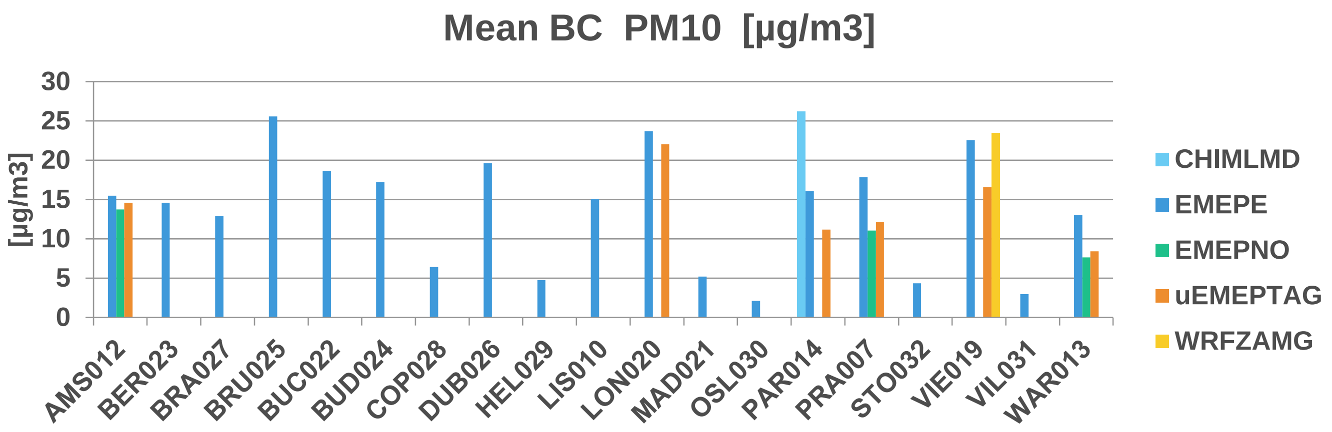
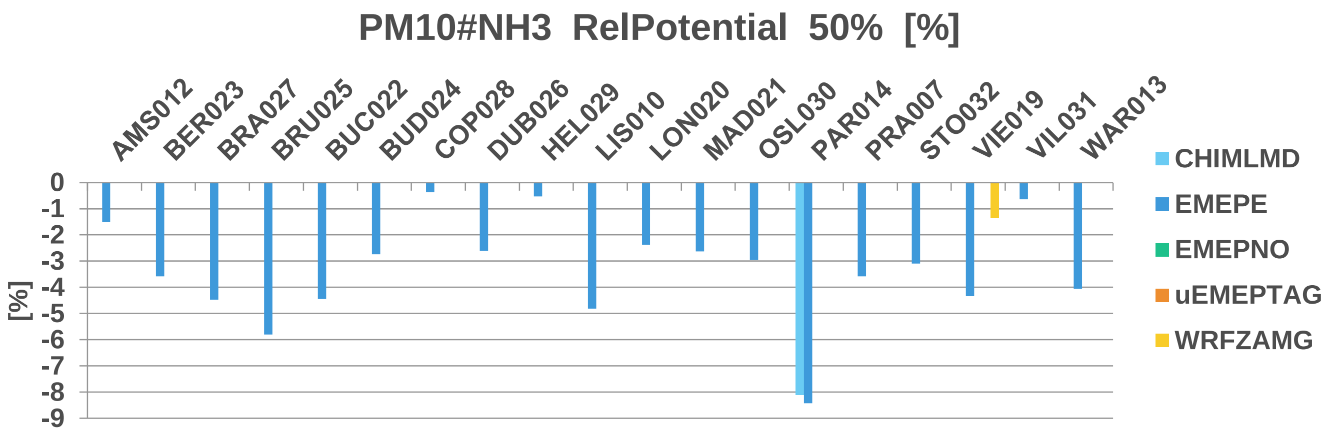
A look at short term

- Idem





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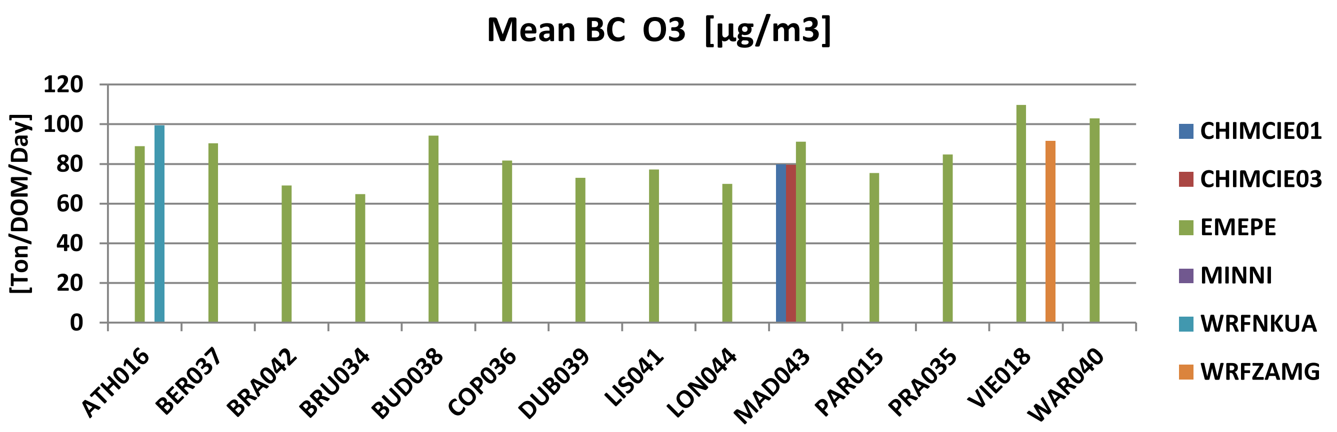
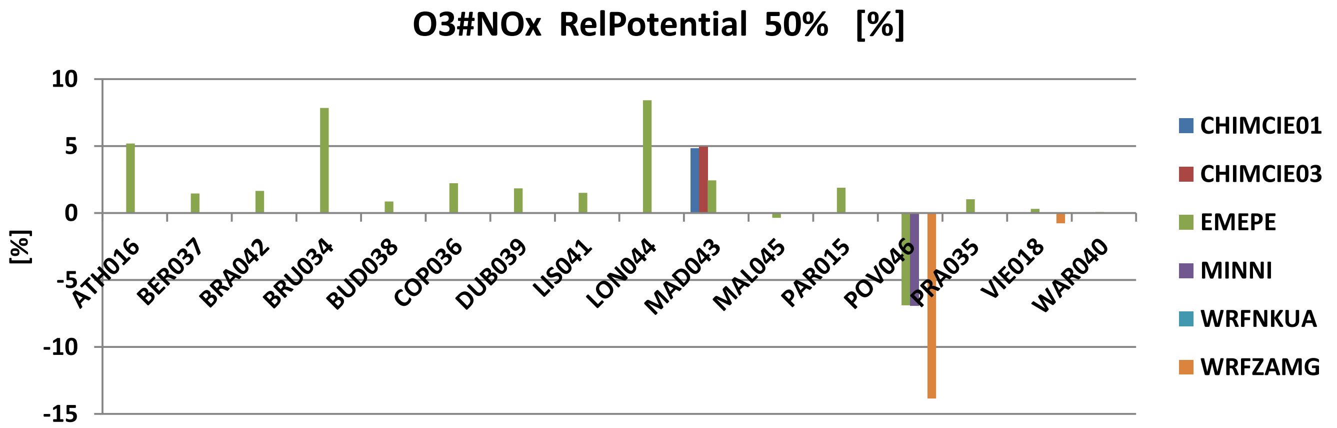
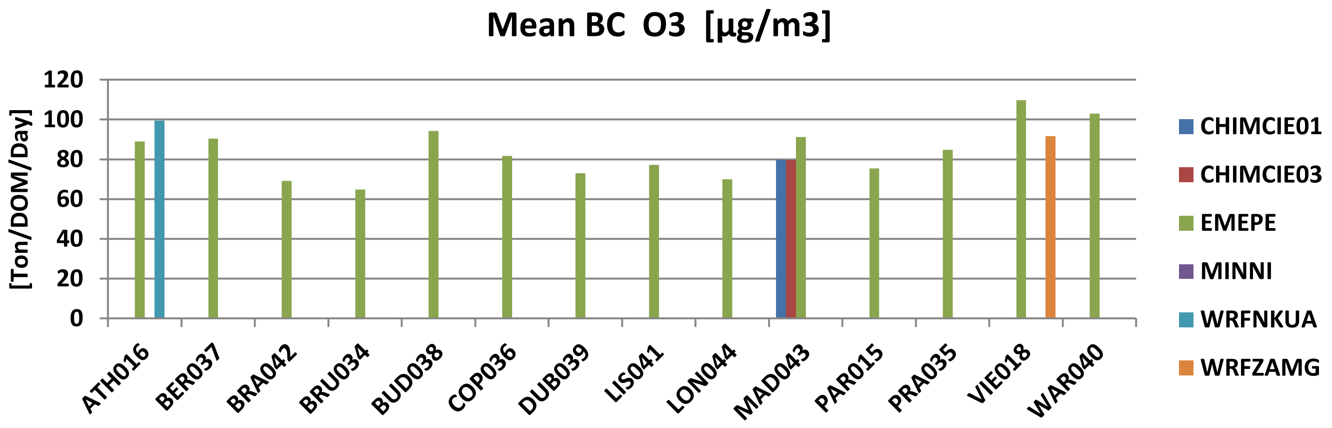
A look at short term for O3 episodes

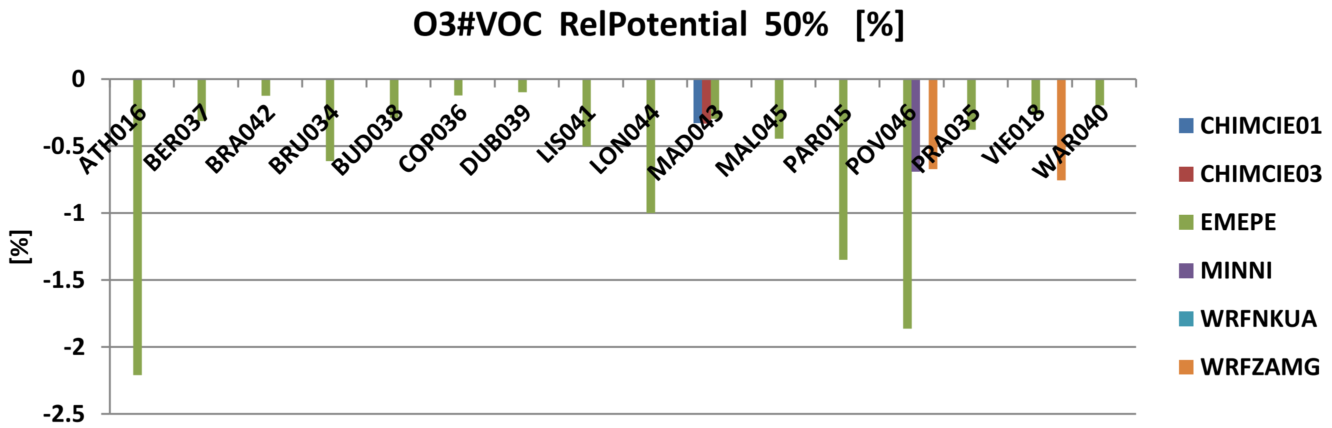
- Weak impact of resolution in Madrid case with a slight increase of the RPI from 1 to 3km
- Increase everywhere except over the Po Valley





A look at short term for O3 episodes

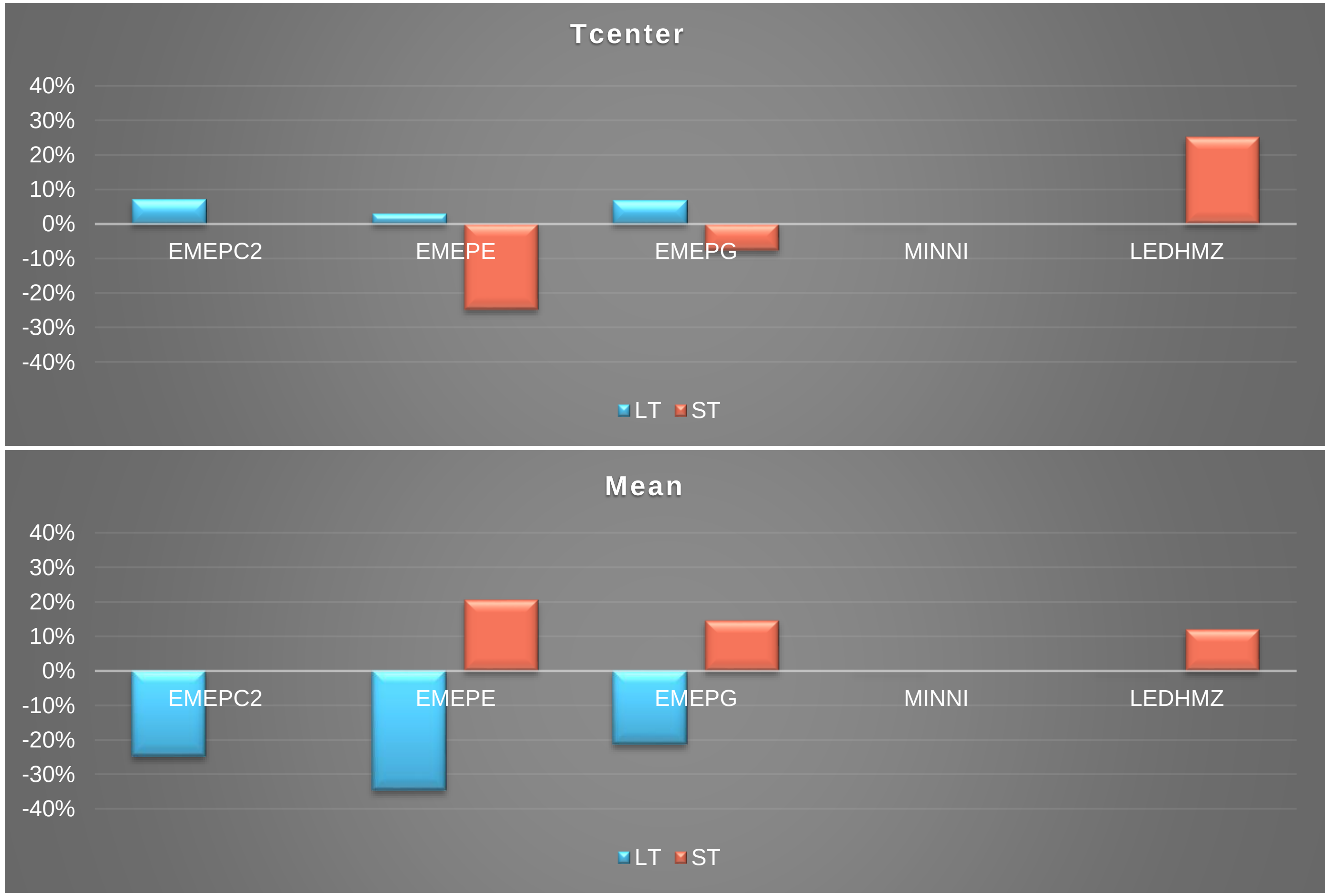




Linearities over the Po valley for Short Term versus Long Term

- Long Term (LT) versus Short Term (ST) O3 episodes
- Averaging remove more local non linearities in time and space

Deviation to linearity of API50%/AP25% for O3#NOx



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Concluding remarks

- A sufficient database to play with but we need more scenarios on Short Term and more emission reductions
- Indicators: API, RPI, APy
- Many simulations remains to be performed particularly for episodes
- Variability based on NSD:
  - Less variability on O3 Mean than PM10 Mean (4 versus 8 % on average for LT)
  - Variability of RPI << API (less clear for O3) - 10 to 25% depending on the indicator
  - Extent of the target domain where emissions are reduced could be important
  - More variability looking at specific location (TC) and shorter timeframe (ST)
- Indicators are sensitive to seasons
- Non linearity effects clearly highlighted for secondary species
- **Open exercize: other modelling teams are still welcome** ☺

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Ideas for the next steps (I/II)

- **Continue to populate the database**
  - Yearly simulation for variability assessment and seasonality
  - Short term simulations for variability analysis and prepare next phases
- More data will be necessary to analyse the ST simulations (more hourly concentrations for many species at least at the first level)
- *Other indicators to calculate?*
- *API, RPI, APy, NSD for variability of indicator: Other?*
- *Are taking the mean, TC, P95 adapted?*

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Ideas for the next steps (II/II)

If a team performed all requested simulations for this first step then prepare the next phase to understand the delta of concentrations

- Creation of sub-groups to understand this large variability with Short Term simulations over episodes
  - One or several models change only one setting (on a target area) that could be:
    1. Emissions (including the impact of vertical profile distribution, biogenic emissions: NO and VOC)
    2. Horizontal resolution
    3. Physics and chemistry schemes
    4. Lateral and boundary conditions (link with vertical diffusion schemes) particularly for O3
    5. General model setting (Domain nesting strategy, numerical schemes)
    - ✓ **Other?**
  - **We need leaders to frame each activity (i, ii, iii, iv, v,…)**

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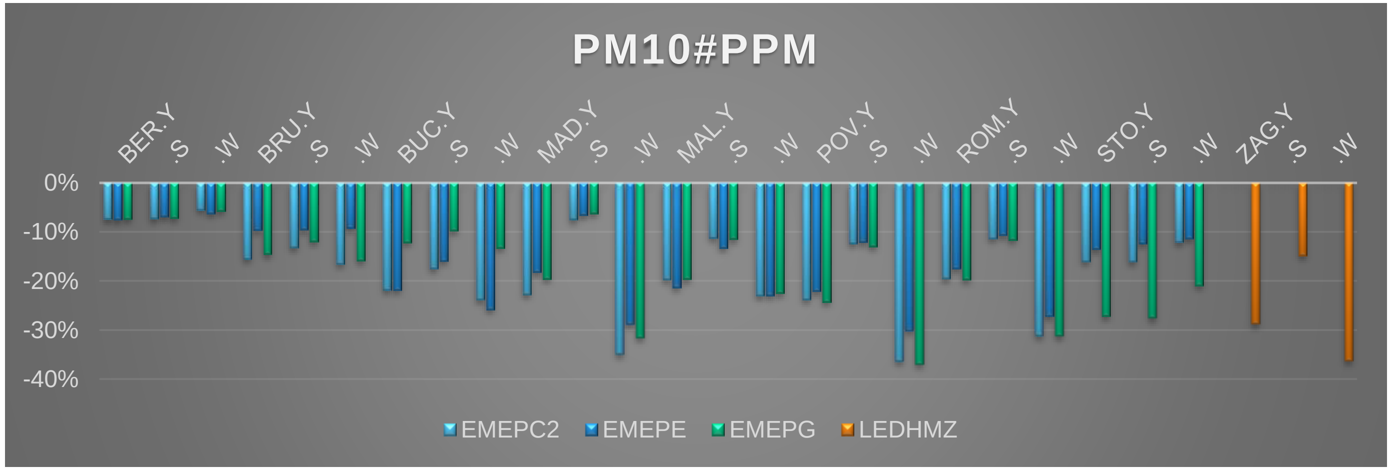
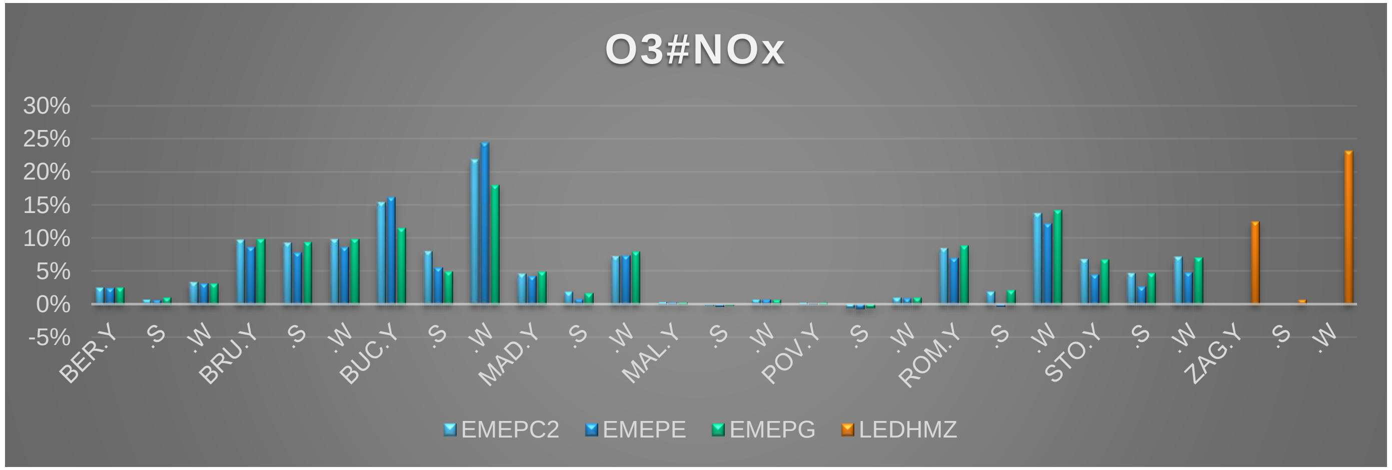
The end

Additional slides

Seasonality of RPI on mean values

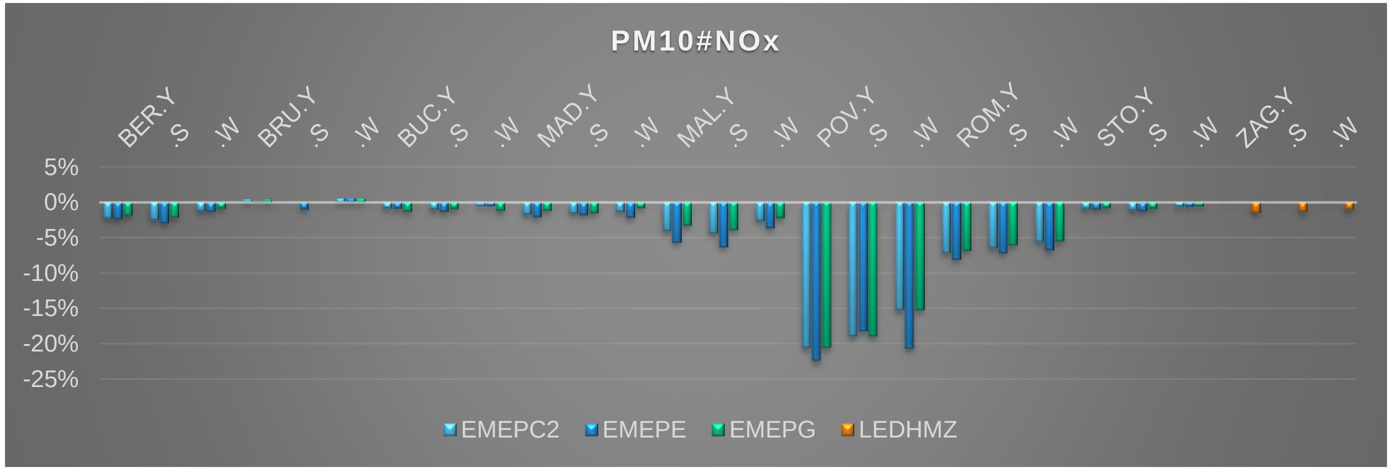
- Yearly (Y), Winter (W as DJF), Summer (S as JJA)
- A clear winter(W) vs summer (S)
  - Negative Delta S < W for PM10 with PPM reduction
  - Positive Delta S < W for O3 with NOx reduction

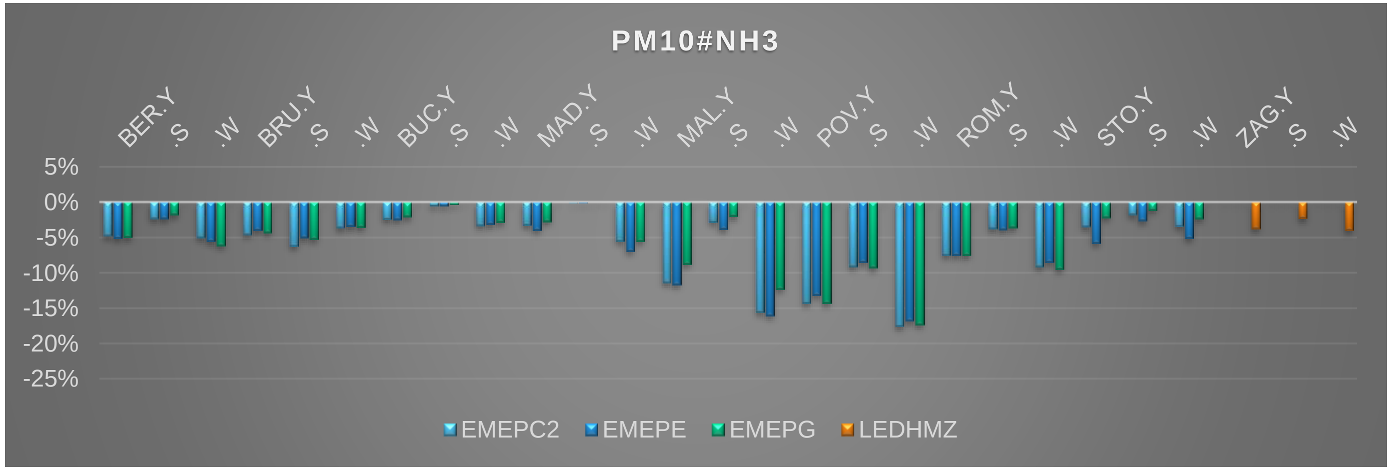




Seasonality of RPI on mean values

- Difficult to have a general behaviour, it depends on cities and chemical regimes





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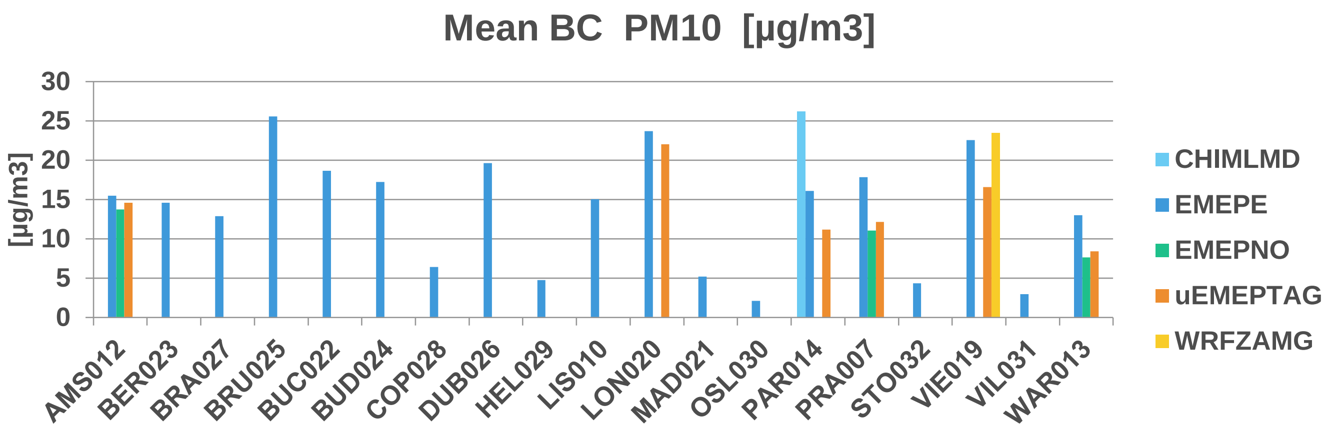
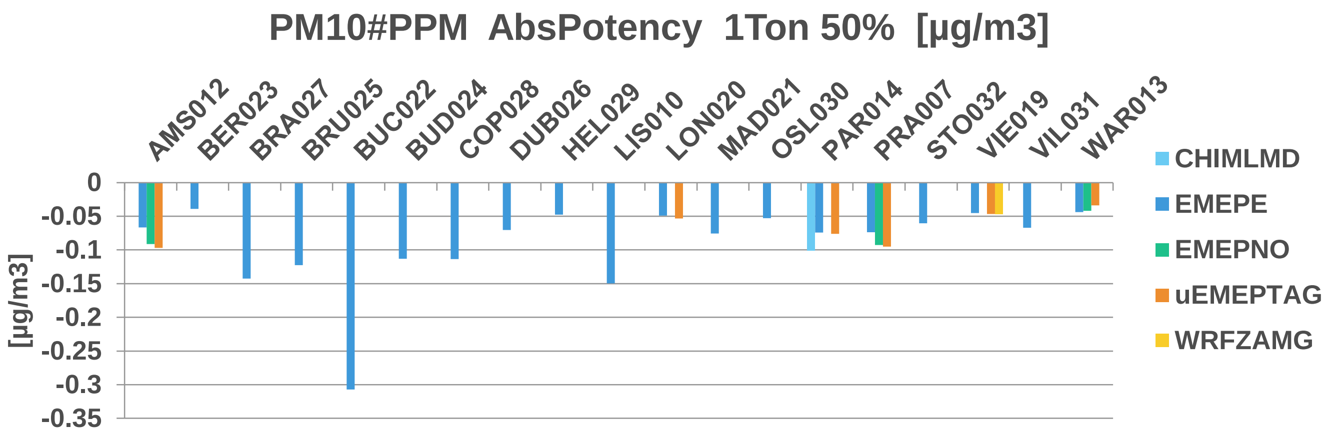
A look at short term





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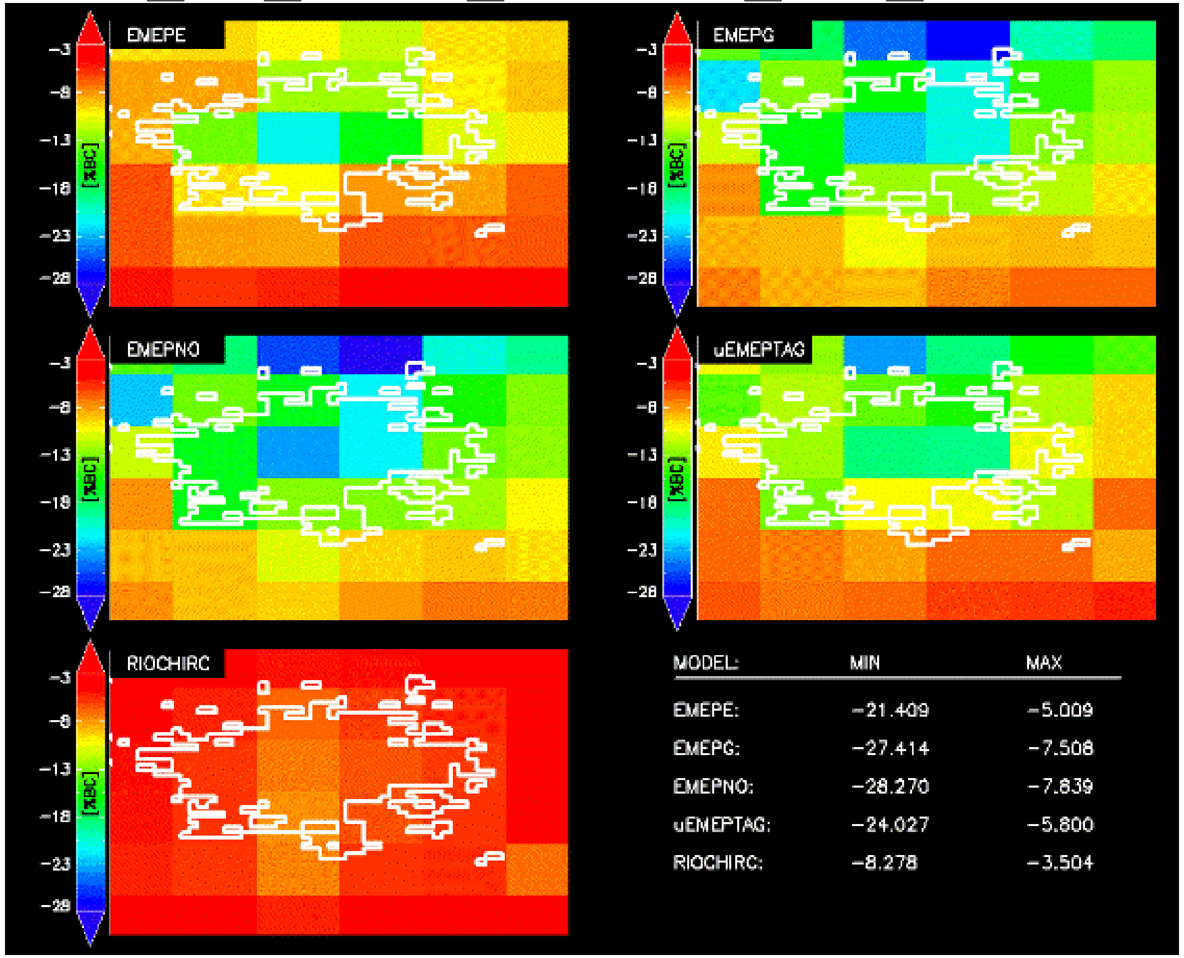
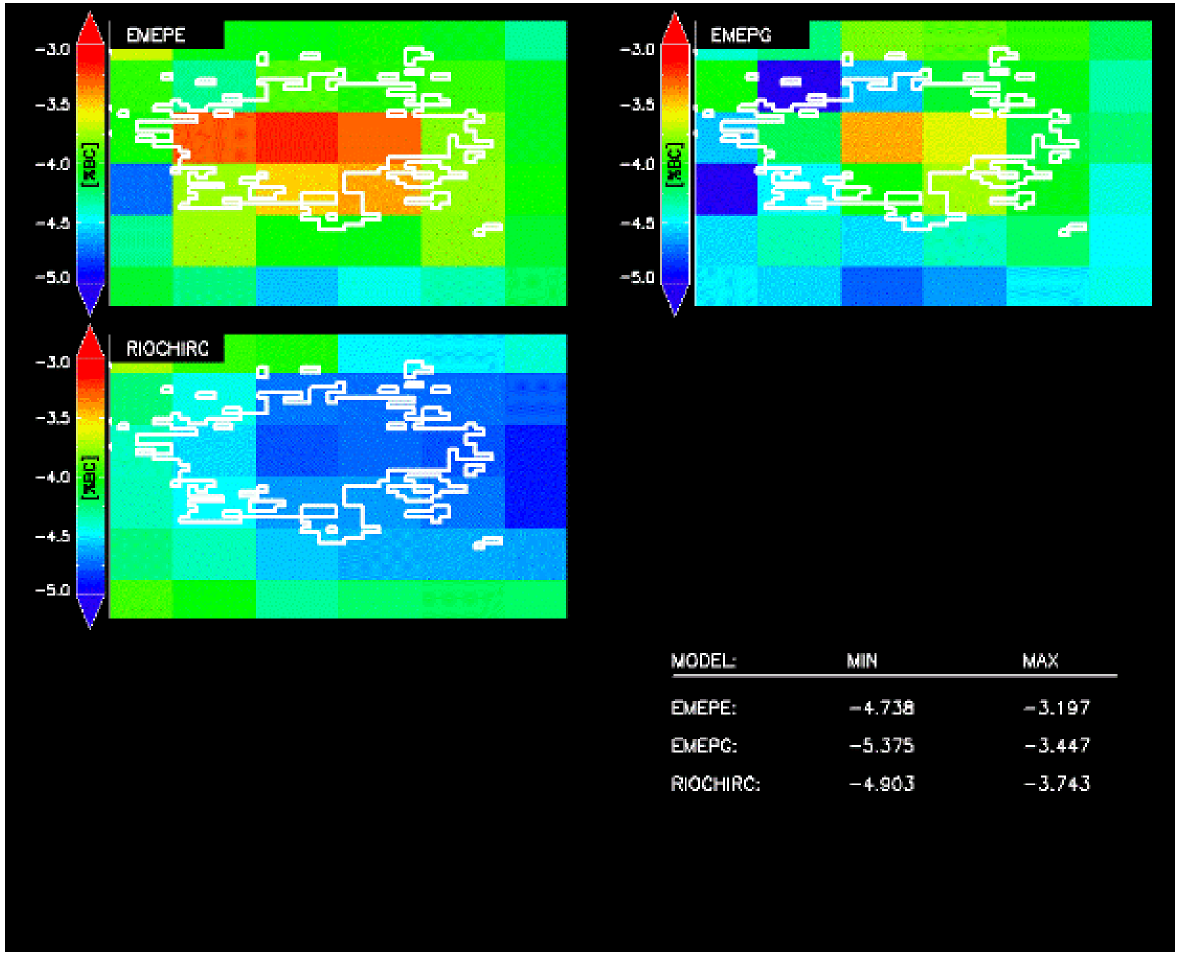
Non linearities in models?

PICT_2D_PM10_BRU003_RPI_50%PPM



Non linearities in models?

PICT_2D_PM10_BRU003_RPI_50%NH3



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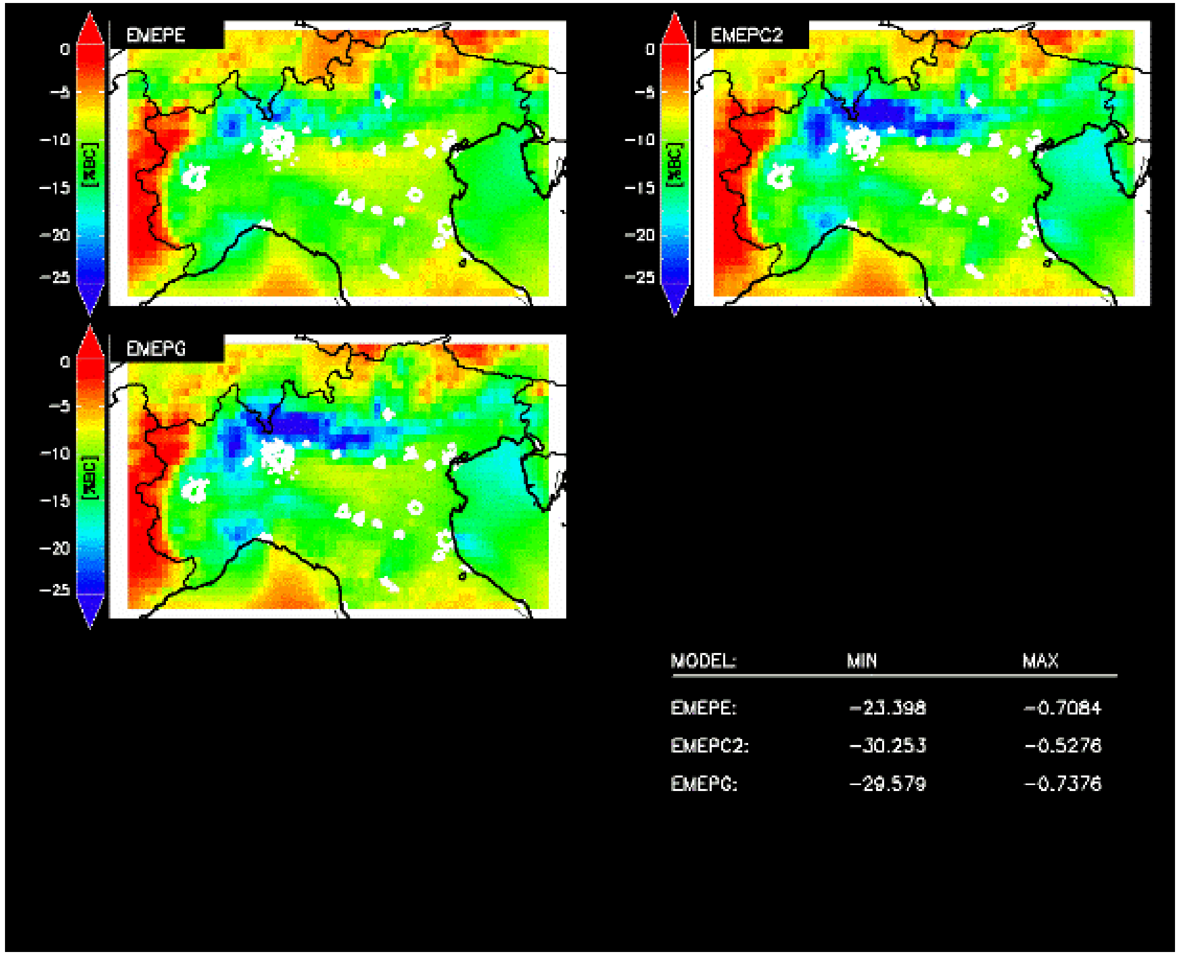
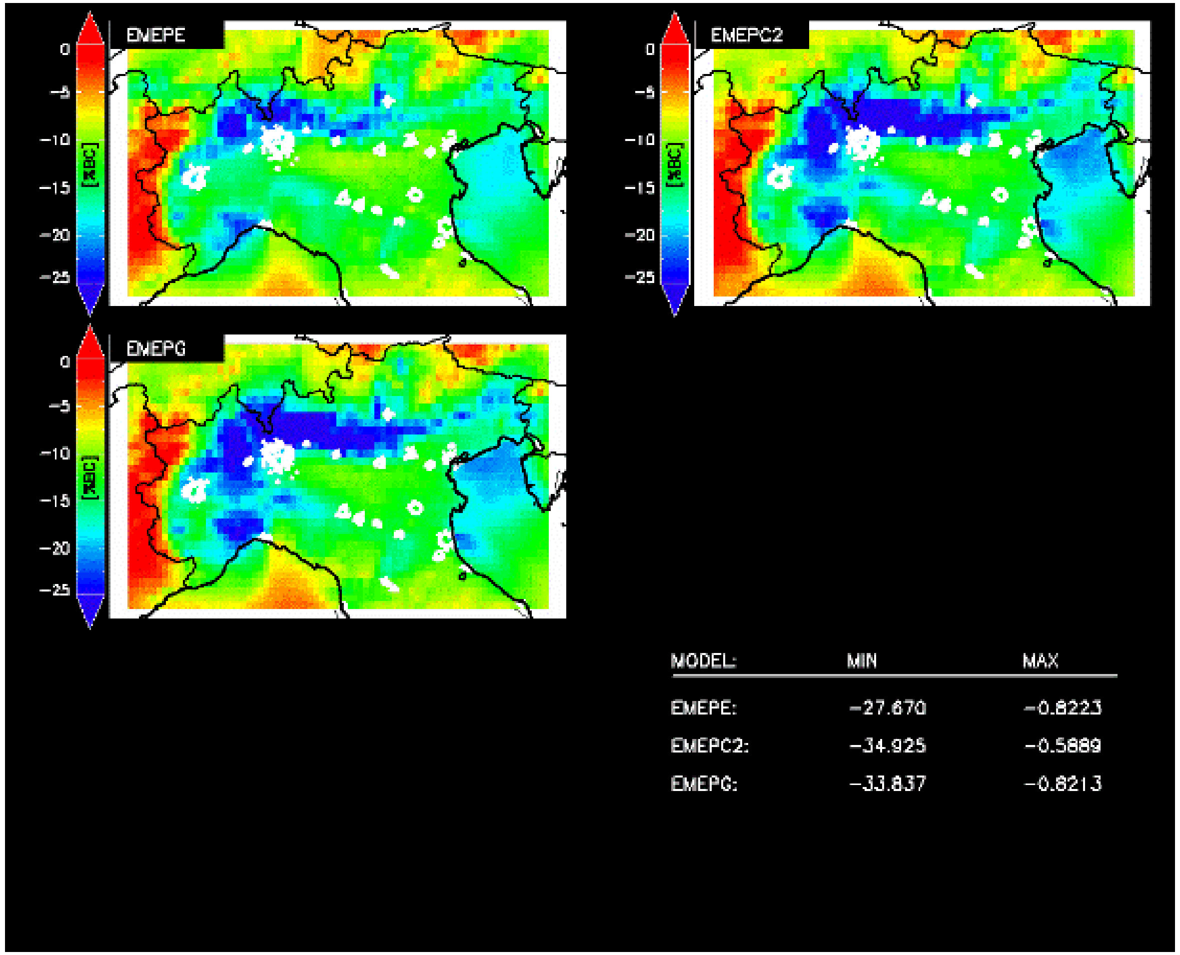
Spatial variability with 2D plots - Linearity

PICT_2D_PM10_POV002_RPI_25%NH3



Spatial variability with 2D plots - Linearity

PICT_2D_PM10_POV002_RPI_**50%**NH3

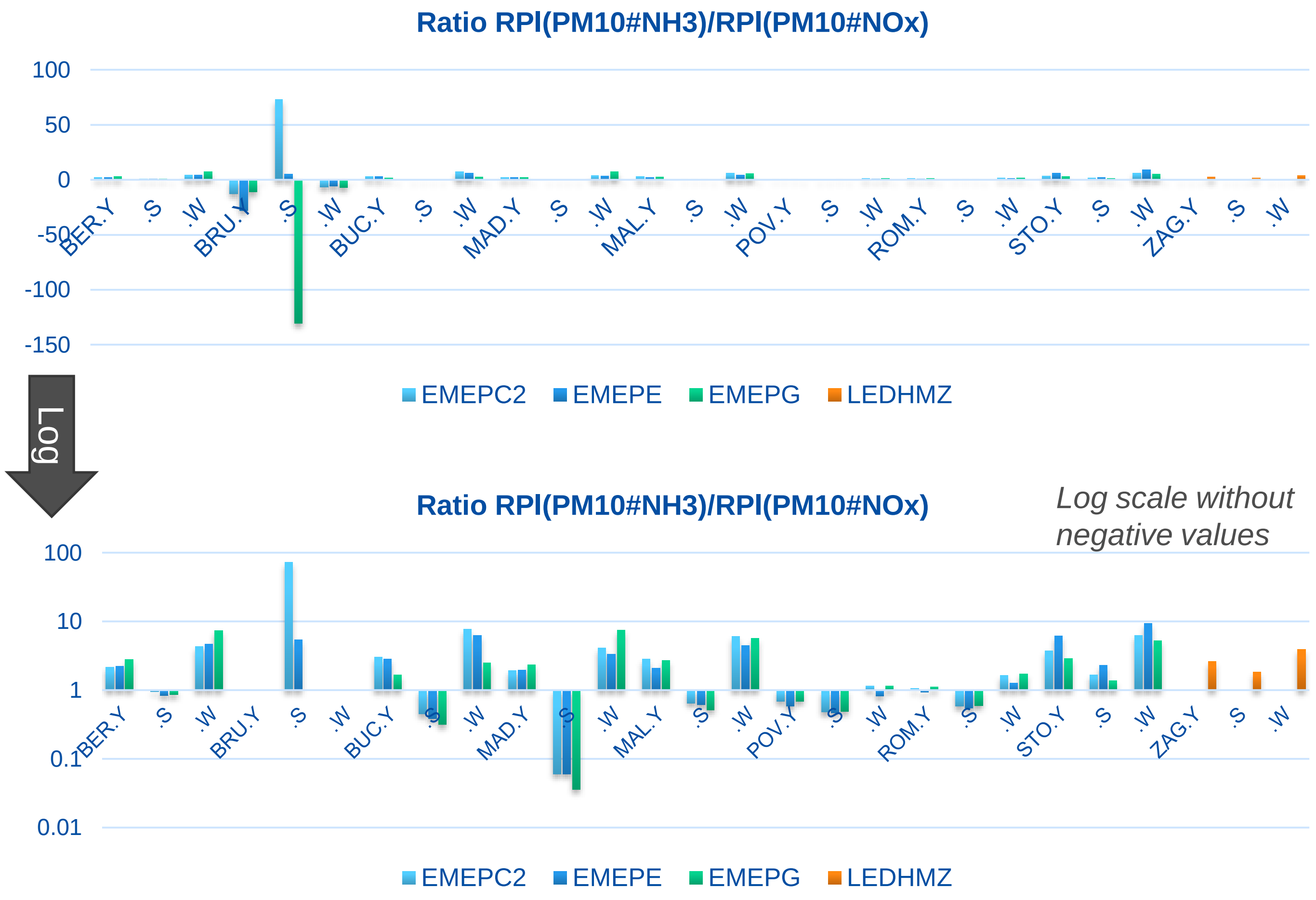


Indicators I/II

- k — Zone of emission reductions
- n — Precursor as NOx, VOC, PPM, SOx, NH3
- m — Pollutant: O3, NO2, PM10,…
- s — Simulation scenario named as 50%NOx, etc. … or base case BC
- α — Emission reduction (25 or 50%)
- $E^{m,k,s}$ — Total emission of precursor *m* over zone k for simulation s
- $e_{i,j}^{m,k,s}$ — Emission of precursor *m* over zone k for grid cell $(i,j) \in A_k$ for simulation s
- $C^{n,k,s}$ — Averaged concentration of pollutant n over zone k for simulation s
- $c_{i,j}^{m,k,s}$ — Concentration of pollutant n over zone k for grid cell $(i,j) \in A_k$ for simulation s

Seasonality of RPI on mean values

- Ratio of RPI between NOx and NH3 reductions
- Usually same sign of concentration reductions except in Brussels
- Usually higher RPI from ammonia emission reduction scenario except in summertime



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