

Analyse of sequential coupling error in a
multiscale urban air quality model.

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Model coupling for urban air quality

- High spatial variability of pollutant concentrations in the urban environment → need for a "local" description
- The background contribution remains significant for most of pollutants (NO_2 , $\text{PM}_{2.5}$, ...) → need for a "regional" description



Paris (almost) from the sky...



Paris from the ground...

Need for a 'multiscale' modelling framework that can be based on model coupling.

Regional scale - the CHIMERE-WRF coupled model

WRF v4.1

Provide meteorological fields over the 3 nested domains ("one-way" nesting).

- Use of the SLUCM urban canopy model (Kusaka et al., 2001) with CORINE land cover data (3 urban classes) and urban fraction.

CHIMERE (Menut et al. 2024)

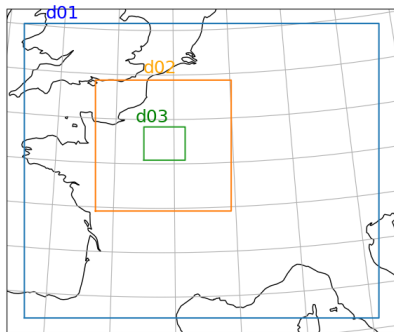
Provide background concentrations.

- EMEP and Airparif inventories
- MEGAN for biogenic emissions
- LMDz-INCA for IC/BC

Simulation

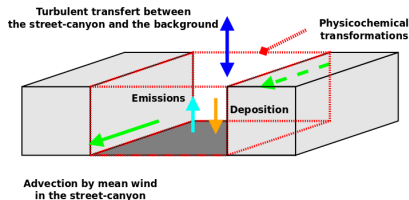
period : February 2014

	d01	9 km × 9 km
domains :	d02	3 km × 3 km
	d03	1 km × 1 km

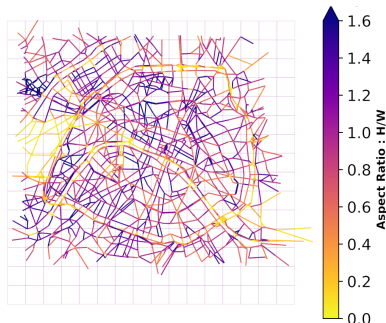


Simulated domains.

Local scale - the MUNICH street network model



- Homogeneous concentration in streets.
- Wind profile and turbulent exchanges parameterised from meteorological variable above street.
- A non-stationary chemistry modelled (Melchior and SSH-aerosol).



Simulated street network in Paris and its inner suburbs.

Solve a system of mass conservation equations for each street segment of the simulated network (Soulhac et al., 2011; Kim et al., 2018; Lugon et al. 2020; Kim et al. 2022)

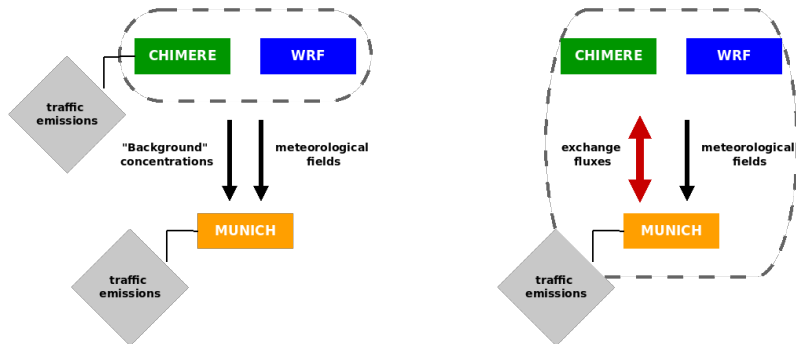
$$\frac{\partial c_i^s}{\partial t} = Q_{\text{inflow}}(\{c_i^{s\pm}\}, c_i^{bi}) - Q_{\text{outflow}} + Q_{\text{vert}}(c_i^s, c_i^{bs}) + Q_{\text{chem}} - Q_{\text{dep}} + S_i$$

with

c_i^s , the concentration of species i for the street s , $\{c_i^{s\pm}\}$, those in the upstream streets.

c_i^{bs} , c_i^{bi} the background concentrations of the street s and of the the upstream intersection = **boundary conditions** for MUNICH.

"One-way" vs "two-way" coupling



(Squarcioni et al., 2024)

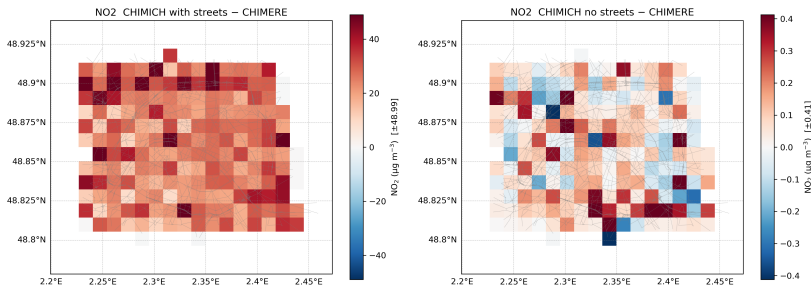
- Limiting errors due to the numerical dilution of pollutants supposed maintained in urban street canyons and its consequences on "background" concentrations evaluation.
- Avoiding errors due to the integration of traffic emissions both in the regional model and in the local model.
- ! The "two-way" coupling involves explicitly distributing the atmospheric volume between CHIMERE and MUNICH.

Impact on regional scale concentrations

"CHIMICH with streets" : Total mass of pollutants (streets + background) diluted in the cell volume.

"CHIMICH no streets" : Mass of pollutants in the background diluted in the cell volume.

"CHIMERE" : usual estimation of the regional model.



Difference of NO₂ average concentrations for February 2014.

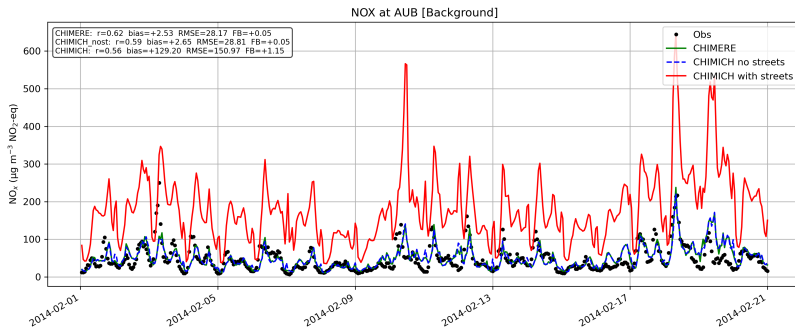
→ A traditional regional Eulerian model do not distinguish between 'average' and 'background' concentrations, the values provided are **only** representative of **background concentrations**.

Impact on regional scale concentrations

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"CHIMERE" : usual estimation of the regional model.



Time evolution of NO_x concentrations during February 2014 for a background monitoring site (Airparif).

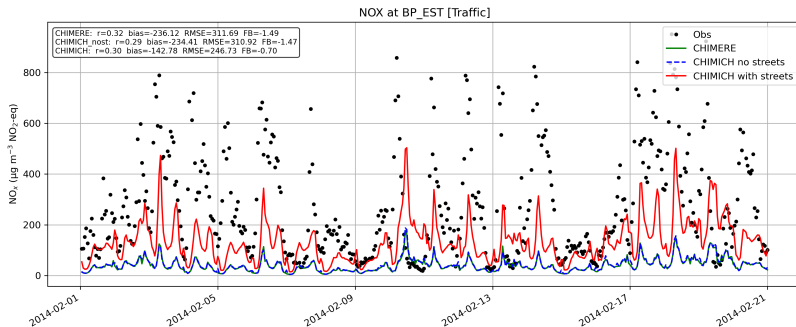
→ The average concentrations is not representative of in-situ observation stations.

Impact on regional scale concentrations

"CHIMICH with streets" : Total mass of pollutants (streets + background) diluted in the cell volume.

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"CHIMERE" : usual estimation of the regional model.



Time evolution of NO_x concentrations during February 2014 for a traffic monitoring site (Airparif).

→ The average concentrations is not representative of in-situ observation stations.

? The average concentration could be comparable to that observed by satellite.

Vertical distribution of street emission fluxes

$$Q_{\text{vert}} = \frac{\sigma_w l_m}{H} \frac{C_{\text{street}} - C_{\text{background}}}{H}$$

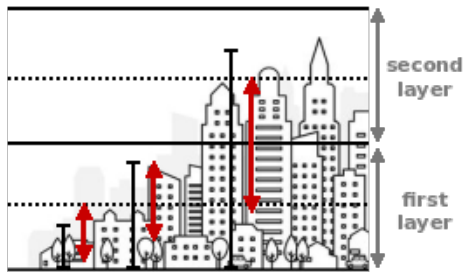
with

σ_w : standard deviation of vertical wind

l_m : a mixing length

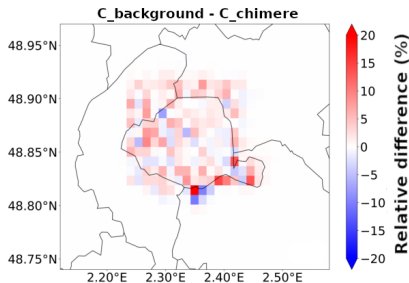
H : the average height of the buildings

Which $C_{\text{background}}$ for which H ?



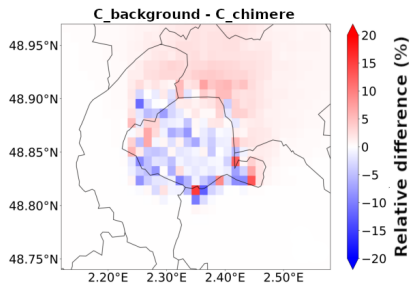
Schematic representation of the vertical discretisation
of the Eulerian regional model.

Vertical distribution of street emission fluxes



Coupling limited to the first layer.

diff. : **1.4%** [-11%; 26%]



Coupling with the first two layers.

diff. : **0.08%** [-14%; 17%]

- The numerical dilution error and the emission vertical distribution error partially offset each other.

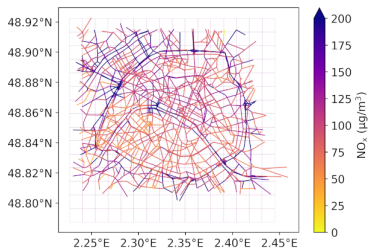
Impact on NO_x local scale concentrations

Sites		FB	R	NMSE
BP_EST	seq.	-0.11	0.52	0.47
	dyn.	-0.03	0.55	0.42
AUT	seq.	-0.28	0.72	0.33
	dyn.	-0.25	0.65	0.41
RN2	seq.	-0.17	0.59	0.40
	dyn.	-0.34	0.65	0.52
SOULT	seq.	0.10	0.68	0.27
	dyn.	0.02	0.68	0.28
CELES	seq.	0.36	0.70	0.42
	dyn.	0.35	0.70	0.42
ELYS	seq.	-0.22	0.74	0.23
	dyn.	-0.22	0.73	0.24
HAUS	seq.	-0.17	0.69	0.29
	dyn.	-0.13	0.7	0.25
BONAP	seq.	-0.37	0.75	0.40
	dyn.	-0.39	0.75	0.42

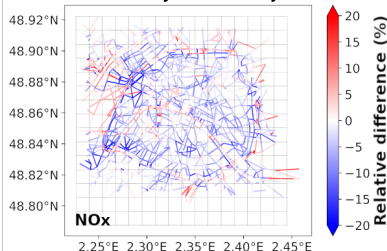
Table 1: Statistical indicators for NO_x hourly concentrations.

- Slight overestimation of sequential coupling by 2% on average.
- Fair statistical scores in both cases.
- The differences are correlated to building heights.

"Two-way" NO_x average - feb. 2014



"Two-way" - "One-way"

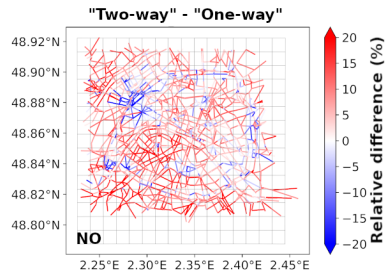
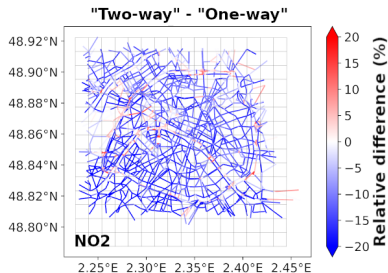


Impact on NO₂ and NO local scale concentrations

Sites		FB	R	NMSE
BP_EST	seq.	0.10	0.54	0.21
	dyn.	0.15	0.55	0.24
AUT	seq.	-0.24	0.69	0.21
	dyn.	-0.24	0.64	0.25
RN2	seq.	0.01	0.50	0.17
	dyn.	-0.21	0.66	0.17
SOULT	seq.	0.18	0.71	0.15
	dyn.	0.02	0.72	0.12
CELES	seq.	0.39	0.72	0.27
	dyn.	0.21	0.75	0.17
ELYS	seq.	0.09	0.70	0.10
	dyn.	0.06	0.71	0.10
HAUS	seq.	0.11	0.71	0.10
	dyn.	0.09	0.72	0.12
BONAP	seq.	0.05	0.70	0.10
	dyn.	-0.15	0.73	0.13

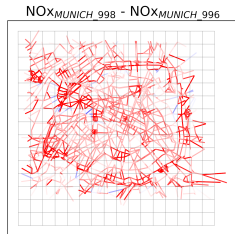
Table 2: Statistical indicators for NO₂ hourly concentrations.

- Stronger overestimation for NO₂ (8.5%) and underestimation for NO (5%).
- Fair statistical scores in both cases.

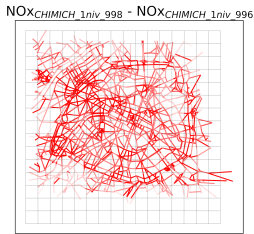


Sensitivity to vertical discretisation

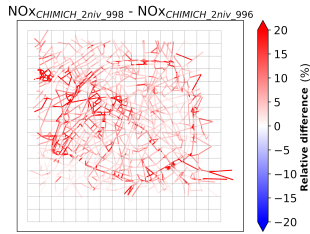
Two different vertical discretisation considered for Chimere
first layer at 998 hPa (~ 16 m) vs at 996 hPa (~ 32 m)



"One-way"
Average bias : $11.5 \mu\text{g.m}^{-3}$



"Two-way", one level.
Average bias : $18 \mu\text{g.m}^{-3}$



"Two-way", two levels.
Average bias : $10 \mu\text{g.m}^{-3}$

- Sensitivity to the thickness of the first layer remains high.
- Coupling on 2 levels helps to limit it slightly.

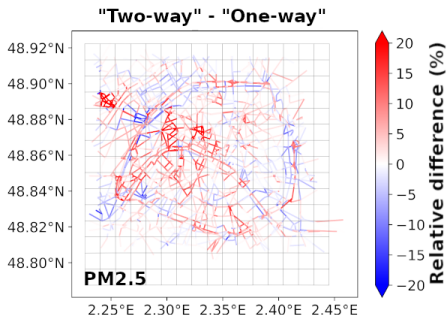
Conclusions and prospects

A multiscale modelling framework has been implemented by dynamically coupling **CHIMERE** and **MUNICH**.

- Limit numerical dilution error for regional scale simulation.
 - Moderate impact on NO_x local concentrations but more visible impact on NO_2 and $\text{PM}_{2.5}$.
 - Possibility of reducing the sensitivity of local results to the vertical discretisation of the regional model.
- Implementation currently improved by Myrto Valari (thanks!!!)
- Improve the meteorological "downscaling" and extend the multi-layer implementation to meteorological fields.

Extend the analysis:

- for different periods,
- for different pollutants :
particle chemical compounds.
UFP and particles number
concentrations.
- for comparison to satellite data?



Thank you for your attention!

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