ENHANCING URBAN AIR POLLUTION MODELLING THROUGH A NETWORK SCIENCE APPROACH

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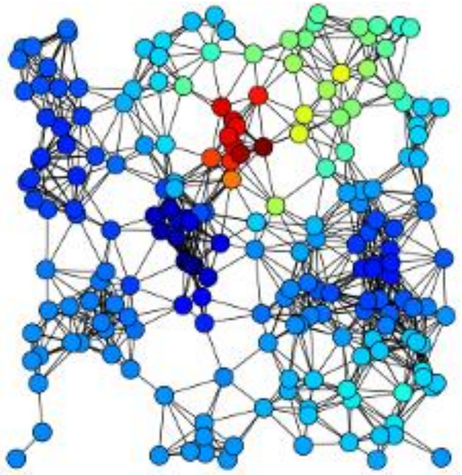
What is the optimal place to reduce transport emissions?

Photo by Gabriel Bouys/AFP

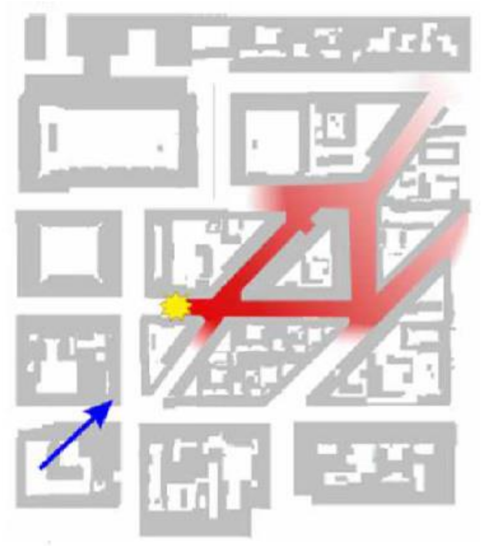
AIR QUALITY PLANS TO MEET AIR QUALITY STANDARDS IN CITIES

WHERE TO IMPOSE TRAFFIC RESTRICTIONS?

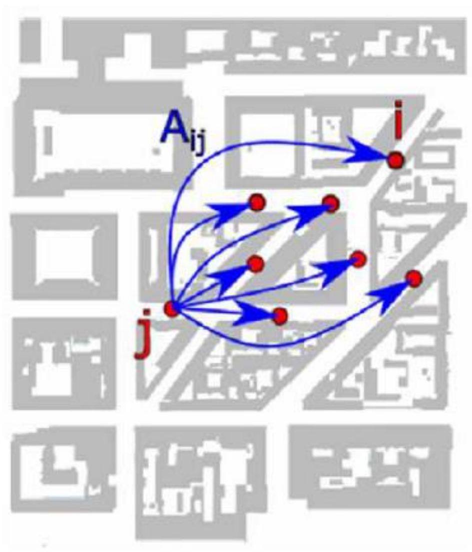


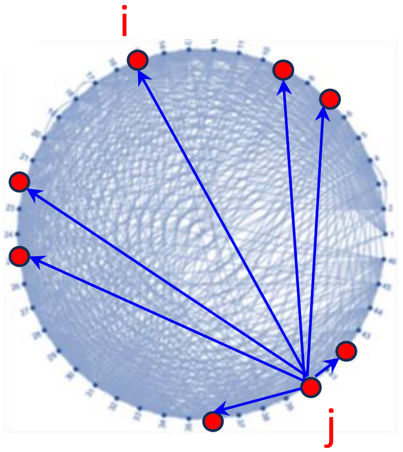
NETWORK APPROACH

Network representation

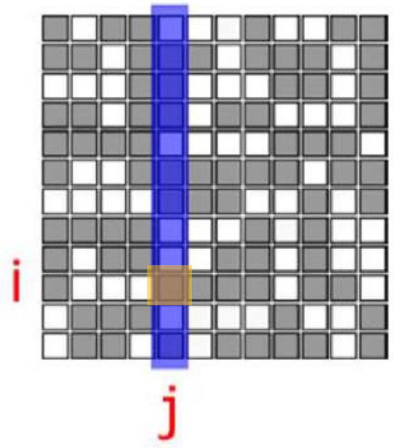


Dispersion from an emission source





The emission-receptor network

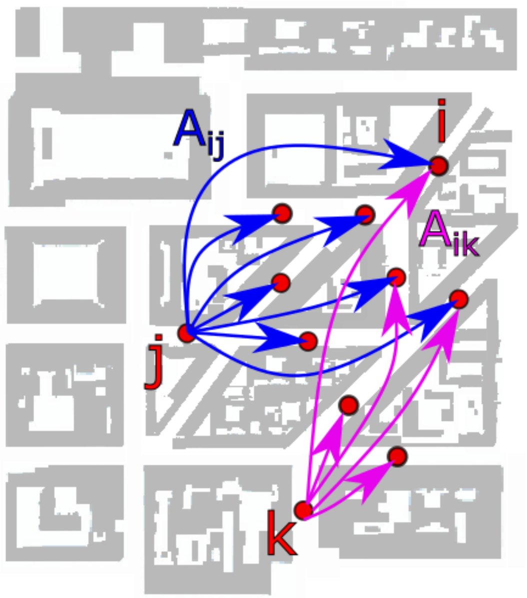


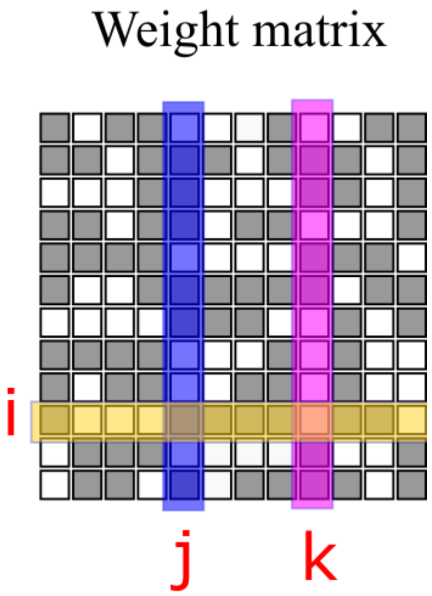
The weight matrix A

Streets → Nodes
Emission-Impact → Links

Emission-Impact quantification

The linear assumption

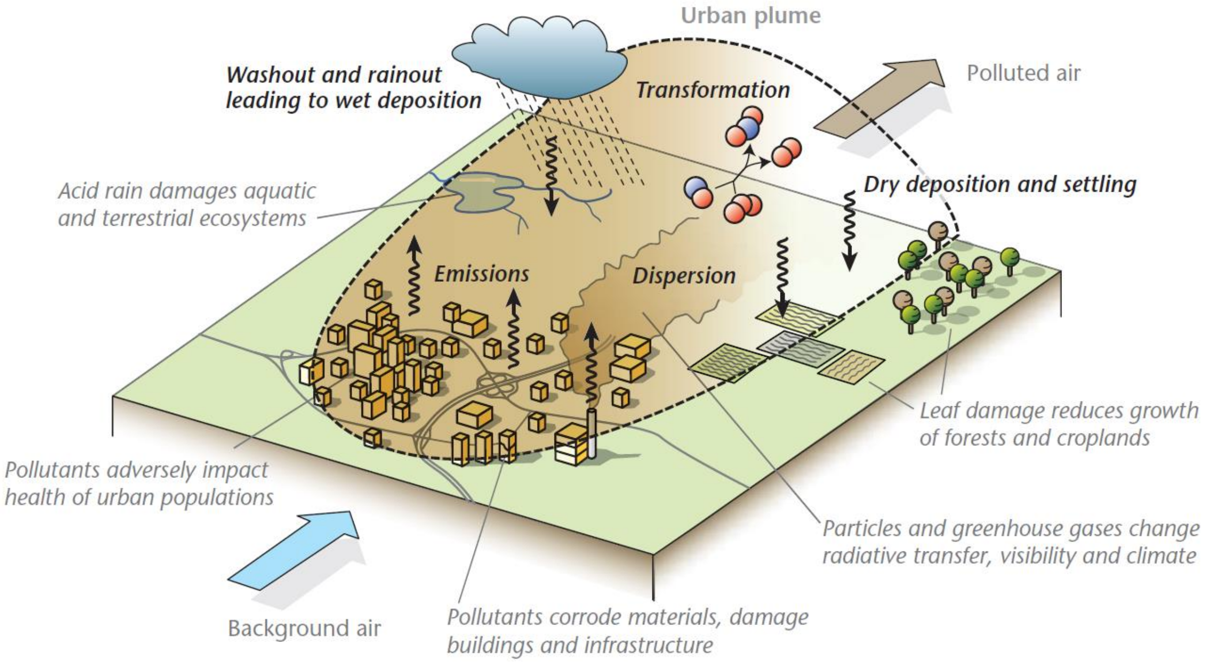




$$\boldsymbol{C_i} = A_{ij}Q_j + A_{ik}Q_k$$

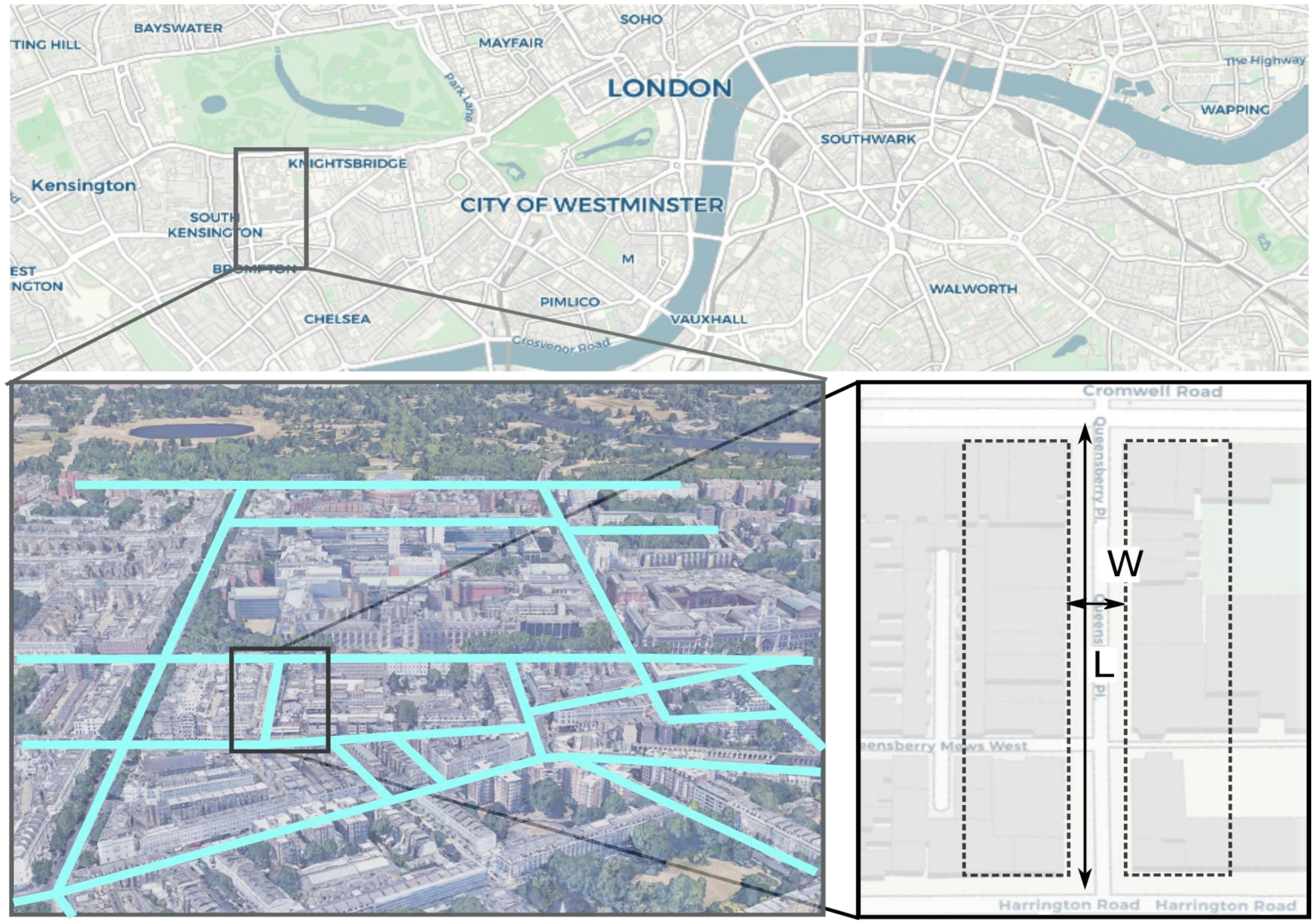
$$\boldsymbol{C} = A\boldsymbol{Q}$$?

Linear relation between emissions and concentrations in the street network

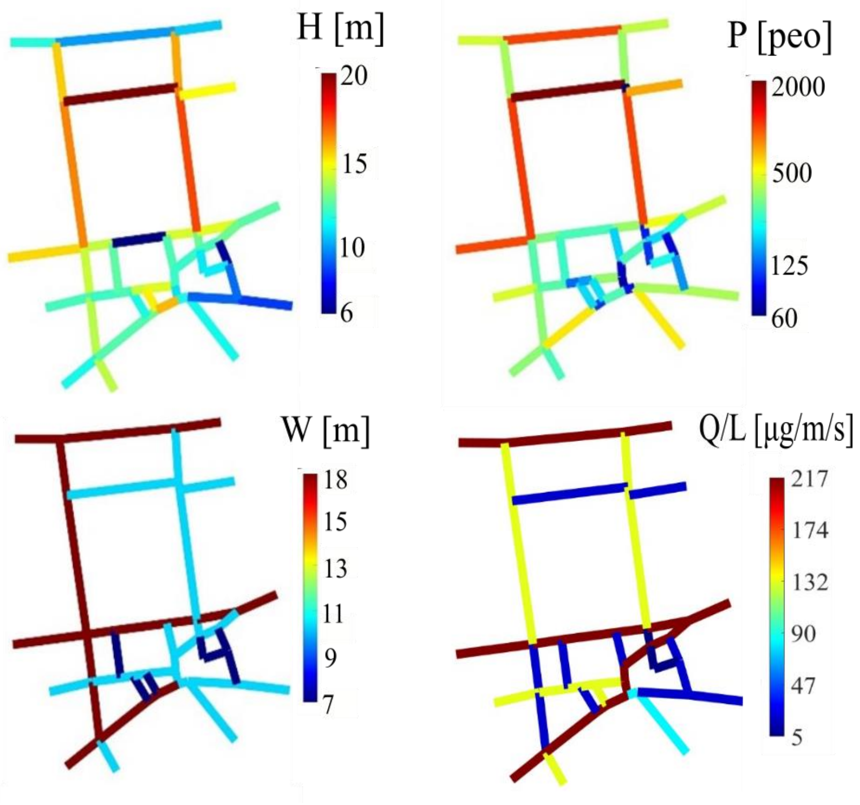


Oke, Timothy R., et al. *Urban climates*. Cambridge University Press, 2017.

South Kensington case study



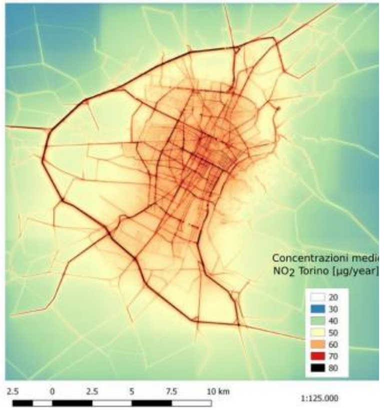
46 streets → 46 nodes → 46x46 matrix **A** and **E**



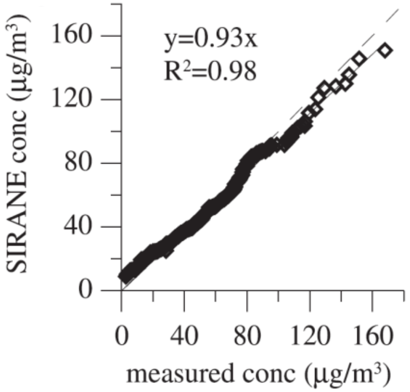
Average values of NOx emissions for 2021 from traffic simulation software and emission model

Building matrix A

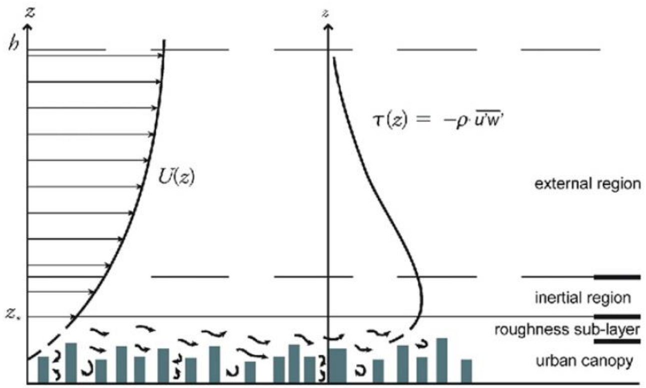
SIRANE software: NO2 concentration in the city of Lyon



Validation in Lyon (NO2)

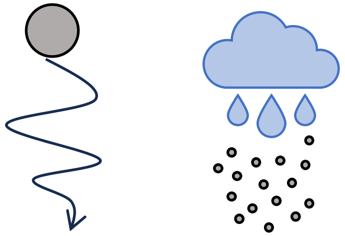


METEOROLOGICAL PREPROCESSOR

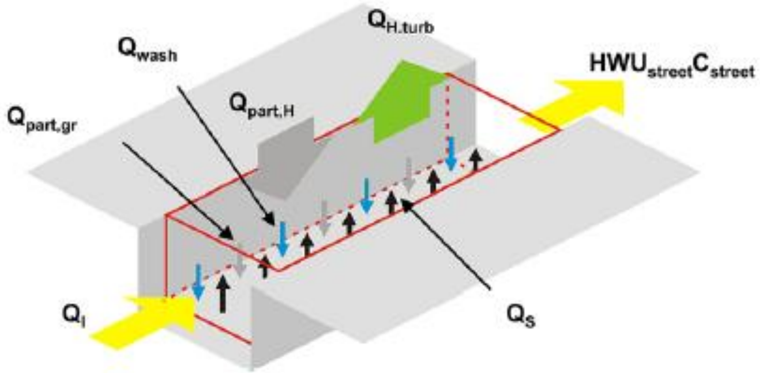


PHYSICO-CHEMICAL PROCESSES

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

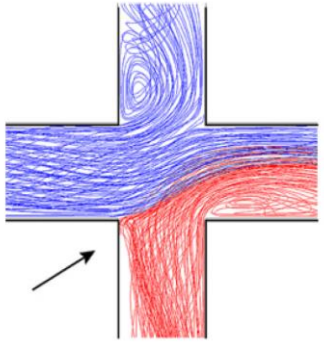


MASS BALANCE IN EACH STREET CANYON



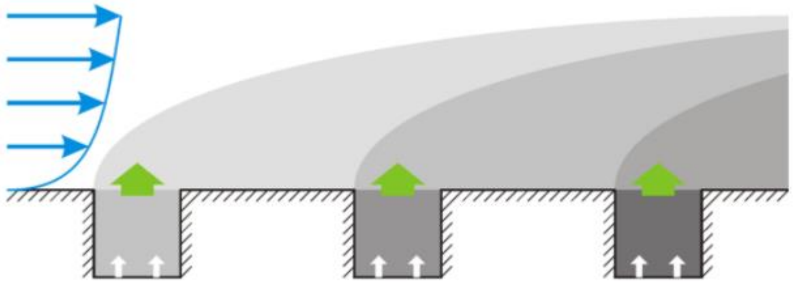
$$Q + Q_I = Q_{H,turb} + Q_{adv} + Q_{part} + Q_{wash}$$

EXCHANGE MODEL AND MASS BALANCE IN STREET INTERSECTIONS



$$Q_{I,j} = \sum_i P_{i,j}(\phi_0) C_{street_i} + P_{ext \to j} C_{I,ext}$$

GAUSSIAN PLUME MODEL ABOVE ROOF LEVEL

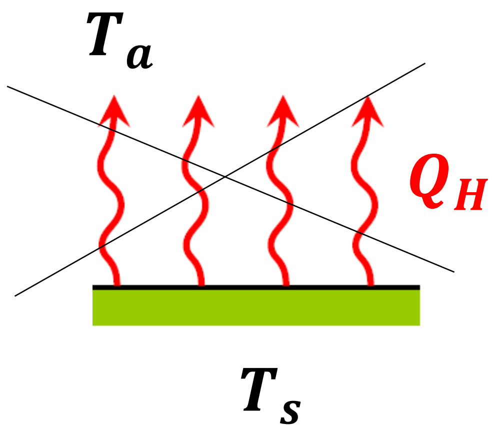


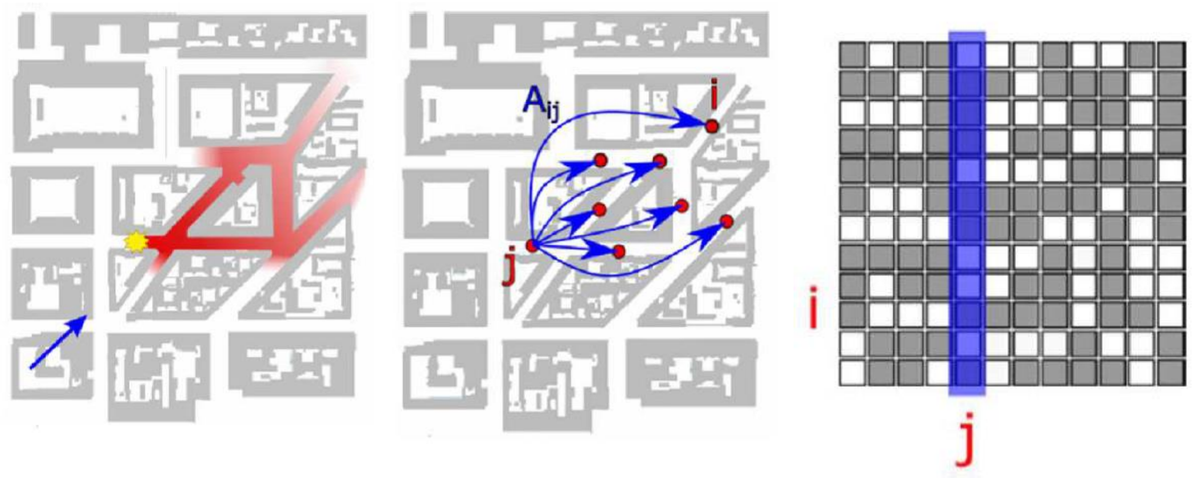
Soulhac, Lionel, et al. "The model SIRANE for atmospheric urban pollutant dispersion; part I, presentation of the model." *Atmospheric environment* 45.39 (2011): 7379-7395.

Building matrix A

SIRANE
Urban Air Quality Model

- **Inert** tracer emission (O3+ Night+ No precipitation)
- Null **background** concentration
- **Neutrally** stratified boundary layer →Albedo=1
- External **wind** U_0, Φ





Emission-Impact matrix *A*

$$\boldsymbol{C} = A\boldsymbol{Q}$$

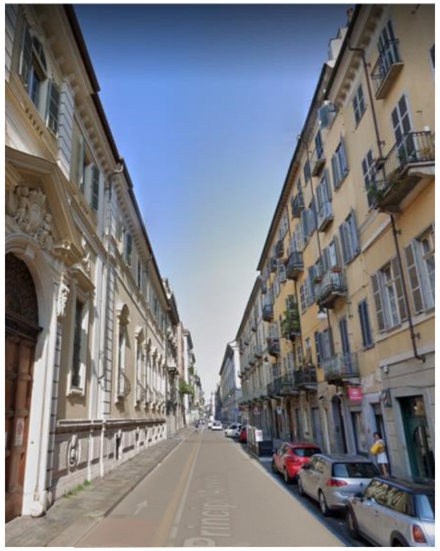
- **Unit** passive scalar emission from street j ($Q_j = 1$)

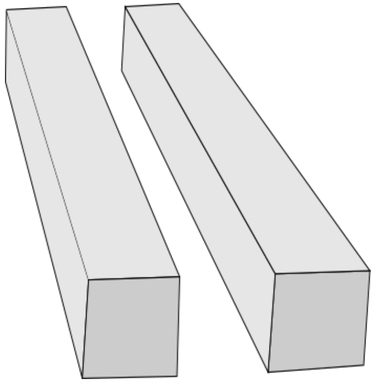
  ↓

  column j is filled ($C_{.j}$)

- 1 h simulation for **each** j to fill the entire matrix $A(U_0, \phi)$
- Simulations are repeated for **8 wind directions**

Building the exposure matrix E



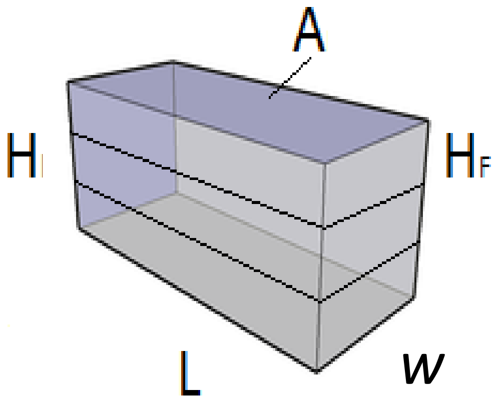


People in a street (p_i)

$$S_i = 2\frac{H_i L_i w}{H_F}$$ Total living space for street

$$S_p = \frac{\sum_j 2H_j L_j w/H_F}{n_{TOT}}$$ Living space for a resident

$$p_i = 2\frac{H_i L_i w}{H_F}\frac{n_{TOT}}{2\,w\sum_j H_j L_j/H_F} = \frac{H_i L_i}{\sum_j H_j L_j} n_{TOT}$$



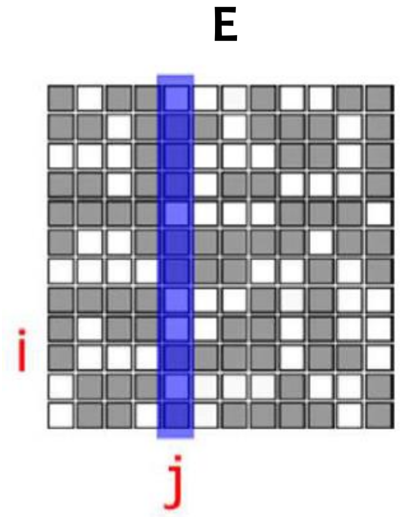
Exposure matrix E

$$e_i = q p_i C_i \quad [\mathrm{g/h}]$$

$$\boldsymbol{e} = q\boldsymbol{p} \circ \boldsymbol{C} = q\boldsymbol{p} \circ A\boldsymbol{Q} = E\boldsymbol{Q}$$

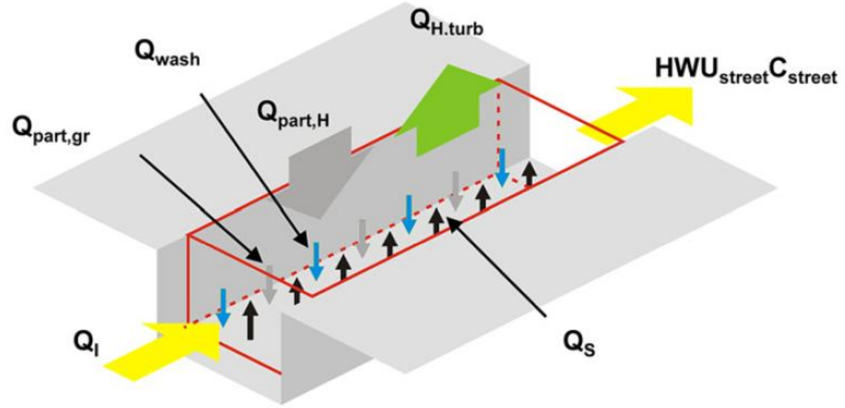
Inhalation rate

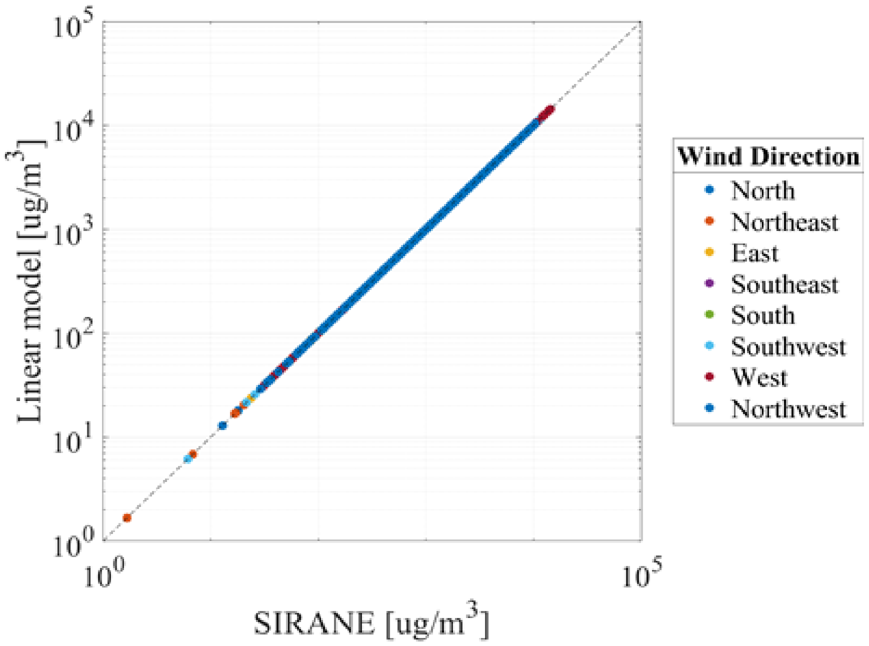
$(q = 0.57\,\frac{m^3}{h})$



Testing the linear assumption for the inert scenario

I. Construction of matrix $A(U_0, \Phi)$
II. Random n emissions **Q** and find **C** with **linear model:** $\boldsymbol{C} = A\boldsymbol{Q}$
III. Simulations with **SIRANE** for same **Q**
IV. Comparison of concentrations
V. Test repeated 20 times for each Φ





Why does the linear assumption hold?

$$Q + Q_I = Q_{H,turb} + Q_{adv} + Q_{part} + Q_{wash}$$

Negligible re-entrainment from roofs

$$Q + U_S W H C_{up} = u_d W L C + U_S W H C$$

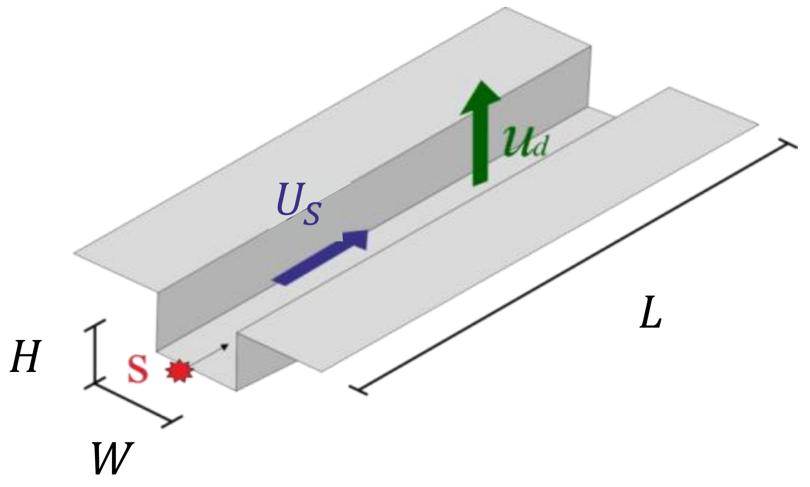
$$C_{up} \propto \boldsymbol{Q}$$

! Once matrix $A(U_0, \Phi)$ is built, all the possible emission scenarios in the city can be easily computed!

Wind speed correction

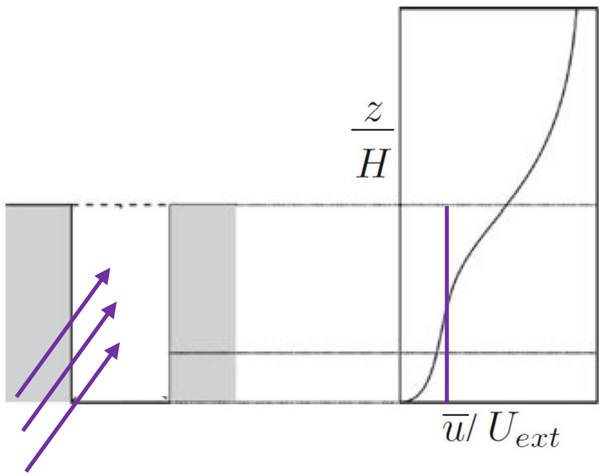
$$\boldsymbol{C} = A\boldsymbol{Q} \qquad A(U_0, \Phi)$$

$$Q + U_S WHC_{up} = u_d WLC + U_S WHC$$



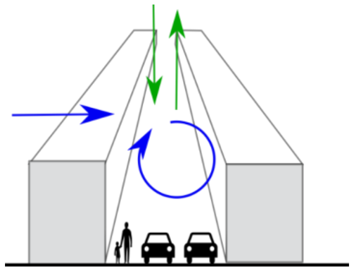
Longitudinal mean velocity in a street canyon

$$U_S \propto u_*$$



Vertical exchange velocity at roof level

$$u_d \propto \sigma_w \propto u_*$$



$$U_S, u_d \propto u_* \propto U \longrightarrow A \propto \frac{1}{U}$$

$$A(U, \Phi) = \frac{U_0}{U} A_0(\phi)$$

Dispersion matrix for a general wind intensity

Wind speed correction

I. Construction of one matrix $A_0(\Phi)$ for **single wind intensity** U_0
II. Construction of matrix $A(U, \Phi)$ using wind correction:

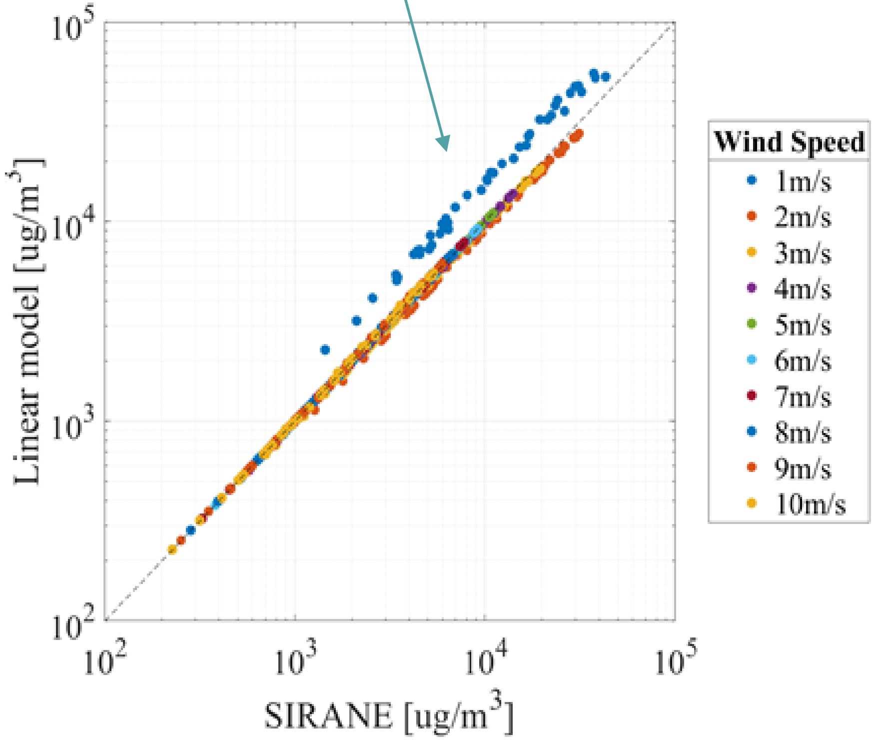
$$A(U, \Phi) = \frac{U_0}{U} A_0(\phi)$$

III. Random n emissions **Q** and find **C** with **linear model**:

$$\boldsymbol{C} = A\boldsymbol{Q}$$

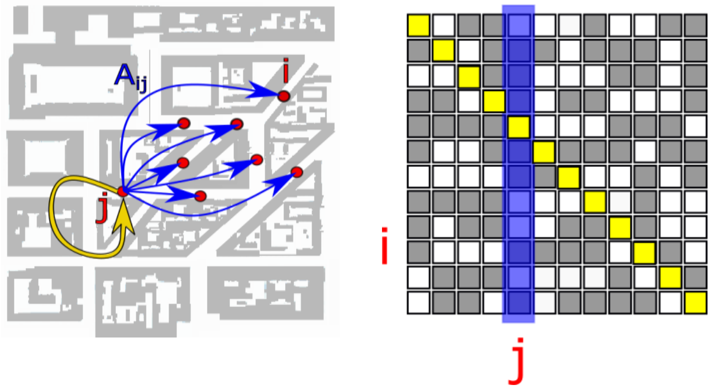
IV. Simulations with **SIRANE** for same **Q** *and simulating different* U
V. **Comparison** of concentrations
VI. For each U simulations are **repeated** for different wind directions Φ

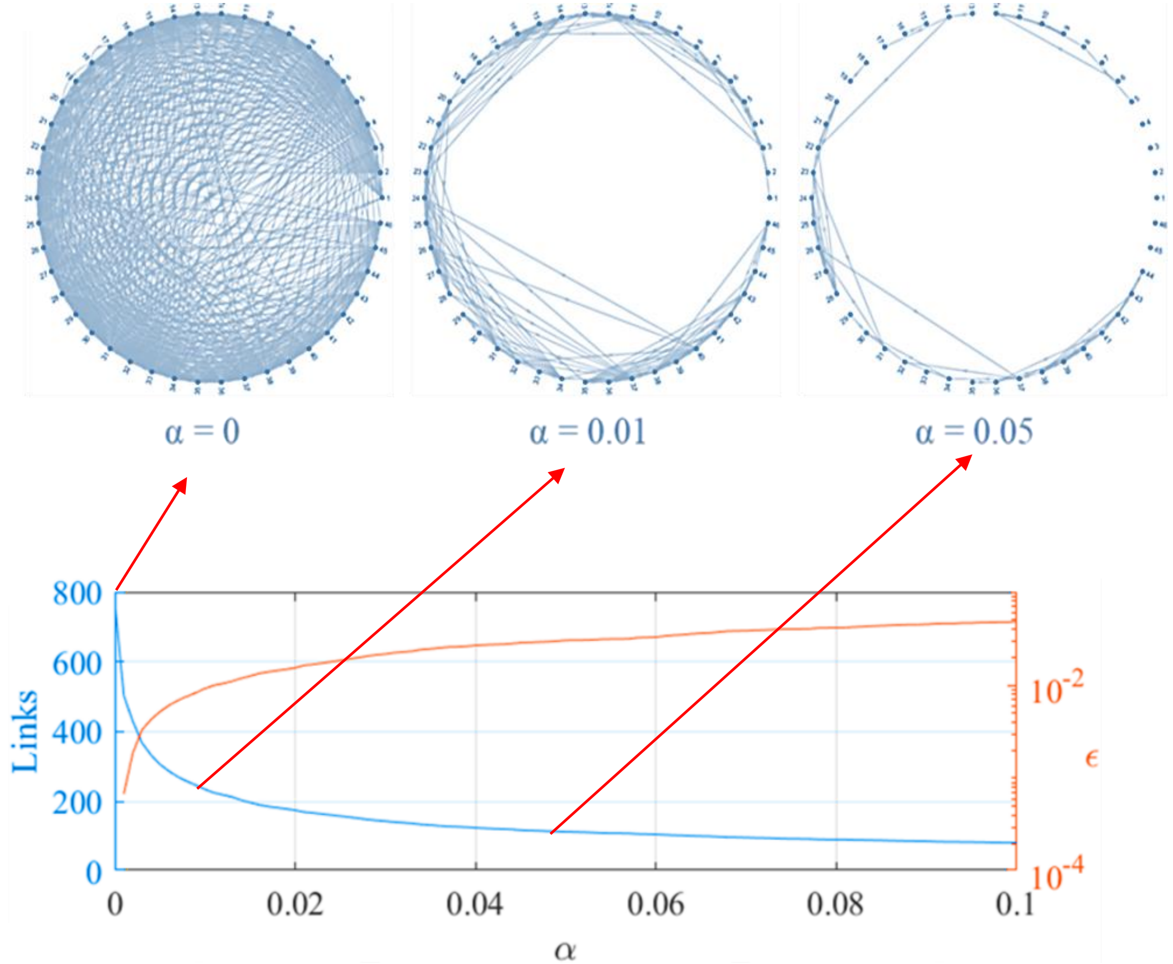
SIRANE prescribes a minimum u_*



! Once a single matrix $A_0(\Phi)$ is built, all the possible emission scenarios in the city can be easily computed also for different wind intensities!

Reducing network complexity





Simplified matrix $\breve{A}$

$$\breve{A}_{ij} = \begin{cases} A_{ij}, & if\ A_{ij} > \alpha \left(\prod_{1}^{N} A_{ii} \right)^{\frac{1}{N}} \\ 0, & \text{otherwise} \end{cases}$$

Error in reducing complexity

$$\epsilon = \frac{\|\boldsymbol{C} - \breve{\boldsymbol{C}}\|_2}{\|\boldsymbol{C}\|_2} = \frac{\|(A - \breve{A})\boldsymbol{Q}\|_2}{\|A\boldsymbol{Q}\|_2} \approx \frac{\|A - \breve{A}\|_2}{\|A\|_2}$$

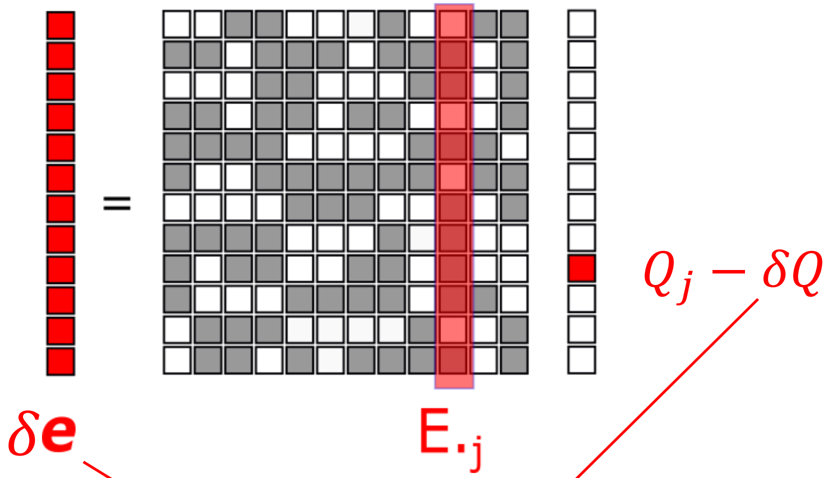
! The number of links in the network can be severely reduced without significantly alter the results.

Where to reduce emissions?

Perturbation of emission-exposure model

$$\boldsymbol{e} = q\boldsymbol{p} \circ \boldsymbol{C} = q\boldsymbol{p} \circ A\boldsymbol{Q} = E\boldsymbol{Q}$$

$$\delta\boldsymbol{e} = E\delta\boldsymbol{Q}$$

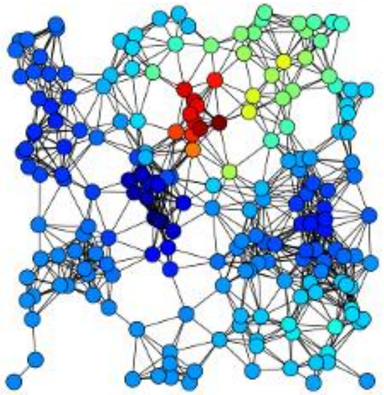


$$R_j = -\sum_i \delta e_i = \delta Q \boxed{\sum_i E_{ij}}$$

Outdegree of node j

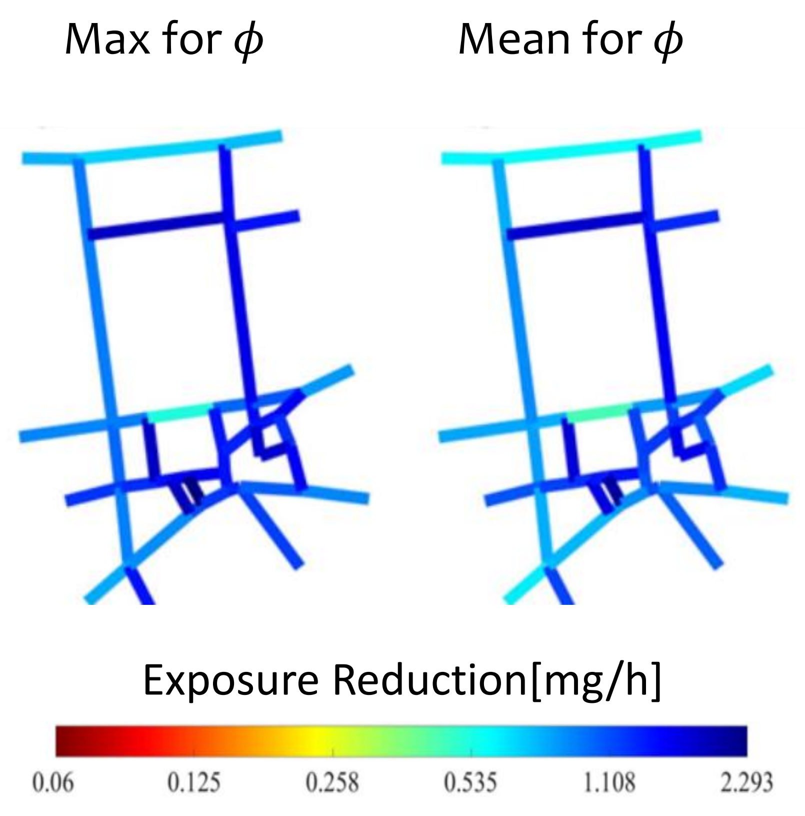
Total exposure reduction obtained by reducing emission in **street j**

OUTDEGREE in NETWORK SCIENCE



Where to reduce emissions?

$$R_j = -\sum_i \delta e_i = \delta Q \sum_i E_{ij}$$

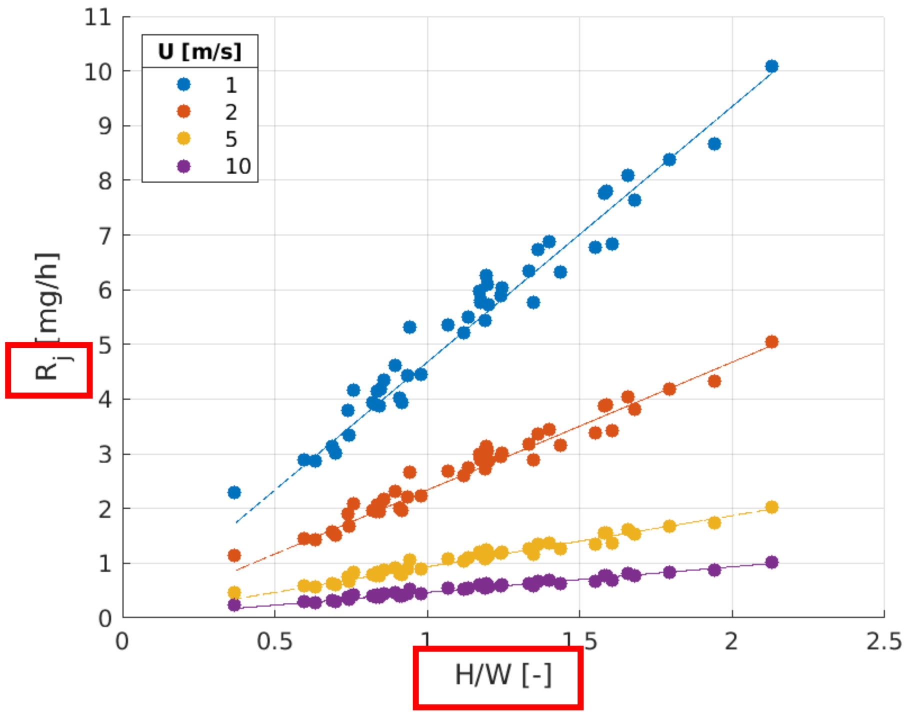


Weak dependence on wind direction since A is diagonally dominant

$$R_i \approx \delta Q\, E_{ii} = \delta Q\, q\, p_i\, A_{ii} = \delta Q\, q\, p_i \frac{U_0}{U} A_{0,ii}$$

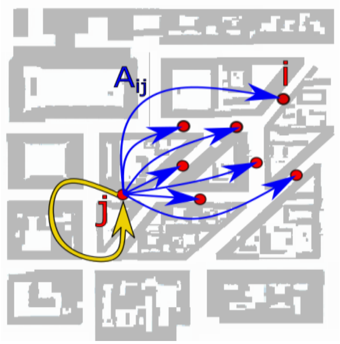
$$Q_i + U_{S,i} W_i H_i C_{i,up} = u_{d,i} W_i L_i C_i + U_{S,i} W_i H_i C_i \longrightarrow A_{0,ii} = \frac{1}{u_d W L}$$

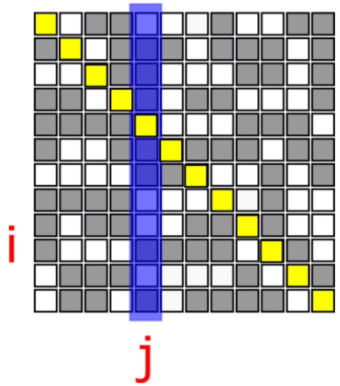
$$R_i \approx \delta Q E_{ii} = \frac{U_0}{U} \frac{\delta Q\, q\, n_{TOT}}{u_{d0} \sum_j H_j L_j} \frac{H_i}{W_i}.$$



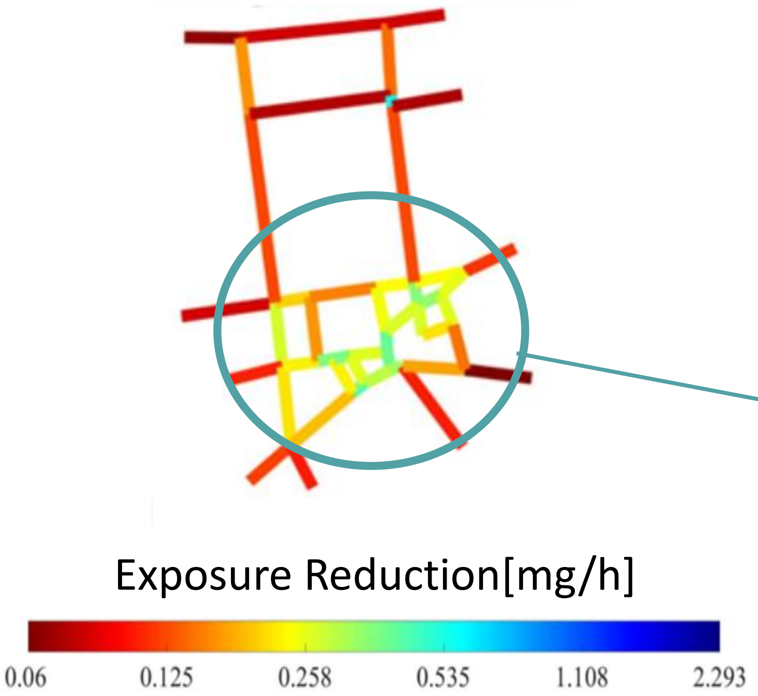
Where to reduce emissions?

Consider all the connections except the self-interactions





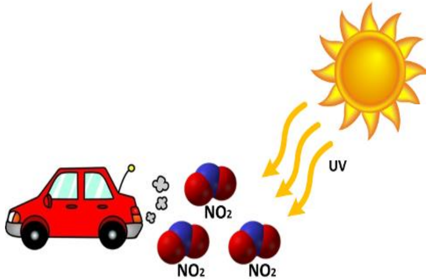
Mean for ϕ
(no self-interactions)



$$R_j = -\sum_i \delta e_i = \delta Q \sum_i E_{ij}$$

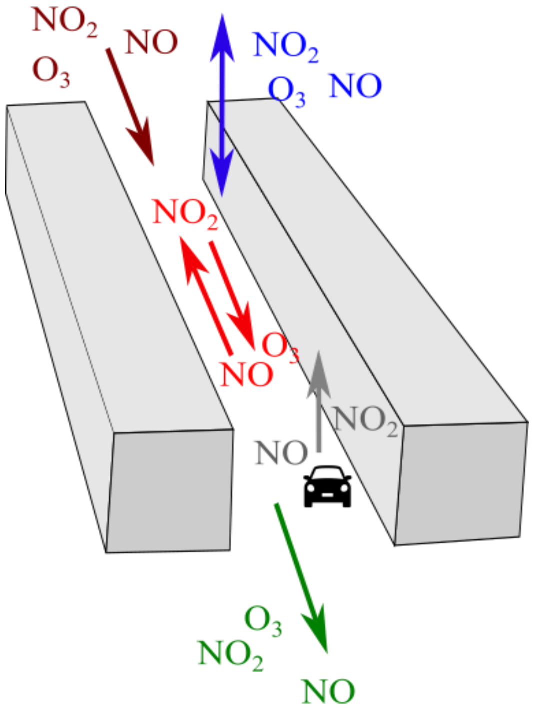
Strong interconnectivity

Extension to photochemical smog



- Driven by solar radiation
- Due to traffic emissions (NO_x)
- Irritate the eyes and the respiratory tract
- Complex chemical reactions that can be simplified in the $NO_2 - NO - O_3$ cycle

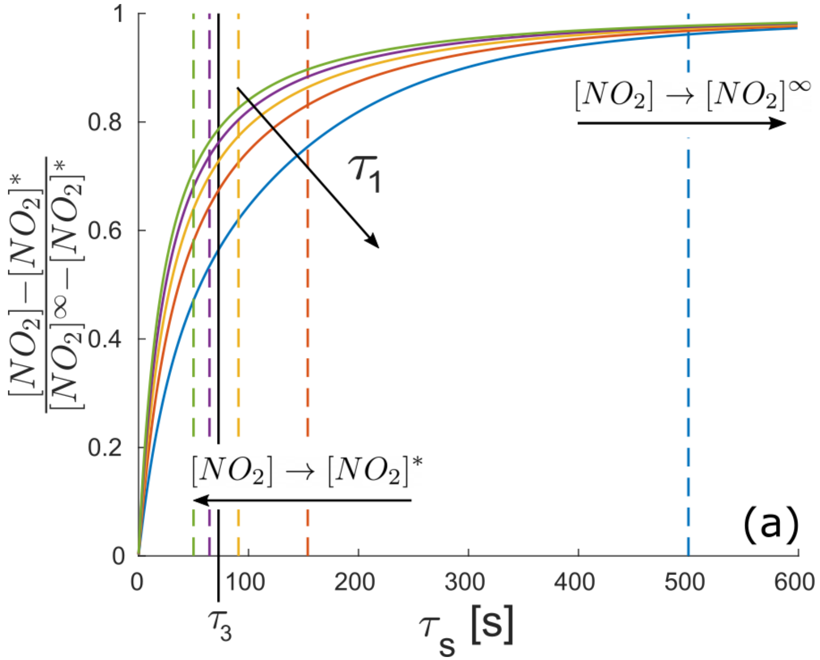
$$\begin{cases} NO_2 + h\nu \xrightarrow{k_1} NO + O\bullet \\ O\bullet + O_2 \xrightarrow{k_2} O_3 \\ NO + O_3 \xrightarrow{k_3} NO_2 + O_2 \end{cases}$$



PHOTOSTATIONARY ASSUMPTION

The **timescales of chemical reactions** are very short compared to the **timescales of turbulent transport.**

Chemical reactions can be applied **after** transport.



Soulhac, Lionel, et al. "Evaluation of Photostationary and Non-Photostationary Operational Models for NOX Pollution in a Street Canyon." Atmospheric Environment 297 (2023): 119589.

Extension to photochemical smog

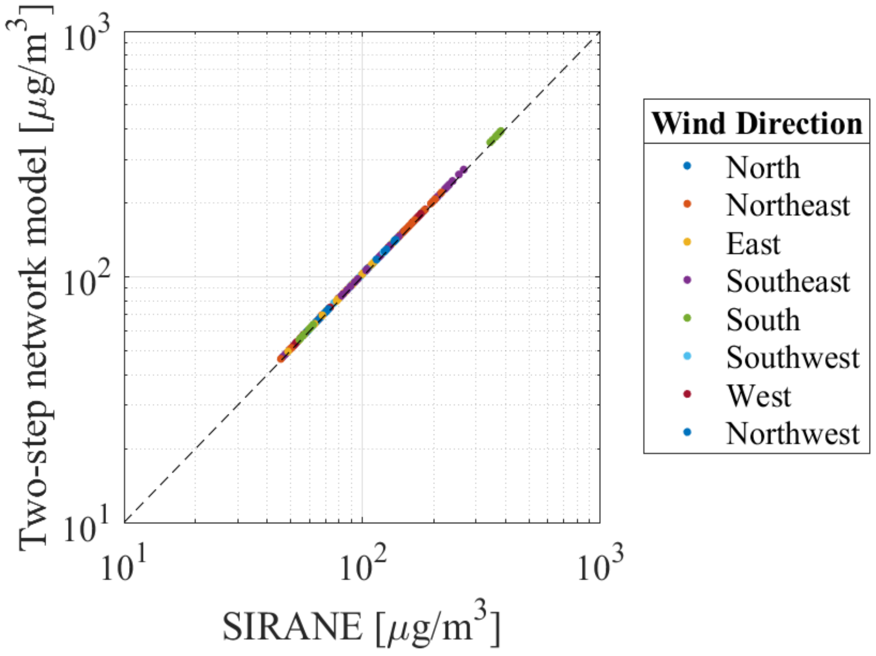
I. TRANSPORT as PASSIVE SCALARS

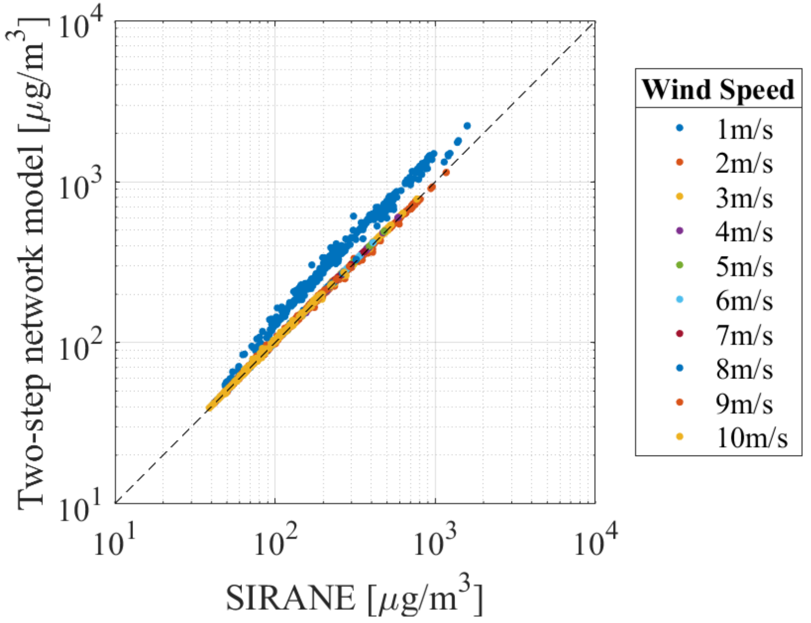
$$\widetilde{\boldsymbol{C}}_{NO_2} = A\boldsymbol{Q}_{NO_2},$$
$$\widetilde{\boldsymbol{C}}_{NO} = A\boldsymbol{Q}_{NO},$$
$$\widetilde{\boldsymbol{C}}_{O_3} = A\boldsymbol{Q}_{O_3}$$

II. NULL-CYCLE **CHEMISTRY**

$$\boldsymbol{C} = \boldsymbol{f}(\widetilde{\boldsymbol{C}}) = \boldsymbol{g}(\widetilde{\boldsymbol{C}}_{NO_X})$$

III. COMPARISON WITH SIRANE
SIMULATIONS FOR DIFFERENT WIND DIRECTIONS AND WIND INTENSITIES (ADOPTING VELOCITY CORRECTION)





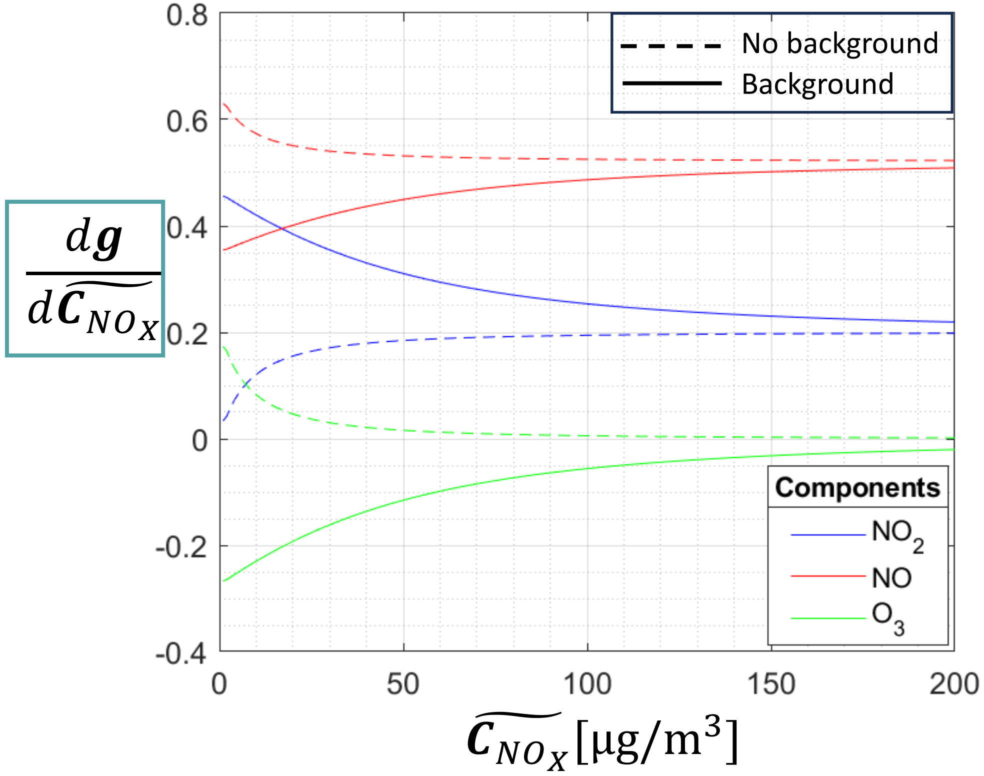
! Multiple scenarios of chemical pollutant dispersion can be achieved starting from a single transport matrix A

Where to reduce emissions considering chemical reactions?

Perturbation of emission-exposure model

$$\boldsymbol{e} = q\boldsymbol{p} \circ \boldsymbol{C} = q\boldsymbol{p} \circ A\boldsymbol{Q} = E\boldsymbol{Q} \longrightarrow \boldsymbol{e} = q\boldsymbol{p} \circ \boldsymbol{C} = q\boldsymbol{p} \circ f(\widetilde{\boldsymbol{C}}) = q\boldsymbol{p} \circ f(A\boldsymbol{Q})$$

$$\delta\boldsymbol{e} = E\delta\boldsymbol{Q} \longrightarrow \delta\boldsymbol{e} = q\boldsymbol{p} \circ \delta\boldsymbol{C} = q\boldsymbol{p} \circ \delta\boldsymbol{f}(\widetilde{\boldsymbol{C}}) = q\boldsymbol{p} \circ \delta\boldsymbol{f}(A\boldsymbol{Q})$$



TAYLOR SERIES EXPANSION

$$\delta\boldsymbol{e} = \boldsymbol{e} - \boldsymbol{e_0} \approx q\boldsymbol{p} \circ \frac{\partial \boldsymbol{f}}{\partial \widetilde{\boldsymbol{C}}} A\delta\boldsymbol{Q}$$

$$\delta\boldsymbol{e} = E\delta\boldsymbol{Q} \quad \text{where} \quad E = q\boldsymbol{p} \circ \frac{\partial \boldsymbol{f}}{\partial \widetilde{\boldsymbol{C}}} A$$

$$\frac{\partial \boldsymbol{f}}{\partial \widetilde{\boldsymbol{C}}} = \frac{d\boldsymbol{g}}{d\widetilde{\boldsymbol{C}_{NO_X}}} \left((\boldsymbol{1} - \boldsymbol{a}) \ \frac{\boldsymbol{M_{NO}}}{\boldsymbol{M_{NO_2}}} \ \boldsymbol{a} \ \boldsymbol{0}\right)$$

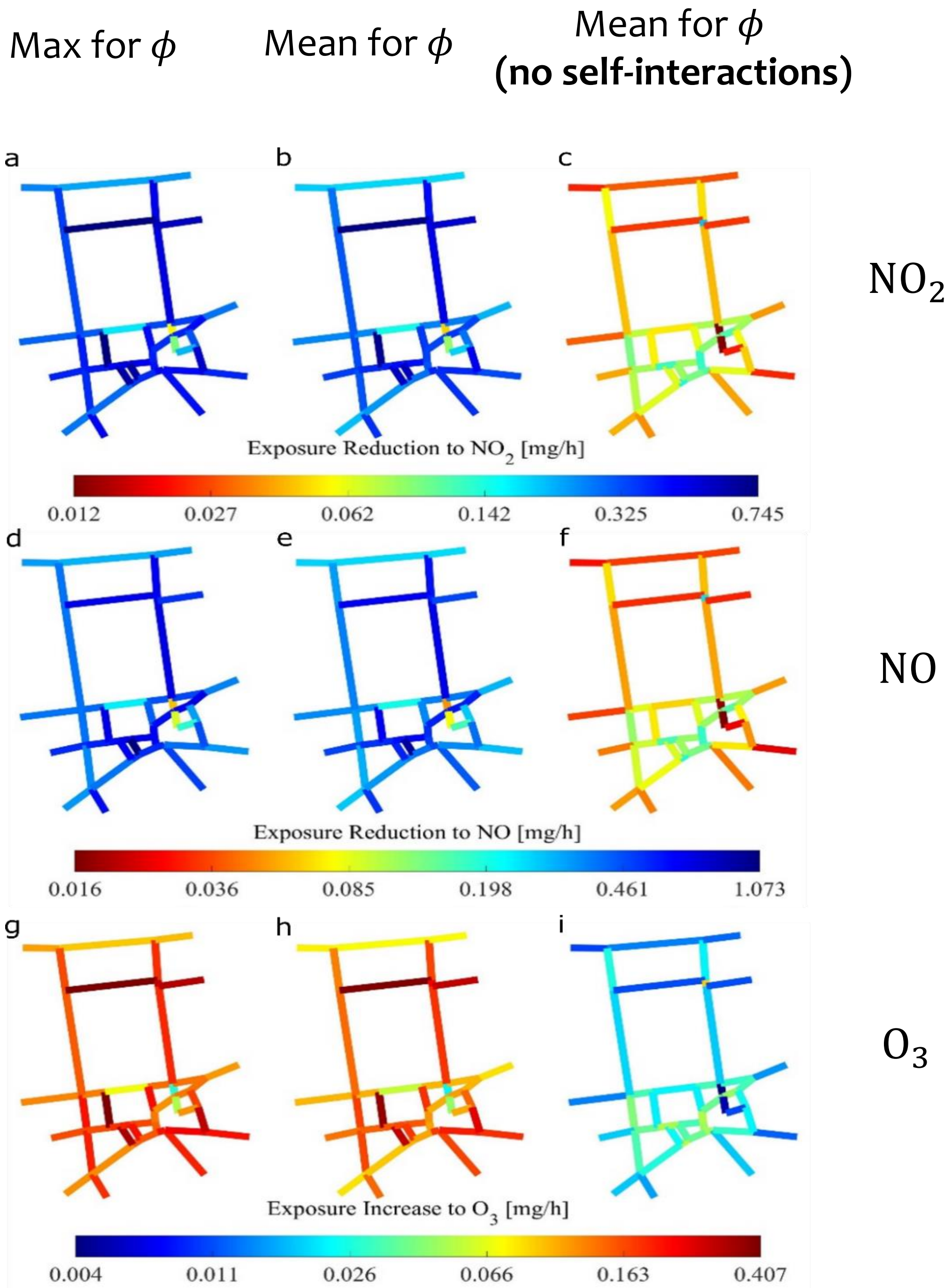
When the emitted and avected nitrogen oxides ($\widetilde{NO_x}$) are large, the relation between before-after reaction concentrations is almost **linear**

Where to reduce emissions?

Exposure Reduction/Increase[mg/h] to NO_2, NO, O_3 by decreasing the emission of NO_2, NO (NO_x)

$$R_j = -\sum_i \delta e_i$$

- Exposure reductions are **linear functions** of the passive scalar case
- A reduction in NO_x emission is responsible for a **concentration increase** of ozone



Conclusions

I. MULTIPLE SCENARIOS FROM A SINGLE TRANSPORT MATRIX (A)

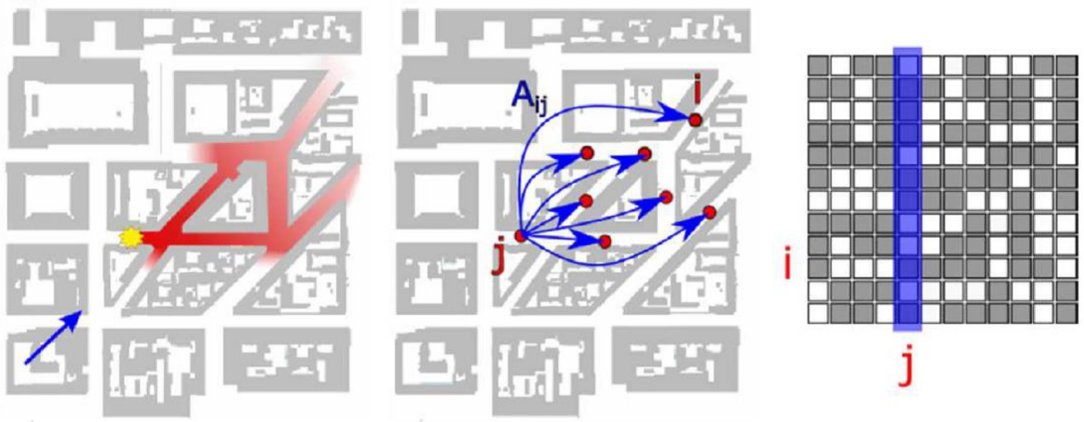
II. LINEAR SCALING FOR VELOCITY INTENSITY

III. NETWORK REDUCTION

IV. OUTDEGREE OF EXPOSURE MATRIX (E) PROVIDES BEST PLACE WHERE TO REDUCE EMISSIONS

V. EXTENSION TO CHEMISTRY

VI. SIMPLE AND MODULAR MODEL



and perspectives…

I. TRANSPORT MATRIX (A) FROM LES SIMULATIONS

II. TEST FOR DIFFERENT STABILITY CONDITIONS AND CHEMICAL MODELS

III. BETTER EXPOSURE MODEL