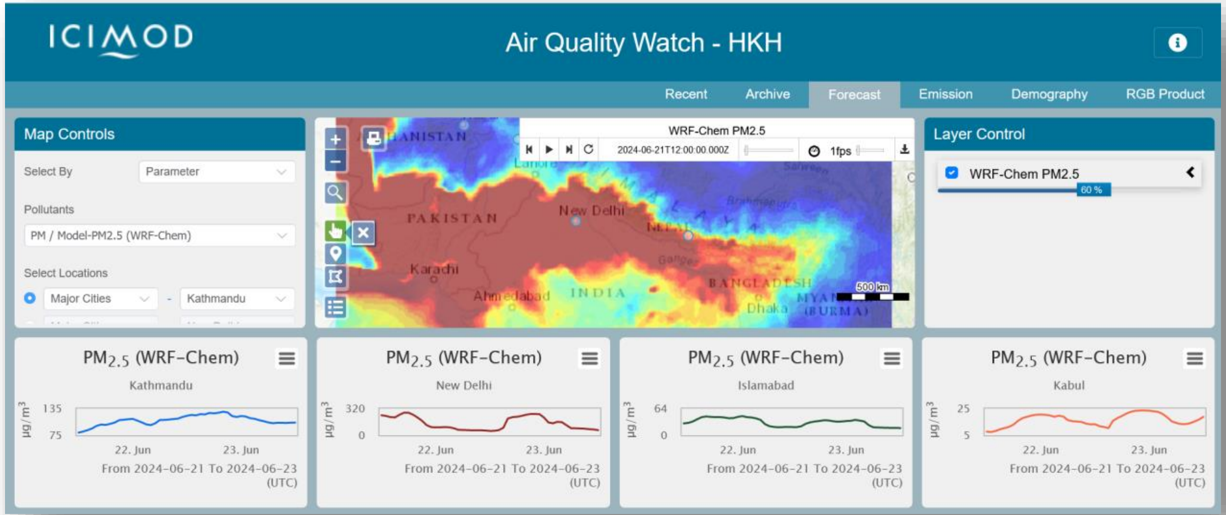
ICIMOD

Air Quality Modelling

Bertrand Bessagnet (PhD Habil.)
Action Area Coordinator – Air Quality

Models in the Air Quality Management strategy

- **Modelling** as one of the pillars of the management strategy (with Emissions and Observations)
- Models are used for Forecasting, Assessment of Mitigation strategies, Planning, Policy support
- Different models:
  - **Air Quality models**: use Emission models, Meteorological Models
  - **Metamodels** : a simplification of complex models
  - **Integrated models**: Simulate the full chain from emissions to impacts



Different types of models

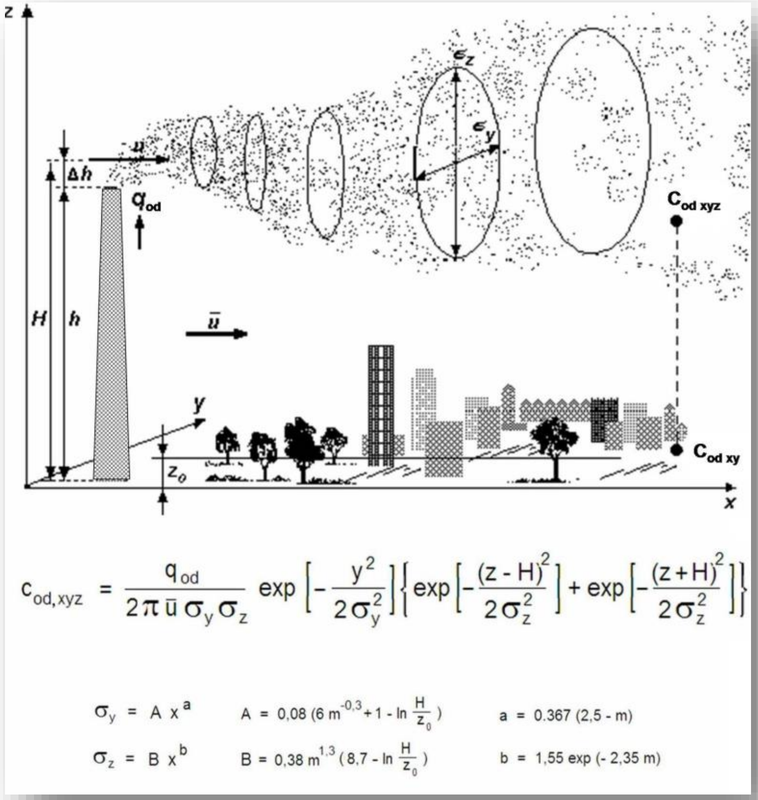
- ➢Lagrangian models of atmospheric dispersion
- ➢**Eulerian models of atmospheric dispersion (Chemistry Transport Model)**
- ➢Gaussian models
- ➢Street-canyon models (ADMS, SIRANE)

Chemistry Transport Model

- *WRF-Chem*
- *CHIMERE*
- *CMAQ*
- *CAMx*
- *LOTOS*

- *MOZART*
- *GEOS-Chem*

Gaussian models



Chemistry Transport Models (CTM)

Input

Emissions

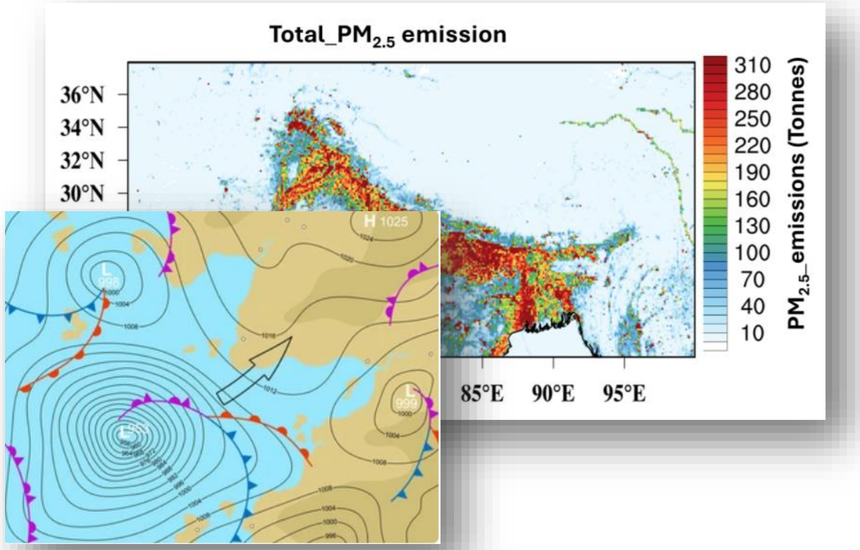
Meteorology

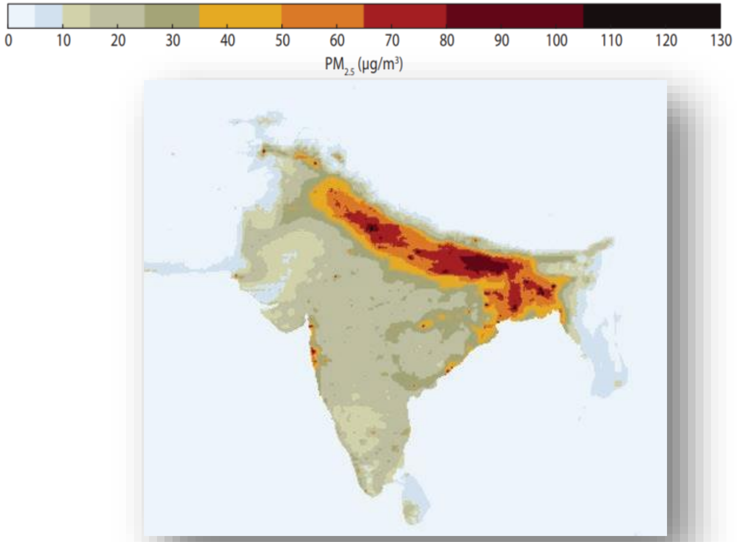
Chemistry Transport Model

Ouput

Concentrations PM2.5, Ozone…

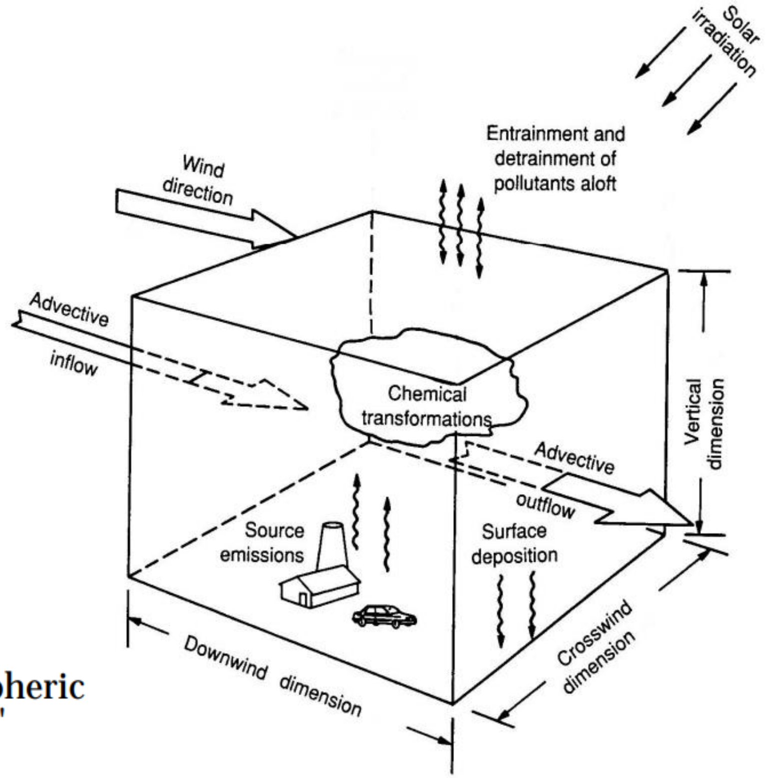
Physics, chemistry processes

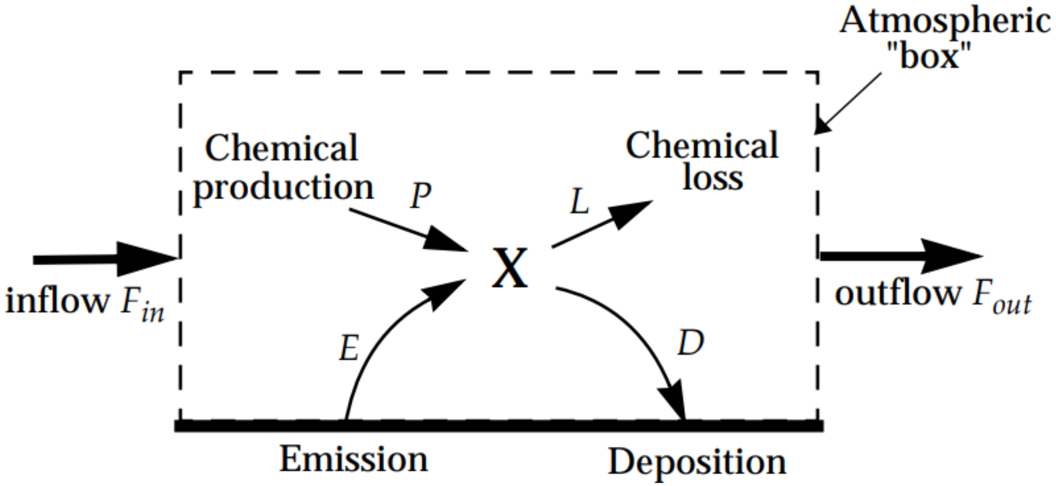




Eulerian models or Chemistry Transport Models

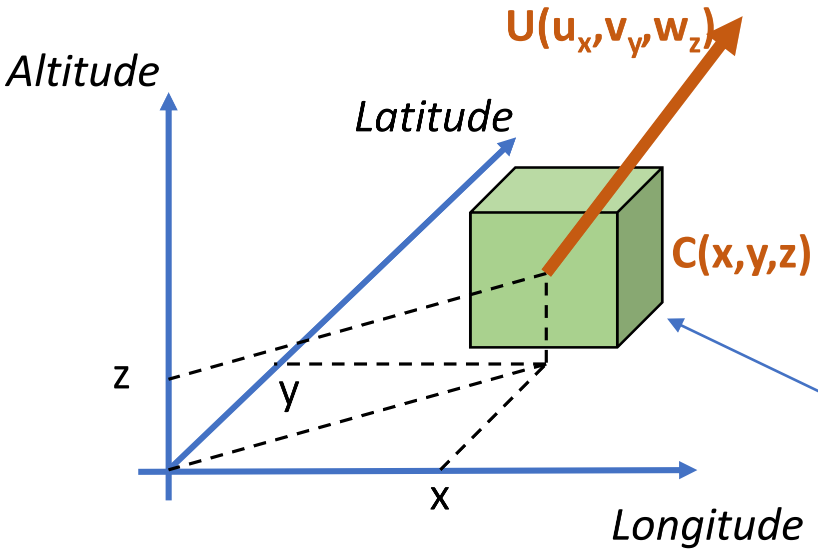
- The chemical-transport equation (also called the atmospheric diffusion equation or the **mass conservation equation**) does not have an analytical solution
- For very simple cases (for example in the case of a steady-state gaussian plume) that are typically not representative of the atmosphere at regional or global scales.
- Therefore, a numerical solution is needed. It is generally solved via a **discretization** of the chemical-transport equation.



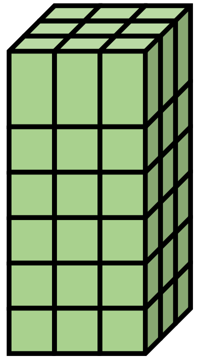


For those who like fundamentals: Base Equation of CTM

$$\overbrace{\frac{\partial C}{\partial t}}^{\text{Concentration change}} = \underbrace{-u\frac{\partial C}{\partial x} - v\frac{\partial C}{\partial x}}_{\text{Horizontal advection}} - \underbrace{w\frac{\partial C}{\partial z}}_{\text{Vertical advection}} + \overbrace{\frac{\partial}{\partial x}\left(k_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(k_y\frac{\partial C}{\partial y}\right)}^{\text{Horizontal diffusion}} + \overbrace{\frac{\partial}{\partial z}\left(k_z\frac{\partial C}{\partial z}\right)}^{\text{Vertical diffusion}} + \overbrace{P - L}^{\text{Chemistry}} + \underbrace{E}_{\text{Emissions}} - \overbrace{D}^{\text{deposition}}$$

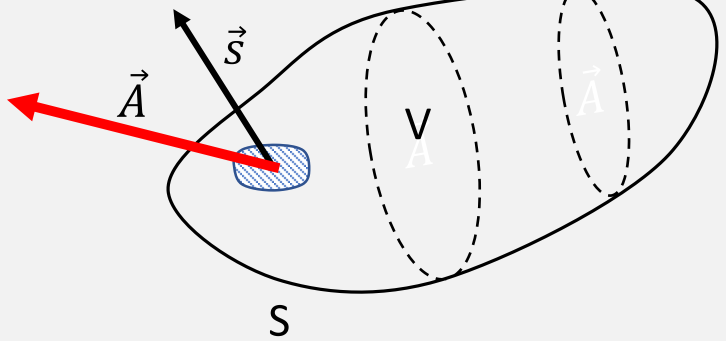


C: concentration
U: wind of components (u,v,w)
k: diffusion (turbulent)
P-L: Production - Loss



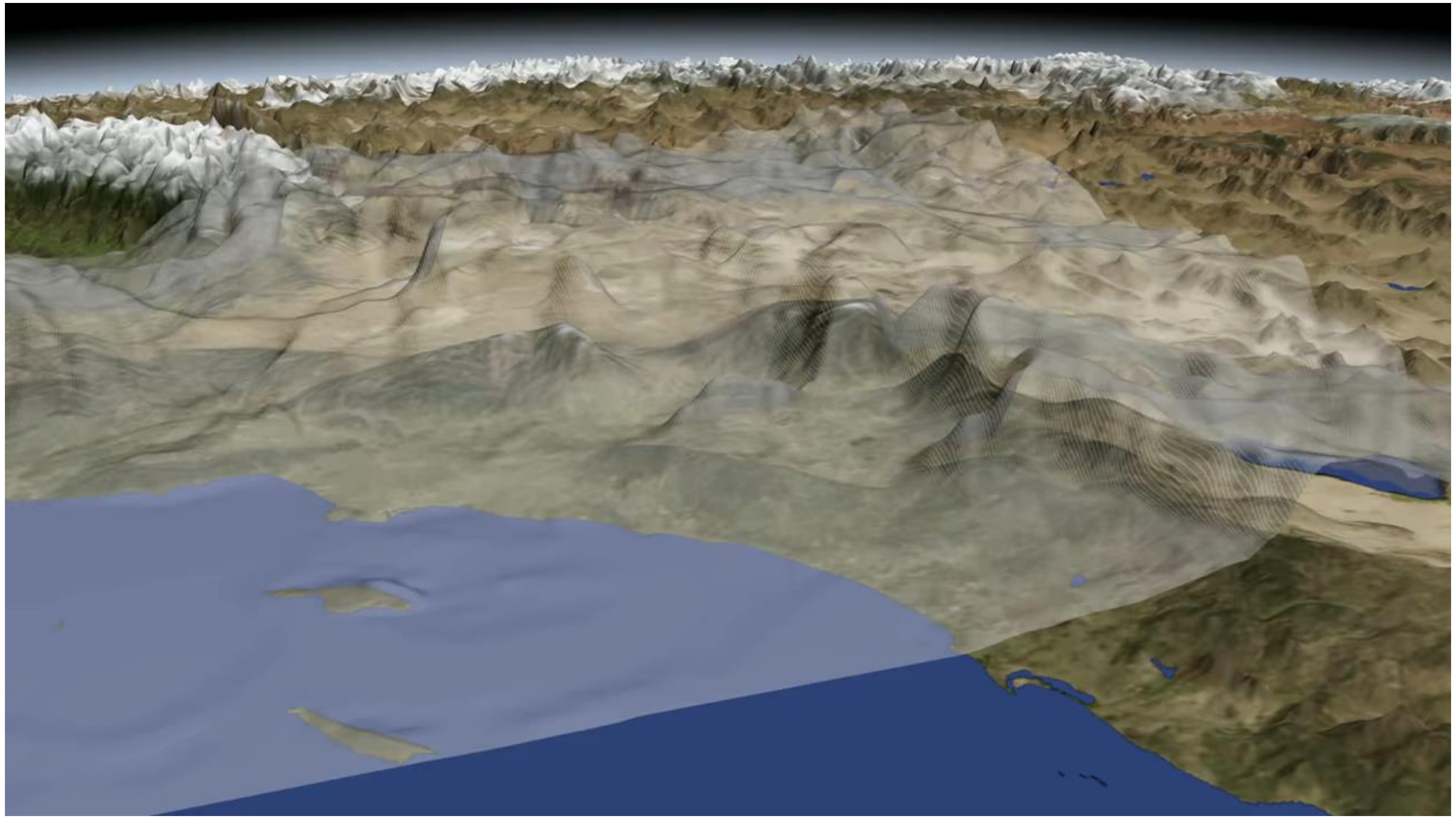
Green Ostrogradski Theorem

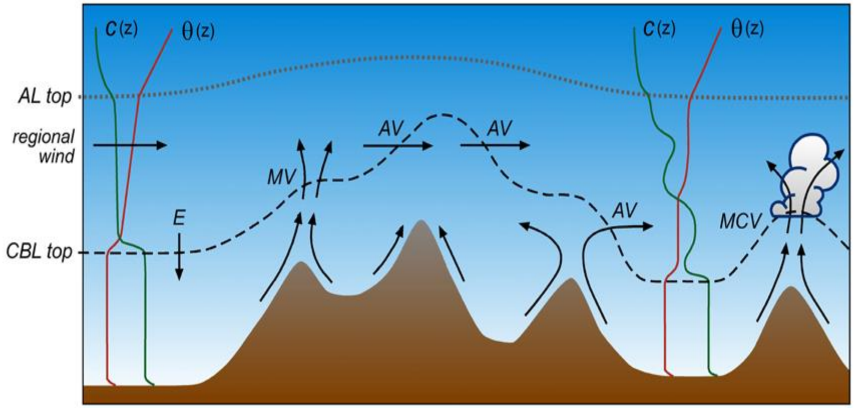
$$\oiint_S \vec{A} \cdot \vec{dS} = \iiint_V \operatorname{div} \vec{A} \cdot dV$$



Planetary boundary Layer (PBL)

- PBL governed by the level of turbulences (influenced by rugosity on the ground, and temperature)
- PBL lower over seas
- PBL maximum in the afternoon

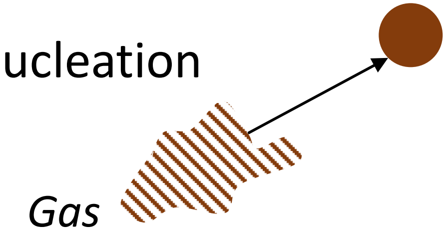




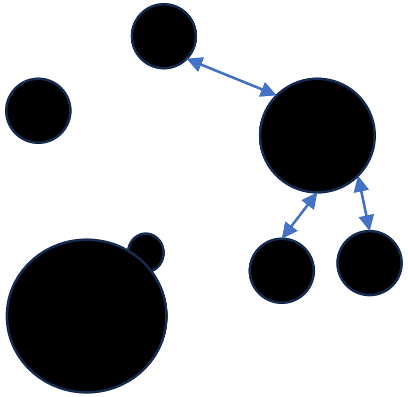
Schematic illustration of mountain induced exchange processes between the convective boundary layer and the overlying atmosphere. E, entrainment; AV, advective venting; MV, mountain venting; and MCV, mountain-cloud venting. Vectors indicate airflow while c(z) and θ(z) indicate vertical profiles of pollutant concentration and potential temperature, respectively. The dotted and dashed line indicate the top of the aerosol layer (AL) and the CBL, respectively

Processes related to particles

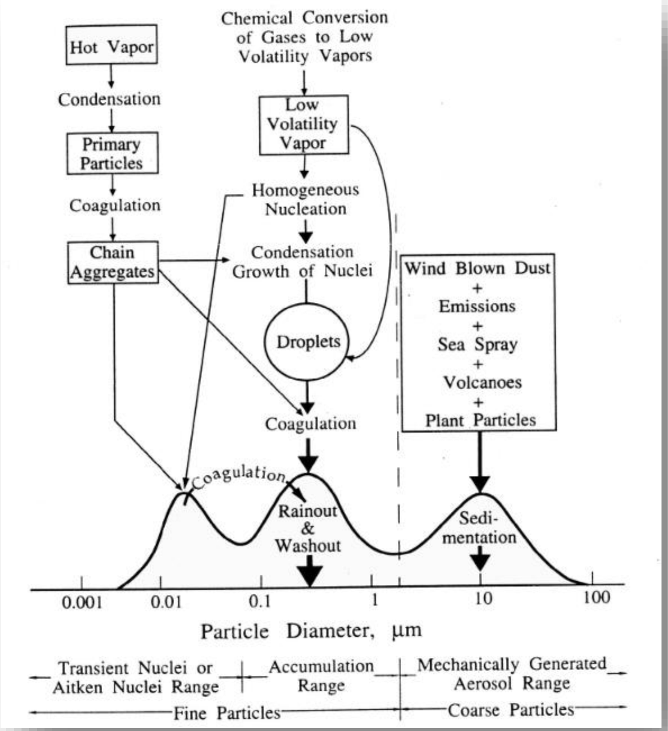
➢ Nucleation



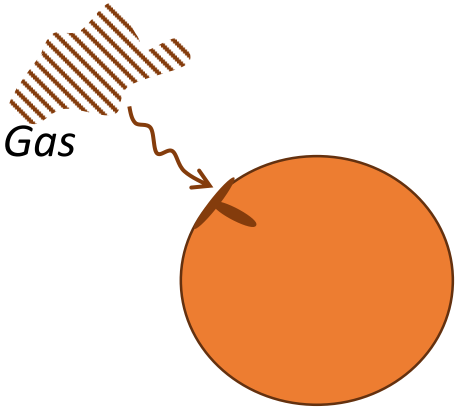
➢ Coagulation/Coalescence



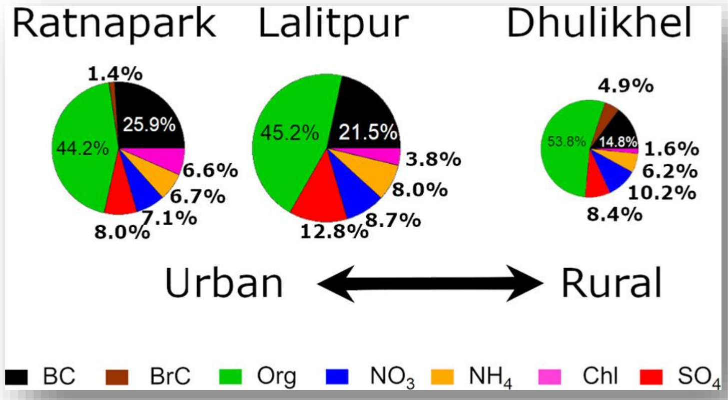
General Size Distribution



➢ Condensation/Absorption



Composition (Werden et al., 2023)



Secondary production of particles

Sulfate

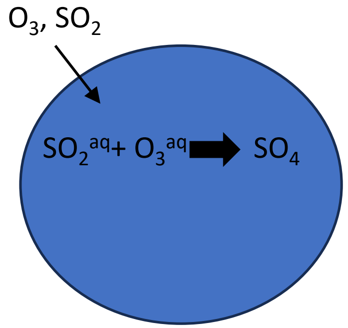
$$SO_2^{aq} + O_3^{aq} \rightarrow SO_4^{2-}$$

$$HSO_3^{-} + O_3^{aq} \rightarrow SO_4^{2-}$$

$$SO_3^{2-} + O_3^{aq} \rightarrow SO_4^{2-}$$

$$SO_2^{aq} + H_2O_2^{aq} \rightarrow SO_4^{2-}$$

$$SO_2^{aq} + NO_2^{aq} \rightarrow SO_4^{2-}$$



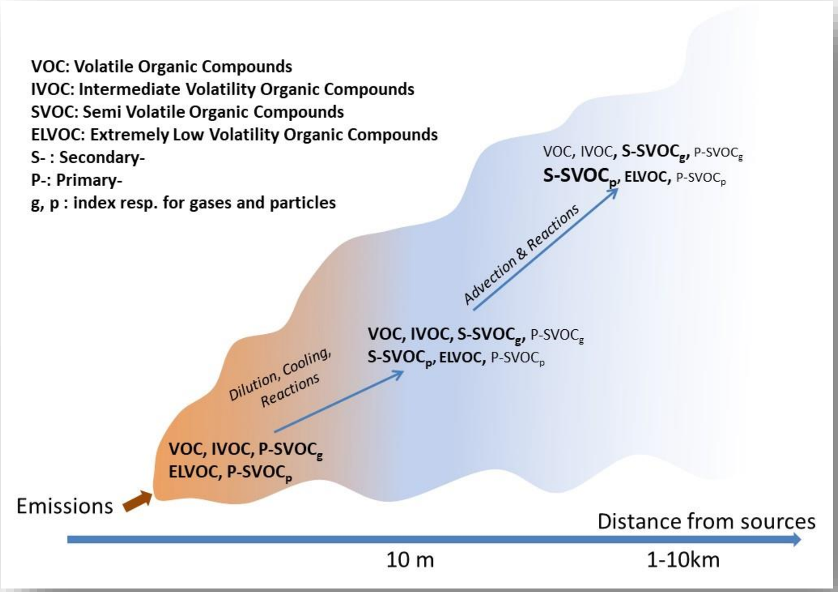
Organics

Reactions	Kinetic rates (*molecules cm*$^{-3}$ *s*$^{-1}$)
TOL+OH → 0.004×AnA0D + 0.001×AnA1D + 0.084×AnBmP + 0.013×AnBlP	1.81×10^{-12}exp(355/T)
TMB+OH → 0.002×AnA0D + 0.002× AnA1D + 0.001×AnA2D + 0.088×AnBmP + 0.006×AnBlP	9.80×10^{-9}/T
NC4H10+OH → 0.07×AnBmP	1.36×10^{-12}exp(190/T)$^{-2}$
API+OH → 0.30×BiA0D + 0.17×BiA1D + 0.10×BiA2D	1.21×10^{-11}exp(444/T)
API+O3 → 0.18×BiA0D + 0.16×BiA1D + 0.05×BiA2D	1.01×10^{-15}exp (−732/T)
API+NO3 → 0.80×BiBmP	1.19×10^{-12}exp(490/T)
BPI+OH → 0.07×BiA0D + 0.08×BiA1D + 0.06×BiA2D	2.38×10^{-11}exp(357/T)
BPI+O3 → 0.09×BiA0D + 0.13×BiA1D + 0.04×BiA2D	1.50×10^{-17}
BPI+NO3 → 0.80×BiBmP	2.51×10^{-12}
LIM+OH → 0.20×BiA0D + 0.25×BiA1D + 0.005×BiA2D	1.71×10^{-10}
LIM+O3 → 0.09×BiA0D + 0.10×BiA1D	2×10^{-16}
TPO+OH → 0.70×BiA0D + 0.075×BiA1D	5.10×$^{-8}$/T
TPO+O3 → 0.50×BiA0D + 0.055×BiA1D	7.50×10^{-14}/T
TPO+NO3 → 0.70×BiA0D + 0.075×BiA1D	4.30×10^{-9}/T
ISO+OH → 0.232×ISOPA1 + 0.0288×ISOPA2	2.55×10^{-11}exp(410/T)

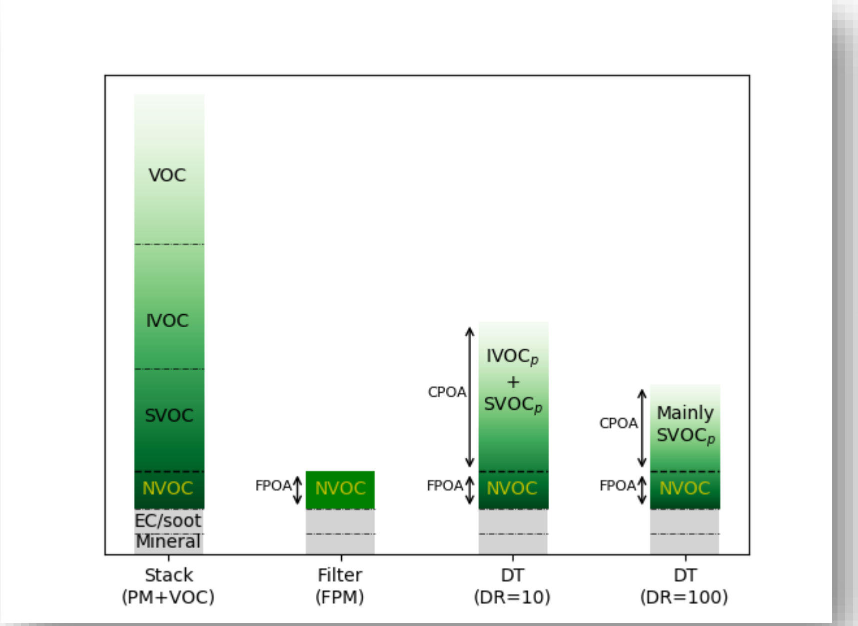
The surrogate SOA compounds consist of six hydrophilic species that include an anthropogenic non-dissociative species (AnA0D), an anthropogenic once-dissociative species (AnA1D), an anthropogenic twice-dissociative species (AnA2D), a biogenic non-dissociative species (BiA0D), a biogenic once-dissociative species (BiA1D) and a biogenic twice-dissociative species (BiA2D), three hydrophobic species that include an anthropogenic species with moderate saturation vapor pressure (AnBmP), an anthropogenic species with low saturation vapor pressure (AnBlP) and a biogenic species with moderate saturation vapor pressure (BiBmP), and two surrogate compounds for the isoprene oxidation products (ISOPA1, ISOPA2). T is the temperature in K.

The issue of Semi Volatile Organic Compounds

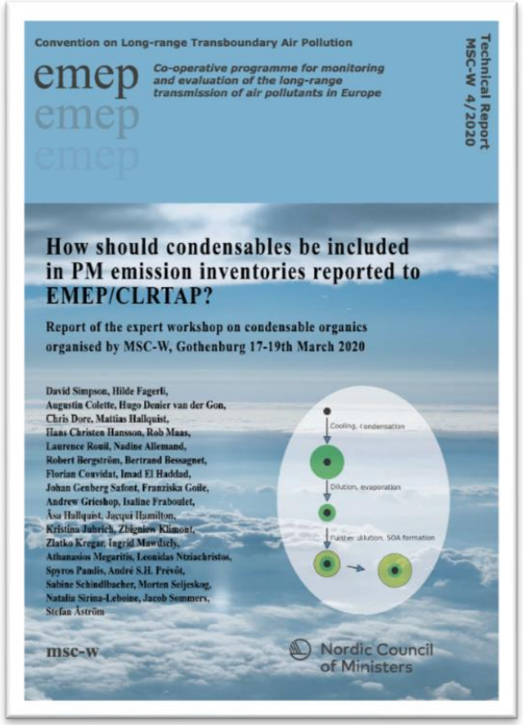
Secondary organic formation



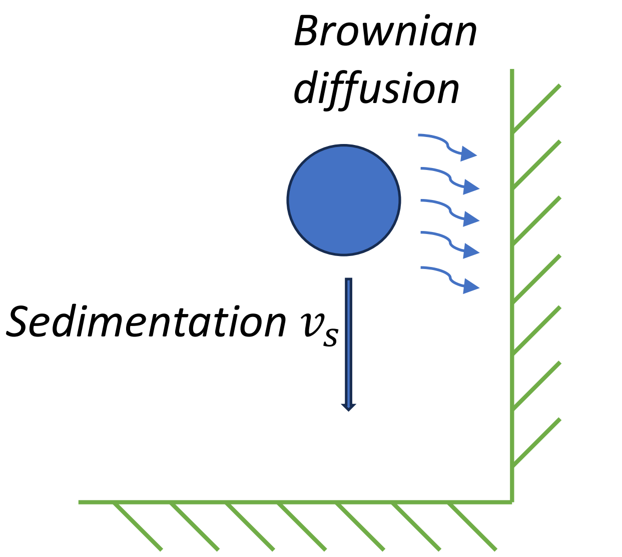
Emissions



Methods to calculate Emission Factors



Dry deposition of particles



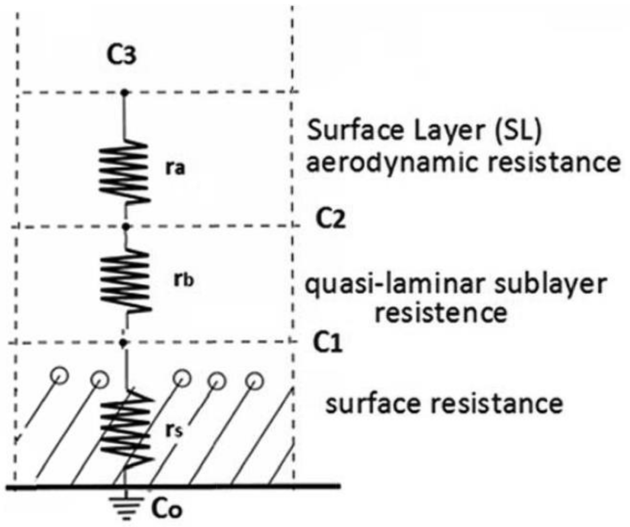
Concept of Deposition Velocity (Vd)

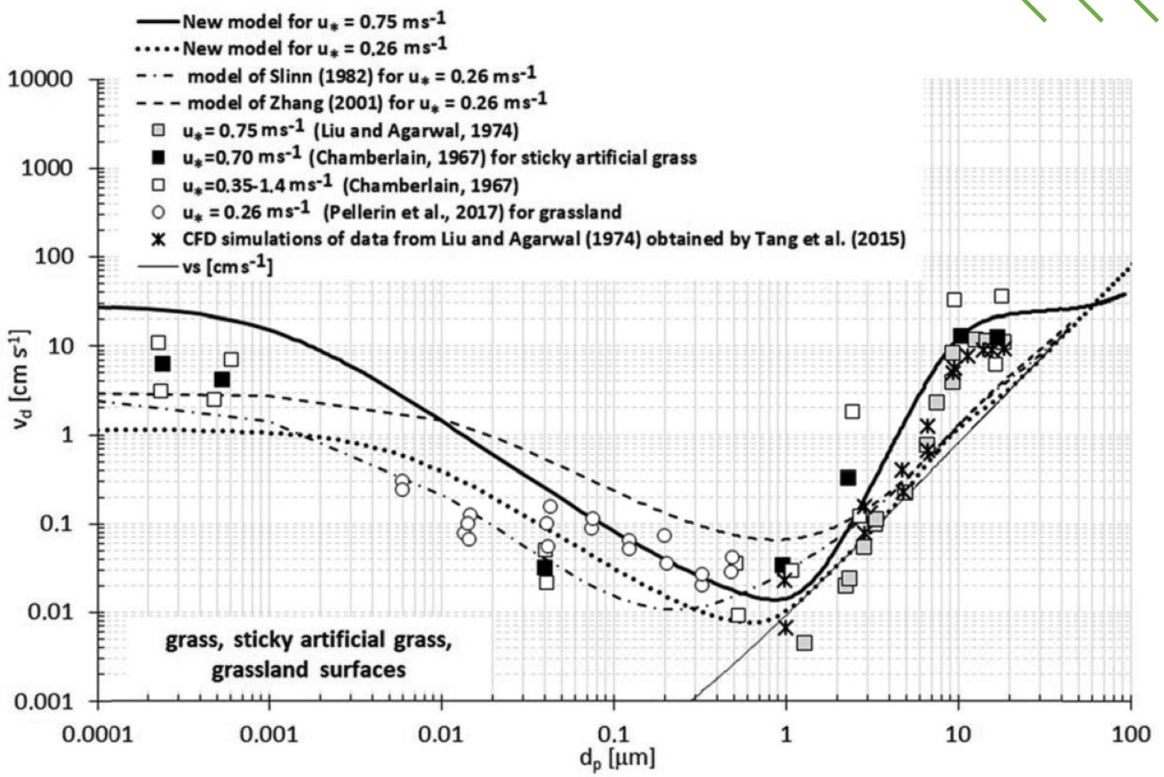
$$F = v_d \times C$$

$$v_d = \frac{1}{r_a + r_s + r_a \times r_s \times v_s} + v_s$$

$$V_S = \frac{\rho_p d_p^2}{18\mu} g$$

Resistance model for gas

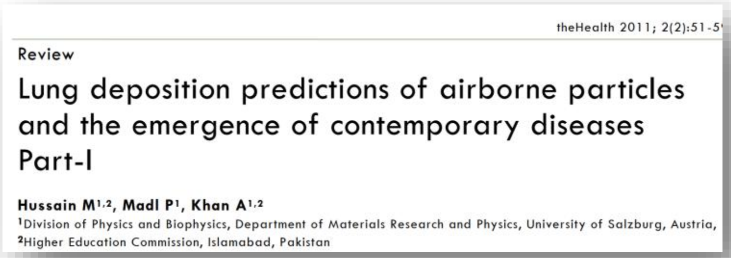


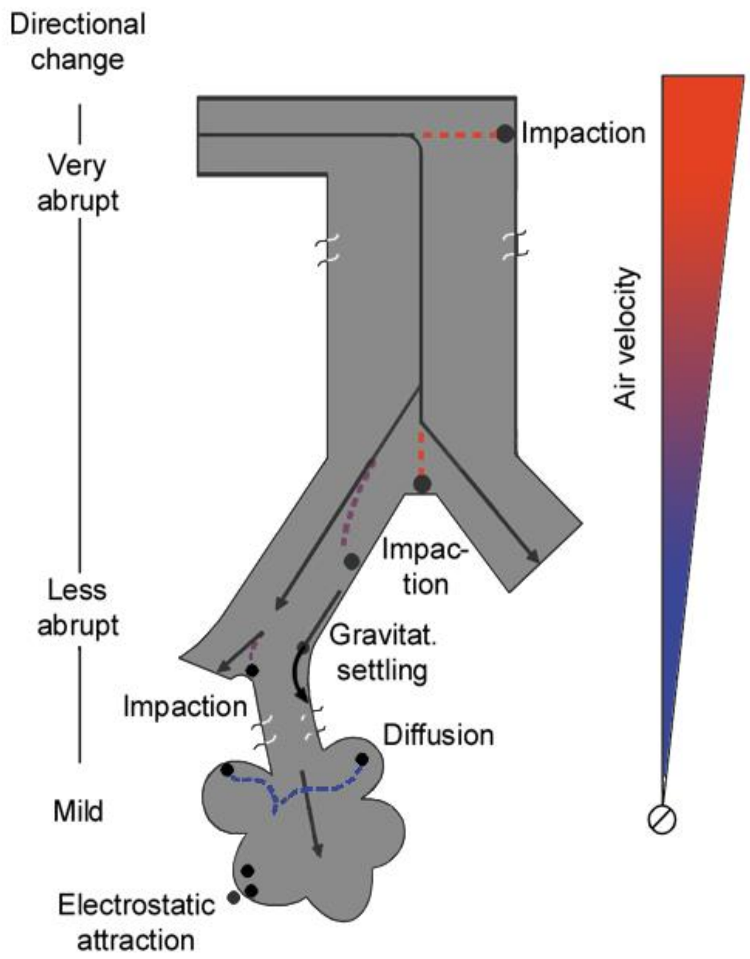


Deposition of particles in the respiratory systems

$$Stk = (\rho_p d_p^2 u)/(18\mu d) \quad (1)$$

where d_p and ρ_p are the particle diameter and density, respectively; u and μ are the mean velocity and dynamic viscosity of the carrier gas, respectively; and d is a characteristic length equal to the diameter of the airway. The higher the Stokes' number, the more efficient the inertial transport and the more likely that particles will deposit by inertial impaction.


theHealth 2011; 2(2):51-5
Review
Lung deposition predictions of airborne particles and the emergence of contemporary diseases Part-I
Hussain M[1,2], Madl P[1], Khan A[1,2]
[1]Division of Physics and Biophysics, Department of Materials Research and Physics, University of Salzburg, Austria,
[2]Higher Education Commission, Islamabad, Pakistan

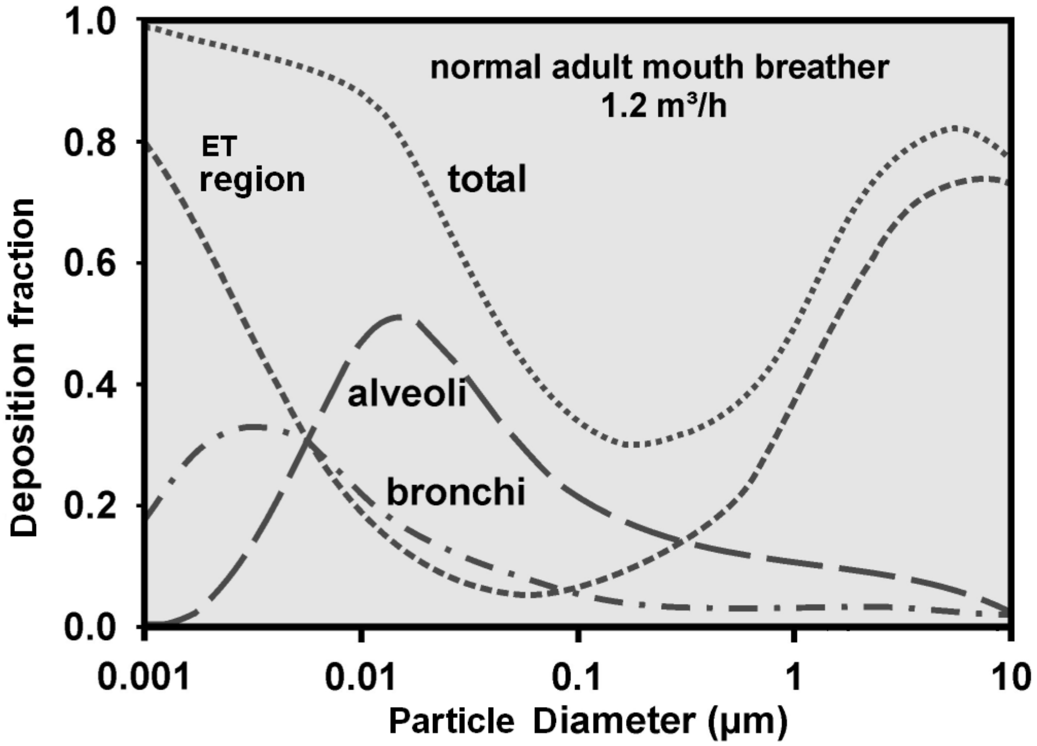


Throat

Bronchi

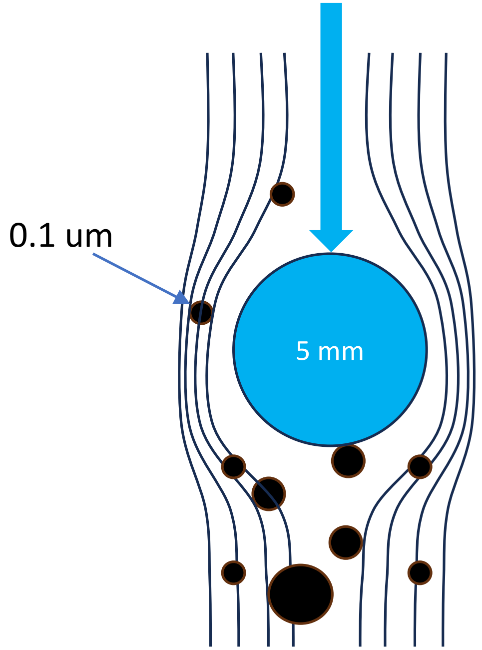
Lung/Alveoli

Average predicted total and regional lung deposition

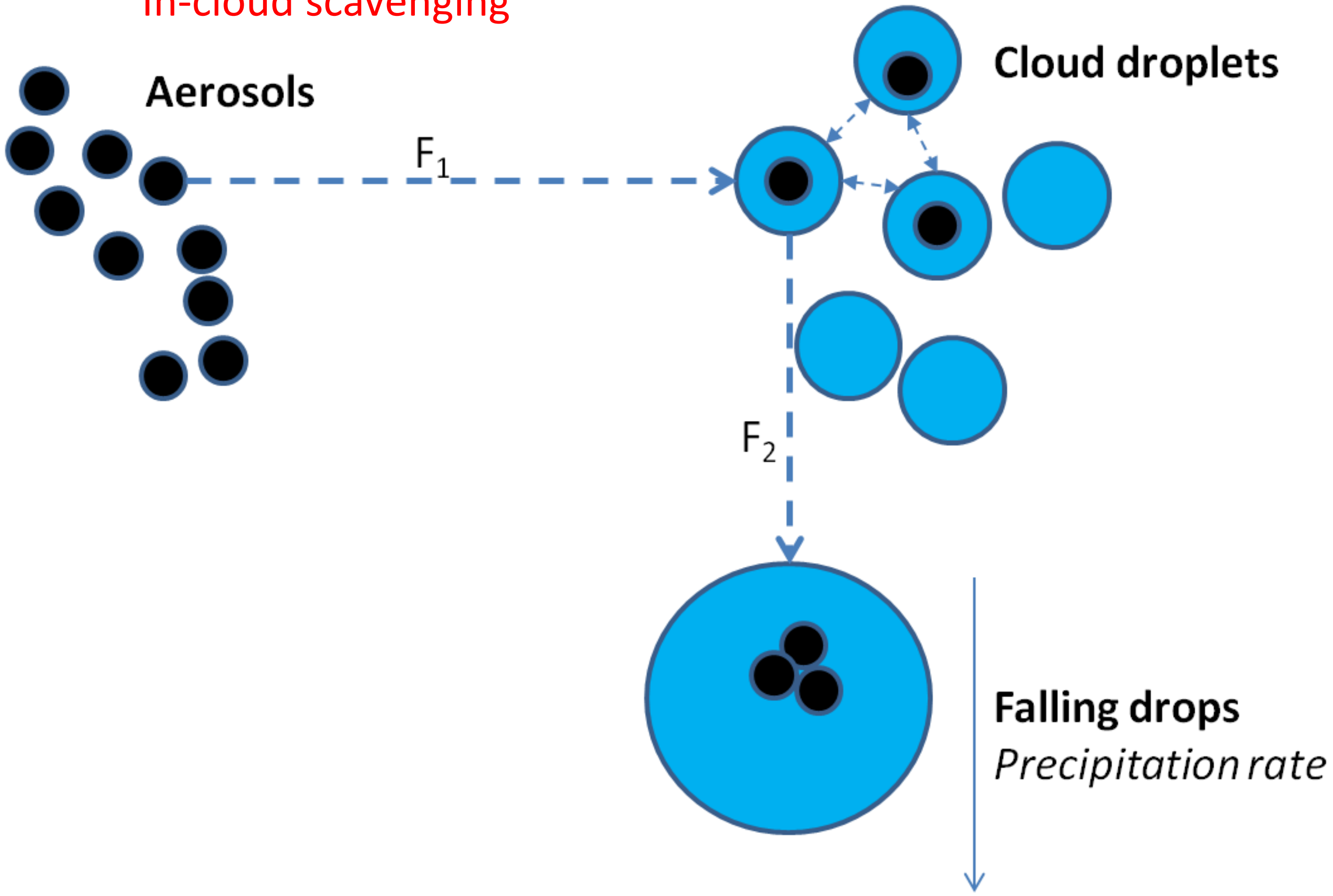


Wet scavenging of particles

Below-cloud scavenging

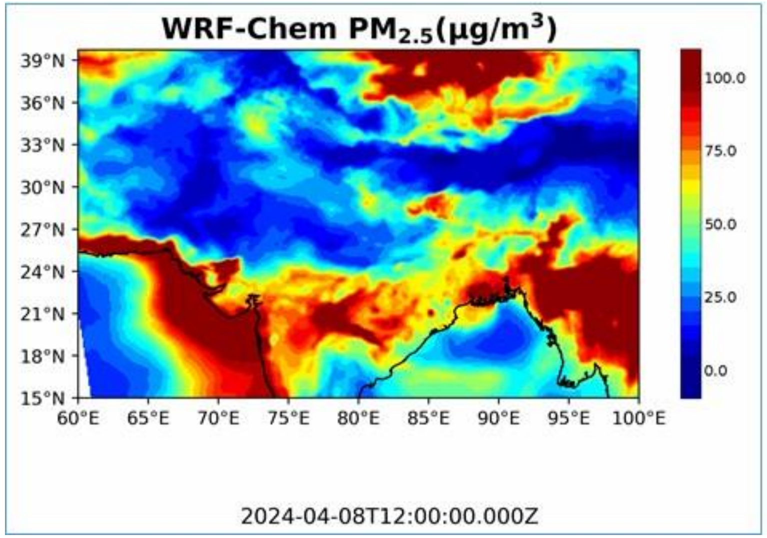


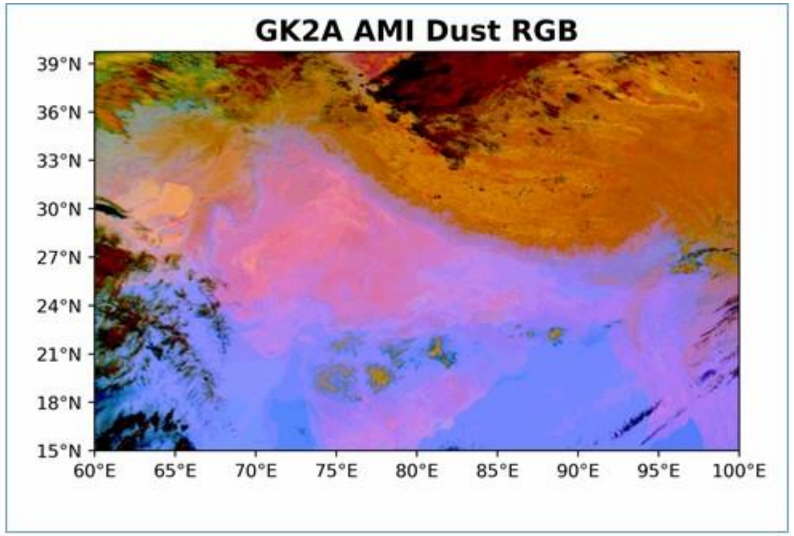
In-cloud scavenging

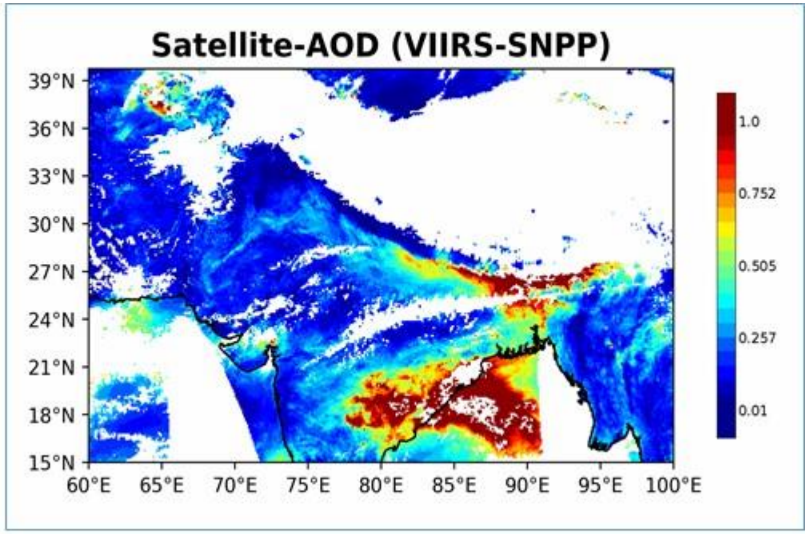


AQ monitoring over HKH at ICIMOD

Air Quality Data Products



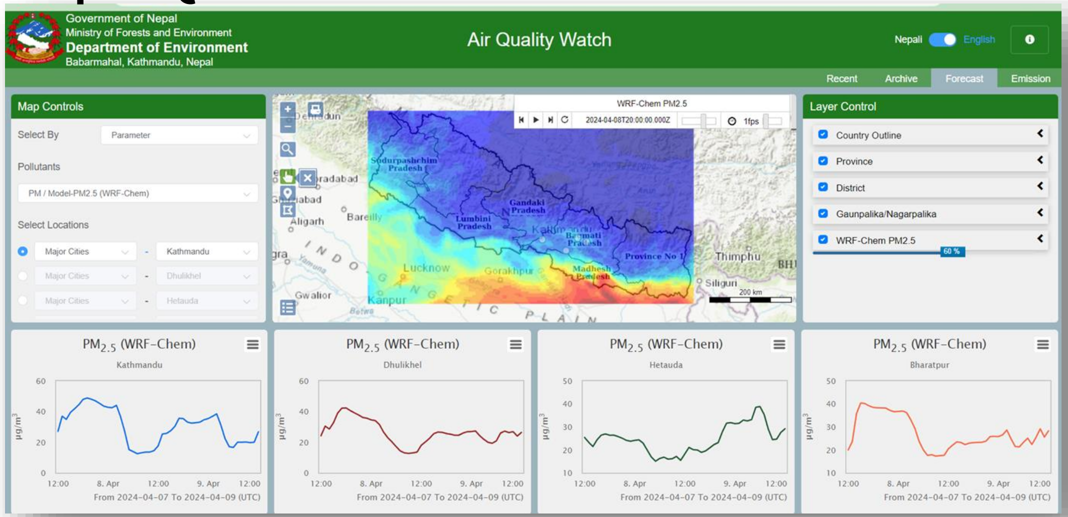




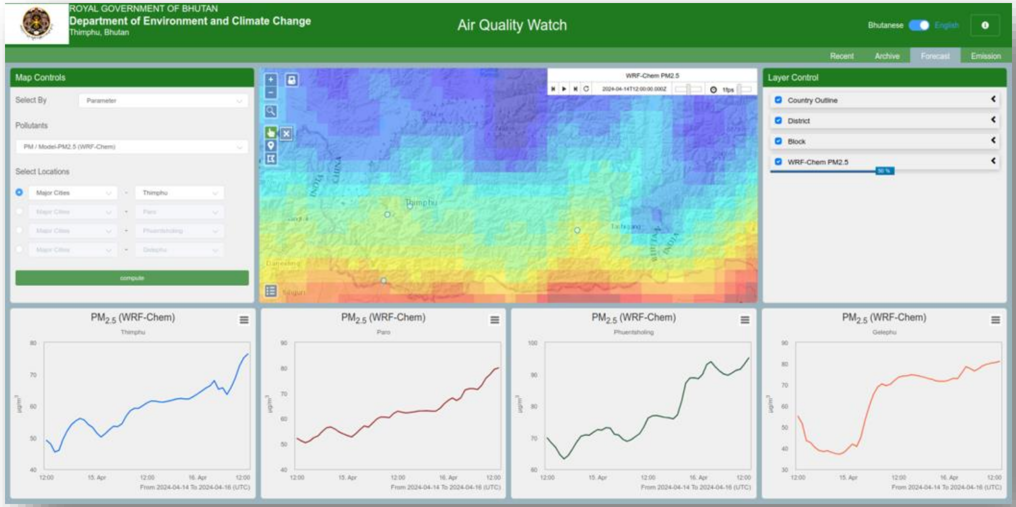
http://smog.icimod.org/apps/airquality/

http://smog.spatialapps.net/apps/airqualitynp/recent/?lang=en

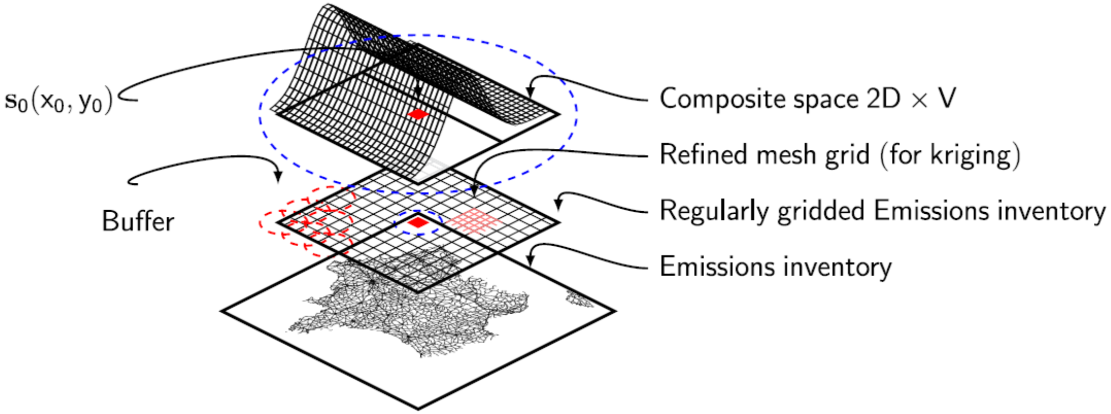
Nepal AQ Dashboard



Bhutan AQ Dashboard

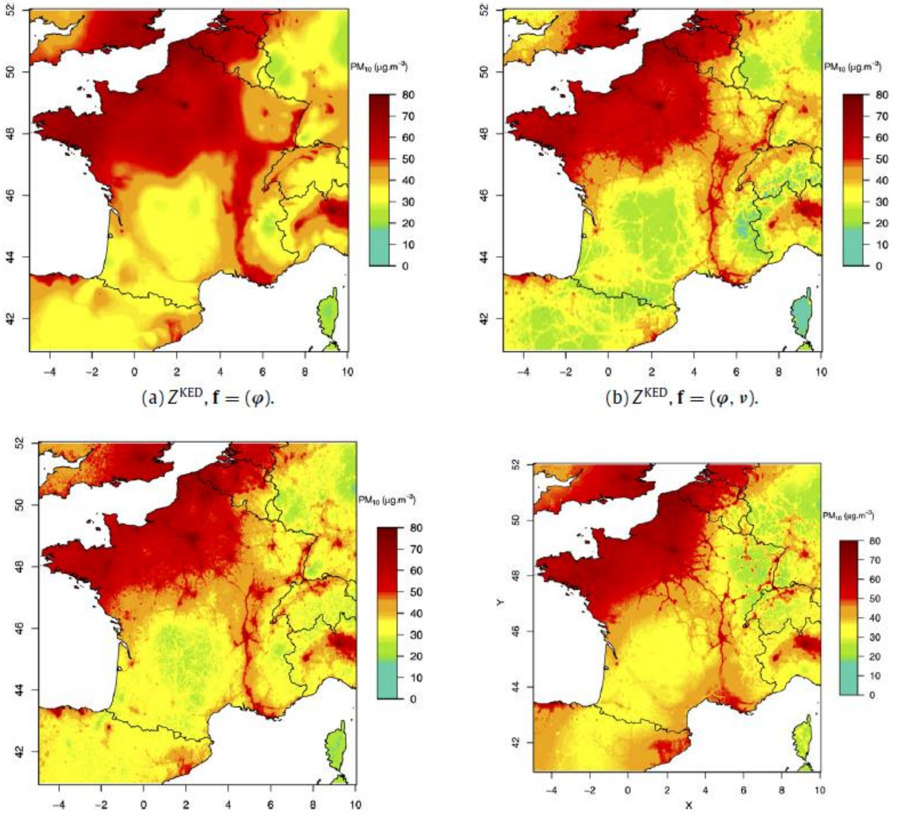


Model output statistics MOS



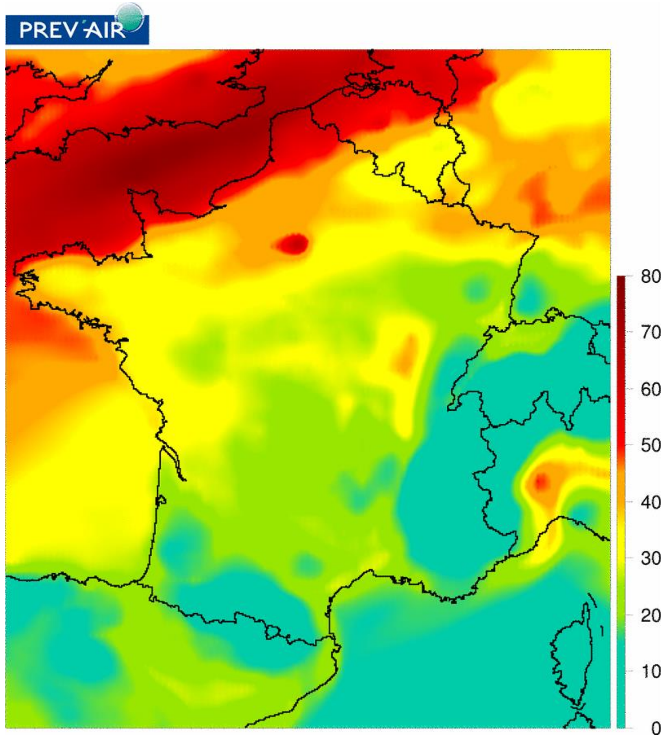
- **Correction of model outputs – Post simulation assimilation**
- Kriging methods
  - Include observations
  - Emission inventory
- Statistical correction based on past performances for forecast
- Machine learning techniques now

M. Beauchamp et al. / Spatial Statistics 22 (2017) 18–46

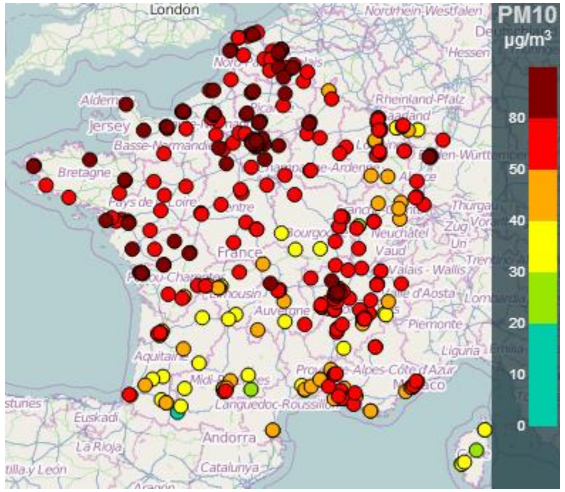


(a) Z^{KED}, $\mathbf{f} = (\varphi)$. (b) Z^{KED}, $\mathbf{f} = (\varphi, \nu)$. (c) Z^{KED}_{psm}, $\mathbf{f} = (\varphi)$. (d) Z^{KED}_{m}, $\mathbf{f} = (\varphi)$.

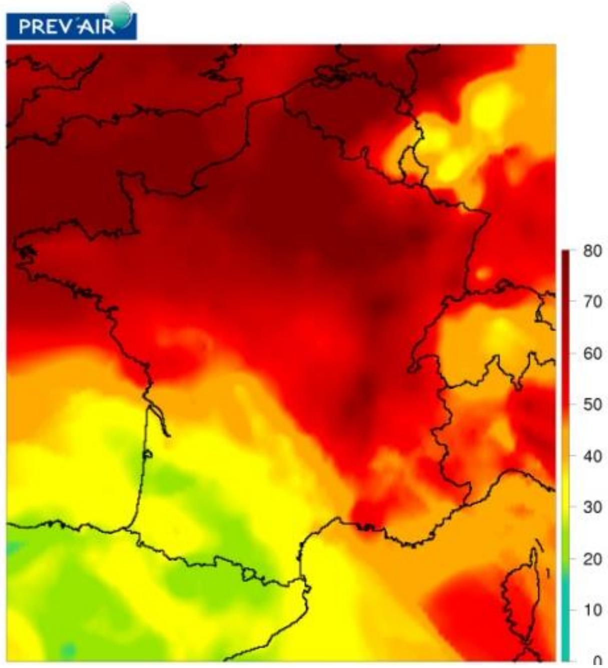
Example in France for PM2.5



+



=



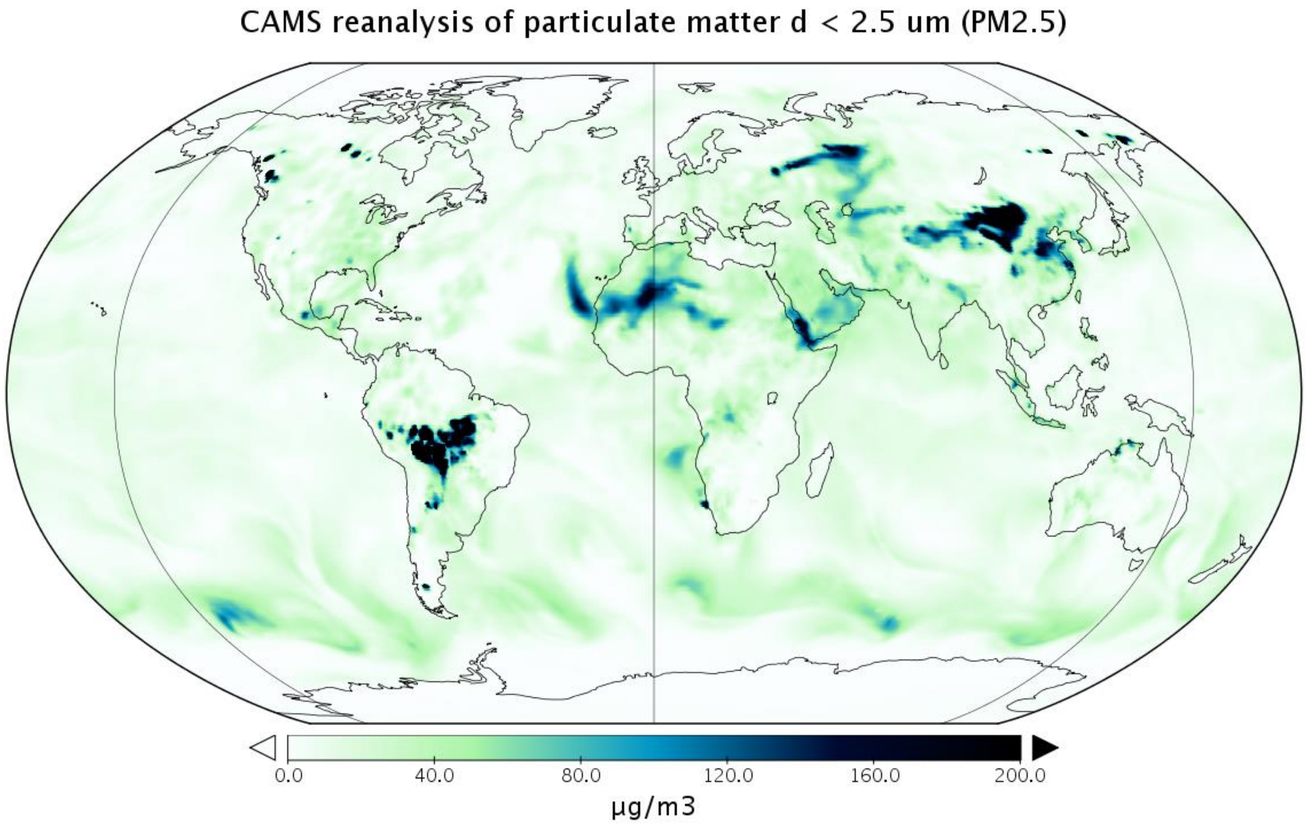
Raw model simulation

Observations

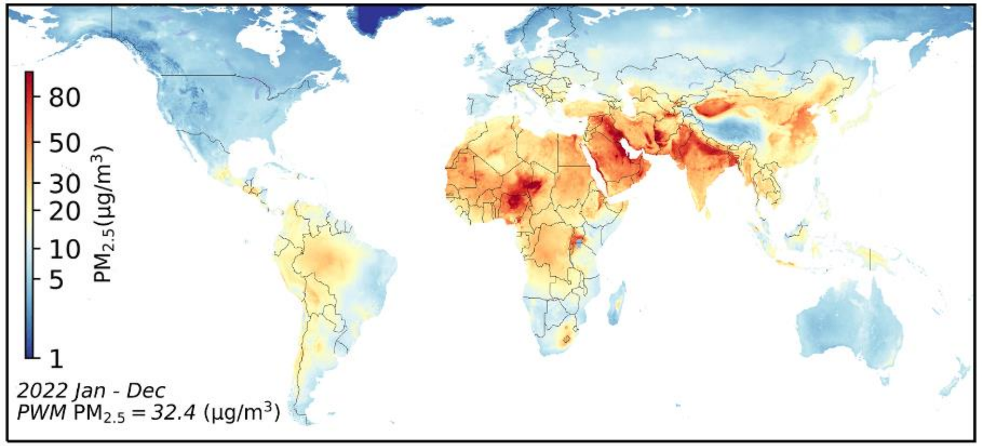
Krigged map

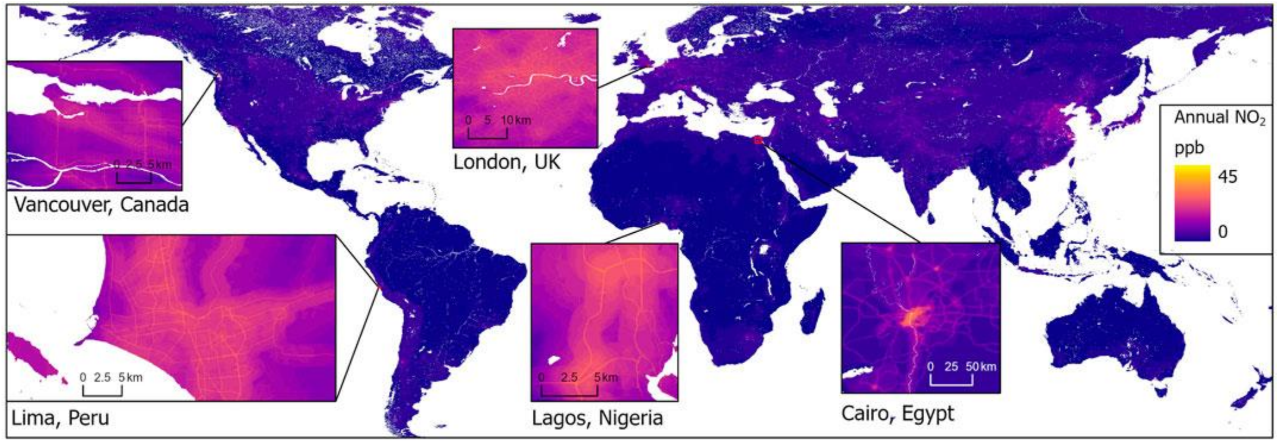
Global model dataset with satellite data assimilation

- https://www.copernicus.eu/en/access-data/copernicus-services-catalogue/cams-global-reanalysis-eac4



Global Satellite-model dataset





https://www.frontiersin.org/journals/environmental-science/articles/10.3389/fenvs.2023.1125979/full

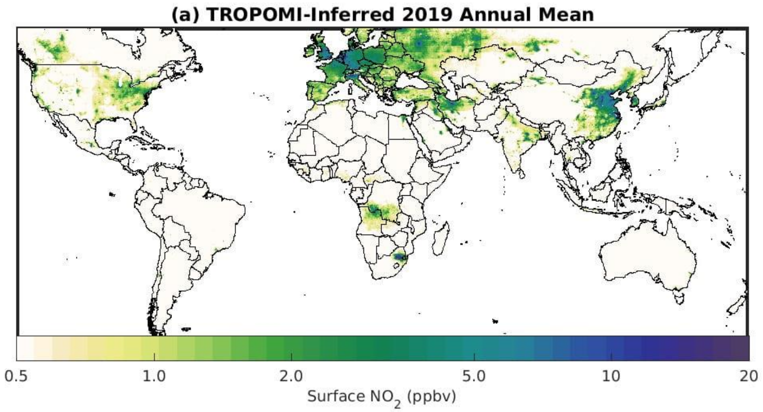
Environ. Res. Lett. 15 (2020) 104013 https://doi.org/10.1088/1748-9326/aba3a5

Environmental Research Letters

LETTER

Inferring ground-level nitrogen dioxide concentrations at fine spatial resolution applied to the TROPOMI satellite instrument

Matthew J Cooper, Randall V Martin, Chris A McLinden and Jeffrey R Brook

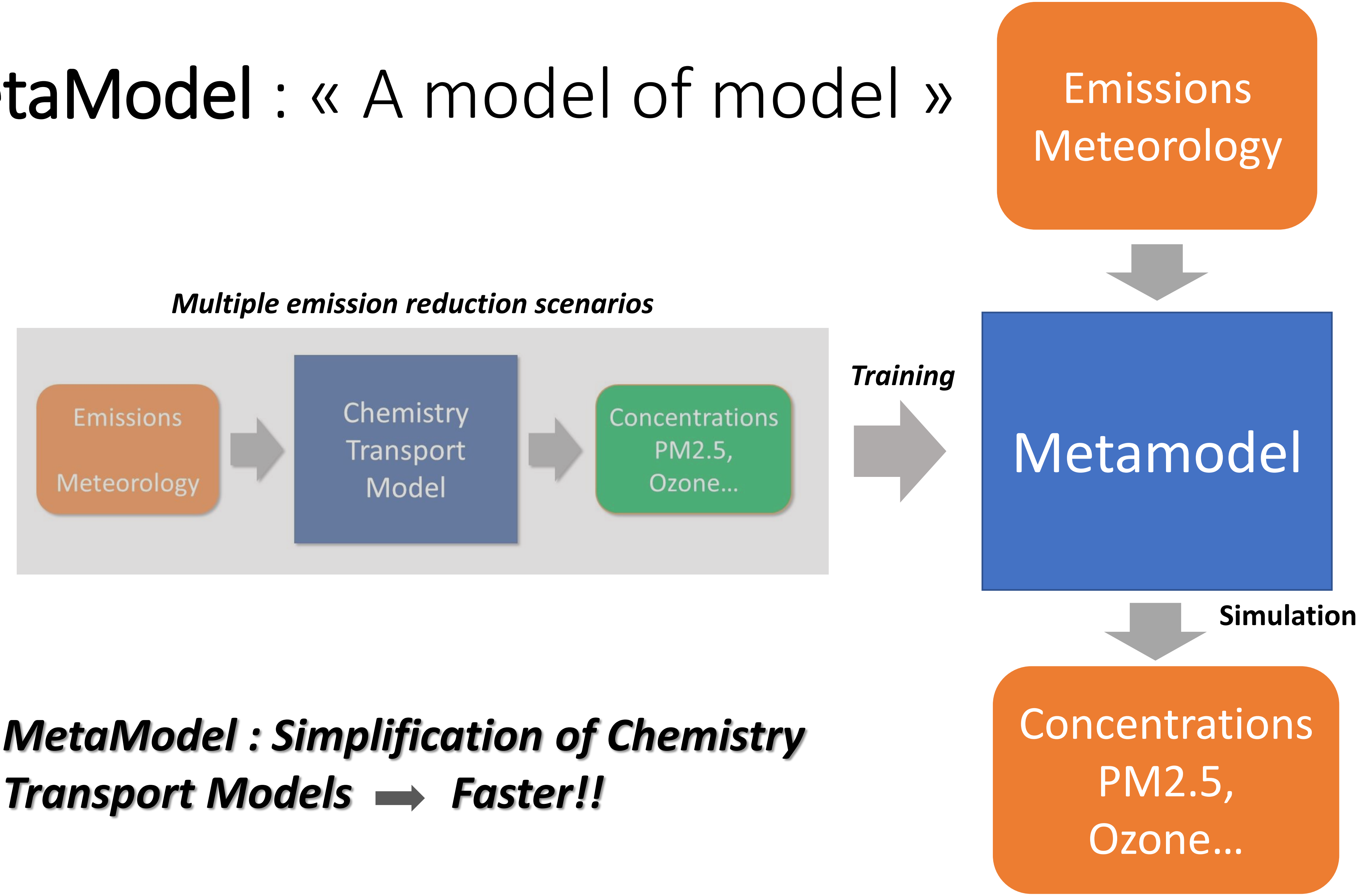


A global spatial-temporal land use regression model for nitrogen dioxide air pollution

Andrew Larkin[1*], Susan Anenberg[2], Daniel L. Goldberg[2], Arash Mohegh[2], Michael Brauer[3,4] and Perry Hystad[1]

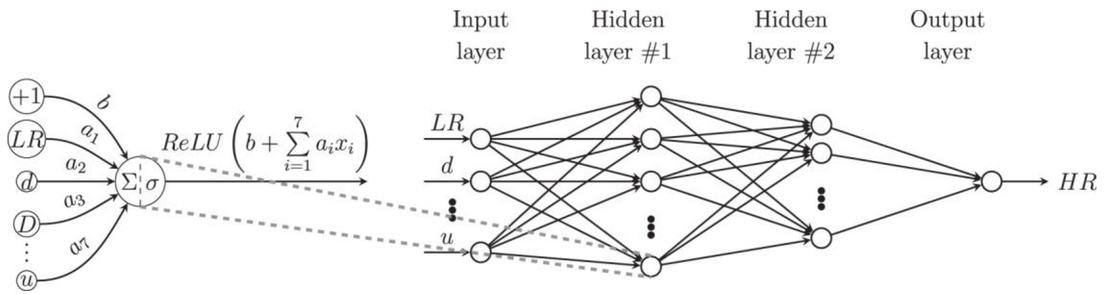
Shen, S. Li, C. van Donkelaar, A. Jacobs, N. Wang, C. Martin, R. V.: Enhancing Global Estimation of Fine Particulate Matter Concentrations by Including Geophysical a Priori Information in Deep Learning. (2024) ACS ES&T Air. DOI: 10.1021/acsestair.3c00054

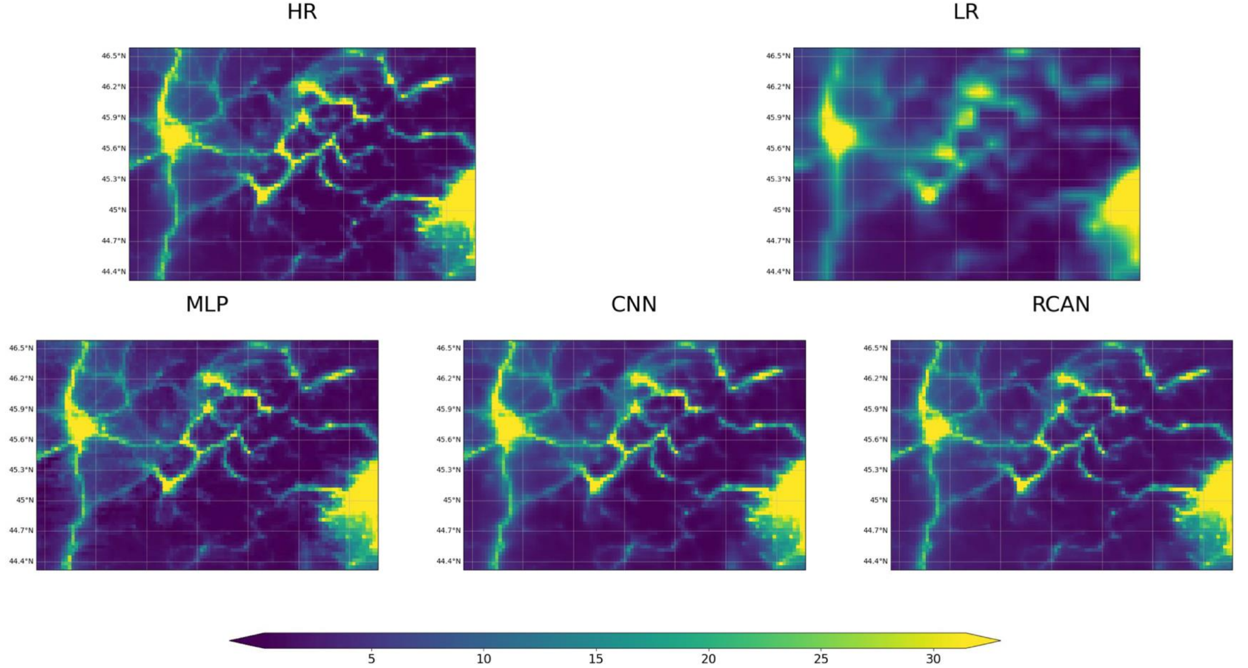
MetaModel : « A model of model »



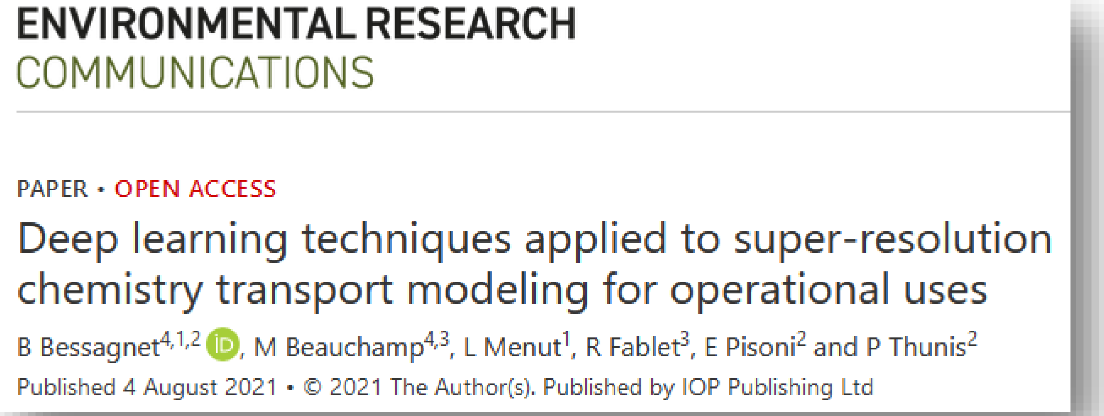
MetaModel : Simplification of Chemistry Transport Models → Faster!!

MetaModel with Machine Learning techniques





NO2 mean concentrations (μg m^{-3}) over the validation period for CHIMERE high-resolution and coarse resolution (top line) and 3 NN-based super resolution architectures (bottom line): from left to right, pixel-based independent multi-layer perceptron (MLP), Convolutional neural network (CNN) and Residual channel attention network (RCAN).


ENVIRONMENTAL RESEARCH
COMMUNICATIONS

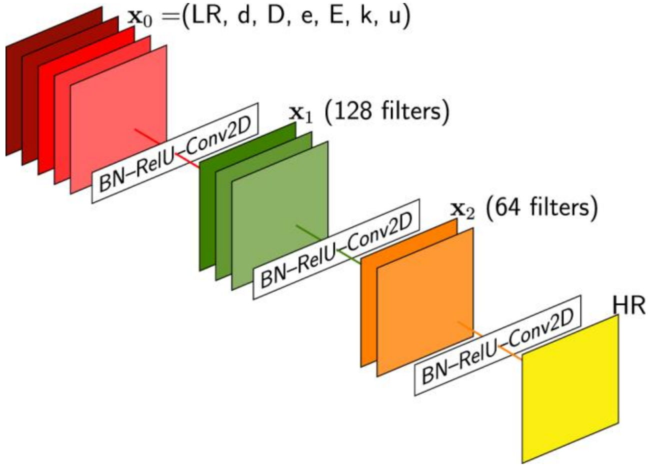
PAPER • OPEN ACCESS

Deep learning techniques applied to super-resolution chemistry transport modeling for operational uses

B Bessagnet[4,1,2], M Beauchamp[4,3], L Menut[1], R Fablet[3], E Pisoni[2] and P Thunis[2]

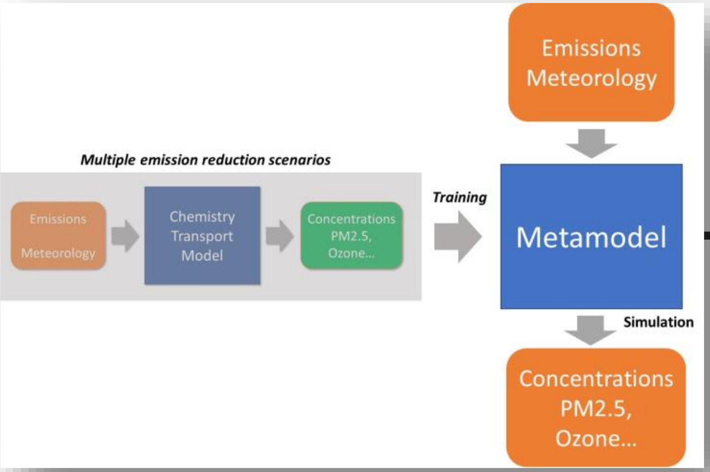
Published 4 August 2021 • © 2021 The Author(s). Published by IOP Publishing Ltd

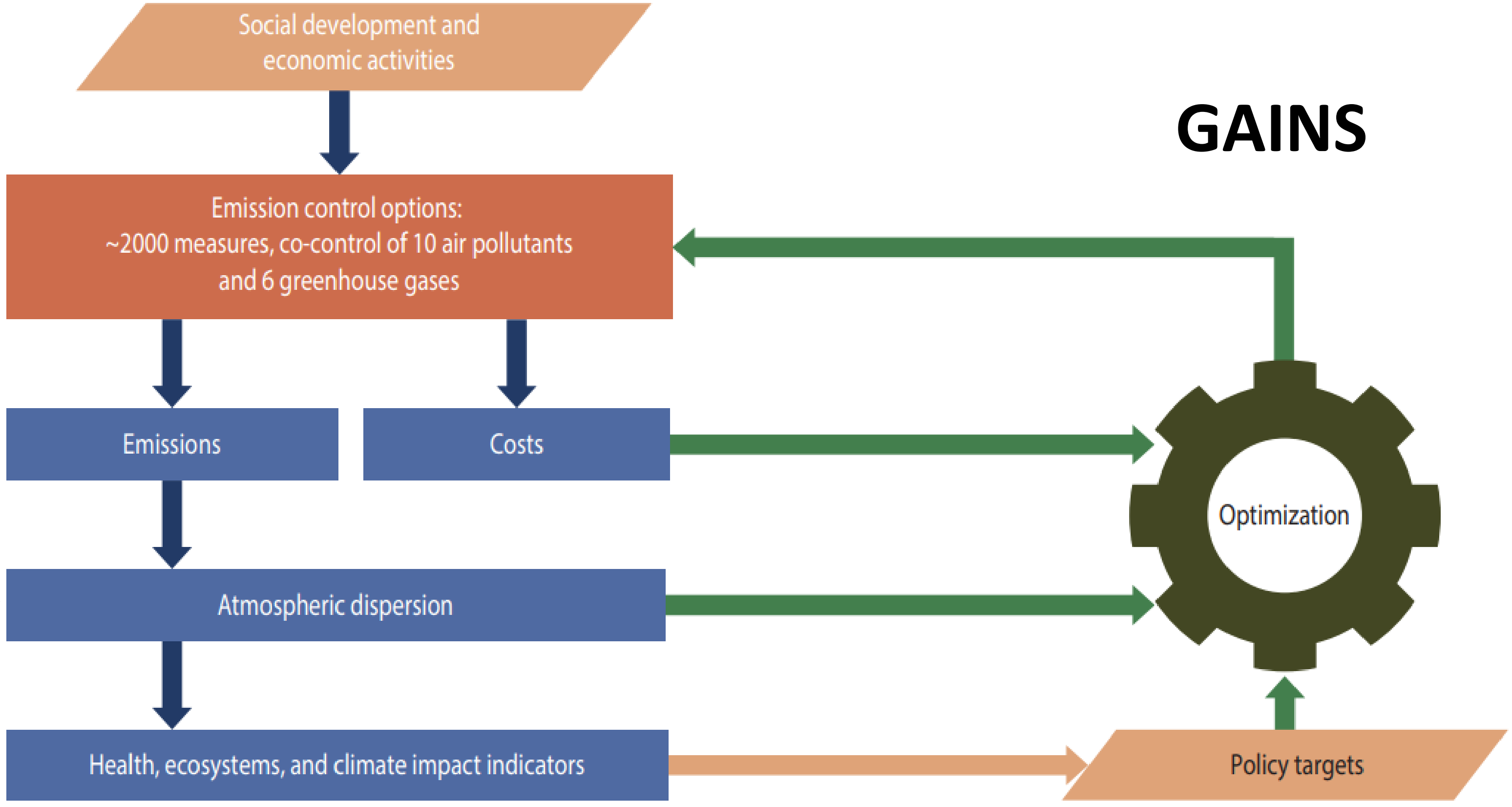
Convolutional Neural Network (CNN) architecture



Integrated modelling to find the best strategies (Example of GAINS model by IIASA)

Atmospheric modelling

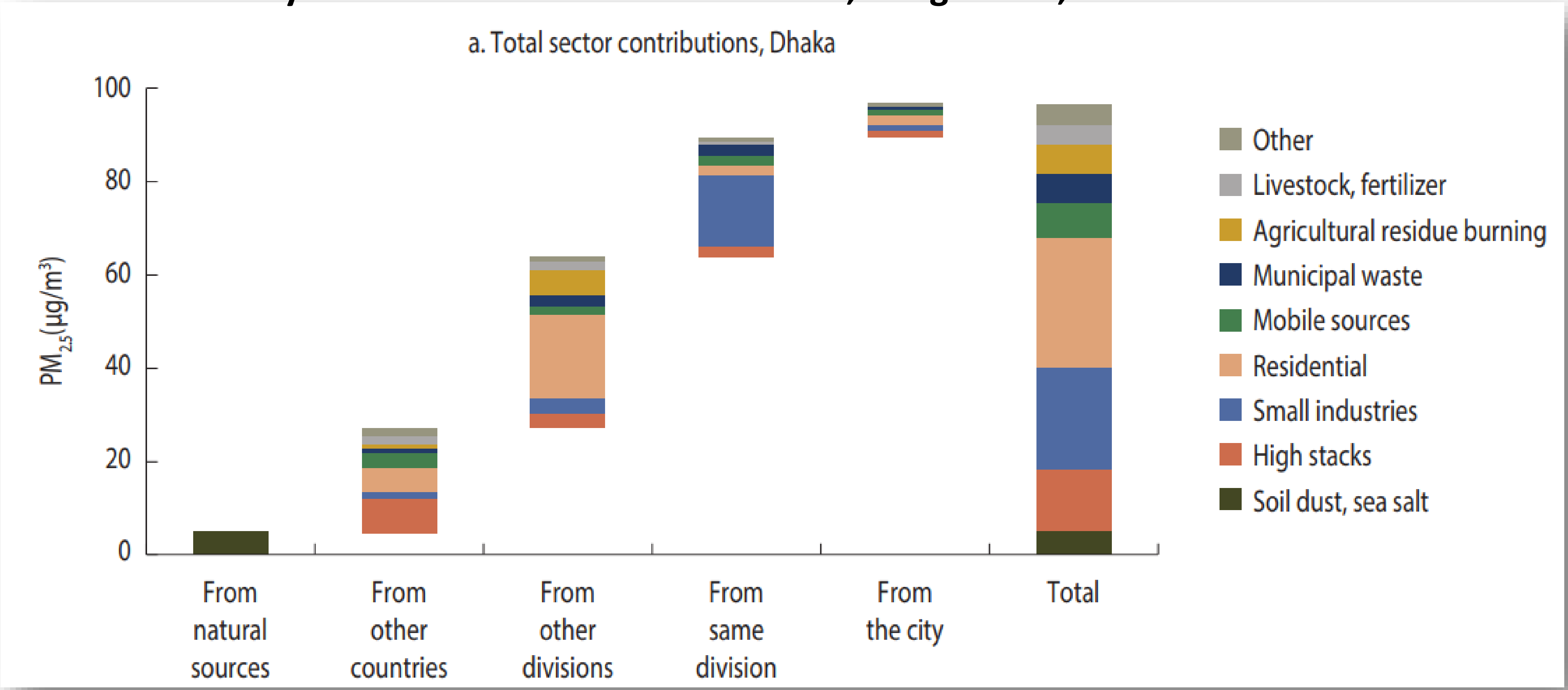




Source: International Institute for Applied Systems Analysis.
Note: GAINS = Greenhouse Gas and Air Pollution Interactions and Synergies.

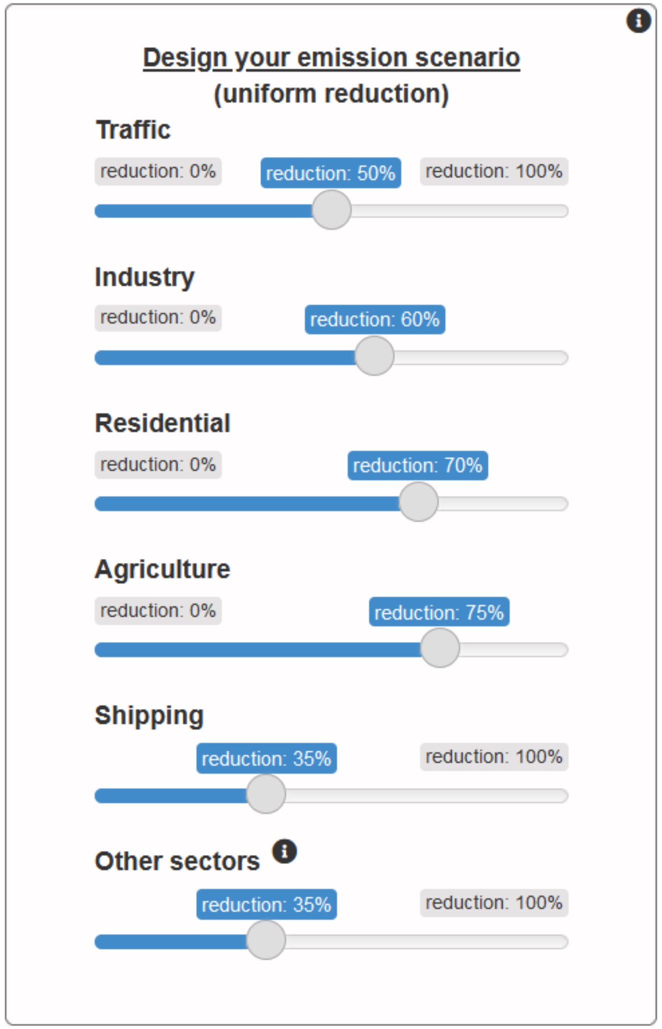
Example with the integrated model GAINS

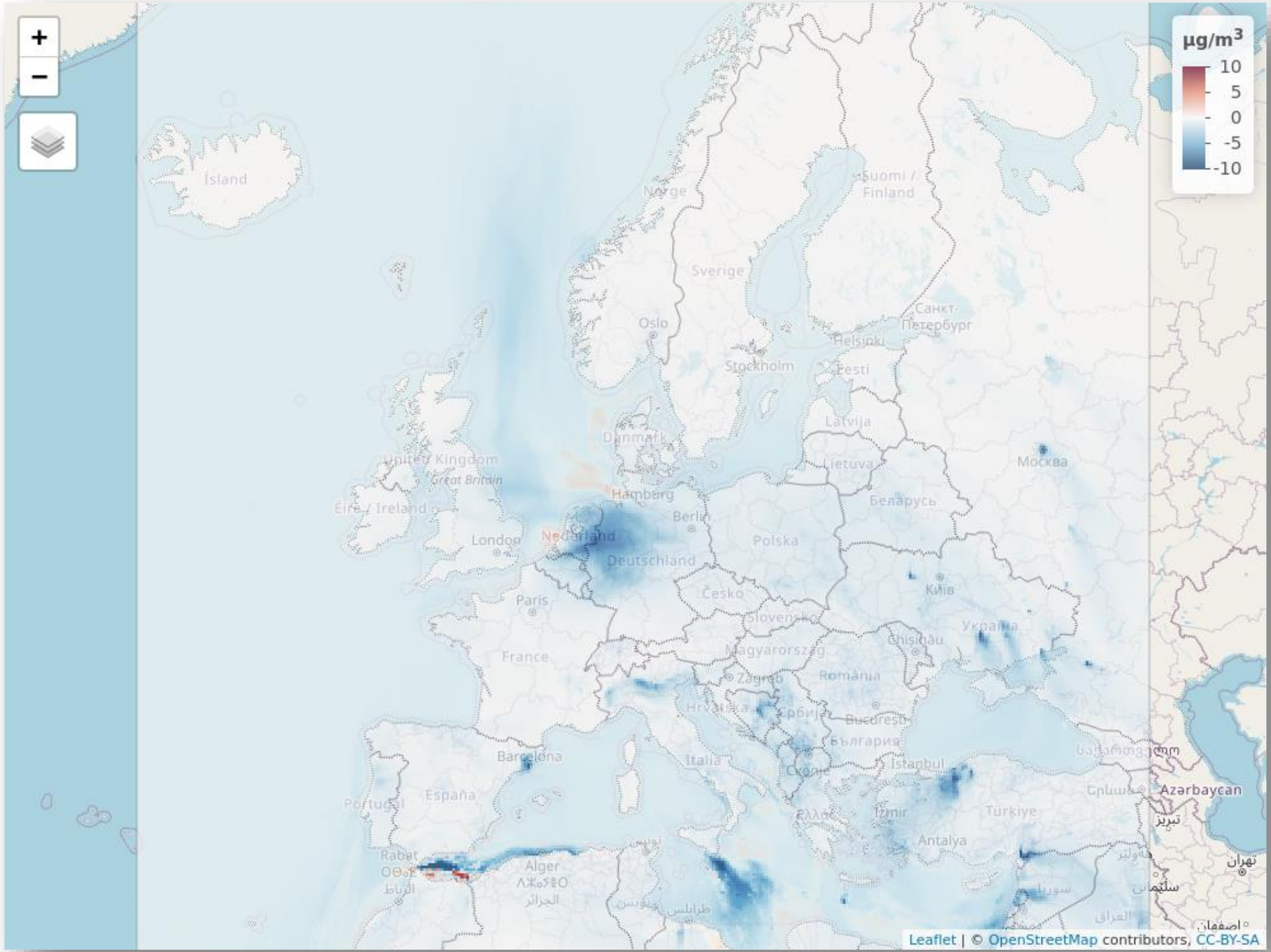
Source Allocations of Population Exposure to Total Fine Particulate Matter and Primary versus Secondary Fine Particulate Matter in Dhaka, Bangladesh, 2018



“Striving for Clean Air” – World Bank report 2023

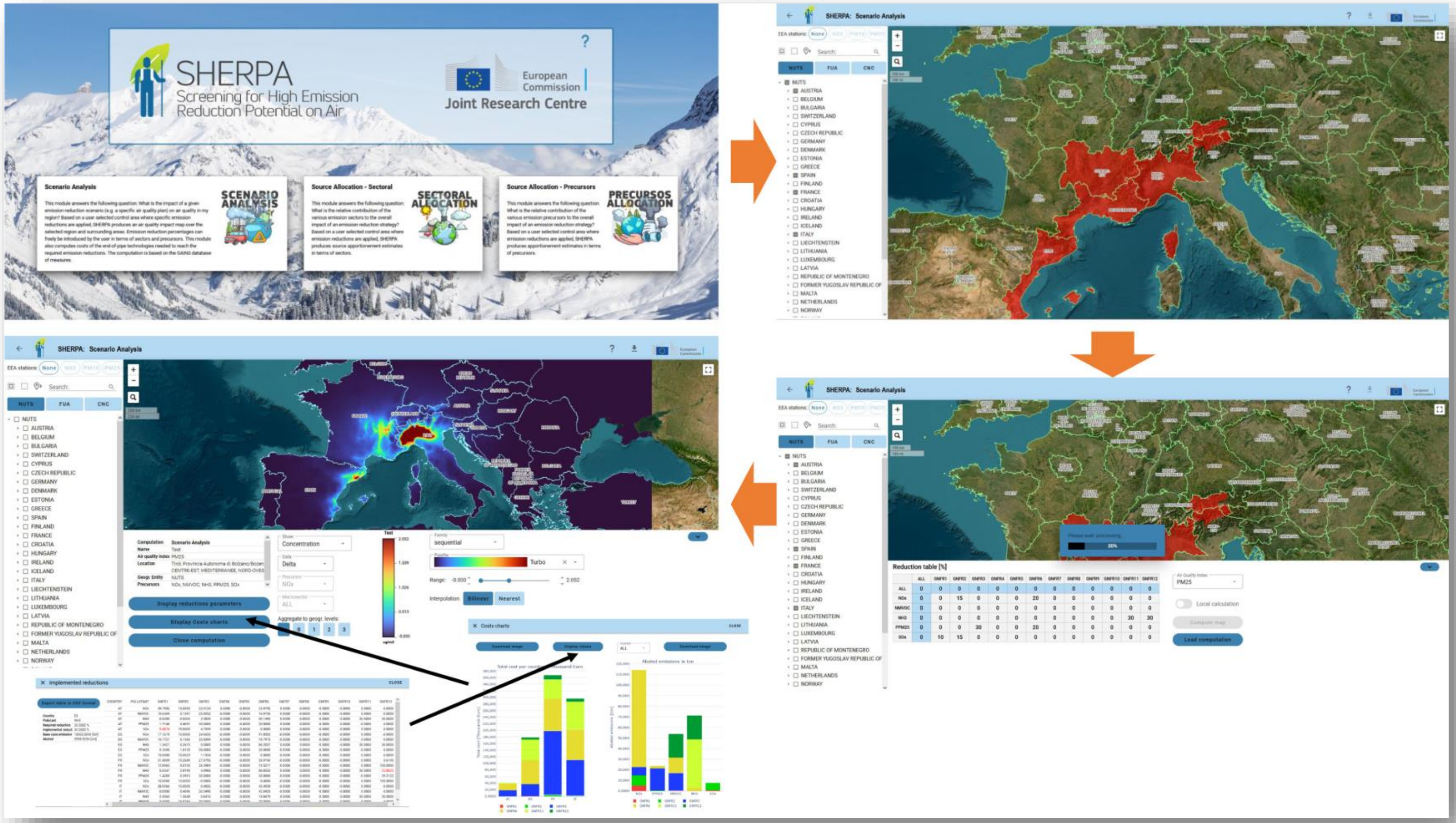
COPERNICUS: **CAMS-ACT** online tool





https://policy.atmosphere.copernicus.eu/

SHERPA: A tool to analyse regional and local Air Quality plans



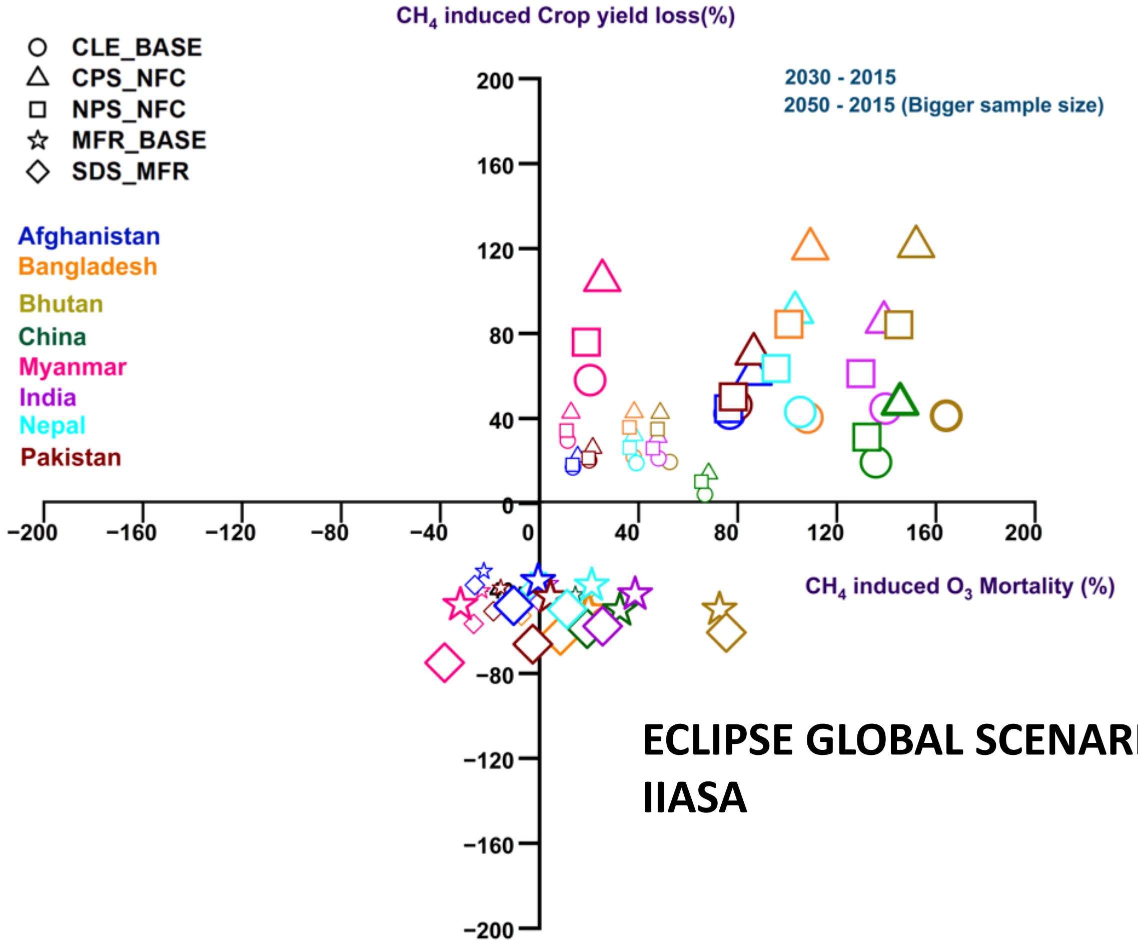
An online web app
User friendly interface
adapted for policy makers

To be adapted in the region…

European Commission

https://jeodpp.jrc.ec.europa.eu/eu/dashboard/voila/render/SHERPA/Sherpa.ipynb

FASST-TM5: a global scale tool (metamodel) to analyse global and regional scenarios



ECLIPSE GLOBAL SCENARIO
IIASA

Scenario analysis

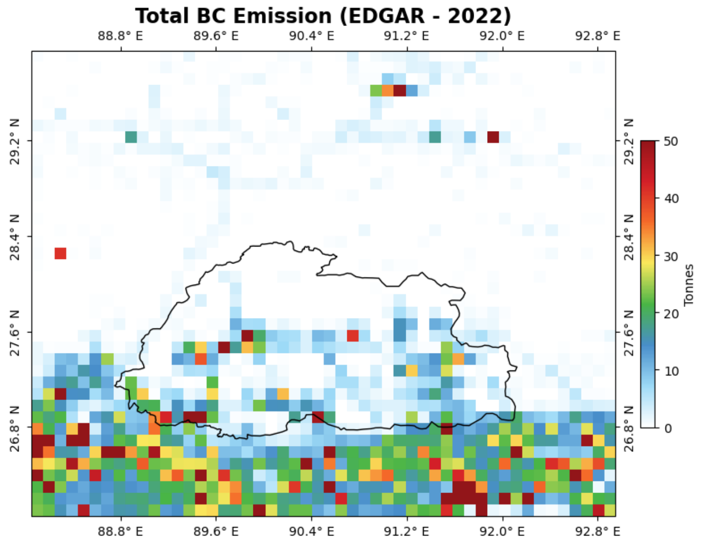
Changes in mortalities due to CH4-O_3 exposure in 2030, relative to exposure of the year 2015 O_3 level and their percentage difference.

Source JRC (Claudio Belis) from FASST-TM5 model
Processed by ICIMOD: Arshini Saikia

https://tm5-fasst.jrc.ec.europa.eu/

Some conclusions

- Several Air Quality Management numerical tools already exist and in use in HKH
- The IGP-HF region is specific and these tools must be adapted to the local context:
    - *Emissions (crop residue burning, forest fires, open burning of wastes, road dust resuspension)*
    - *Meteorology (orography, monsoon)*
    - *The role of Black Carbon, mineral dust on glacier melting*
    - *Impact of heavy pollution on local meteorology and then hydrology, agriculture*



- **Emissions** of pollutants is the key to manage Air Quality, an effort of knowledge and data **sharing**, **harmonization and development** is crucial

THANK YOU

#SaveOurSnow

Keep mountains on the global agenda

Sign the declaration

Spread the word

Share stories and photos of climate impacts on mountains

www.icimod.org/saveoursnow