Assessing Population Exposure with Air Quality Modelling

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French National Institute for Industrial Environment and Risks

Integrated Environmental Health Impact Assessment of Air Pollution and Climate Change in Mediterranean Areas

International Centre for Theoretical Physics, Trieste, Italy 23-27 April, 2018

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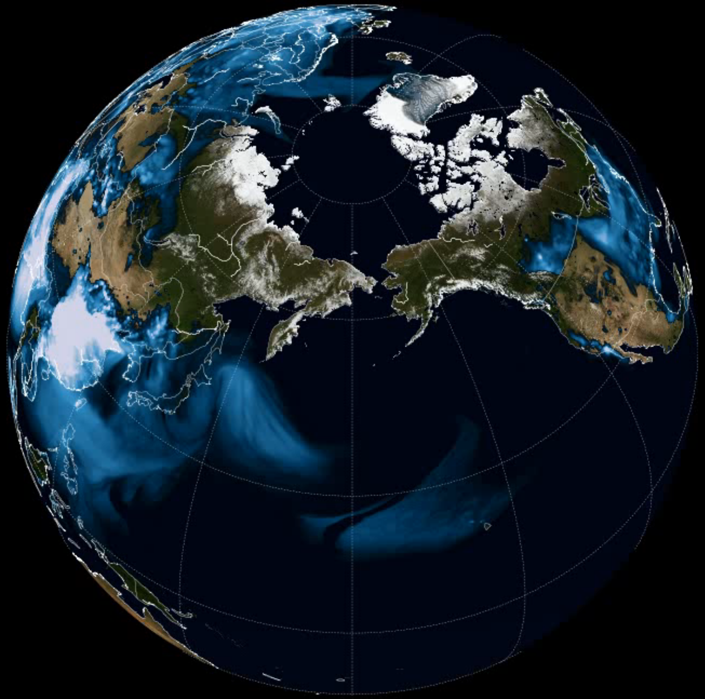

Risk Assessment

Accidental Risk = f(hazard , probability)

Chronic Risk = f(toxicity , exposure)

Integrated Assessment

Exposure to ambient air pollution

Scales

Spatial

- Individual
- Urban
- Country
- Continent
- Global

Temporal

- Day to day
- Annual
- Lifetime

Tools

Observations

- Citizen monitors
- Regulatory network
- Satellites

Algorithm

- Air quality models
- Land use Regression
- Data Assimilation
- Data fusion

Air Quality Modelling

	Chemistry-Transport (deterministic)	Geostatistical regressions (statistics)
Pros	• More physical • Sensitivity to changing conditions	• Well fitted / calibrated
Cons	• Complex • Prone to model biases	• Lower sensitivity to changes

Of noteworthy importance for air quality:

- Non-linear chemistry, production of secondary species (O3, PM)
- Long range transport of air pollutants

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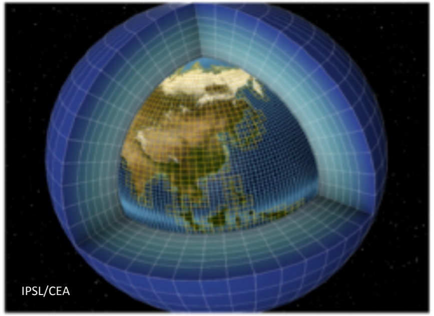
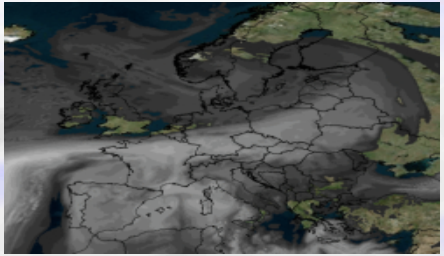
Chemistry-Transport Modelling

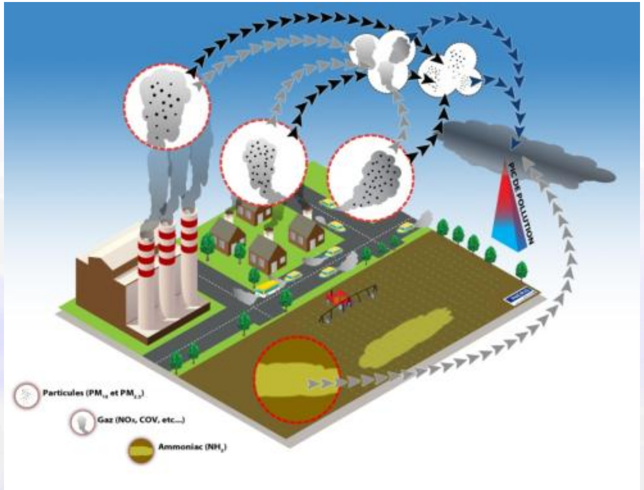
Global Chemistry



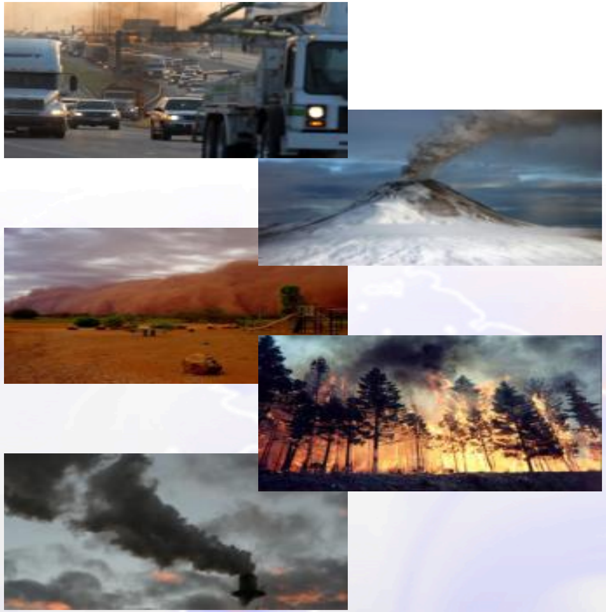
Regional Meteorology



Regional Chemistry Transport



Emissions of Trace species



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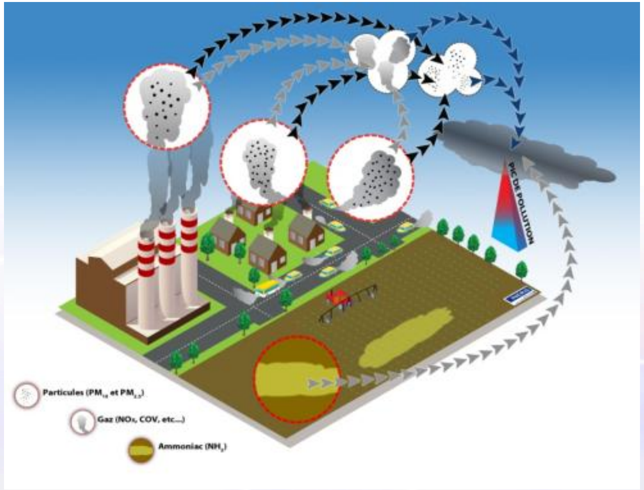
Regional Chemistry Transport model: what's inside ?

- The physics & chemistry

$$\partial c/\partial t = \mathbf{u}\nabla c + Production - Loss$$

advection, diffusion

chemistry, emission, deposition



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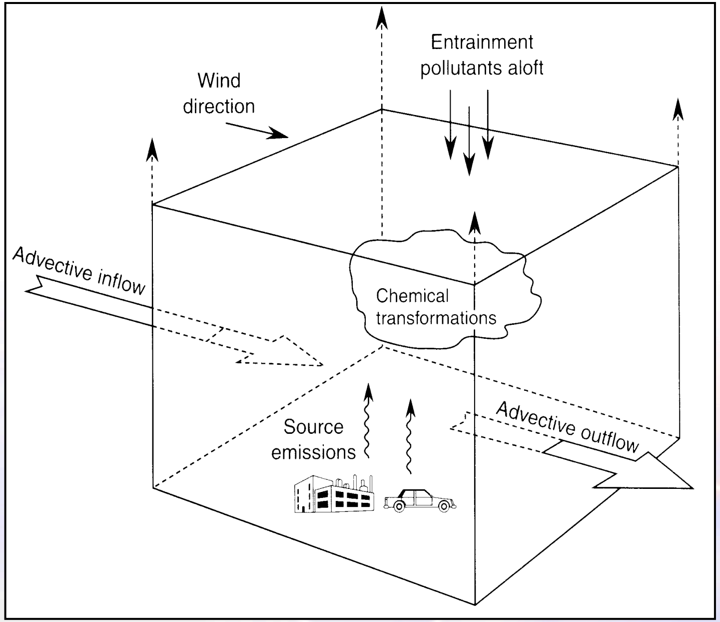
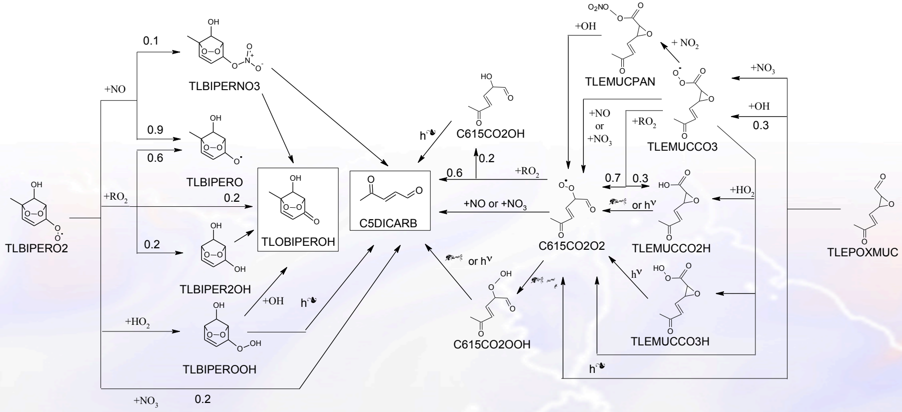
Regional Chemistry Transport model: what's inside ?

- Transport
  - Advection (laminar flow)
  - Mixing / Turbulence
    - Planetary boundary layer
    - Large scale convection
- Deposition
  - Dry:
    - air/surface interaction at the ground, role of vegetation and subsequent impacts
  - Wet:
    - scavenging of hydrophilic species (gas or aerosols)
    - In cloud (inc. fog), or in precipitation (removal)



Regional Chemistry Transport model: what's inside ?

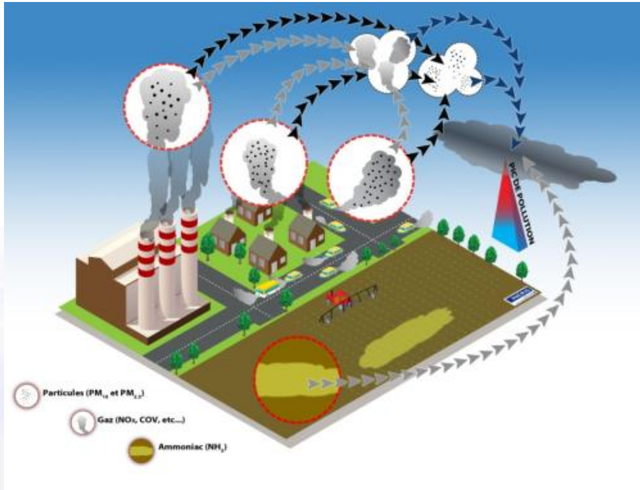
- Chemistry
  - Gas-phase
    - ~100-300 species / reactions
  - Aerosols
    - Chemistry: ~5-50 species / reactions
    - Microphysics: Nucleation, Coagulation, Condensation
    - Organics, Inorganics (sulphate, nitrate, ammonium), Naturals (ash, dust, sea salts)
  - Heterogeneous chemistry
- Photochemistry
  - Solar irradiance (role of clouds)



G. Lanzafame

Regional Chemistry Transport model: what's inside ?

- Chemistry
  - Altitude dependance
    - Planetary Boundary Layer
    - Tropospheric
    - Stratospheric
  - Surface dependance
    - Urban
    - Snow
    - Forests
    - Deserts

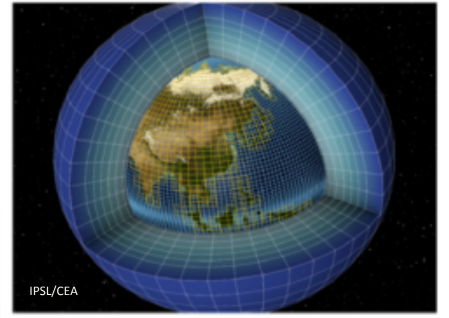


Regional Chemistry Transport model: the engine

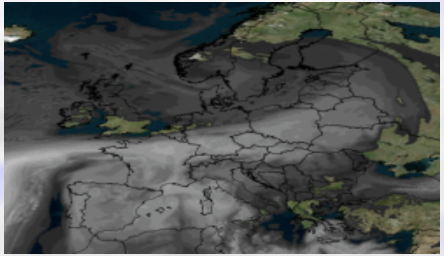
- Many available tools:
  - A few regional CTMs : CMAQ, CAMx, EMEP, CHIMERE, LOTOS, WRF-CHEM, Polair3D, MOCAGE, MATCH, SILAM, …
- ~50,000 lines of numerical code (fortran, c++, python)
- Runs on high performance computers (100-5000 CPUs)
- A specificity of CTMs: large amount of i/o
- Runtime
  - Assessment:
    - Europe low-res (50km): 1yr simulated in 1 day / 100 CPUs
  - Forecast:
    - Europe high-res (10km): 5 days simulated in 3 hrs / 300 CPUs

Chemistry-Transport Modelling

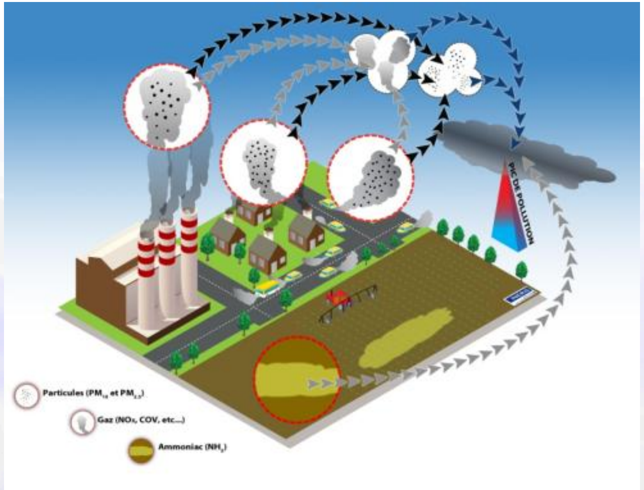
Global Chemistry



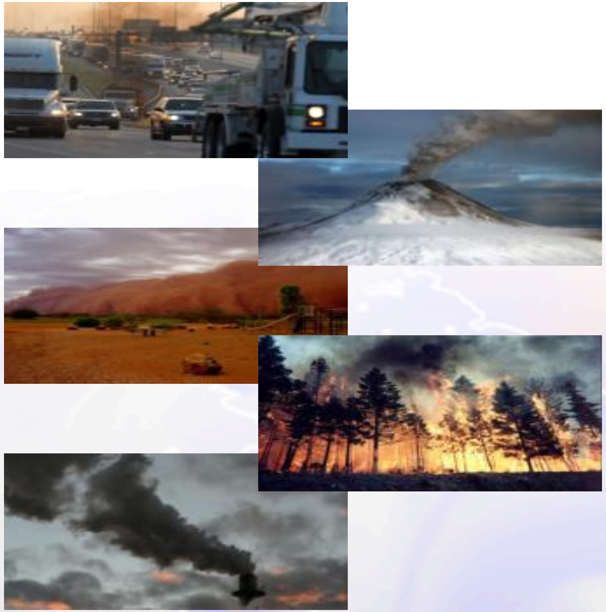
Regional Meteorology



Regional Chemistry Transport



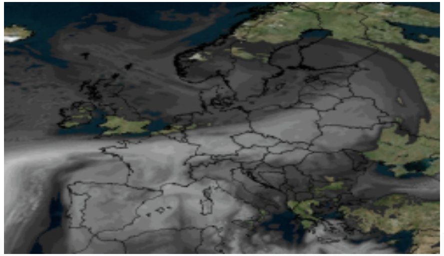
Emissions of Trace species



Regional Chemistry Transport model: input data METEOROLOGY

- Meteorology
  - Prognostic:
    - u, v, t, q, P
  - Diagnostic:
    - u* Surface friction
    - PBL depth
    - Turbulent mixing
    - Precipitation
    - Solar irradiance

- Temporal scale
  - Day to day forecast
  - Annual assessment
  - Decadal/Century (Climate)
- Sources
  - Operational weather centres (NCEP, ECMWF)
  - In-house (e.g. open source WRF)
  - Climate projections (IPCC)



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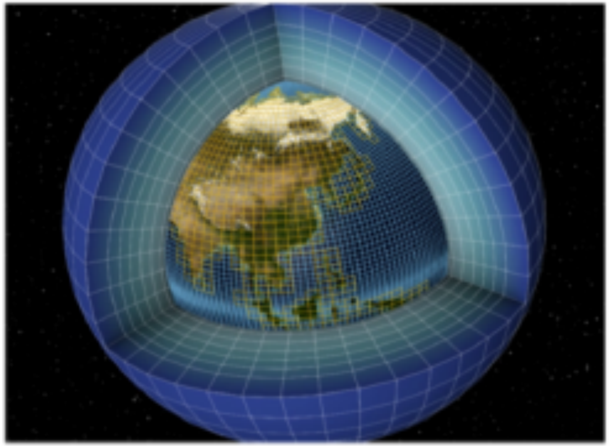
Regional Chemistry Transport model: input data GLOBAL CHEMISTRY

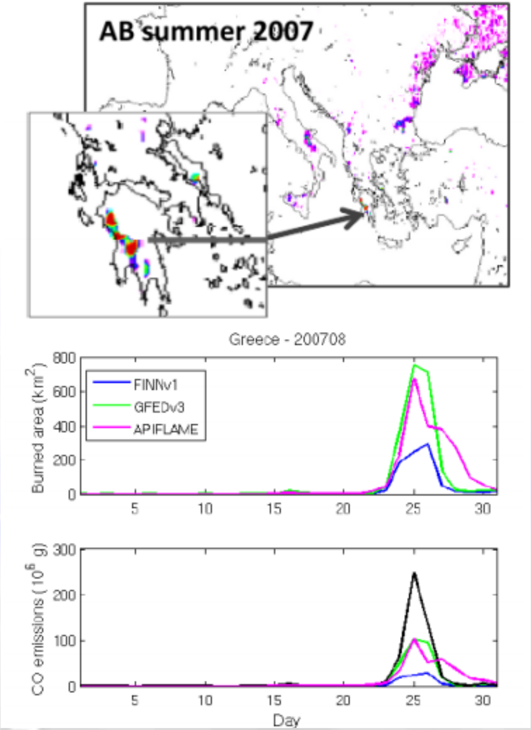
- Global Chemistry
  - Specific need for regional/local air quality model
  - Large scale inflow
    - Intercontinental pollution plumes
    - Desert dusts
    - Stratospheric intrusions
- Temporal scale
  - Day to day (ex: plumes)
  - Monthly averages
- Sources
  - Operational /Research Centres (NCAR, ECMWF)
  - Climate (ACCMIP, CCMI)



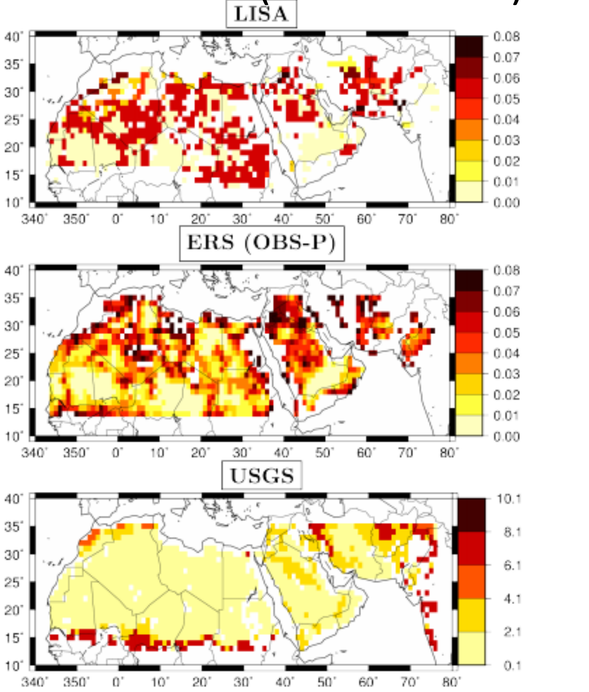
Regional Chemistry Transport model: input data: EMISSIONS

- Natural processes
  - Desert dust:
    - Landuse maps + erosion
  - Volcanoes
    - Continuous & sporadic
  - Biogenic VOCs
    - Ecosystem models
  - Pollens
    - Ecosystem models
  - Wildfires
    - Sporadic location & intensity

Wildfires (Turquety et al.)



Desert Dusts (Menut et al.)



Comparison of roughness length from LISA (African data), ERS (global satellite) and USGS (global model).

Regional Chemistry Transport model: input data: EMISSIONS

- Anthropogenic activities (« pollution »)
  - SOx, NOx, COV, primary PM, NH3, CO, CH_4
  - Industry, Residential, Traffic, Agriculture, Waste, Shipping, Aircrafts

- Spatialisation
  - Emission fluxes generaly provided as country totals
  - Spatilized using proxies:
    - Population
    - Traffic
    - Large point sources

Figure 2.4 Contribution to EU-28 emissions from main source sectors in 2015 of SO_x, NO_x, PM_{10}, $PM_{2.5}$, NH_3, NMVOCs, CO and BC

Note: For CH_4, please see Figure 3.4.

Sources: EEA, 2017c, 2017e.

Non-road transport · Road transport · Energy production and distribution · Commercial, institutional and households
Energy use in industry · Industrial processes and product use · Agriculture · Waste · Other

Regional Chemistry Transport model: input data: EMISSIONS

- Sources
  - Databases of officially reported fluxes
    - Activity data
    - Emission factors
  - Inversion (satellite + models)
    - Observationally constrained
    - Useful to benchmark reported fluxes
    - Not linked to activity
  - Long term projections
    - Policy targets
    - Technology
    - Macro-economics

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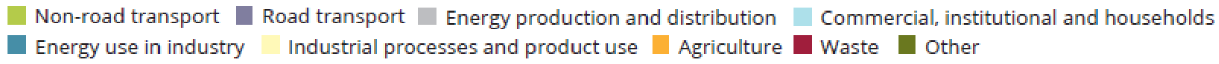
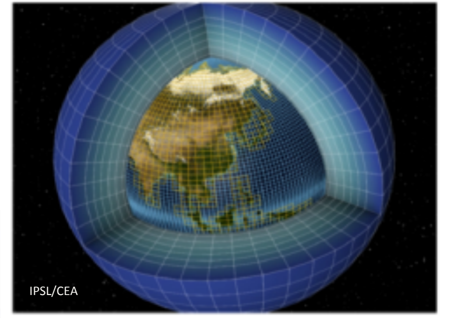
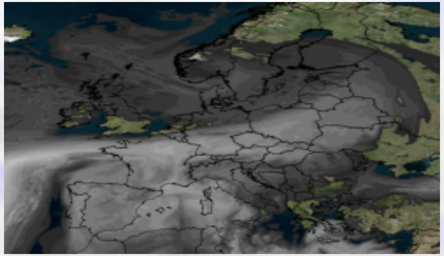


Chemistry-Transport Modelling

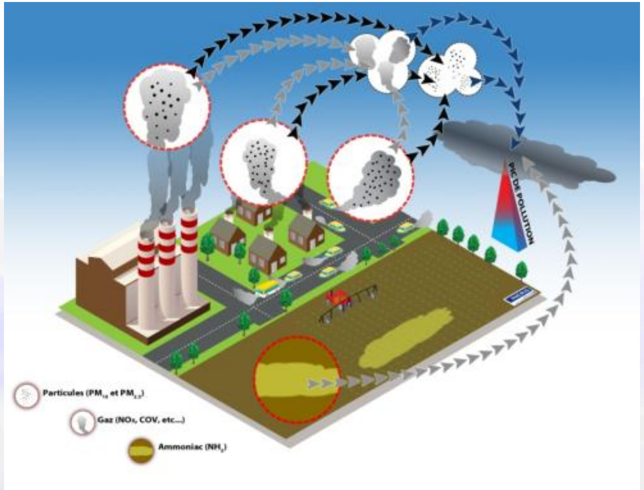
Global Chemistry



Regional Meteorology



Regional Chemistry Transport



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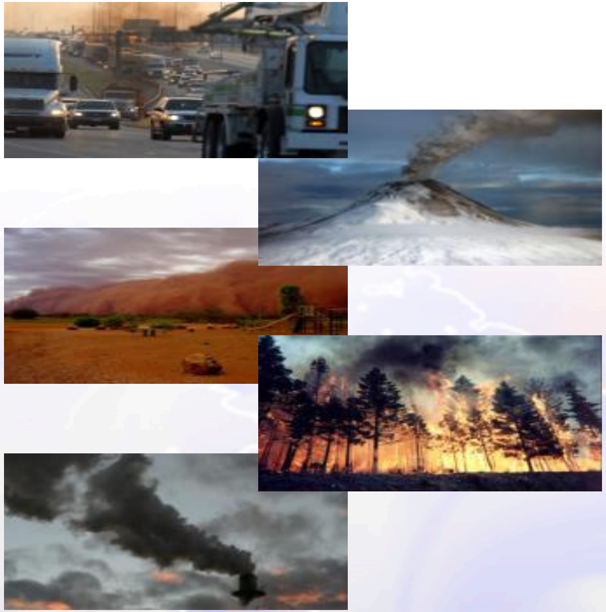
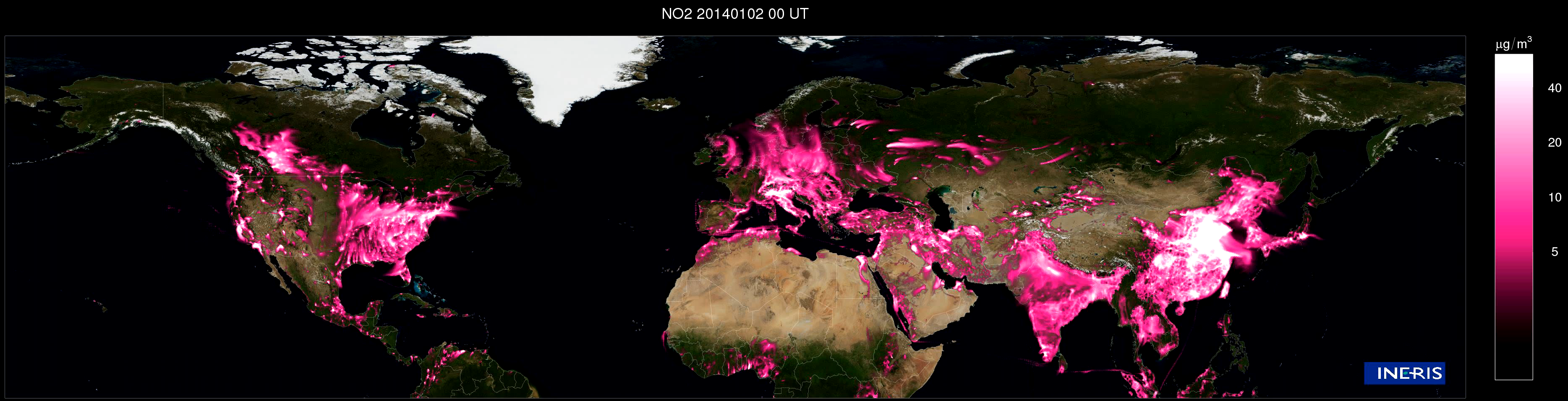
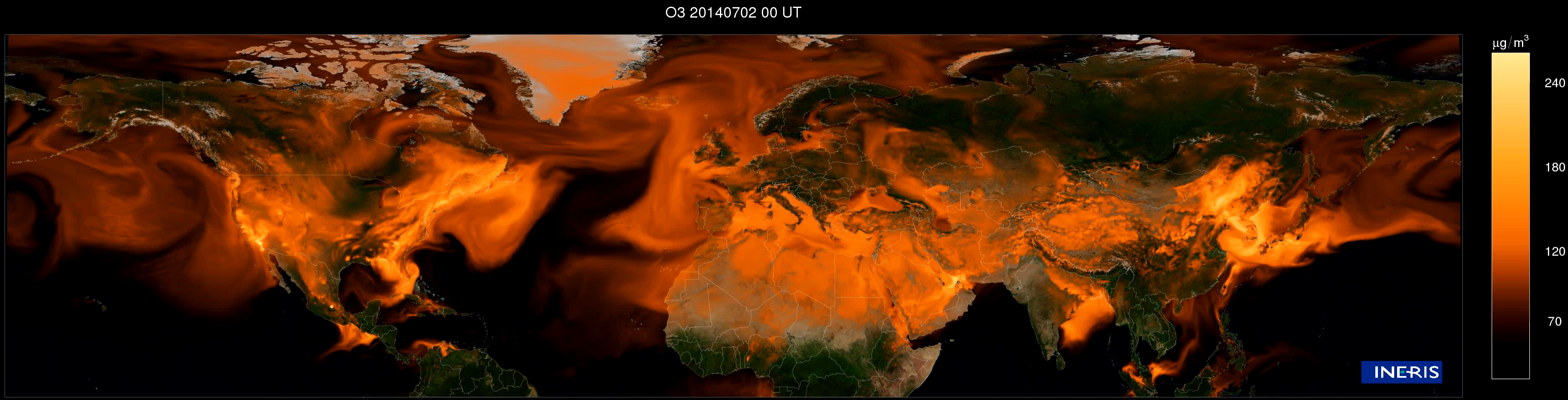


Nitrogen oxides (NOx) have a short lifetime and are thus located close to the main emission sources



Ozone (O_3) is found over much larger areas because of its longer lifetime



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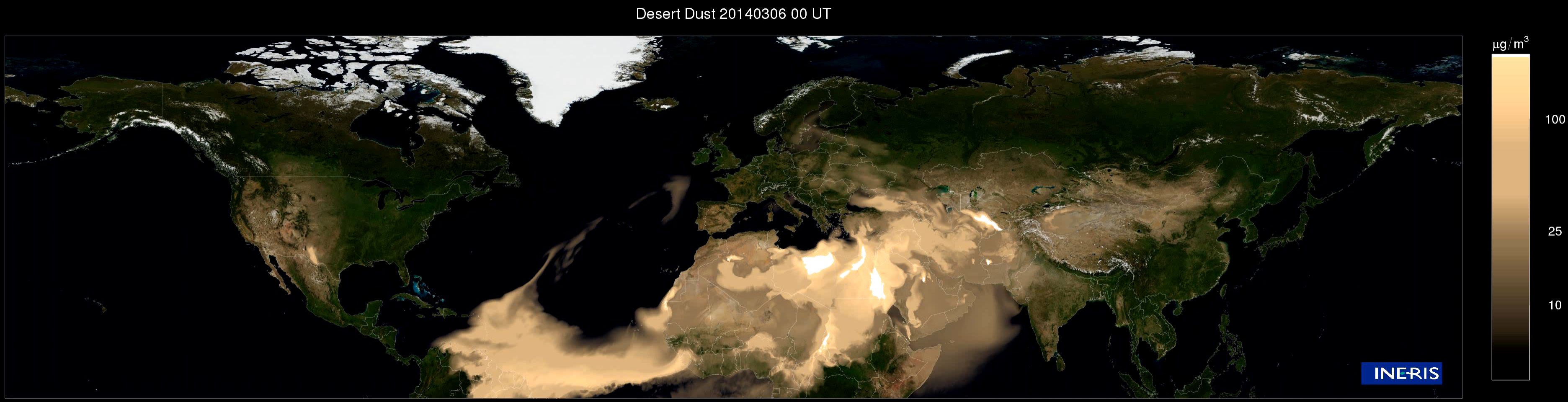
Desert dust are present in the natural atmosphere. The source is so massive that it can also remain in the atmosphere over long distances



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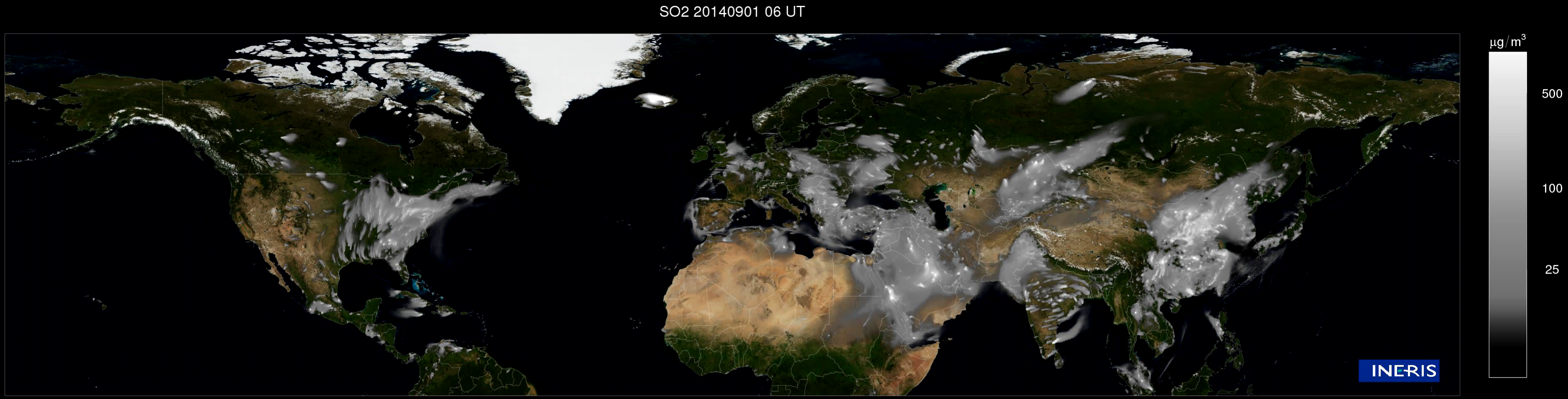
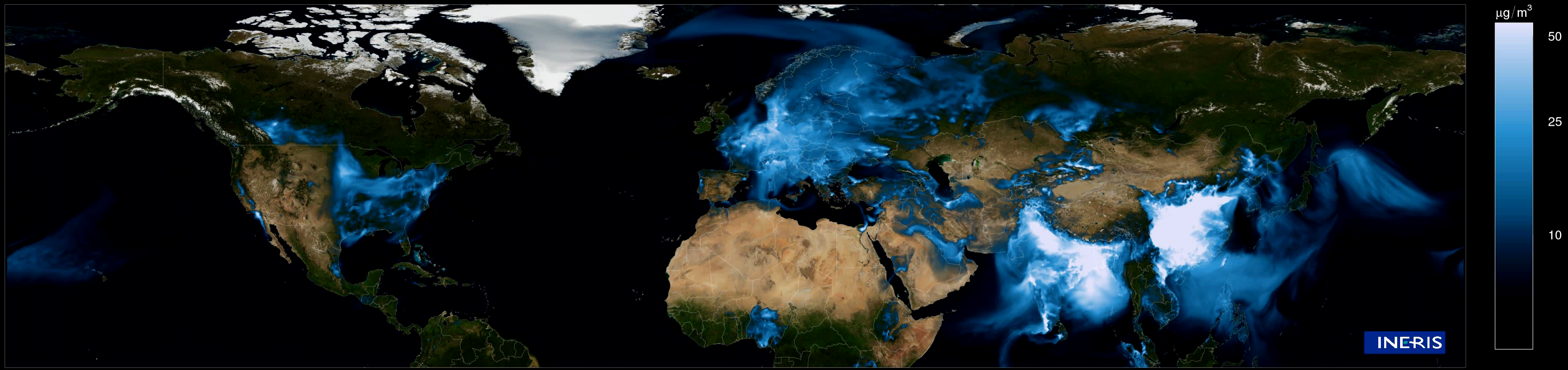
Volcanic eruption constitute a massive source of ash, or here sulphur dioxide (SO_2).



Anthropogenic fine particulate matter (PM2.5) are today the main threat to human health

PM25 anthropogenic 20140306 00 UT



Models and Observations

- Validation
- Assimilation
- Fusion

Model validation

- Comparing observations to models interpolated in time & space

- Typology of observations
  - Surface: Regulatory AQ networks (Note: low cost sensors not yet mature enough for validation)
  - Profiles: balloon sounding, aircrafts, lidar
  - 3D: satellite

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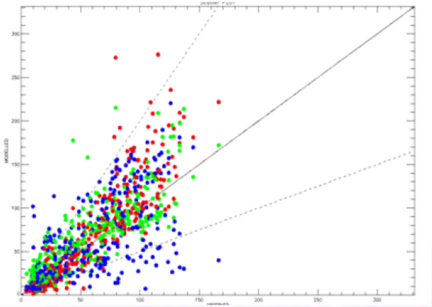
Model validation

- Variety of statistical indicators
  - e.g. fairmode.jrc.ec.europa.eu

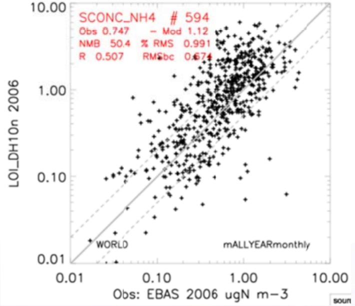
Mean	$\overline{M} = \frac{1}{N}\sum_{i=1}^{N} M_i$, $\overline{O} = \frac{1}{N}\sum_{i=1}^{N} O_i$
Standard Deviation	$\sigma_M = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(M_i - \overline{M})^2}$, $\sigma_O = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(O_i - \overline{O})^2}$
Mean Bias	$MBias = \frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)$
Mean Fractional Bias	$MFB = \frac{1}{N}\sum_{i=1}^{N}\frac{M_i - O_i}{(M_i + O_i)/2}$
Mean Fractional Error	$MFE = \frac{1}{N}\sum_{i=1}^{N}\frac{\lvert M_i - O_i\rvert}{(M_i + O_i)/2}$
RootMeanSquare Error	$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)^2}$
Ratio of Systematic and unsystematic RMSE	$RMSE_S / RMSE_U = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\hat{M}_i - O_i)^2} \Big/ \sqrt{\frac{1}{N}\sum_{i=1}^{N}(M_i - \hat{M}_i)^2}$ *where* $\hat{M}_i = a + bO_i$ *are the regressed model values, estimated from a least square fit to observations;* $RMSE^2 = RMSE_S^2 + RMSE_U^2$.
Target	$RMSE / \sigma_O = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)^2} \Big/ \sqrt{\frac{1}{N}\sum_{i=1}^{N}(O_i - \overline{O})^2}$
Pearson Correlation Coefficient	$R = \sum_{i=1}^{N}(M_i - \overline{M})\cdot(O_i - \overline{O}) \Big/ \sqrt{\sum_{i=1}^{N}(M_i - \overline{M})^2} \cdot \sqrt{\sum_{i=1}^{N}(O_i - \overline{O})^2}$
Index of Agreement	$IOA = 1 - N \cdot RMSE^2 \Big/ \sum_{i=1}^{N}\left(\lvert M_i - \overline{O}\rvert + \lvert O_i - \overline{O}\rvert\right)^2$
Relative Directive Error and its maximum	$RDE = \frac{\lvert O_{LV} - M_{LV}\rvert}{LV}$ *where* O_{LV} *is the closest observed concentration to the limit value concentration (LV) and* M_{LV} *is the correspondingly ranked modelled concentration.* *MRDE=Max (RDE over 90% of stations)*
Relative Percentile Error and its maximum	$RPE = \frac{\lvert O_p - M_p\rvert}{O_p}$ *where* p *is the percentile corresponding to the allowed number of exceedances of the limit value* *MRPE=Max (RPE over 90% of stations)*
Factor of modelled values within a factor of two of observations	$FAC2 = \frac{1}{N}\sum n_i$ *with* $n_i = \begin{cases} 1 \text{ for } 0.5 \le \lvert M_i / O_i\rvert \le 2 \\ 0 \text{ else} \end{cases}$
Centred Root Mean Square error	$CRMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left[(M_i - \overline{M}) - (O_i - \overline{O})\right]^2}$
Model Efficiency Score	$MEF = 1 - RMSE^2$

Model validation

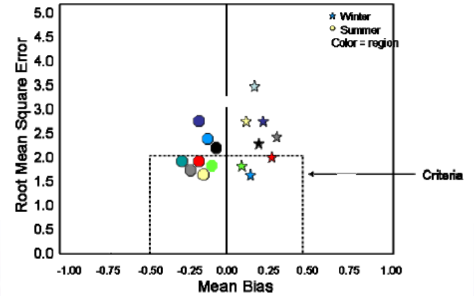
Scatterplots



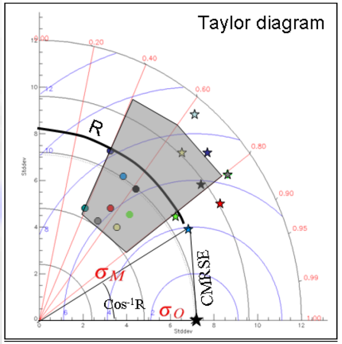
Log/log scatterplots



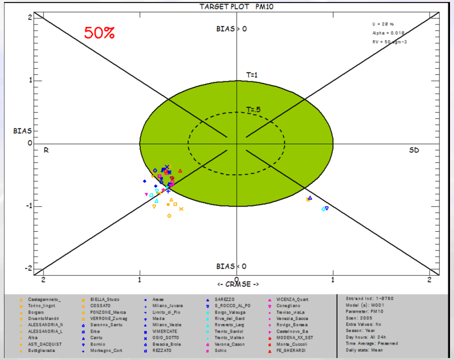
Soccer plots



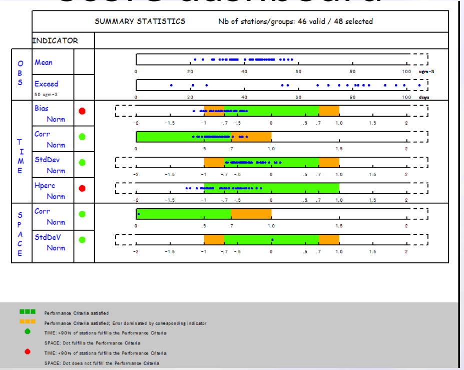
Taylor plots



Target plots



Score dashboard



Fairmode/JRC

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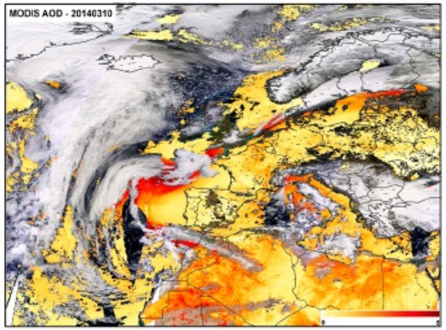
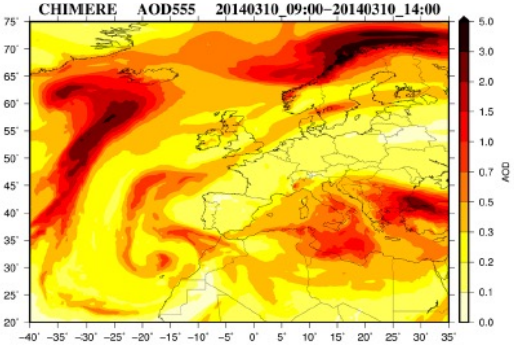
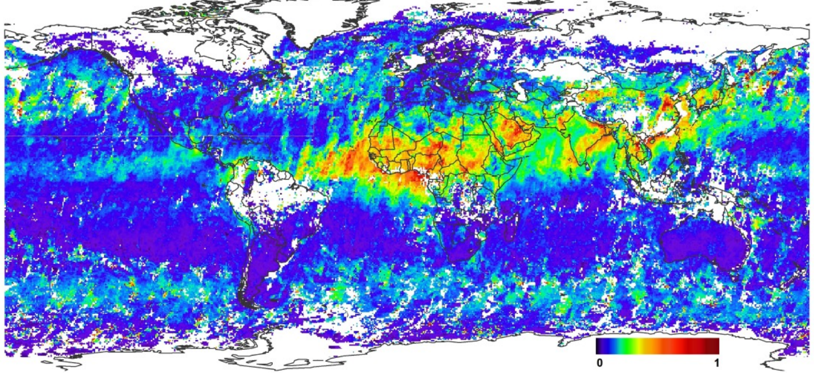
Model validation

Instantaneous comparison of AOD





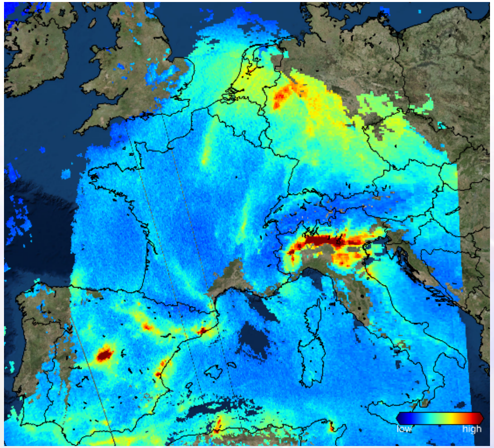
long term average to minimise cloud effect



New perspectives:

TropOMI

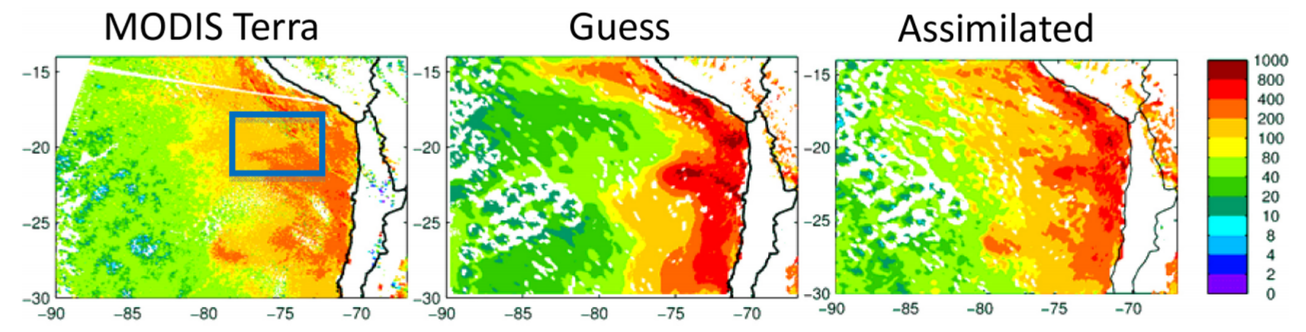
Sentinel 5P launched 2017



Data Assimilation

- Feeding the model online with observations (in situ, satellite…)

- Various approaches :
  - Ensemble (Kalman Filter)
  - Variationnal (3D-Var, 4D-Var):
    - need for a derivation of the model

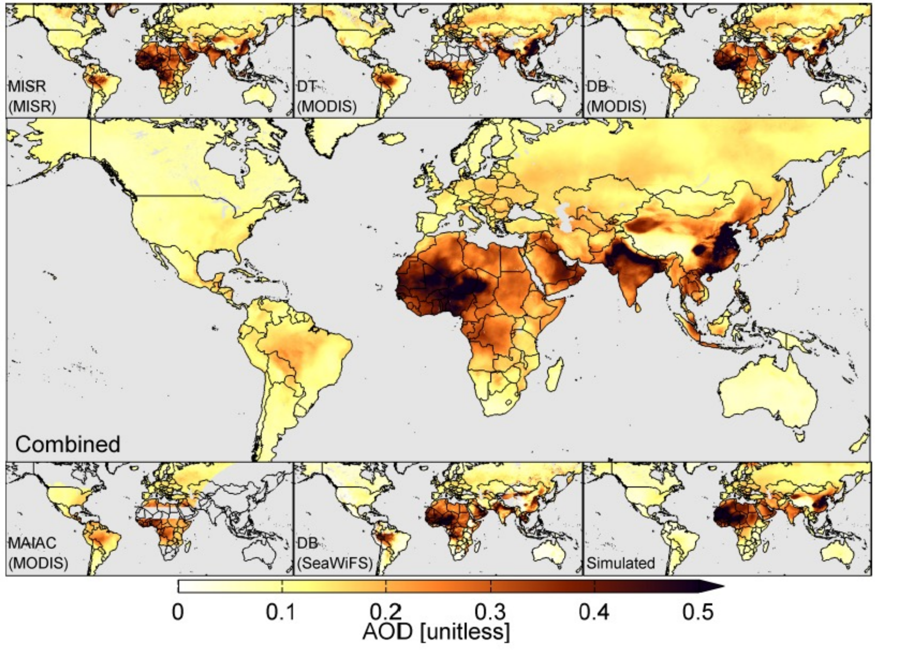


Bocquet et al., ACP 2015

Data fusion

- Correct the model offline (postprocessing) with observations

- Optimal interpolation: Geostatistics (kriging) using a combination of
  - Model
  - In situ
  - Satellite



Von Donkelaar, EST, 2016

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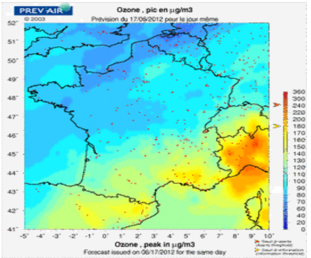
Statistical adaptation

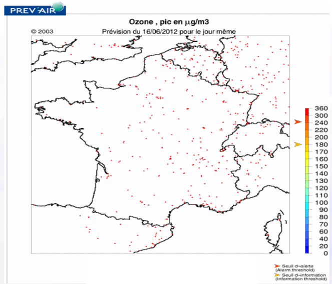
- Weather Forecast
- Emissions
- Landuse
- Boundary Conditions

AQ Model



Deterministic forecast

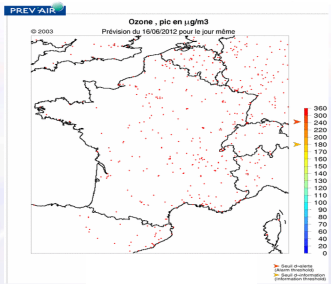
D+1



D+0

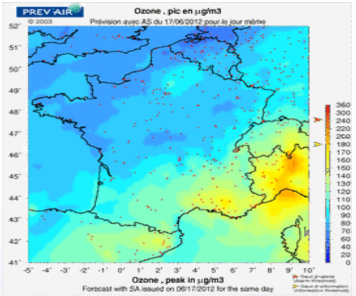
Statistical FC

Statistical forecast at stations



D+1

Hybrid FC



D+1

Combining point statistical forecast to 2D deterministic model with geostastical kriging

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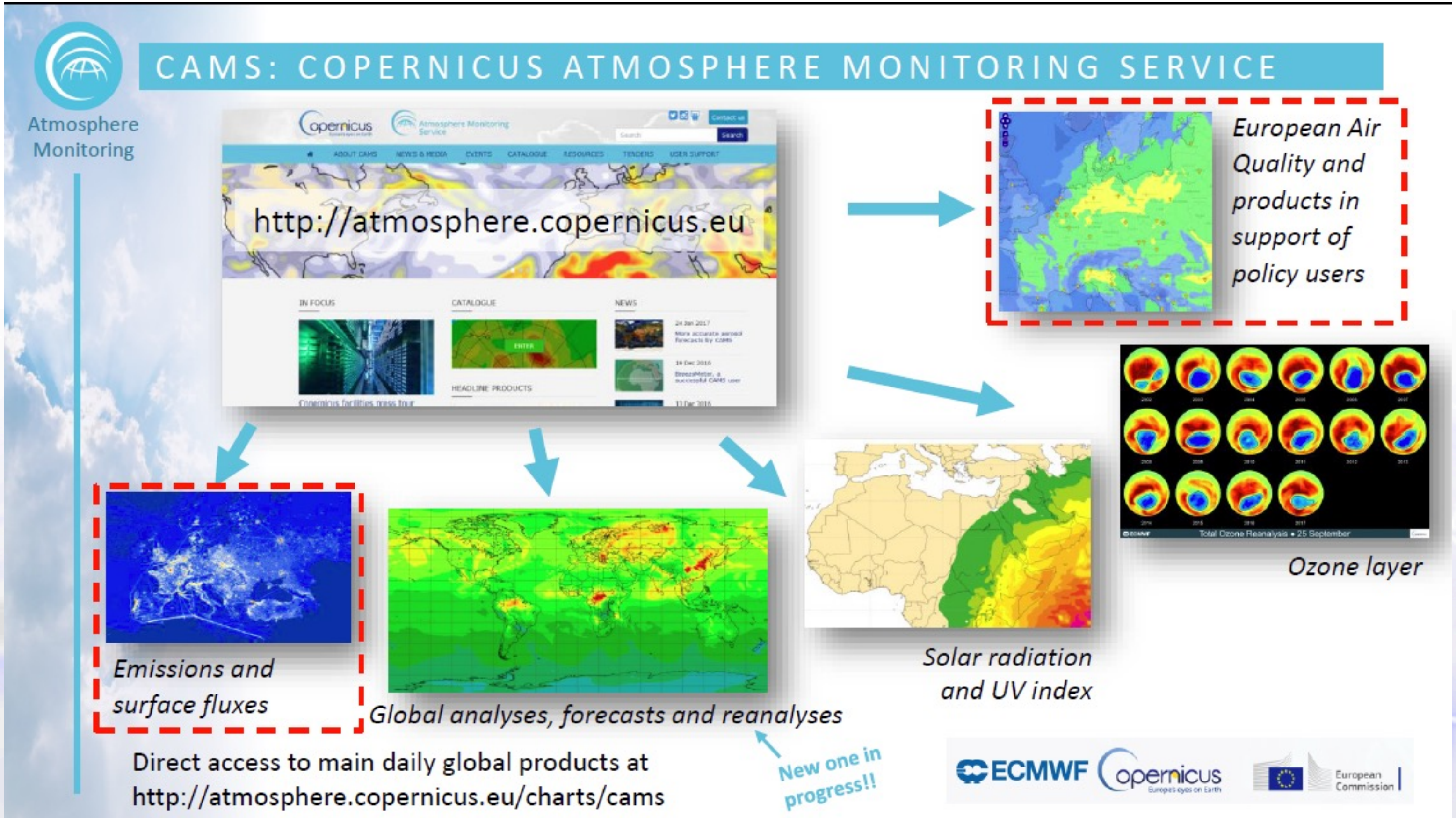
Model use cases

Forecasts: Copernicus Atmospheric Monitoring Service



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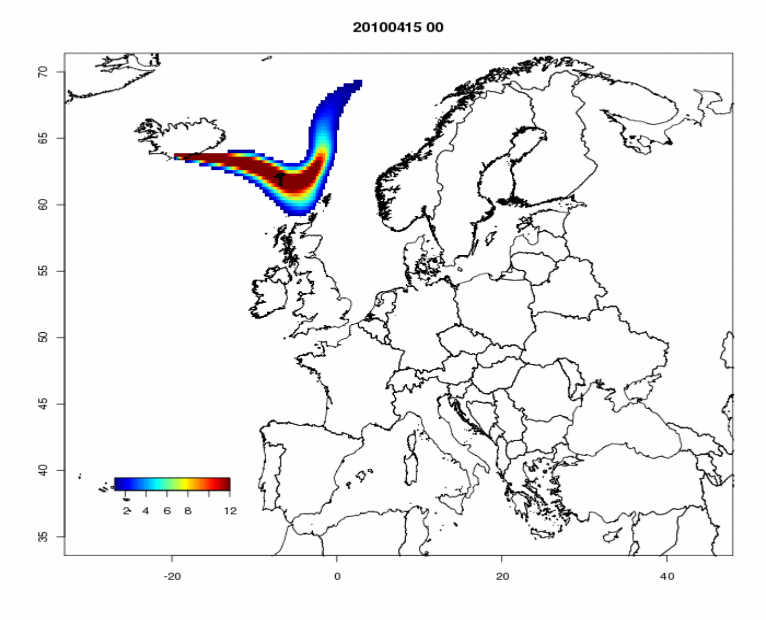
pour un développement durable

Emergency Support

Eyjafjallajökull volcanic eruption, Iceland, 2010



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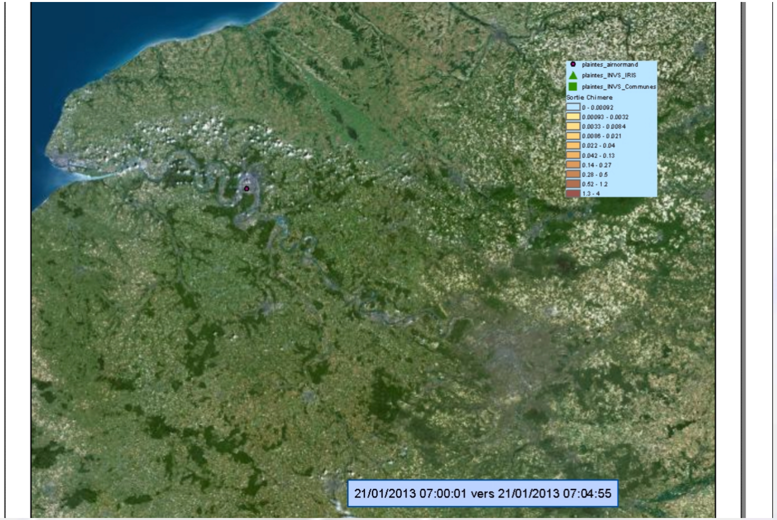
maîtriser le risque
pour un développement durable

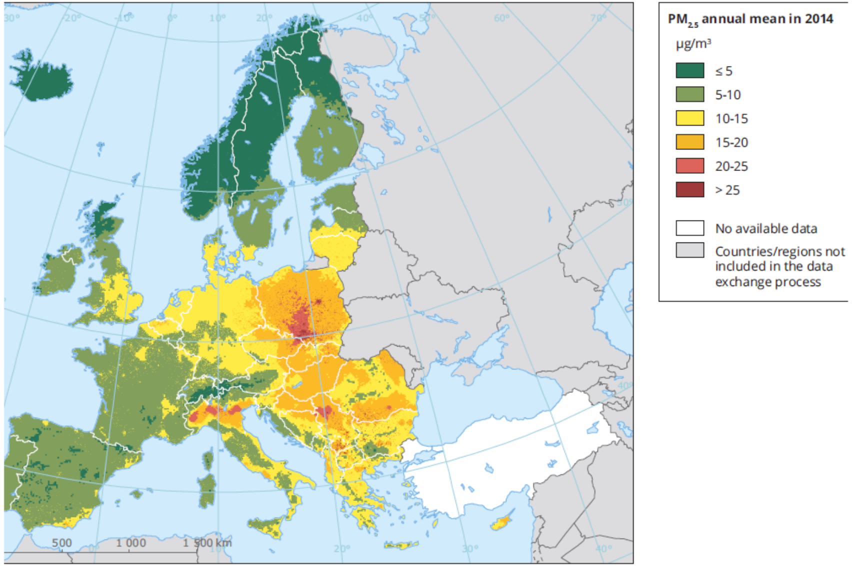
Emergency Support

Lubrizol, industrial mercaptan leak, 2013

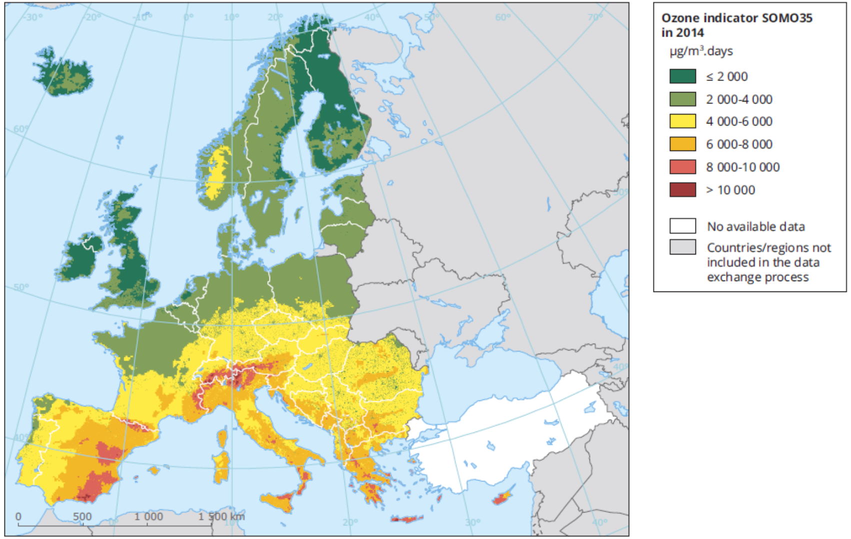


Assessment: long term exposure

PM2.5



Ozone



Sources: ETC/ACM, 2017b, 2017d.

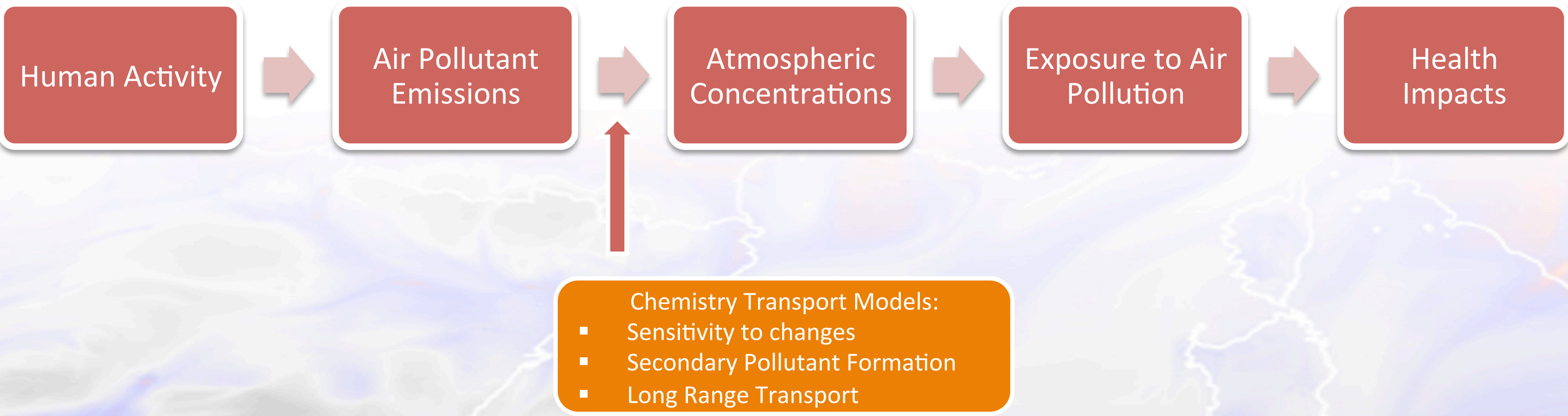
European Environment Agency, 2017 AQ Report

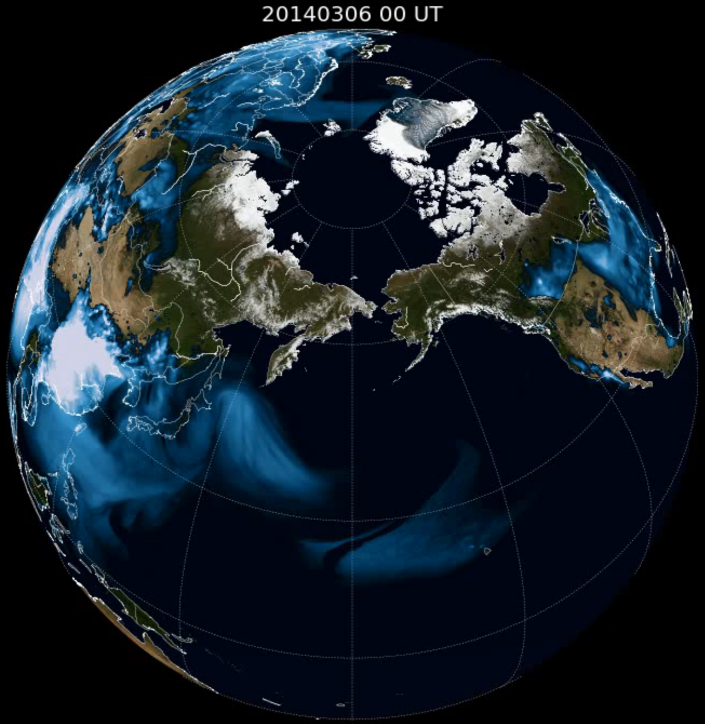
Wrap-Up

- Deterministic air quality models:
  - Complex numerical tools
  - Prone to biases
    - require validation / data fusion / assimilation

- Why using air quality models to assess exposure?

Integrated Assessment





INERIS Youtube Channel
https://youtu.be/xuUsEOL0Lj8