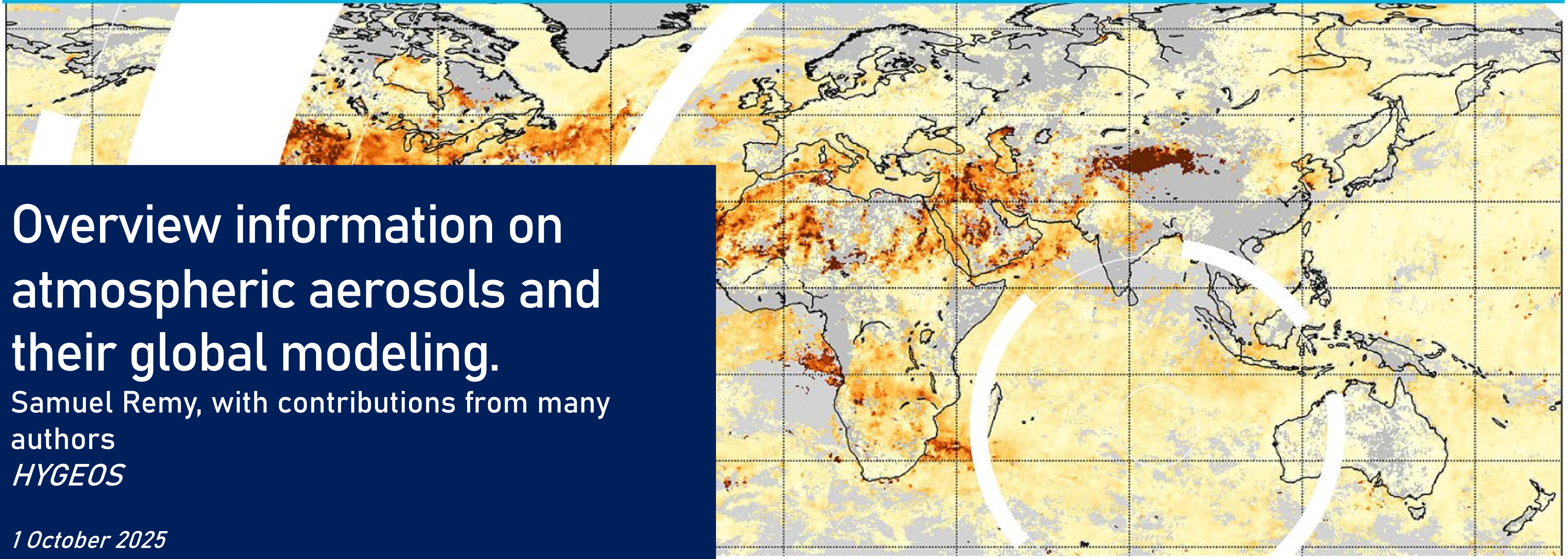
PROGRAMME OF THE EUROPEAN UNION

IMPLEMENTED BY

JOINT TRAINING IN ATMOSPHERIC COMPOSITION

13 -17 OCTOBER 2025, BRUSSELS



Overview information on atmospheric aerosols and their global modeling.

Samuel Remy, with contributions from many authors

HYGEOS

1 October 2025

Agenda

Introduction

Aerosols – why do they matter?

Introduction to CAMS

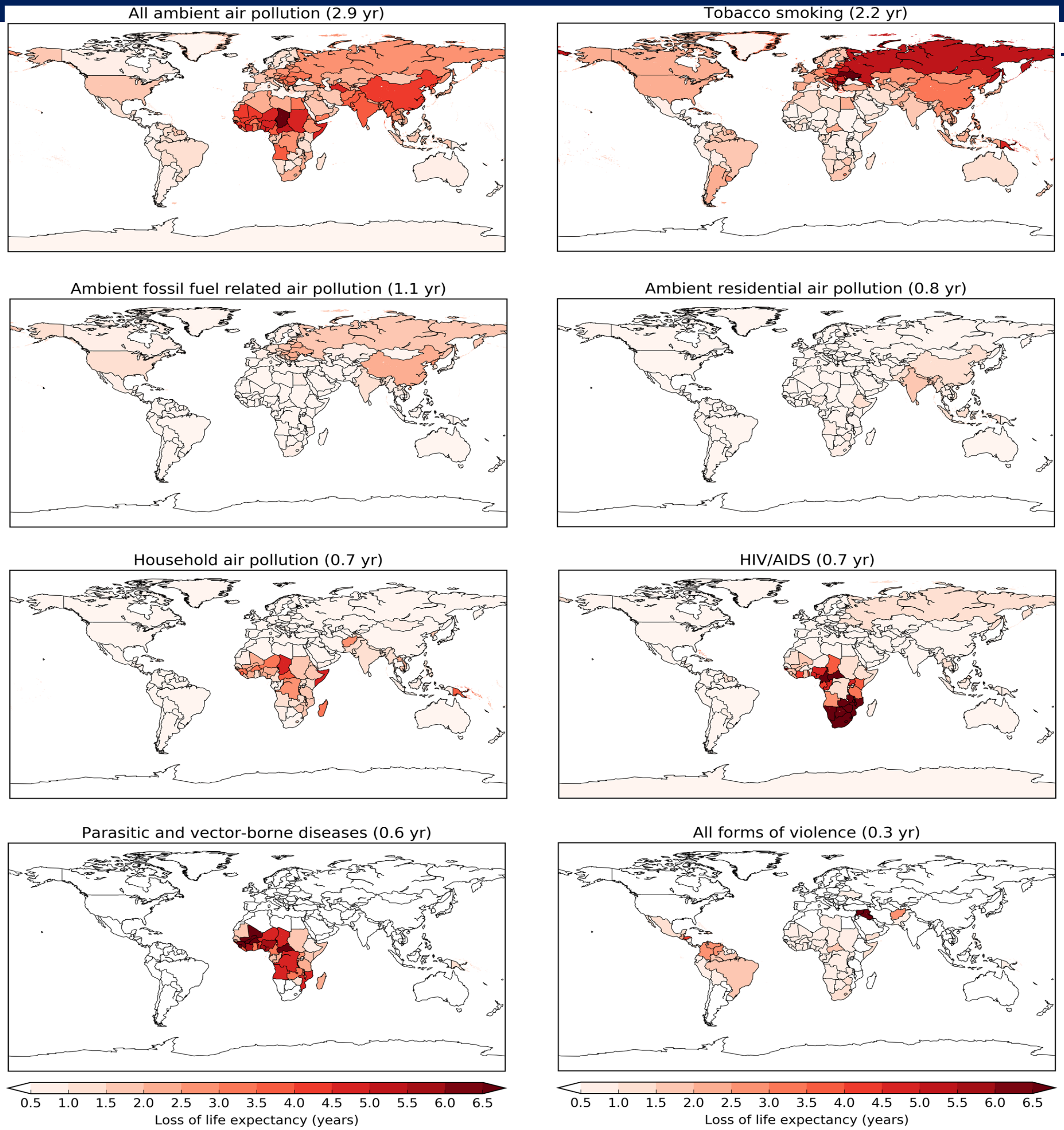
Different aspects of global atmospheric composition modelling

AI/ML for aerosol modelling

Aerosols – why do they matter?

- Aerosols represent a major public health issue
- Estimated loss in life expectancy because of air pollution (PM) :

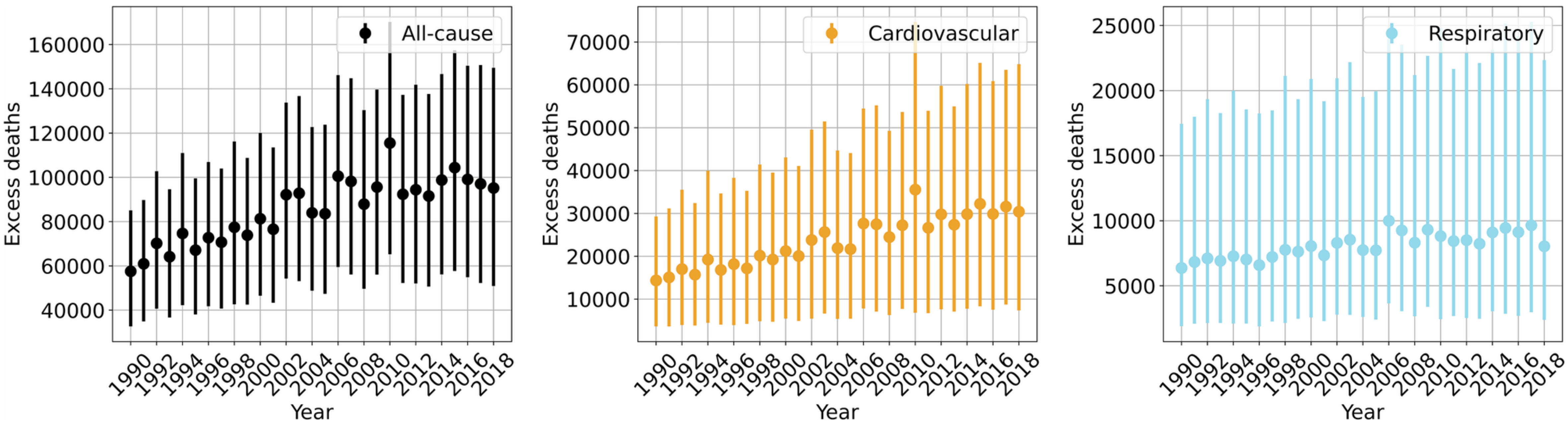
Mean global and country-level loss of life expectancy from different causes of death referring to the year 2015. Household air pollution is from the indoor use of solid biofuels. Ambient residential air pollution is mostly from household sources and can include fossil and biofuel use. Parasitic and vector-borne diseases include malaria, leishmaniasis, rabies, dengue, yellow fever, and others. Violence includes interpersonal, collective conflict, and armed intervention.



Lelieveld et al. 2020: Loss of life expectancy from air pollution compared to other risk factors: a worldwide perspective

Aerosols – why do they matter?

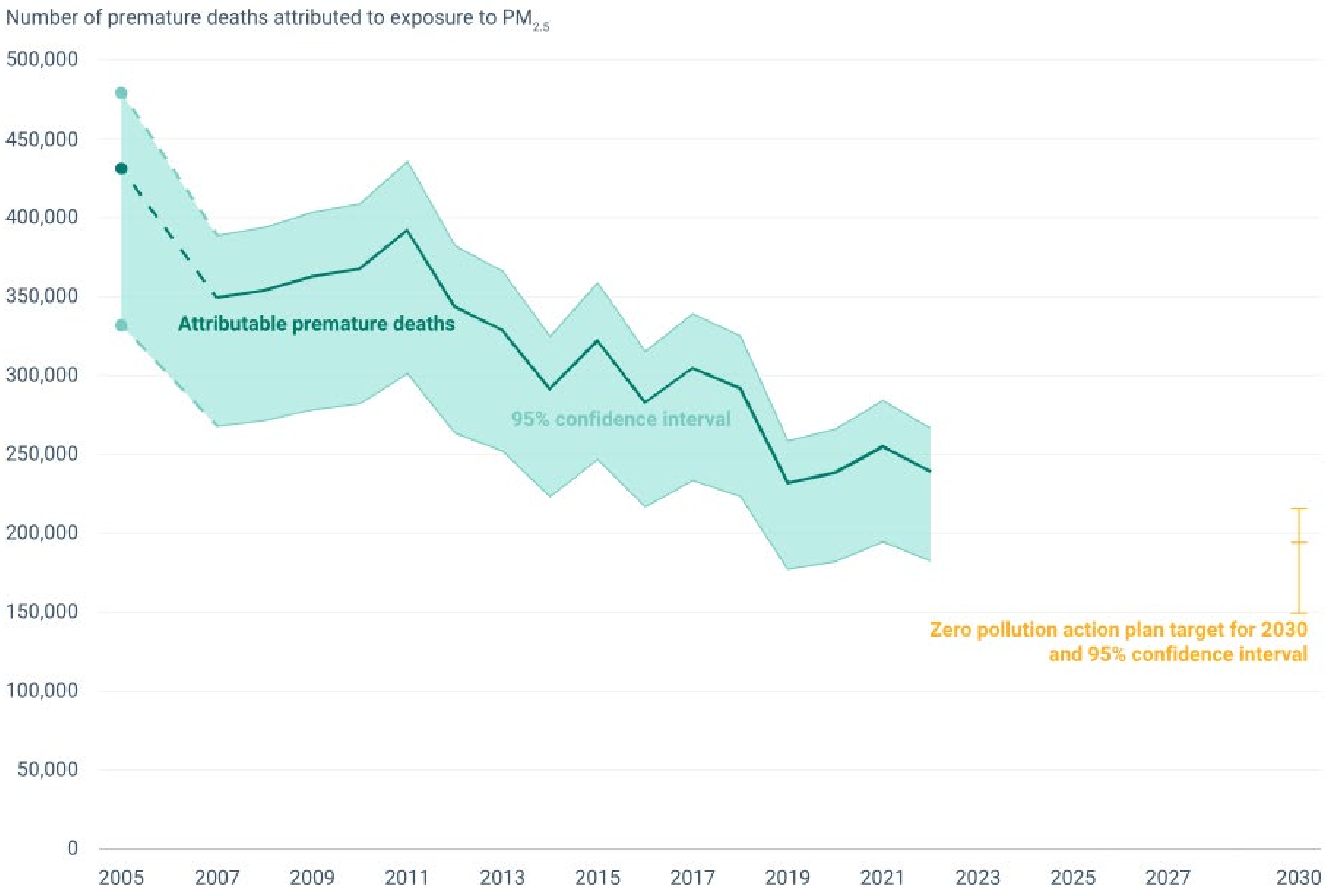
- Aerosols represent a major public health issue
- Estimated excess deaths from exposure to acute fire PM:



Chowdury et al. 2025: Global health burden from acute exposure to fine particles emitted by fires

Aerosols – why do they matter?

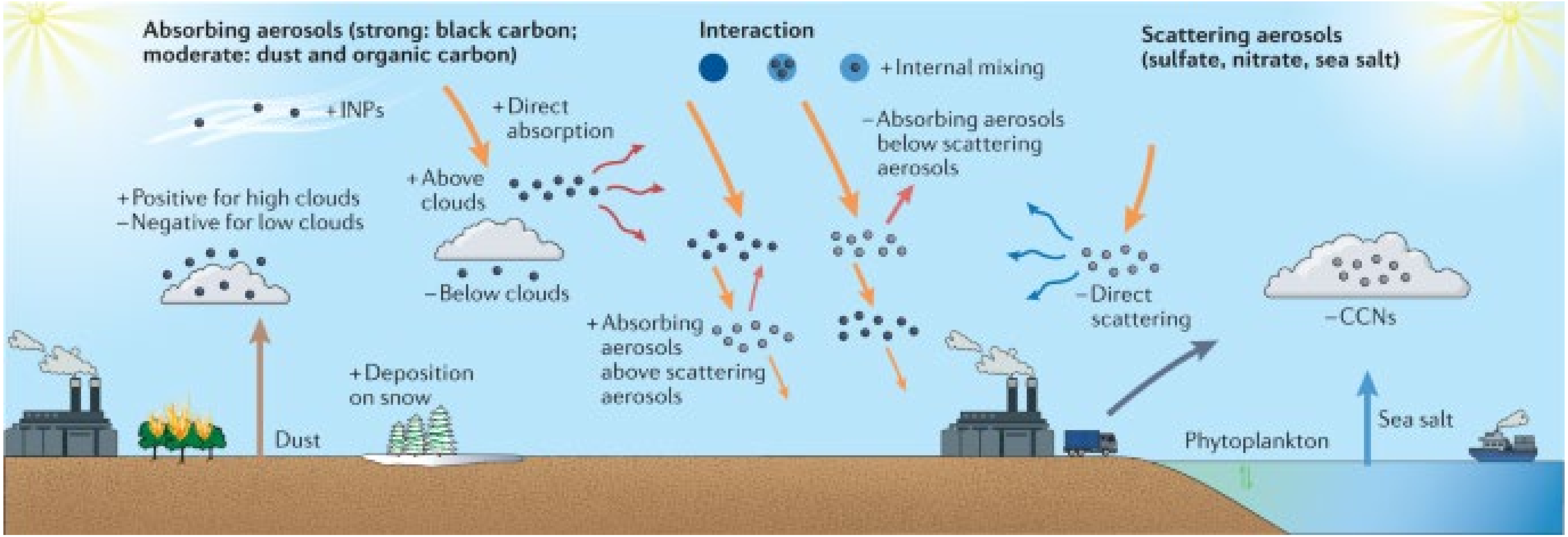
- Aerosols represent a major public health issue
- Premature deaths attributable to exposure to fine particulate matter ($PM_{2.5}$), EU



https://www.eea.europa.eu/en/analysis/indicators/health-impacts-of-exposure-to

Aerosols – why do they matter?

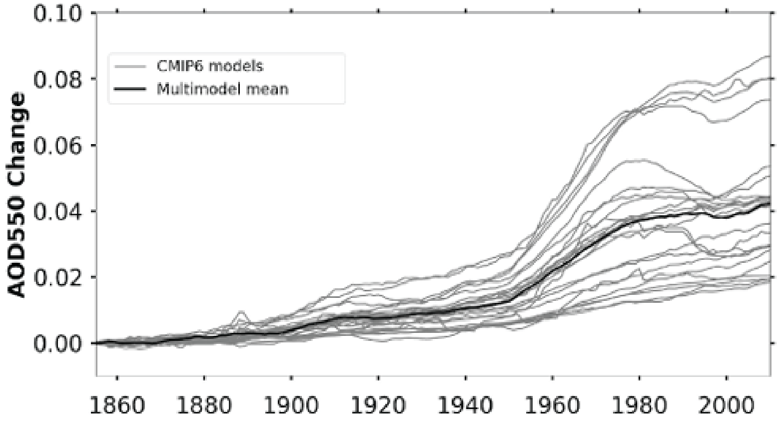
- Aerosols interact with weather – radiation and clouds



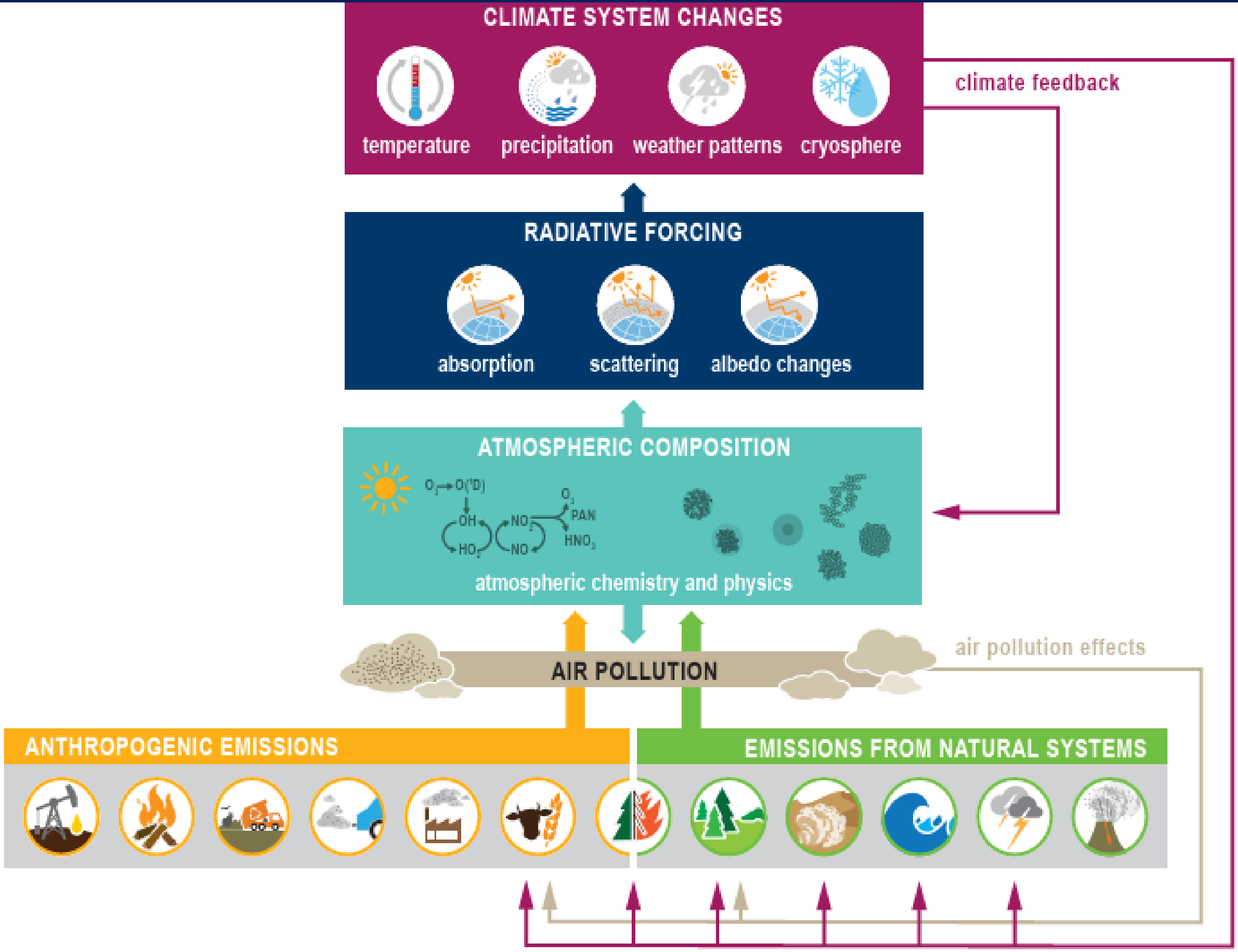
Li et al. 2022: Scattering and absorbing aerosols in the climate system

Aerosols – why do they matter?

- Aerosols interact with weather – radiation and clouds



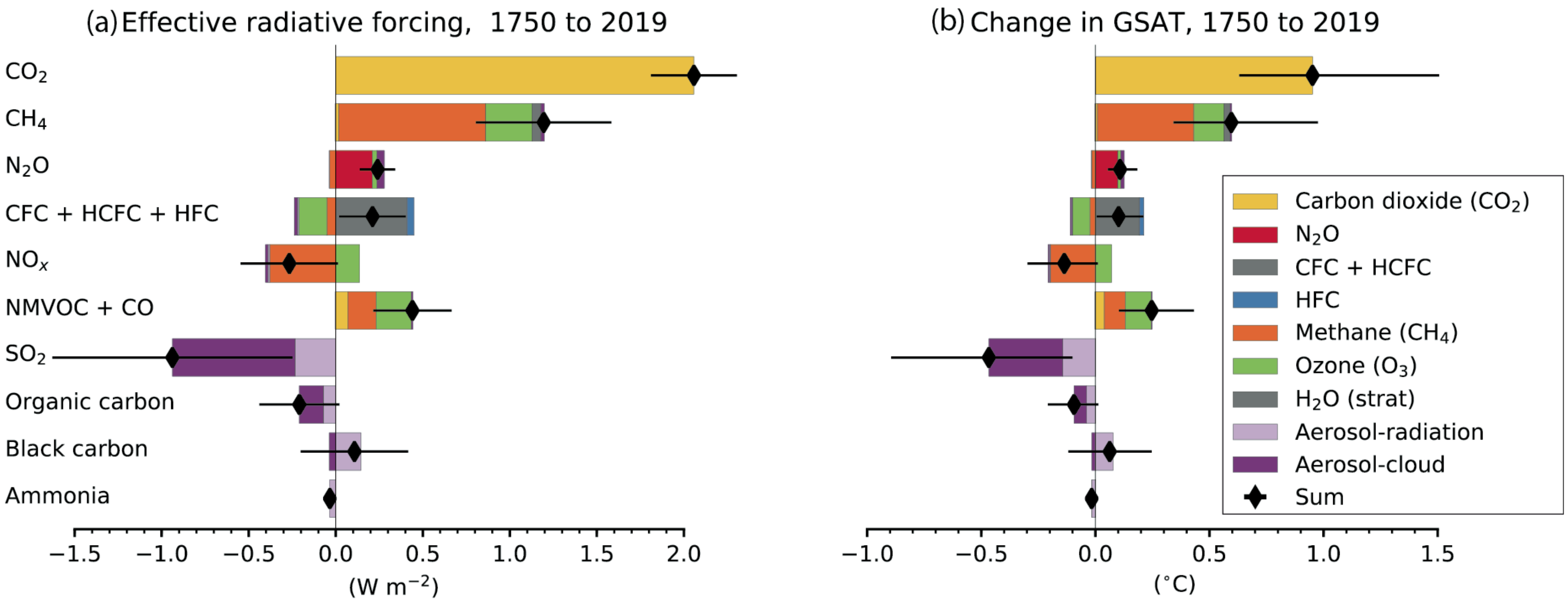
Time evolution of changes in global mean aerosol optical depth (AOD) at 550 nm



IPCC AR6 (Short Lived climate forcers) – Szopa et al 2021

Aerosols – why do they matter?

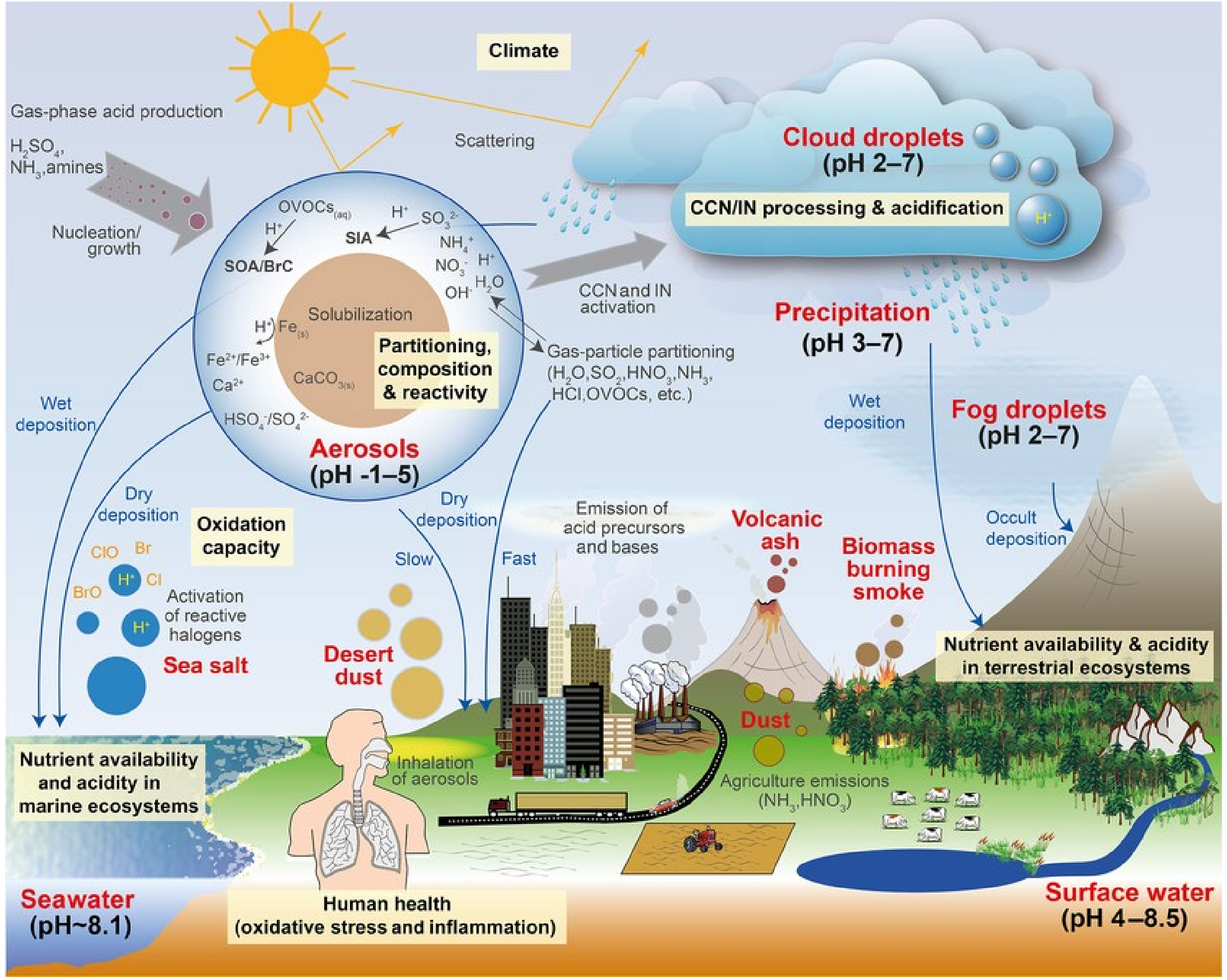
- Aerosols interact with weather – radiation and clouds



IPCC AR6 (Short Lived climate forcers) – Szopa et al 2021

Aerosols – why do they matter?

- Aerosols and gases impact the acidity of precipitation

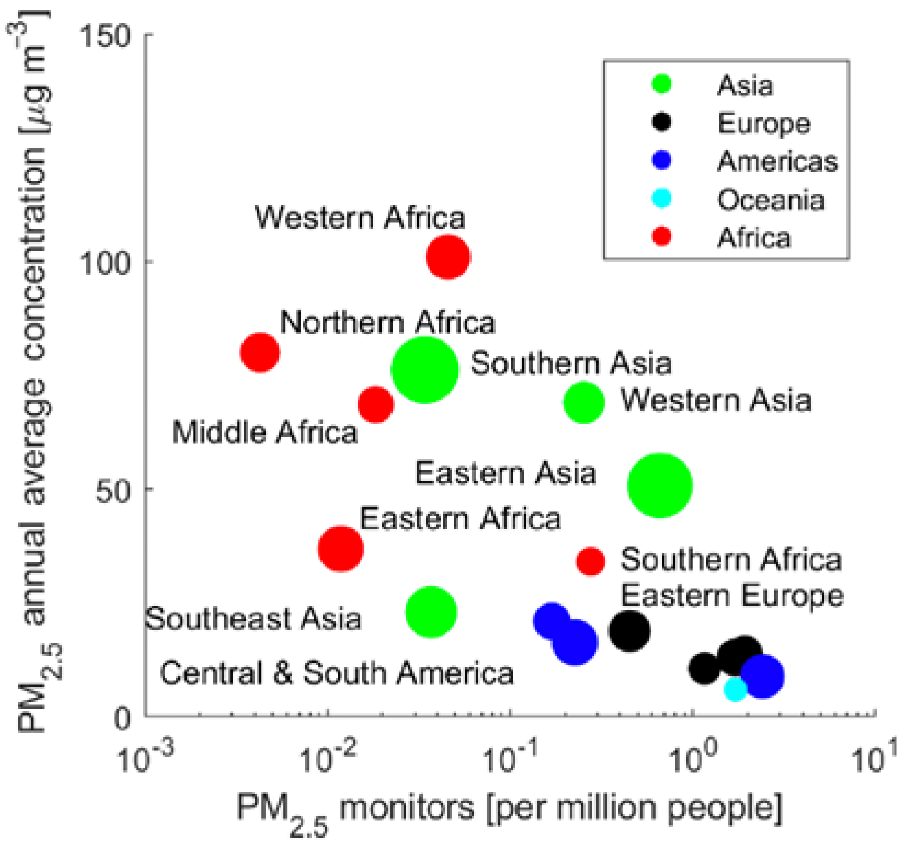


Pye et al (2020)

Sources and receptors of aerosol and cloud droplet acidity. Major primary sources and occurrence in the atmosphere are identified in bold red text: sea salt, dust, and biomass burning (sources); and aerosols, fog droplets, cloud droplets, and precipitation (occurrence). Key aerosol processes are indicated by arrows and gray text: nucleation/growth, light scattering, cloud condensation nuclei (CCN) and ice nuclei (IN) activation, and gas-particle partitioning. Sinks (wet, dry, and occult deposition) are indicated by blue lines and text. The effects that aerosols have in the atmosphere, and on terrestrial and marine ecosystems and human health, are highlighted in pale yellow boxes. Approximate pH ranges of aqueous aerosols and droplets, seawater, and terrestrial surface waters are also given.

Why do we need atmospheric composition models?

- Test our theories and understanding
- Provide air quality information in areas with a lack of observations
  - Spatial coverage
  - Temporal coverage (consistent time series)
  - Species and processes not well observed such as deposition
- Make air pollutions forecasts for the next days (or historic periods)
- Support air quality policy measures (impact emission reductions)
- Test and support validity of observations and support satellite retrievals



Estimated annual PM2.5 concentration versus density of (regulatory-grade) monitoring stations). Figure from Malings et al (2020).

Why do we need atmospheric compo

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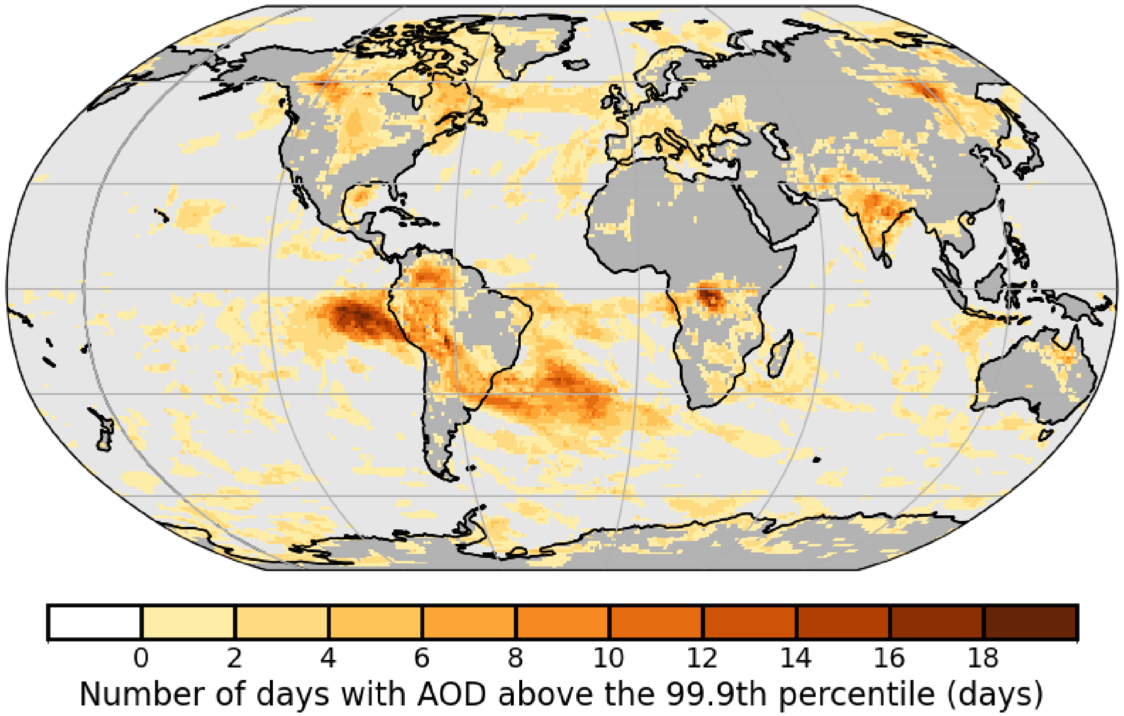
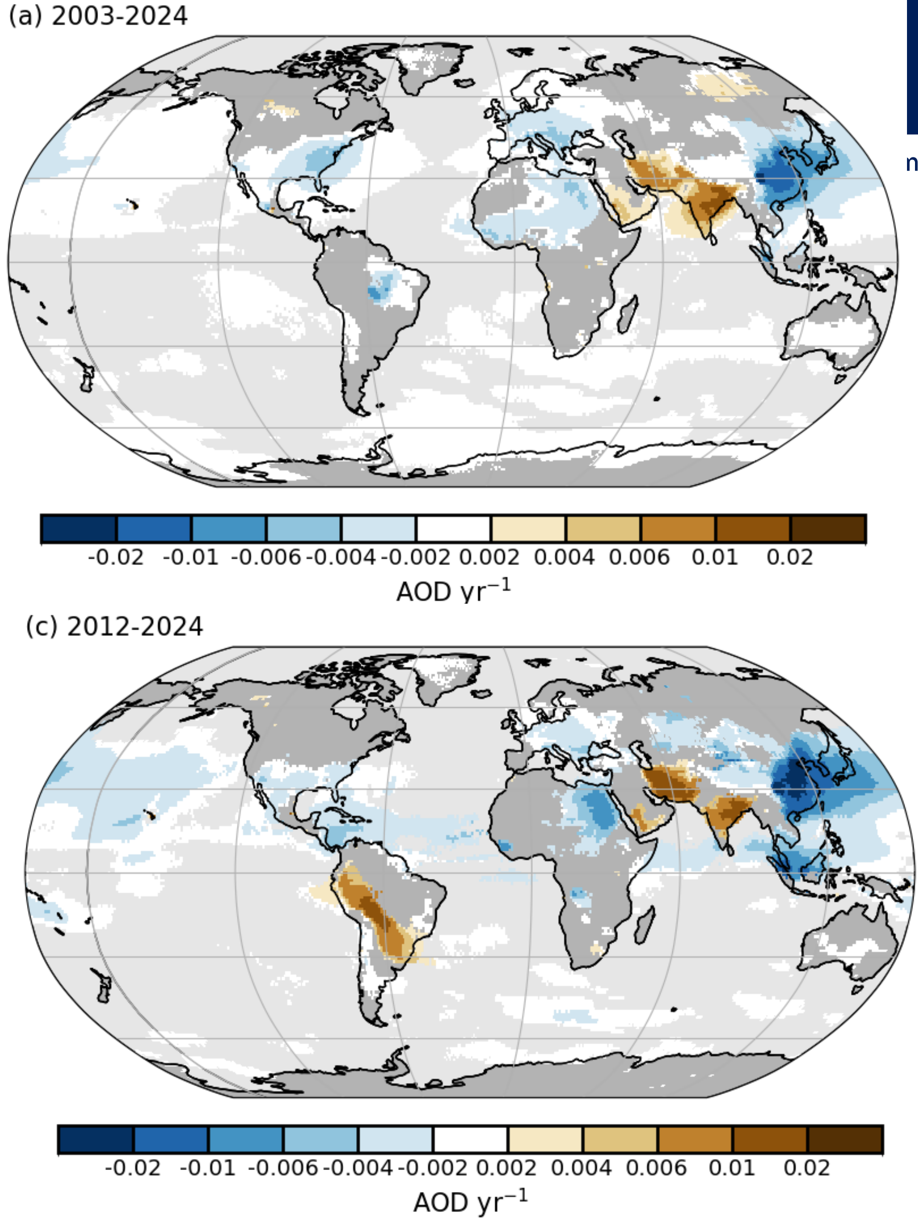
- **Temporal coverage (consistent time series)**



Number of extreme AOD at 550nm days from the CAMS Reanalysis. Aerosol section of the BAMS State of the climate 2024



AOD at 550nm trend sin 2003-2024 and 2012-2024 from the CAMS Reanalysis. Aerosol section of the BAMS State of the climate 2024

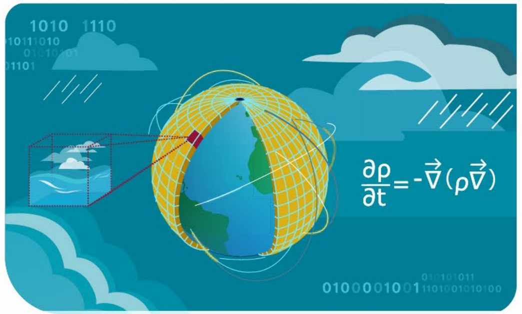
Copernicus Atmosphere Monitoring Service

CAMS is one of six thematic information services provided by the Copernicus Earth Observation Programme of the European Union.

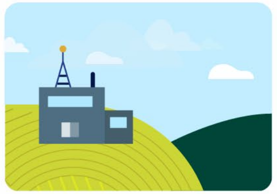
CAMS provides consistent and quality-controlled information related to air pollution and health, solar energy, greenhouse gases and climate forcing, everywhere in the world.

AIR QUALITY OBSERVATIONS

MODELLING



OUTPUTS



1. Monitoring the current situation

- Air quality
- Solar radiation
- Greenhouse gases
- Fire emissions

2. Forecasts for the next few days

- Global
- Europe

3. Tools to explore further

- Emissions and impact of reductions
- Origins of pollution
- Annual air quality assessments

USERS

- Industry
- Businesses
- Government and policymakers
- Scientific community
- The public

CAMS Workflow

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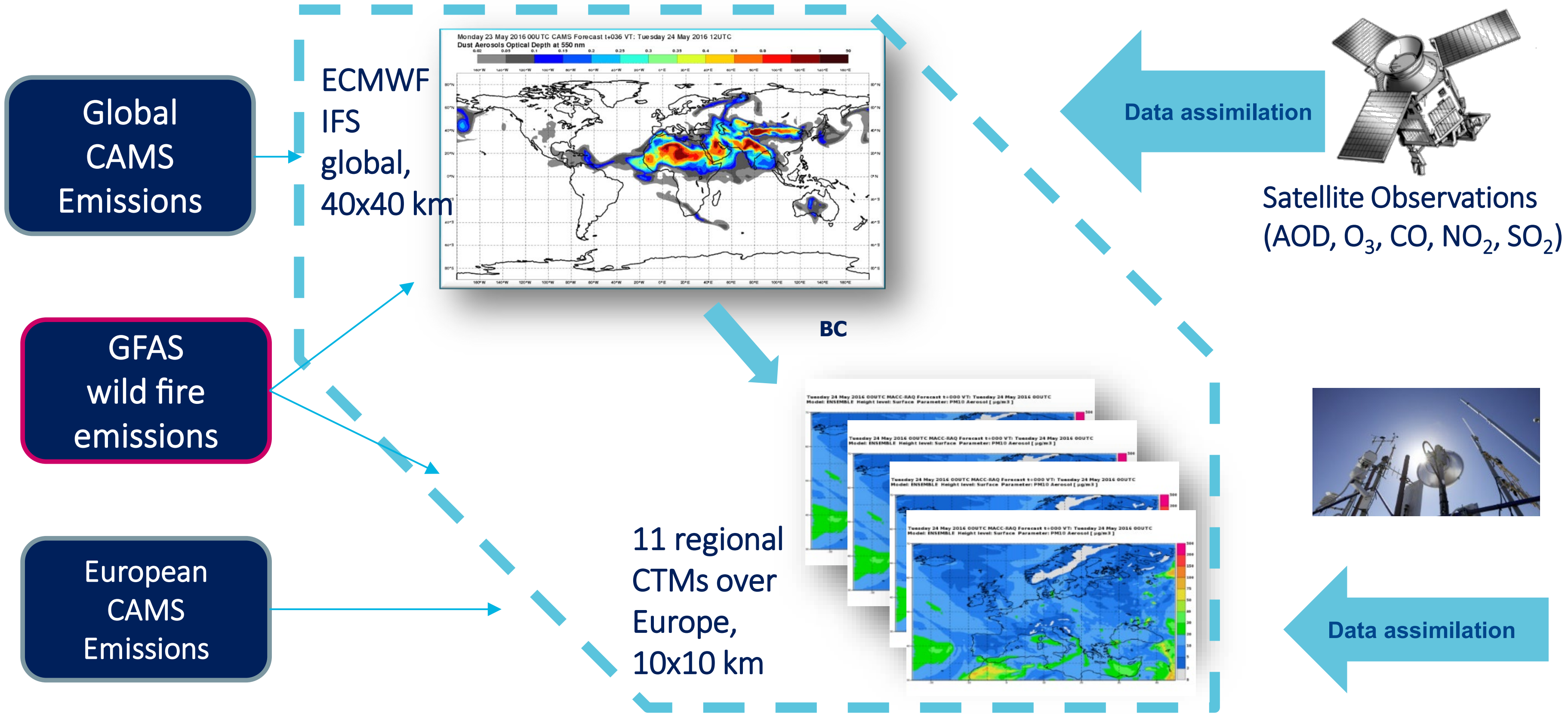
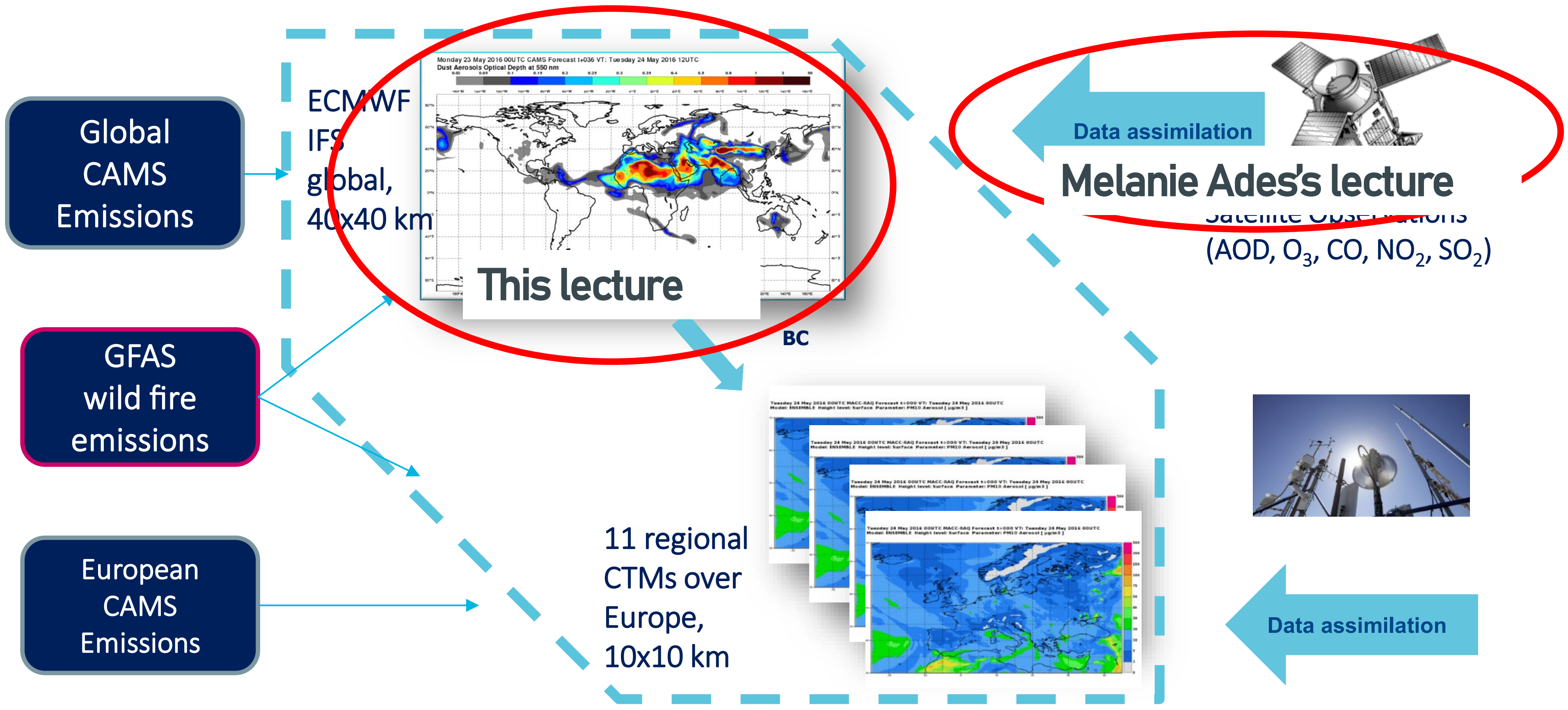
CAMS includes a global and a regional component

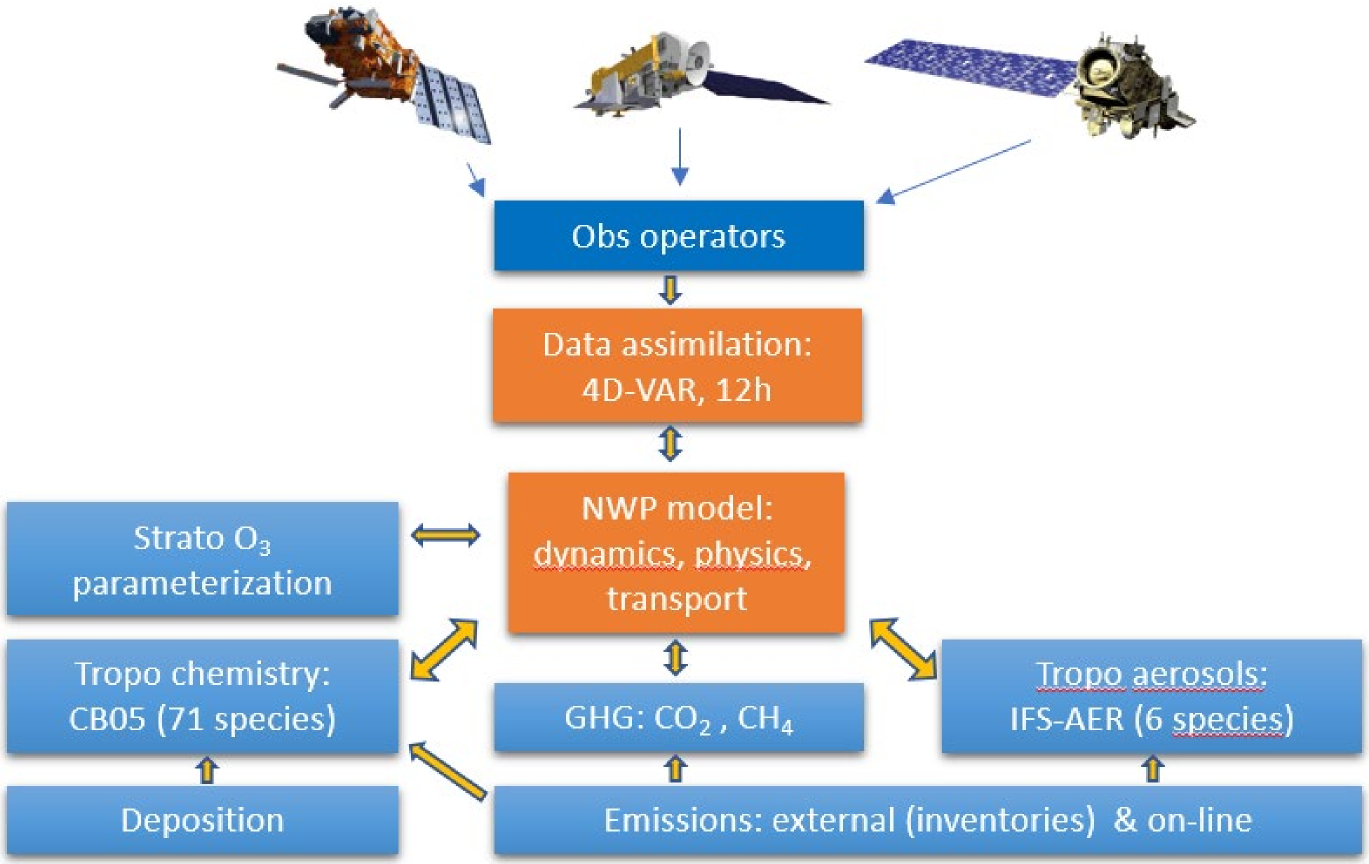


CAMS includes a global and a regional component



The CAMS global system : IFS-COMPO

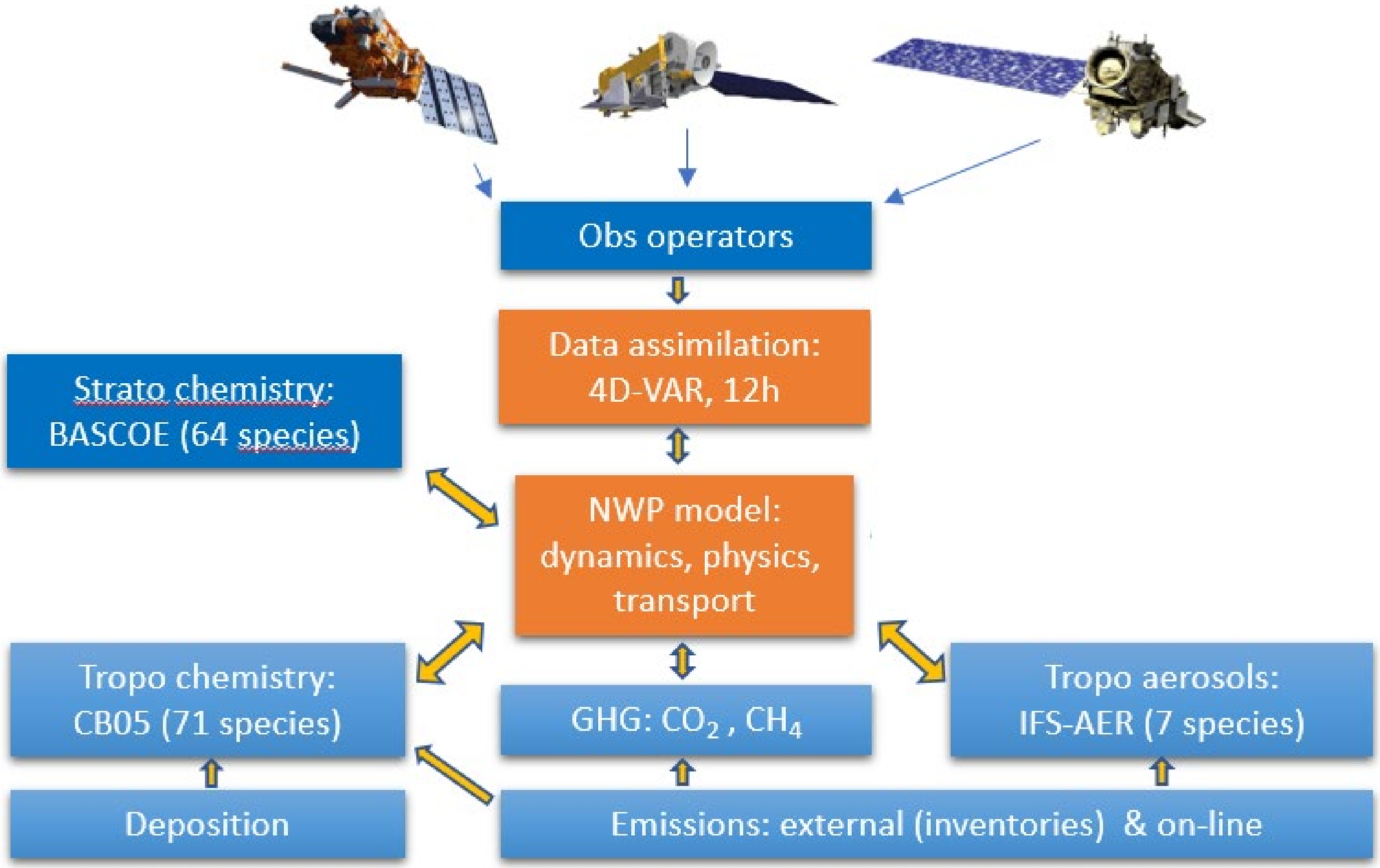
IFS-COMPO is the ECMWF Integrated Forecasting System (IFS – the Numerical Weather Prediction system) with atmospheric composition extensions



Cycle 47R3 IFS-COMPO (operational July 2021 – June 2023)

The CAMS global system : IFS-COMPO

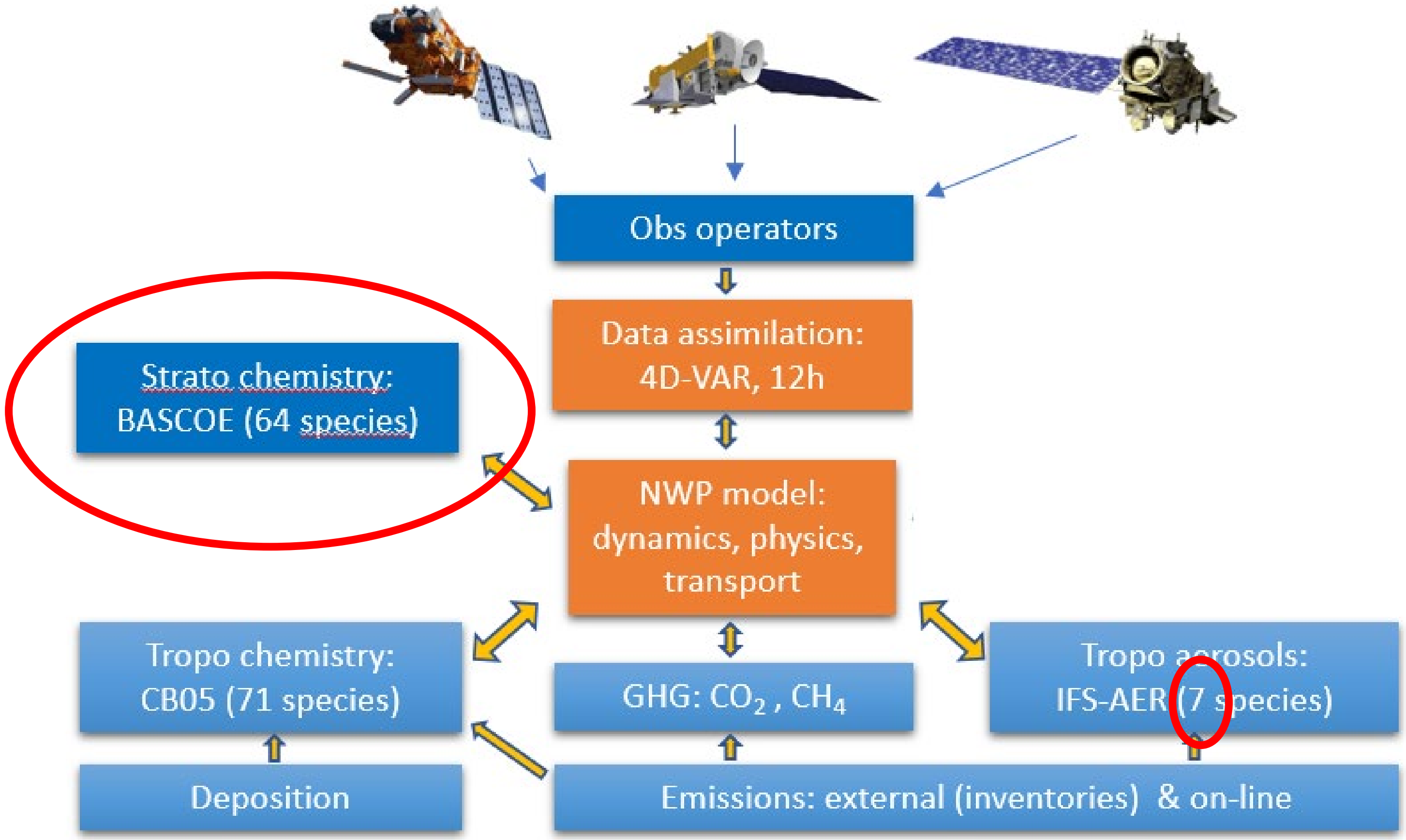
IFS-COMPO is the ECMWF Integrated Forecasting System (IFS – the Numerical Weather Prediction system) with atmospheric composition extensions



Cycle 48R1 IFS-COMPO (operational June 2023 – November 2024)

The CAMS global system : IFS-COMPO

IFS-COMPO is the ECMWF Integrated Forecasting System (IFS – the Numerical Weather Prediction system) with atmospheric composition extensions



Cycle 48R1 IFS-COMPO (operational June 2023 – November 2024)

The CAMS global system : IFS-COMPO

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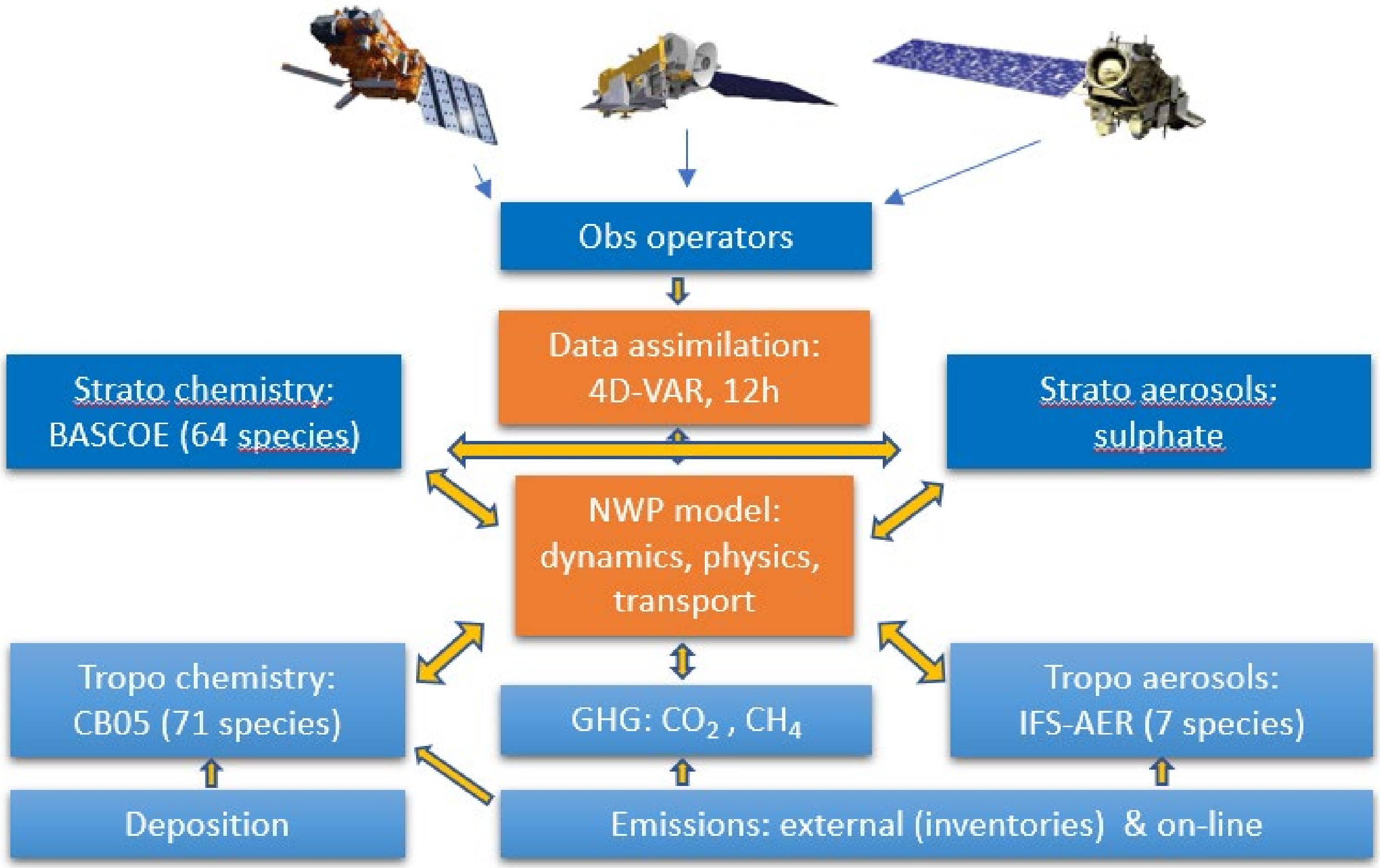
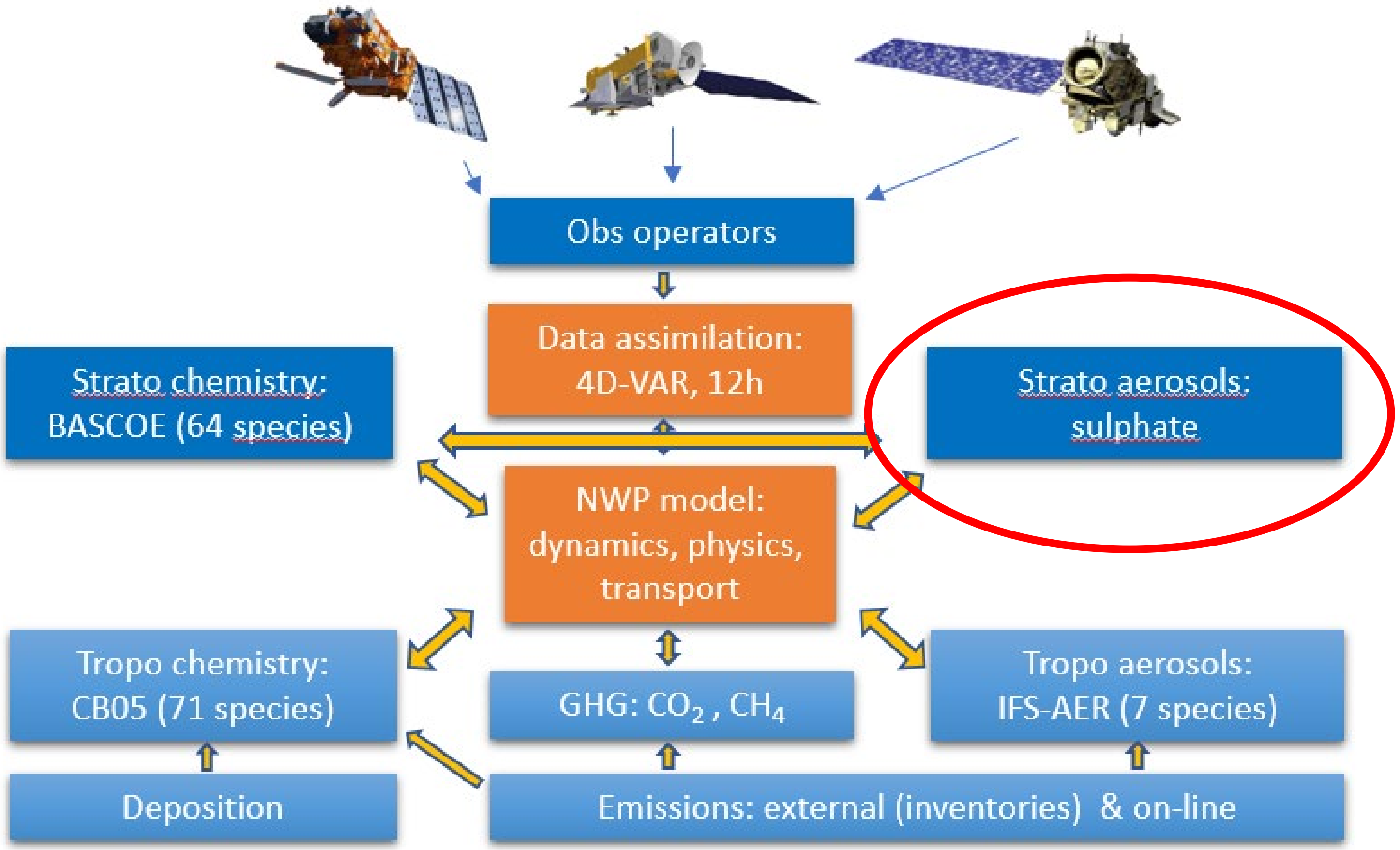
IFS-COMPO is the ECMWF Integrated Forecasting System (IFS – the Numerical Weather Prediction system) with atmospheric composition extensions



Cycle 49R1 IFS-COMPO (operational November 2024 -)

The CAMS global system : IFS-COMPO

IFS-COMPO is the ECMWF Integrated Forecasting System (IFS – the Numerical Weather Prediction system) with atmospheric composition extensions



Cycle 49R1 IFS-COMPO (operational November 2024 -)

The CAMS global system : IFS-COMPO

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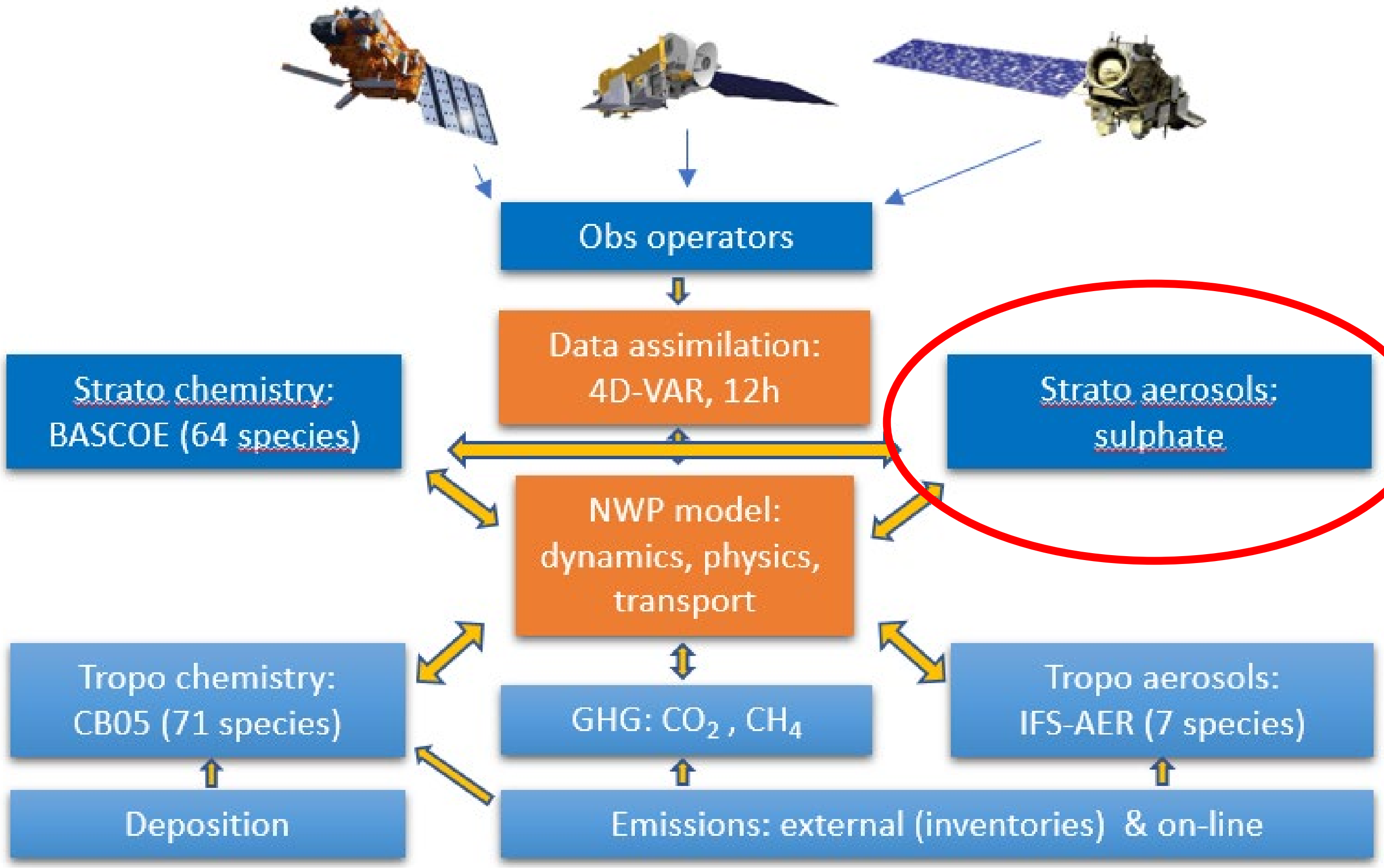


More about stratospheric aerosols in the talk by V. Sofieva.

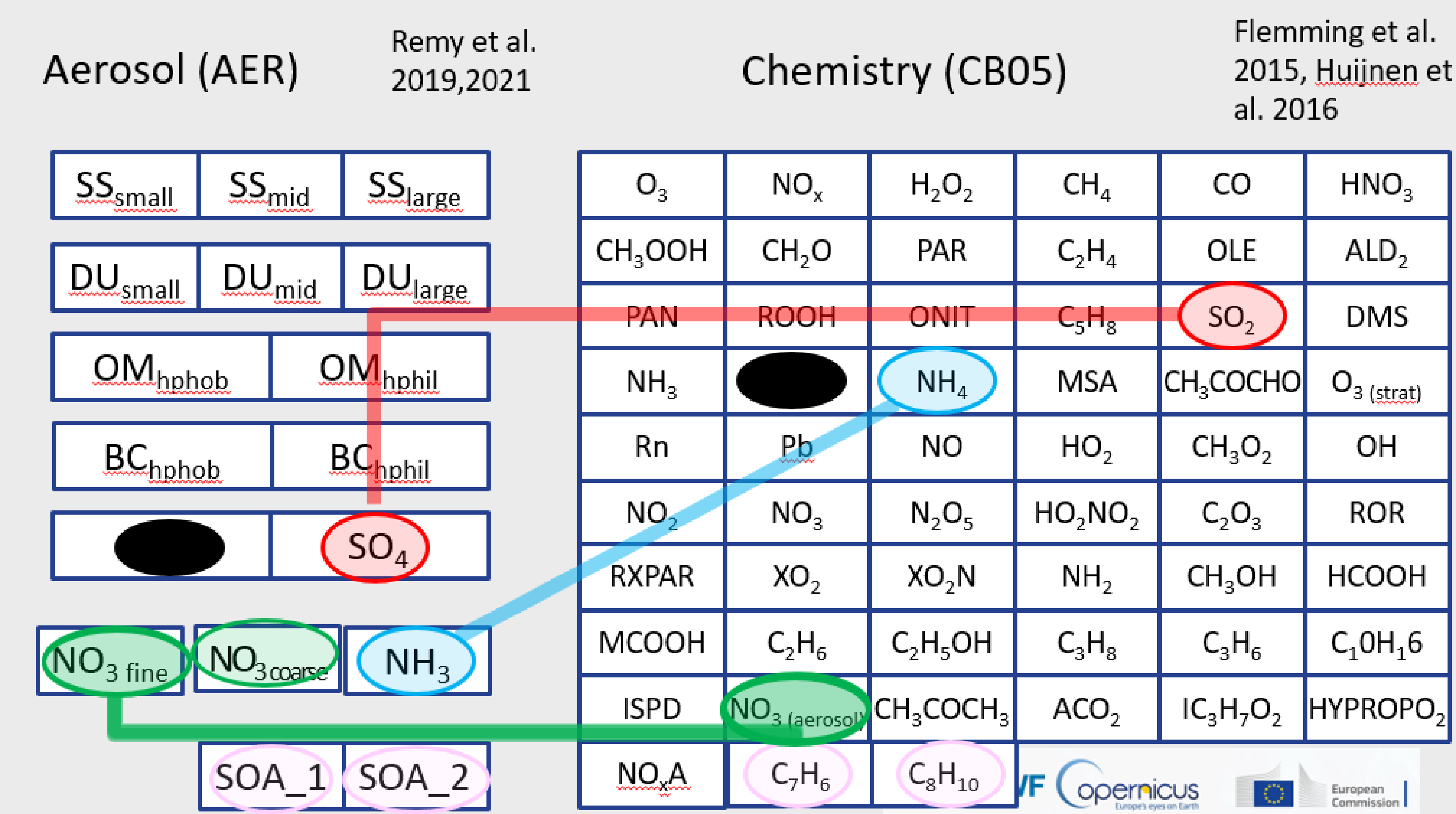
Cycle 49R1 IFS-COMPO (operational November 2024 -)

Aerosols in IFS-COMPO

- 8 species considered:
  - Desert dust (DD): 3 tracers
  - Sea-salt aerosol (SS): 3 tracers
  - Organic Matter (OM): 2 tracers
  - Black carbon (BC): 2 tracers
  - Sulfate (SO4) + precursor SO2 when running uncoupled from chemistry
  - Nitrate: 2 tracers (from gas/particle partitioning, and from het. reactions) since cycle 46R1
  - Ammonium: 1 tracer since cycle 46R1
  - SOA: 2 tracers (biogenic and anthropogenic) since cycle 48R1
- Bulk/bin approach : bulk for OM/BC/SO4, 3 size bins for SS/DD
- For OM and BC, hydrophobic (fresh) and hydrophilic (aged) components are considered
- Sea-salt aerosol and Sulfate are also hydrophilic
- 16 tracers representing dry aerosol mass mixing ratio **except for sea-salt aerosol: mass mixing ratio at 80% RH**
- IFS-AER is relatively cheap: in its cycle 48R1 version, it represents only 0.8% of the computing cost of a model integration (including tropospheric and stratospheric chemistry)
- AER variants are implemented in the IFS, in OpenIFS/AC (cycle 43R3) and in the CNRM climate model (TACTIC, Michou et al. 2015)

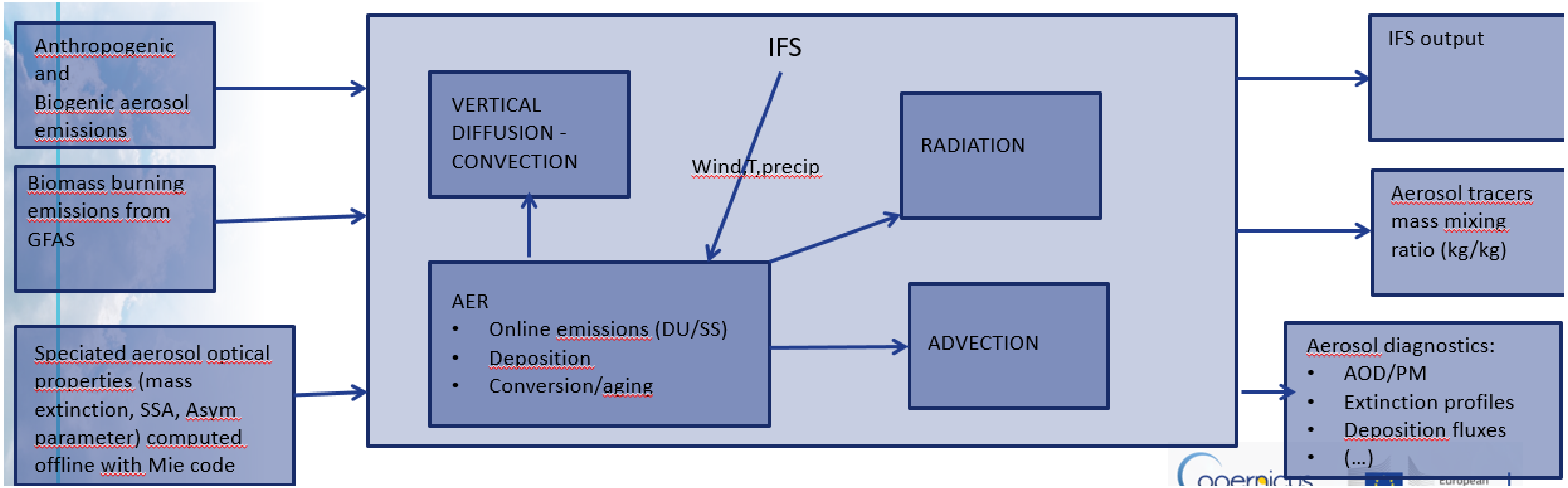
Aerosols and chemistry coupling in IFS-COMPO

- Originally aerosols were standalone in IFS-COMPO – no interaction with chemistry
- Production rates of sulphate and SOA are provided by chemistry
- Production rate of nitrate/ammonium are computed by EQSAM4Clim using gaseous and particulate inputs
- Other couplings : use of aerosol input in chemical photolysis and heterogeneous reactions



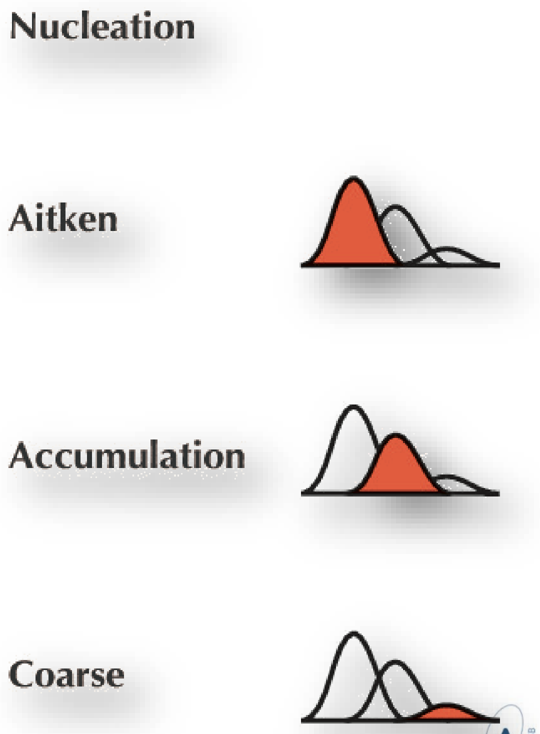
Aerosols in IFS-COMPO

- Originally developed by J.J. Morcrette and O. Boucher during the GEMS project (2006-2008)
- Designed as a part of the ECWMF Integrated Forecasting System (IFS)
- First versions were standalone, ie not coupled with chemistry
- Coupling with radiation (direct effect) implemented from the start
- No coupling with clouds/microphysics

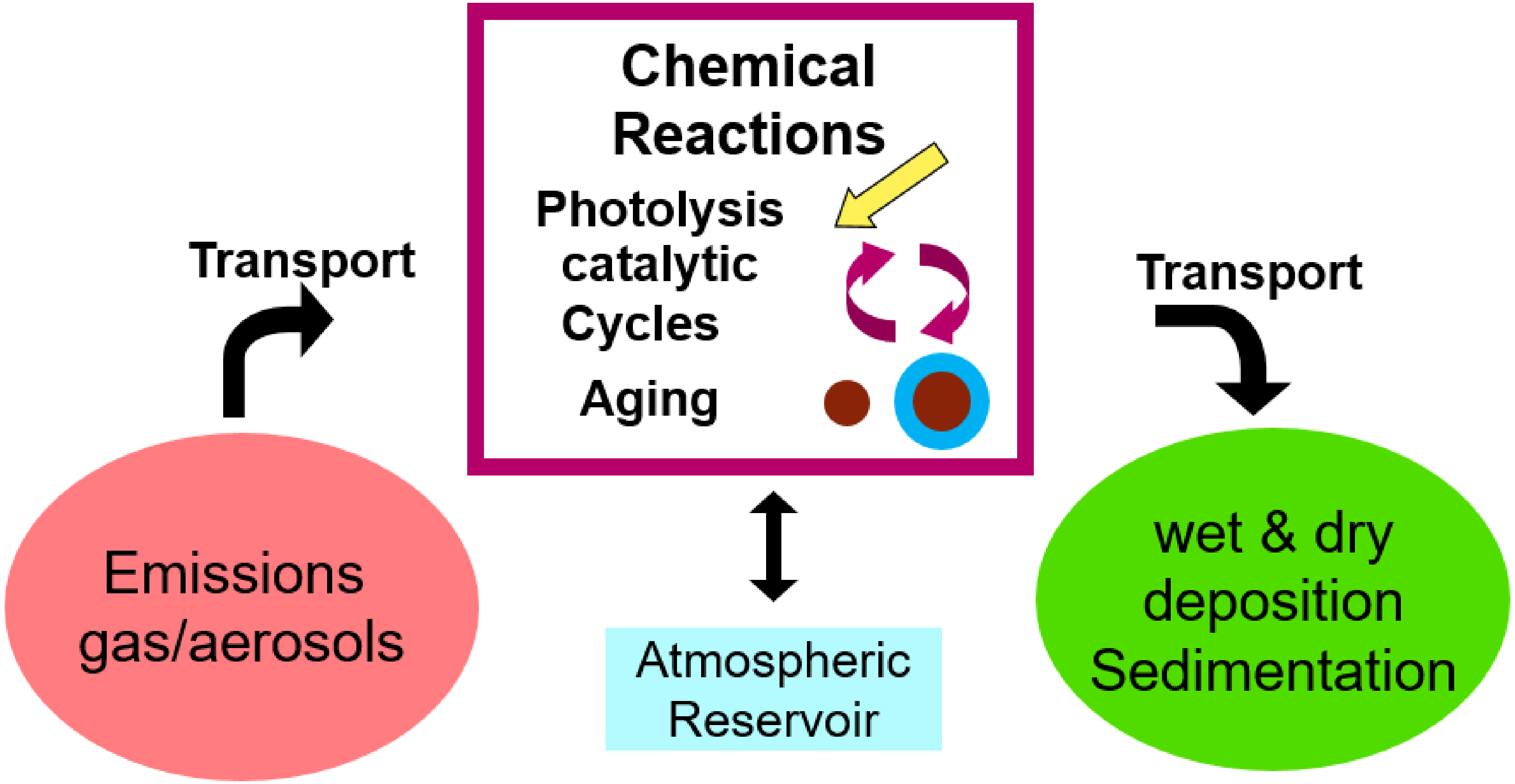


Aerosol modelling : sectional versus modal approach

- Modal approach is often closer to observed reality
- Modal approach allows for an easier coupling with clouds and microphysics
- Sectional/bulk approach can be cheaper computationally
- Modal approach often more complex, but additional complixity doesn't always translate in improved skill!



General processes in Atmospheric composition



Mass balance equation for chemical and aerosol species

$$\frac{\partial c_i}{\partial t} + \mathbf{V}_h.\nabla_h c_i + \frac{\partial}{\partial z} w_c c_i - \frac{\partial}{\partial z} K_Z \frac{\partial c_i}{\partial z} = E + R - D$$

Advection | Turbulent Mixing | Source and Sinks

c_i concentration of species i

$E_i \neq f(c_i)$ ... Emission

$R_i = f(c_i, c_j, c_k, c_{m,} ...)$ ... Chemical conversion

$D_i = l_{Dep} c_i$ ... Deposition

Emissions

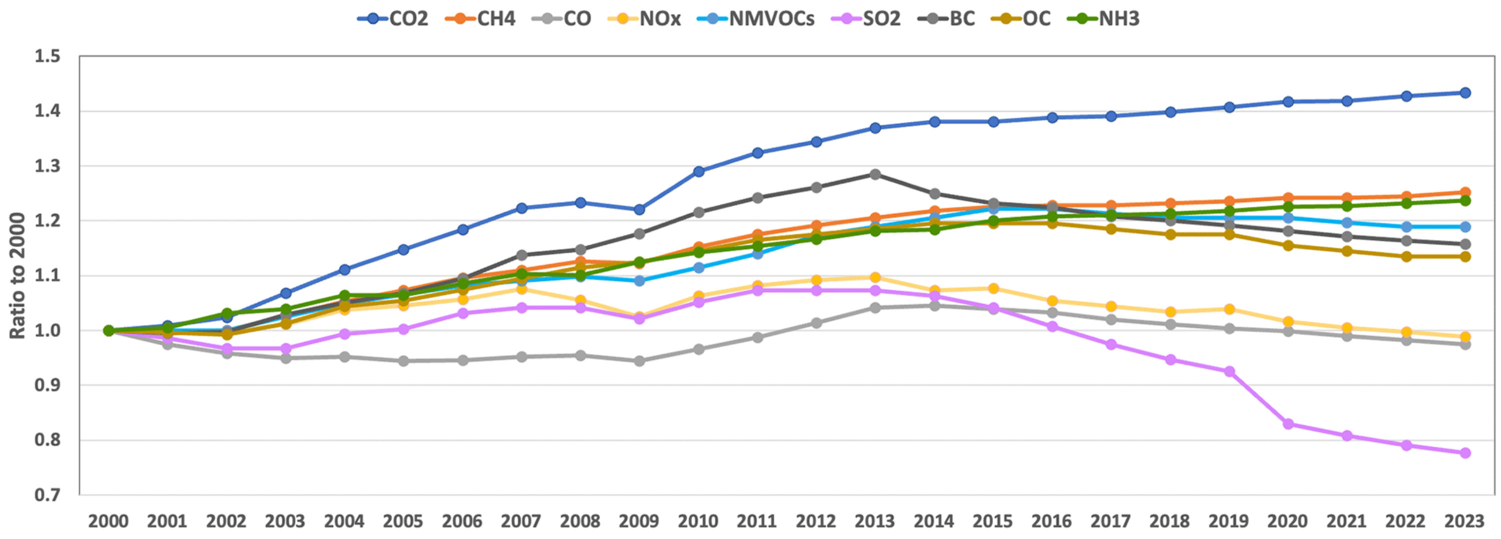
- Anthropogenic emissions (industry, power generation, traffic, transport, aviation)
  - provided as inventories based on socio economic data
  - Specific for base years with projections for future
  - Large variety between different inventories
- Wildfire emissions
  - based on fire radiative power or burned area satellite observations
- Natural Emissions from soils, oceans and volcanoes
  - Desert dust suspension, sea salt aerosol, NOx soil emissions, DMS emissions from oceans, NOX emissions from lightning
  - strong dependency on meteorology and land surface
  - modelled on-line
- Biogenic emission of volatile organic compounds - e.g. isoprene
  - Strong dependency on temperature, PAR and LAI and vegetation types
  - Modelled – online but also with dedicated BVOC models (MEGAN)
- **Emissions are often considered the most important input parameter to AC models**

Emissions – CAMS_GLOB_ANT dataset

- Global emissions inventories for anthropogenic, biogenic, shipping, volcanic outgassing, soil NOx
- Geographical and sectoral temporal profiles
- Regular updates to include, e.g., specific information on regional (including China, India, & SE Asia) emissions
- Public releases and documentation available via CAMS Atmosphere Data Store

https://ads.atmosphere.copernicus.eu/cdsapp#!/dataset/cams-global-emission-inventories

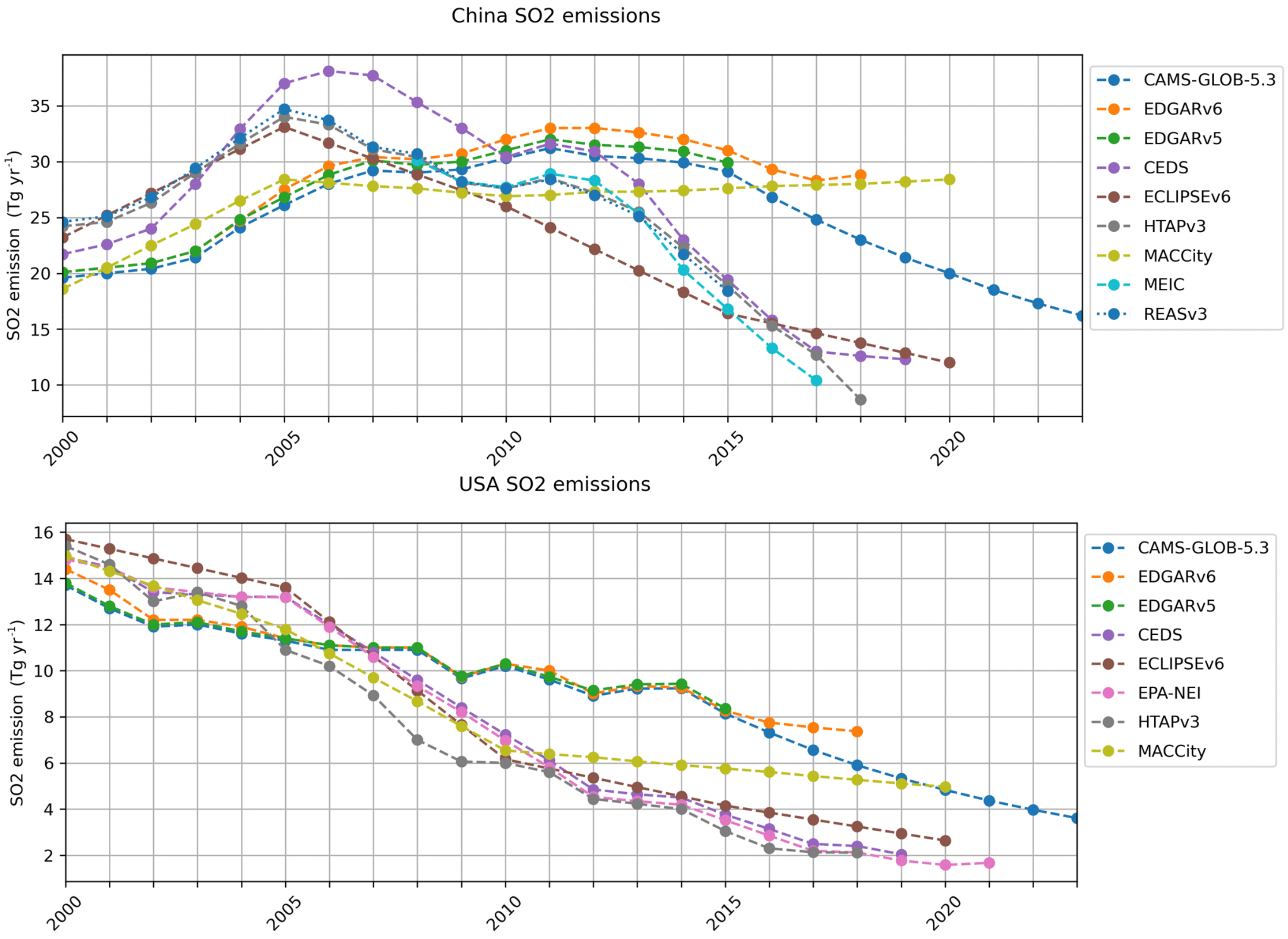
https://eccad.aeris-data.fr/



From Soulié et al (2023), CAMS_GLOB_ANT emission inventory, relative change of emissions of various species relative to 2000

Emissions

Large uncertainties and variability between different emissions datasets



From Soulié et al (2023), CAMS_GLOB_ANT emission inventory SO2 emissions compared to other inventories over China and the USA

Online emissions – desert dust

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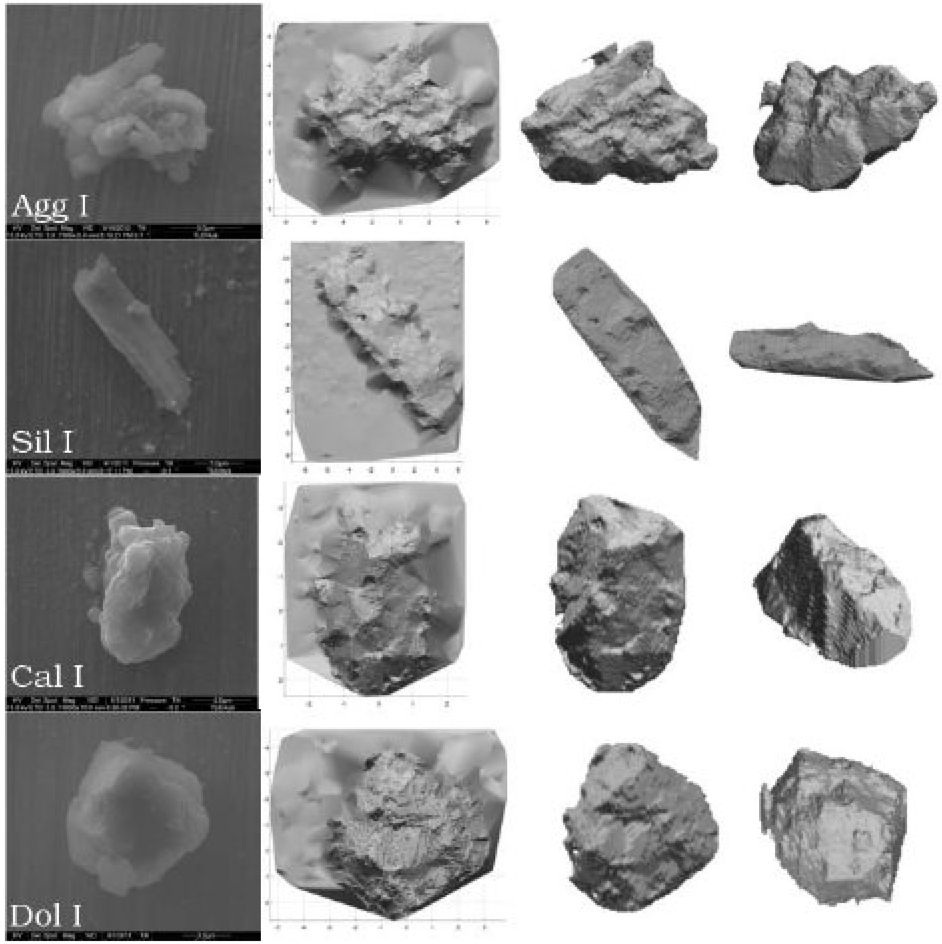
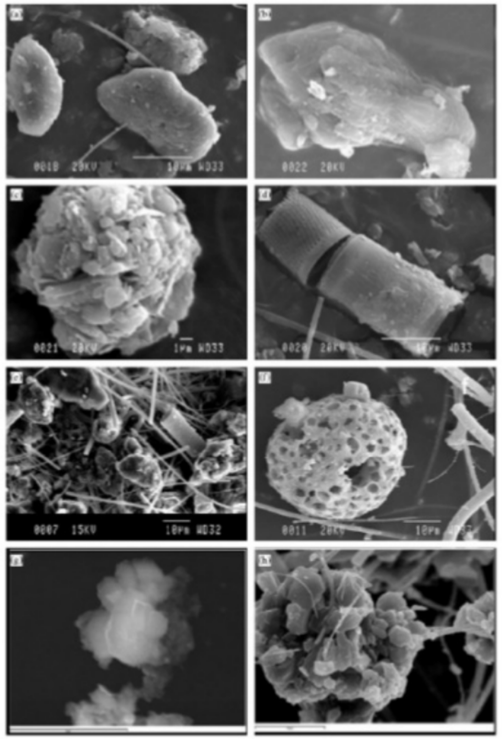
Dust is composed of aggregates of a wide variety of minerals: quartz, feldspar, dolomite, illite, smectite, hematite, kaolinite, etc. with different shapes, colors, etc.



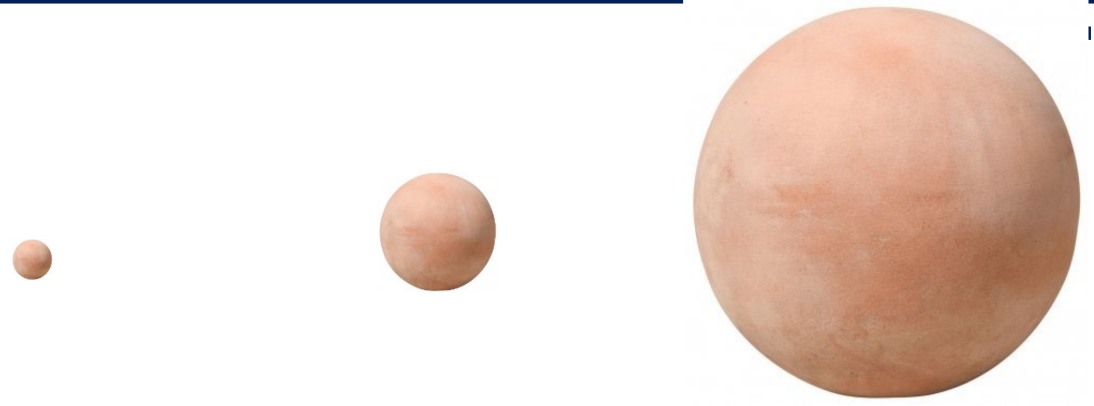
Lindqvist et al (2014)



Alastuey et al (20105

Online emissions – desert dust

- Desert dust in cycle 48R1 IFS-COMPO : three size bins, assumed spheres



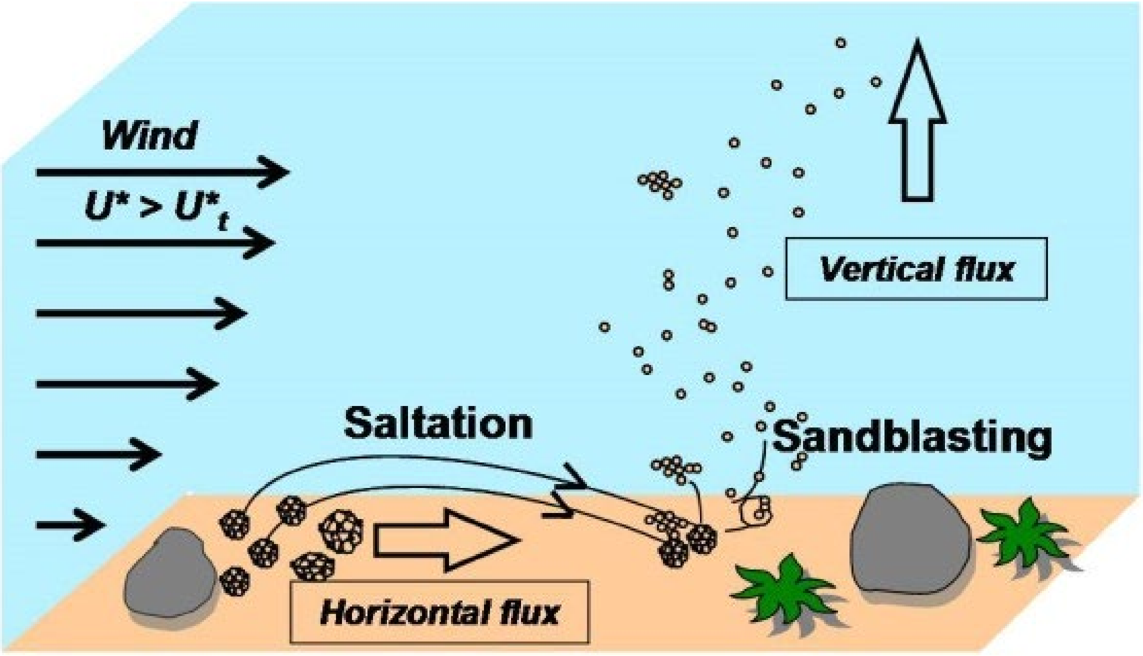
- Desert dust in cycle 49R1 : three size bins, spheroids with aspect ratio 1.6

- Desert dust in future cycle 51R1 : six size bins, spheroids with aspect ratio 1.6

Online emissions – desert dust

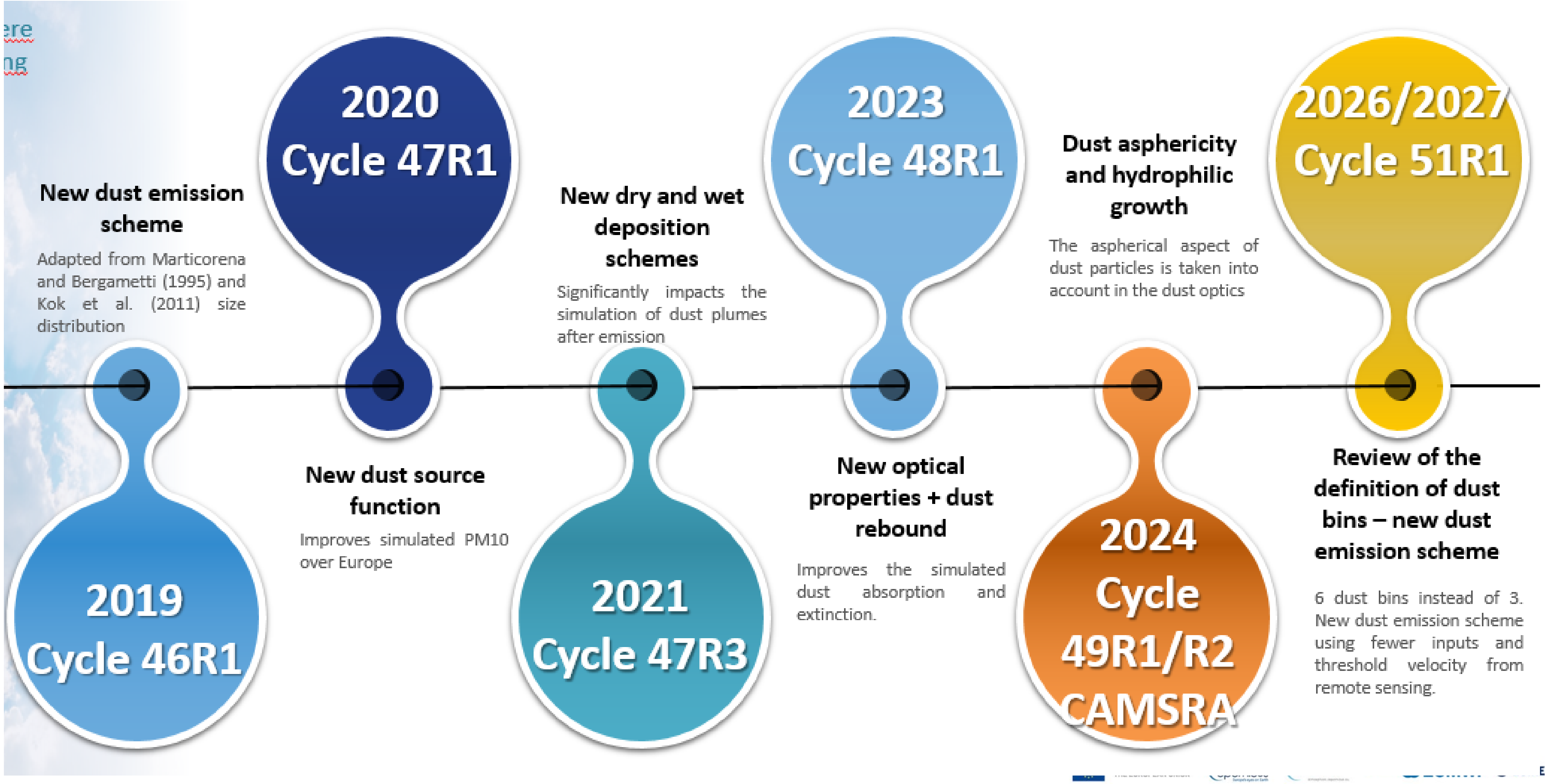
- Dust is emitted in the atmosphere through the saltation and sandblasting processes,
- These processes depend on meteorological (friction velocity) and surface (soil wetness, silt/sand/clay fraction) parameters,
- In CAMS, we use the Marticorena and Bergametti (1995) scheme to represent saltation and sandblasting, associated with a Kok et al (2011) dust size distribution at emissions,
- Several challenges:
    - Uncertainty of some inputs (soil typology in particular)
    - Representation of small scale processes with a 40x40km grid cell
    - Mismatch between the complexity of dust species and its representation as a single species

Observations are key! See talk by S. Vandenbussche this afternoon



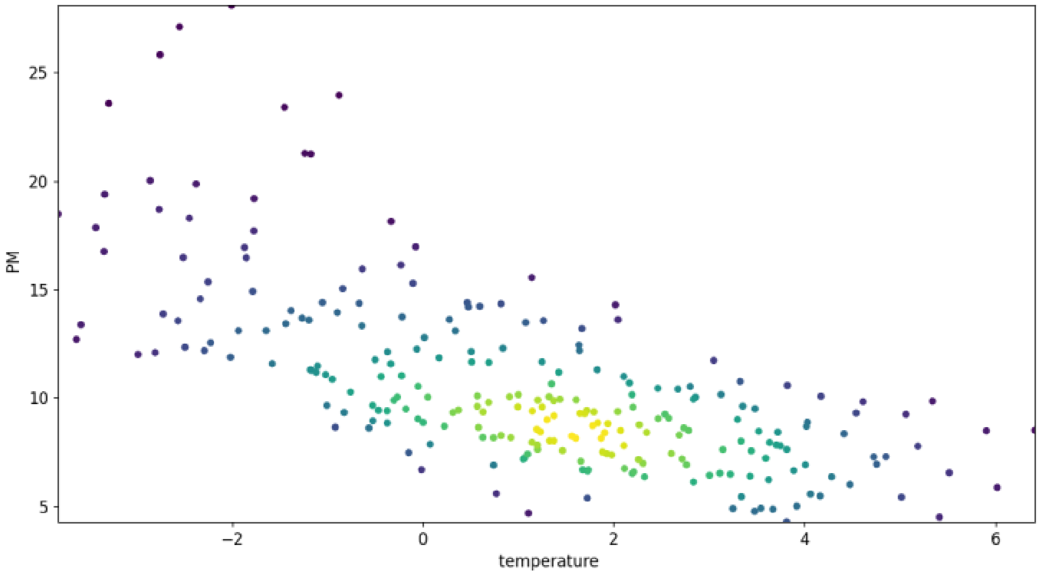
Schematic from LISA representing the key processes for the production of desert aerosols.

Desert dust is subject to frequent updates in IFS-COMPO



Online emissions – residential emissions

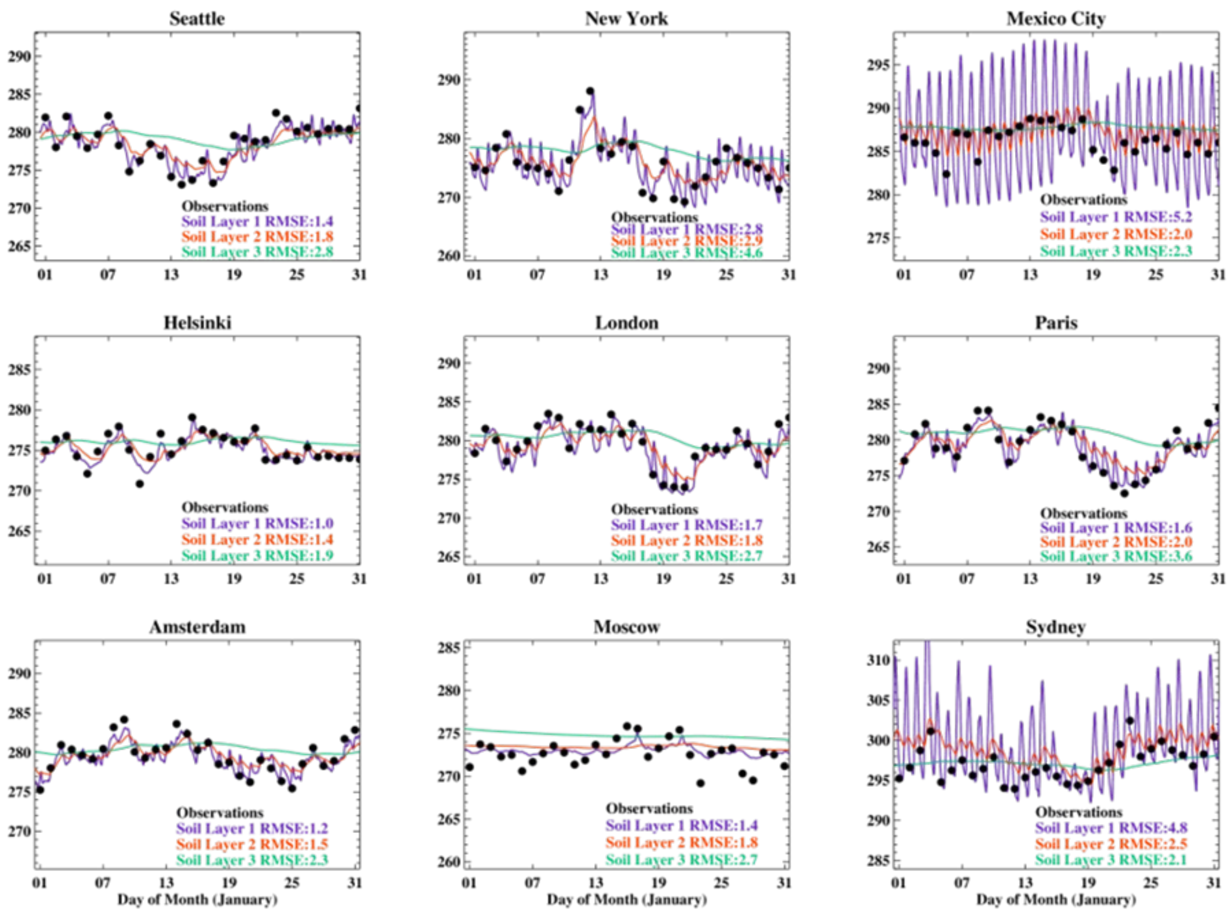
- Residential emissions are provided by emissions inventories as monthly or yearly averages
- However, they are known to be highly dependent on temperature in wintertime
- This results in some correlation between temperature and PM2.5 over some regions in wintertime
- Online modulation of residential emissions by temperature could yield some benefits



January 2019, simulated daily lowest model level temperature vs observed PM2.5 over background urban stations in Europe

Online emissions – residential emissions

- Tests with a « Heat Degree Day approach » - HDD following Guevara et al (2020)
- A difficulty – daily mean 2m temperature is required, but not know in the model
- A solution – use soil temperature (2nd level) as a proxy for daily mean 2m temperature



Guevara et al 2020, Copernicus Atmosphere Monitoring Service TEMPOral profiles (CAMS-TEMPO): global and European emission temporal profile maps for atmospheric chemistry modelling

from Mc Norton et al. (2023): A comparison of hourly IFS modelled soil temperature for different layers with the daily mean observed 2 m temperature for January, 2020.

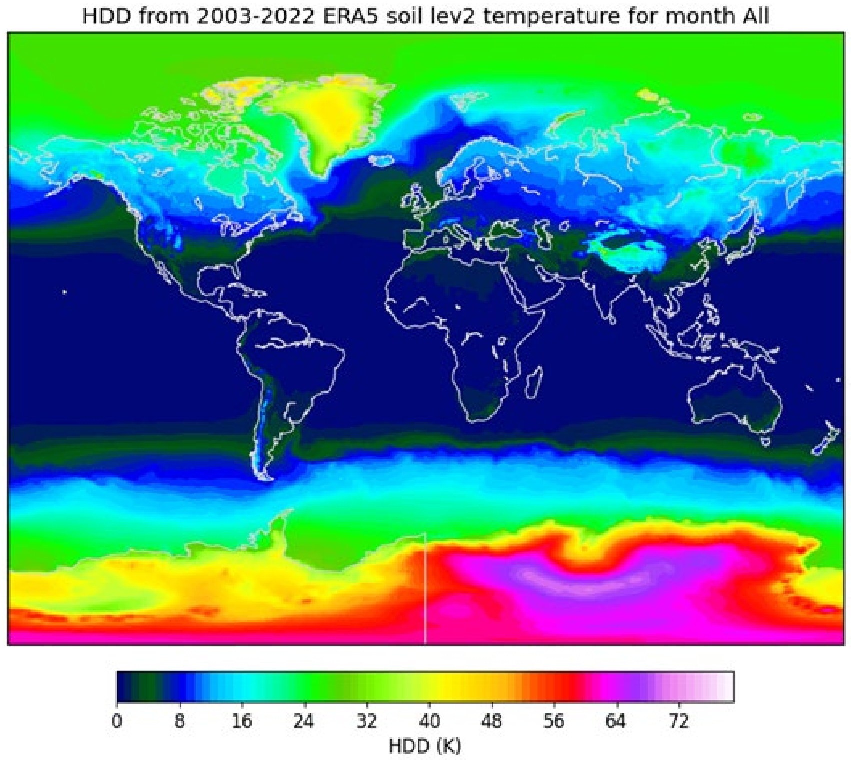
Online emissions – residential emissions

HDD depends on two parameters : Tb – threshold temperature of 15.5°c, and offset f=0.2 based on the European household energy statistics reported by Eurostat

$$HDD_{clim} = \sum_{d=1/1/2003}^{d=31/12/2022} \max(T_b - T_{s2}(d), 1)$$

$$HDD_t = \max(T_b - T_{s2}(t), 1)$$

$$EMIS_{res,t} = EMIS_{res,y} * \frac{HDD_t + f * HDD_{clim}}{(1+f)HDD_{clim}}$$



2003-2022 Climatological HDD from ERA5 computed using soil level 2 temperature

Online emissions – residential emissions

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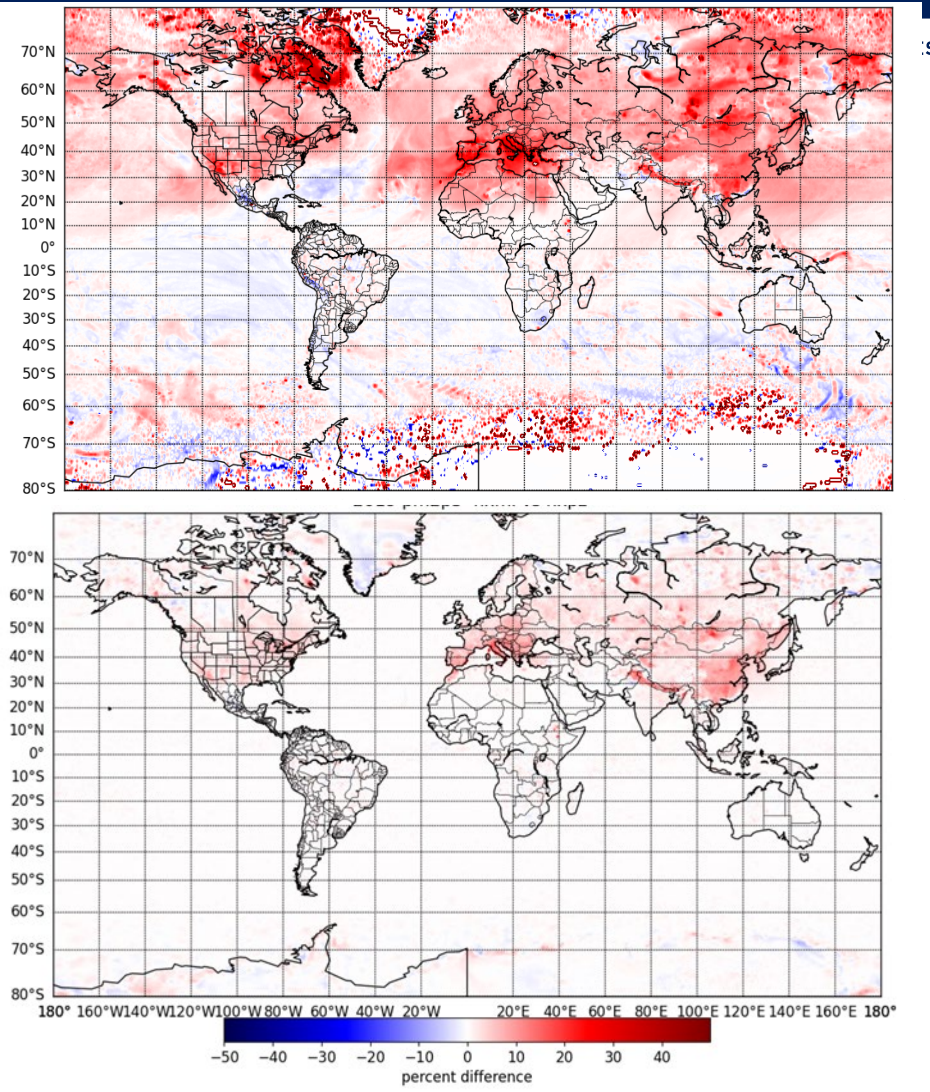
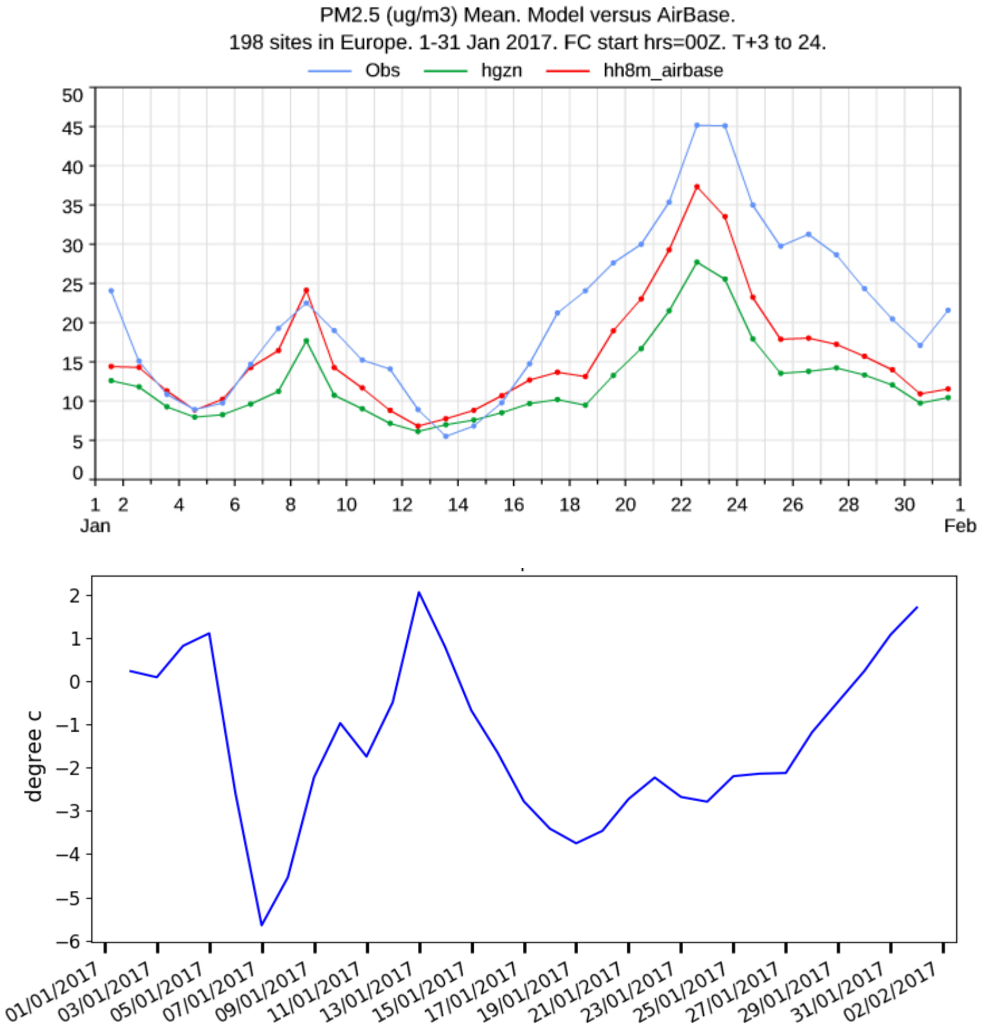
Significant impact on simulated organic matter at surface and PM2.5



January 2019, relative difference of a simulation using HDD versus a reference simulation in simulated surface organic matter (top) and PM2.5 (bottom)

Online emissions – residential emissions

Significant impact on simulated organic matter at surface and PM2.5



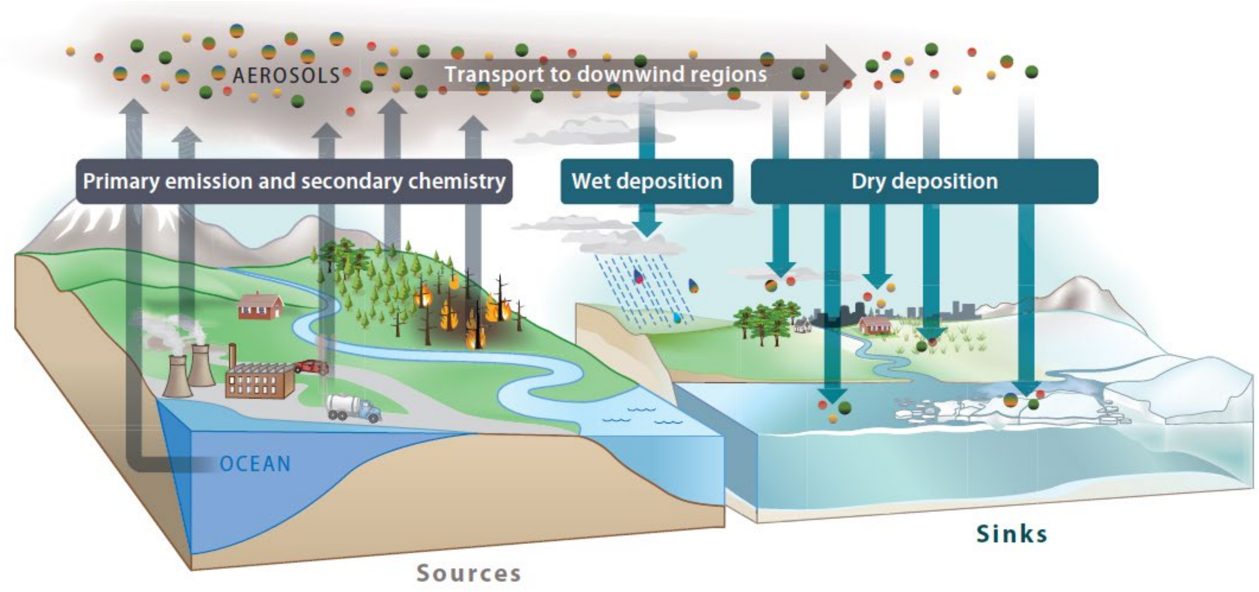
January 2017, observed and simulated PM2.5 (top), and simulated mean daily 2m temperature over Europe (bottom).

Deposition processes

On average, deposition matches the emissions.

At first order, deposition of particles are modulated by:

- Wind speed, surface type, particle diameter and concentration for dry deposition
- Precipitation rate, particle diameter and concentration over the vertical (burden) for wet deposition
- (Particle diameter)², air density and concentration over the vertical (burden) for sedimentation



Schematic of emissions and deposition from Farmer et al (2021)

Dry deposition

$F_{DD} = V_{DD} * C$

Sedimentation

$F_S = V_S * C$

Wet deposition

$F_{WD} = F_P * C_{res}$

C = Concentration

V_{DD} = dry deposition velocity = F (Diffusion, surface and canopy)

V_S = sedimentation velocity = F ((particle diameter)², meterology)

C_{res} = scavenging rate = F (solubility, transfer to droplet)

F_p precipitation flux

Dry deposition is the combination of several physical processes

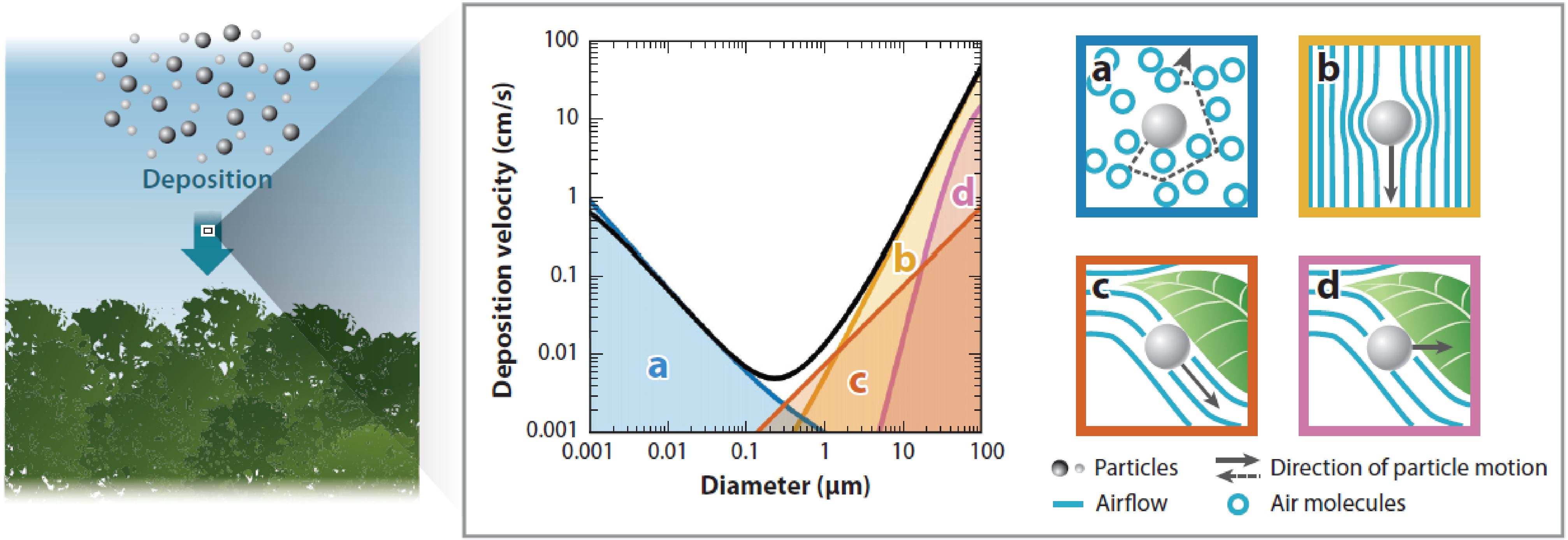


Figure 2

Dry deposition velocities of particles are a function of particle diameter and are driven by a combination of processes, including (*a*) Brownian diffusion (*blue*), (*b*) gravitational settling (*yellow*), (*c*) interception (*orange*), and (*d*) impaction (*purple*). The relative importance of these processes varies with particle size and surface type, with the graph providing an example of these processes and the total calculated deposition velocity (*thick black line*) for a conifer forest. The direction of airflow in panels *a*–*d* is indicated by solid blue lines; the direction of particle motion is indicated by gray arrows. In the case of Brownian diffusion, particle movement is random, as indicated by the dashed gray arrow. The size of particles relative to gases is not drawn to scale.

Farmer et al (2021)

Dry deposition

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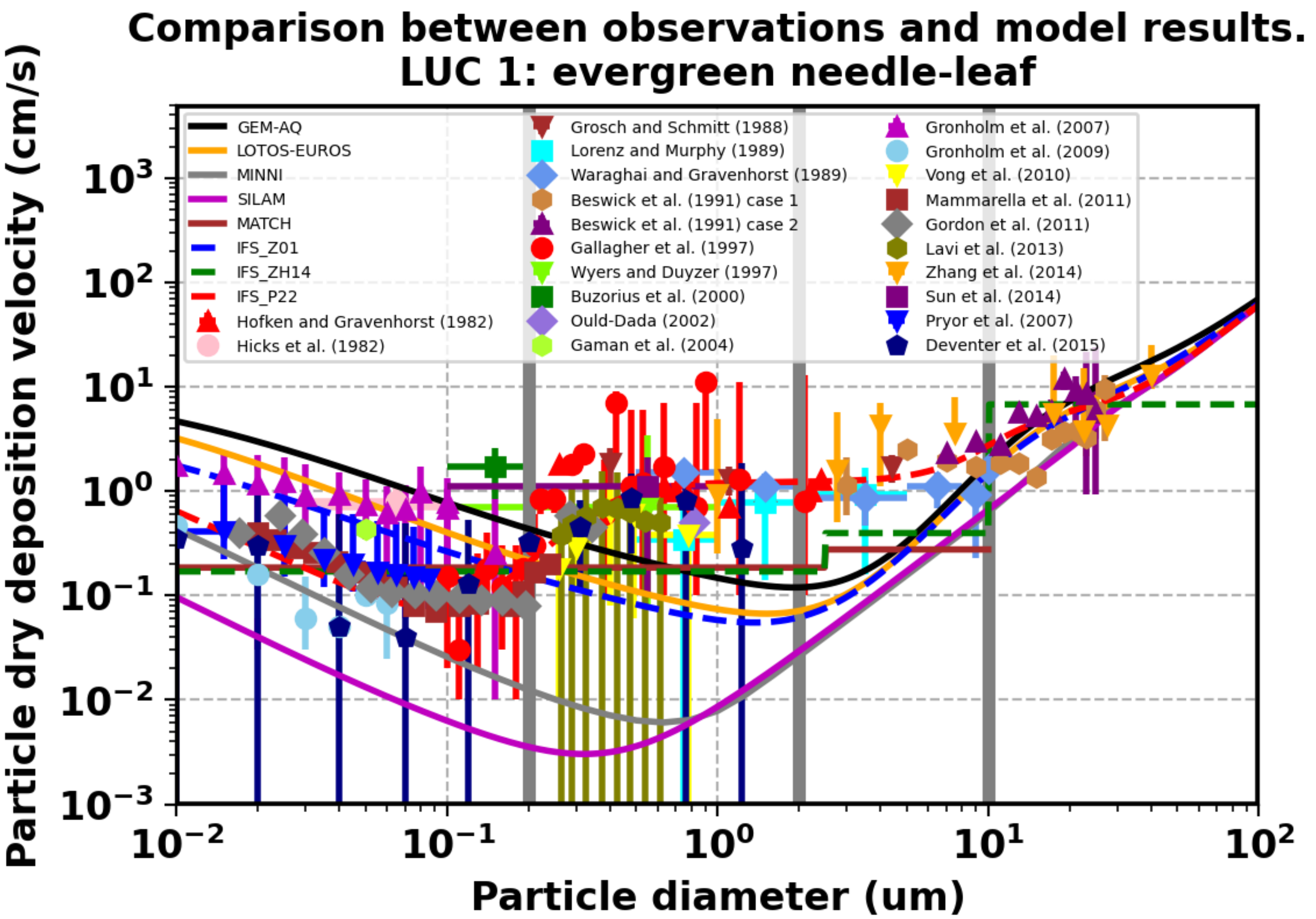
Large variability in how dry deposition is represented between models

Intercomparison of dry deposition carried out in the CAMAERA HE project



CAMAERA

Dry deposition

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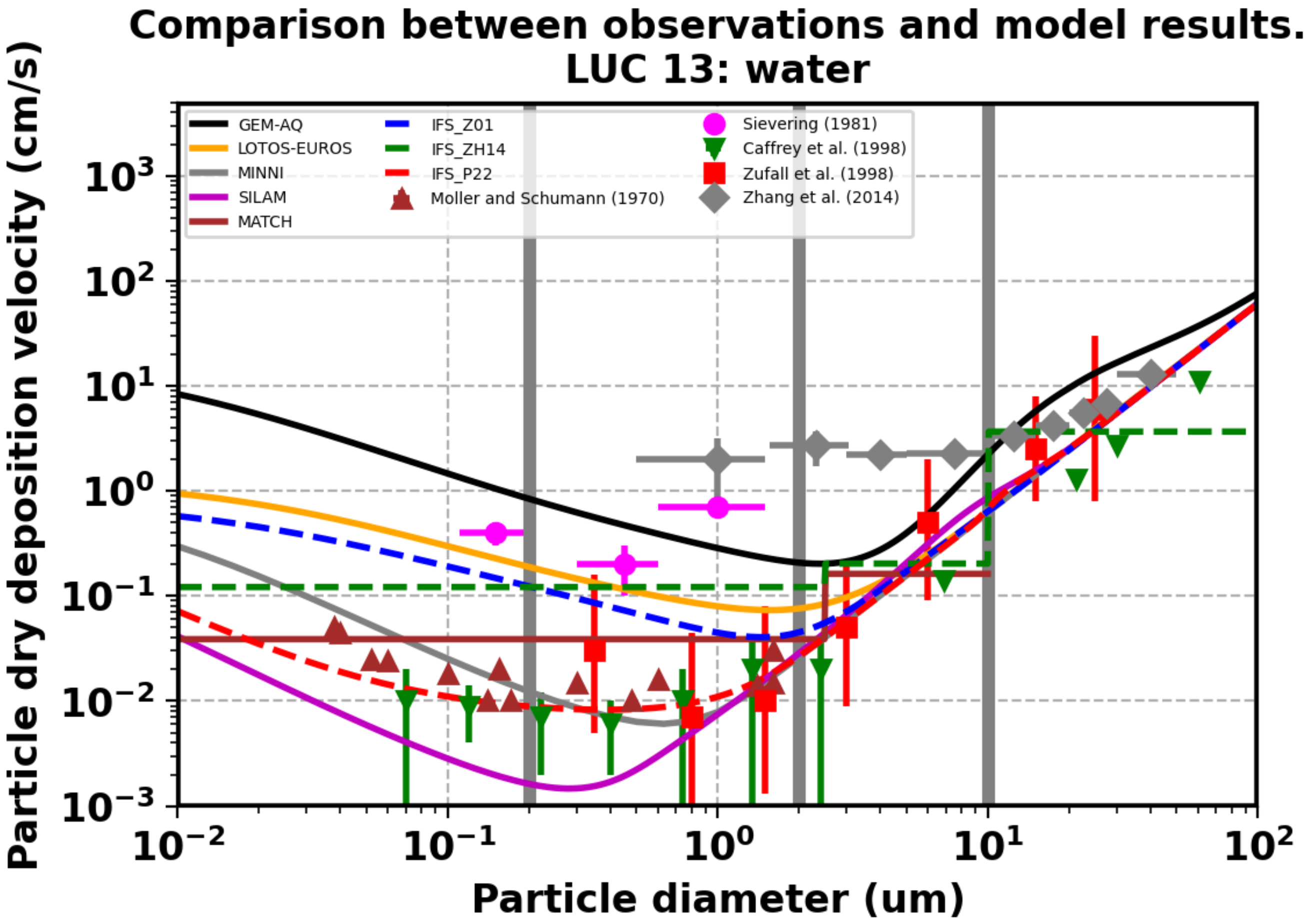
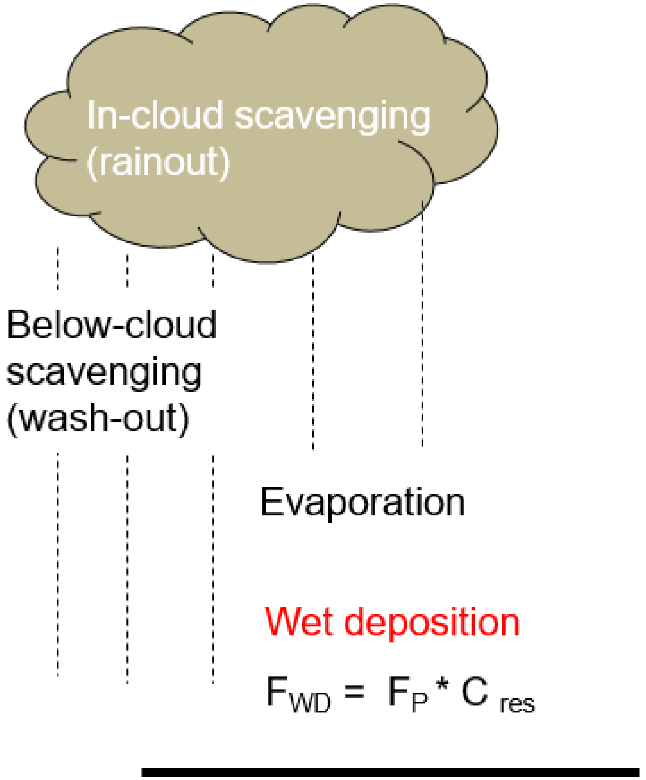


CAMAERA

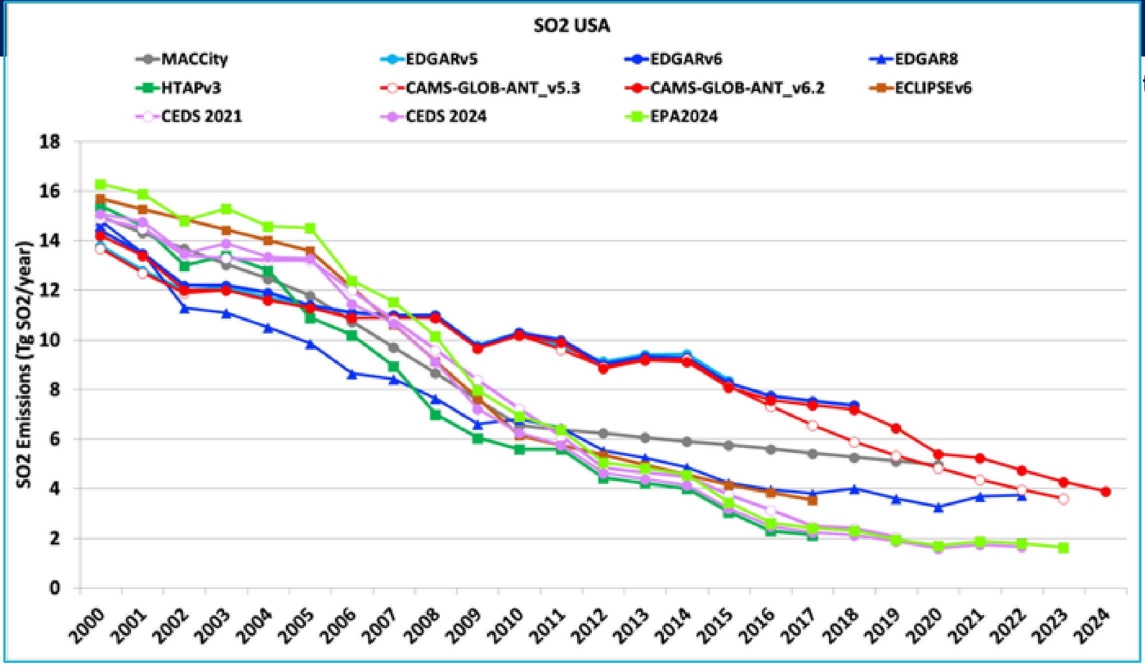
Wet deposition

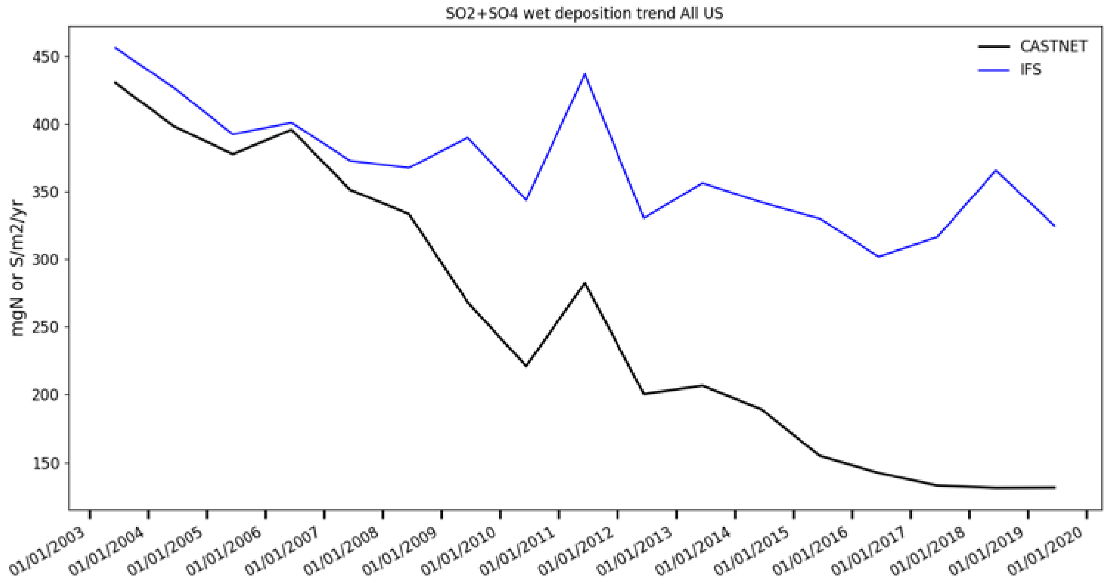
- Wet deposition is also the combination of several physical processes
- Wet deposition trends of nitrogen and sulphur are monitored and the subject of many papers
- Wet deposition can be used to assess emissions also, as done in long IFS-COMPO simulations to prepare for next reanalysis



Wet deposition

- Wet deposition can be used to assess emissions also, as done in long IFS-COMPO simulations to prepare for next reanalysis
- Simulation first done with CAMS_GLOB_ANT emissions
- Then, use of scaling factors over US and China; over US, use of EPA2024 emissions as a reference





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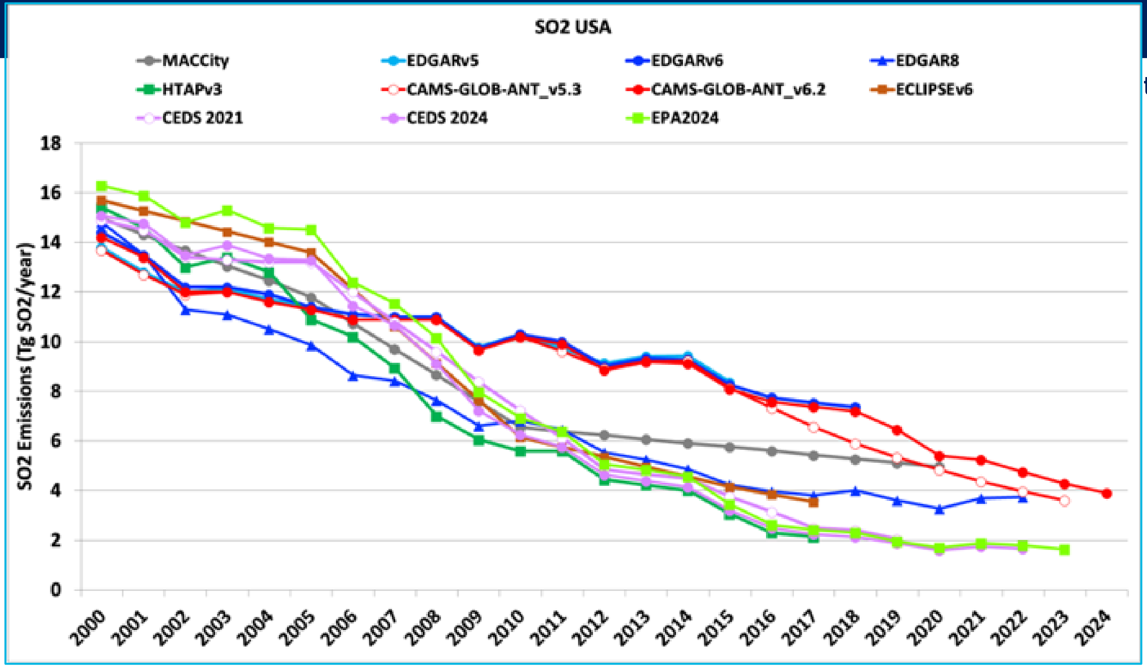

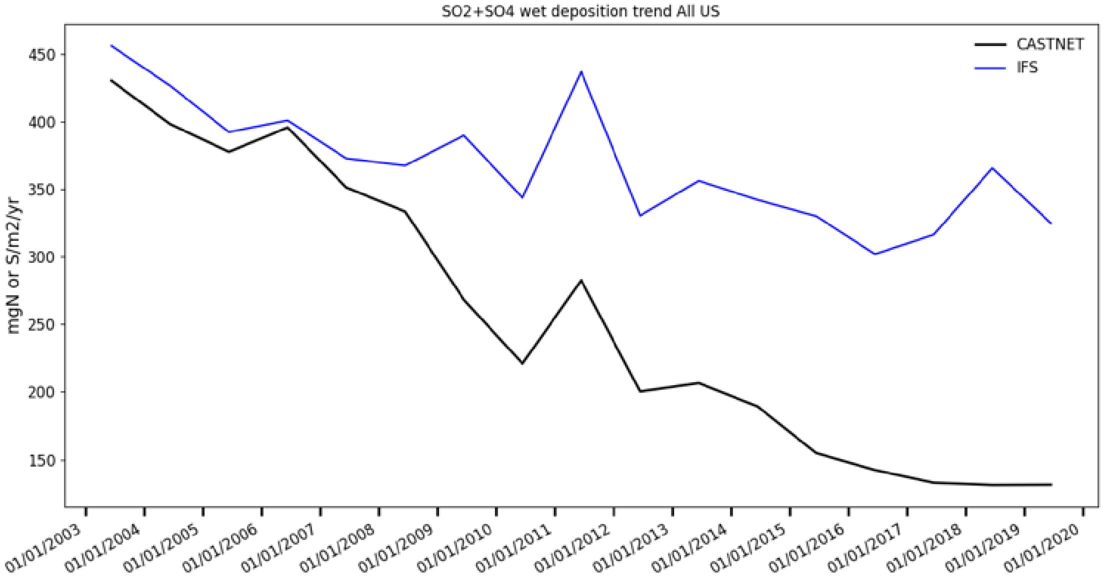

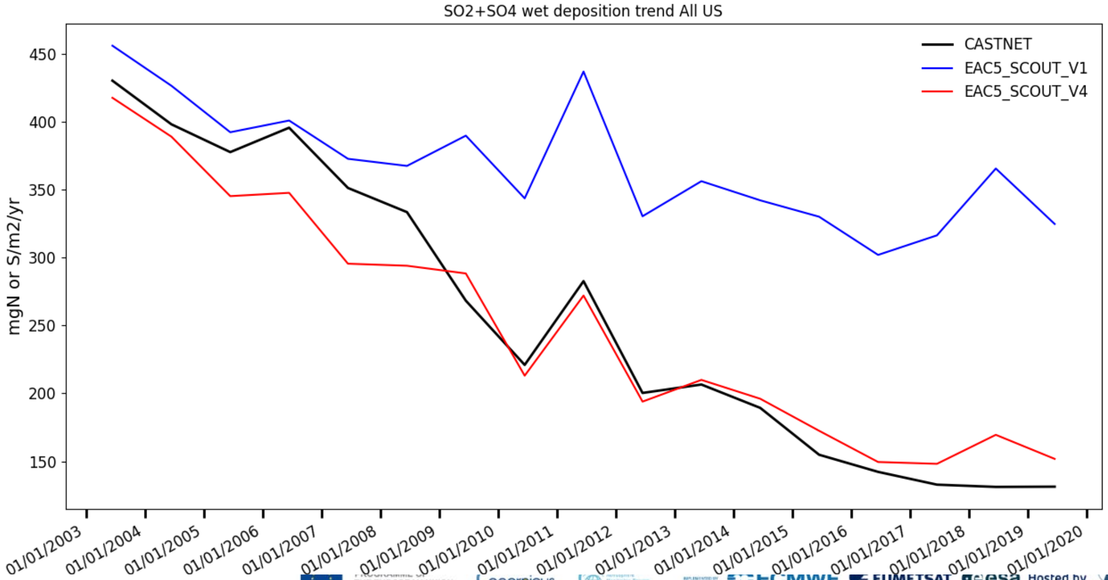

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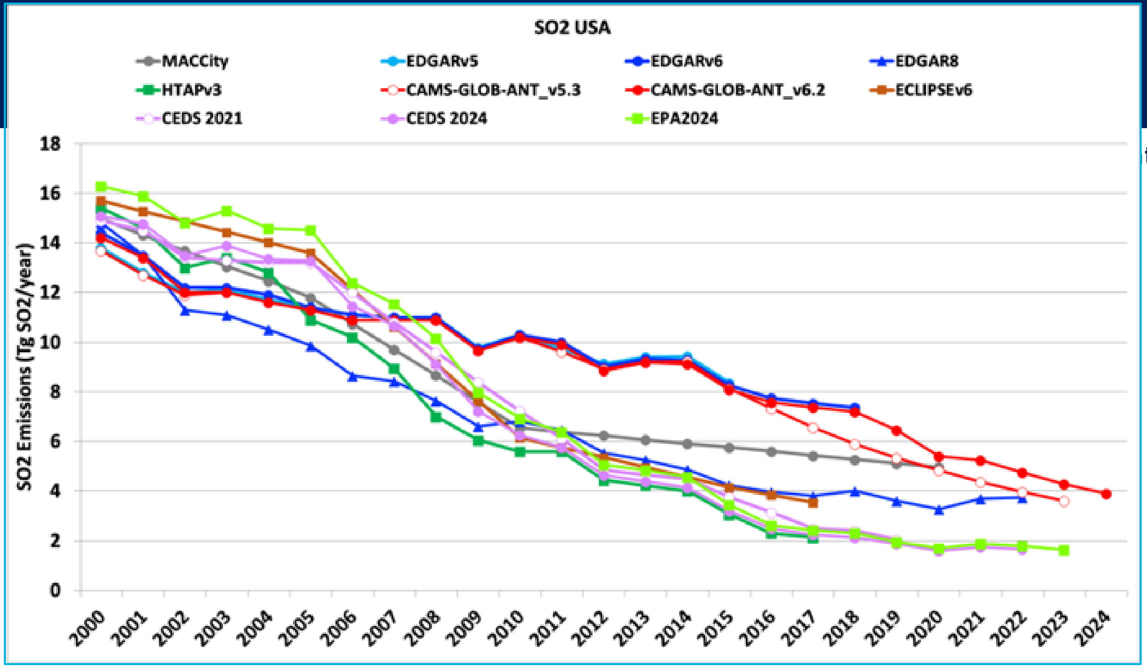
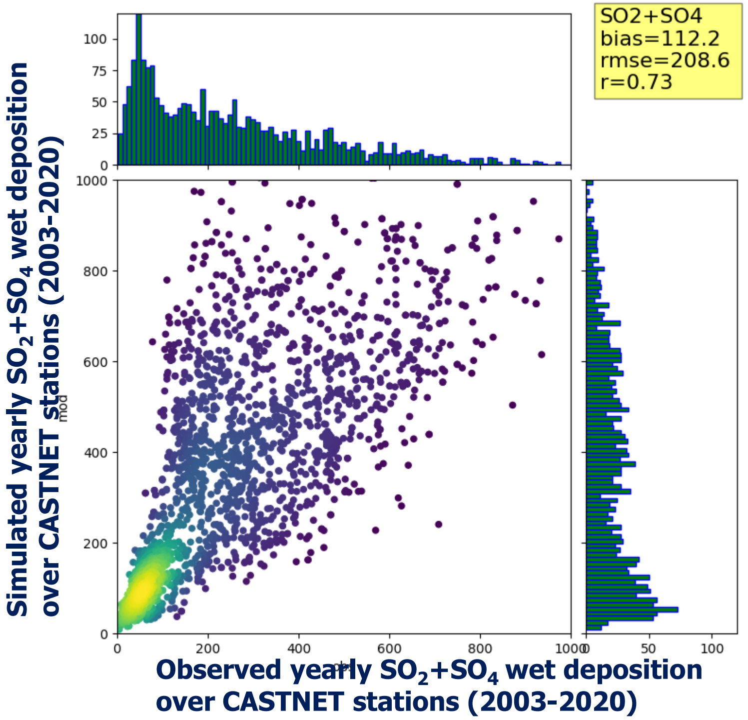
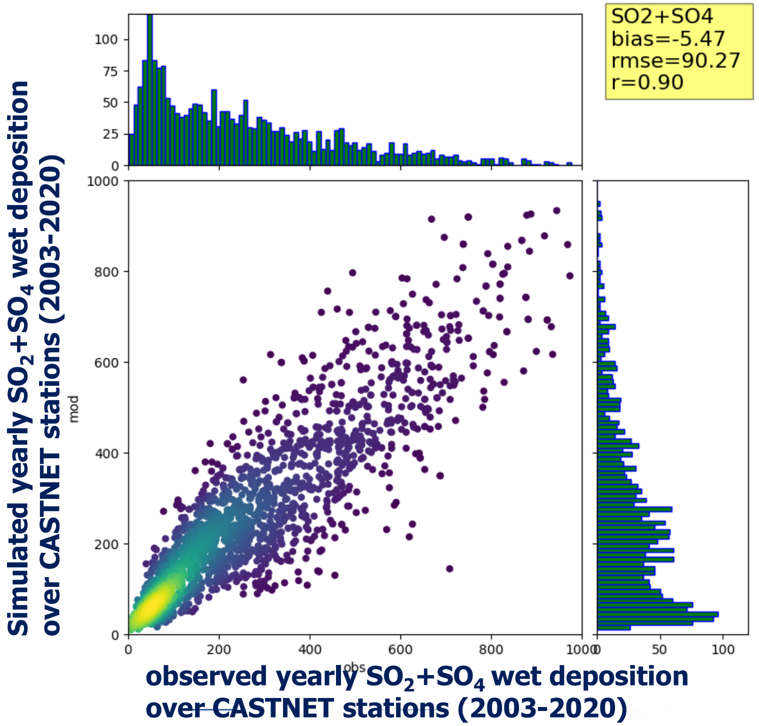






Outlook : AI/ML for atmospheric composition modeling

- AI/ML more and more used in AC modeling, in particular to replace Mie code:
  - NeuralMie (Geiss et al 2025)
  - Mie AI (Kumar et al 2024)
- Two ongoing activities to implement ML in IFS-COMPO
- Replace selected processes by ML (HE project CAMAERA). Focus on:
  - Whitecap fraction and sea-salt aerosol emissions
  - Desert dust emissions (just started)
- Replace the whole model + DA by ML (ECMWF – Paula Harder)
  - A first prototype of AIFS-COMPO

More ML application in talk by O Hasekamp

Outlook : AI/ML for atmospheric composition modeling

- Replace selected processes by ML (HE project CAMAERA). Focus on:
  - Whitecap fraction and sea-salt aerosol emissions

Current status of sea-salt aerosol emissions in cycle 49R1 IFS-COMPO:

- The whitecap fraction (WF) is estimated by the **Albert** et al. (2016) parameterization:

$$\boldsymbol{WF = a(SST)[WSP + b(SST)]^2}$$

- Sea-salt aerosol emissions are derived using the **Gong** (2003) assumed size distribution

$$(WSP, SST) \xrightarrow{\text{A16}} WF \xrightarrow{\text{Gong}} Sea\text{-}Salt$$

Our objective : Estimation of whitecap fraction and sea-salt emissions in IFS-COMPO with deep neural networks (DNN) by :

1. Training offline a DNN model to estimate whitecap fraction
2. Integrating this DNN model into IFS-COMPO

Outlook : AI/ML for atmospheric composition modeling

- Replace selected processes by ML (HE project CAMAERA). Focus on:
  - Whitecap fraction and sea-salt aerosol emissions

Dataset description

Ground truth : Whitecap fraction (WF) at **10.7** and **37** GHz derived from remote sensing (Anguelova et al 2019)

Time range : 2 years of data with an hourly resolution

Predictors : 8 predictors collected

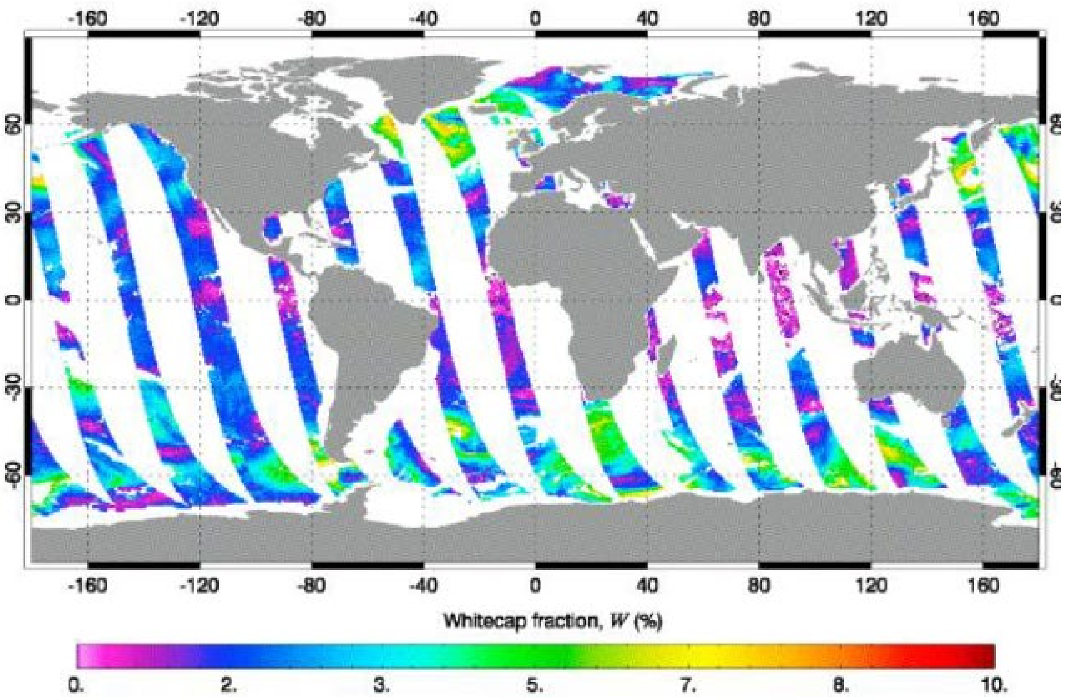
From ERA5 :

- Wind Speed
- Wind Direction
- Sea Surface Temperature
- Mean Wave Period
- Significant Wave Height

From HINDCAST :

- Total Wave Height
- Significant Wave Height
- Dissipation of turbulent energy from breaking waves

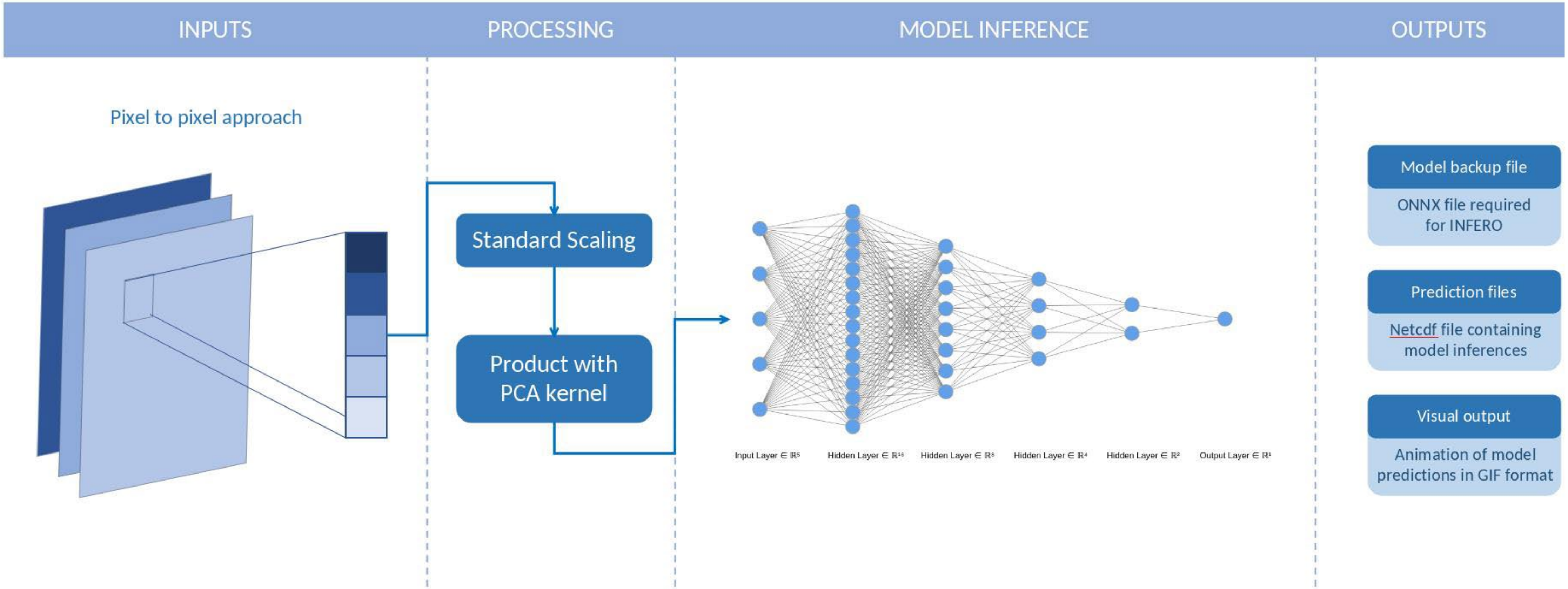
Dimension : around 200 million pixels



Example of daily map of whitecap fraction from Windsat acquisition [Anguelova et al.]

Outlook : AI/ML for atmospheric composition modeling

- Replace selected processes by ML (HE project CAMAERA). Focus on:
  - Whitecap fraction and sea-salt aerosol emissions



Outlook : AI/ML for atmospheric composition modeling

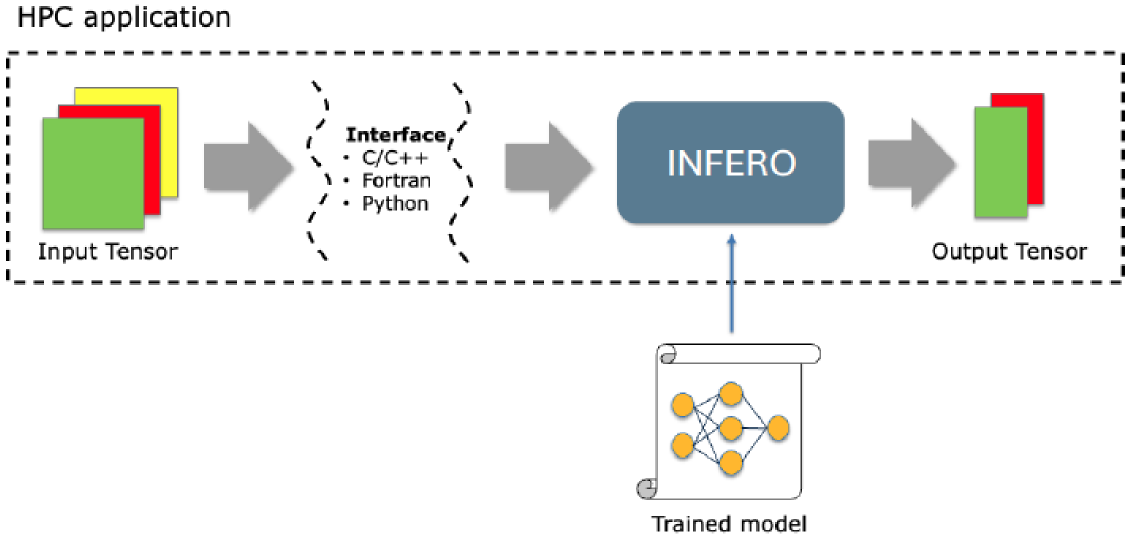
- Replace selected processes by ML (HE project CAMAERA). Focus on:
  - Whitecap fraction and sea-salt aerosol emissions

Incorporation of an **exported version (ONNX format)** of the DNN to compute whitecap fraction and sea-salt aerosol emissions online in IFS-COMPO.

The **INFERO** library has been integrated into IFS-COMPO to interface with Deep Learning models

Interest : runs a learning model in ONNX format from a Fortran script

Representation of the incorporation of our model into IFS



Outlook : AI/ML for atmospheric composition modeling

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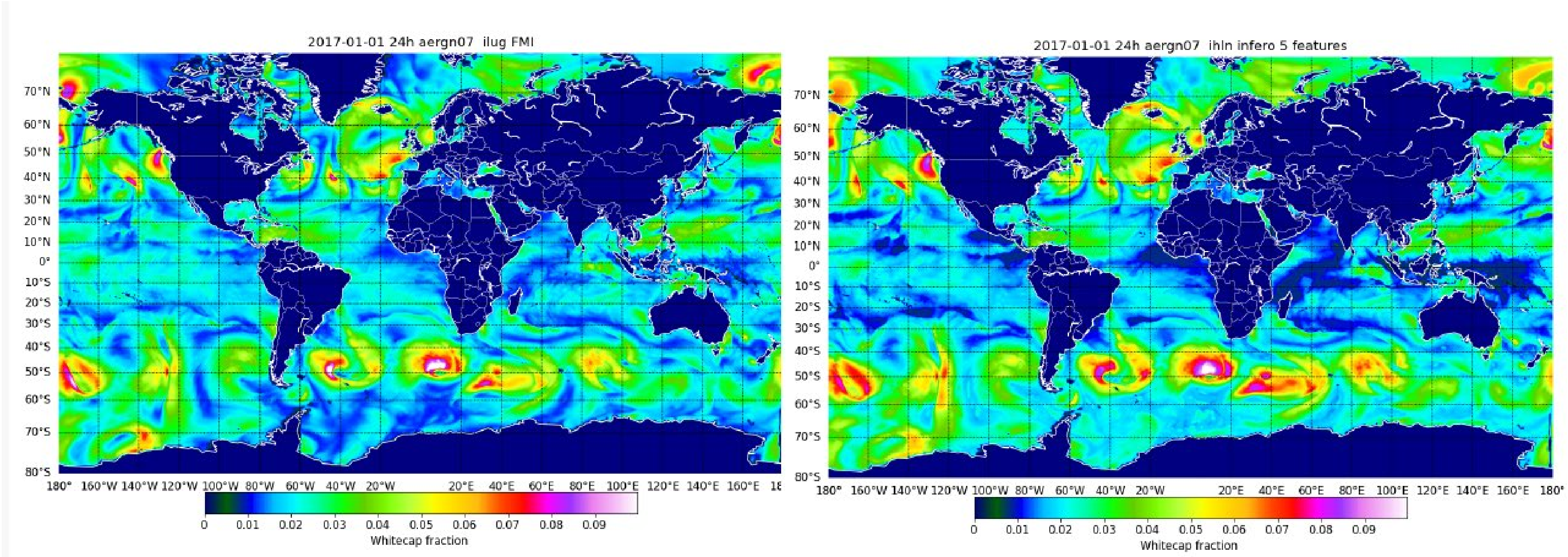
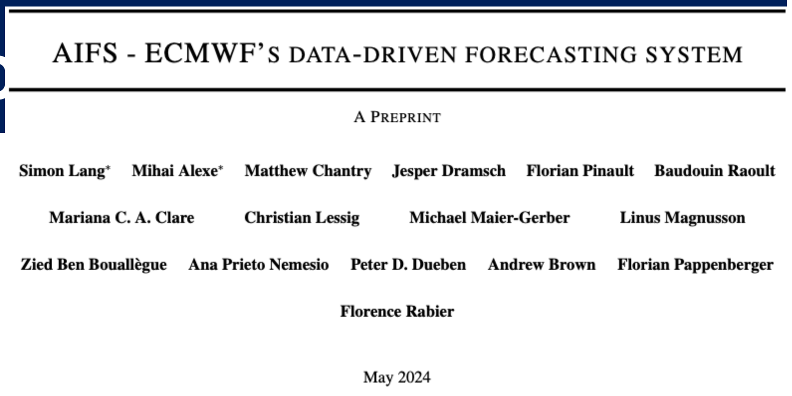


Simulated whitecap fraction by IFS-COMPO on 1/1/2017 0UTC, using the newly developed FMI scheme (left), and with deep learning model (using 5 predictors) enabled through the INFERO library (right).

Outlook : AI/ML for atmospheric compositio


AIFS - ECMWF's DATA-DRIVEN FORECASTING SYSTEM

A PREPRINT

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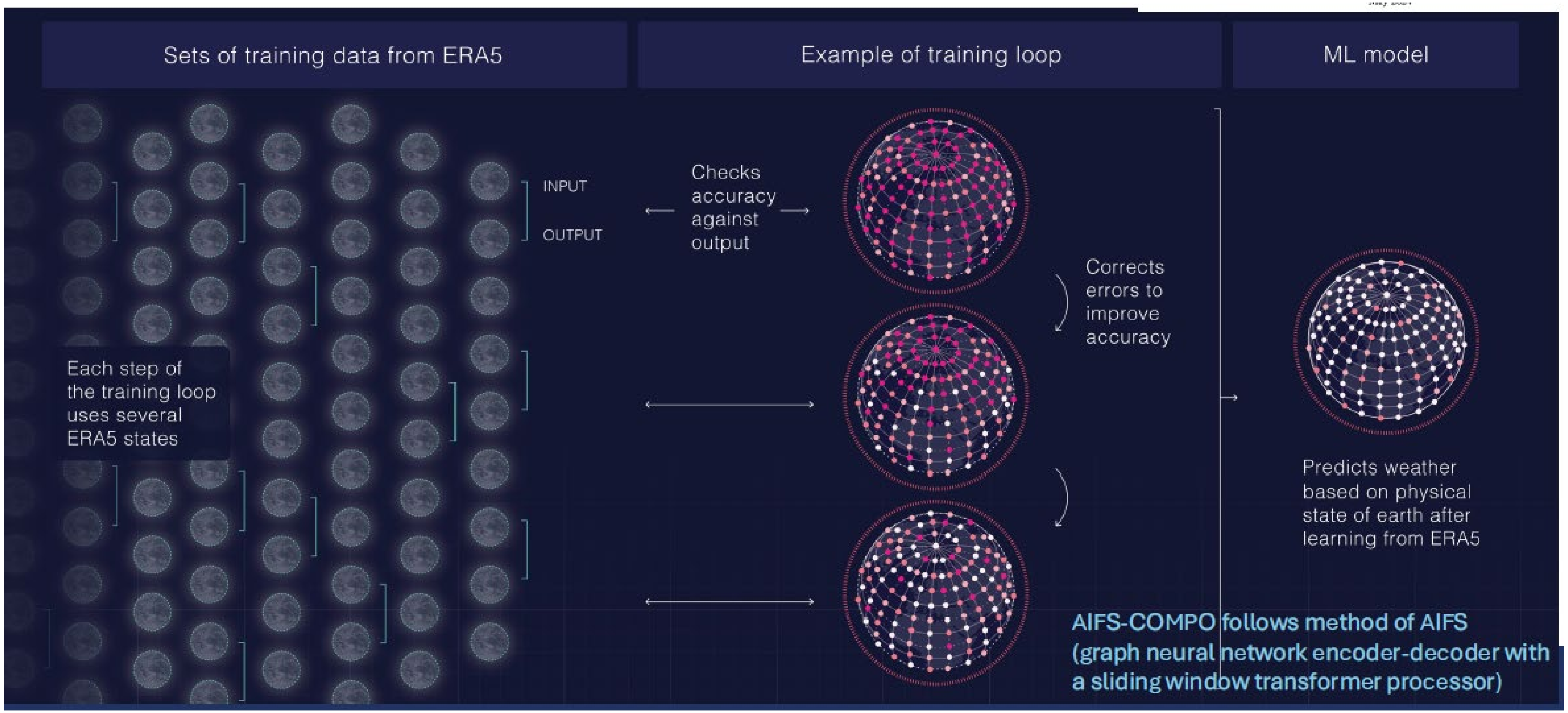
Mariana C. A. Clare Christian Lessig Michael Maier-Gerber Linus Magnusson
Zied Ben Bouallègue Ana Prieto Nemesio Peter D. Dueben Andrew Brown Florian Pappenberger
Florence Rabier

May 2024

Replace the whole model + DA by ML (ECMWF – Paula Harder)

- A first prototype of AIFS-COMPO

AIFS-COMPO follows method of AIFS



AIFS-COMPO follows method of AIFS (graph neural network encoder-decoder with a sliding window transformer processor)

Outlook : AI/ML for atmospheric composition modeling

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Replace the whole model + DA by ML (ECMWF – Paula Harder)

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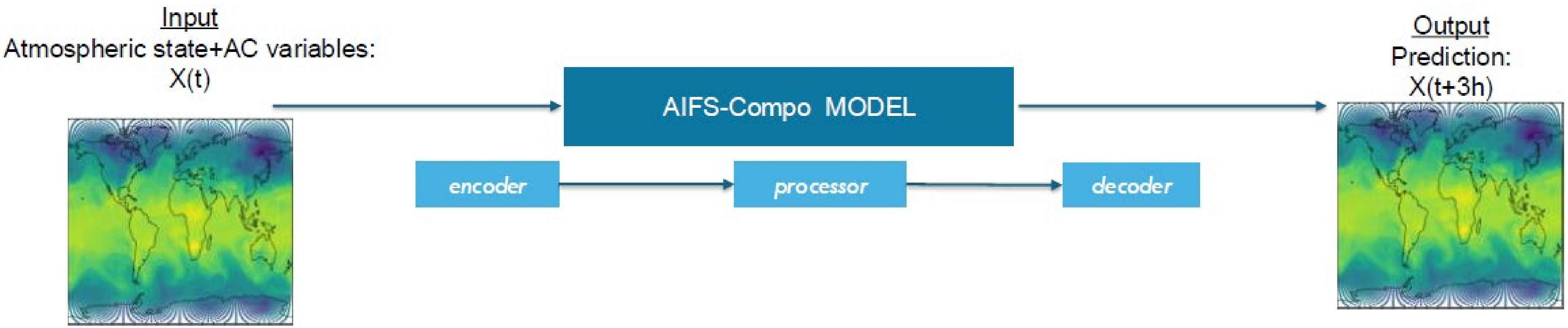
From AIFS to AIFS-COMPO



Variables:
- Atmospheric composition variables
  - AOD, PMs, Reactive gases
  - Mixing ratio at pressure levels
- Upper-air variables at 13 pressure levels (t,v,u,w,z)
- Surface variables (temperature, winds, pressure, radiation)
- Static geographical features, location and time information as input forcing

Training Scheme:
1. Train on EAC4
2. Fine-tune on operational analysis/forecast and lead times up to 36h

Outlook : AI/ML for atmospheric composition modeling

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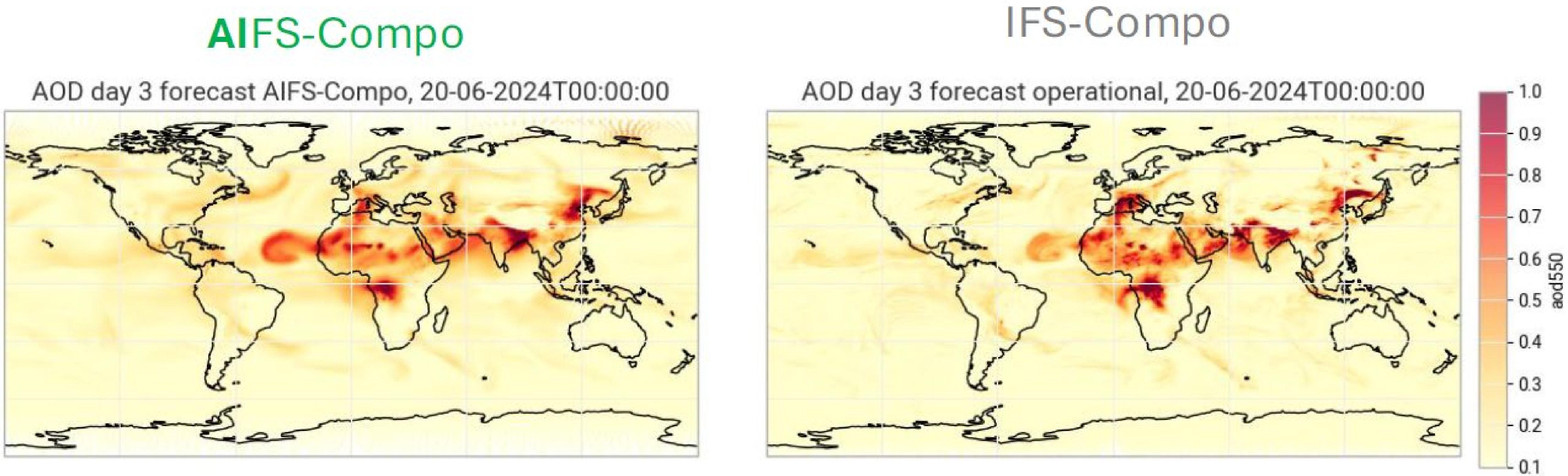
Replace the whole model + DA by ML (ECMWF – Paula Harder)

- A first prototype of AIFS-COMPO

Results: AOD



Outlook : AI/ML for atmospheric composition modeling

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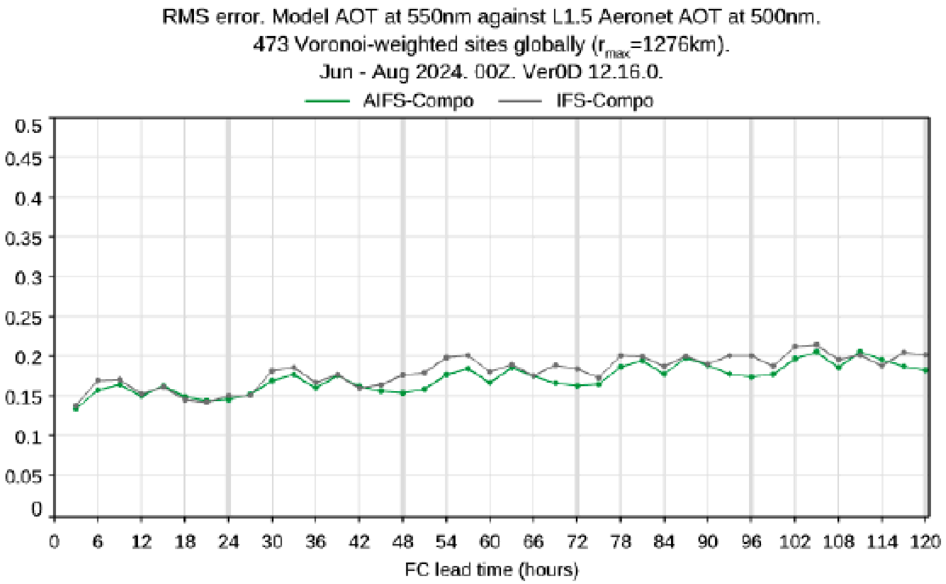
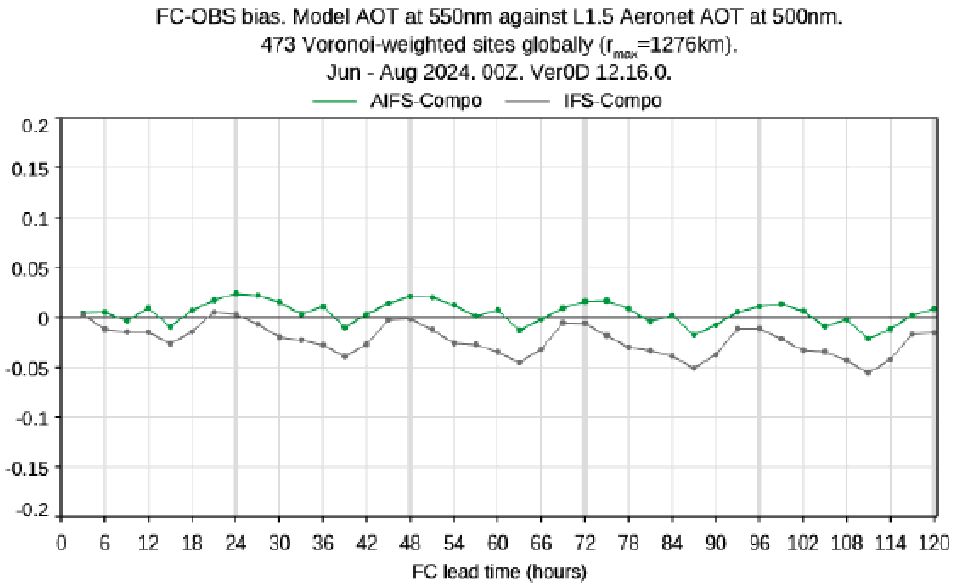
- A first prototype of AIFS-COMPO

Results: AOD

RMSE against observations



Bias against observations



Conclusion : how to improve Atmospheric Composition models?

- Improve emissions
  - Better knowledge of emission processes (EF, activity data, on-line calculation)
  - Use concentration observations to constrain emissions in models
- Increase model complexity
  - Better modelling of chemistry, aerosols, deposition and transport
  - Grid-box resolution
  - More coupling of processes (NWP-AC)
- Build Machine learning based models:
  - Replace components ACM with ML – for example chemistry schemes
  - Emulate ACM results directly – e.g. much faster forecasting
- Combine observations with modelling – data assimilation (**talk by Mel Ades)**
- Use new information from remote sensing for evaluation, in particular Earthcare and S4/S5 data (**talks by R. Lindsrat and A. Hoffmann)**

Thank you!

Questions are welcome.