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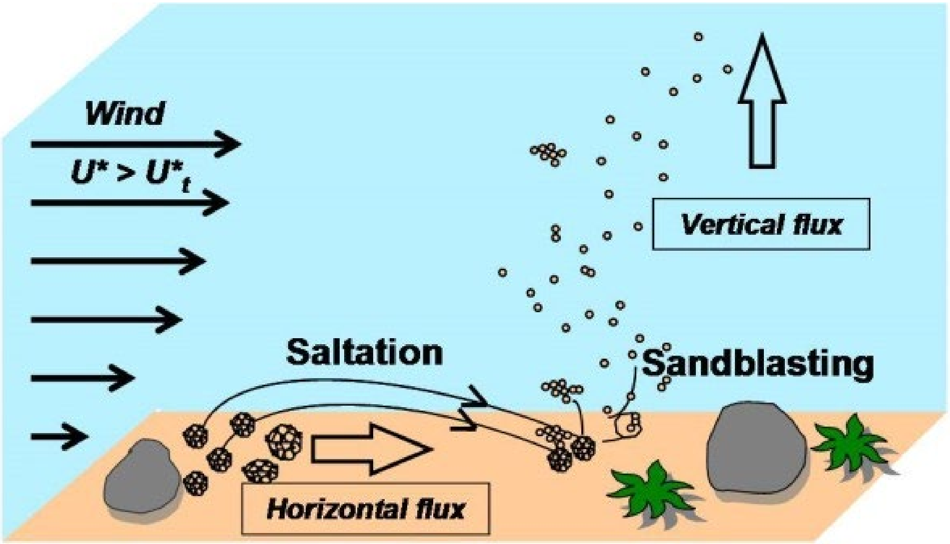
A first attempt at predicting desert dust emissions with neural networks in IFS-COMPO

Samuel Remy, Nathan Capon, Rose-Cloé Meyer (HYGEOS)
Jeronimo Escribano (BSC – now ECMWF)

Why use ML for desert dust emissions?

CAMAERA

- Computational cost small compared to other processes (photolysis, wet deposition, etc.)
- But many sources of uncertainties impact desert dust emissions (inputs, resolution, representativeness, processes, etc.)
- In CAMAERA, we want to explore if there a possibility to train a statistical approach on a dataset of dust emissions that merges simulations and observations – a dust emissions analysis
- So the objective here is to improve **skill**, not **speed.**



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

Work plan

- Some desert dust emission datasets from flux inversion exist (Escribano et al 2017), but estimates depend a lot from model to model, so probably not applicable here.
- A first task is to create a reference dust emission analysis, computed with an offline ensemble Kalman smoothing applied to IFS-COMPO emissions.
- This offline dust inversion methodology can also have other uses:
  - Provides information on systematic/frequent biases of the dust emission scheme
  - Provides a comparison point to the future dust emissions from the IFS-COMPO emission inversion framework (work of Michael and Mel)
- Then, use this reference dust emission data to train a ML/NN algorithm offline.
- Finally implement in IFS-COMPO the capacity to call the inference model computed offline in order to estimate dust emissions

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Offline inversion of desert dust emissions

Jeronimo Escribano, Samuel Remy

Offline dust emission inversion how?

- **Data assimilation** of remote sensing dust AOD or AOD at 550nm to estimate dust emissions
- Modified workflow of the **Local Ensemble Transform Kalman Filter (LETKF)** used at BSC
- Provides scaling factors of the prior emissions (3 days temporal resolution, grid point spatial resolution)

Assimilated DOD
VIIRS SNPP Deep Blue

IFS-COMPO Ensemble

20 members with perturbed emissions at the time

100 *active* members

LETKF (smoother)

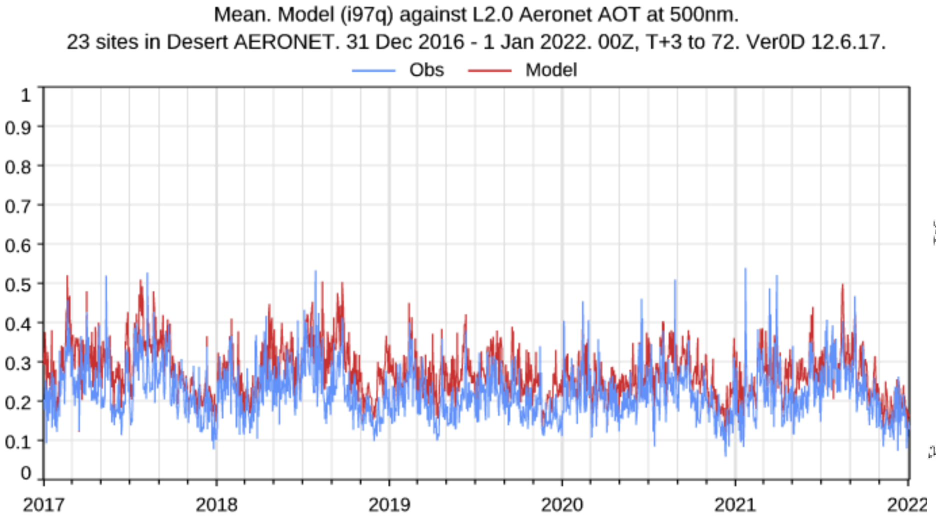
Control: dust emission
- 3 days temporal resolution
- Model horizontal resolution

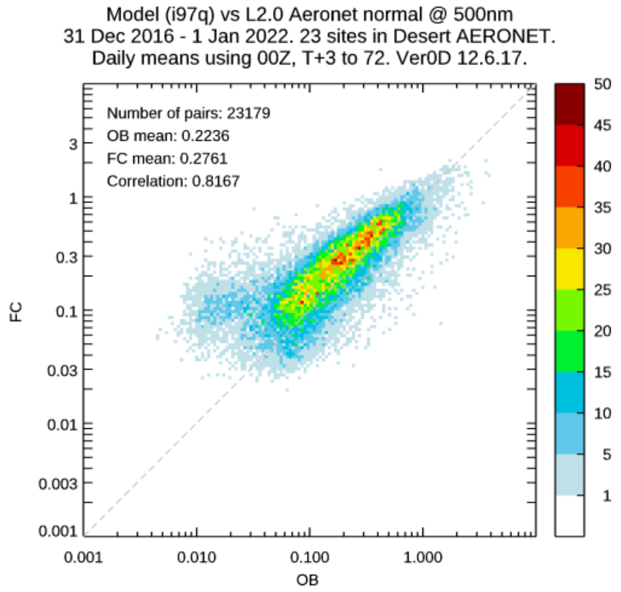
Observations: Dust AOD or AOD 550nm

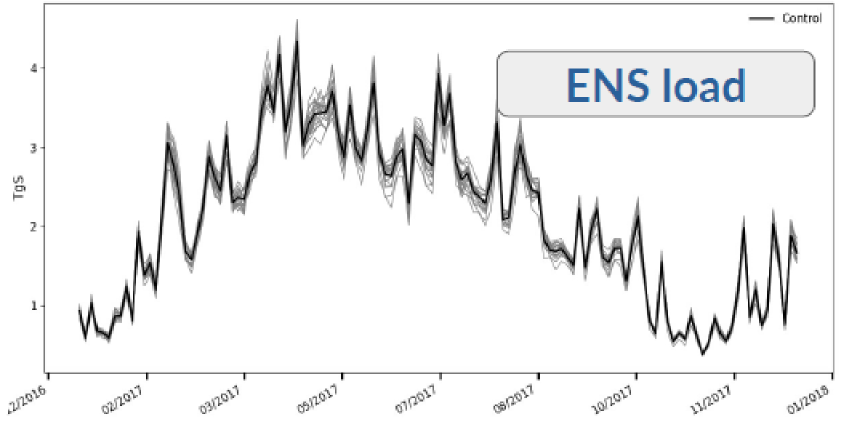
(BSC – J Escribano)

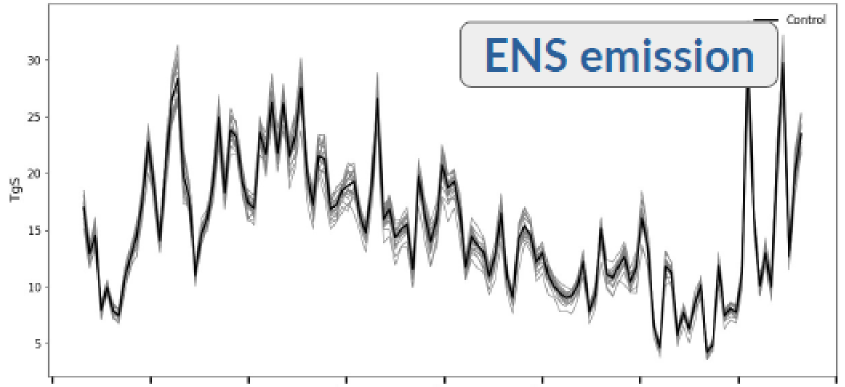
Control run and ensemble

- 1 control and 20 perturbed members
- 15 days forecasts, cycling every 3 days, no data assimilation
- Meteorology nudged to ERA-5 during the forecast
- Perturbations of dust emissions applied in the first three days
- T511 (~50km grid cell) L137 resolution
- Aerosol only IFS-COMPO, pre cycle 50R1, no chemistry configuration
- Processed from 31/12/2016 to 1/1/2022







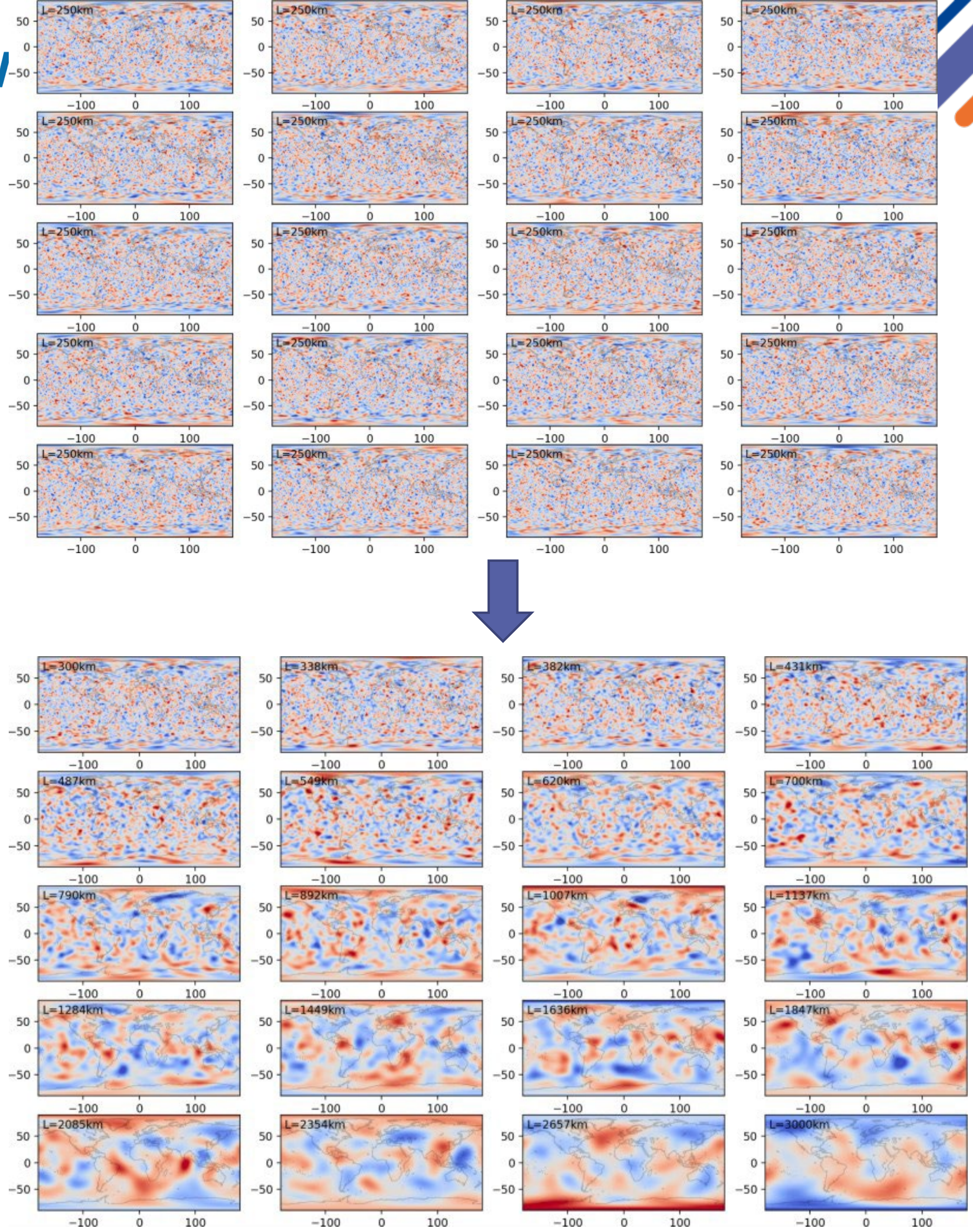


(BSC – J Escribano)

Ensemble versions

- Version 1 with currently operational dust emission scheme and fixed correlation length of ensemble perturbations (250km)
- Version 2 with new dust emission scheme from CAMAERA WP5 (adapted from SILAM dust emission scheme), and with varying correlation length (300-3000km)
- Results of V2 shown

(BSC – J Escribano)



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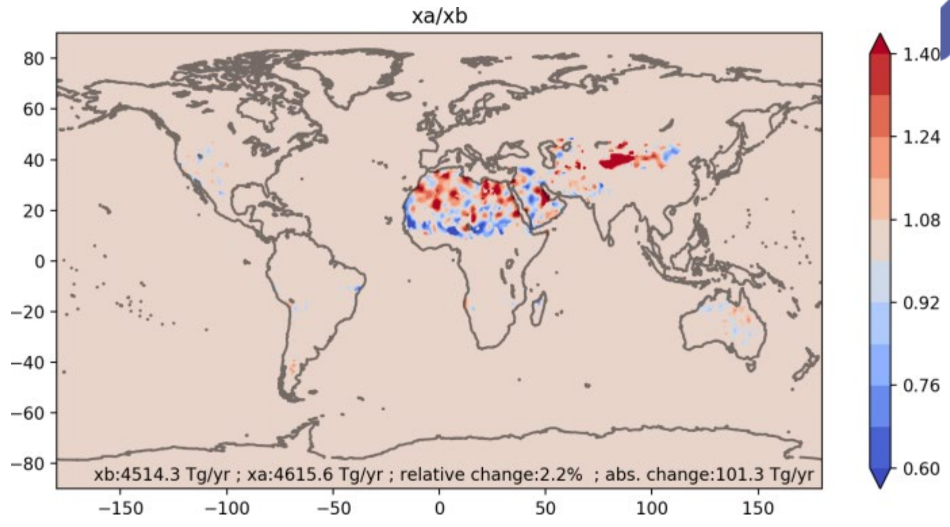

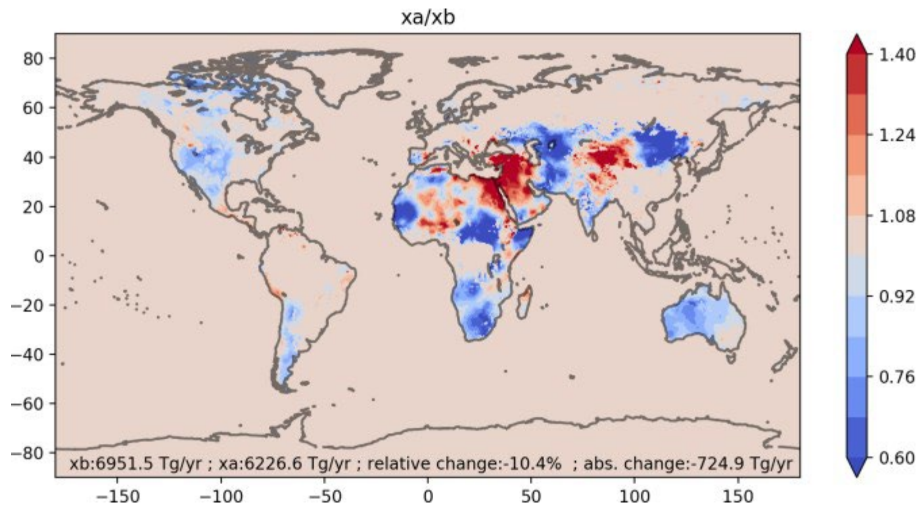

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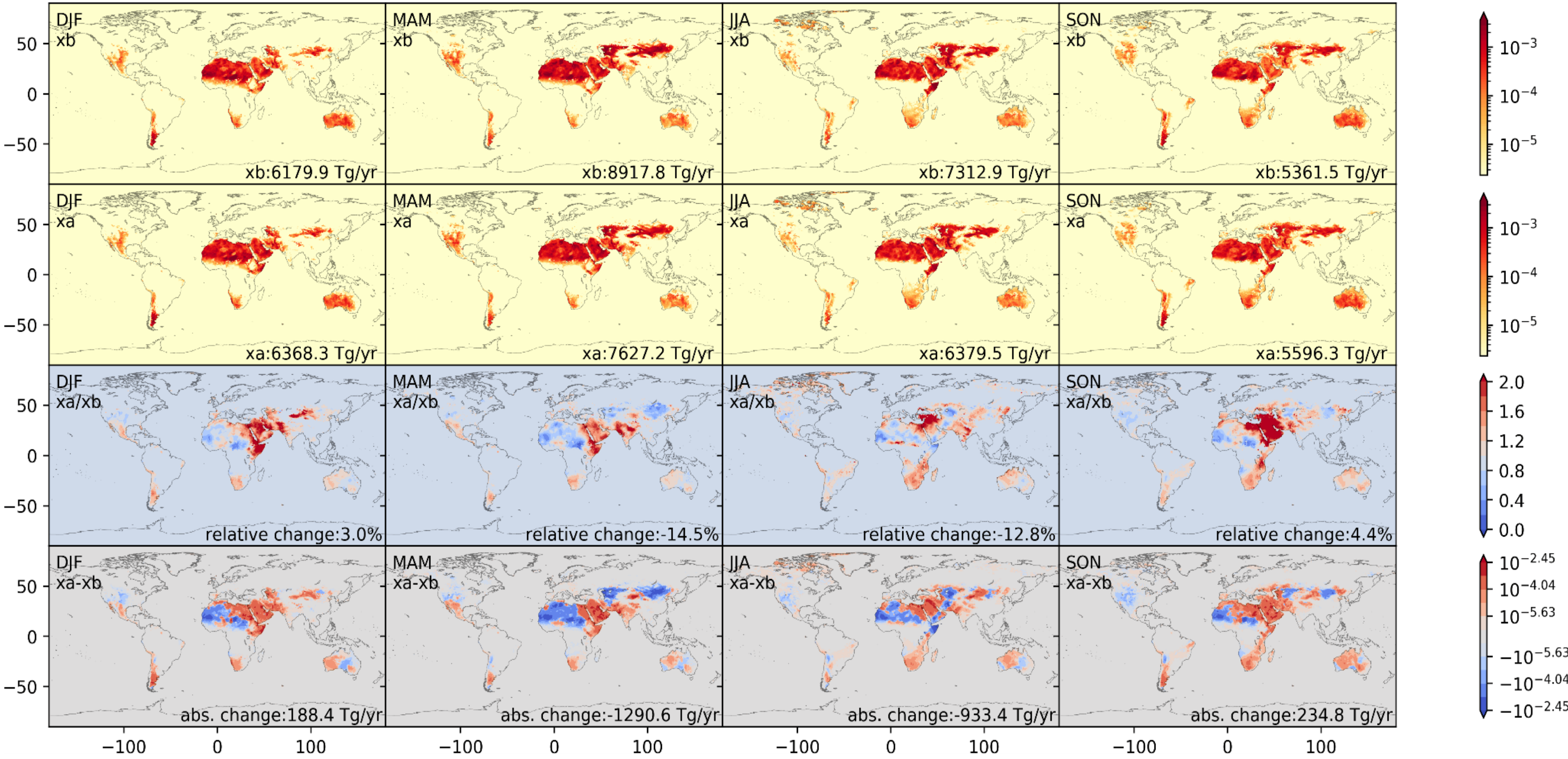
Results: emission changes

2017 only

Assimilation of DODx1.5



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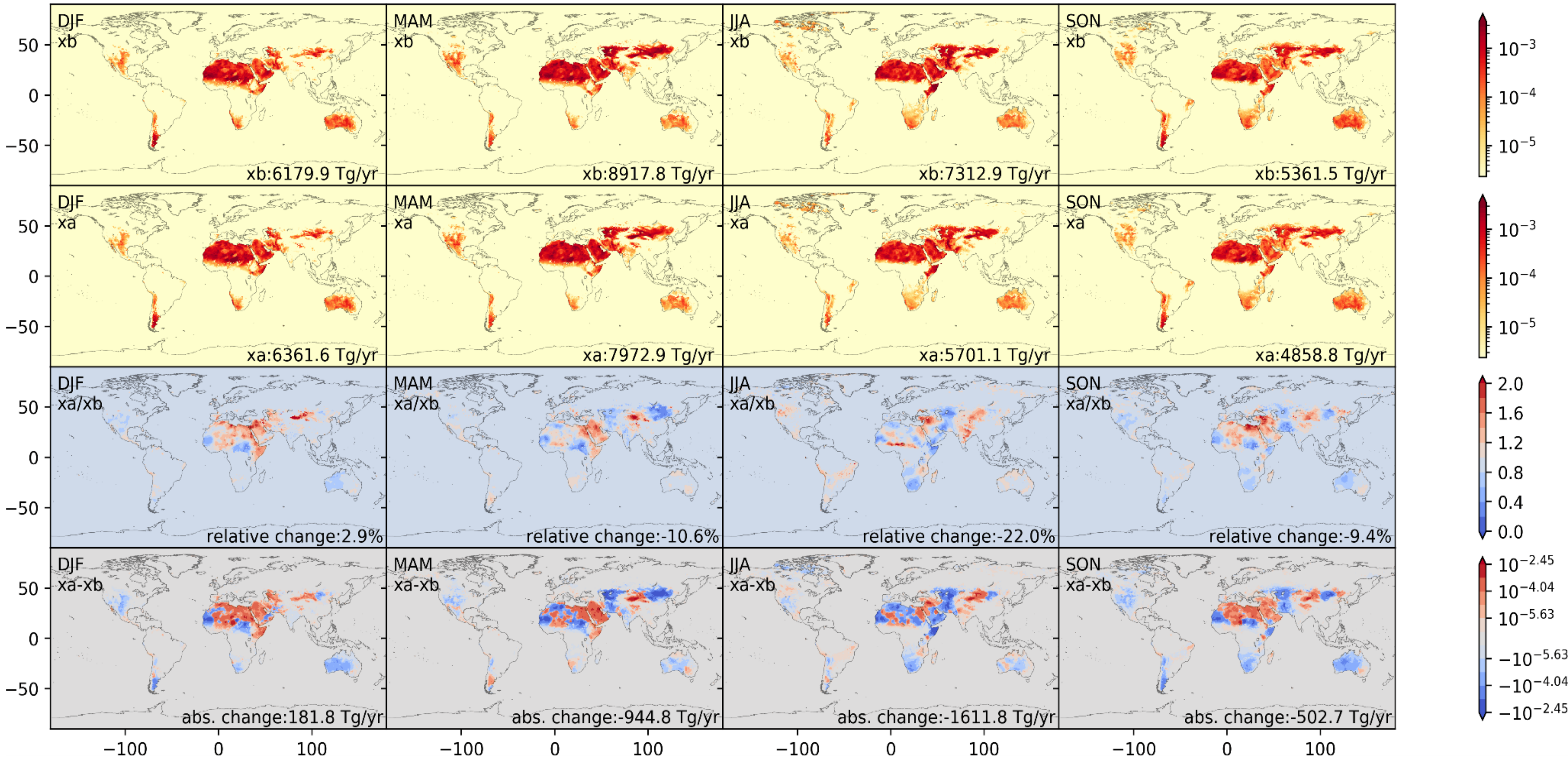
Results: emission changes

2017 only

Assimilation of AOD



(BSC – J Escribano)

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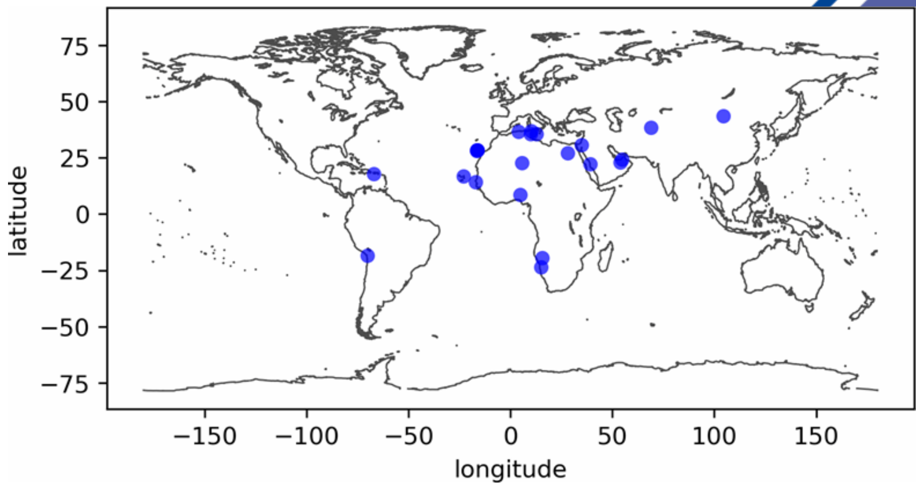
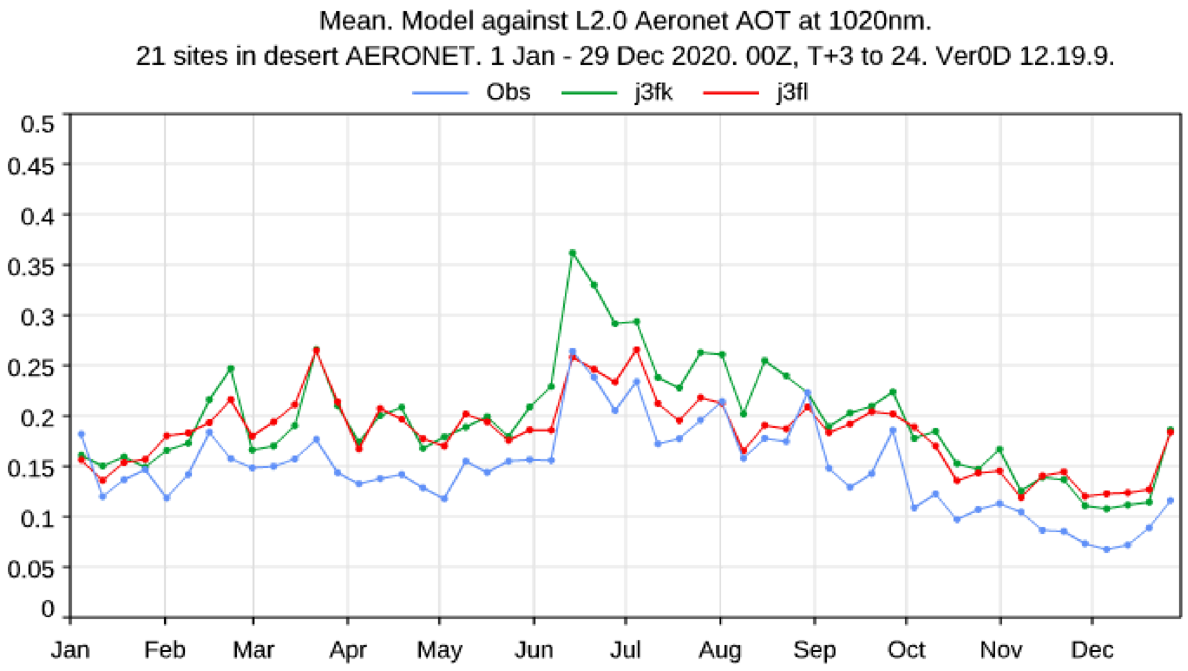
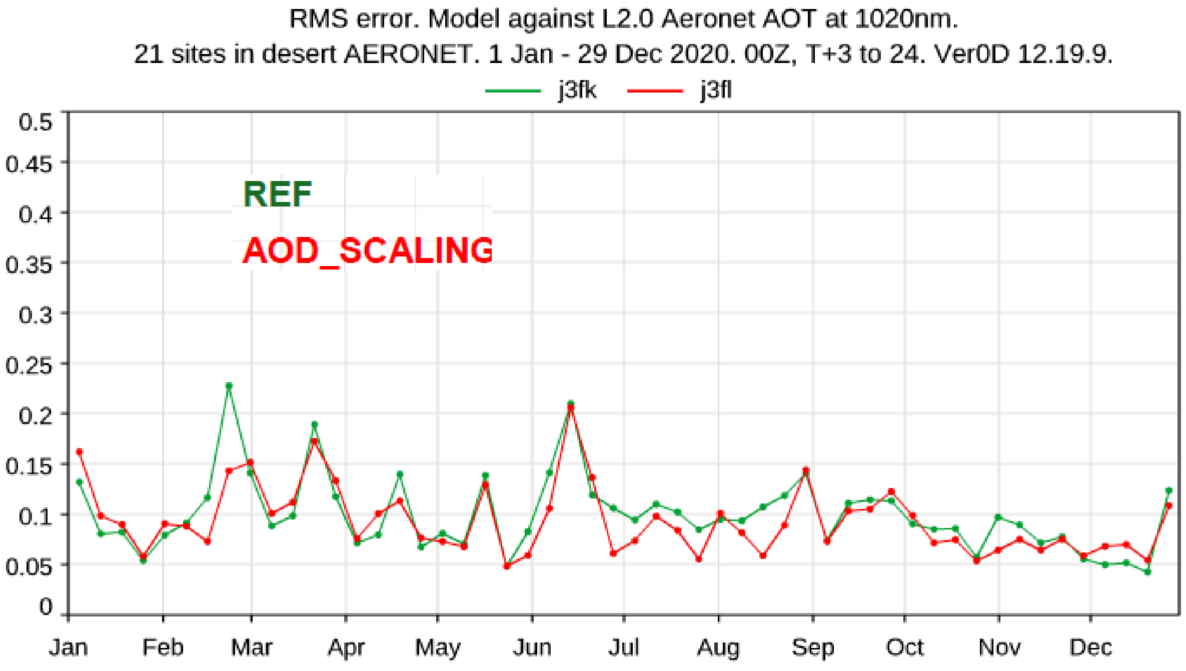
Use of scaling factors in IFS-COMPO

- Use of daily desert dust emissions scaling factors in IFS-COMPO dust emissions
- Test in forecast only (no DA) simulations over several years
- Often lower emissions in summertime
- RMSE vs AERONET improved in summertime
- No improvement in correlation







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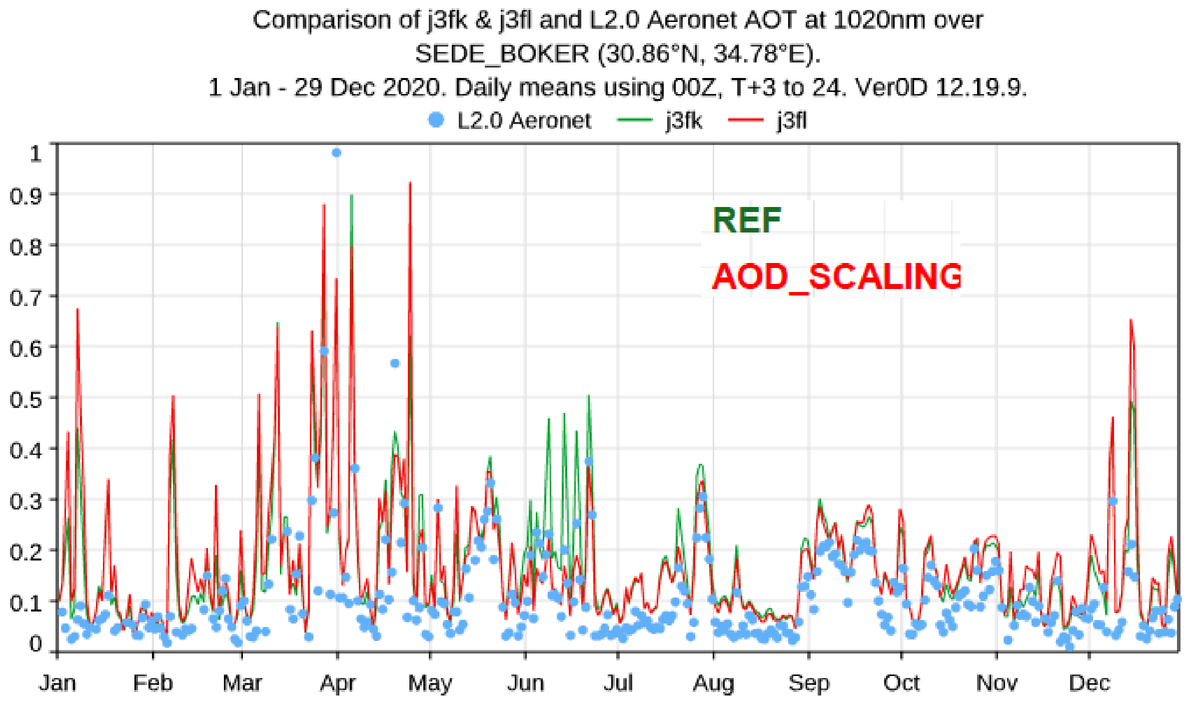

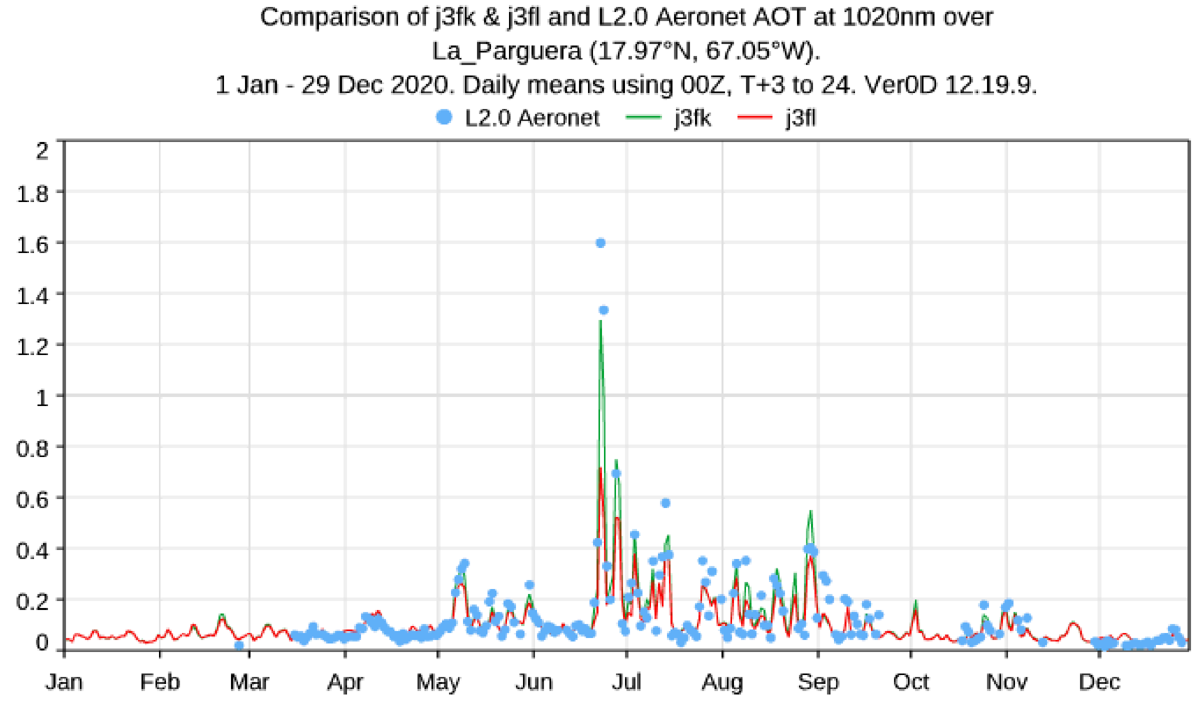

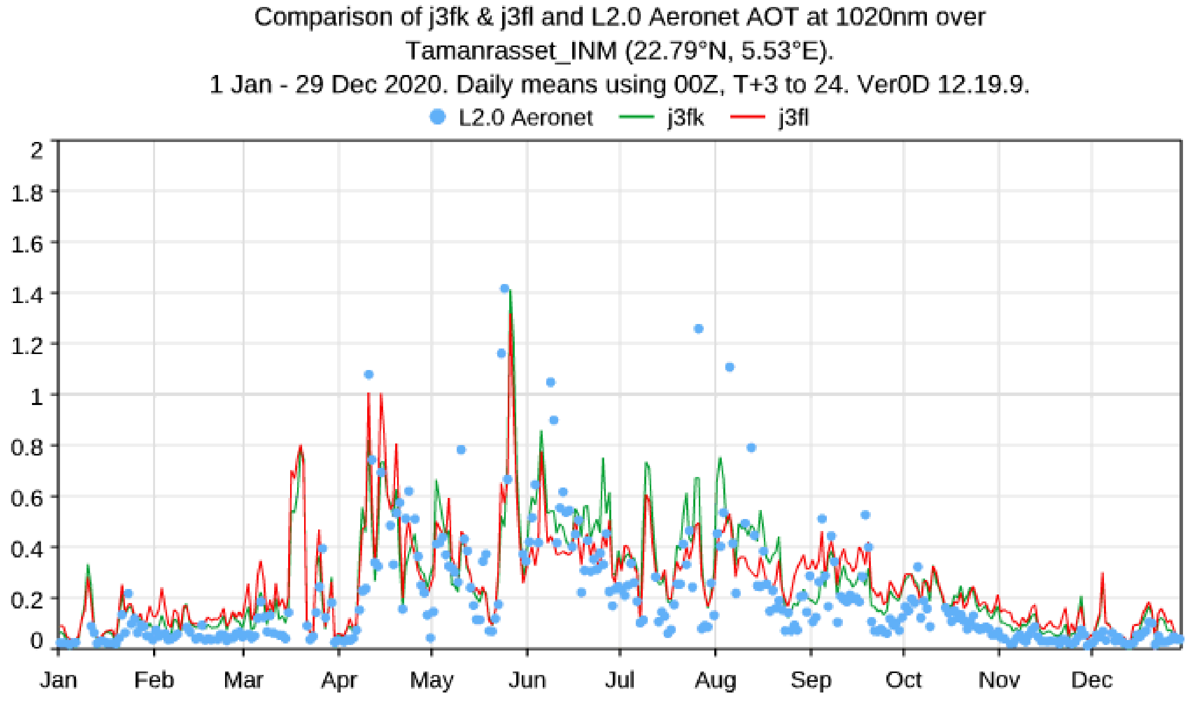

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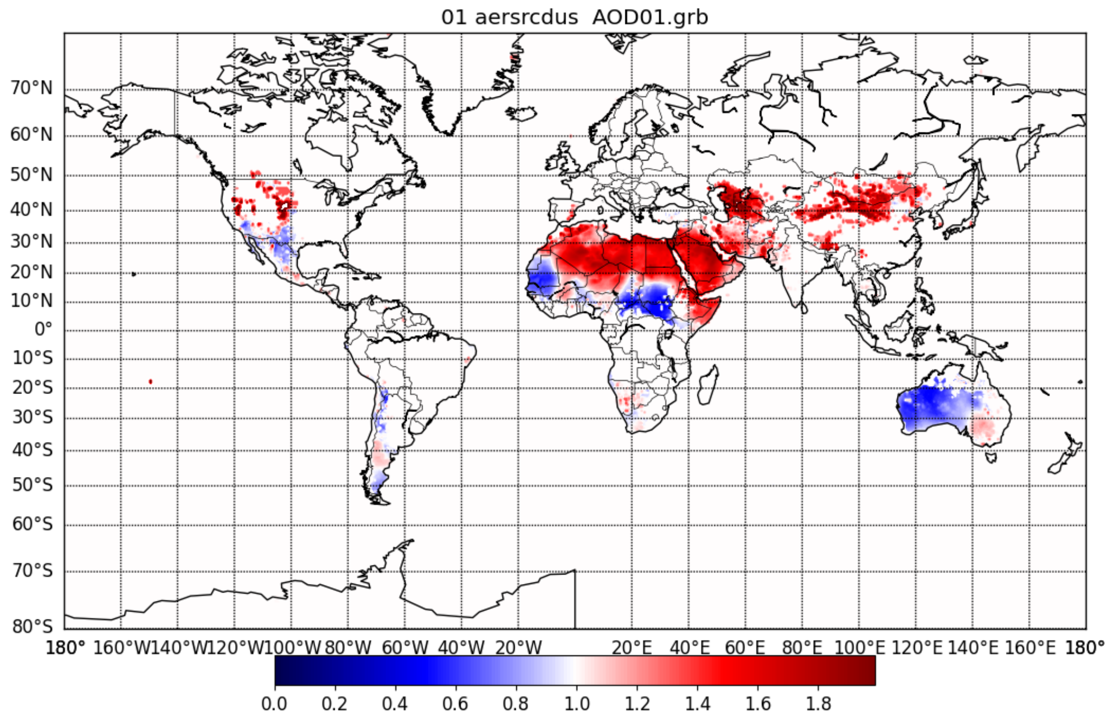
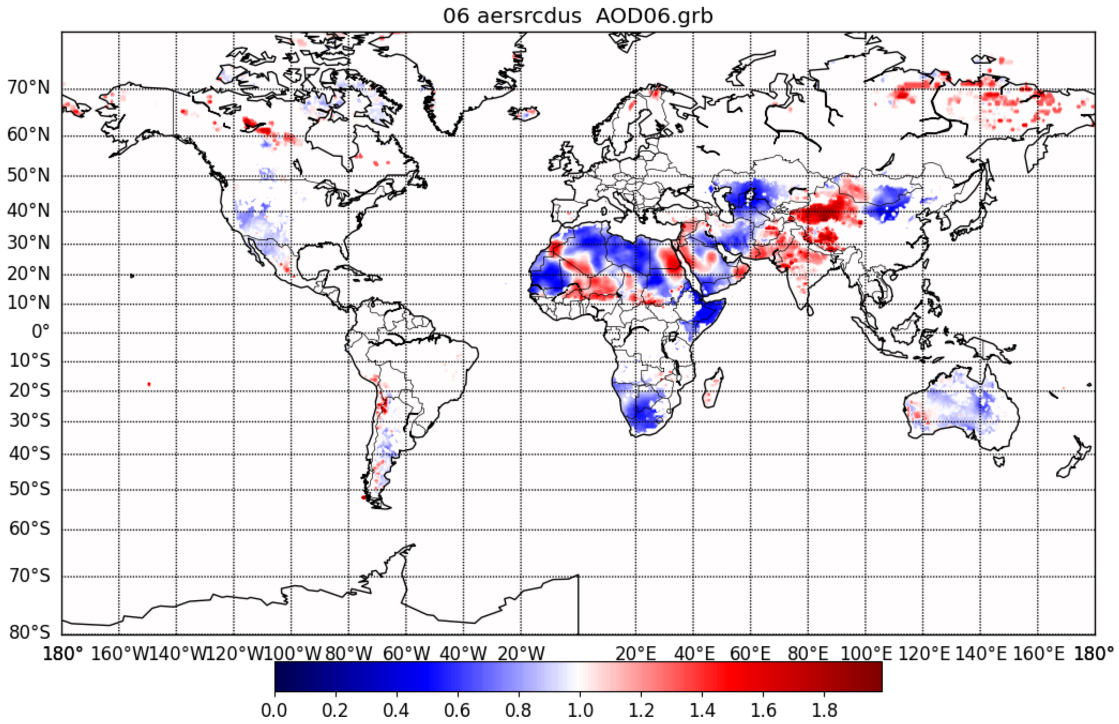
Computation of mean monthly emissions weighted scaling factors

- Could be used to debias IFS-COMPO dust emissions
- Currently being tested



January



June

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Training of a neural network to estimate desert dust emissions

Nathan Capon

Inference model versions

- V0 (technical test) with 5 predictors – March 2026
- V1 with 15 predictors – End of April 2026
- V2 with various updates and use of log (dust emissions) as reference – June 2026

Input data - predictors

- 15 predictors from cycle 50R1 IFS-COMPO simulations
- The inputs include meteorological variables, surface properties (fixed), climatological input

Wind	Static Soil	Seasonal Soil	State Variables
Wind speed	Clay fraction	Roughness length	Soil moisture
Wind gusts	Sand fraction	Surface albedo	Snow depth
Friction velocity	Bare soil fraction	LAI (Leaf Area Index)	
Threshold velocity	Orography std. dev.		

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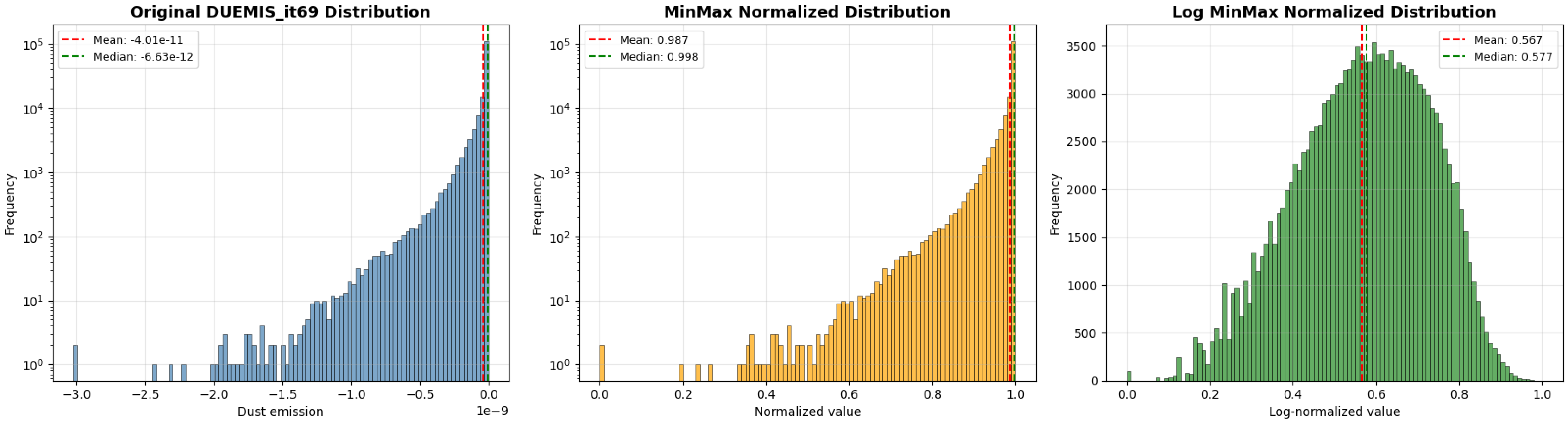
Input data - reference

- Data from the dust emissions analysis – AOD control variable
  - Training: 2018–2020 (36 monthly files) → 90% train / 10% validation
  - Test: 2017 (12 monthly files)
  - Grid: 361 × 720 = 260K spatial locations per timestep
- Dataset heavily tilted towards small values
- In a v2, in order to reduce the relative weight of small values, use of log(normalized emissions) as a reference



Model selection

- Three constraints guided the choice of a model

Constraint	Implication	Excluded Models
IFS-COMPO parallelization	Only local pixel values accessible	CNNs, UNets, Transformers
Continuous output	Smooth predictions required	Decision trees, Random Forests, GBDT
Non-linear relationships	Complex feature interactions	Ridge, Lasso, Linear Regression

- The most suitable model is a feed-forward Neural Network (DNN)

Hyperparameter optimisation

Finding the best hyperparameters is like searching for the highest point in a mountain range without a map (in foggy conditions)

Hyperparameter optimisation

Hyperparameters:

Category	Parameters
Architecture	Layers, Hidden dim, Activation, Dropout
Training	Batch size, LR, Weight decay, Grad clip
Optimizer	Type, Scheduler
Normalization	MinMax, Standard
Loss	MSE, MAE, R^2

Possible approaches:

Approach	How it works	Problem
Random Search	Sample randomly	Wastes trials on already-explored regions
Grid Search	Test every combination	Too slow (combinatorial explosion)
Bayesian Optimisation	Learn from past trials	Smart & efficient exploration

Key idea: Build a probabilistic model (surrogate) of the objective function Use it to decide where to sample next. 100 trials executed.

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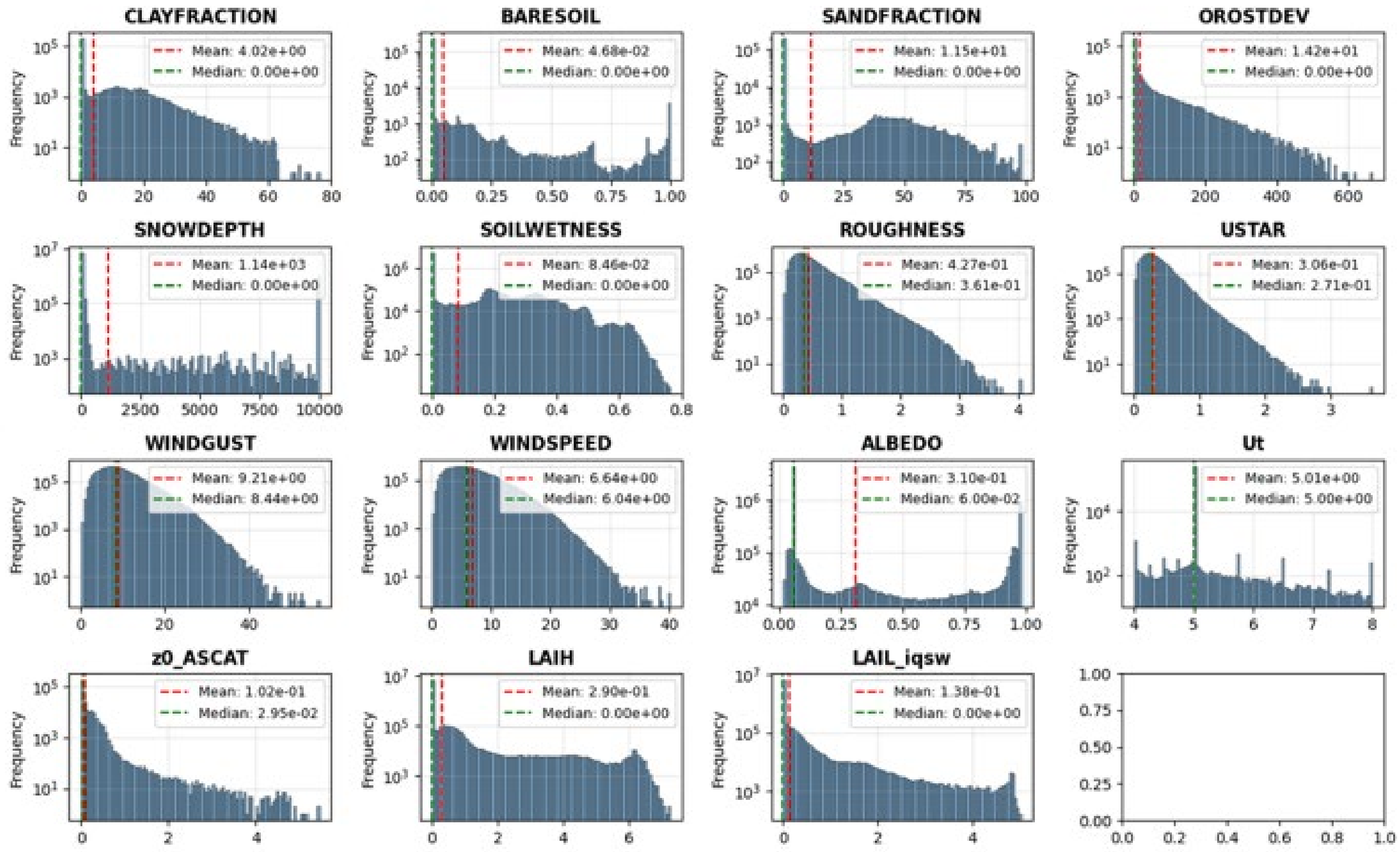
Hyperparameter optimization – input norm

Min-Max normalization preferred over Standard (z-score) normalization

Why? Our predictors do not follow a Gaussian distribution. Applying z-score normalization would not be appropriate, making Min-Max scaling the better choice for input features.



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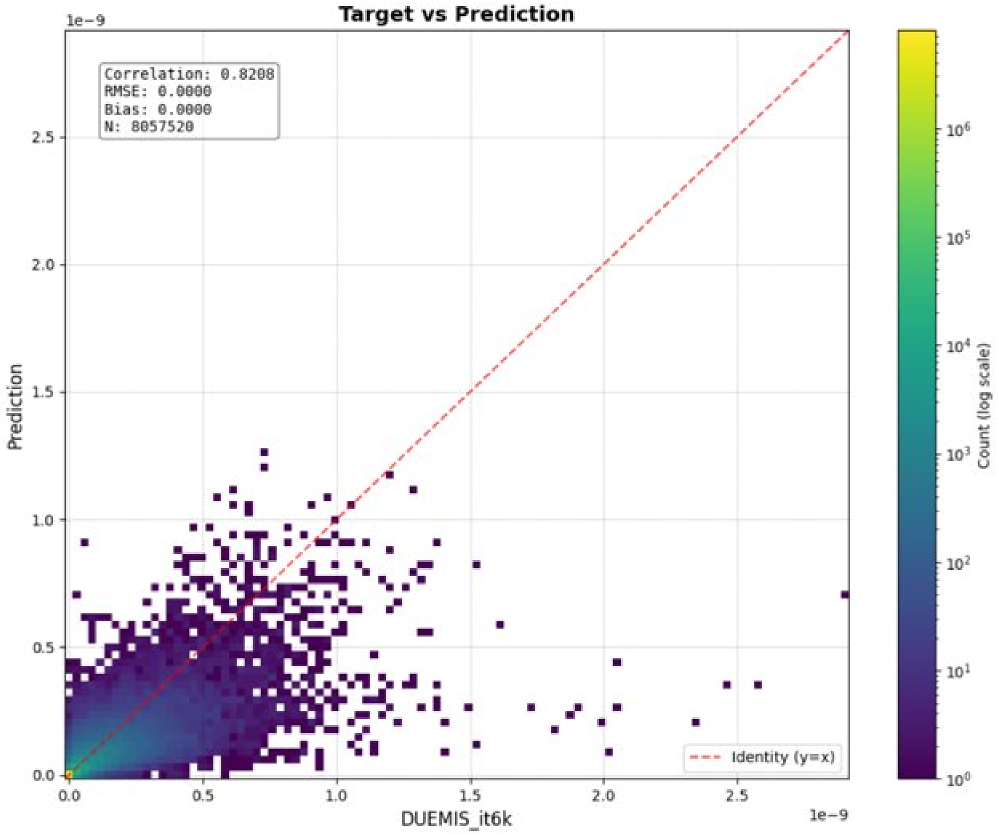
Final pre-trained inference model architecture

Final configuration for our DNN model:

Hyperparameter	Value
Layers	[256,256,256]
Activation	GeLU
Normalisation	Inputs & Output
Dropout	0.2
Loss	r2
Optimizer	AdamW
learning rate	1e-4
batch size	256



Final pre-trained inference model architecture –v2

Final configuration for our DNN model:

Hyperparameter	Value
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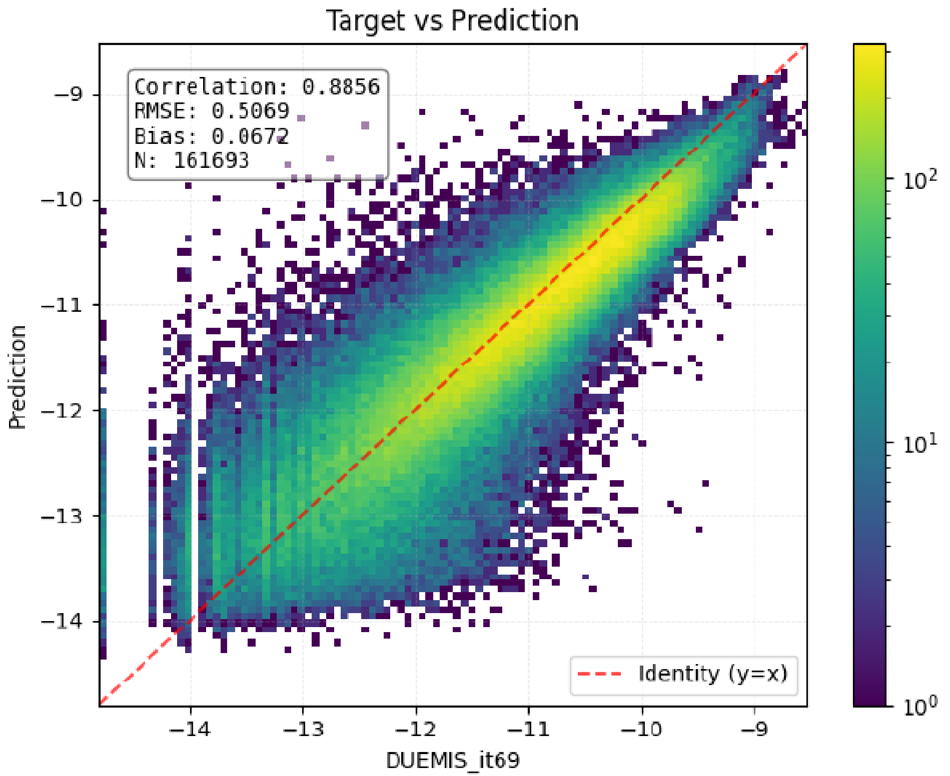
Normalisation	Inputs & Output
Dropout	0.2
Loss	r2
Optimizer	AdamW
learning rate	1e-4
batch size	256



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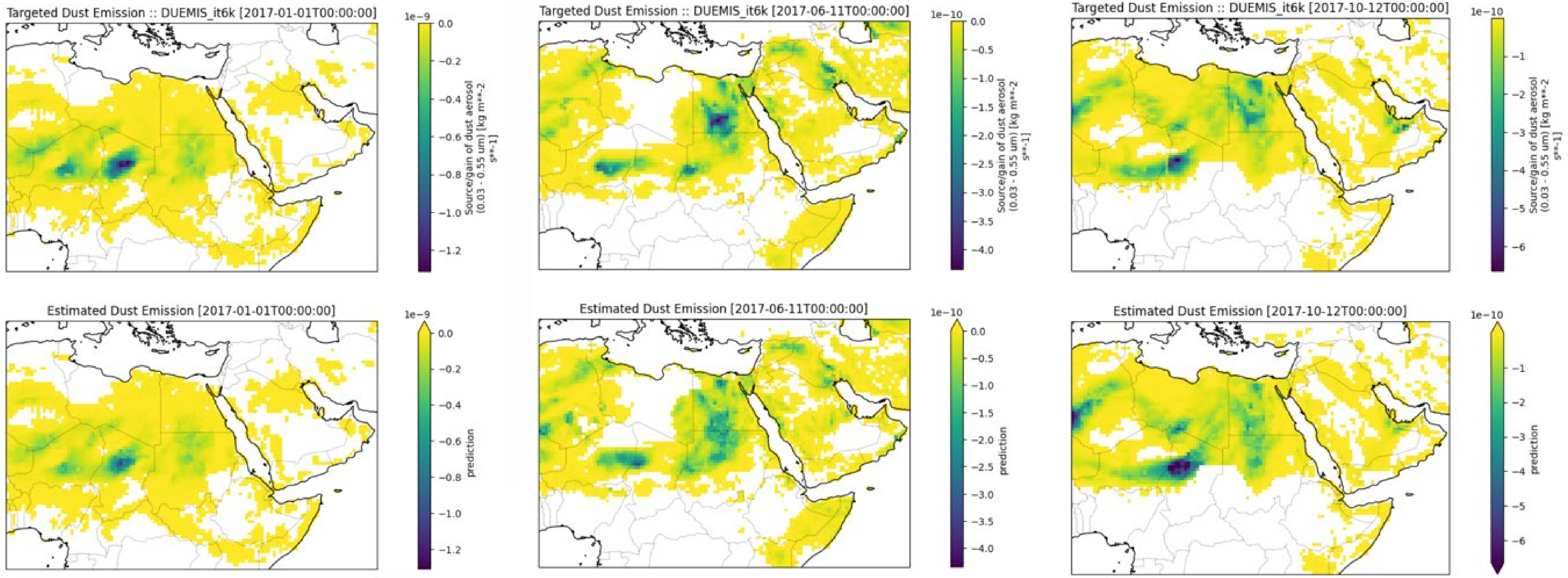

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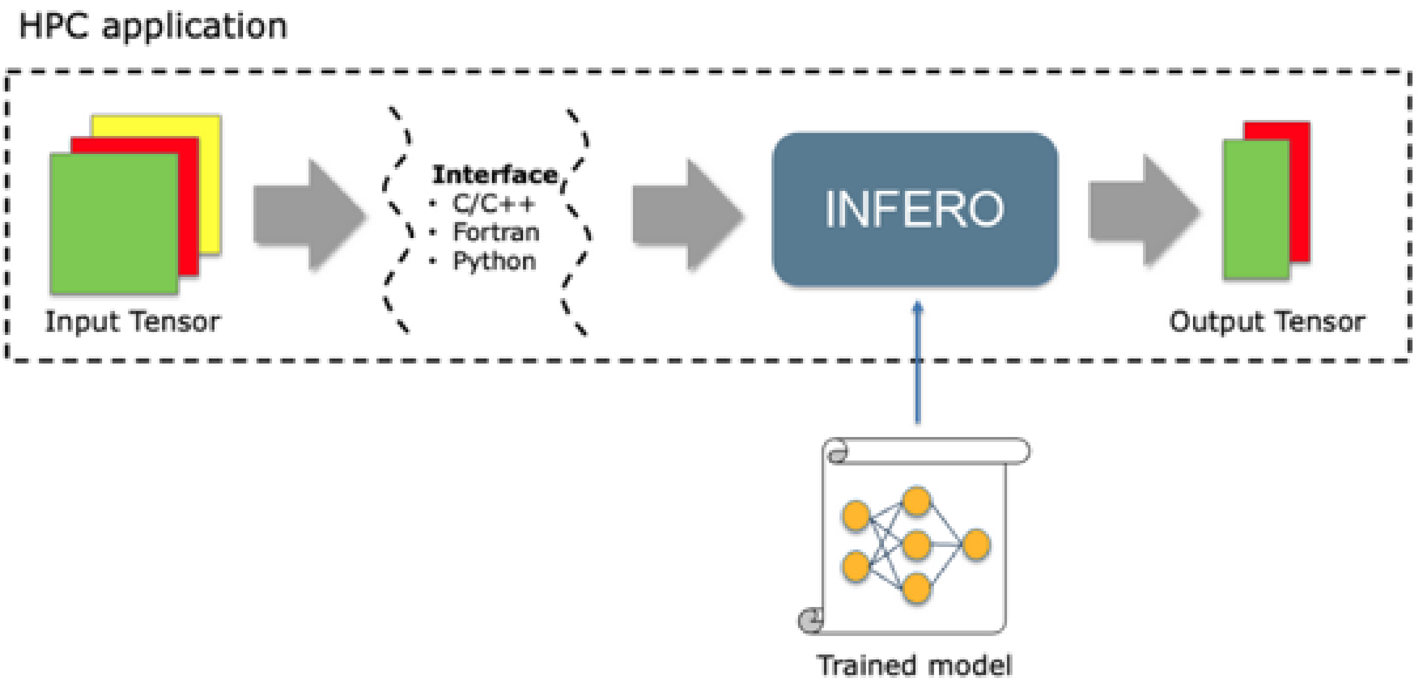
Implementation of desert dust emissions from neural network in IFS-COMPO

Rose-Cloé Meyer, Samuel Remy

Use of the inference model in IFS-COMPO

- Use of the ECMWF INFERO library in cycle 50R1 IFS-COMPO (https://infero.readthedocs.io/en/latest/)
- INFERO allows to run a pre trained inference model (exported in ONNX format) in IFS-COMPO



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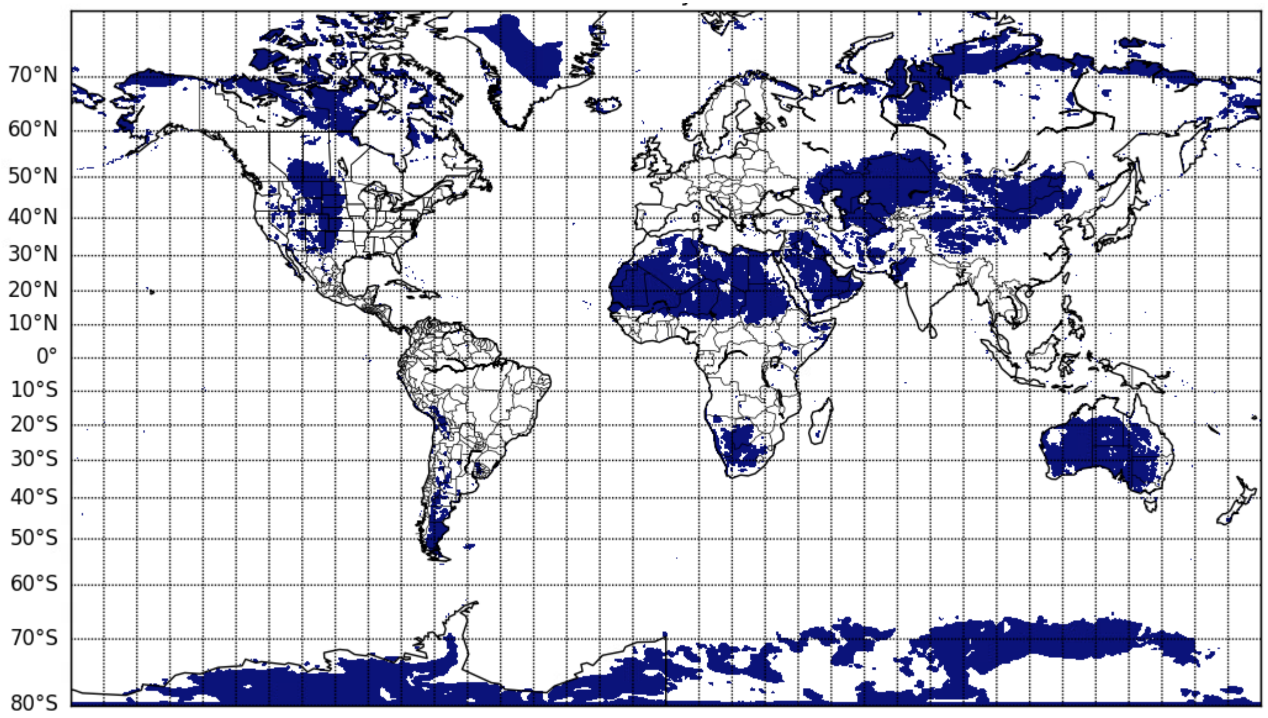
Use of the inference model in IFS-COMPO

The use of desert dust emissions from NN has been tested into IFS-COMPO forecast only experiments with the following specifics :

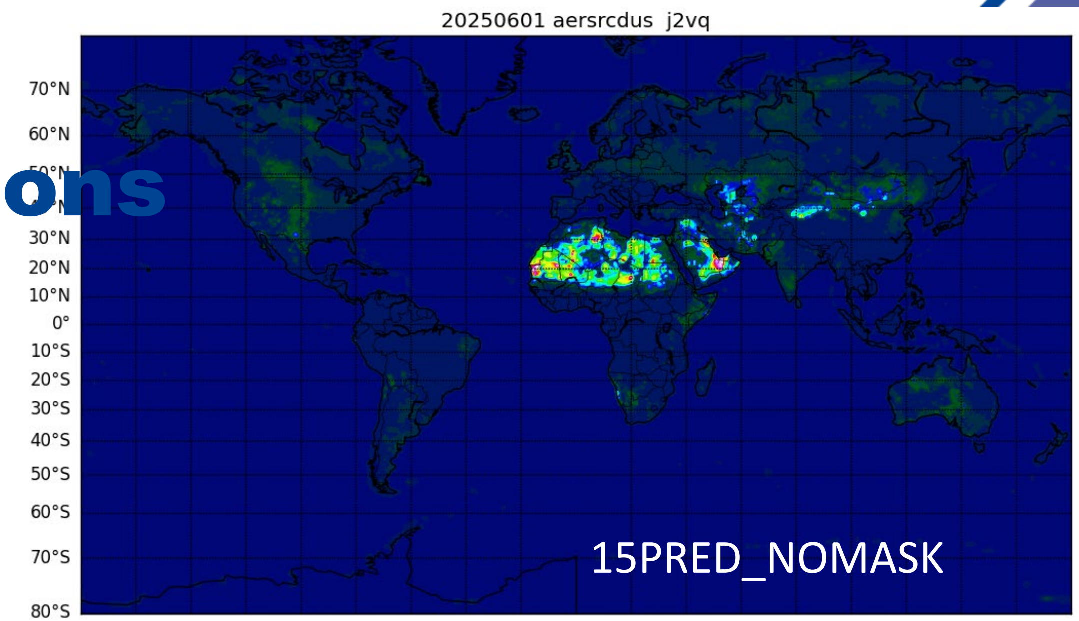
- Cycle 50R1 + new dust emission scheme from CAMAERA WP5, adapted from SILAM + new dry deposition (proposed for 51R1)
- 2017 and second half of 2025 tested

Three experiments are shown:

- reference experiment using the physical scheme
- experiment using the full 15 predictors neural network for dust emissions
- experiment using a similar configuration but only in the blue area – outside, desert dust emissions are always null.

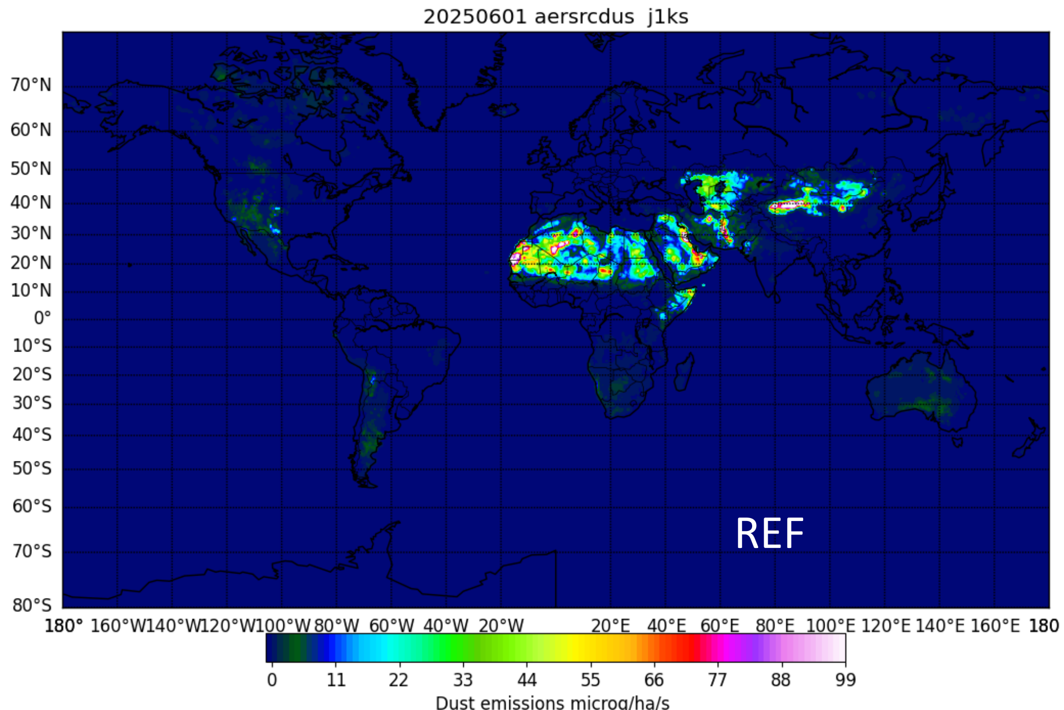


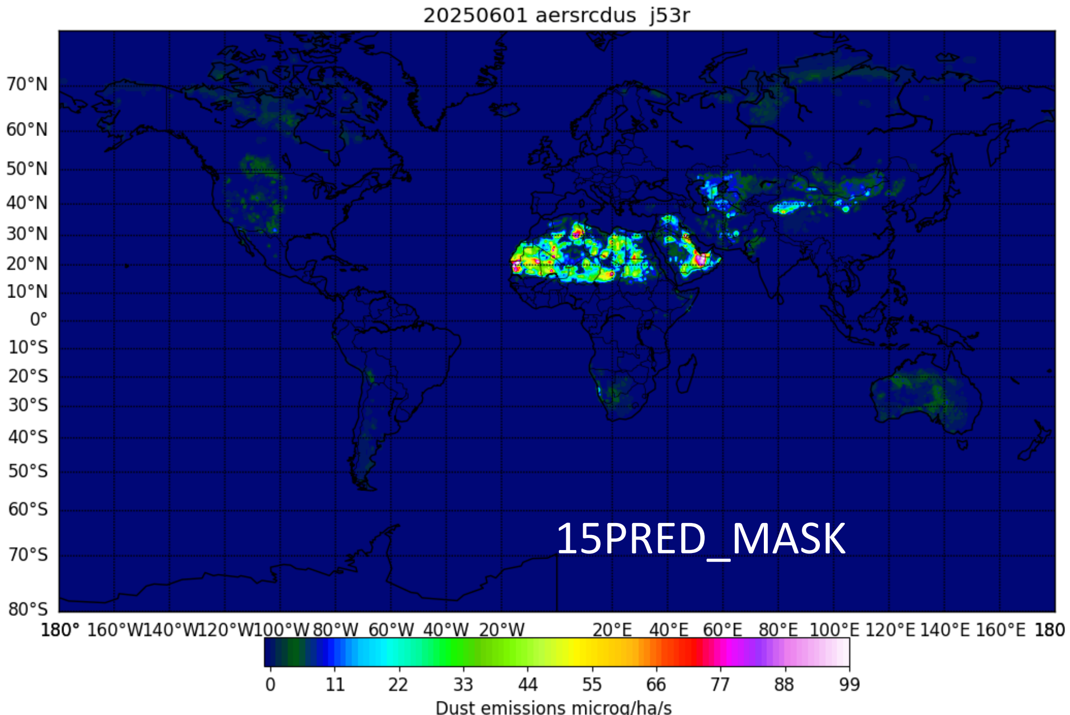
Simulated desert dust emissions



Simulated dust emissions averaged in June 2025:

- General features are quite similar
- High latitude dust sources visible over Canada
- NN predicts lower emissions over Taklimakan
- For experiment with (15 predictors, no mask), large areas with low but non null emissions

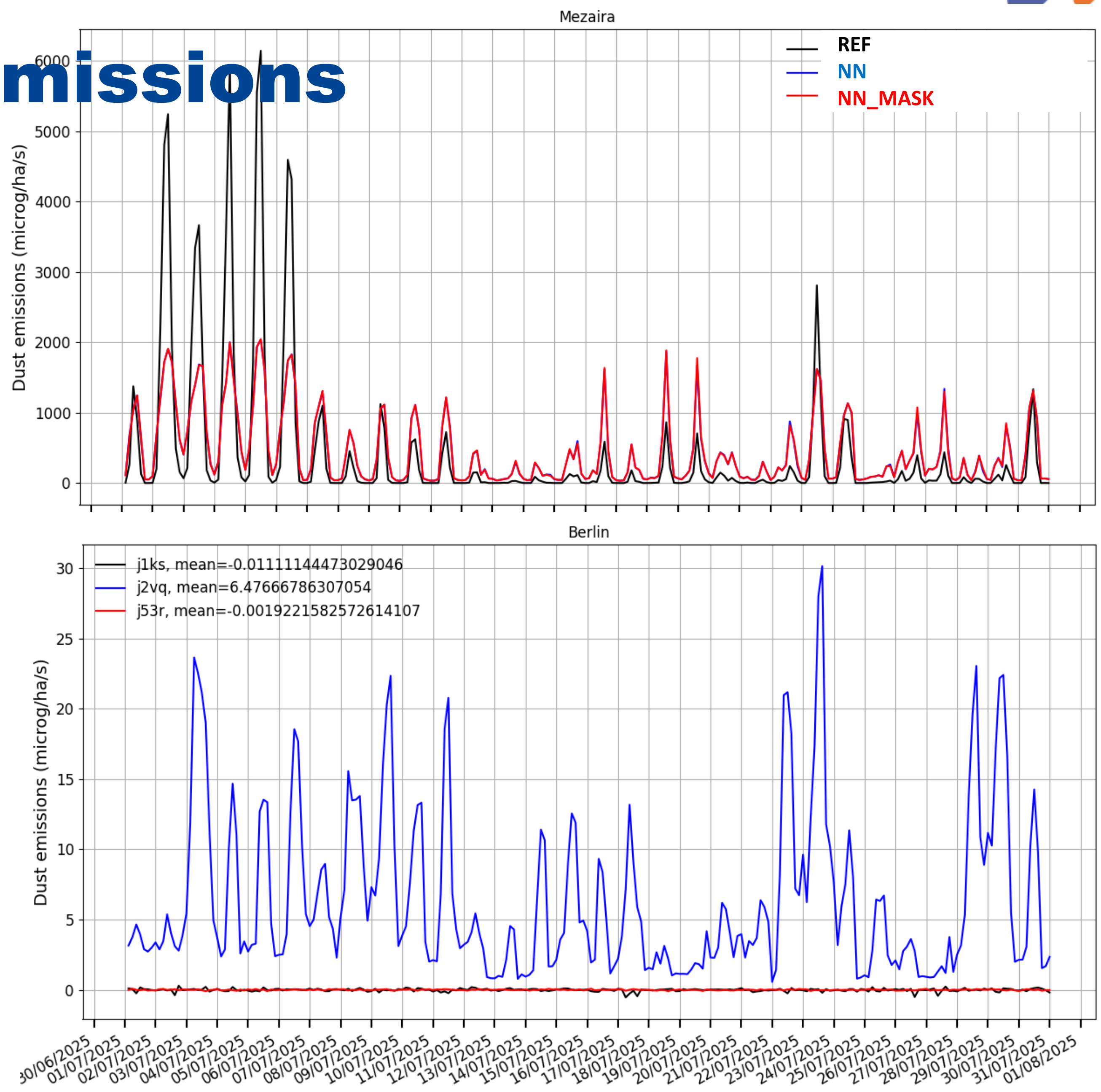




Simulated desert dust emissions

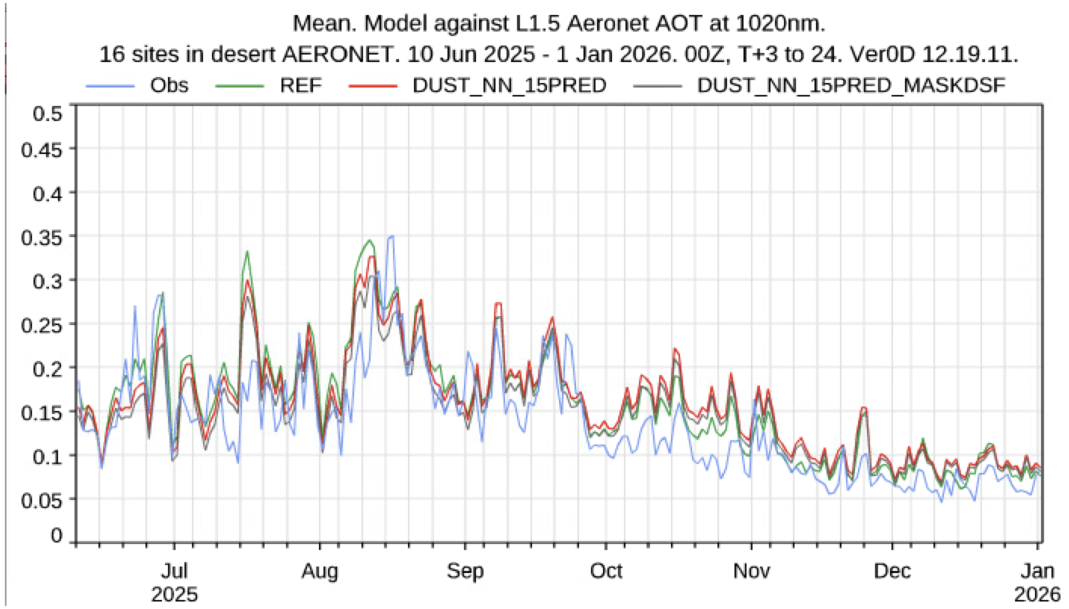
Timeseries of simulated dust emissions over Mezaira (UAE – dusty region) and Berlin (Germany, not dusty!) show:

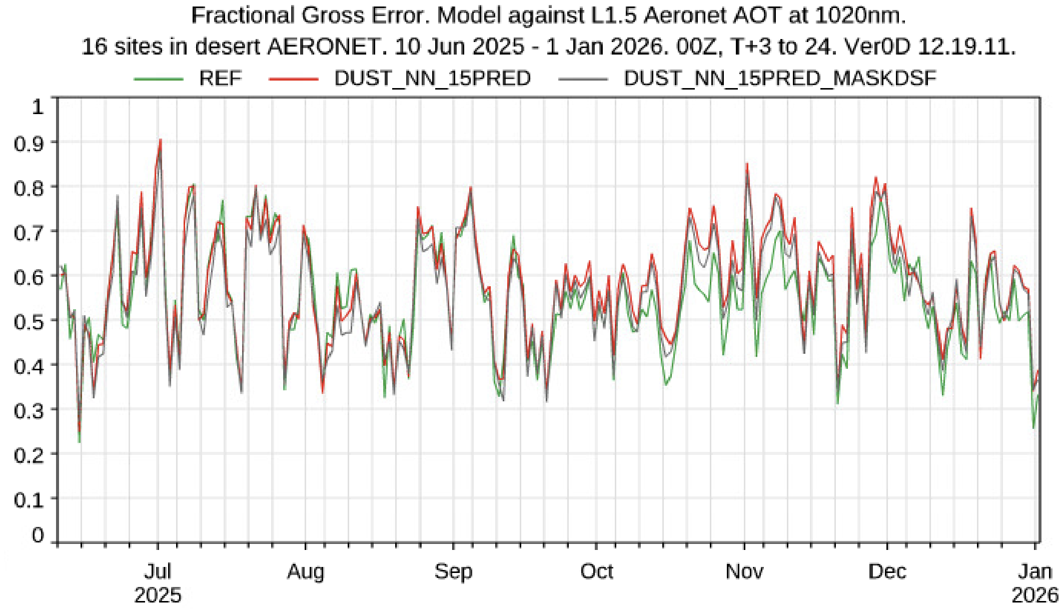
- NN without mask predicts low but still significant dust emissions over Berlin, effectively masked out with the use of a DSF based mask
- The occurrence of dust emissions in Mezaira is forecasted in quite a similar way
- The diurnal cycle shows a lower amplitude with NN : no null values at night, lower maxima in daytime

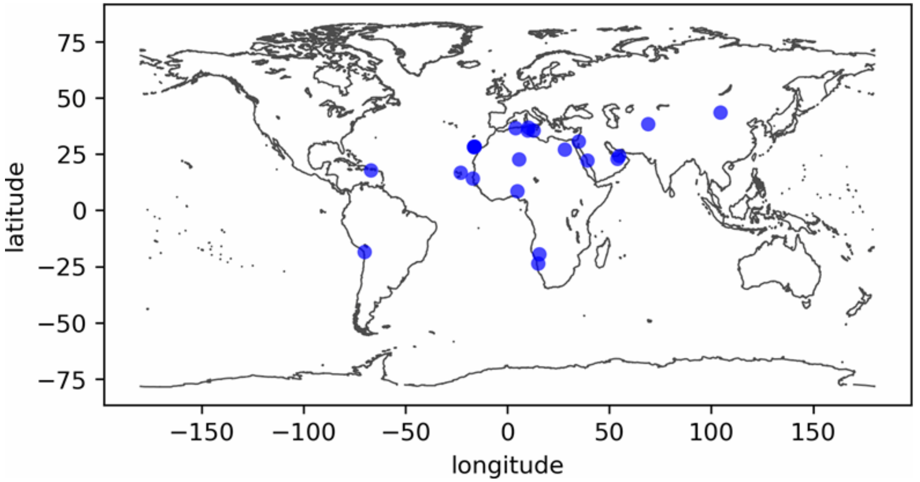


Impact on simulated AOD

- A comparison of simulated AOD at 1020nm over a selection of « dusty » AERONET stations show comparable results
- No strong signal on error – sometimes better, sometimes worse

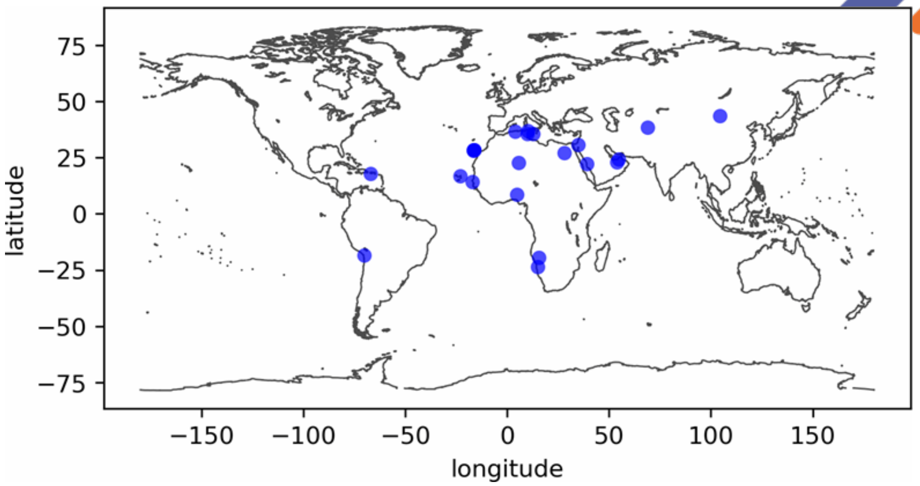


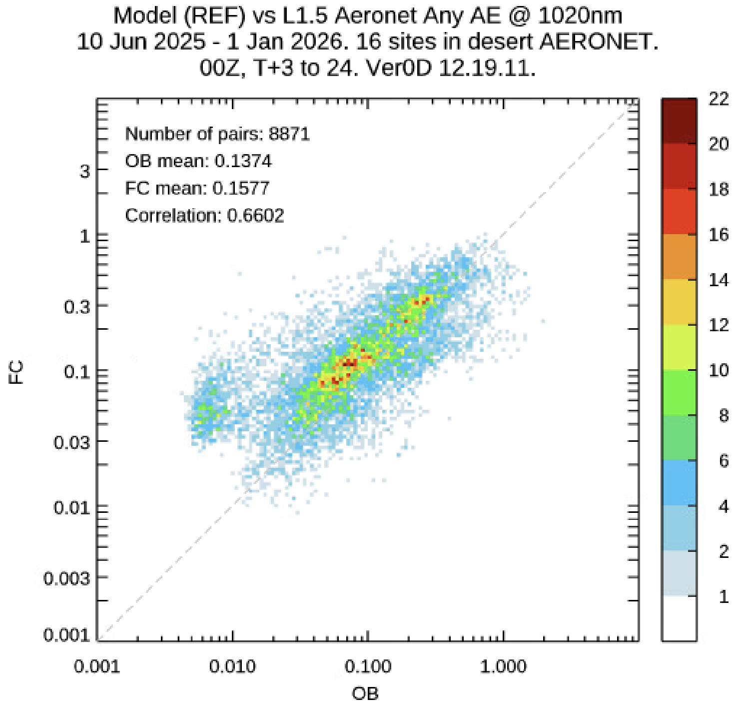


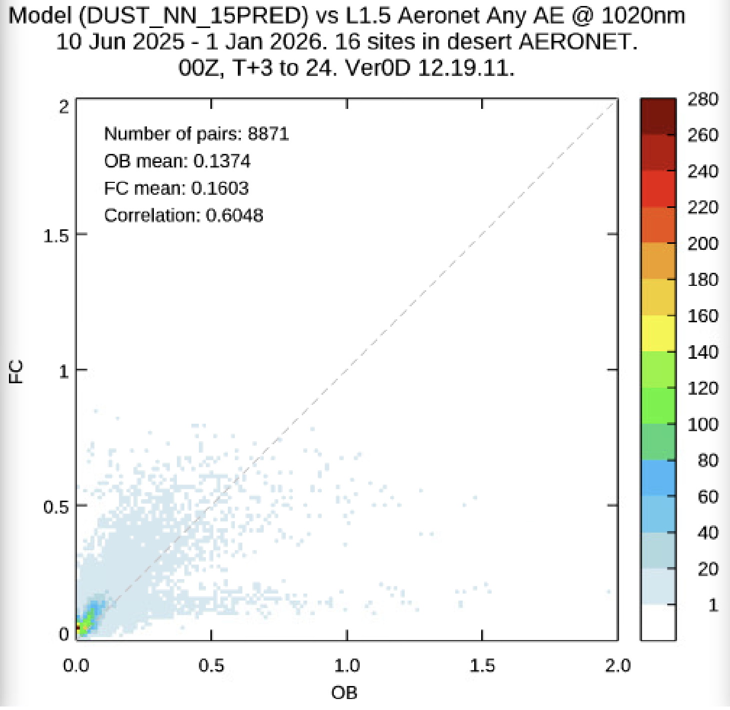


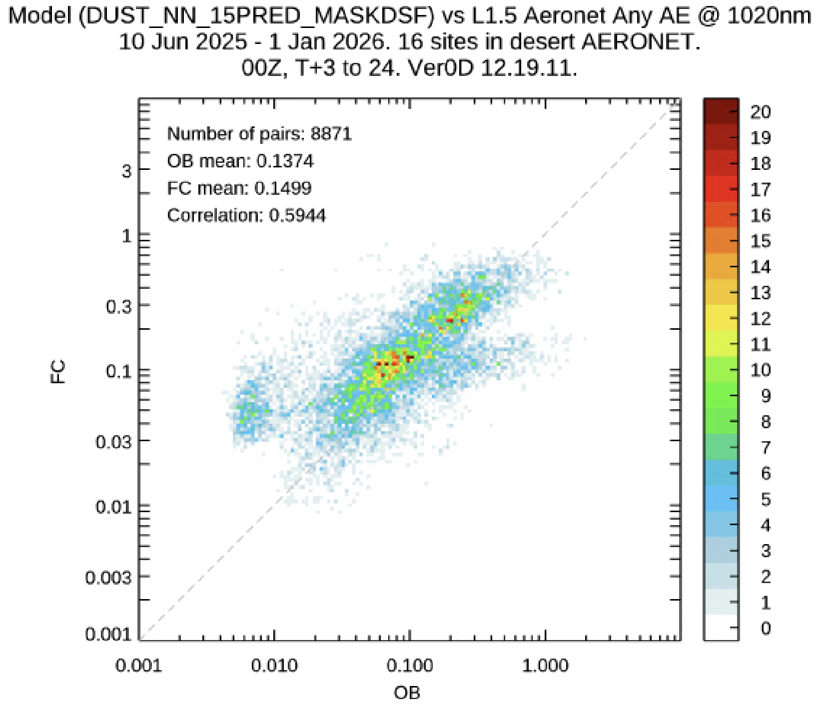
Impact on simulated AOD

- A comparison of simulated AOD at 1020nm over a selection of « dusty » AERONET stations show comparable results
- No strong signal on error – sometimes better, sometimes worse
- Correlation is clearly degraded









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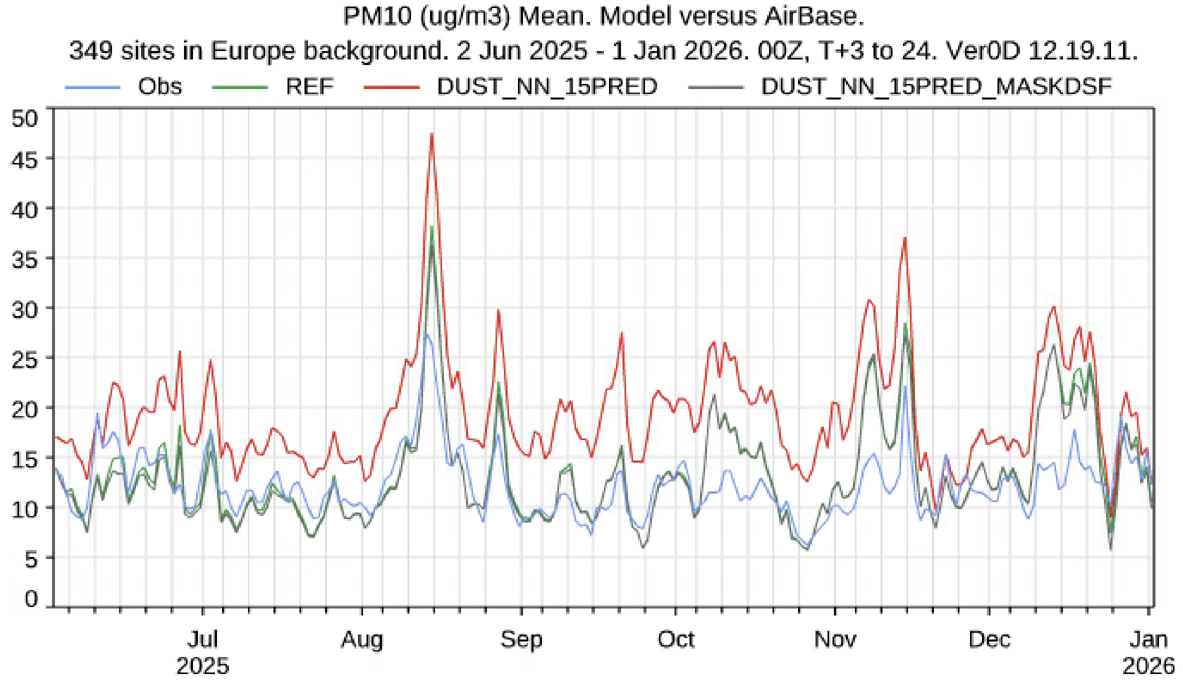
Impact on simulated PM10 in Europe

A comparison of simulated vs observed PM10 over background rural stations in Europe show:

- A clear degradation from the small and persistent emissions with the NN
- Problem easily removed by the masking
- Skill scores very close



Conclusion – what we have learnt and ongoing work

- NN dust emissions is possible but hard – much harder then whitecap fraction (for SS emissions) : skill scores on the test dataset are much lower than the training/validation
- The training is done on an analysis of (non null) desert dust emissions – which means that the NN doesn't know about null emissions => this needs to be taken into account elsewhere
- Theoretically, it could be possible to train a model including null emissions, but not sure it is worth it – probably better/easier to use NN only in areas where desert dust emissions are supposed to happen
- So some information from IFS-COMPO is useful/needed to use NN desert dust emissions => towards a "mixed" approach, NN with some physical constraints
- Ongoing work and next steps:
  - Retrain offline inference model with updated hyperparameters – error metric
  - Work on feature analysis – which predictors have more weight and "why"?
  - Work on predictors : some should be removed, and maybe some should be added, such as $(u - u_t)^3$ for example?
  - Test convolution approach (U-Net) – not implementable in IFS-COMPO but could be informative