Recent and planned developments on the ECMWF's CAMS data assimilation suite: A focus on surface flux inversions

Atmosphere Monitoring

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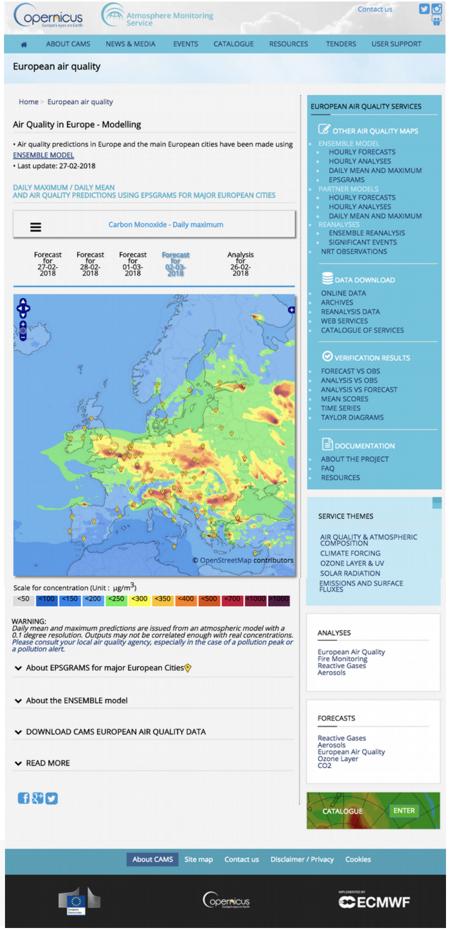
Motivations and outline

- The European Union's Copernicus Atmosphere Monitoring Service (CAMS) operationally provides analyses and forecasts of global atmospheric composition and regional AQ. Parameters include: GHG, Reactive gases and aerosols

- There is a need to monitor emissions/fluxes in addition to the 3D representation of the atmospheric composition. The implementation needs to be real time or "near" real time emission estimates, given constrains on the ECMWF IFS system and the observations available.

- Life time of species are several orders of magnitude apart! CO_2 (100years) vs NO_2 (few hours). This makes the idea of an integrated system particularly challenging and interesting…

- Outline:
  - Methodology on emission inversion
  - Emission sensitivities using the EDA
  - Work on improving **B** for composition.
  - The new Sentinel 5p TROPOMI instrument



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Variational surface flux inversion options…

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Model: $x_t = \mathcal{M}(x_{t-1}, \varepsilon_{t-1})$

With concentrations (observed) and surface flux rates (unobserved)

With x concentrations (observed) and ε surface flux rates (unobserved)

Separate minimizations:

$$J(\delta x) = J_b(\delta x) + J_o(\delta x)$$

$$J(\delta \varepsilon) = J_b(\delta \varepsilon) + J_o(\delta \varepsilon)$$

Flexibility such as window length, algorithm, but can add complexity such as communication/consistency between the analyzes and code management…

Single joint minimization:

Full augmentation

$$X = \begin{pmatrix} x \\ \varepsilon \end{pmatrix} \qquad J(\delta X) = J_b(\delta X) + J_o(\delta X)$$

Would need compromises on assimilation window length for **long-lived** species. Using cross-correlated inference on co-emitted **short-lived** species will help.

Augmentation using "balance"

$$X = \begin{pmatrix} x \\ \varepsilon \end{pmatrix} \qquad J(\delta X) = J_b(\delta X) + J_o(\delta x)$$

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Surface flux sensitivity

The adjoint sensitivity of $\frac{\partial \delta \varepsilon}{\partial \delta x}$ could be difficult to calculate, many processes involved such as: convection, turbulent mixing, deposition, injection heights, chemistry, emission temporal profile, etc…

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Combining the ensemble information within variational minimization:

"the ensemble sensitivity is the projection of the analysis-error covariance matrix onto the adjoint-sensitivity field divided by the variance" (Ancell & Akim 2007)

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"the ensemble sensitivity is the projection of the analysis-error covariance matrix onto the adjoint-sensitivity field divided by the variance" (Ancell & Akim 2007)

$$\frac{\partial \delta \boldsymbol{\varepsilon}}{\partial \delta \boldsymbol{x}} \approx \frac{\boldsymbol{\sigma}_{\varepsilon x}}{\boldsymbol{\sigma}_{xx}}$$

Whether we choose to attack the problem from J_o or J_b. The ensemble information is valuable to provide the sensitivities between model parameters.
Here: 3D chemical fields to surface fluxes.

Testing on CAMS CO configuration EDA

Ensemble of Data Assimilation:

- Is an ensemble of 4DVar IFS cycles (Isaken et al., 2010), currently 25 members operationally.
- After each cycle statistics are calculated to specify **B** (hybrid or online see Bonavita et al., 2015)

Testing the EDA for emissions:

- 12 hour window
- Low resolution T159
- 2 outer-loops
- 30 members
- Focus on **CO only**: Linear CO chemistry (lifetime 1 month)

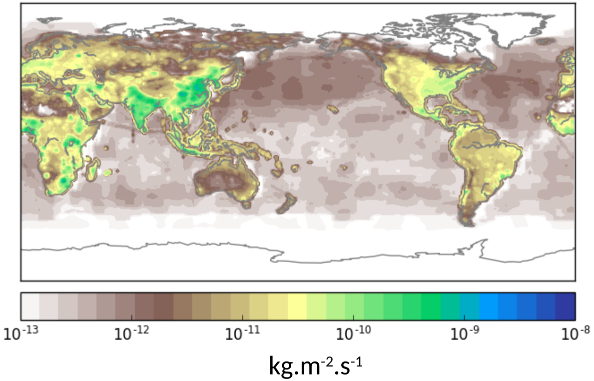
Perturbations:

- Sea Surface Temp
- Physical tendencies
- Observations (no CO obs)
- **Adding Surf. Flux**

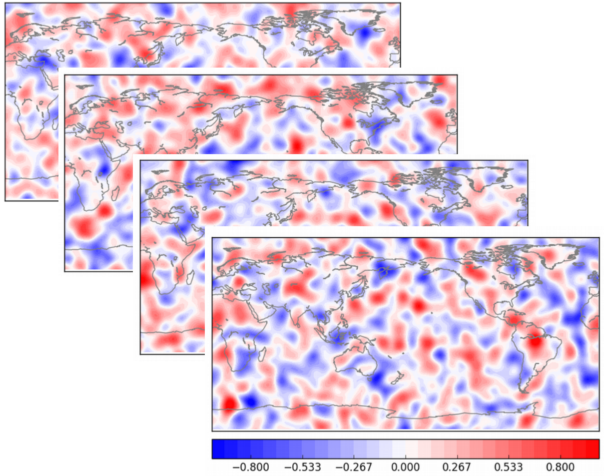
Emission perturbations

Pseudo random perturbation: correlated perturbation over space, similar to SPPT

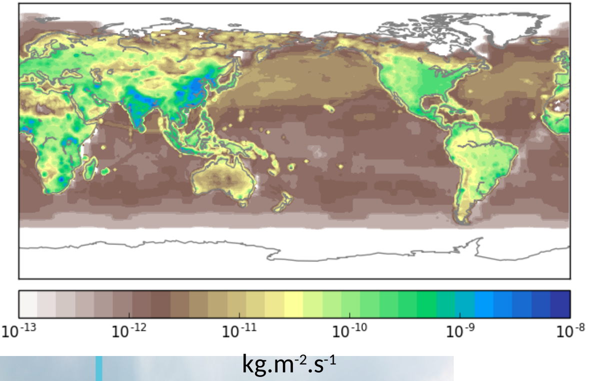
CO emission spread, 30% approx.



Perturbations, 30 members



CO emission totals from inventory



Each emission sectors could be perturbed independently to retrieve a separate sensitivity. **First things first…We are not there yet….**

CO Ensemble spread. After 15 days (20170515)

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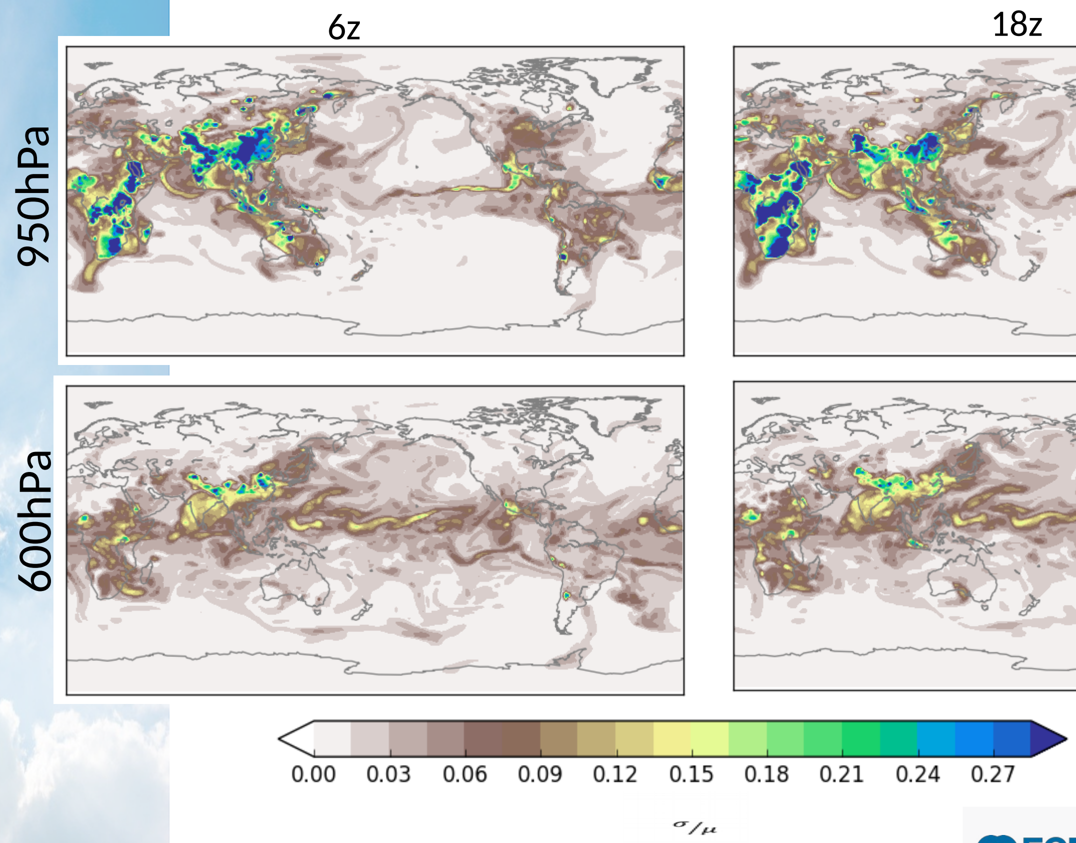

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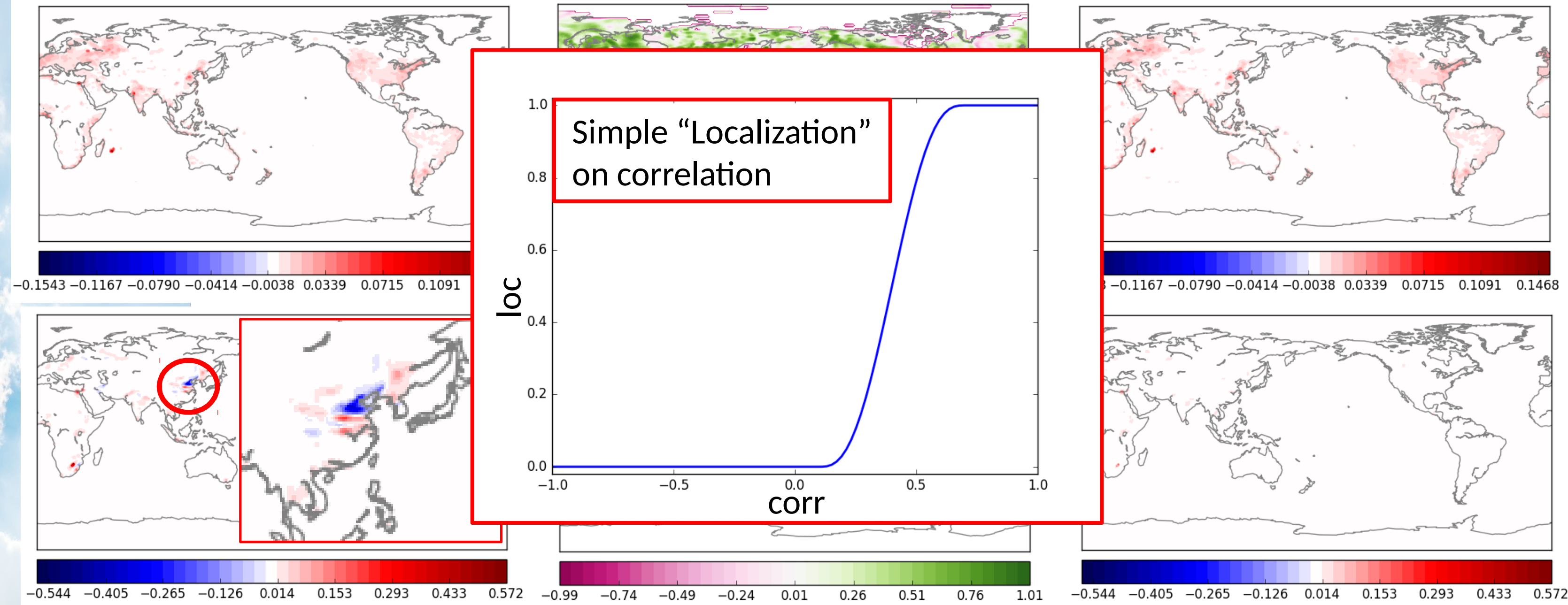
Sensitivity: CO to surface fluxes

$$\frac{\partial \delta \varepsilon}{\partial \delta x} \approx \frac{\sigma_{\varepsilon x}}{\sigma_{xx}} = r_{\varepsilon x} \frac{\sigma_{\varepsilon}}{\sigma_{x}}$$

spread ratio could be very large in the upper trop leading to strong spurious sens. Needs filtering.



Unfiltered sens.: $kg.m^{-2}.s^{-1}.ppm^{-1}$

Correlation

Filtered sens.: $kg.m^{-2}.s^{-1}.ppm^{-1}$

Sensitivity: CO to surface fluxes

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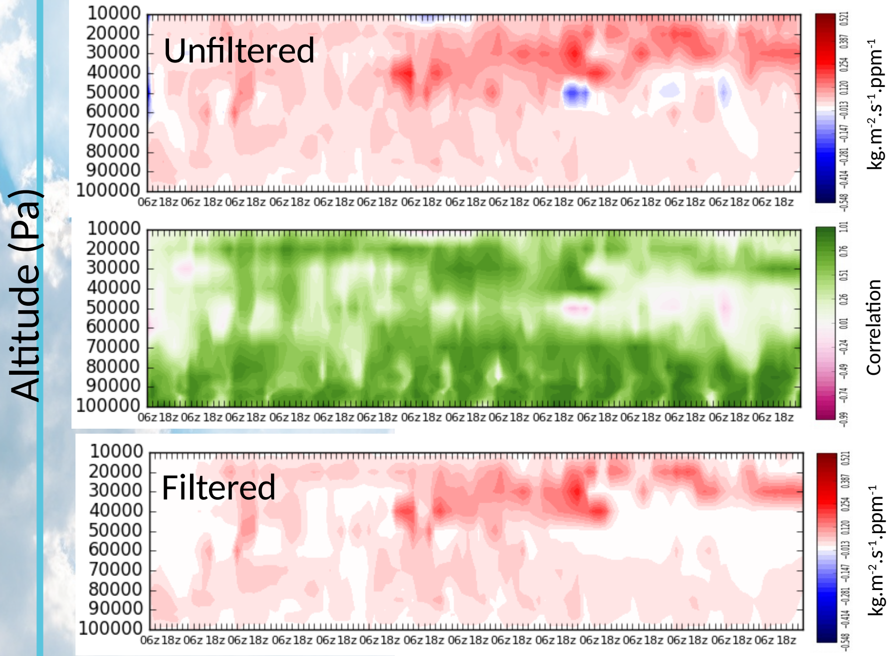
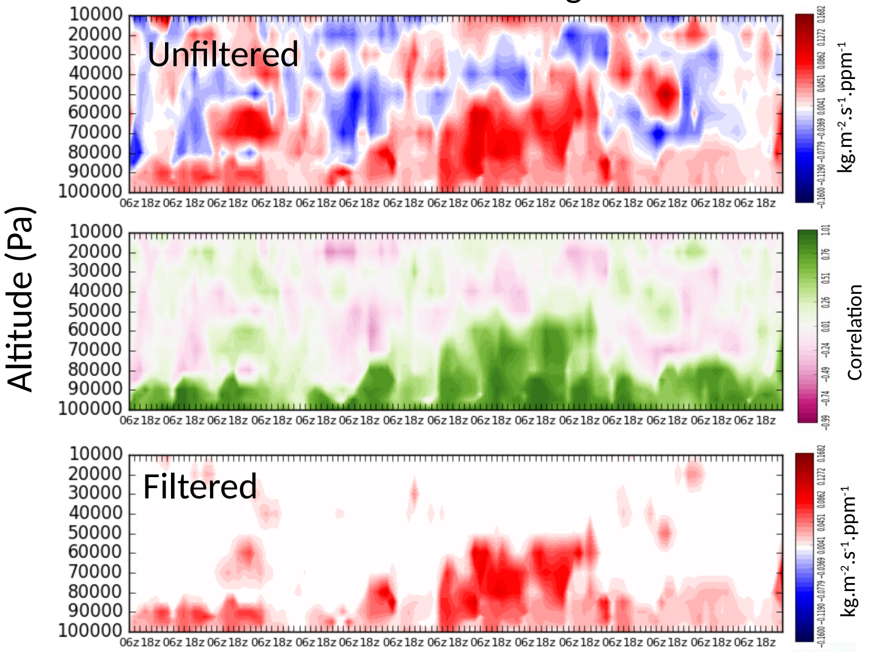
East Java Indonesia



2017-05-01 2017-05-15

St Petersburg



2017-05-01 2017-05-15

Conclusions form preliminary work

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- Using ensemble information for emissions has possible advantages, replace the TL/AD where it is missing or lacking information. Possibly computationally cheaper with full chemistry (non linear system with a lot variables)

- Concerning emission inversion it seems that the nature of the sensitivity is quite variable in space and time. Ensemble statistics are useful to retrieve those but require large number of members

- Filtering techniques have to be envisioned but filtering (sampling error correction, NMC-like,etc.) or climatological hybrid estimates could degrade the variability

- Currently, to what level of accuracy we need to represent the emission sensitivity?
    - What is the Nature of the error on emissions?,
    - Depends also lifetime of a chemical compound,
    - Observation network: revisit & vertical sensitivity of observations, etc…

Improving Standard deviations using NMC statistics

Courtesy of **Melanie Ades**

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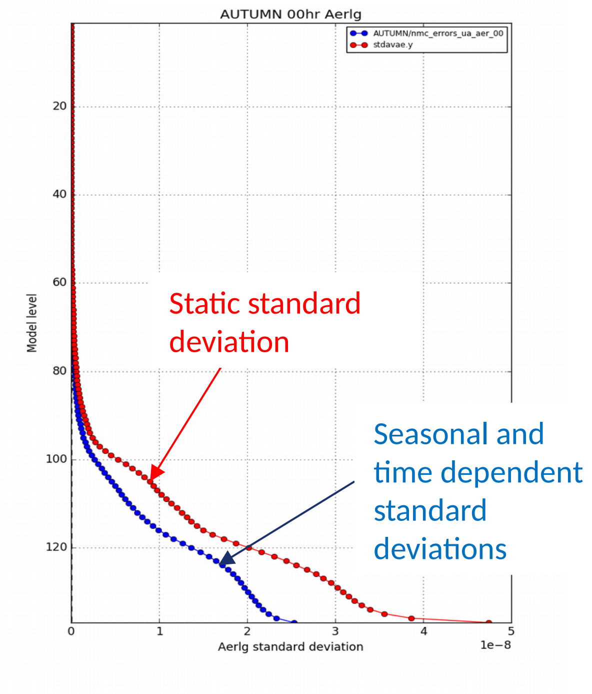
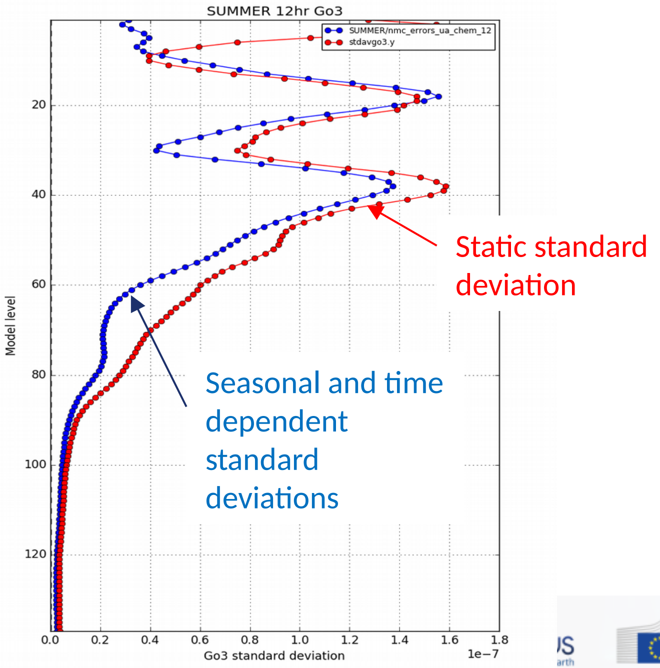
Standard deviations calculated seasonally for the 0z and 12z windows

Aerosols – autumn 00z



Ozone – summer 12z



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Aerosol verification using independent observations

Courtesy of **Melanie Ades**

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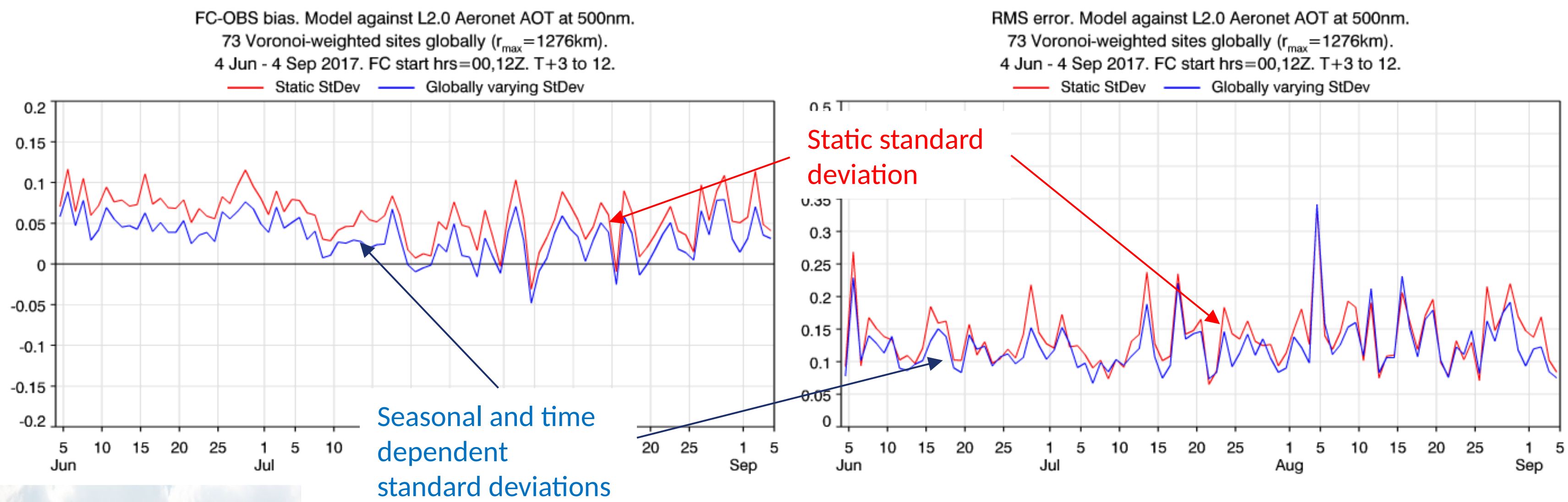
- Significant bias improvement on forecasted AOD.
- Slightly better on RMS error



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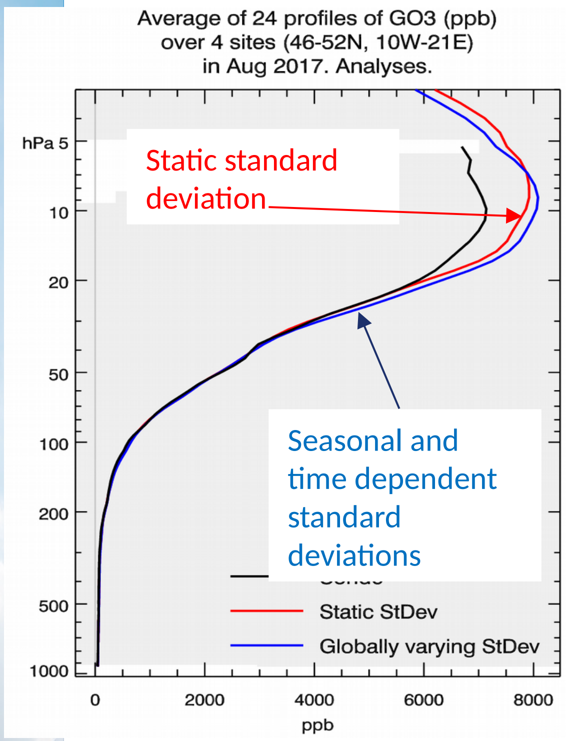
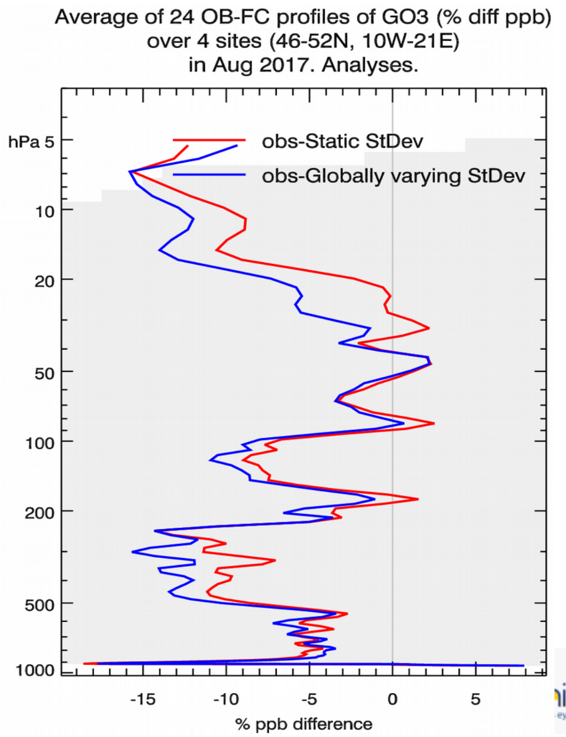
Ozone verification using independent Sonde profiles

Courtesy of **Melanie Ades**

Ozone improvement is not so obvious, work in progress…





The sentinel 5p satellite: Monitoring and assimilation

Courtesy of **Antje Inness**

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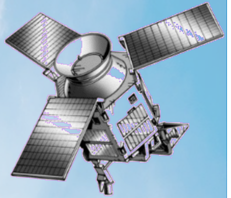


S5p: LEO specific focus on Composition,
(launched oct 2017)

L1b data

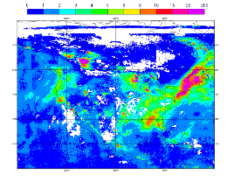
Retrieval teams

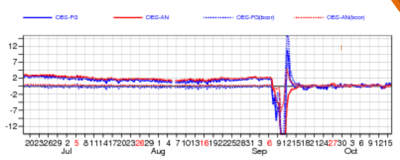
L2 data

CAMS analysis and monitoring tools

Statistics and plots

Feedback

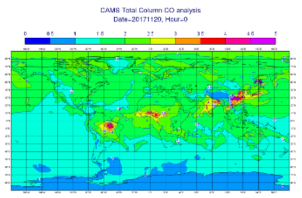




Good data

Assimilation tests

NRT assimilation



Downstream services and users

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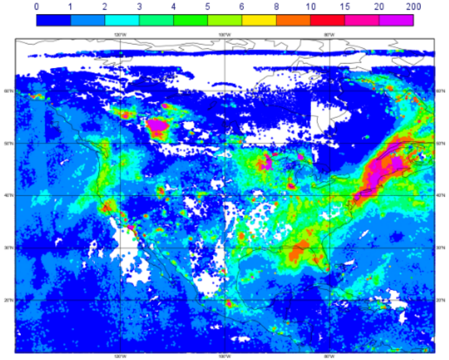
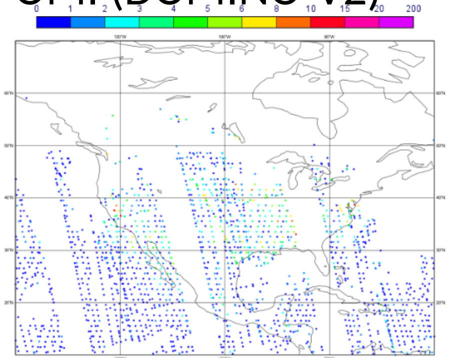
The sentinel 5p satellite: Monitoring and assimilation

Courtesy of **Antje Inness**

TROPOMI (all data)

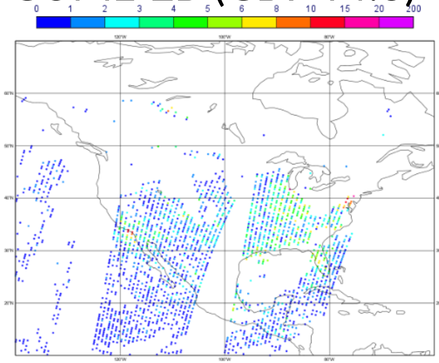


OMI (DOMINO-V2)

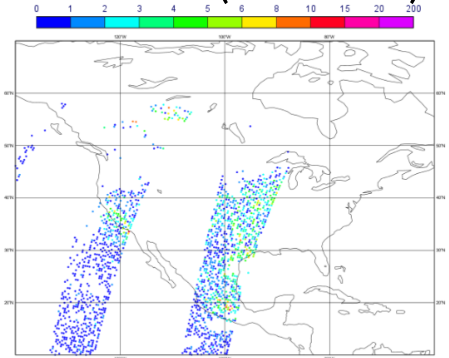


S5P **test data** provided by Henk Eskes (KNMI)

GOME-2B (GDP v4.8)



GOME-2A (GDP v4.8)



GOME-2 and OMI thinned to 0.5° x 0.5° and cloud cleared

Disclaimer: The presented work has been performed in the frame of the Sentinel-5 Precursor Validation Team (S5PVT) or Level 1/Level 2 Product Working Group activities. Results are based on preliminary (not fully calibrated/validated) Sentinel-5 Precursor data that will still change.

Acknowledgement: Sentinel-5 Precursor is a European Space Agency (ESA) mission on behalf of the European Commission (EC). The TROPOMI payload is a joint development by ESA and the Netherlands Space Office (NSO). The Sentinel-5 Precursor ground-segment development has been funded by ESA and with national contributions from The Netherlands, Germany, and Belgium.

- First S5P test data look promising with amazing resolution.
- NRT monitoring and assimilation tests will follow when NRT S5P data become available

Conclusions

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- NRT emission inversions developments will be carried out the next few years
  - With strong collaborations with the EU CHE project on CO_2 anthropogenic emissions
  - Big challenge of having an integrated system for long and short lived species
  - Real interest and need of using co-emited/cross-correlated species inference

- A lot of work has to be done and is currently going on for improving **B** for composition

- The new generation of satellites for atmospheric composition will change the data assimilation prospective for composition, with better sensitivity at the surface, and drastic change on coverage/revisit.

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Backup slides…

4DVar Assimilation & Inversion compared

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$$J(\delta x_0) = \frac{1}{2}(\delta x_0)^T \mathbf{B}^{-1}(\delta x_0) + \frac{1}{2}\Sigma_{t=i}(\mathbf{H}_i(\delta x_i) - d_i)^T \mathbf{R}^{-1}(\mathbf{H}_i(\delta x_i) - d_i)$$

$$\mathbf{M}^T = \prod_{i=0}^{p} \left(\frac{\partial \delta x_i}{\partial \delta x_{i-1}}\right)^T$$

$$\nabla J(\delta x_0) = \mathbf{B}^{-1}(\delta x_0) + \Sigma\, \mathbf{H}_i^T \mathbf{R}^{-1}(\mathbf{H}_i(\delta x_i) - d_i)$$

$$\mathbf{H}^T = \mathbf{M}^T \mathcal{H}^T \qquad \mathbf{M}^T = \mathbf{C}^T \mathbf{T}^T$$

Assimilation window length can vary. It is 12 hours in the current IFS configuration.

$$J(\delta \varepsilon_0) = \frac{1}{2}(\delta \varepsilon_0)^T \mathbf{B}^{-1}(\delta \varepsilon_0) + \frac{1}{2}\Sigma_{t=i}(\mathbf{H}_i(\delta \varepsilon_i) - d_i)^T \mathbf{R}^{-1}(\mathbf{H}_i(\delta \varepsilon_i) - d_i)$$

$$\mathbf{M}^T = \prod_{i=0}^{p} \left(\frac{\partial \delta \varepsilon_i}{\partial \delta x_i}\right)^T \left(\frac{\partial \delta x_i}{\partial \delta x_{i-1}}\right)^T$$

$$\nabla J(\delta \varepsilon_0) = \mathbf{B}^{-1}(\delta \varepsilon_0) + \Sigma\, \mathbf{H}_i^T \mathbf{R}^{-1}(\mathbf{H}_i(\delta \varepsilon_i) - d_i)$$

$$\mathbf{H}^T = \mathbf{M}^T \mathcal{H}^T \qquad \mathbf{M}^T = \mathbf{E}^T \mathbf{C}^T \mathbf{T}^T$$

Assimilation window hence requires different length depending on observation network and species. E.g. weeks for GHG vs only several hours for short-lived species (NO_2).

$\mathbf{E}^T$ *emission adj.*
$\mathbf{C}^T$ *chemistry adj.*
$\mathbf{T}^T$ *transport adj.*

Joint state 4DVar Inversion

In the case of a **monitoring system** i.e. assimilating/inverting **NRT** do we choose to have a joint state 3D fields + emissions minimization or two separated minimizations at different times and windows?

In the case of the joint minimization we have the augmented state:

$$\underline{\nabla} J(\delta X_0) = B^{-1}(\delta X_0) + \sum H_i^T R^{-1}(H_i(\delta X_i) - d_i)$$

$$\boldsymbol{X} = \begin{pmatrix} \boldsymbol{x} \\ \boldsymbol{\varepsilon} \end{pmatrix} \qquad \mathbf{M}^T = \begin{pmatrix} \mathbf{C}^T\mathbf{T}^T \\ \mathbf{E}^T\mathbf{C}^T\mathbf{T}^T \end{pmatrix}$$

$$\mathbf{M}^T = \begin{pmatrix} \prod_{i=0}^{p} \left(\frac{\partial \delta x_i}{\partial \delta x_{i-1}}\right)^T \\ \prod_{i=0}^{p} \left(\frac{\partial \delta \varepsilon_i}{\partial \delta x_i}\right)^T \left(\frac{\partial \delta x_i}{\partial \delta x_{i-1}}\right)^T \end{pmatrix}$$

For GHG (**long-lived** species) this probably implies inferring sources using cross-correlation between species. For example using NO_2 (**short lived**) emission factors to infer anthropogenic CO_2 emissions.

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Alternative joint state - the balance operator

Instead of using the sensitivities/jacobians into J_o can we thing of inserting the equivalent information into J_b using cross-correlation or balance operators. (J_o does not need to be augmented.)

$$X = \begin{pmatrix} x \\ \varepsilon \end{pmatrix}$$

$$\nabla J(\delta X) = B^{-1}(\delta X_0) + \sum H^T R^{-1}(H(\delta x) - d)$$

Correlation: $\mathbf{C} = \begin{pmatrix} \mathbf{C}_x & 0 \\ 0 & \mathbf{C}_\varepsilon \end{pmatrix}$

Variance: Σ

$$\mathbf{B} = \mathbf{K}^{-1/2}\Sigma^{1/2}\mathbf{C}\Sigma^{1/2}\mathbf{K}^{-T/2}$$

Then formulate a **K** balance operator so that $\delta\varepsilon = \mathbf{K}\delta x$. At a given time ε is 2D (in most cases) whereas x is 3D, so level integrated such as: that $\delta\varepsilon = \sum_l \mathbf{K}_l \delta x_l$

$\mathbf{K}_l$ or the sensitivities $\left(\frac{\partial \delta\varepsilon_0}{\partial \delta x_0}\right)_l$ need to be computed per model level and stored beforehand (wavelet formulation?)

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