



Atmosphere Monitoring

# Exploring synergies in composition and NWP data assimilation

*Antje Inness (ECMWF)*

*Workshop on data assimilation (Bonn): 9 April 2025*

With thanks to: Johannes Flemming, Noureddine Semane,  
Ziga Zaplotnik, Sebastien Massart, Marco Matricardi, ....



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## Outline

1. CAMS overview
2. Stratospheric humidity analysis (*Noureddine Semane*)
3. Impact of using interactive aerosols (*Johannes Flemming*)
4. Wind information from tracers (*Ziga Zaplotnik, Sebastien Massart, Noureddine Semane*)
5. Using CAMS CO<sub>2</sub> in RTTOV (*Marco Matricardi*)
6. Summary





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# COPERNICUS ATMOSPHERE MONITORING SERVICE (CAMS)

Within the 6 Copernicus Services, CAMS mandate is to deliver **consistent and quality-controlled information** related to **the chemical composition of the atmosphere**, its drivers (**air pollutants and GHG**) and its impact on air quality and health, solar energy, climate forcing, in Europe and everywhere in the world.



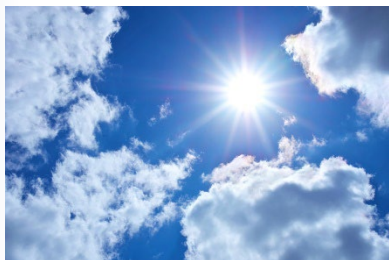
Air quality



Policy tools



Solar energy



Ozone layer and UV radiation



Emissions and surface Fluxes



Climate forcing



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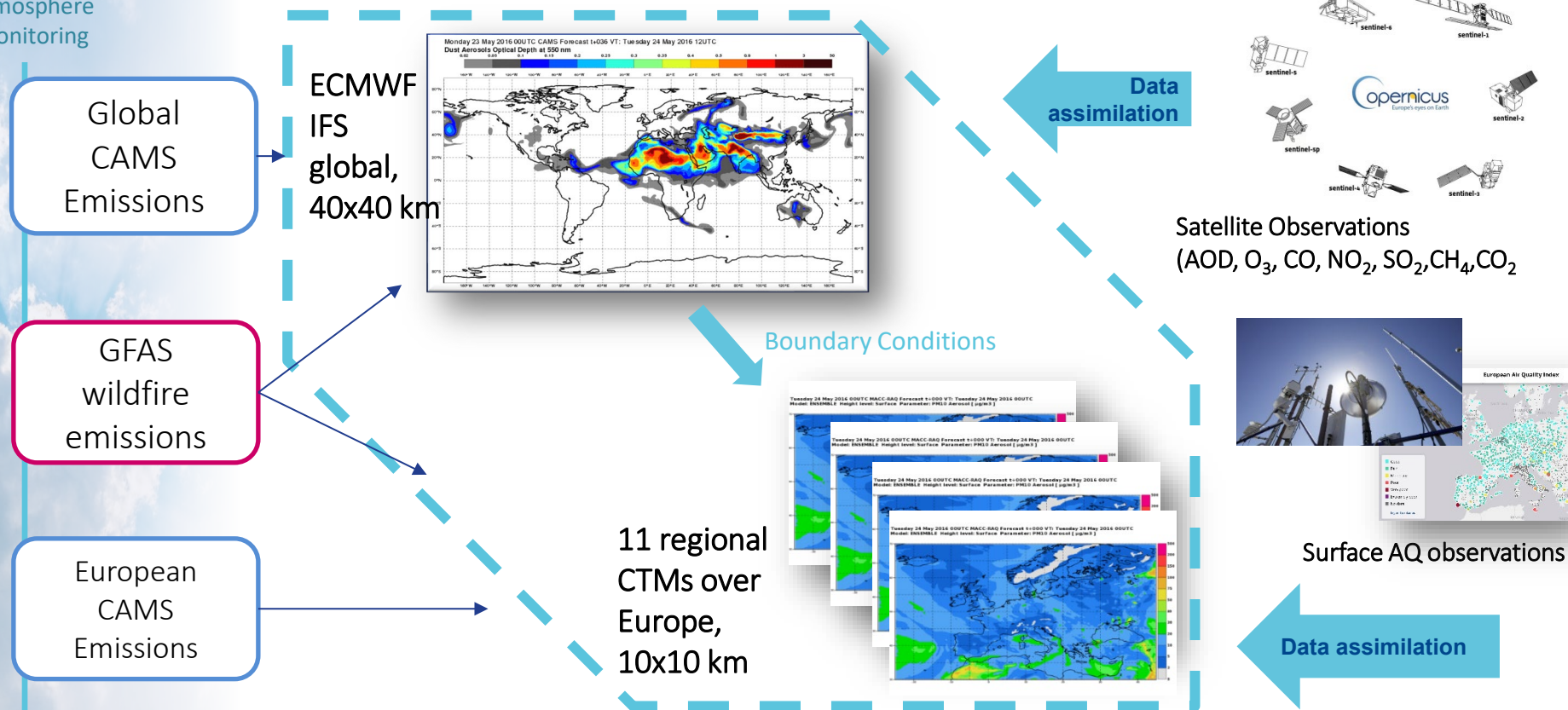
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# CAMS integrated framework



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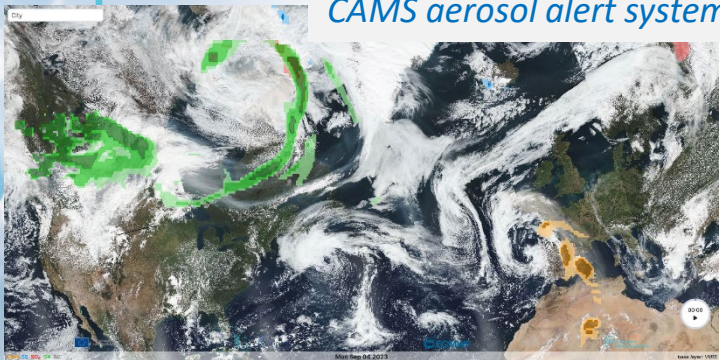


# Examples of CAMS services

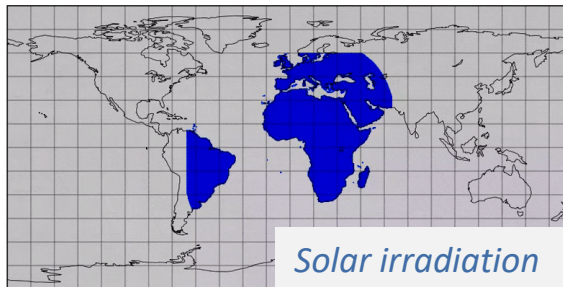
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<https://aerosol-alerts.atmosphere.copernicus.eu>

*CAMS aerosol alert system*



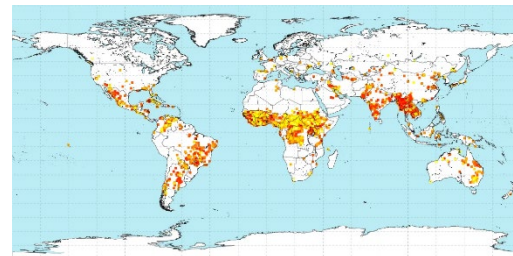
global shortwave downward irradiation received over an horizontal plane  
Time: 2022-06-01 00:15:00



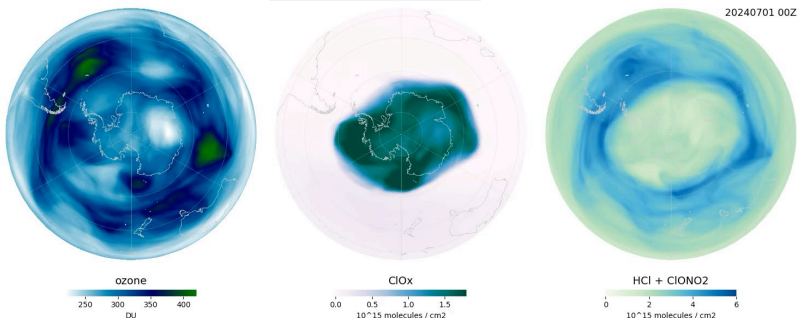
*Solar irradiation*

global shortwave downward irradiation received over an horizontal plane (W h m<sup>-2</sup>)  
0.0 50.0 100.0 150.0 200.0 250.0  
Data Min = 0.0, Max = 0.0, Mean = 0.0

*Wildfires*

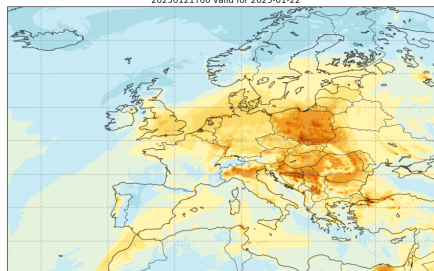


*Ozone hole*



*European air quality*

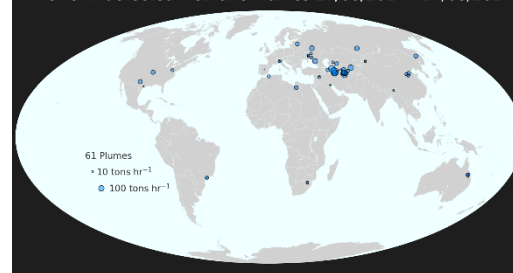
CAMS Regional Ensemble Forecast daily max pm2p5 conc at 0m:  
20250121T00 valid for 2025-01-22



0 2 5 10 20 30 40 50 75 100 150 200 300  
µg m<sup>-3</sup>  
ECMWF

*Methane Hot-spots*

TROPOMI-detected Methane Plumes 17/08/2024 - 24/08/2024



61 Plumes  
• 10 tons hr<sup>-1</sup>  
• 100 tons hr<sup>-1</sup>

Data  
provided  
by SRON

<https://apps.atmosphere.copernicus.eu/methane-explorer>

<https://atmosphere.copernicus.eu/monitoring-ozone-layer>



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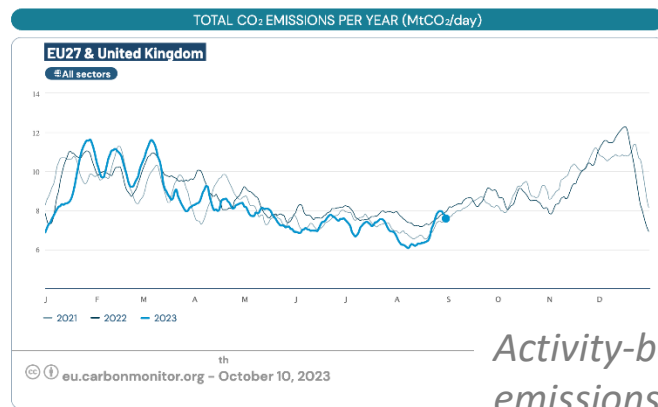
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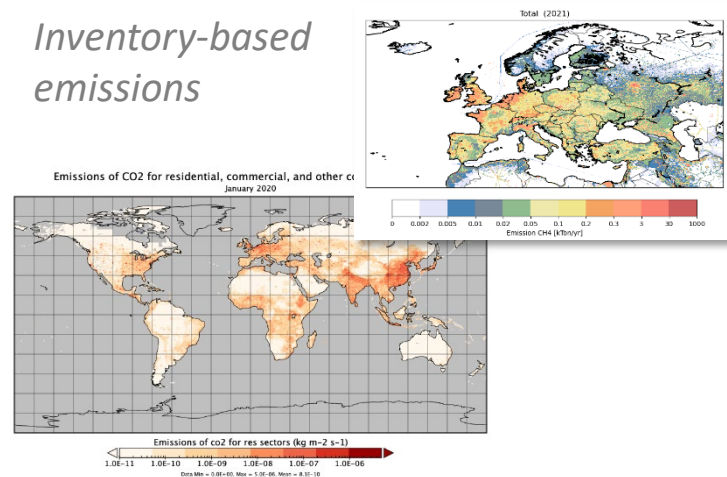
# CAMS current offer on GHG information products

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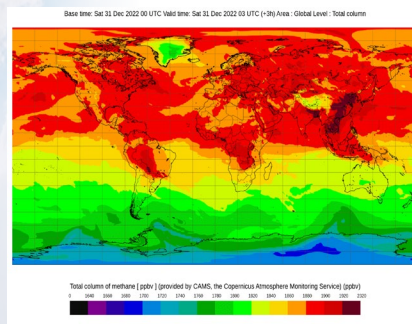


Activity-based  
emissions

Inventory-based  
emissions



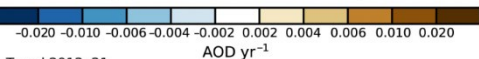
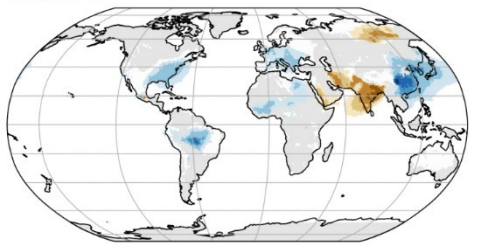
Daily global forecasts of atmospheric CO<sub>2</sub> and  
CH<sub>4</sub> concentrations at high resolution



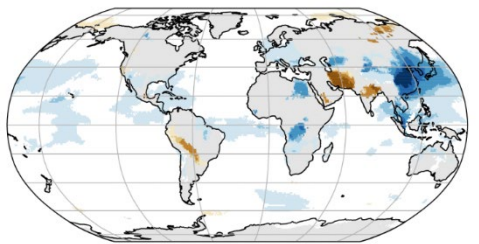


# CAMS reanalysis of atmospheric composition (EAC4)

Trend 2003–21

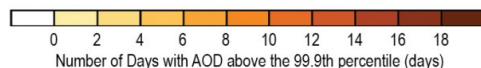
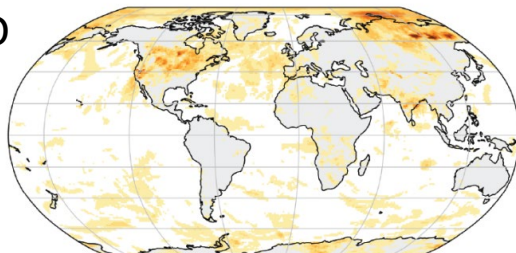


Trend 2012–21



CAMS reanalysis linear trends of total AOD for 2003–2021 and 2012–2021

AOD



Remy et al. (2022),  
STOC 2021

CAMS reanalysis data have been used for almost a decade to contribute to BAMS State of the Climate reports

## Comparison of xCO with TCCON at Parkfalls

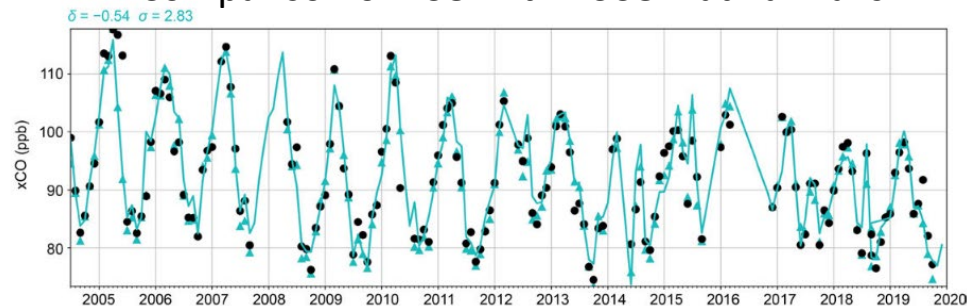
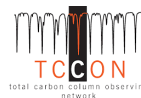


Fig. 2.62. Column-averaged CO (xCO, in ppb) at the Park Falls TCCON station. Monthly mean observations are shown by the black dots, and corresponding monthly mean xCO columns calculated using the TCCON-averaging kernels are shown by the blue triangles. The continuous blue line is the monthly xCO from the CAMS reanalysis.

Flemming et al. (2020), STOC 2019

TCCON data from:  
<https://tccondata.org/>



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Europe's eyes on Earth

Extreme AOD days in 2021 correspond to extreme boreal fire events, including transport to the Arctic

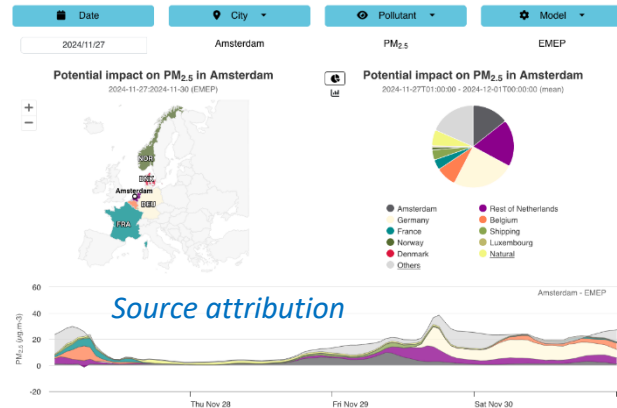




# Interactive policy tools

<https://policy.atmosphere.Copernicus.eu>

What is the potential impact of local and country emissions reduction on  $PM_{10/2.5}$ , ozone and  $NO_2$ ?



## CAMS regional service

How would different policy scenarios of emission reductions affect current air quality?

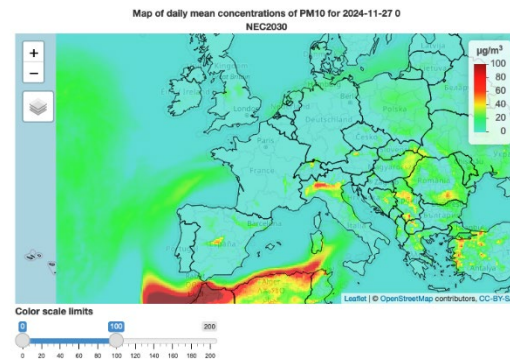
### Policy scenarios

Pollutant:  $PM_{10}$  mean

Day: 2024-11-27

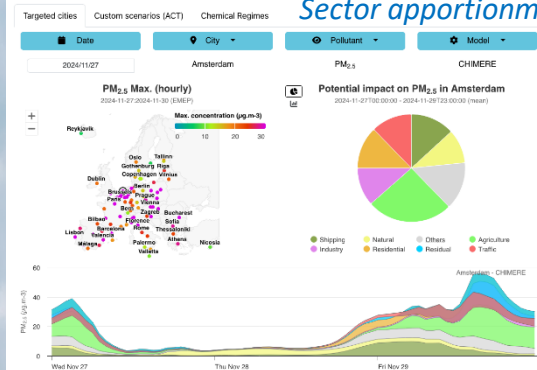
Forecast day: D+0

Scenario: NEC2030



What is the potential impact of different measures affecting sector emissions?

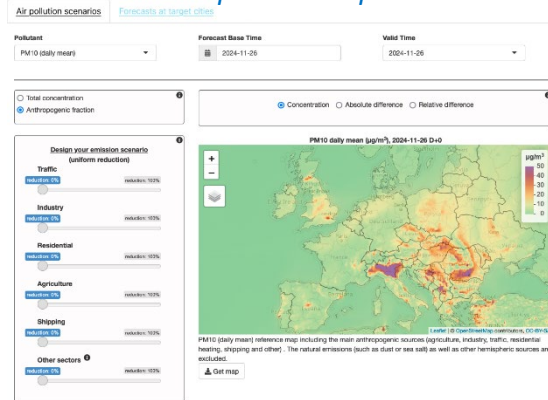
### Sector apportionment



### Air Quality Reports

Find reports on **major air pollution episodes** in Europe (fine particles, ozone, forest fires, ...), as well as **annual assessment reports**.

### CAMS ACT: Atmospheric composition toolbox



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Copernicus  
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ECMWF

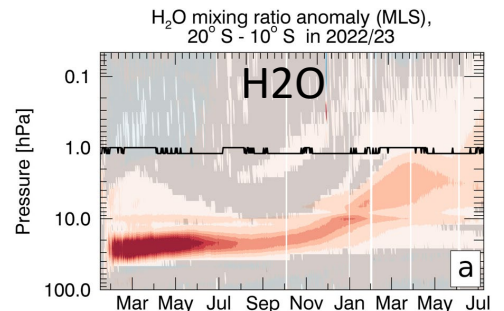
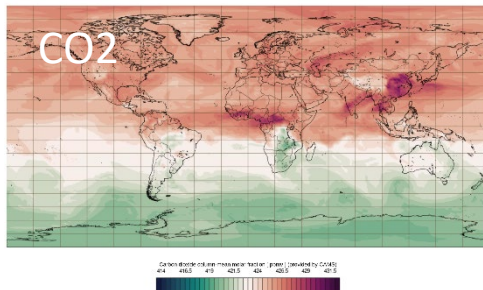
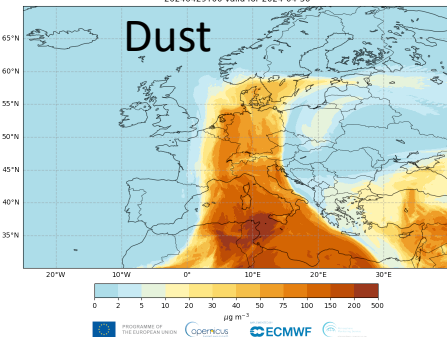




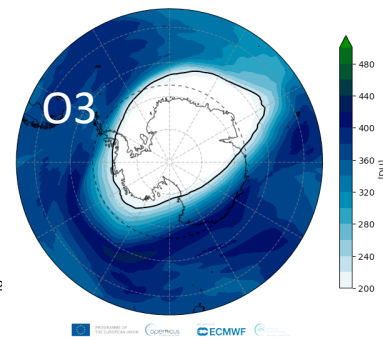
# Potential impact of atmospheric composition on NWP

Atmosphere

CAMS Regional Ensemble Forecast daily max dust at 3000m:  
20240423T00 valid for 2024-04-30



CAMS Forecast Daily Max Total Column Ozone  
20231023T00 valid for 20231023T00

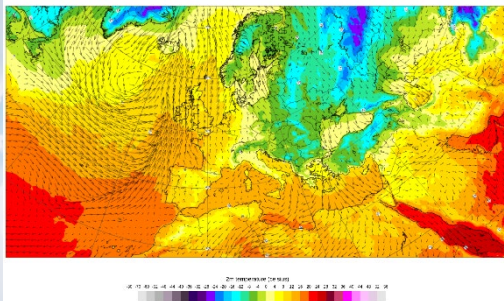


Niemeier et al. (2023)  
<https://doi.org/10.1029/2023GL106482>



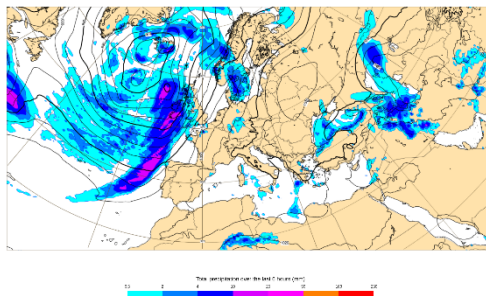
2 m temperature and 30 m wind

Obs time: Fri 23 Feb 2024 06:00 UTC (0600 UTC) R: 23 Feb 2024 09:00 UTC (0900 UTC) Europe



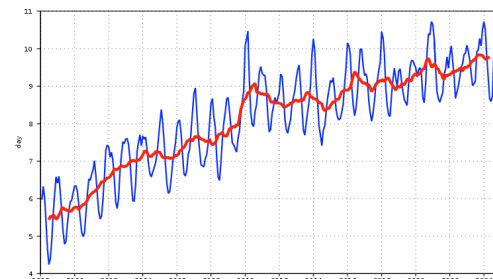
Rain and mean sea level pressure

Obs time: Fri 23 Feb 2024 06:00 UTC (0600 UTC) R: 23 Feb 2024 09:00 UTC (0900 UTC) Europe



850hPa temperature | NHem Extratropics

Lead time of Continuous ranked probability skill score reaching 25%



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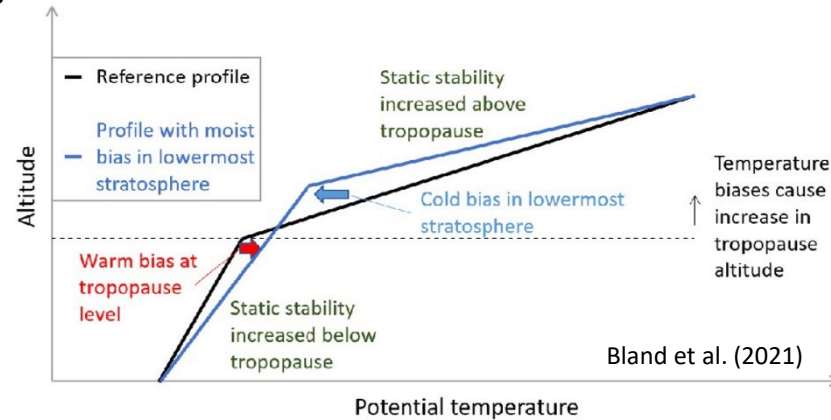
Copernicus  
Europe's eyes on Earth

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## 2. Stratospheric humidity analysis

- ECMWF's stratospheric humidity field currently not updated by 4D-Var (CY49R1)
  - Analysis increments forced to be zero above the model tropopause.
- Humidity above tropopause is changed only to remove supersaturation caused by a temperature increment.
- This was introduced in 2003 to avoid spurious humidity increments in the stratosphere that degraded forecast scores
- Humidity levels in lowermost stratosphere are overestimated in IFS (Bland et al., 2021)
  - ⇒ Excessive longwave radiative cooling
  - ⇒ Increasing cold bias in temperature forecasts, with a cooling rate of  $-0.2$  K per day





# Experiment setup: stratospheric humidity analysis

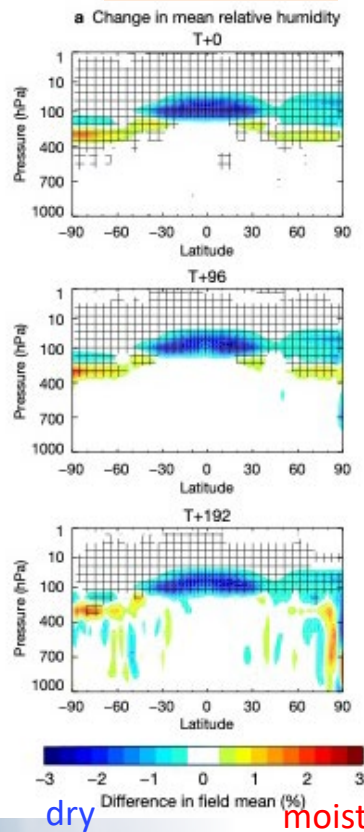
Credit: N. Semane

Exp	Description
CTL	CY49R1 humidity analysis <ul style="list-style-type: none"><li>• Radiosonde humidity profiles</li><li>• GNSS-RO bending angles</li><li>• Radiances from satellite microwave and infrared sounders</li><li>• No stratospheric humidity increments</li></ul>
QIN	CTL + analysis of stratospheric humidity
MLS	QIN + <ul style="list-style-type: none"><li>• Radiosonde RS41 humidity obs up to 60 hPa</li><li>• Assimilate EOS-Aura Microwave Limb Sounder (MLS) H2O retrievals</li></ul>

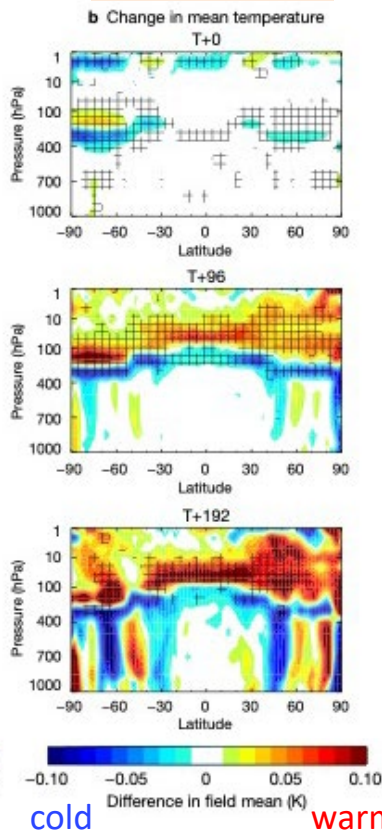


# Change in relative humidity and temp (MLS – CTL)

## Rel humidity



## Temperature



- Enabling stratospheric humidity analysis and assimilating MLS & extended sonde humidity observations leads to
  - ⇒ a drying of the lower stratosphere and moistening below tropopause
  - ⇒ a warming of the lower stratosphere and cooling of upper troposphere
- Mitigates known IFS biases
- Sharpens the tropopause (weak & diffuse tropopause is also a known issue in ECMWF forecasts/analyses - Krüger et al. (2023))

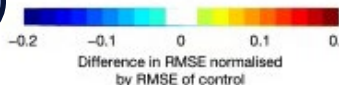
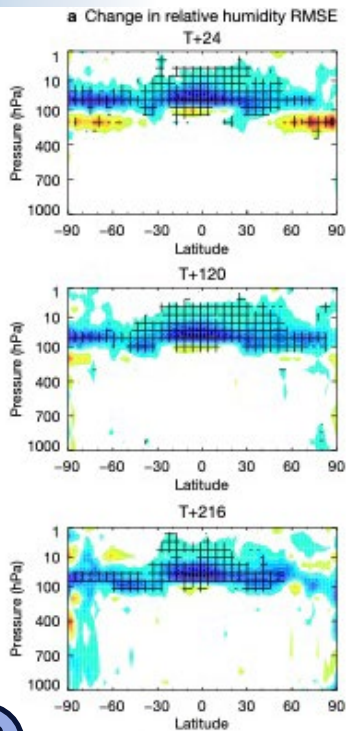
Credit: N. Semane (ECMWF newsletter 183)



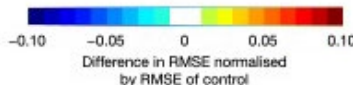
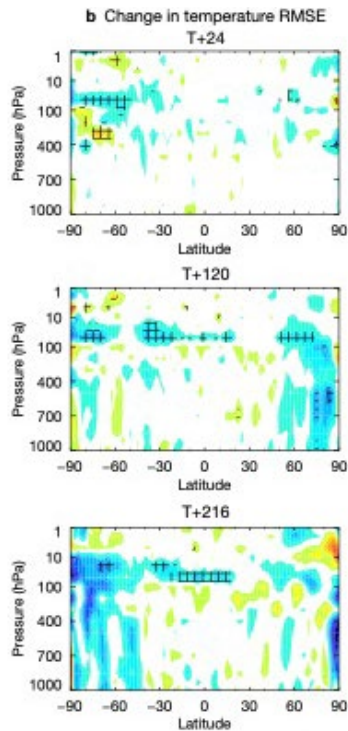


# Impact on forecast scores (MLS – CTL)

## Rel humidity



## Temperature



- Improved forecasts across all lead times.
- Enhancements most pronounced in UTLS
- Indications that improvements propagate into troposphere with increasing lead time.
- **Stratospheric humidity analysis will be activated in CY50R1**



Credit: N. Semane (ECMWF newsletter 183)



### 3. Use of interactive aerosols

- ECMWF's NWP system currently uses a monthly aerosol climatology (Bozzo et al., 2020; GMD)
- CAMS uses prognostic aerosols interactively in the radiation scheme
- What is the benefit of using prognostic aerosol in the IFS radiation scheme compared to using the aerosol climatology?



Pete Laing/BC Wildfire Service



Pavliha/iStockphoto



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# Mean Difference between climatological and prognostic aerosols (Total column mass) JJA 2019

Credit: J. Flemming

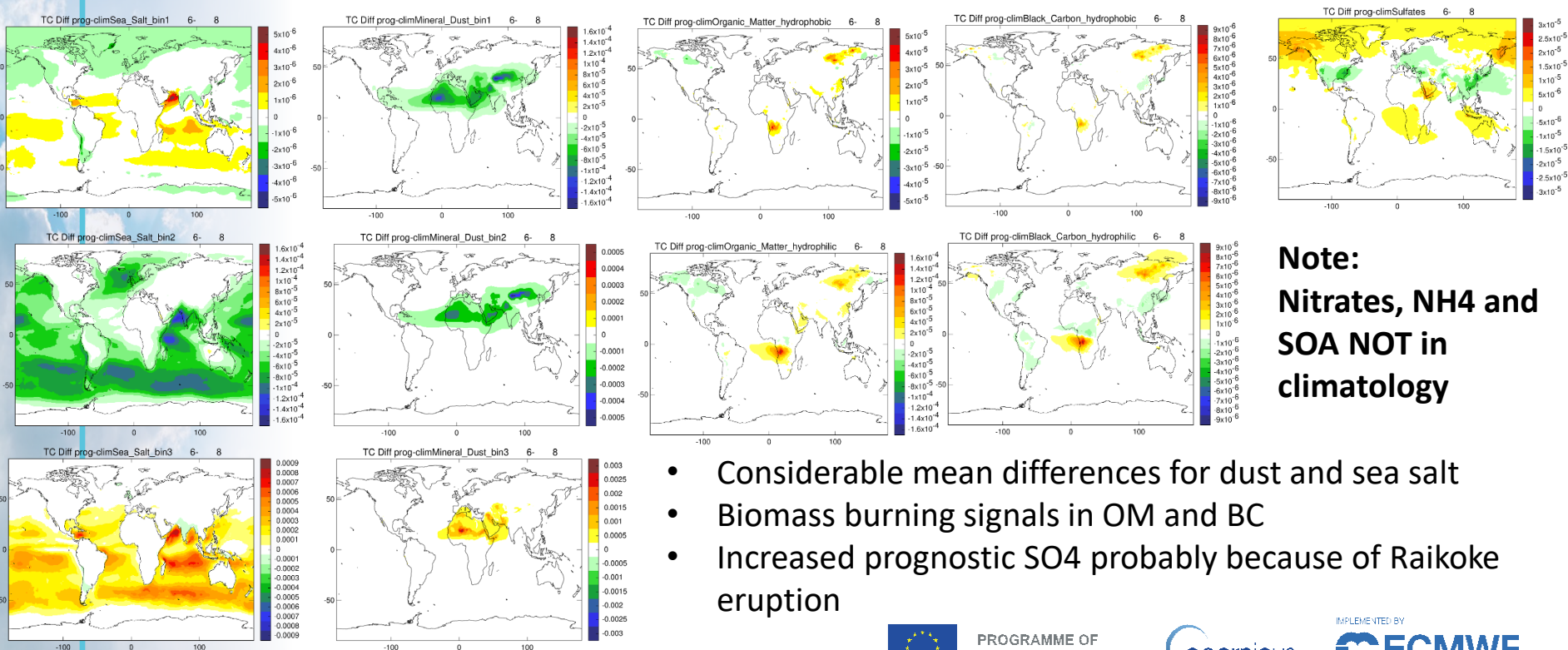
Sea Salt

Dust

OM

BC

SO4



**Note:**  
Nitrates, NH<sub>4</sub> and  
SOA NOT in  
climatology

- Considerable mean differences for dust and sea salt
- Biomass burning signals in OM and BC
- Increased prognostic SO4 probably because of Raikoke eruption



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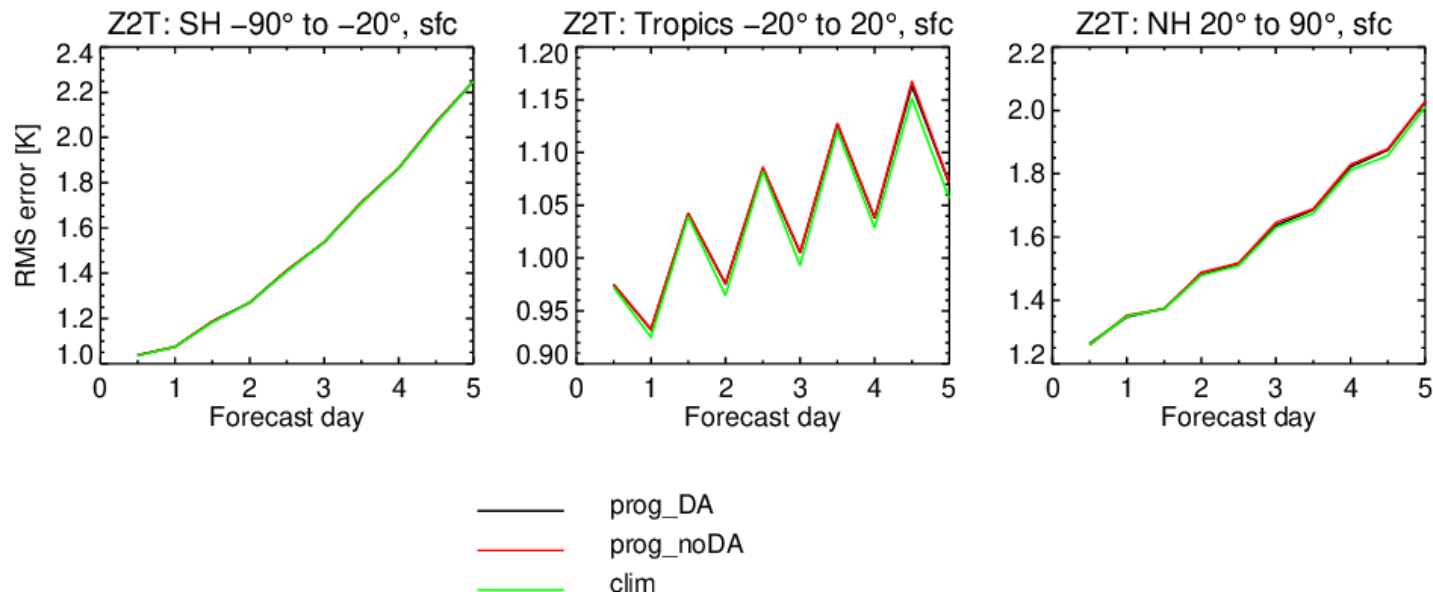
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1-Jun-2021 to 31-Aug-2021 from 87 to 92 samples. Verified against 0001.

No statistical significance testing applied



Using prognostic aerosol makes no noticeable difference for “average” NWP scores, e.g. RMS 2mT with lead time



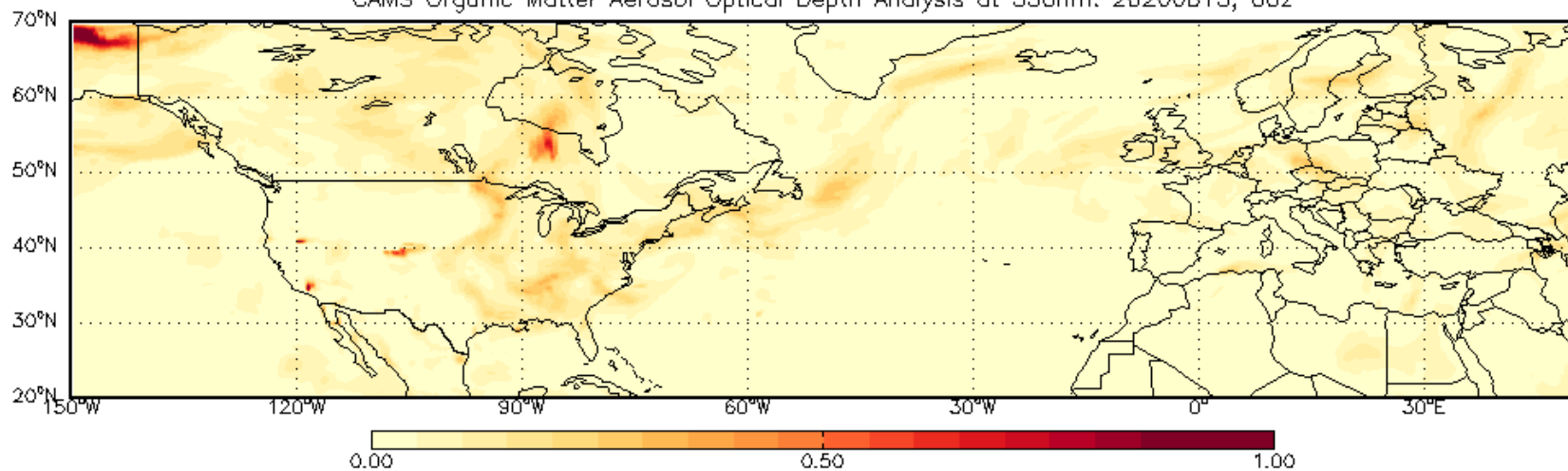


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# California and Western US fires 2020

## Smoke transport from wildfires

CAMS Organic Matter Aerosol Optical Depth Analysis at 550nm: 20200815, 00z



Mark Parrington  
CAMS Weather Room



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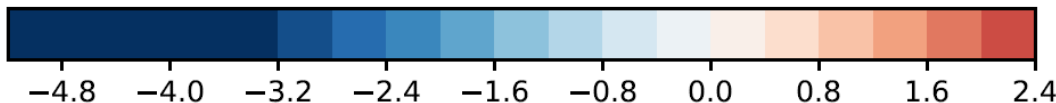
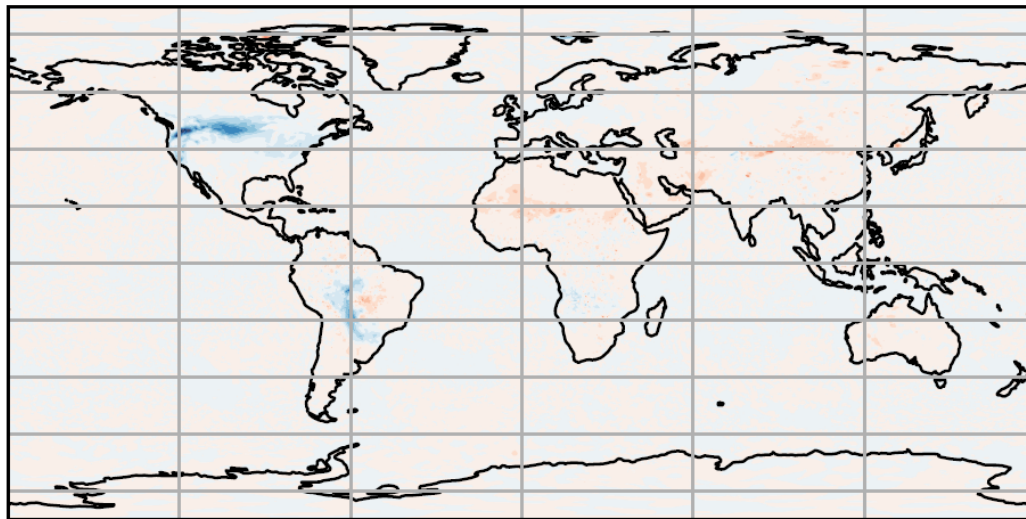




## 2 m T difference: prognostic aerosols

Credit: J. Flemming

t2m prognostic - climatology 20200915[6, 12, 18, 24]



CAMS o-suite (prog Aerosol) minus CAMS-CLIM (clim aerosol)

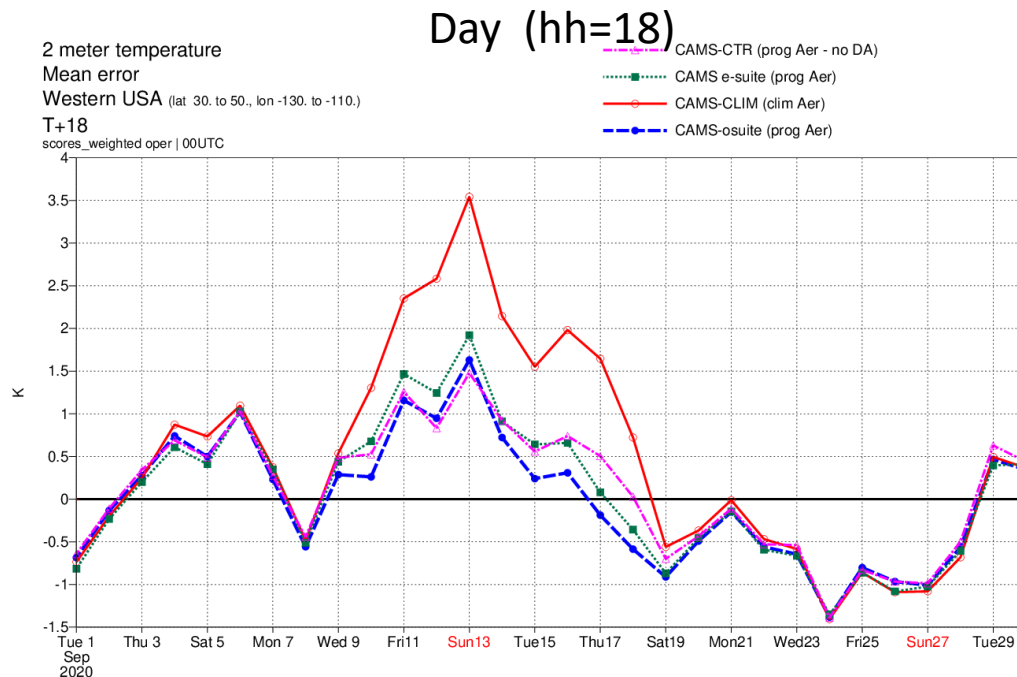
Up to 5 K reduction  
in daily mean 2mT

**CAMS o-suite uses  
prognostic aerosol and  
ozone in radiation scheme**

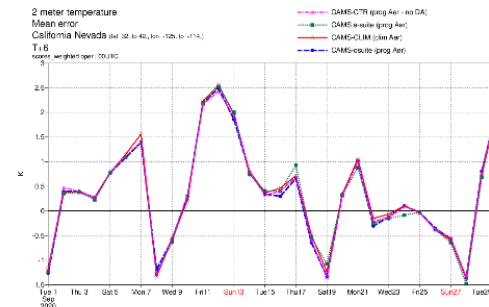
CAMS-CLIM control  
forecast (00) using aerosol  
and ozone climatology tun  
in NRT



clim Aero  
prog Aero DA (47r1)  
prog Aero DA (46r1)  
prog\_Aero noDA (46r1)



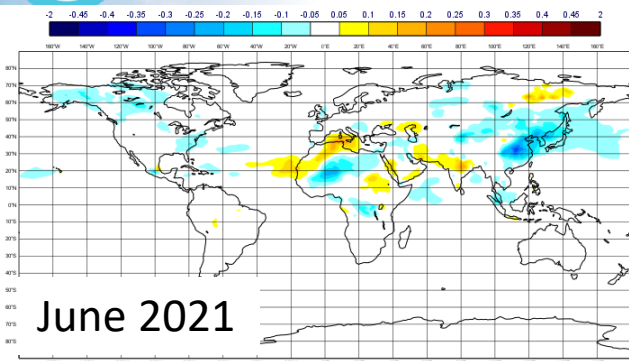
Night (hh=6)



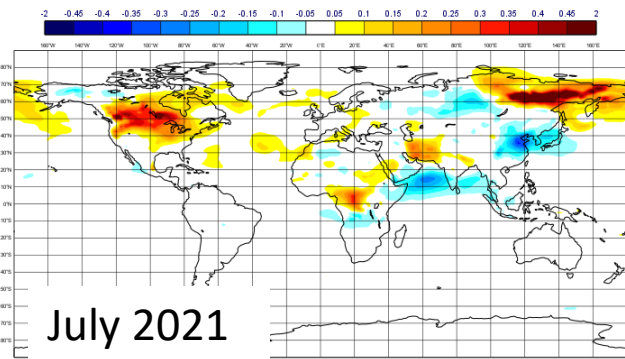
Increased positive bias with aerosol climatology in CAMS-CLIM CTR



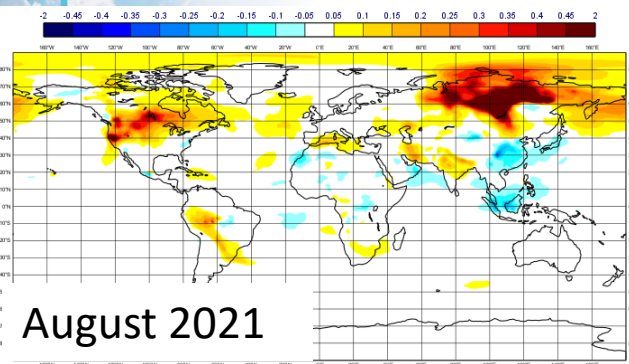
# AOD anomalies and boreal wildfires 2021



June 2021



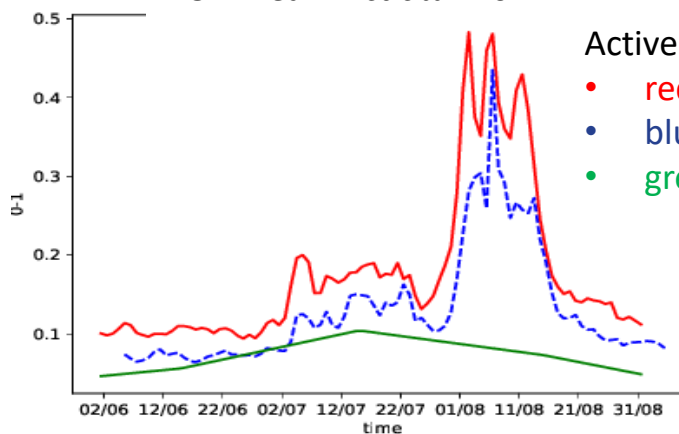
July 2021



August 2021

AOD anomalies due to  
Siberian and N-American  
wildfires in JJA 2021

## AOD mean Arctic JJA 2021



Active vegetation fires in Siberia

- red: AOD analysis,
- blue: 108 h forecast
- green: climatology

Anomalies calculated against 2003-2020  
monthly means from CAMS reanalysis



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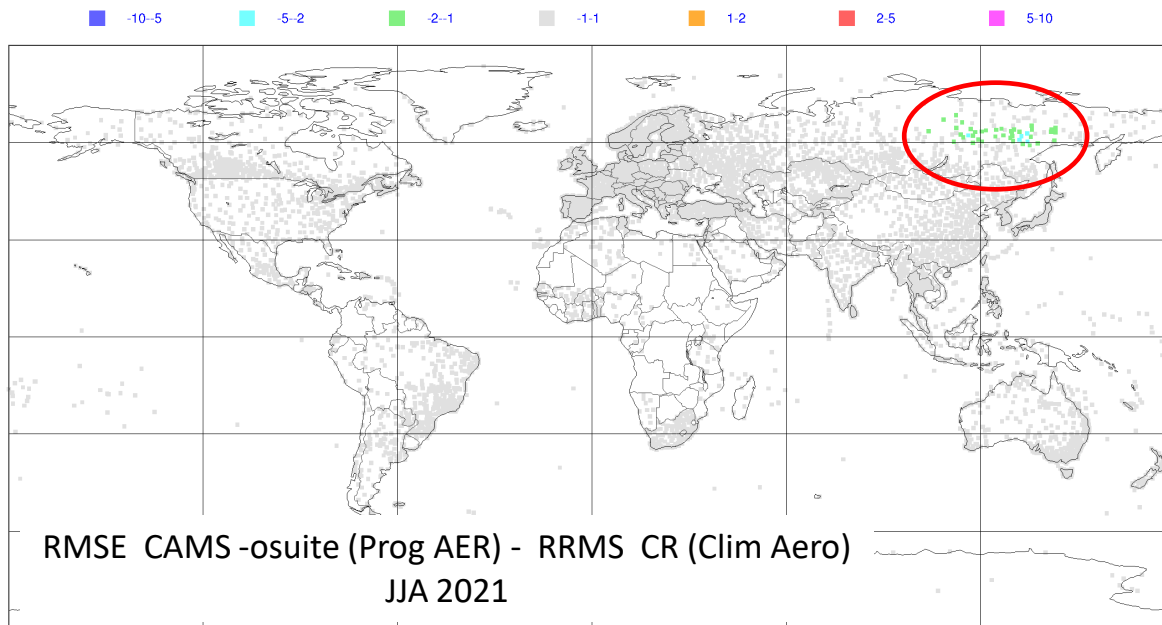




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# Impact on Arctic wildfires on 2m temperature forecasts (JJA 2021)

Credit: J. Flemming



Magics 4.3.3 (64 bit) - lysander - naj - Tue Sep 21 21:11:48 2021

ECMWF

Using prognostic aerosols leads to decrease in 2mT RMSE against synop observations

Credit: Johannes Flemming



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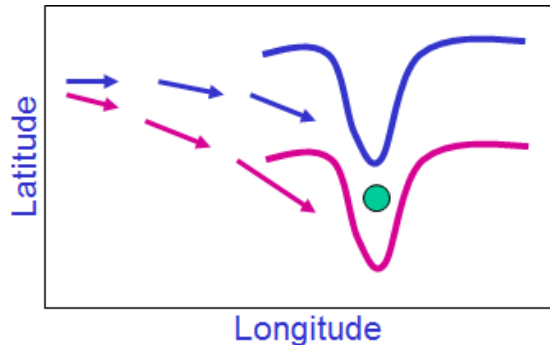
## Summary interactive aerosols

- Compared to using the CAMS/ECMWF aerosol climatology:
  - Cooling of several K in the case of large AOD anomalies
  - Clear indication of improved 2mT forecast against synop observations in case of large fire events (US, Canada, Siberia)
  - No overall improvement in standard NWP scores
- Prognostic aerosol in IFS for NWP purposes is ongoing research topic at ECMWF
- Potential to improve medium-range and monthly seasonal forecast recognised



## 4. Wind information from tracers

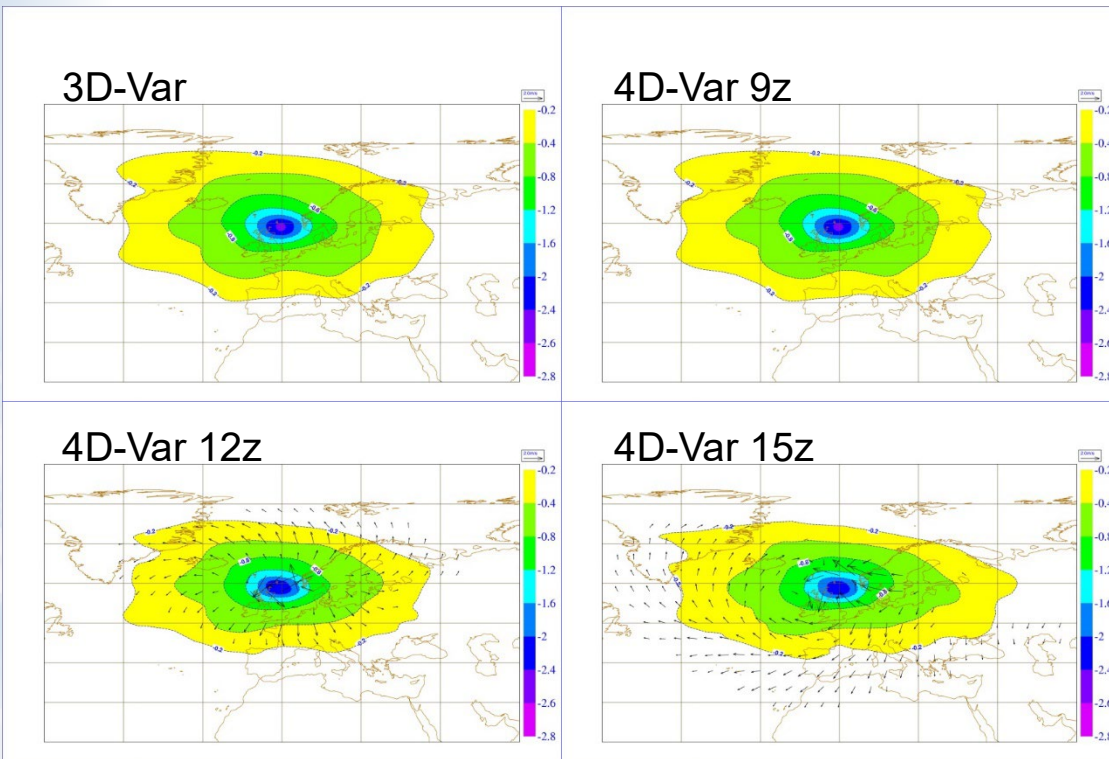
- Prospect to extract wind information from long lived tracers in stratosphere and upper troposphere, e.g. O<sub>3</sub>, H<sub>2</sub>O, N<sub>2</sub>O
- Similar to cloud track winds but data coverage worse
- Potential was demonstrated a long time ago in early studies for H<sub>2</sub>O (Thépaut 1992) and O<sub>3</sub> (Daley 1995; Riishojgaard 1996; Holm 1999; Peuch et al. 2000).
- Could compliment existing wind observations and help in areas where there is a lack of adequate global wind profile data
- Potential to extract wind info indirectly through TL and AD of tracer advection





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# Single observation experiment: O<sub>3</sub> and wind increments



Level 20,  
≈ 30 hPa

Impact in 6h 4D-Var [window from 9z-15z] from single obs at 9z, 12z or 15z



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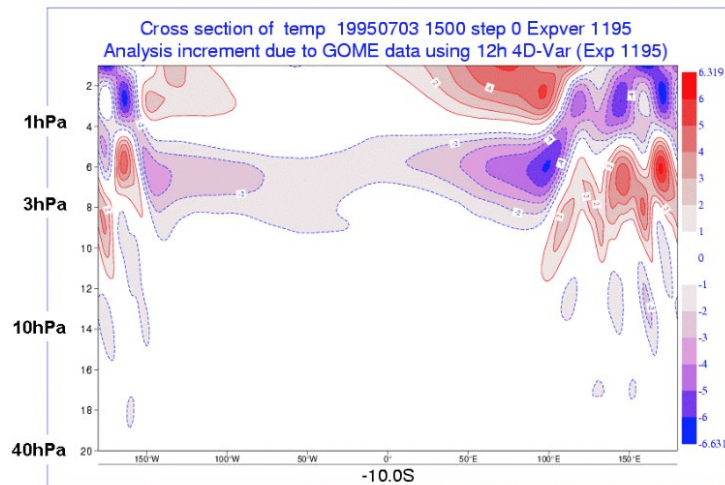




Year 2007, Slide courtesy of Dick Dee

## 4D-Var ozone assimilation

The impact of the ozone data on the temperature analysis at 10S



## Ozone assimilation

Can 4D-Var infer stratospheric winds from ozone data?

- The answer is: **Not yet.**
- Assimilation of ozone profile data causes large and unrealistic T/U/V increments near the stratopause to accommodate the observed discrepancies between background and data



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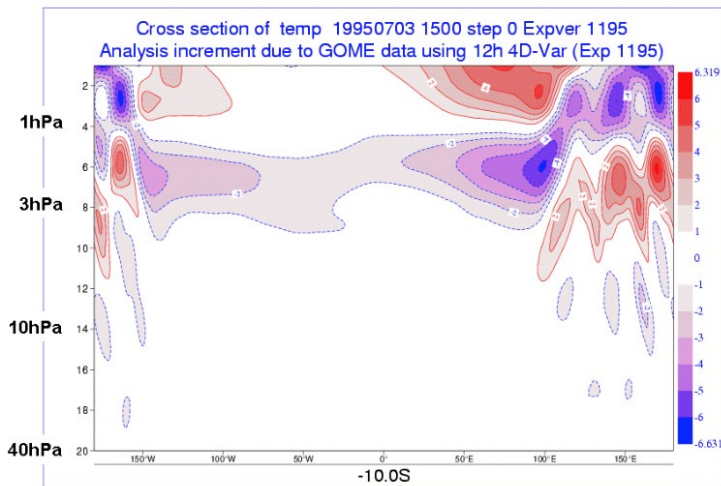
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## Year 2007, Slide courtesy of Dick Dee

### 4D-Var ozone assimilation

The impact of the ozone data on the temperature analysis at 10S



### Ozone assimilation

Can 4D-Var infer stratospheric winds from ozone data?

• The answer is: **Not yet.**

• Assimilation of ozone profile data causes large and unrealistic T/U/V increments near the stratopause to accommodate the observed discrepancies between background and data

## Year 2024

- Wind-tracer coupling in 4D-Var via the TLM integration:

$$\frac{\partial \delta \mathbf{v}}{\partial t} = -(\delta \mathbf{v} \cdot \nabla) \mathbf{v} - (\mathbf{v} \cdot \nabla) \delta \mathbf{v}$$

$$\frac{\partial \delta c}{\partial t} = -\gamma(x, y, t) (\nabla \cdot (\delta \mathbf{v} c)) - \nabla \cdot (\mathbf{v} \delta c)$$

... and the backwards ADM integration:

$$-\frac{\partial \delta \mathbf{v}^*}{\partial t} = (\mathbf{v} \cdot \nabla) \delta \mathbf{v}^* - (\nabla \otimes \mathbf{v}) \delta \mathbf{v}^* + \gamma(x, y, t) (-\delta c^* \nabla c + c \nabla \delta c^*)$$

$$-\frac{\partial \delta c^*}{\partial t} = -\nabla \cdot (\delta c^* \mathbf{v}) + \frac{\partial J}{\partial c}$$

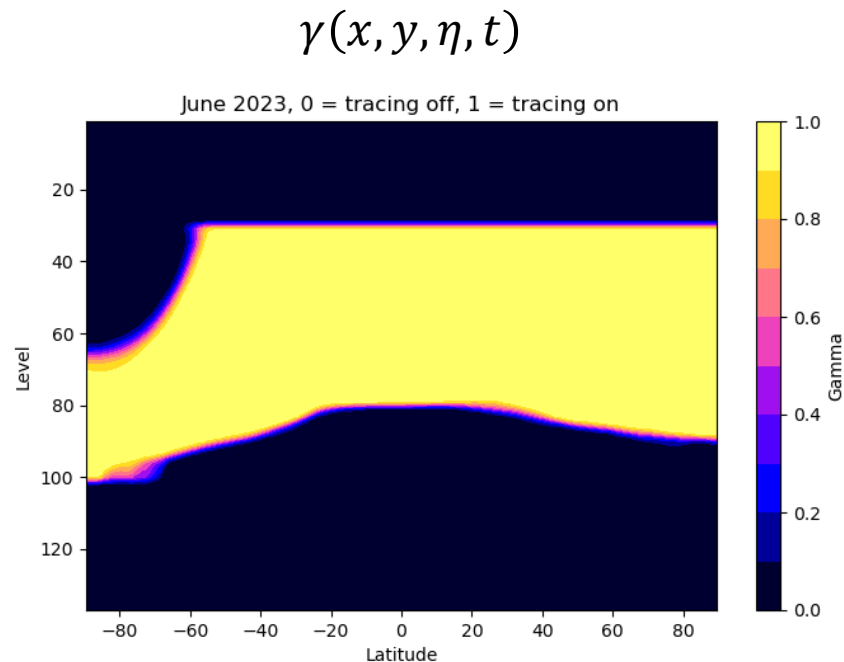
Parameter  $\gamma$  controls the “level” of tracer-wind coupling in the assimilation.

$\gamma=1$ : on  
 $\gamma=0$ : off

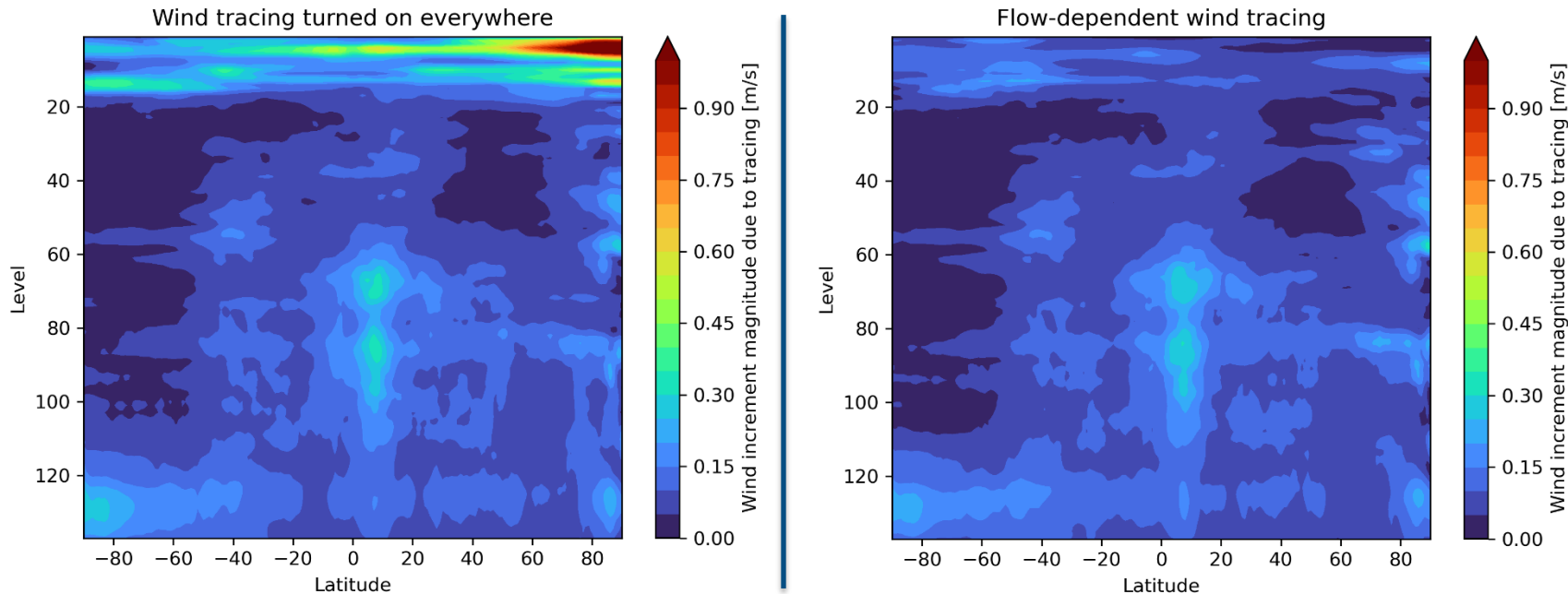
Zaplotnik, Ž., Žagar, N. & Semane, N.(2023) Flow-dependent wind extraction in strong-constraint 4D-Var. QJRM, 149(755, 2107–2124

Tracing turned off:

- In the mid- and lower-troposphere
- In the 4D-Var sponge layer (above 10 hPa)
- In the areas with  $T < 195$  K, where less predictable heterogeneous chemistry is an important contributor to  $\partial r(O_3)/\partial t$  in the nonlinear model
- Different  $\gamma$  for each month based on ERA5 climatology
- Fully flow-dependent  $\gamma$  based on latest background implemented and being tested

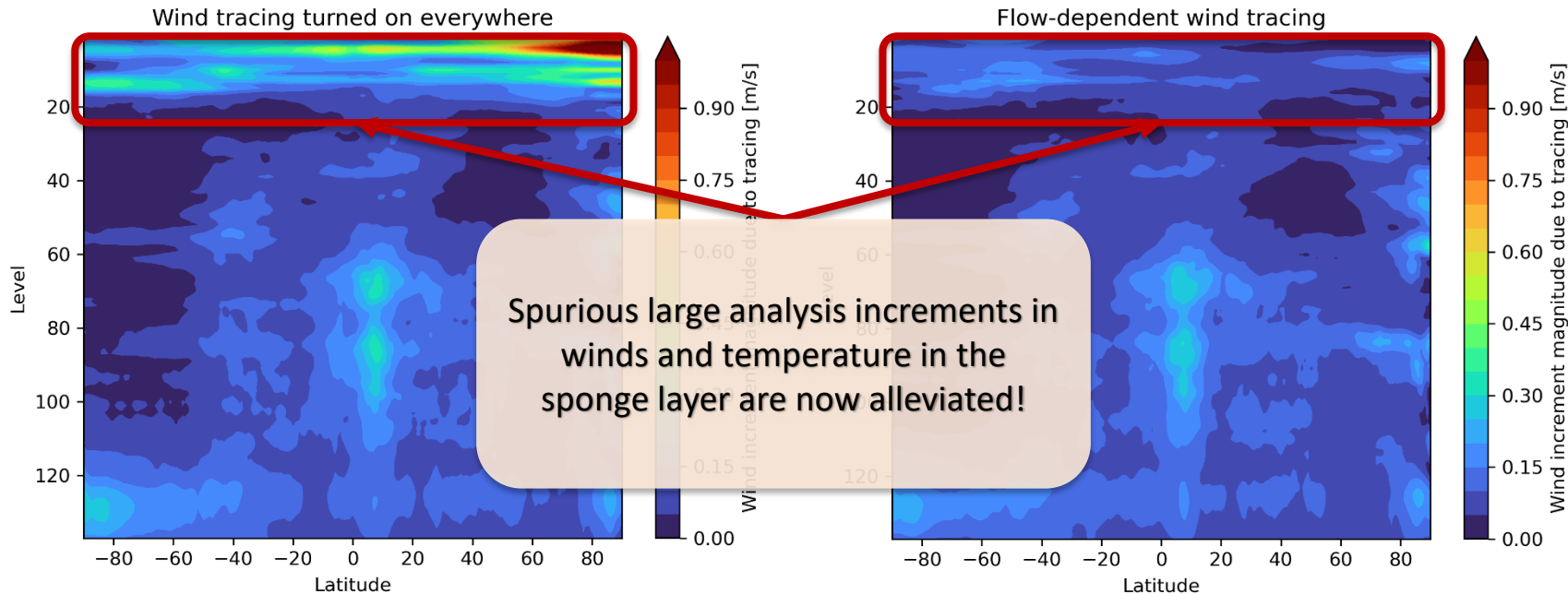


Zaplotnik, Ž., Žagar, N. & Semane, N.(2023) Flow-dependent wind extraction in strong-constraint 4D-Var. Quarterly Journal of the Royal Meteorological Society, 149(755), 2107–2124



- Positive impact on O-B statistics for ozone-sensitive channels (IASI, CRIS, AIRS), neutral-to-positive impact on other O-B statistics
- Ozone-wind tracing is undergoing testing for CY50R1



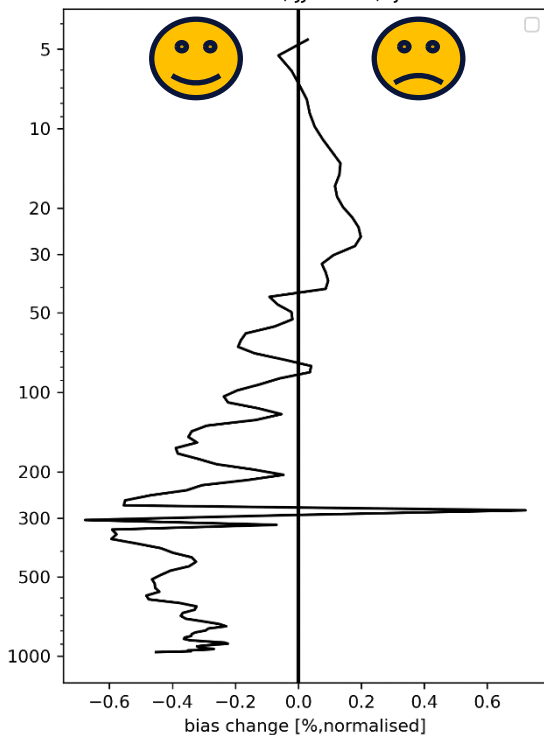


- Positive impact on O-B statistics for ozone-sensitive channels (IASI, CRIS, AIRS), neutral-to-positive impact on other O-B statistics



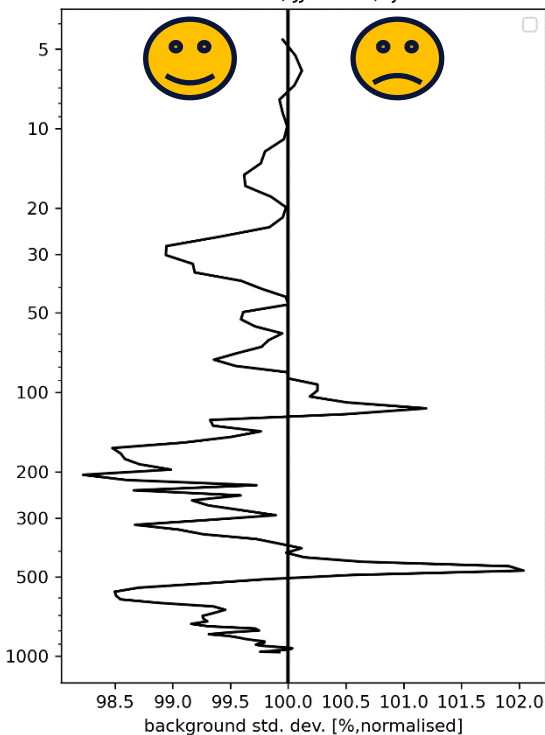
## Change in bias

Normalised change in bias,  
vs. ozone sondes, JJA2022, ij25 vs. i9fs



## Change in stdv

Normalised change in standard deviation,  
vs. ozone sondes, JJA2022, ij25 vs. i9fs

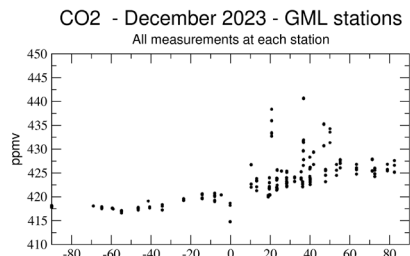
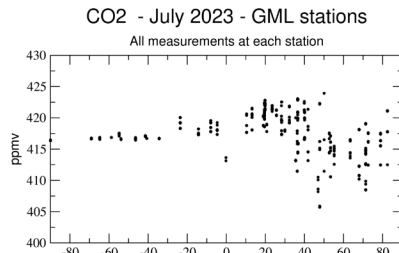


- Improved fit to ozone sondes with flow-dependent wind tracing
- **Ozone-wind tracing will be activated in CY50R1**

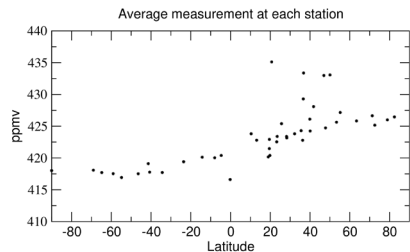
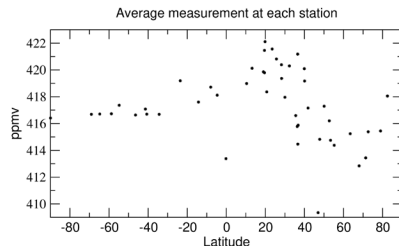


- RTTOV calculations are carried out with a fixed CO<sub>2</sub> profile (no change with latitude or month) with values  $\sim 401$  ppmv in troposphere
- Testing of using varying CO<sub>2</sub> profiles in the RTTOV calculations, obtained from a bi-dimensional monthly mean climatology derived from one year of CAMS reanalysis (EGG4)  
=> CO<sub>2</sub> mixing ratios used in the RTTOV calculation vary with altitude, latitude and month

All obs



Average



Surface CO<sub>2</sub> obs from  
Global Monitoring  
Laboratory network



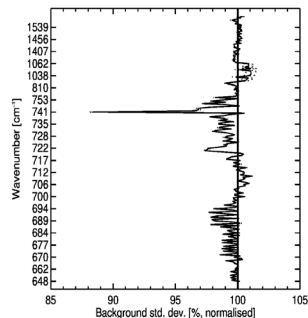
Atmosphere  
Mo

# Impact on fit to observations

Credit: M. Matricardi

## IASI

Instrument(s): METOP-B/C - IASI - TB Area(s): N.Hemis S.Hemis Tropics  
From 00Z 15-Jun-2022 to 12Z 26-Feb-2023

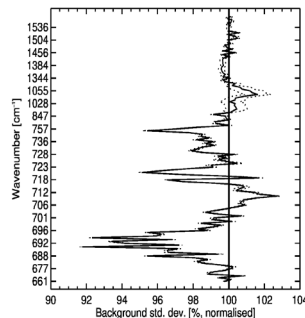


Possibly invalid -  
numbers are different by 2%

CO2CLIM\_FAIL\_EXP  
100% = CONTROL

## CrIS

Instrument(s): NOAA-20; NPP - CRIS - TB Area(s): N.Hemis S.Hemis Tropics  
From 00Z 15-Jun-2022 to 12Z 26-Feb-2023

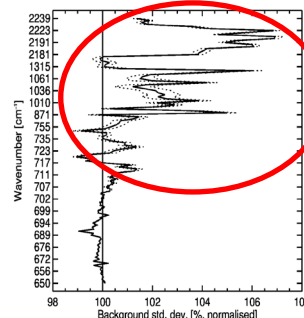


Possibly invalid -  
numbers are different by 2%

CO2CLIM\_FAIL\_EXP  
100% = CONTROL

## AIRS

Instrument(s): AQUA - AIRS - TB Area(s): N.Hemis S.Hemis Tropics  
From 00Z 15-Jun-2022 to 00Z 25-Feb-2023



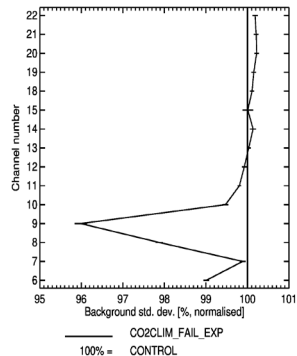
Possibly invalid -  
numbers are different by 6%

CO2CLIM\_FAIL\_EXP  
100% = CONTROL

In this spectral region the  
main absorber is  $N_2O$ , not  $CO_2$

## ATMS

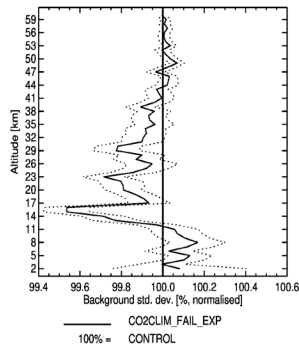
Instrument(s): NOAA-20; NPP - ATMS - TB Area(s): N.Hemis S.Hemis Tropics  
From 00Z 15-Jun-2022 to 12Z 26-Feb-2023



CO2CLIM\_FAIL\_EXP  
100% = CONTROL

## RO

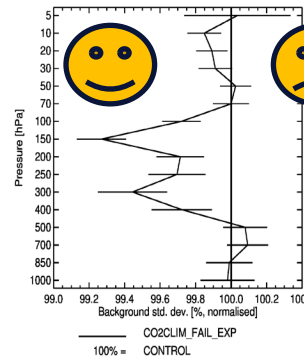
2E6; GRACE-C; KOMPSAT-5; METOP-1.3; SENTINEL-6A; SPIRE-LEMUR-3U; TANDEM  
Area(s): N.Hemis S.Hemis Tropics  
From 00Z 15-Jun-2022 to 12Z 26-Feb-2023



CO2CLIM\_FAIL\_EXP  
100% = CONTROL

## Radiosonde - T

Instrument(s): TEMP - T Area(s): N.Hemis S.Hemis Tropics  
From 00Z 15-Jun-2022 to 12Z 26-Feb-2023



CO2CLIM\_FAIL\_EXP  
100% = CONTROL

Better fit to the  
hyperspectral data  
affected by the  $CO_2$   
changes and better  
fit to independent  
observations

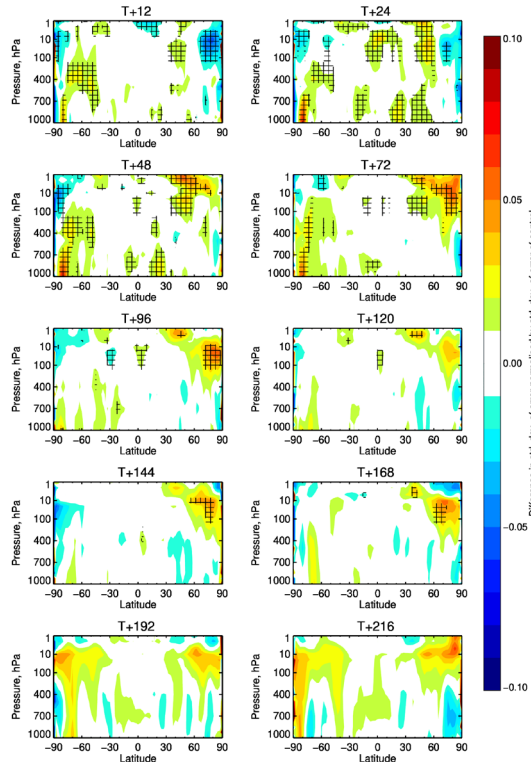




Z

Change in std. dev. of error in Z (CO2CLIM\_FAIL\_EXP-CONTROL)

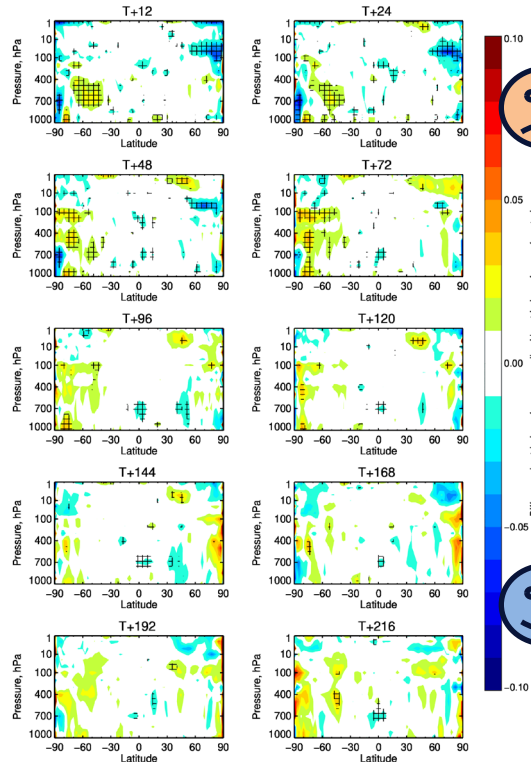
15-Jun-2022 to 28-Feb-2023 from 262 to 300 samples. Verified against own-analysis.  
Cross-hatching indicates 95% confidence with Sidak correction for 50 independent tests.



T

Change in std. dev. of error in T (CO2CLIM\_FAIL\_EXP-CONTROL)

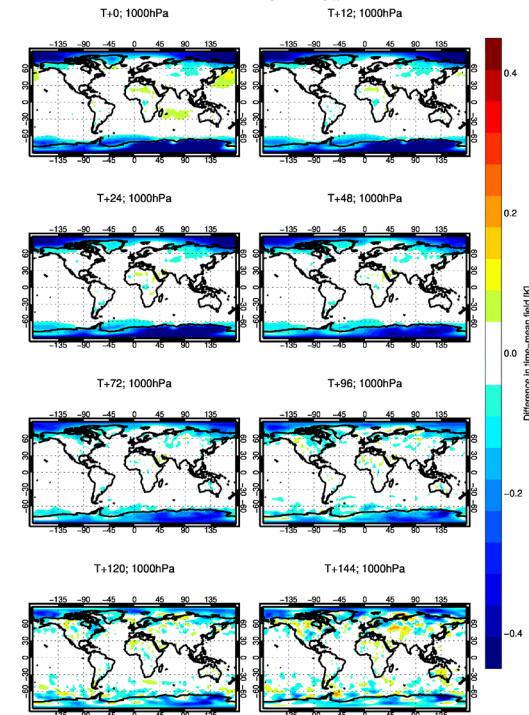
15-Jun-2022 to 28-Feb-2023 from 262 to 300 samples. Verified against own-analysis.  
Cross-hatching indicates 95% confidence with Sidak correction for 50 independent tests.



## Difference in mean T

Difference in time-mean T (CO2CLIM\_FAIL\_EXP - CONTROL)

25-Jun-2022 to 28-Feb-2023 from 262 to 282 samples. Combining own-analysis and forecast  
No statistical significance testing applied



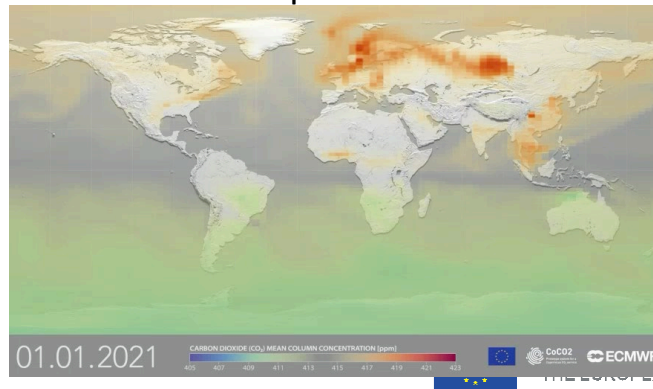
Difference in std. dev. of error normalised by std. dev. of error of control





- The system based on the CO<sub>2</sub> climatology produces an analysis that, overall, is better than the analysis produced by the operational system
  - => Better fit to the hyperspectral data affected by the CO<sub>2</sub> changes and fit to independent observations
- Medium range forecast scores launched from the improved analysis do not improve the operational scores.
- The system based on the climatological CO<sub>2</sub> seems to cool the atmosphere at the poles.
- More work to come, e.g. exploring use of NRT CO<sub>2</sub> data from CAMS instead of climatology

Atmospheric CO<sub>2</sub>





## 6 . S u m m a r y

- CAMS provides a wide range of atmospheric composition products
  - Useful in their own right and freely available
- Exciting potential to improve NWP forecasts with atmospheric composition information. E.g.
  - Stratospheric humidity analysis (active in CY50R1)
  - Ozone wind tracing (active in CY50R1)
  - Using aerosols interactively in the radiation scheme
  - Using variable CO2 in RTTOV

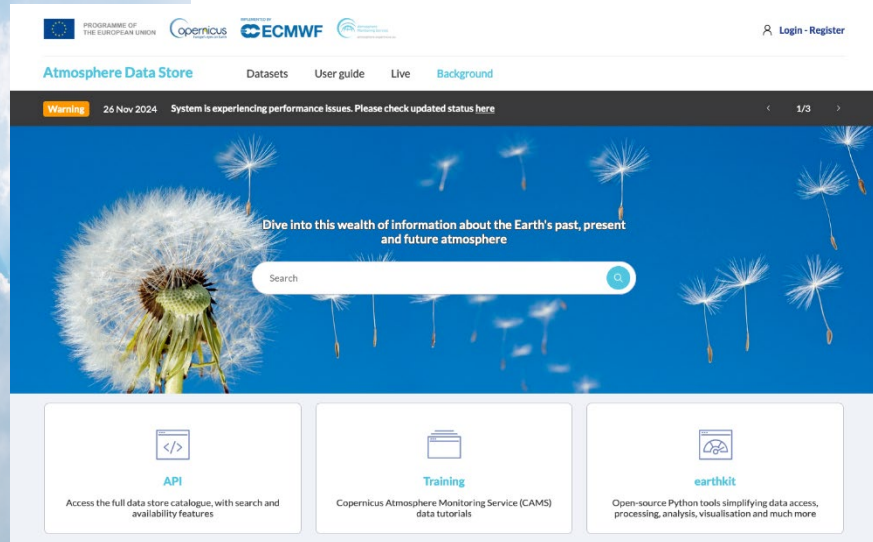




Atmosphere  
Monitoring

# The Atmosphere Data Store (ADS)

All CAMS data are freely available: <https://ads.atmosphere.copernicus.eu/>



Copernicus EU



Copernicus ECMWF



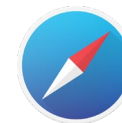
@CopernicusEU  
@CopernicusECMWF



@copernicusecmwf



Copernicus EU  
Copernicus ECMWF



[www.copernicus.eu](http://www.copernicus.eu)  
[ads.atmosphere.copernicus.eu](https://ads.atmosphere.copernicus.eu/)

## Documentation of atmospheric composition in IFS:

<https://www.ecmwf.int/en/elibrary/81374-ifs-documentation-cy48r1-part-viii-atmospheric-composition>

## Validation reports from:

<https://atmosphere.copernicus.eu/quality-assurance>



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Atmosphere Monitoring

# Thank you !



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