

Atmosphere Monitoring

Satellite data assimilation of atmospheric composition *Melanie Ades (ECMWF)*

Contributions from: Nicolas Bousserez, Antje Inness, Johannes Flemming, Richard Engelen





Why atmospheric composition at an operational weather prediction centre?

Atmosphere Monitoring

- Poor air quality is a major public health issue in many countries.
- Local authorities need accurate and timely information to implement effective air pollution mitigation measures.
- Accurate air quality forecasts require accurate transport models.
- Can leverage sophisticated data acquisition infrastructures implemented at operational weather prediction centers.
- Atmospheric composition also impacts the weather and forecasts.



YEAR



Why this lecture?

Atmosphere Monitoring

- Basic data assimilation theory is the same for atmospheric composition, but...
 - Radiance assimilation is not always feasible (yet)
 - Atmospheric composition data assimilation is much more influenced by additional factors such as emissions and chemistry than by the initial values
 - With many species not being observed, the problem is even more underdetermined than the standard NWP case
 - Atmospheric composition impacts the basic NWP problem as well





Atmosphere Monitoring

1. Copernicus Atmosphere Monitoring Service (CAMS)







What the Copernicus Atmosphere Monitoring Service has to offer

Atmosphere Monitoring









This is done by assimilating atmospheric composition data into the IFS (in addition to meteorological observations)

https://atmosphere.copernicus.eu

The CAMS portfolio includes Earth Observation based information products about:

- global atmospheric composition;
- the ozone layer;
- air quality in Europe;
- emissions and surface fluxes of key pollutants and greenhouse gases;
- solar radiation;
- climate radiative forcing.
- reanalysis of atmospheric composition (back to 2003)

Quarterly validation reports of global and regional outputs.



CAMS Global System

Atmosphere Monitoring



40km horizontal resolution at 137 model levels; two 5-day forecasts at 00z and 12z UTC each day

- Aerosols (AOD and concentrations): e.g. biomass burning, dust, sea-salt, sulphate, ...
- Reactive gases: CO, HCHO, NO₂, O₃, SO₂

9km horizontal resolution at 137 model levels; one 5-day forecast per day (CO₂, CH₄, linear CO)

CECMWF

European



Atmosphere Monitoring

2. Data assimilation methodology for atmospheric composition





Cost function

Atmosphere Monitoring Data assimilation for atmospheric composition is in principle no different from NWP data assimilation data assimilation

 $J(x) = (x - x_b)^T B^{-1}(x - x_b) + \sum_{i=0}^n (y_i - H_i[x_i])^T R_i^{-1}(y_i - H_i[x_i])$ J_b J_b J_b J_o J_o J

x: control vector

x_b: model background (short forecast)

B: Background error covariance matrix

y: Observations

H[x]: Model equivalent of observations R: Observation error covariance matrix

- Strong constraint 4D-Var assumes perfect model over assimilation period
- Weak constrained 4D-Var includes a model error term

opernic

Europear



Atmosphere Monitoring

Data assimilation for atmospheric composition is in principle no different from NWP data assimilation

$$J(x) = (x - x_b)_{Control variables}^{TB^{-1}}(x - x_b) + \sum_{i=0}^{n} (y_i - H_i[x_i])^T R_i^{-1}(y_i - H_i[x_i])$$

$$NWP$$

$$Vorticity
divergence
temperature
surface pressure (logarithm)
specific humidity
Atmospheric Composition
$$OTE
carbon monoxide
nitrogen dioxide
formaldehyde
sulphur dioxide
carbon dioxide
methane
aerosol mixing ratio$$$$







Combining the AC and NWP models

Atmosphere

Monitoling Atmospheric composition models can be run coupled to NWP or fully integrated.

NWP with aerosols NWP Physics with prognostic aerosols Physics Radiation Radiation Aerosol sources Vertical diffusion Dry deposition IFS Sedimentation Mass-Flux convection In the IFS the atmospheric composition Vertical diffusion Large-scale condensation and NWP models are fully integrated Mass-flux convection Cloud scheme Large-scale condensation Cloud scheme BC/OM aging New routine Conversion SO₂/SO₄ Modified routine Scavenging in- and below clouds Unchanged Aerosol budget Aerosol radiance diagnostics Morcrette et al. 2009, JGR, 114, doi:10.1029/2008JD011235

Data assimilation methodology





Atmosphere Monitoring

3. Observations of atmospheric composition





Global observing system

Atmosphere Monitoring



We want to provide information about nearsurface air quality



European

opernicus

CECMWF

- CAMS assimilates satellite retrievals of atmospheric composition
- CAMS uses ground-based & aircraft data and satellite retrievals for validation

Spectral signature of trace gases





Satellite orbits



www.esa.int

Polar Orbit:

- Low earth orbit (LEO, 600-800 km)
- Sun-synchronous orbit: overpass over given latitude always at the same local time, providing similar illumination
- Global measurements possible, but fixed overpass time & no observation of diurnal cycle
- Global coverage in a few days (in some cases better)

Geostationary Orbit:

- 36000 km flight altitude, equatorial orbit
- Fixed position relative to the Earth,
- Limited area from low to middle latitudes,
- No global measurements possible
- Observations of diurnal cycle
- AC constellation planned (S4, TEMPO, GEMS already launched)



AC Observations used in CAMS

Atmosphere Monitoring

AP

	Aura 272.5 PARASOL	CloudSat Sec. CloudSat 103 sec. CloudSat CCOM-W1 73 sec. CSSS CSSS CSSSS CSSSSS CSSSSSSSSSSSSS
	Species	Instruments
	CAMS Global system	
	O ₃	OMI, SBUV, GOME-2, MLS, OMPS, S5p
	CO	MOPITT, IASI, S5p
	NO ₂	GOME-2, S5P
	Aerosol	MODIS, PMAp, VIIRS, S3
L	CO ₂	GOSAT, IASI, OCO-2
	CH ₄	GOSAT, IASI, S5P
	GFAS fire emissions	MODIS, SEVIRI*, VIIRS, Sentinel-3, GOES-E/W*, HIMAWARI-8*

All from LEOs

Radiances versus retrievals

Atmosphere Monitoring

L2 retrievals generally use same methodology as data assimilation minimize a cost function that contains the observations and some a-priori constraint:

$$J(\mathbf{x}) = \frac{1}{2} (\mathbf{x} - \mathbf{x}_r^b)^{\mathrm{T}} \mathbf{B}_r^{-1} (\mathbf{x} - \mathbf{x}_r^b) + \frac{1}{2} [\mathbf{y}^o - H(\mathbf{x})]^{\mathrm{T}} \mathbf{R}^{-1} [\mathbf{y}^o - H(\mathbf{x})]$$

Simplified solution: $\mathbf{x}_r = \alpha \mathbf{x} + \beta \mathbf{x}_r^b$

The retrieved value will be biased relative to the assimilation model background, when the prior information is different from the model background.

This bias will have a vertical structure based on the vertical sensitivity of the observations.



How do we use retrievals in 2023?

Atmosphere Monitoring

Retrieval \mathbf{x}_r can be written (after linearization) as:

$$\mathbf{x}_r = \mathbf{x}_r^b + \mathbf{A}(\mathbf{x} - \mathbf{x}_r^b) + \varepsilon = \mathbf{A}\mathbf{x} + (\mathbf{I} - \mathbf{A})\mathbf{x}_r^b + \varepsilon$$

With a-priori \mathbf{x}_r^{b} , error covariance matrix \mathbf{S}_r and averaging kernel \mathbf{A} :

$$\mathbf{S}_{r} = \left(\mathbf{K}^{T}\mathbf{R}^{-1}\mathbf{K} + \mathbf{B}^{-1}\right)^{-1}$$
$$\mathbf{A} = \mathbf{S}_{r}\mathbf{K}^{T}\mathbf{R}^{-1}\mathbf{K}$$

R: observation error covariance matrixB: prior error covariance matrixK: weighting function

The averaging kernel **A** describes the vertical structure of the impact of the a priori information.





•Diurnal variations of Tsurf affect retrieval over land.

- CO near surface more detectable during day, AKs shift downwards
- Diurnal variability of AKs largest over e.g. deserts, smallest over sea
- If AKs are not used this can introduce an artificial diurnal CO cycle in the analysis

opernicus

European

Assimilating retrievals: Column retrieval example

Atmosphere Monitoring

We can make use of the averaging kernel **A** in the observation:

$$d = y - H(\mathbf{x}_m) \in \mathbf{x}_r^b + \mathbf{A}(\mathbf{x} - \mathbf{x}_r^b) + \varepsilon + H(\mathbf{x}_m)$$

Without averaging kernels in observation operator

$$d = y - \hat{H}(\mathbf{x}_m) = \mathbf{x}_r^b + \mathbf{A}(\mathbf{x} - \mathbf{x}_r^b) + \varepsilon - (\mathbf{x}_r^b + \mathbf{A}(H(\mathbf{x}_m) - \mathbf{x}_r^b))$$
$$= \mathbf{A}(\mathbf{x} - H(\mathbf{x}_m)) + \varepsilon$$
With averaging kernels in

We remove the influence of the a-priori profile if we use the averaging kernel to sample the model profile according to the assumptions made in the retrieval.



observation operator

s s u e s

- Atmosphere Monitoring • Total column retrievals come with integrated averaging kernels; some information is lost
 - Profile retrievals with full averaging kernels and retrieval errors can become difficult to handle
 - Not all retrieval methods allow the estimation of an averaging kernel; e.g., neural networks
 - Not all data providers use the same definition of averaging kernel in their data files
 - Many different versions of the observation operator needed to deal with all variations
 - We use:
 - Reactive gases: Profiles, columns with and without averaging kernels
 - Aerosols: Columns without averaging kernels, profiles being tested
 - Greenhouse gases: Radiances and columns with averaging kernels



Assimilating retrievals: summary

- Atmosphere Monitoring
- Easier
- No radiative transfer model for some of the species of interest
- Bad experiences with radiance assimilation:

Combination of model bias and VarBC in CO₂ data assimilation from AIRS and IASI radiances caused artificial long-term trend. Tests with IASI/AIRS ozone radiance assimilation led to degraded tropospheric ozone in CAMS

- Retrieval teams can focus their expertise fully on specific observation
- Good communication between data providers and data assimilation users needed
- Good characterization of retrieval is crucial
 - Averaging kernels
 - A priori
 - Error estimates
 - Quality flags





Atmosphere Monitoring

4. Emissions and emission inversion



Initial condition vs boundary problem



- NWP 4D-Var is mostly defined as an initial value problem. Only initial conditions are changed and model error is relatively small.
- AC modelling depends on initial state and surface fluxes

Atmosphere

Monitoring

 Large part of chemical system not sensitive to initial conditions because of chemical equilibrium, but dependent on other parameters (e.g. emissions, deposition, reaction rates, ...) which all might have errors





- Large positive increments from OMI NO2 assim ٠
- Large differences between analyses of ASSIM and CTRL
- Impact is lost during subsequent 12h forecast
- Constraining emissions (in addition of IC) would give a better initial state and persistence of ٠ forecast improvements throughout the DA window

Inness et al. (2015, ACP)

Emissions

Atmosphere Monitoring

- Emissions are one of the major uncertainties in composition modeling (can not be measured directly)
 - The compilation of emissions inventories is a labour-intensive task based on a wide variety of socio-economic and land use data
 - Trends are applied to inventories from previous years to produce future emission datasets
 - Some emissions can be "modeled" based on wind (dust and sea salt aerosol) or temperature (biogenic emissions)
 - Some emissions can be observed indirectly from satellites instruments (Fire radiative power, burnt area, volcanic plumes)
 - "Inverse" methods can be used to correct prior emission estimates using observations of concentrations and models



Examples of emissions

TNO European anthropogenic NOx emissions



MACC-GHG Reanalysis Flux Inversion December 2011 Mean CO2 Fluxes [gC / m2 / day] mean = 0.039 red - sources blue - sinks 100*W 60°E

CO2 fluxes

CAMS GLOB biogenic CO emissions



Volcanic SO2



5 704-7

70-0

5 704-11 5 70e-12



Commission



Biomass burning, 15 October 2017



CAMS_GLOB anthropogenic emissions



How to improve?

Atmosphere Monitoring

31

Adjust emissions as well as concentrations





opernicus

🗭 Joint state/emissions 4D-var inversion system

Atmosphere Monitoring

 $J_{b}: \text{ background constraint for } J_{p}: \text{ constraint for emission scaling factors}$ $J(x,p) = (x) - x_{b})^{T} B^{-1}(x - x_{b}) + (p) - p_{b})^{T} B_{p}^{-1}(p - p_{b})$ Parameter (e.g. scaling factors) $Vector + \sum_{i=0}^{n} (y_{i} - H_{i}[x_{i}, p])^{T} R_{i}^{-1}(y_{i} - H_{i}[x_{i}, p])$

J_o: observation constraint

- Joint optimisation of emissions and initial conditions
- Optimized emissions e.g. CO2, CH4, CO & NO2
- TL/AD of simplified chemistry: link between NO emissions and NO2 observations
- 2D scaling factors p applied to emission fields
- Prior error definition:
 - Global constant or 2D map of standard error
 - Spatial correlation length scale (via B_p)
 - NO/CO2 emission error correlation in B_p -> NO2 obs can contrain CO2 emissions

Credit: Nicolas Bousserez



Impact of Covid lockdown on US anthropogenic emissions

 Differences between posterior emissions May 2020 – May 2019 show impact of covid lockdown

Atmosphere

- Based on CAMS operational emissions in the prior and a fixed prior uncertainty of 40%.
- 10-20% reduction consistent with previous studies (e.g., *Keller et al.* (2020); Liu et al. (2020))
- Provided uncertainties in NO/CO₂ emission ratios are accounted for, topdown NO₂ estimates could help quantify CO₂ emissions variability

NO_x emission changes (%) between May 2020 and May 2019





Atmosphere Monitoring

5. Potential issues when assimilating AC satellite data







Atmosphere Mismatch between modelled and observed

Monitoring



$$+\sum_{i=0}^{n} (y_i - H_i[x_i])^T R_i^{-1} (y_i - H_i[x_i])$$

Only a small subset of all chemical species are observed and therefore included in the control vector. This means the full chemical system is very underconstrained.



Atmosphere Mismatch between modelled and observed variables

Monitoring





Increment from one TC ozone retrieval



Increment from one TC ozone retrieval



An extreme example: Ozone 7 October 2004

Atmosph **GEMS** reanalysis CAMS reanalysis Monitor 100 125 [DU]

- Similar TCO3 analysis from (old) GEMS reanalysis and CAMS reanalysis
- Huge differences between corresponding O3 profiles
- No profile data (MIPAS, MLS) were assimilated in GEMSRA in Oct 2004 and model had a large O3 bias leading to very bad vertical O3 analysis profiles
- Shows importance of using limb sounding data for O3 analysis



Aerosol analysis

Atmosphere Monitoring

- CAMS aerosol model has 14 aerosol bins:
 - 3 size bins each for sea-salt and desert dust
 - 2 bins (hydrophilic and hydrophobic) each for organic matter and black carbon
 - 1 bin for sulphate
 - 2 bins (fine and coarse) for nitrate
 - 1 bin for ammonium
- Assimilated observations are AOD at 550 nm from MODIS (Aqua and Terra) and VIIRS (SNPP and NOAA20) over land and ocean & PMAp (Metop-BC) over ocean
- Control variable is formulated in terms of the total aerosol mixing ratio.
- Analysis increments are repartitioned into the species according to their fractional contribution to the total aerosol mixing ratio.
- The repartitioning of the total aerosol mixing ratio increment into the different bins is difficult



Dust storm February 2021



NASA Worldview – MODIS Aqua and Terra AOD 550nm observations for 20210222

The CAMS forecast does a good job of forecasting the AOD plume from Africa over Northern Europe

CAMS Total AOD at 550nm 12hr forecast valid at 20210222 12hr

Aerosol forecasts - Sunday 21 Feb 2021, 00 UTC VT Sunday 21 Feb 2021, 12 UTC Step 12 © ECMWF 2021



Dust test case February 2021





Total AOD at 550nm: 20210222 03hr

- AOD increments are attributed to the different species according to their proportion in the nonlinear forecast.
- If there is no dust in the forecast in a specific location then the increment will be given to whatever species are there – in this case Sulphate



Dust









Sulphate aerosol optical depth at 550nm hipt increme

AOD incr at 550nm

European

Commission

Dust test case February 2021



LMD IASI 10um obs 20210222 12hr

European Commission



Atmosphere Monitoring

6. Potential benefits for NWP





Potential benefit for NWP

- Atmosphere Monitoring
- Prognostic aerosols, feedback on dynamics via radiation scheme: NWP first used Tegen AER climatology in radiation scheme, then CAMS interim climatology from CY43R3 and CAMSRA climatology from 48R1 onwards. CAMS uses aerosols interactively
- Use of O3 (& other fields) in the radiation scheme: MACC climatologies used in NWP. CAMS uses interactive O3.
- RTTOV observation operator: Use of O3, CO2 analysis fields to improve the use of radiances sensitive to O3, CO2: model O3 is used, but climatologies used for other tracers (e.g. fixed CO2 value)
- Dynamical coupling with wind/T through TL and AD: turned off
- Multivariate JB: Correlations between tracers and dynamical variables, e.g. O3 and vorticity; correlations between chemical species: univariate



Impact of prognostic aerosols

AOD anomalies and boreal wildfires summer 2021



Atmosphere Monitoring

Anomalies calculated against 2003-2020 monthly means from CAMS reanalysis



Atmosphere Impact on Artic wildfires on 2m temperature forecasts (JJA 2021)

-10--5 -1-1 1-2 2-5 5-10 RMSE CAMS -osuite (Prog AER) - RRMS CR (Clim Aero) JJA 2021

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

Monitoring

CECMWF

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

Credit: Johannes Flemming



Wind information from tracers

- Atmosphere Monitoring
- Prospect to extract wind information from long lived tracers in stratosphere and upper troposphere, e.g. O3, H2O, N2O.
- Similar to cloud-track winds but data coverage worse.
- Two ways:
 - Directly through cross correlations between tracer and other variables in background error covariance matrix
 - Indirectly as adjoint of tracer continuity equation propagates the tracer sensitivities over the analysis time window. E.g. O3 observations can influence the winds indirectly as the system attempts to reduce the O3 innovations via both wind and O3 increments
- Potential was demonstrated in early studies for H2O (Thepaut 1992) and O3 (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



Ozone and wind increments

Atmosphere

Monito



Single observation experiments

Level 20, ≈ 30 hPa

Observation at T0: 4D-Var = 3D-Var

Observation at T3: wind increments

Observation at T6: wind increments

6h assimilation window





Monitoring

Requirements to extract wind info from tracers

- Complete data coverage (3D), frequent observations.
 - Accurate observations
 - High quality background field
 - No bias between observations and background
 - Depends on accuracy of TL model compared to full model (better for passive tracers/ long chemical lifetime) => E.g. extracting wind information from O3 is more difficult in the tropics and summer hemisphere where photochemical lifetime is shorter
 - Studies have looked at this in idealized experiments (e.g. Daley 1995; Riishojgaard 1996; Peuch et al. 2000; Allen et al. 2013, 2014, 2018) focusing on long-lived tracers O3, H2O, N2O and found positive impact for perfect (and frequent) observations.
 - Few studies used real data (e.g. MLS O3, Semane et al. 2009) and positive results are less clear for 'not perfect' or infrequent observations



Example from ERA-Interim (it went wrong)



GOME 15-layer profiles (~15,000 per day) SBUV 6-layer profiles (~1,000 per day) The stratosphere is not well constrained by observations:

- Ozone profile data generate large temperature increments
- 4D-Var adjusts the flow where it is least constrained, to improve the fit to observations
- => IFS O3 analysis is completely uncoupled now



52



Atmosphere Monitoring







What we have seen today...

Atmosphere Monitoring

- Basic Data Assimilation theory is the same
- Particular challenges related to DA for atmospheric composition
 - Boundary conditions (emissions) as well as initial conditions; inversions
 - Mismatches between modelled and observed variables
 - Fast reactions and short life-time of some species
 - Cost of using chemical processes in the minimization (i.e., in the TL/AD models)
- Atmospheric composition has the potential to improve various aspects of NWP
- CAMS produces useful global and regional European Atmospheric Composition forecasts and analyses, freely available from <u>atmosphere.copernicus.eu</u>



The Atmosphere Data Store (ADS)

Atmosphere Monitoring All CAMS data are freely available

https://atmosphere.copernicus.eu/data



http://atmosphere.copernicus.eu

@CopernicusECMWF

@CopernicusEU





References: Reactive gases

Atmosphere Baklanov, A., D. Brunner, G. Carmichael, J. Flemming, S. Freitas, M. Gauss, Ø. Hov, R. Mathur, K.H. Schlünzen, C. Seigneur, and B. Vogel, 2017: Monitoring Key Issues for Seamless Integrated Chemistry–Meteorology Modeling. Bull. Amer. Meteor. Soc., 98, 2285–2292, https://doi.org/10.1175/BAMS-D-15-00166.1

N. Elguindi, H. Clark, C. Ordóñez, V. Thouret, J. Flemming, O. Stein, V. Huijnen, P. Moinat, A. Inness, V.-H. Peuch, A. Stohl, S. Turquety, G. Athier, J.-P. Cammas, and M. Schultz (2010): Current status of the ability of the GEMS/MACC models to reproduce the tropospheric CO vertical distribution as measured by MOZAIC. Geosci. Model Dev., 3, 501-518, 2010

Flemming, J., Benedetti, A., Inness, A., Engelen, R. J., Jones, L., Huijnen, V., Remy, S., Parrington, M., Suttie, M., Bozzo, A., Peuch, V.-H., Akritidis, D., and Katragkou, E.: The CAMS interim Reanalysis of Carbon Monoxide, Ozone and Aerosol for 2003–2015, Atmos. Chem. Phys., 17, 1945-1983, doi:10.5194/acp-17-1945-2017, 2017.

Flemming, J. and A. Inness, 2021: Carbon Monoxide [in "State of the Climate in 2020"]. Bull. Amer. Meteor., 102 (8), S101–S102, https://doi.org/10.1175/BAMS-D-21-0098.1. (also 2015, 2016, 2017, 2018, 2019)

Flemming, J., Huijnen, V., Arteta, J., Bechtold, P., Beljaars, A., Blechschmidt, A.-M., Josse, B., Diamantakis, M., Engelen, R. J., Gaudel, A., Inness, A., Jones, L., Katragkou, E., Marecal, V., Peuch, V.-H., Richter, A., Schultz, M. G., Stein, O., and Tsikerdekis, A.: Tropospheric chemistry in the integrated forecasting system of ECMWF, Geosci. Model Dev. Discuss., 7, 7733-7803, doi:10.5194/gmdd-7-7733-2014, 2014.

Flemming, J., and A. Inness (2013), Volcanic sulfur dioxide plume forecasts based on UV satellite retrievals for the 2011 Grímsvötn and the 2010 Eyjafjallajökull eruption, J. Geophys. Res. Atmos., 118, doi:10.1002/jgrd.50753.

Flemming, J., Inness, A., Jones, L., Eskes, H. J., Huijnen, V., Schultz, M. G., Stein, O., Cariolle, D., Kinnison, D., and Brasseur, G. (2011): Forecasts and assimilation experiments of the Antarctic ozone hole 2008, Atmos. Chem. Phys., 11, 1961-1977, doi:10.5194/acp-11-1961-2011

J. Flemming, Inness, A., Flentje, H., Huijen, V., Moinat, P., Schultz, M.G. and Stein O. (2009): Coupling global chemistry transport models to ECMWF's integrated forecast system. Geosci. Model Dev., 2, 253-265, 2009. <u>www.geosci-model-dev.net/2/253/2009/</u>





References: Reactive gases

Atmospher Monitoring Huijnen, V., Pozzer, A., Arteta, J., Brasseur, G., Bouarar, I., Chabrillat, S., Christophe, Y., Doumbia, T., Flemming, J., Guth, J., Josse, B., arydis, V. A., Marécal, V., and Pelletier, S.:Quantifying uncertainties due to chemistry modelling – evaluation of tropospheric composition simulations in the CAMS model (cycle 43R1), Geosci. Model Dev., 12, 1725–1752, https://doi.org/10.5194/gmd-12-1725-2019, 2019.

Huijnen, V., M. J. Wooster, J. W. Kaiser, D. L. A. Gaveau, J. Flemming, M. Parrington, A. Inness, D. Murdiyarso, B. Main and M. van Weele. Fire carbon emissions over maritime southeast Asia in 2015 largest since 1997. Sci. Rep. 6, 26886; doi: 10.1038/srep26886 (2016).

Huijnen, V., Flemming, J., Kaiser, J. W., Inness, A., Leitao, J., Heil, A., Eskes, H. J., Schultz, M. G., Benedetti, A., Hadji-Lazaro, J., Dufour, G., and Eremenko, M. (2012). Hindcast experiments of tropospheric composition during the summer 2010 fires over western Russia. Atmos. Chem. Phys., 12:4341–4364.

Inness, A., Ades, M., Balis, D., Efremenko, D., Flemming, J., Hedelt, P., Koukouli, M.-E., Loyola, D., and Ribas, R.: Evaluating the assimilation of S5P/TROPOMI near real-time SO2 columns and layer height data into the CAMS integrated forecasting system (CY47R1), based on a case study of the 2019 Raikoke eruption, Geosci. Model Dev., 15, 971–994, https://doi.org/10.5194/gmd-15-971-2022, 2022.

Inness, A., Chabrillat, S., Flemming, J., Huijnen, V., Langenrock, B., Nicolas, J., et al. (2020). Exceptionally low Arctic stratospheric ozone in spring 2020 as seen in the CAMS reanalysis. Journal of Geophysical Research: Atmospheres, 125(23), e2020JD033563.

Inness, A., Ades, M., Agustí-Panareda, A., Barré, J., Benedictow, A., Blechschmidt, A.-M., Dominguez, J. J., Engelen, R., Eskes, H., Flemming, J., Huijnen, V., Jones, L., Kipling, Z., Massart, S., Parrington, M., Peuch, V.-H., Razinger, M., Remy, S., Schulz, M., and Suttie, M.: The CAMS reanalysis of atmospheric composition, Atmos. Chem. Phys., 19, 3515–3556, https://doi.org/10.5194/acp-19-3515-2019, 2019.

Inness, A., Flemming, J., Heue, K.-P., Lerot, C., Loyola, D., Ribas, R., Valks, P., van Roozendael, M., Xu, J., and Zimmer, W.: Monitoring and assimilation tests with TROPOMI data in the CAMS system: near-real-time total column ozone, Atmos. Chem. Phys., 19, 3939–3962, https://doi.org/10.5194/acp-19-3939-2019, 2019.

Inness, A., Blechschmidt, A.-M., Bouarar, I., Chabrillat, S., Crepulja, M., Engelen, R. J., Eskes, H., Flemming, J., Gaudel, A., Hendrick, F., Huijnen, V., Jones, L., Kapsomenakis, J., Katragkou, E., Keppens, A., Langerock, B., de Mazière, M., Melas, D., Parrington, M., Peuch, V. H., Razinger, M., Richter, A., Schultz, M. G., Suttie, M., Thouret, V., Vrekoussis, M., Wagner, A., and Zerefos, C.: Data assimilation of satellite retrieved ozone, carbon monoxide and nitrogen dioxide with ECMWF's Composition-IFS, Atmos. Chem. Phys., 15, 5275-5303, doi:10.5194/acp-15-5275-2015, 2015.



References: Reactive gases

Atmosphere

Monitoring Inness, A., Baier, F., Benedetti, A., Bouarar, I., Chabrillat, S., Clark, H., Clerbaux, C., Coheur, P., Engelen, R. J., Errera, Q., Flemming, J., George, M., Granier, C., Hadji-Lazaro, J., Huijnen, V., Hurtmans, D., Jones, L., Kaiser, J. W., Kapsomenakis, J., Lefever, K., Leita o, J., Razinger, M., Richter, A., Schultz, M. G., Simmons, A. J., Suttie, M., Stein, O., Th'epaut, J.-N., Thouret, V., Vrekoussis, M., Zerefos, C., and the MACC team (2013). The MACC reanalysis: an 8 yr data set of atmospheric composition. Atmos. Chem. Phys., 13(8):4073–4109.

Inness, A., Benedetti, A., Flemming, J., Huijnen, V., Kaiser, J. W., Parrington, M., and Remy, S.: The ENSO signal in atmospheric composition fields: emission-driven versus dynamically induced changes, Atmos. Chem. Phys., 15, 9083-9097, doi:10.5194/acp-15-9083-2015, 2015.

Inness, A., Flemming, J., Suttie, M. and Jones, L., 2009: GEMS data assimilation system for chemically reactive gases. ECMWF RD Tech Memo 587. Available from http://www.ecmwf.int.

C. Ordonez, N. Elguindi, O. Stein, V. Huijnen, J. Flemming, A. Inness, H. Flentje, E. Katragkou, P. Moinat, V-H. Peuch, A. Segers, V. Thouret, G. Athier, M. van Weele, C. S. Zerefos, J-P. Cammas, and M. G. Schultz (2009): Global model simulations of air pollution during the 2003 European heat wave. Atmos. Chem. Phys., 10, 789-815, 2010. www.atmos-chem-phys.net/10/789/2010/

Stein, O., Flemming, J., Inness, A., Kaiser, J. W., and Schultz, M. G. (2012). Global re- active gases forecasts and reanalysis in the MACC project. Journal of Integrative Environmental Sciences, 1:1–14

Min Huang, Gregory R. Carmichael, R. Bradley Pierce, Duseong S. Jo, Rokjin J. Park, Johannes Flemming, Louisa K. Emmons, Kevin W. Bowman, Daven K. Henze, Yanko Davila, Kengo Sudo, Jan Eiof Jonson, Marianne Tronstad Lund, Greet Janssens-Maenhout, Frank J. Dentener, Terry J. Keating, Hilke Oetjen, and Vivienne H. Payne, Impact of intercontinental pollution transport on North American ozone air pollution: an HTAP phase 2 multi-model study, Atmos. Chem. Phys., 17, 5721-5750, https://doi.org/10.5194/acp-17-5721-2017, 2017

Zerefos, C. S., Eleftheratos, K., Kapsomenakis, J., Solomos, S., Inness, A., Balis, D., Redondas, A., Eskes, H., Allaart, M., Amiridis, V., Dahlback, A., De Bock, V., Diémoz, H., Engelmann, R., Eriksen, P., Fioletov, V., Gröbner, J., Heikkilä, A., Petropavlovskikh, I., Jarosławski, J., Josefsson, W., Karppinen, T., Köhler, U., Meleti, C., Repapis, C., Rimmer, J., Savinykh, V., Shirotov, V., Siani, A. M., Smedley, A. R. D., Stanek, M., and Stübi, R.: Detecting volcanic sulfur dioxide plumes in the Northern Hemisphere using the Brewer spectrophotometers, other networks, and satellite observations, Atmos. Chem. Phys., 17, 551-574, doi:10.5194/acp-17-551-2017, 2017.





References: Aerosols

Atmosphe Bellouin, N., J. Quaas, J.-J. Morcrette, and O. Boucher, 2013: Estimates of radiative forcing from the MACC re-analysis. Atmos. Chem. Phys., 13, 2045-2062.

Benedetti, A. et al, 2014: Operational dust prediction. Chapter 10 in: Knippertz, P.; Stuut, J.-B. (eds.), Mineral Dust – A Key Player in the Earth System, Springer Netherlands, 223–265, ISBN 978-94-017-8977-6. doi:10.1007/978-94-017-8978-3_10

Benedetti, A., Morcrette, J.-J., Boucher, O., Dethof, A., Engelen, R. J., Fisher, M., Flentje, H., Huneeus, N., Jones, L., Kaiser, J. W., Kinne, S., Manglold, A., Razinger, M., Simmons, A. J., and Suttie, M. (2009). Aerosol analysis and forecast in the European Centre for Medium-Range Weather Forecasts Integrated Forecast System: 2. Data assimilation. J. Geophys. Res., 114(D13):D13205

Benedetti, A., Kaiser, J. W., and Morcrette, J.-J. (2012). Global aerosols [in "State of the climate in 2011"]. Bull. Amer. Meteor. Soc., 93(7):S44–S46. (Also for subsequent years)

Huneeus, N., M. Schulz, Y. Balkanski, J. Griesfeller, S. Kinne, J. Prospero, S. Bauer, O. Boucher, M. Chin, F. Dentener, T. Diehl, R. Easter, D.
Fillmore, S. Ghan, P. Ginoux, A. Grini, L. Horowitz, D. Koch, M.C. Krol, W. Landing, X. Liu, N. Mahowald, R. Miller, J.-J. Morcrette, G. Myhre, J.
Penner, J. Perlwitz, P. Stier, T. Takemura, and C. Zender, 2011: Global dust model intercomparison in AEROCOM phase I. Atmos. Chem. Phys., 11, 7781-7816, doi:10.5194/acp-11-7781-2011.

Mangold, A., H. De Backer, B. De Paepe, S. Dewitte, I. Chiapello, Y. Derimian, M. Kacenelenbogen, J.-F. Léon, N. Huneeus, M. Schulz, D. Ceburnis, C. O'Dowd, H. Flentje, S. Kinne, A. Benedetti, J.-J. Morcrette, and O. Boucher, 2011: Aerosol analysis and forecast in the European Centre for Medium-Range Weather Forecasts Integrated Forecast System: 3. Evaluation by means of case studies, J. Geophys. Res., 116, D03302, doi: 10.1029 /2010JD014864.

Rémy, S., Kipling, Z., Flemming, J., Boucher, O., Nabat, P., Michou, M., Bozzo, A., Ades, M., Huijnen, V., Benedetti, A., Engelen, R., Peuch, V.-H., and Morcrette, J.-J.: Description and evaluation of the tropospheric aerosol scheme in the European Centre for Medium-Range Weather Forecasts (ECMWF) Integrated Forecasting System (IFS-AER, cycle 45R1), Geosci.Model Dev., 12, 4627–4659, https://doi.org/10.5194/gmd-12-4627-2019, 2019.



Atmosphere Morcrette, J.-J., Boucher, O., Jones, L., Salmond, D., Bechtold, P., Beljaars, A., Benedetti, A., Bonet, A., Kaiser, J. W., Razinger, M., Schulz, M., Monitoring Serrar, S., Simmons, A. J., Sofiev, M., Suttie, M., Tompkins, A. M., and Untch, A. (2009). Aerosol analysis and forecast in the European Centre for Medium-Range Weather Forecasts Integrated Forecast System: Forward modeling. J. Geophys. Res., 114(D6):D06206.

Morcrette, J.-J., O. Boucher, L. Jones, D. Salmond, P. Bechtold, A. Beljaars, A. Benedetti, A. Bonet, J.W. Kaiser, M. Razinger, M. Schulz, S. Serrar, A.J. Simmons, M. Sofiev, M. Suttie, A.M. Tompkins, A. Untch, and the GEMS-AER team, 2009: Aerosol analysis and forecast in the ECMWF Integrated Forecast System: Forward modelling. J. Geophys. Res., 114, D06206, doi: 10.1029 /2008JD011235.

Morcrette, J.-J., A. Beljaars, A. Benedetti, L. Jones, and O. Boucher, 2008: Sea-salt and dust aerosols in the ECMWF IFS. Geophys. Res. Lett., 35, L24813, doi:10.1029/2008GL036041.

Morcrette, J.-J., A. Benedetti, L. Jones, J.W. Kaiser, M. Razinger, and M. Suttie, 2011: Prognostic aerosols in the ECMWF IFS: MACC vs. GEMS aerosols. ECMWF Technical Memorandum, 659, 32 pp.

Morcrette, J.-J., A. Benedetti, A. Ghelli, J.W. Kaiser, and A.P. Tompkins, 2011: Aerosol-cloud-radiation interactions and their impact on ECMWF/MACC forecasts. ECMWF Technical Memorandum, 660, 35 pp.

Nabat, P., S. Somot, M. Mallet, I. Chiapello, J.-J. Morcrette, F. Solmon, S. Szopa, and F. Dulac, 2013: A 4-D climatology (1979-2009) of the monthly aerosol optical depth distribution over the Mediterranean and surrounding regions from a comparative evaluation and blending of remote sensing and model products. Atmos. Meas. Tech., 6, 1287-1314, doi:10.5194/amt-6-1287-2013.

Peubey, C., A. Benedetti, L. Jones, and J.-J. Morcrette, 2009: GEMS-Aerosol: Comparison and analysis with GlobAEROSOL data. In GlobAEROSOL User Report, October 2009, 11-20.





References: Greenhouse gases

Atmosphere Monitoring

Agusti-Panareda, A., Diamantakis, M., Bayona, V., Klappenbach, F., and Butz, A.: Improving the inter-hemispheric gradient of total column atmospheric CO2 and CH4 in simulations with the ECMWF semi-Lagrangian atmospheric global model, Geosci. Model Dev., 10, 1-18, doi:10.5194/gmd-10-1-2017, 2017.

A. Agusti-Panareda; S. Massart; F. Chevallier; G. Balsamo; S. Boussetta; E. Dutra; A. Beljaars A biogenic C02 flux adjustment scheme for the mitigation of large-scale biases in global atmospheric CO2 analyses and forecasts. ECMWF Technical Memorandum, no 773, 2015 http://www.ecmwf.int/en/elibrary/technical-memoranda

Agusti-Panareda, A., S.Massart, F.Chevallier, S.Boussetta, G.Balsamo, A.Beljaars, P.Ciais, N.M.Deutscher, R.Engelen, L.Jones and R.Kivi, J.-D.~Paris, V.-H. Peuch, V.Sherlock, A.T.Vermeulen, P.O.Wennberg, D.Wunch, 2014: Forecasting global atmospheric CO2, Atmospheric Chemistry and Physics ,14, 11959-11983, doi:10.5194/acp-14-11959-2014

Chevallier, F., R. J. Engelen, C. Carouge, T. J. Conway, P. Peylin, C. Pickett-Heaps, M. Ramonet, P. J. Rayner, and I. Xueref-Remy, 2009. AIRS-based vs. flask-based estimation of carbon surface fluxes. J. Geophys. Res., 114, D20303, doi:10.1029/2009JD012311.

Chevallier, F., R. J. Engelen, and P. Peylin, 2005. The contribution of AIRS data to the estimation of CO2 sources and sinks. Geophys. Res. Lett., 32, L23801, doi:10.1029/2005GL024229.





References: Greenhouse gases

Atmosphere Engelen, R.J., S. Serrar, and F. Chevallier, 2009. Four-dimensional data assimilation of atmospheric CO2 using AIRS observations. J. Monitoring Geophys. Res., 114, D03303, doi:10.1029/2008JD010739.

Engelen, R.J. and A. P. McNally, 2005. Estimating atmospheric CO2 from advanced infrared satellite radiances within an operational fourdimensional variational (4D-Var) data assimilation system: Results and validation. J. Geophys. Res., 110, D18305, doi:10.1029/2005JD005982

Massart et al. (2016) Ability of the 4-D-Var analysis of the GOSAT BESD XCO2 retrievals to characterize atmospheric CO2 at large and synoptic scales. Atmos. Chem. Phys., 16, 1653–1671, www.atmos-chem-phys.net/16/1653/2016/ doi:10.5194/acp-16-1653-2016. http://www.atmos-chem-phys.net/16/1653/2016/acp-16-1653-2016.pdf

Massart, S. and Agusti-Panareda, A. and Aben, I. and Butz, A. and Chevallier, F. and Crevoisier, C. and Engelen, R. and Frankenberg, C. and Hasekamp, O., 2014: Assimilation of atmospheric methane products in the MACC-II system: from SCIAMACHY to TANSO and IASIO, Atmospheric Chemistry and Physics, 14, 6139–6158,10.5194/acp-14-6139-2014.

Tang, W., Arellano, A. F., DiGangi, J. P., Choi, Y., Diskin, G. S., Agustí-Panareda, A., Parrington, M., Massart, S., Gaubert, B., Lee, Y., Kim, D., Jung, J., Hong, J., Hong, J.-W., Kanaya, Y., Lee, M., Stauffer, R. M., Thompson, A. M., Flynn, J. H., and Woo, J.-H.: Evaluating High-Resolution Forecasts of Atmospheric CO and CO2 from a Global Prediction System during KORUS-AQ Field Campaign, Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2018-71, in review, 2018.

Verma, S., Marshall, J., Parrington, M., Agustí-Panareda, A., Massart, S., Chipperfield, M. P., Wilson, C., and Gerbig, C.: Extending methane profiles from aircraft into the stratosphere for satellite total column validation using the ECMWF C-IFS and TOMCAT/SLIMCAT 3-D model, Atmos. Chem. Phys., 17, 6663-6678, https://doi.org/10.5194/acp-17-6663-2017, 2017.





References: Fires

Atmosphere

Monitoring Kaiser, J. W., Heil, A., Andreae, M. O., Benedetti, A., Chubarova, N., Jones, L., Morcrette, J.-J., Razinger, M., Schultz, M. G., Suttie, M., and van der Werf, G. R. (2012). Biomass burning emissions estimated with a global fire assimilation system based on observed fire radiative power. Biogeosciences, 9:527–554.

Kaiser, J. W. and van der Werf, G. R. (2012). Global Biomass Burning [in "State of the Climate in 2011"]. Bull. Amer. Meteor. Soc., 93(7):S54–S55. (also for other years)

Kaiser, J.W., M. Suttie, J. Flemming, J.-J. Morcrette, O. Boucher, and M.G. Schultz, 2009: Global real-time fire emission estimates based on space-borne fire radiative power observations. AIP Conf. Proc., 1100, 645-648.

Rémy, S., Veira, A., Paugam, R., Sofiev, M., Kaiser, J. W., Marenco, F., Burton, S. P., Benedetti, A., Engelen, R. J., Ferrare, R., and Hair, J. W.: Two global data sets of daily fire emission injection heights since 2003, Atmos. Chem. Phys., 17, 2921-2942, doi:10.5194/acp-17-2921-2017, 2017.





References: General

Atmosphere

Monitoring Granier, C., Bessagnet, B., Bond, T., D'Angiola, A., Dernier van der Gon, H., Frost, G., Heil, A., Kaiser, J., Kinne, S., Klimont, G., Kloster, S., Lamarque, J.-F., Liousse, C., Masui, T., Meleux, F., Mieville, A., Ohara, T., Raut, J.-C., Riahi, K., Schultz, M., Smith, S., Thompson, A., van Aardenne, J., van der Werf, G., and van Vuuren, D. (2011). Evolution of anthropogenic and biomass burning emissions of air pollutants at global and regional scales during the 1980–2010 period. Climatic Change, 109(1-2):163–190.

Hollingsworth, A., Engelen, R. J., Textor, C., Benedetti, A., Boucher, O., Chevallier, F., Dethof, A., Elbern, H., Eskes, H., Flemming, J., Granier, C., Kaiser, J. W., Morcrette, J.-J., Rayner, P., Peuch, V.-H., Rouil, L., Schultz, M. G., and Simmons, A. J. (2008). Toward a monitor- ing and forecasting system for atmospheric composition: The GEMS project. Bull. Amer. Meteor. Soc., 89(8):1147–1164.

