Atmospheric composition assimilation
Antje Inness (ECMWF)
Thanks to the ECMWF CAMS team
Outline

• MACC/CAMS

• Data assimilation with the Composition-IFS
  • C-IFS model
  • CAMS composition data assimilation
  • Examples

• Concluding remarks
• Copernicus Atmosphere Monitoring Service (CAMS)
• Operational delivery of atmospheric composition services funded by the EU
• Initial period from 2015 – 2020
• ECMWF is in charge of implementation
• Heritage from GEMS, MACC, -II, -III, PROMOTE
• Global and European regional scale
Data assimilation with the Composition-IFS (C-IFS)

- Chemistry schemes included in ECMWF’s IFS
- Use ECMWF’s 4D-Var to assimilate observations of atmospheric composition
- Assimilated data: Satellite retrievals
- Assimilated species: O3, CO, NO2, SO2, HCHO (AOD, CO2, CH4)
Assimilation of CO observations in a global model

Carbon Monoxide (CO) is a tracer of combustion sources
Composition-IFS (C-IFS) model

- Over the last decade IFS has been extended with modules for atmospheric composition (aerosols, reactive gases, greenhouse gases)
- At first a “Coupled System”, now composition fully integrated into IFS (more efficient)
- Data assimilation of AC data to provide best possible IC for subsequent forecasts
- AC benefits from online integration and high temporal availability of meteorological fields
- C-IFS provides daily analyses and 5-day forecasts of atmospheric composition in NRT
C-IFS chemistry schemes

**TM5 (CB05) chemical mechanism**
- Tropospheric scheme with 54 species and 126 reactions
- Stratospheric O3: Cariolle and Teyssèdre parametrisation
- Dry deposition climatological fields from MOCAGE
- Harvard wet deposition scheme
- Anthropogenic emissions: MACCity
- Fire emissions: GFAS
- Biogenic emission: POET data base, isoprene emissions from MEGAN2.1

**MOZART chemical mechanism**

**MOCAGE chemical mechanism**

**TM5 (CB05) + BASCOE chemical mechanism**

Flemming et al. (2015, GMD)
CAMS 4D-Var data assimilation system

Extra information:
- Emissions (e.g. GFAS)
- Fluxes

IFS control variables
- CHEM: O3, NO2, SO2, CO, HCHO
- AER: single or dual control variables (total or fine & coarse mode aerosol mixing ratio)
- GHG: CO2, CH4

Meteorological variables
- Aerosol model with 12 bins (no TL or AD)
- GHG fields

Observations
- Observation operators
- Bias correction
- Background error statistics

Chemistry solvers included in IFS e.g. TM5 (CB05)
54 species, 126 reactions
photolysis, dry and wet deposition (no TL + AD of chemistry)
# Data used in CAMS NRT system (2015)

<table>
<thead>
<tr>
<th>Instrument</th>
<th>Satellite</th>
<th>Satellite operator</th>
<th>Data provider</th>
<th>Species</th>
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+ meteorological data
Reactive gases data availability in MACC NRT system: 20140901, 12z

**CO**

- IASI Metop-A
- IASI Metop-B
- MOPITT TERRA

**O3**

- GOME-2 Metop-A
- GOME-2 Metop-B
- OMI, MLS AURA
- SBUV/2 NOAA-19

**Tropospheric NO2**

- OMI AURA
- GOME-2 Metop-A
- GOME-2 Metop-B
- HCHO
- SO2
- GOME-2 Metop-A
- OMI AURA
- GOME-2 Metop-A
- GOME-2 Metop-B

Legend:
- assimilated
- monitored
Challenges for composition DA

- Quality of NWP depends predominantly on initial state
- AC modelling depends on initial state (lifetime) and surface fluxes
- Large part of chemical system not sensitive to initial conditions because of chemical equilibrium, but dependent on model parameters (e.g. emissions, deposition, reaction rates,...)
- Data assimilation is challenging for short lived species (e.g. NO2)
- CTMs have larger biases than NWP models
- Most processes take place in boundary layer, which is not well observed from space
- Only a few species (out of 100+) can be observed
- Data availability
- More complex and expensive, e.g. atmospheric chemistry, aerosol physics
- Concentrations vary over several orders of magnitude
Chemical Lifetime vs. Spatial Scale

After Seinfeld and Pandis [1998]
Emission processes

- Combustion related (CO, NO$_x$, SO$_2$, VOC, CO$_2$)
  - fossil fuel combustion
  - biofuel combustion
  - vegetation fires (man-made and wild fires)
- Fluxes from biogeochemical processes (VOC, Methane, CO$_2$, Pollen):
  - biogenic emissions (plants, soils, oceans)
  - agricultural emissions (incl. fertilisation)
- Fluxes from wind blown dust and sea salt (from spray)
- Volcanic emissions (ash, SO$_2$, HBr ...)

- In CAMS we use **GFAS fire emissions** (Kaiser et al. 2012) and **MACCity anthropogenic emissions** (Granier et al. 2011)
- Biomass burning accounts for ~ 30% of total CO and NO$_x$ emissions, ~10% CH4
Importance of fire emissions for tropospheric NO$_2$

GFAS emissions for January used by mistake in IFS-MOZ during 2011
Importance of emissions (Russian fires 2010)

Huijnen et al. (2012, ACP)

- Assimilation of IASI TCCO leads to improved fit to MOPITT TCCO
- TCCO from Assim and Assim-GFAS are very similar

Daily maximum surface O3 and CO

GFAS emissions are needed to get peak in surface concentrations in GFAS and Assim-GFAS
Short lived memory of NO2 assimilation

OMI NO2 analysis increment [%]

- Large positive increments from OMI NO2 assim
- Large differences between analyses of ASSIM and CTRL
- Impact is lost during subsequent 12h forecast
- It might be more beneficial to adjust emissions (instead of IC)

Inness et al. (2015, ACP)
C-IFS ozone analysis

Assimilated data:

• MLS ozone profiles
• SBUV/2 partial columns
• OMI, GOME-2 (SCIAMACHY) total columns

➔ Profile data very important
➔ Combination of stratospheric profiles and TCO3 also allows some corrections in the troposphere (as residual of the two)

Inness et al. (2015, ACP)
Importance of height resolved observations

- Background errors determine how increment is spread out from a single observation to neighbouring grid points/levels
- Maximum impact for O3 around L20 (~35 hPa)
- Profile data are important to obtain a good vertical analysis profiles
Ozone hole in GEMS reanalysis: Cross section along 8E over South Pole, 4 Oct 2003

ASSIM (MIPAS)

CTRL

70S

Assimilation with profile data

Assimilation with total column data
Ozone assimilation tests (March 2011): Bias against O3 sondes

MACC NRT (f93i) used NRT MLS V2 data and TCO3 data (useful range down to 68 hPa)
- MLS V3: useful range down to 261 hPa
- It is beneficial for the ozone analysis to have the extra MLS levels down to 261 hPa
- Assimilating MLS and TCO3 data (including OMI) improves the fit to sondes in the troposphere and does not change the fit much in the stratosphere where the analysis is well constrained by MLS

Lefever et al. (2015, ACP)
Evolution of CAMS NRT system:
CAMS Ozone score at Neumayer

Better

Worse

2009
Problems during O3 hole
2010
2011
2012
2013
2014
2015

Improvement with time

Switch to MLS v3.4

CIFS
Ozone: Impact of assimilation

Average of 77 profiles of GO3 (mPa) over Ny-Aalesund in 2008. Analyses.

Average of 126 profiles of GO3 (mPa) over Hohenpeissenberg in 2008. Analyses.

Average of 65 profiles of GO3 (mPa) over South_Pole in 2008. Analyses.

Improved fit to ozonesondes in ASSIM in stratosphere and UTLS, less impact in lower troposphere.
Stratospheric ozone: Impact of assimilation

- Large improvements in stratosphere in ASSIM compared to CTRL relative to ACE and MIPAS data
- C-IFS provides good O3 analysis field despite simple stratospheric O3 parameterisation (similar to old coupled system used in MACC REAN)

S. Chabrillat
Tropospheric ozone: Impact of assimilation

- Improved fit of ASSIM to ozonesondes in UT compared to CTRL
- Some improvement in ASSIM in MT during winter/spring.
- Not much impact in LT
- New data (IASI O3 profiles?) might help to improve tropospheric O3 analysis
Sulphur Dioxide assimilation

- In CAMS we only assimilate SO2 for volcanic eruptions
- Volcanic eruptions can have impact on aviation
- SO2 is often considered a proxy for volcanic ash
- Conversion of SO2 to sulphate is the cause for secondary aerosol formation in the plume
- Forecasting SO2 plumes is important
Use of GOME-2 data for SO2 plume forecasts for 2011 Grímsvötn and 2010 Eyjafjallajökull eruptions

Two ways to forecast SO2 plumes:

- Estimate source strength and injection height and simulate transport with model ("CTM"-style)
- Assimilate initial SO2 fields (initial conditions) and model transport ("NWP"-style)

- Use GOME-2 data to estimate volcanic SO2 emissions and injection heights
- Assimilate GOME-2 SO2 data to provide initial conditions for SO2 forecasts
- Both methods allow NRT SO2 forecasts for volcanic eruptions

Flemming and Inness (2013, JGR)
Estimated plume strength and height information from satellite observations

1. Release test tracer ($E_{\text{test}} = 1$ t/s) at different levels - find best match in position

2. Scale emissions of test tracer and observations to get emission estimate

Plume top height obs from a synoptic radar at Keflavik airport (Petersen et al. 2012)
The initialization with GOME-2 SO2 analyses (INI and INIEMI) improved in particular the forecast of the Grímsvötn plume after the end of the eruption.

More in Flemming and Inness (2013, JGR)
GOME-2 SO2 assimilation: 23 April -8 June 2015

- GOME-2A and GOME-2B assimilated in CAMS e-suite
- Volcanic flags provided by DLR following the SACS (Support to Aviation Control) method
- CAMS assimilates all data that are flagged as volcanic
- Provides NRT 5-day SO2 forecasts (assumptions have to be made about injection height)
Credit: DWD

GFAS

CO profiles →

CO @ 500 hPa
Ceilometer, obs. & simul.

July 2013

CO assimilation

Credit: DWD
Concluding remarks

• Copernicus Atmospheric Monitoring Service (CAMS) provides analyses and 5-day forecasts of atmospheric compositions on regional and global scale in NRT

• Chemistry schemes have been included in ECMWF’s IFS to create the Composition-IFS

• Atmospheric composition variables have been included in ECMWF’s 4D-Var data assimilation scheme, e.g. O3, CO, NO2, SO2, HCHO

• Atmospheric composition retrievals are being assimilated

• 10-year reanalysis of atmospheric composition (2003-2012), see Inness et al. (2013, ACP)

• Data are freely available from:
  
  http://www.copernicus-atmosphere.eu

• For questions contact:
  
  info@copernicus-atmosphere.eu