Regional Scale Air Quality Modelling
Evaluation & Applications

Stephan Henne, Dominik Brunner

- COSMO-ART model system
- Validation
  - Gaseous air pollutants
  - Aerosol chemical composition
  - AQMEII-2 model comparison
- Applications
  - Operational Air Quality Forecasts
  - Nitrate aerosol trends
  - Wildfires
  - Dust
  - Volcanic ash
  - Pollen

COSMO-ART Model System

Online coupled chemistry-meteorology

Gas phase chemistry

RADMK
chemistry scheme

PAPA
online photolysis rates

Online emissions

Biogenic VOCs
Vogel et al., 1995

Sea salt
Lundgren et al., 2006

Dust
Vogel et al., 2006

Pollen
Zink et al., 2014

Data preprocessor

INTLM-ART
preprocessor

Meteorology

COSMO

Inputs

Meteorol. IC/BC
ECMWF

Chemical IC/BC
MOZART, IFS-MOZART

Anthr. emissions
TNO/MACC

Cloud processes

SCAV
cloud & rain chemistry
and wet scavenging

Aerosols

MADEsoot
6 modes, soot ageing

SIA
ISORROPIA-2

SOA
VBS or SORGAM

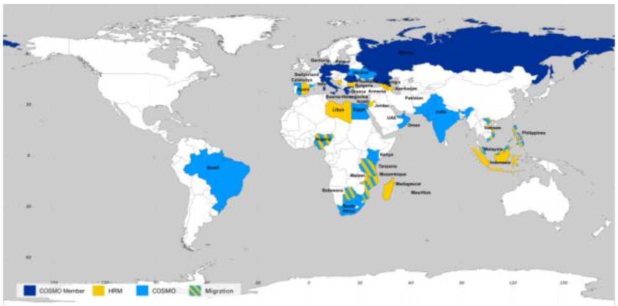
Dry deposition

Wesely
resistance approach

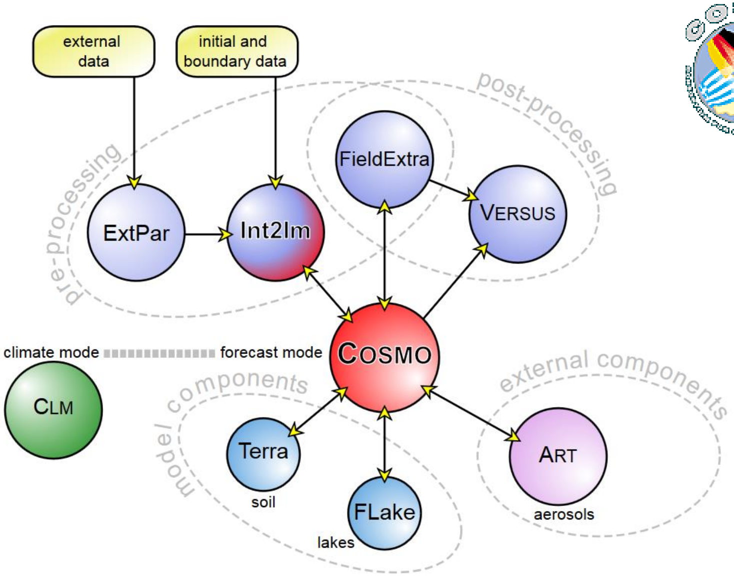
COSMO NWP

http://www.cosmo-model.org

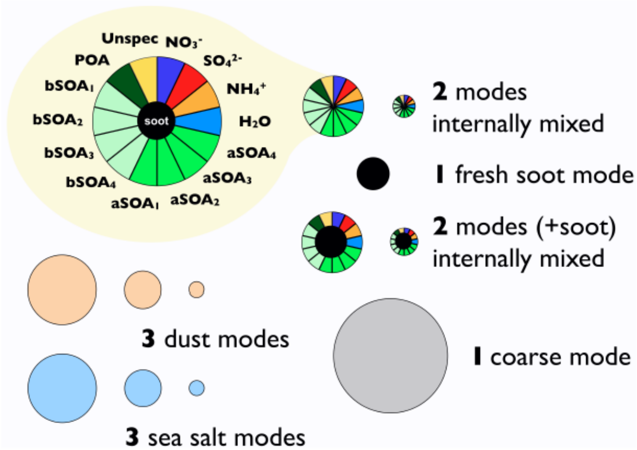
- Non-hydrostatic numerical weather prediction model
- Developed by several national weather services
- Main developmer: German Weather Service (DWD)
- Large scientific user commuity also using COSMO-CLM, COSMO-ART



COSMO Model System Components



Aerosol Representation in COSMO-ART / MADEsoot

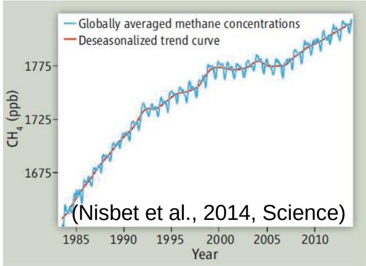


(Vogel et al. 2009, ACP,
Knote et al., 2012, PhD thesis)

Model Evaluation Versus Observations and Model Inter-Comparisons

Data without models are chaos,
but models without data are fantasy

- Patrick Crill, University of Stockholm

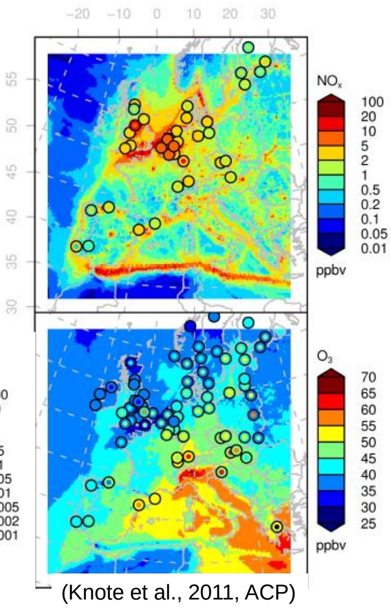


- Provide estimate of associated model uncertainties
- Identify possible weaknesses of model

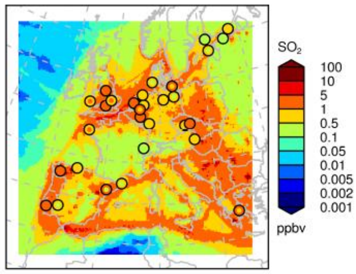
- Confirm adequacy of modelling approach for use in policy driven applications

COSMO-ART Evaluation: Gases

- Focus on periods with continuous observations (AMS) of chemical composition of aerosols (EUCAARI, EUSAAR, EMEP)
- 2 week periods in all seasons
- Spatial variability of O_3 and NO_x captured well, but small O_3 underestimation
- SO_2 generally underestimated (no aqueous chemistry used)



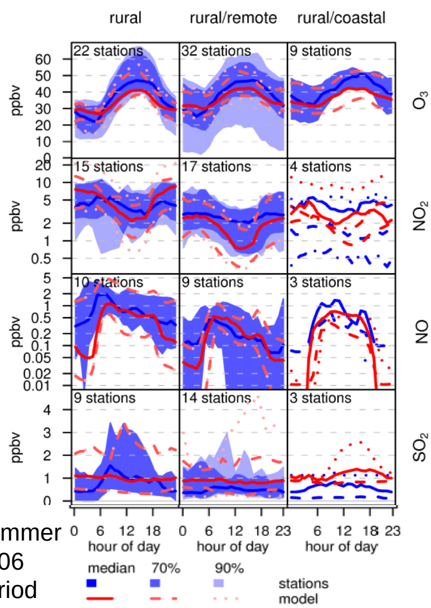
Summer
p.m. values
12-18 UTC
EMEP sites



(Knote et al., 2011, ACP)

COSMO-ART Evaluation: Diurnal Variability

- Good reproduction of O3 diurnal cycle, but indication of slight underprediction of amplitude
- Generally reproduced NO_2 and NO cycle
- Nocturnal NO_2 overestimated at rural sites (resolution issue)
- NO underestimated at night (resolution issue)
- SO_2 overestimated especially at remote and coastal sites (no aqueous chemistry)



Summer
2006
period

(Knote et al., 2011, ACP)

COSMO-ART Evaluation: Satellite NO_2

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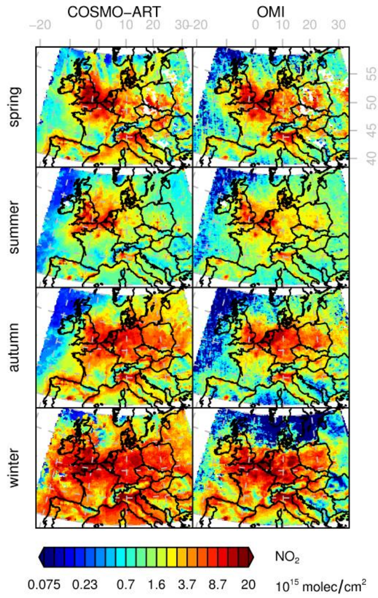
- Comparison with OMI NO_2 total vertical columns (EOMINO, Zhou et al. 2009,2010)
- Spatial variability and absolute amounts captured well during all seasons
- Tendency to overestimate in coastal regions



(Knote et al., 2011, ACP)

COSMO ART Evaluation: Aerosol Chemical Composition

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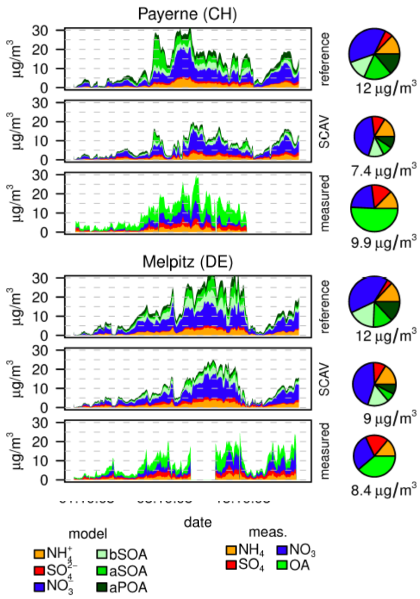
- Aerosol mass spectrometer (AMS) observations: non-refractory PM1 (< 1 μm, organics, SO_4, NH_3, NO_3)
- High temporal resolution
- Without aqueous chemistry SO_4 underestimated and NO_3 overestimated
- With aqueous chemistry comparison improved
- Underestimation of organic aerosol (mostly secondary) in summer (old SOA scheme)



(Knote et al., 2013, ACP)

AQMEII-2 Model Comparison

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Air Quality Model Evaluation International Initiative

Phase 2

- Focus on online coupled model systems
- 16 groups
- 8 different model systems
- 2 domains (Europe, North America)
- Same initial and boundary conditions
  - Chemistry: MACC-II reanalysis
  - Emissions: TNO and US EPA
  - Wildfire: FMI and Environment Canada
- Same model strategy (subsequent 48 h simulations)
- Full year simulations (2010)

AQMEII

http://ensemble2.jrc.ec.europa.eu/aqmeii/

EuMetChem
European Framework for Online Integrated Air Quality and Meteorology Modelling

cost

Supported by COST Action ES1004: European framework for online integrated air quality and meteorology modelling (EuMetChem)

AQMEII-2: Participating Models

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	Groups	Domain	Model	Grid spacing	First layer height (m)	Biogenic model	Gas phase	Photolysis
M1	AT1	EU	WRF-CHEM	23 km	24	MEGAN	RADM2 (Stockwell et al., 1990)	Fast-J (Wild
M2	CH1	EU	COSMO-ART	0.22°	20	Guenther et al., 1993	RADM2K (Vogel et al., 2009)	GRAALS + ST et al., 2009)
M3	DE3	EU	COSMO-MUSCAT	0.25°	20	Guenther et al., 1993	RACM-MIM2 (Karl et al., 2006)	Fast-J
M4	DE4	EU	WRF-CHEM	23 km	24	MEGAN	RADM2 modified (Forkel et al., 2015)	Fast-J
M5	ES1	EU	WRF-CHEM	23 km	24	MEGAN	RADM2	Fast-J
M6	ES2a	EU	NMMB-BSC-CTM	0.20°	45	MEGAN	CB05 (Yarwood et al., 2005)	Fast-J
M7	ES3	EU	WRF-CHEM	23 km	24	MEGAN	CBMZ (Zaveri and Peters, 1999)	Fast-J
M8	IT1	EU	WRF-CHEM	23 km	24	MEGAN	CBMZ	Fast-J
M9	IT2	EU	WRF-CHEM	23 km	24	MEGAN	RACM (Stockwell et al., 1997)	Fast-J
M10	NL2	EU	RACMO LOTOS-EUROS	0.5° × 0.25°	25	Beltman et al., 2013	CB-IV modified (Sauter et al., 2012)	Poppe et al.,
M11	SI1	EU	WRF-CHEM	23 km	25	MEGAN	RADM2	Fast-J
M12	UK4	EU	MetUM-UKCA RAQ	0.22°	20	TNO	UKCA RAQ (Savage et al., 2013)	Fast-J
M13	CA2f	NA	GEM-MACH	15 km	20.66	BEIS	ADOM-II (Lurmann et al., 1986)	Dave, 1972
M14	US6	NA	WRF-CMAQ	12 km	19	BEIS3.14	CB05-TU (Whitten et al., 2010; Sarwar et al., 2011)	Binkowski et
M15	US7	NA	WRF-CHEM	36 km	55–60	MEGAN	MOZART (Emmons et al., 2010; Knote et al., 2013)	fTUV (Tie et
M16	US8	NA	WRF-CHEM	36 km	38	MEGAN	CB05	fTUV

AQMEII-2: Evaluation With Surface Observations

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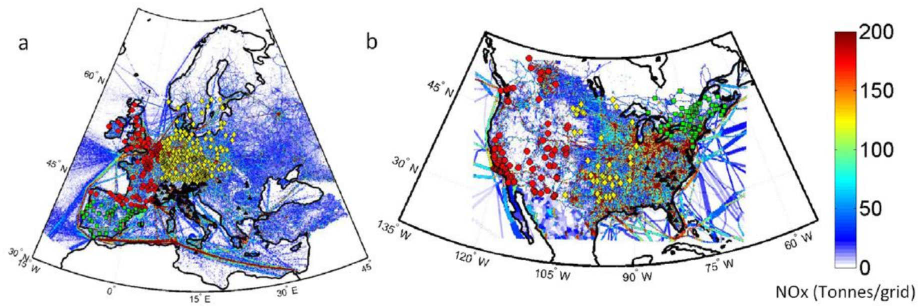

Annual NO_x emissions and surface sites

EU1: North-Western (102 sites)
EU2: Central North-Eastern (277 sites)
EU3: West Mediterranean (30 sites)
EU4: East Mediterranean (101 sites)

(Im, et al., 2015, Atmos. Env.)

AQMEII-2: Ozone Evaluation Europe

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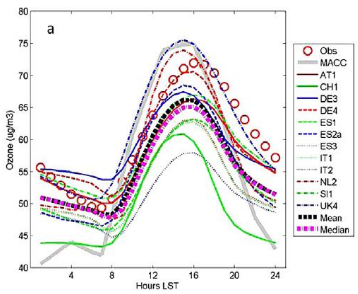
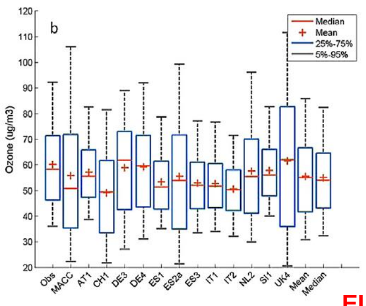
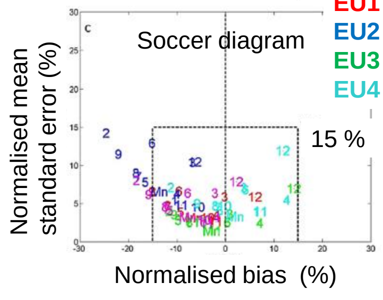




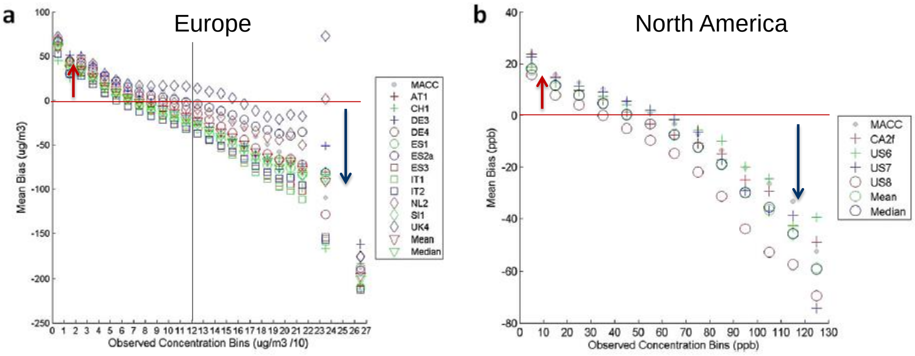
- High temporal correlation coefficients (r > 0.8)
- Dependence on chemistry set-up
- General overestimation in autumn and underestimation in winter
- Annual mean underestimated by about 18% over Europe
- Differences may stem from biogenic emission differences as well

(Im, et al., 2015, Atmos. Env.)



AQMEII-2: O_3 Bias by O_3 Level (max daily 8h mean), May - September

Mean bias from observations



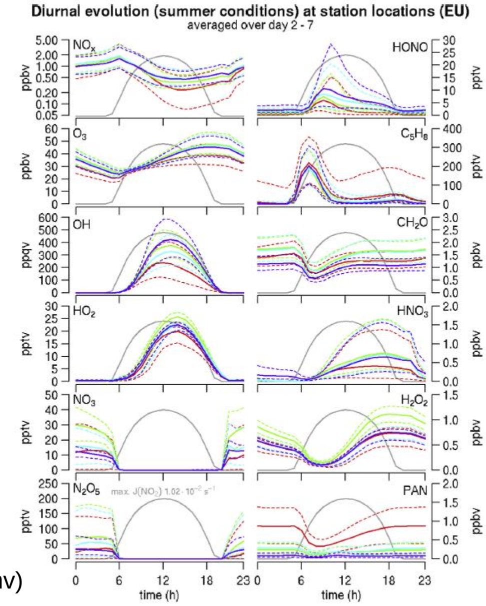
- All model underestimate levels above 120-140 $\mu g\ m^{-3}$
- "Models have a tendency to severely underpredict high O_3 levels that are of concern for air quality forecast and control policy applications"

(Im, et al., 2015, Atmos. Env.)

AQMEII-2: Chemistry Mechanism

- Boxmodel simulations at station locations to study effect of different chemical mechanisms
- Same meteorological conditions
- Same emissions
- Same numerical solver

- O_3 differs by 5 %, NO_x 25 %, isoprene > 100 %, HCHO 20 %
- Key radicals (OH and HO_2) differ by 40 / 25 %
- Differences due to VOC part of mechanism



(Knote et al., 2015, Atmos. Env)

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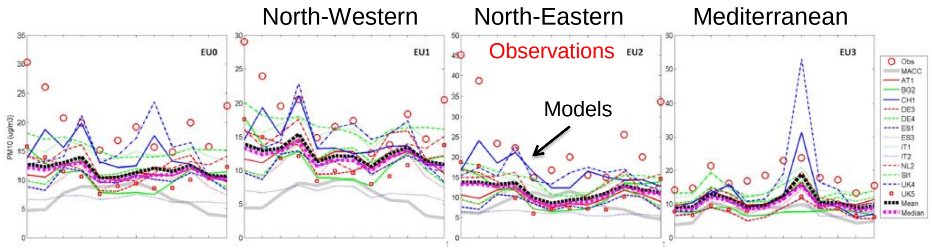
AQMEII-2: PM10 comparison



- Underestimation of PM10 in Mediterranean up to 66 % rural and 75 % for urban
- Due to natural dust emissions
- SO_4^{2-} underestimated
- NO_3^- overestimated
- "Still large challenges and uncertainties in simulating PM levels"

Monthly mean PM10 concentrations
Rural sites

(Im, et al., 2015, Atmos. Env.)

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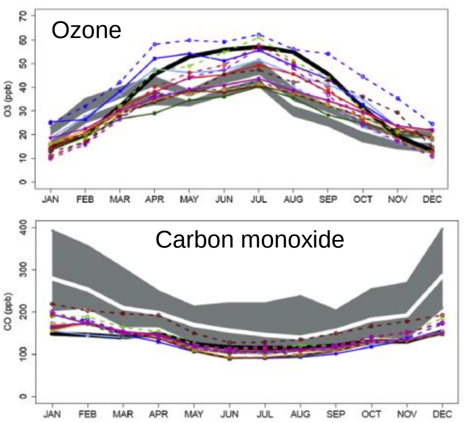
AQMEII-2: Boundary Conditions (BC)

- Regional scale model performance compared to model providing BC (MACC-II reanalysis)
- O_3 overestimation by MACC compensated by region scale models in spring/summer
- BC in winter determine O_3
- CO underestimation due to emissions
- BC have a profound impact on model performance



(Im, et al., 2015, Atmos. Env.)

Operational Air-Quality Forecasts: Copernicus Regional Air Quality (RAQ) Ensemble

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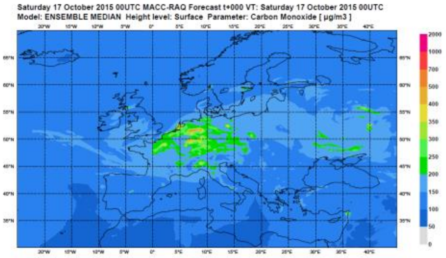
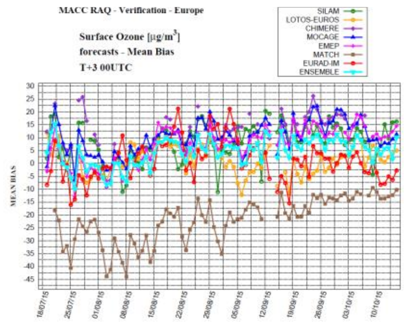
- 7 regional scale models
  - CHIMERE (INERIS, France)
  - EMEP (MET Norway, Norway)
  - EURAD-IM (University of Cologne, Germany)
  - LOTOS-EUROS (KNMI, Netherlands)
  - MATCH (SMHI, Sweden)
  - MOCAGE (Météo-France, France)
  - SILAM (FMI, Finland)
- Daily 4-day forecasts
- Analysed fields using data assimilation of surface obs.
- Model ensemble analysis
- Validation statistics
- http://macc-raq-op.meteo.fr/





Data Assimilation: Copernicus Regional Air Quality (RAQ) Ensemble

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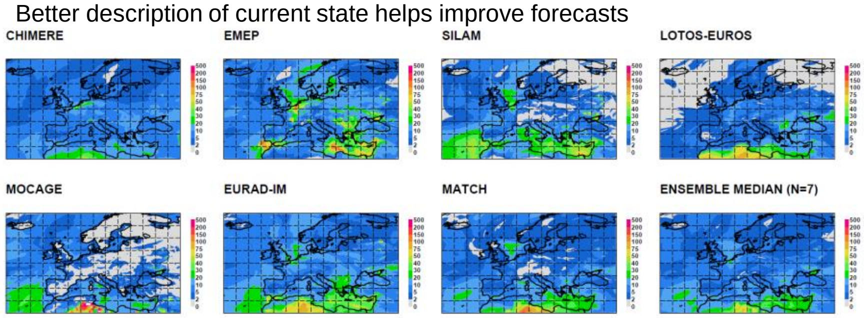
- Data assimilation: combine information from models and observations to generate a most probable representation (*analysis*) of the state of the atmosphere
- Accurate analysis of air pollution distribution helps improve health and ecosystem impact assessments
- Better description of current state helps improve forecasts

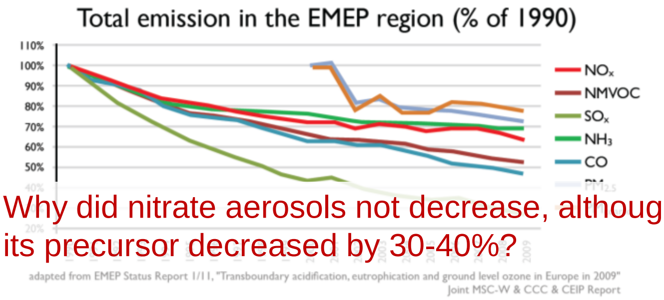


Usage of assimilation:

- Global model IFS-MOZART providing boundary conditions for regional models assimilates satellite observations of O_3, NO_2, CO, PM
- All models provide daily a-posteriori analyses by assimilating surface observartions of the previous day

Nitrate Aerosol Trends in Switzerland

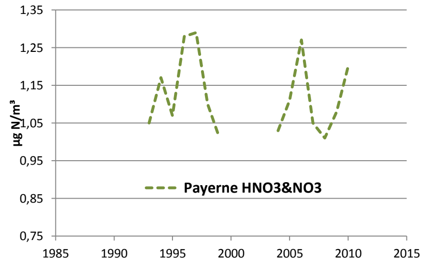
EMPA Materials Science & Technology



Why did nitrate aerosols not decrease, although its precursor decreased by 30-40%?

Species	Emissions	Immissions
SO_2	-70%	-85%
NO_x/NO_2	-45%	-40%
NMVOC	-70%	-65%
NH_3	-13%	≈ const
PM10	-28%	-40%

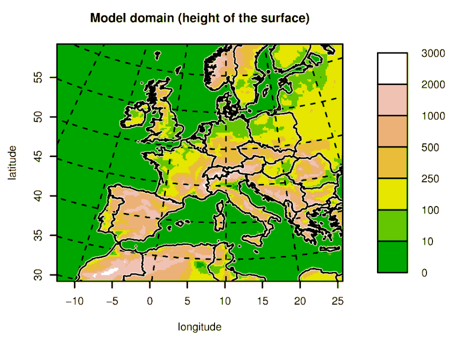
Trends Switzerland (Source: BAFU)



The COSMO-ART Model System

EMPA Materials Science & Technology

- Use of air quality model to simulate observed trends (qualitatively)
- 200 x 190 grid cells with 0.17°
- 40 vertical levels (terrain following)
- Simulation for long period computationally to expensive
- Simulation periods: January
  - 1995 emissions/2009 meteorology
  - 2009 emissions/2009 meteorology
- Use of same meteorology assures to see emission response only and not annual variable influence of meteorology



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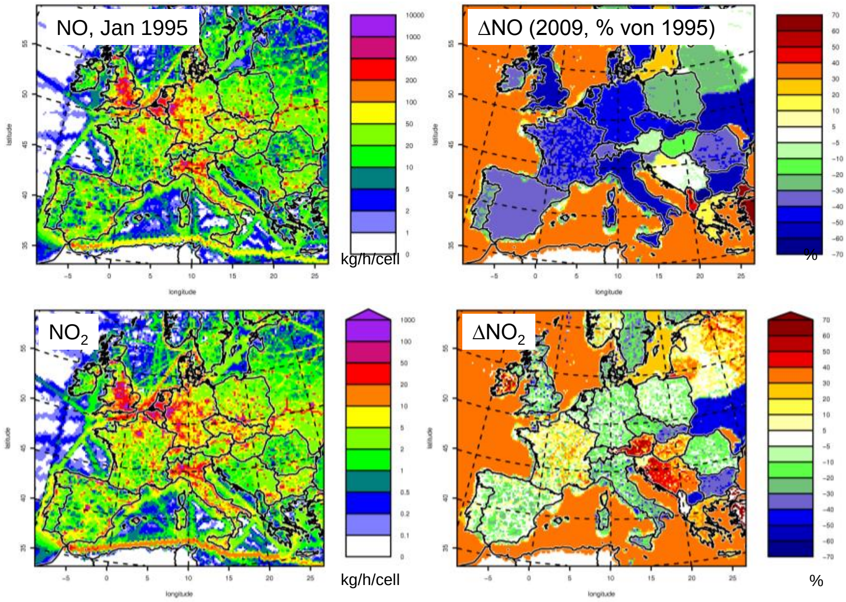
NO_x Emission Changes



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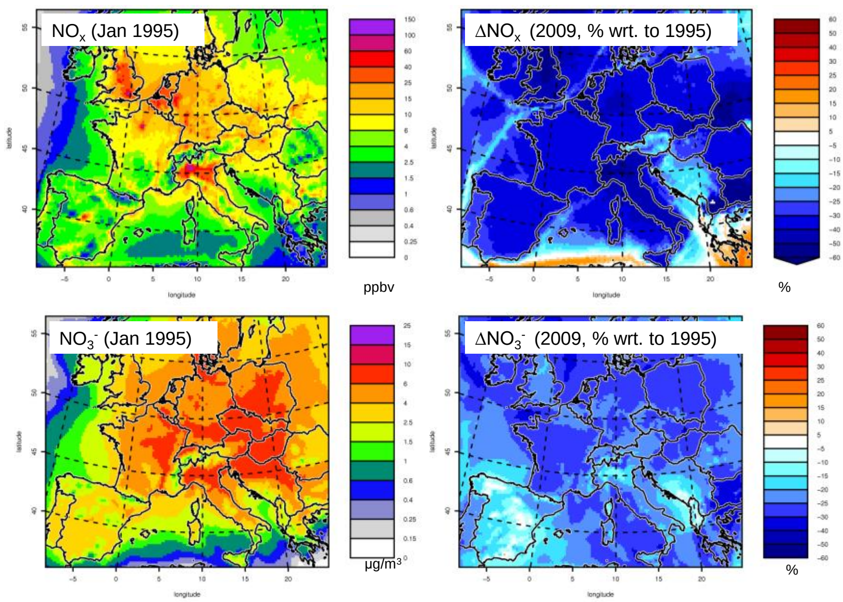
NO_x and Nitrate Reductions



Reasons for Smaller Nitrate Reduction

- In general, reduced nitrate reduction as compared to NO_x reproduced by the model.
- Main difference due to larger availability of surface ozone (less titration) and intensified night-time formation of HNO_3

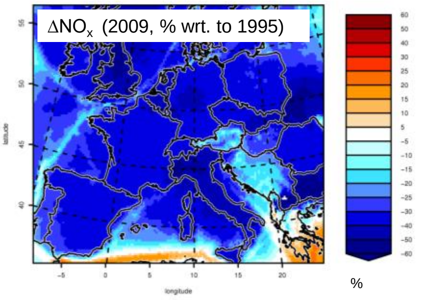
Gas phase

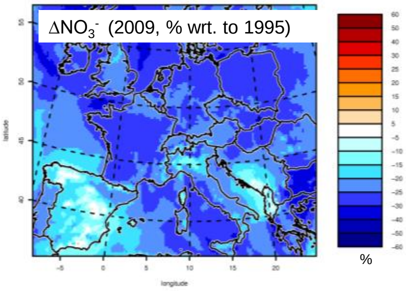
$NO + O_3 \rightarrow NO_2 + O_2$
$NO_2 + O_3 \rightarrow NO_3 + O_2$
$NO_2 + NO_3 + M \leftrightarrow N_2O_5 + M$

Aqueous phase

$N_2O_5(aq) + H_2O \rightarrow 2\ H^+ + 2\ NO_3^-$

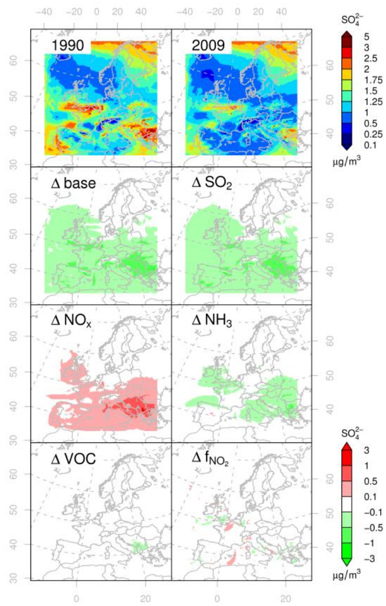
- NH_3 not limiting aerosol formation





NO_x Influences Sulphate Production

- Sulphate reduction when only reducing SO_2 emissions similar to reduction of all precursors
- More linear response as in the case of nitrate and NO_2
- When only reducing NO_x emissions sulphate production increases
- Increased in cloud sulphate production due to increased ozone



Russian Forest Fires 2010

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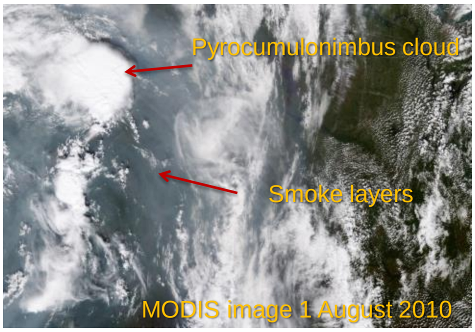
- June to September 2010, peak in early August
- Western Russia
- Heat wave and drought
- Peat and forest fires
- 56,000 premature deaths due to smog and heat
- Destroyed one third of Russia's wheat harvest



COSMO-ART: Aerosol Direct Radiation Effects During Russian Forest Fires 2010

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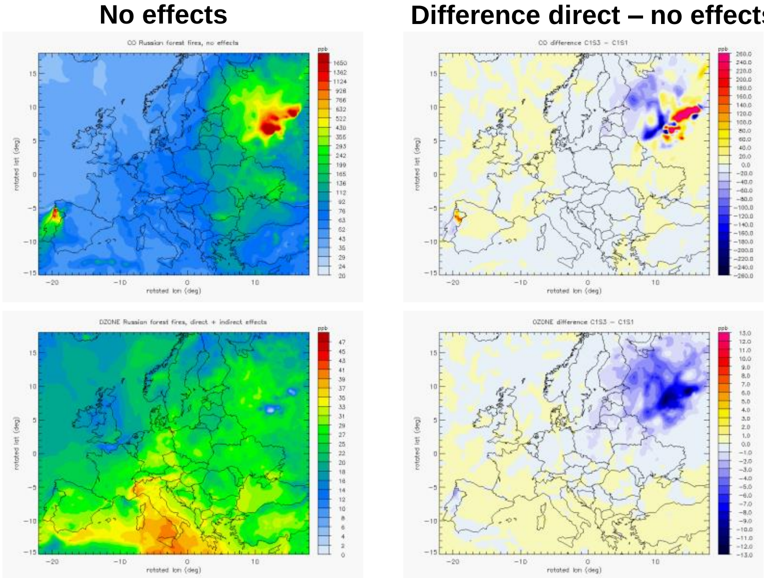
No effects | **Difference direct – no effects**

CO

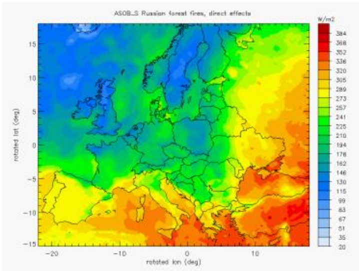
O_3

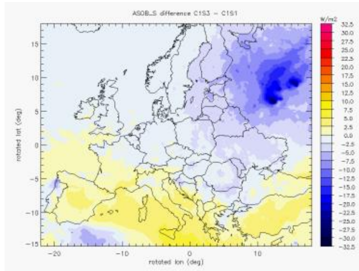


COSMO-ART: Aerosol Direct Radiation Effects During Russian Forest Fires 2010

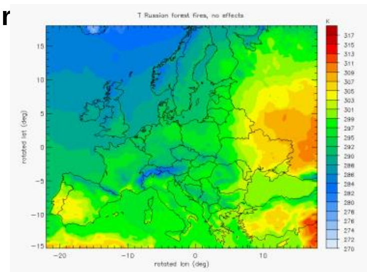
No effects | **Difference direct – no effects**

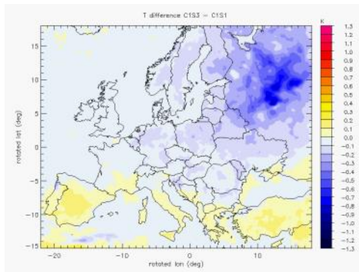
Net SW radiation





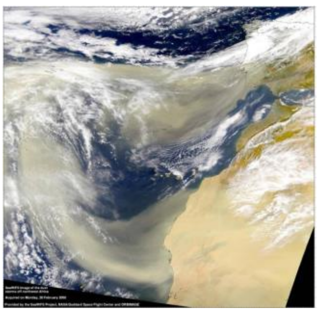
Temperatur

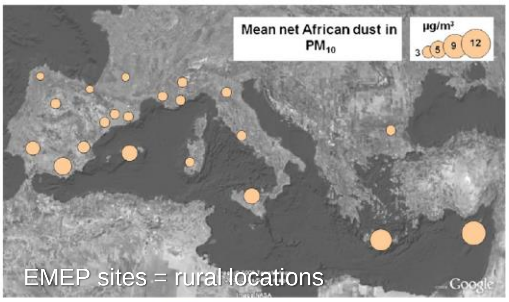


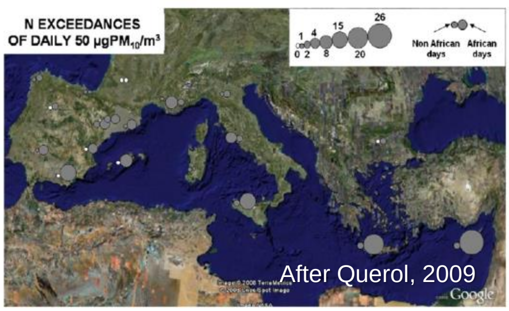


Importance of Saharan Dust

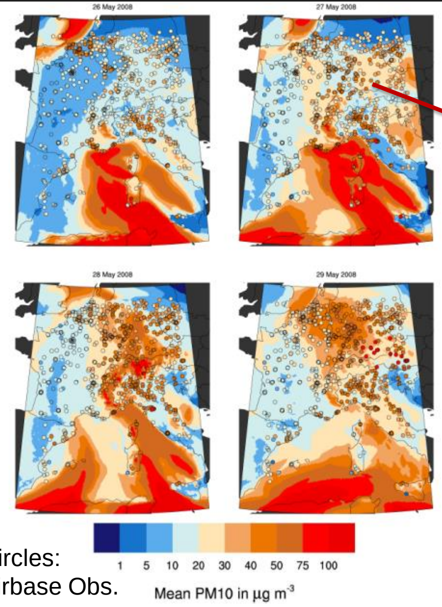
- Contributes significantly to PM concentrations in Mediterranean
- Most exceedances at rural sites caused by dust transport
- Health impact not completely understood



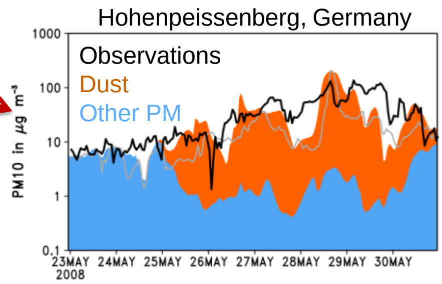




Validation of COSMO-ART During Dust Event



Circles:
Airbase Obs.



- Dust plume transport captured well (magnitude and location)

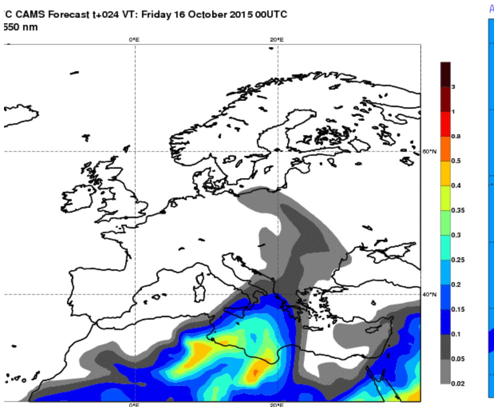
Cloud and radiation impact

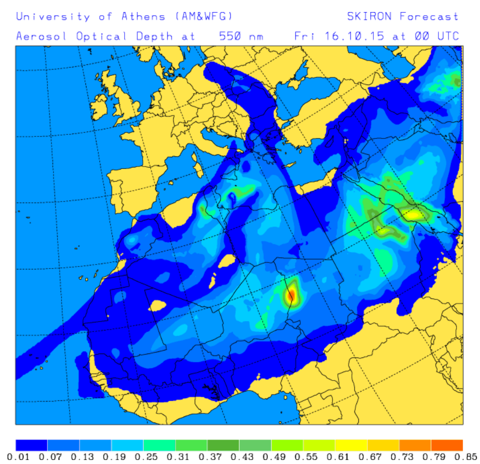
- Doubled number of ice crystals in mixed phase clouds
- Direct and indirect dust effect changed radiation budget
- Impact on surface temperature up to -1.0°C

(Bangert et al., 2012, ACP)

Operational Dust Forecasts

Dust aerosol optical depth: 2015-10-16 00 UTC





Copernicus
http://macc.copernicus-atmosphere.eu
IFS-MACC model (global)

University of Athens
http://forecast.uoa.gr/dustindx.php
SKIRON model

Volcanic Ash Transport

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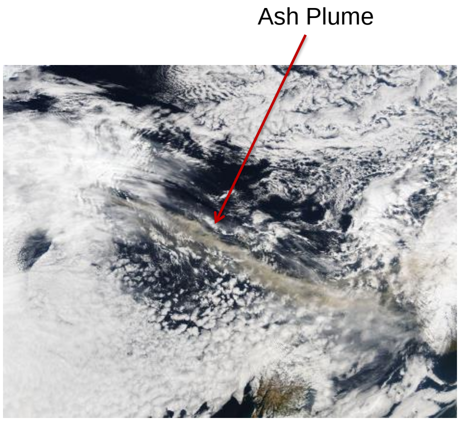
- Eyjafjalla eruption April/May 2010
- 8.3±4.2 Tg fine ash (2.8–28 μm) emitted
- European Air space closed for 10 days
- Estimated loss for airlines 1.7 billion US$



MODIS Aqua, 2010-04-15, 13:30

Volcanic Ash Transport with COSMO-ART

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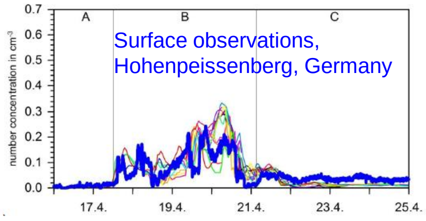
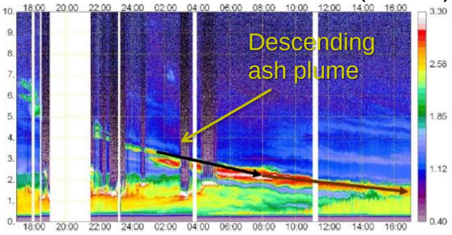
COSMO-ART

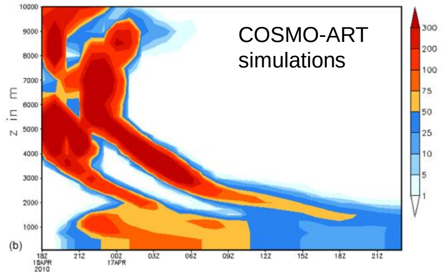
- Online chemistry transport simulations
- Detailed aerosol description (here 6 size bins)
- SO_2 conversion
- Interaction with meteorology

- Good model performance after ‘calibration’
- Required higher vertical model



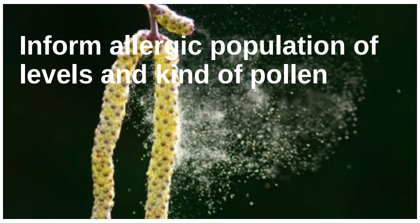
LIDAR backscatter observations (Munich)

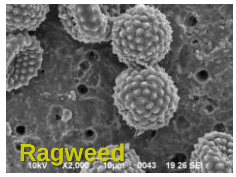




(Vogel et al., 2014, ACP)

Pollen Forecast





Traditional 'forecast'

- Based on pollen measurements, weather forecasts and empirical knowledge
- Low spatial resolution and representativeness
- No account for regional scale transport
- Daily reports

Chemistry transport model

- Explicit transport of pollen as passive aerosols

Pollen in Chemistry Transport Model

Distribution map

Locations and abundances of the pollinating plants.

Dispersion (NWP) model

Parameterization of pollen emission

Pollen emission

Biological and physical processes leading to the release and entrainment of pollen grains.

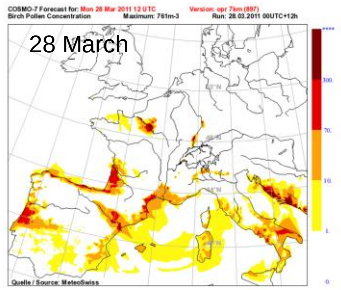
Balance equation for pollen

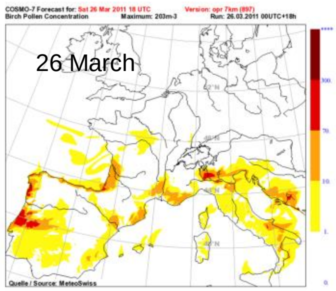
Pollen concentration

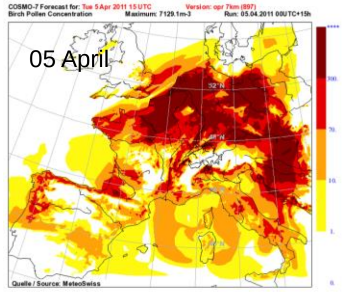
Transport with the mean wind, vertical turbulent diffusion, washout, sedimentation, source term.

Operational Pollen Forecast at MeteoSwiss

- Operational forecasts of birch, grass and ragweed pollen using COSMO-ART
- Birch pollen season 2011
- Resolution 7 km
- Advancement of the pollen season from south to north







(Pauling et al., 2012;
Zink et al., 2013, GMD)

Summary

- Validation
  - Most regional scale air quality models tuned for O_3 simulations (very good correlation with observations, but underestimation of highest O_3 levels relevant for control policy
  - Differences between different chemical mechanisms are still large
  - Emissions and lateral boundary conditions can introduce large biases that regional scale models cannot compensate
  - PM10 differences between models and observations still large
  - Simulation of chemical composition of aerosols depends on realistic simulation of aqueous phase chemistry
- Versatile application to large fields of air quality questions
  - Forecast and impact assessment
  - Nitrate aerosol reductions hampered by increased night-time oxidation
  - Large pollution events (e.g. wildfires, volcanic eruptions, dust) may impact meteorology
  - Detailed and speciated pollen forecast requires understanding of emissions