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JÜLICH
FORSCHUNGSZENTRUM

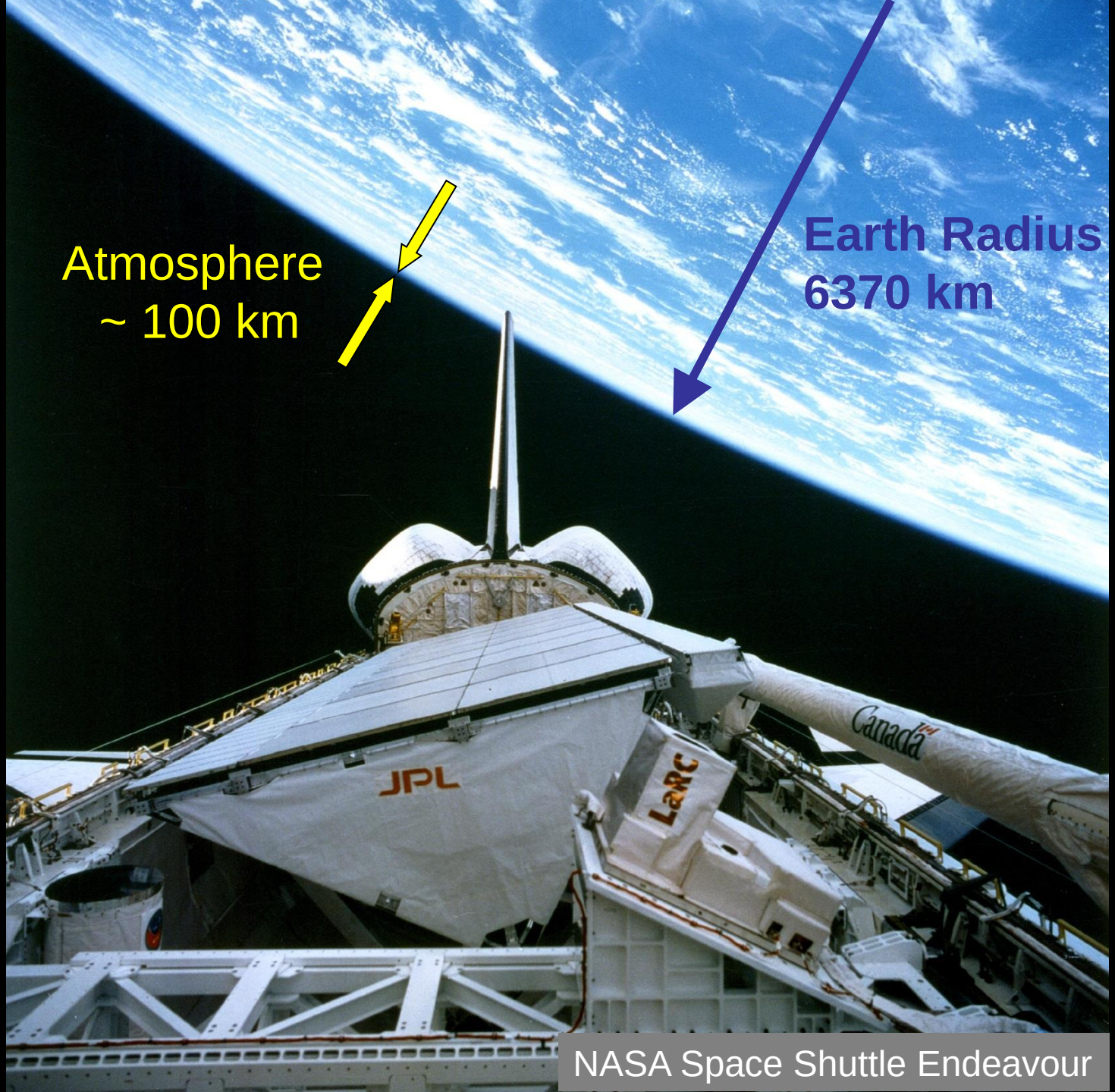
# Institute for Energy und Climate Research : Troposphere (IEK-8)

Prof. Dr. Dr. h.c. Andreas Wahner

Prof. Dr. Astrid Kiendler-Scharr

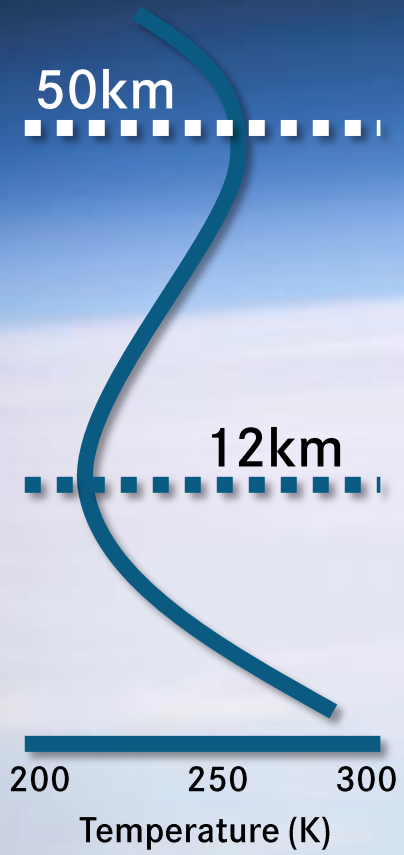
# The Atmosphere

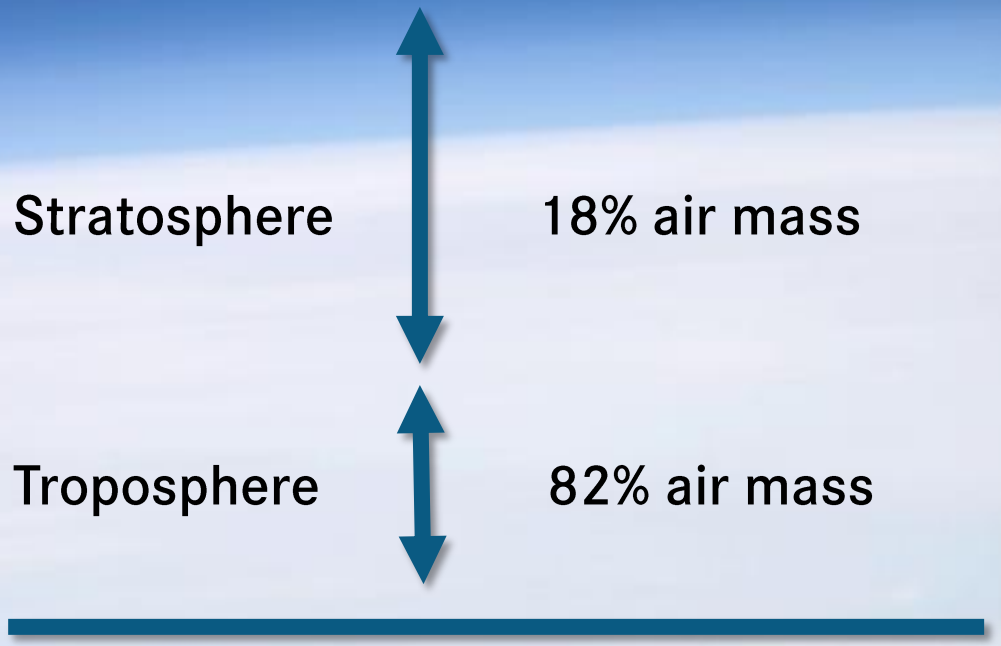

NASA




NASA Space Shuttle Endeavour

# The Atmosphere

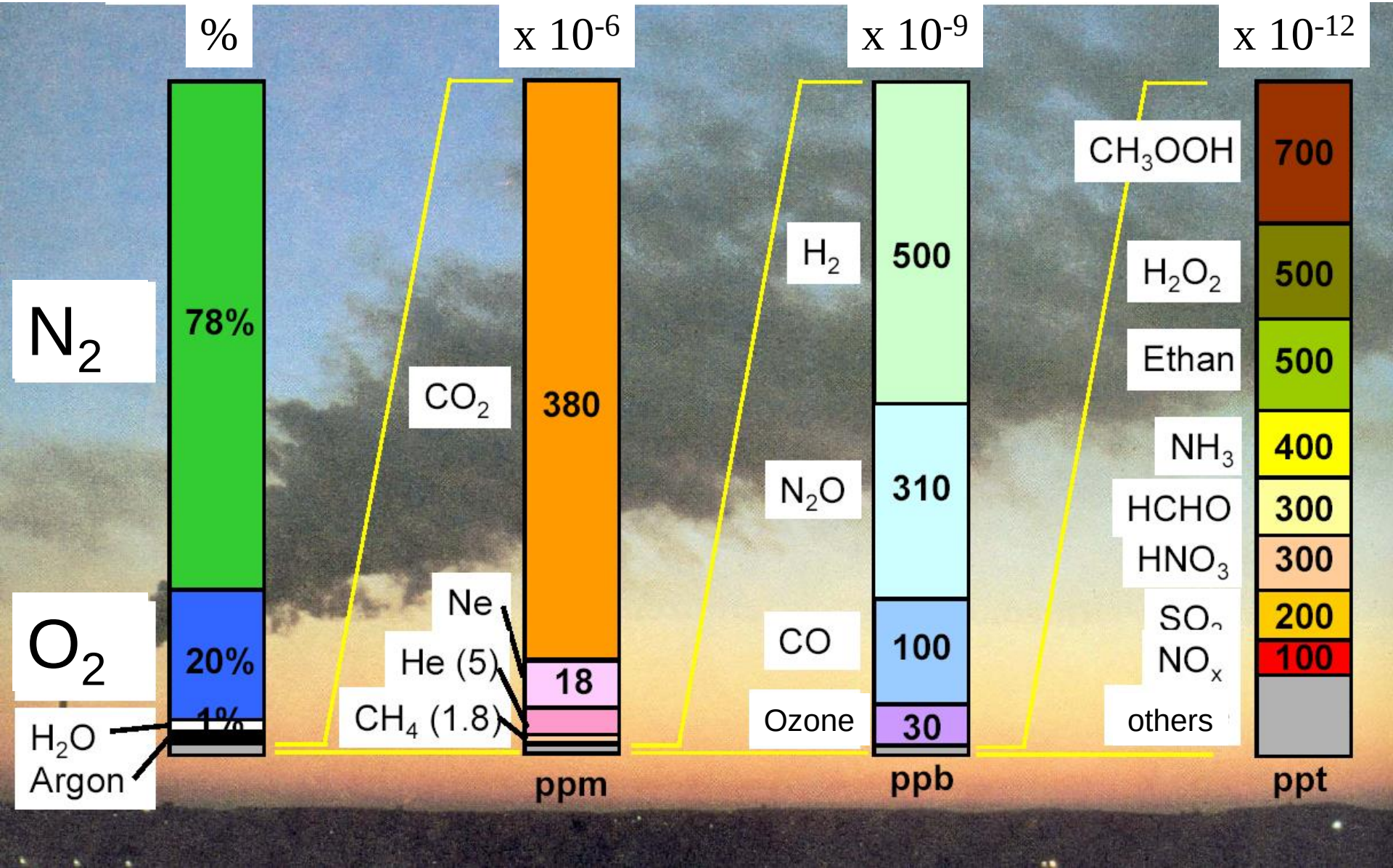


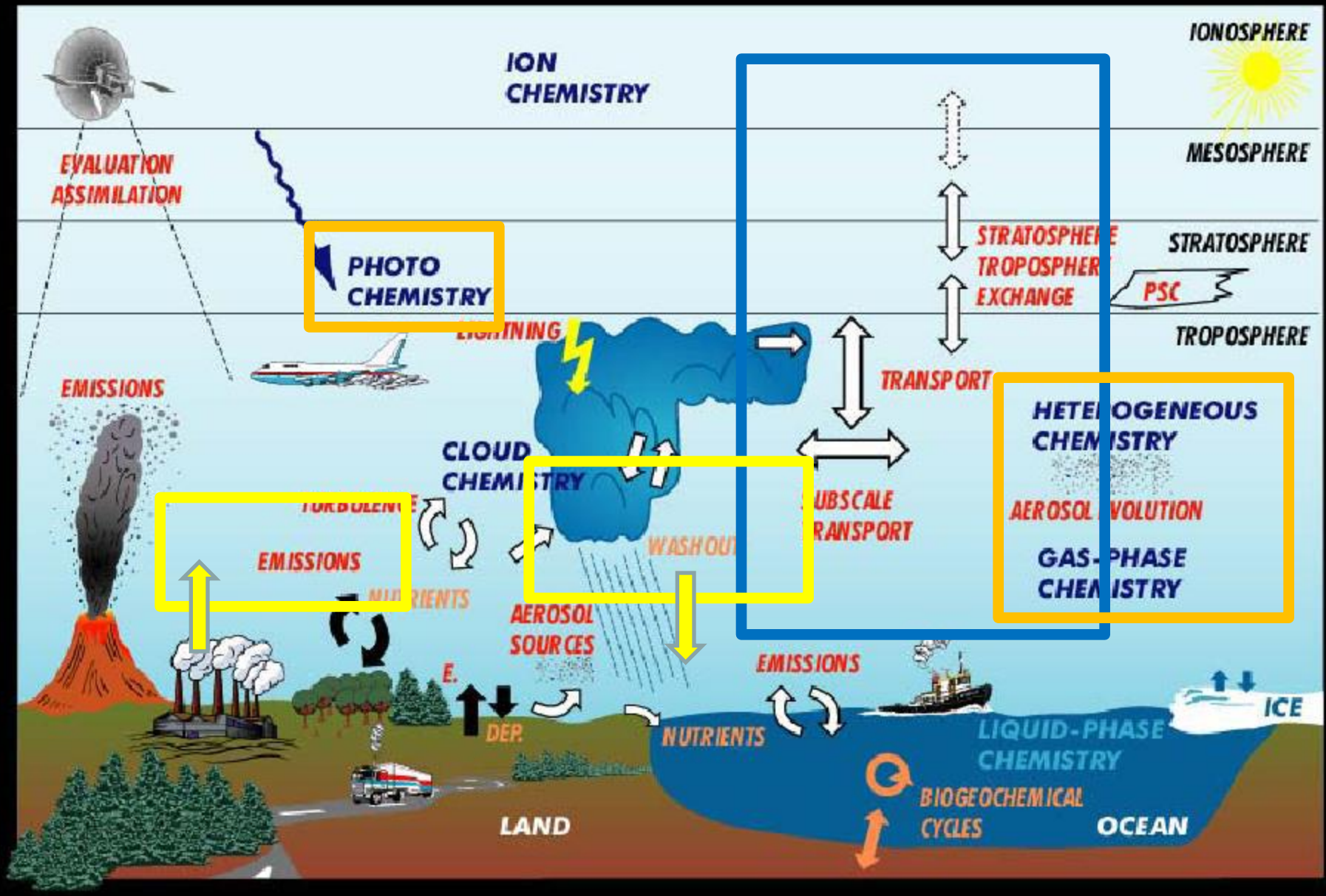

Composition: $N_2$ (78%), $O_2$ (20%), Ar (1%), $H_2O$ (~1%)

trace gases (< 0.05 %)

# Gas Phase Composition of the Atmosphere



# Atmospheric Chemistry and Dynamics



# Oxidative Chemistry

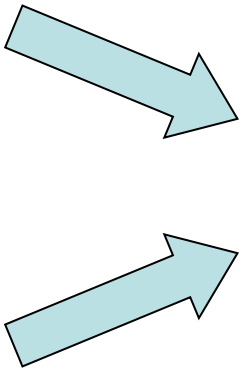
$OH$, $HO_2$, $NO_3$, $O_3$, $XO$

- **Atmospheric Self-Cleaning**

  Oxidative removal of trace gases
  ($CH_4$, HCFCs, VOCs, CO, $SO_2$, $NO_x$)

- **Chemical Transformation**

  Formation of secondary pollutants,
  gaseous + particulate phase
  ($O_3$, $H_2O_2$, $HNO_3$, $H_2SO_4$, OVOCs, SOA)



**Air Quality + Climate Impact**

| | |
|---|---|
| VOC | volatile organic compounds |
| OVOC | oxygenated VOC |
| SOA | secondary organic aerosol |

# Atmospheric Trace Gas Degradation by Oxidation

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| Trace Gas | Global Emission (Million Ton per year) | Degradation by OH-radikals |
|---|---|---|
| CO | 2800 | 85 % |
| Methan | 530 | 90 % |
| Alkane | 20 | 90 % |
| Isoprene | 570 | 90 % |
| Terpene | 140 | 50 % |
| $NO_2$ | 150 | 50 % |
| $SO_2$ | 300 | 30 % |
| $(CH_3)_2S$ | 30 | 90 % |
| $CFCl_3$ | 0,3 | 0 % |

# Self Cleaning of the Atmosphere

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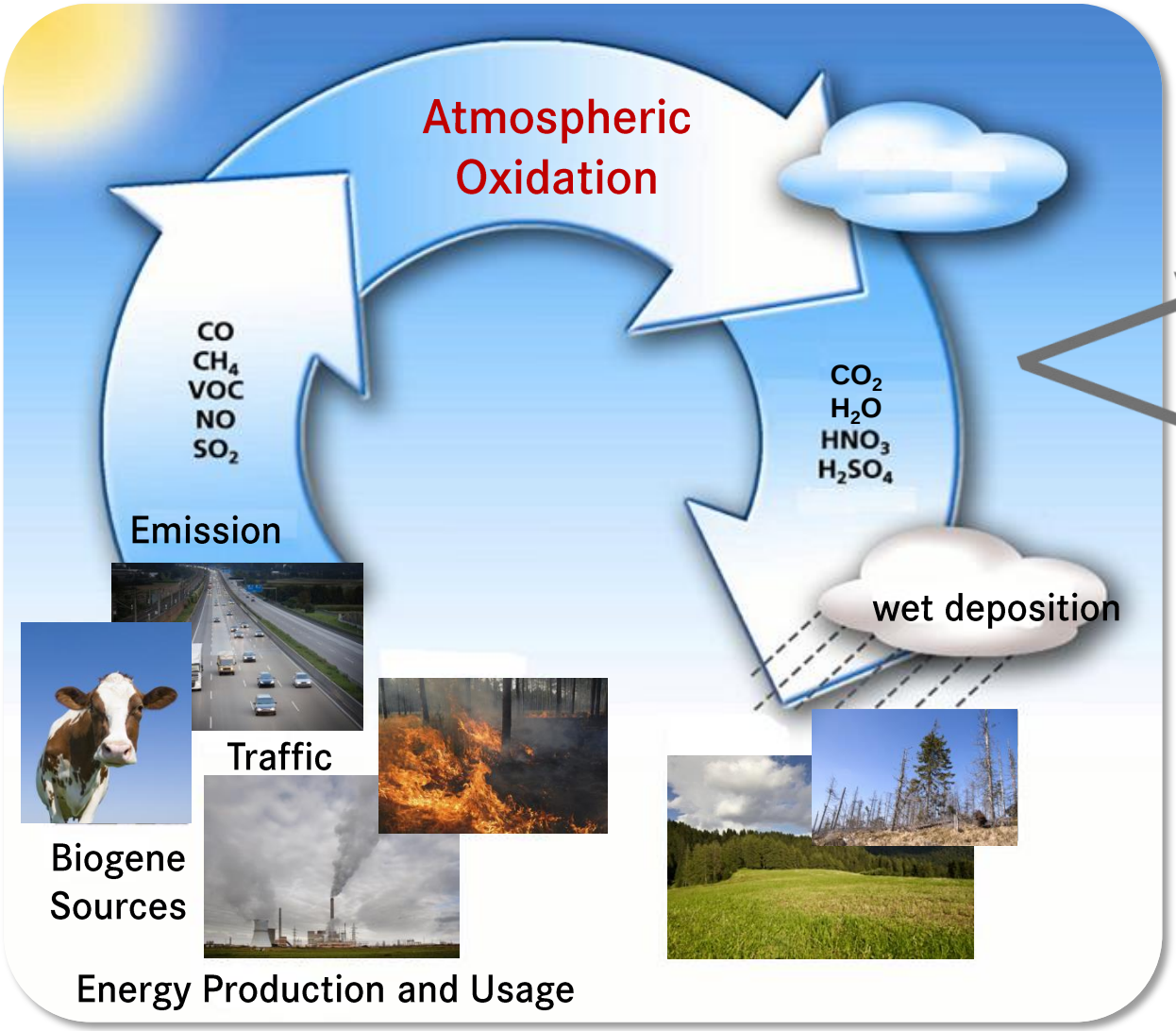
## Health & Climate





# Institute IEK-8: Troposphere

## Chemistry-Climate-Interaction

### Time scales:

**Chemistry – Climate - Interaction**

| days, regional to local | decades, global to regional | centennial, global to regional |
|---|---|---|

**Air Quality** — **long-term Climate Change**

**Ozone, Aerosol, Clouds, Methane, …** — **… Carbon dioxide**

**Energy production and usage lead to emissions**

→ **integrative analysis of the processes between biosphere, troposphere, and stratosphere**

→ **to understand the impact of current and future energy production and usage on atmospheric chemistry and dynamic**

# Institute IEK-8: Troposphere

**observation > process understanding > simulation > societal options**

## unresolved questions

- *self-cleaning of the troposphere;*
- *interaction of biogenic and anthropogenic emissions;*
- *tropospheric ozone production;*
- *formation and aging of aerosol;*
- *night-time chemistry; …*

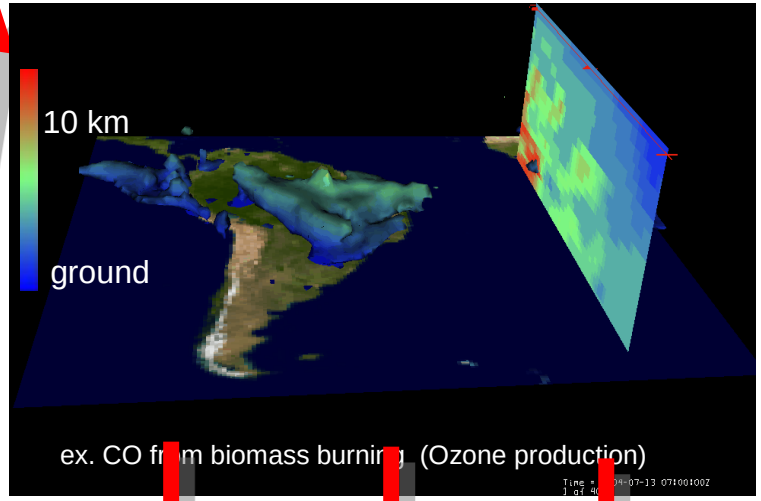
## observation and simulation

- *long-term tropospheric observations*
- *ground based airborne measurements (Zeppelin NT, drones, HALO,…);*
- *atmosphere simulation chamber SAPHIR*
- *plant chamber SAPHIR+ …*

## process understanding

*parameterization of chemical, dynamical and micro-physical processes*

## global and regional simulations and predictions




GEM-AQ

Group on Earth Observations

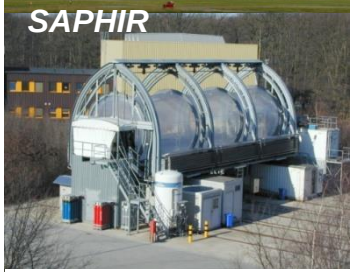
IPCC

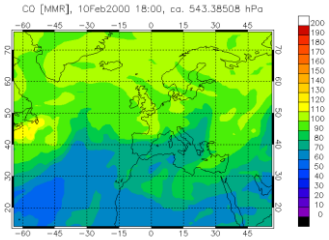
Copernicus Atmosphere Monitoring Service

# IEK-8 research foci

**Emission** ⟷ **atmospheric transformation** ⟷ **Air Quality Climate**






## Focus:

- **Long term observations of tropospheric composition change:** passenger aircraft as part of a global earth observation system
  → **European research infrastructure IAGOS AISBL**
- **Radical chemistry and atmospheric oxidation processes in the lower troposphere:** oxidation capacity and trace gas degradation
  → **Process understanding, Air Quality**
- **Gas to particle conversion, particle formation, and ageing:** quantifying of aerosol processes
  → **Anthroposphere – Biosphere – Atmosphere interaction, Air Quality**
- **Global and regional impacts of atmospheric processes on tropospheric composition and climate:** energy meteorology, operational chemical weather forecast, from science to service
  → **Copernicus Atmospheric Service, GEO, WMO, IPCC**

# In-service Aircraft for a Global Observing System

www.iagos.org

# European Research Infrastructure for Earth Observation using Passenger Aircraft

## Technical Goals

**Equipping 20 long-haul aircraft with scientific instruments for:**

- atmospheric chemical composition ($H_2O$, $O_3$, CO, $NO_x$, $NO_y$, $CO_2$, $CH_4$)
- aerosol and cloud particles

**Long-term deployment (20 years)**

**Global coverage**

**Open data policy (CAMS/GEO/GEOSS)**

**Near real time data provision**

**Deploy the CARIBIC Container**

Large number of species, including those above plus VOCs, CFCs, aerosol chem. composition, $H_2$ isotopes, $SO_2$

## Scientific Objectives

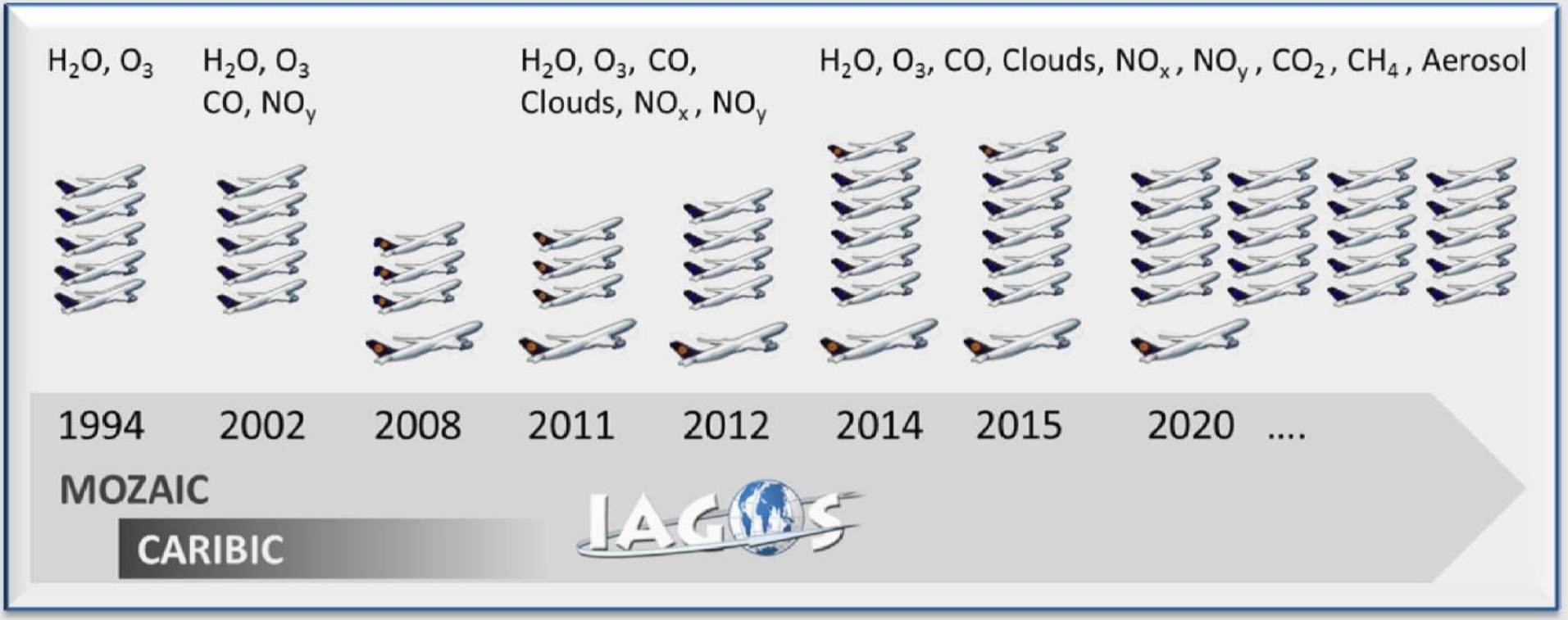
- **Changes in the Tropopause Region**
  - ozone background and trend
  - water vapour background and trend
- **Validation of Atmospheric Models and Satellite Retrievals**
  - tropospheric profiles of $H_2O$, $O_3$, CO, $CO_2$, $CH_4$, $NO_x$, aerosol
- **Global Air Quality**
  - influence of developing regions
  - long-range transport of air pollutants
  - biomass burning, climate change, ...
- **International Transfer Standards**
  - same systems deployed globally

# IN-SERVICE AIRCRAFT FOR A GLOBAL OBSERVING SYSTEM

Association Internationale sans but lucratif

www.iagos.org

## European Research Infrastructure for Earth Observation using Passenger Aircraft

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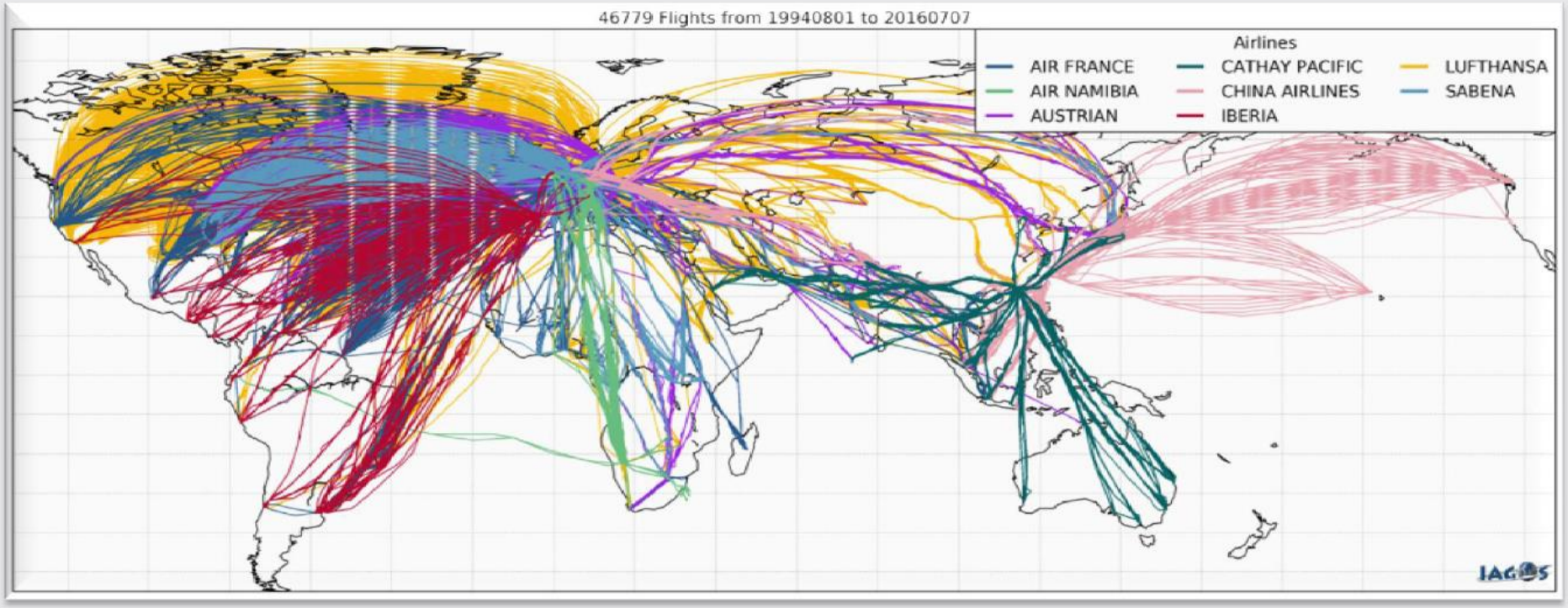
Lufthansa · AIRFRANCE · CHINA AIRLINES · CATHAY PACIFIC · IBERIA

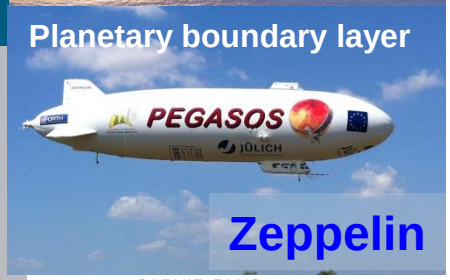
# European Research Infrastructure for Earth Observation using Passenger Aircraft

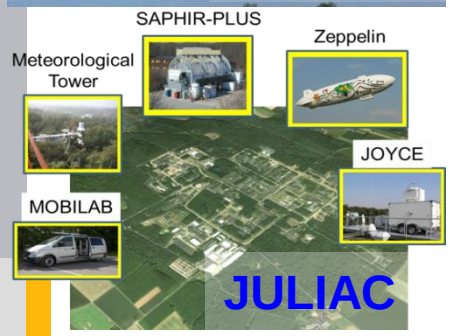



## IAGOS-CORE aircraft schedule:

- In 2016, 7 equipped aircraft in regular operation
- Approx. 500 flights per aircraft per year
- More than 200 airports worldwide visited regularly

# Radical chemistry and atmospheric oxidation processes in the lower troposphere



## Goals

- Atmospheric self-cleaning and air quality
- Experimental determination of entire radical budgets
- Nighttime radical chemistry
- Processes transforming gas phase to secondary organic aerosol

## Field studies ground and airborne

| | |
|---|---|
| Ground | Comprehensive, day / night, seasons (2016/2017); china winter (2015/16); |
| SAPHIR /SAPHIR+ | Aerosol formation and aging; internat. HOx-comp, OH-lifetime; |
| Lower Troposphere | Zeppelin based missions |
| Free Troposphere | HALO missions (OMO-EU (2015), OMO-ASIA (2015)) |

## Key techniques / developments

| | |
|---|---|
| OH, $HO_2$, $RO_2$ | LIF and DOAS |
| OH reactivity | Pump + probe technique |
| $NO_3$, $N_2O_5$ | Cavity ring down technique **(under develop.)** |
| mass-spec and specific sensors for use on drones | |
| Stable isotopes | Isotope-ratio mass spectrometry |

# Atmosphere Simulation Chamber SAPHIR


Volume 270 $m^3$
Double walls (Teflon foil)
Light source: solar radiation
1-min mixing time

## Instrumentation

| | |
|---|---|
| LIF | OH, $HO_2$, $RO_2$, $k_{OH}$ |
| DOAS | OH |
| GC-MS | VOCs |
| PTRMS | VOCs, Isoprene |
| | MVK+MACR ($H_3O^+$), |
| | MACR ($NO^+$ mode) |
| CLD | NO, $NO_2$, $O_3$ |
| RGA | CO |
| LOPAP | HONO |
| Hantzsch | HCHO |
| Radiometry | *j*-values |

# Gas to particle conversion, particle formation and ageing

**Impact**

**cloud formation**

**climate, air quality**

**Transformation**

**chemical ageing**

**atmospheric lifetime**

**multi component aerosols**

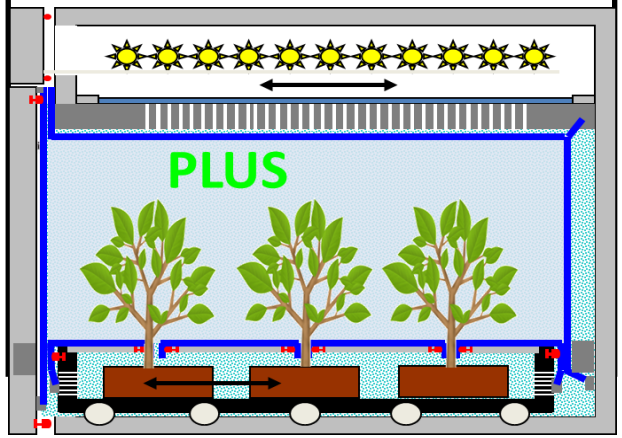
**Formation**

complex emissions

**particle formation potentials**

SAPHIR

SAPHIR+



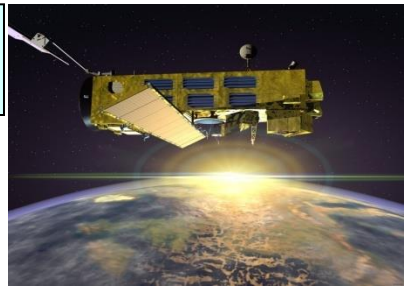

**Goals:**

- **New plant chamber SAPHIR+**
  - **real emissions**
  - **tropospheric radical chemistry**
- **particle suppression by BVOC → nucleation**
- **stress emitted BVOCs**
- **highly oxidized organic multifunctional molecules (HOM)**
- **anthropogenic emissions**

# Regional Air-Quality forecast by Data Assimilation

**Supporting international observing systems**

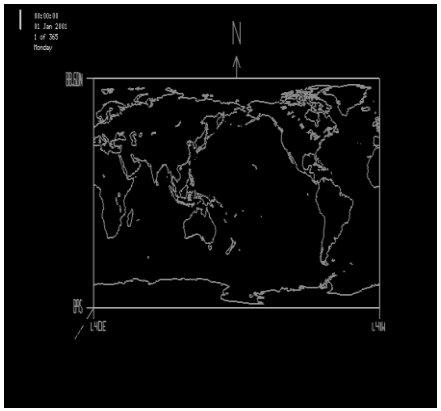
**Satelliten**
PREMIER



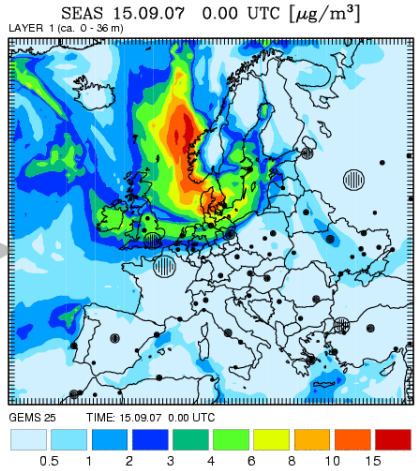
**Linienflugzeuge**
IAGOS-ERI

**Assimilieren**

**Globales Modell**
ECMWF / Jülich



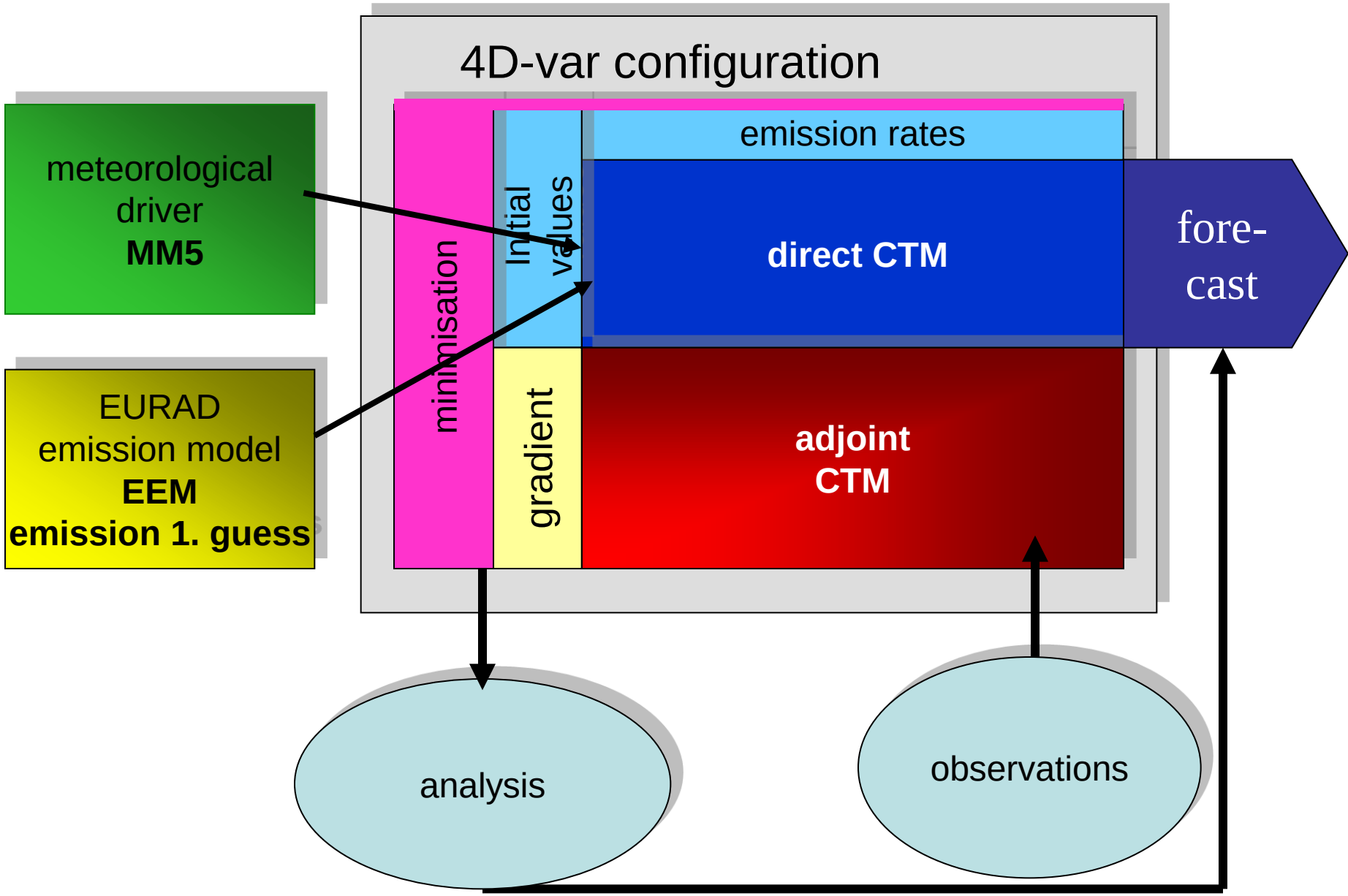
**Randbedingung**




**Regionales Modell**
EURAD

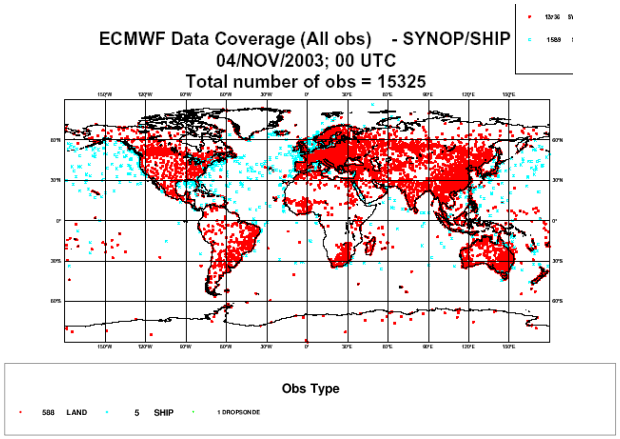
**Global Monitoring of Environment and Security (GMES)**
**GMES Atmospheric Service (GAS) [seit 2013]**

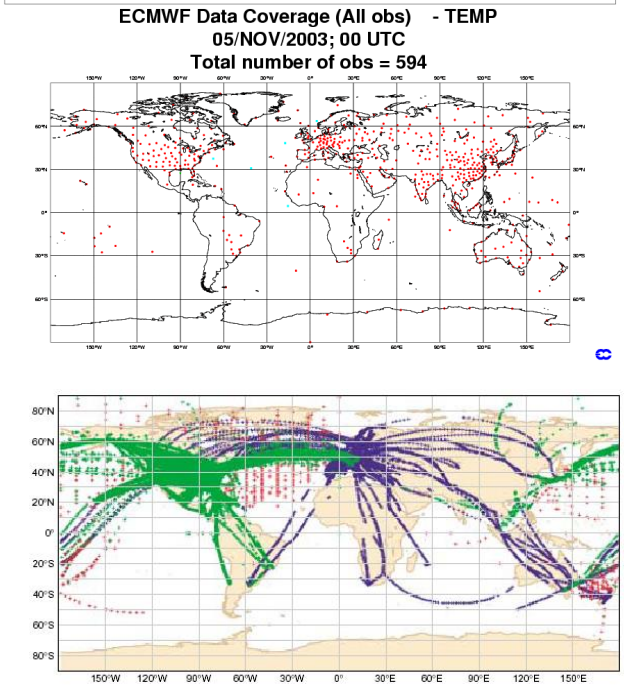
# Mesoscale EURAD 4D-var inverse modelling system



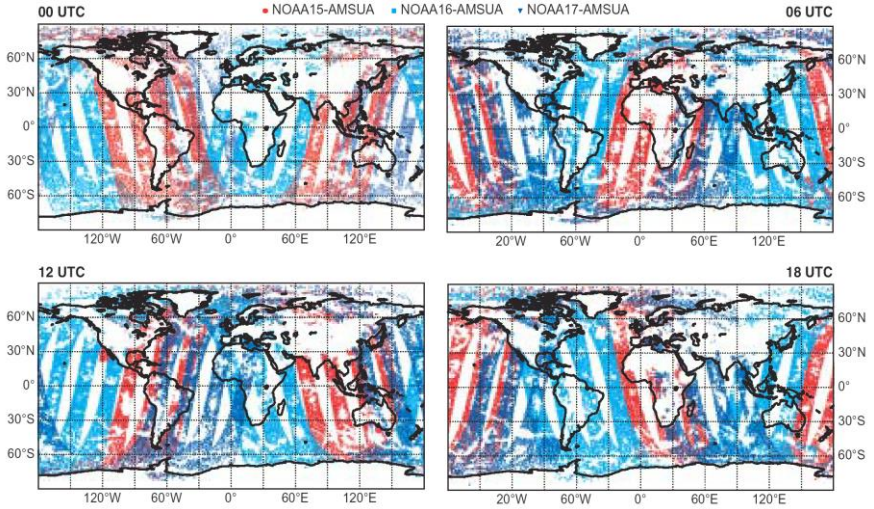
# Observation systems

## In-situ observations

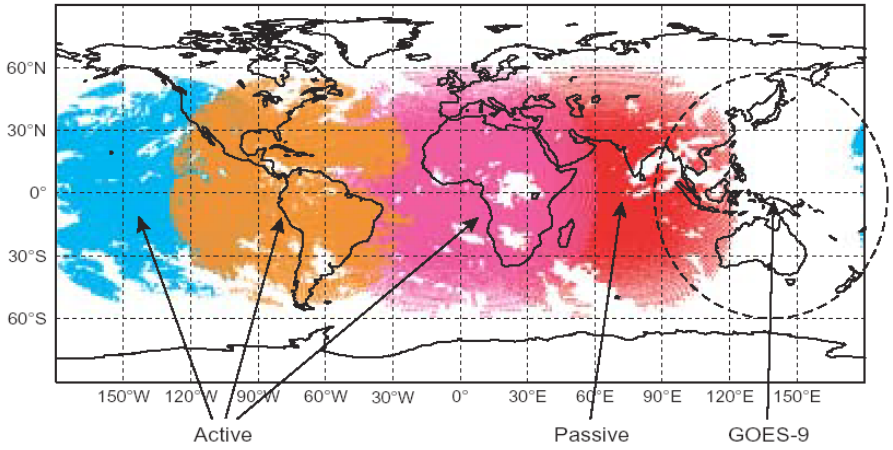


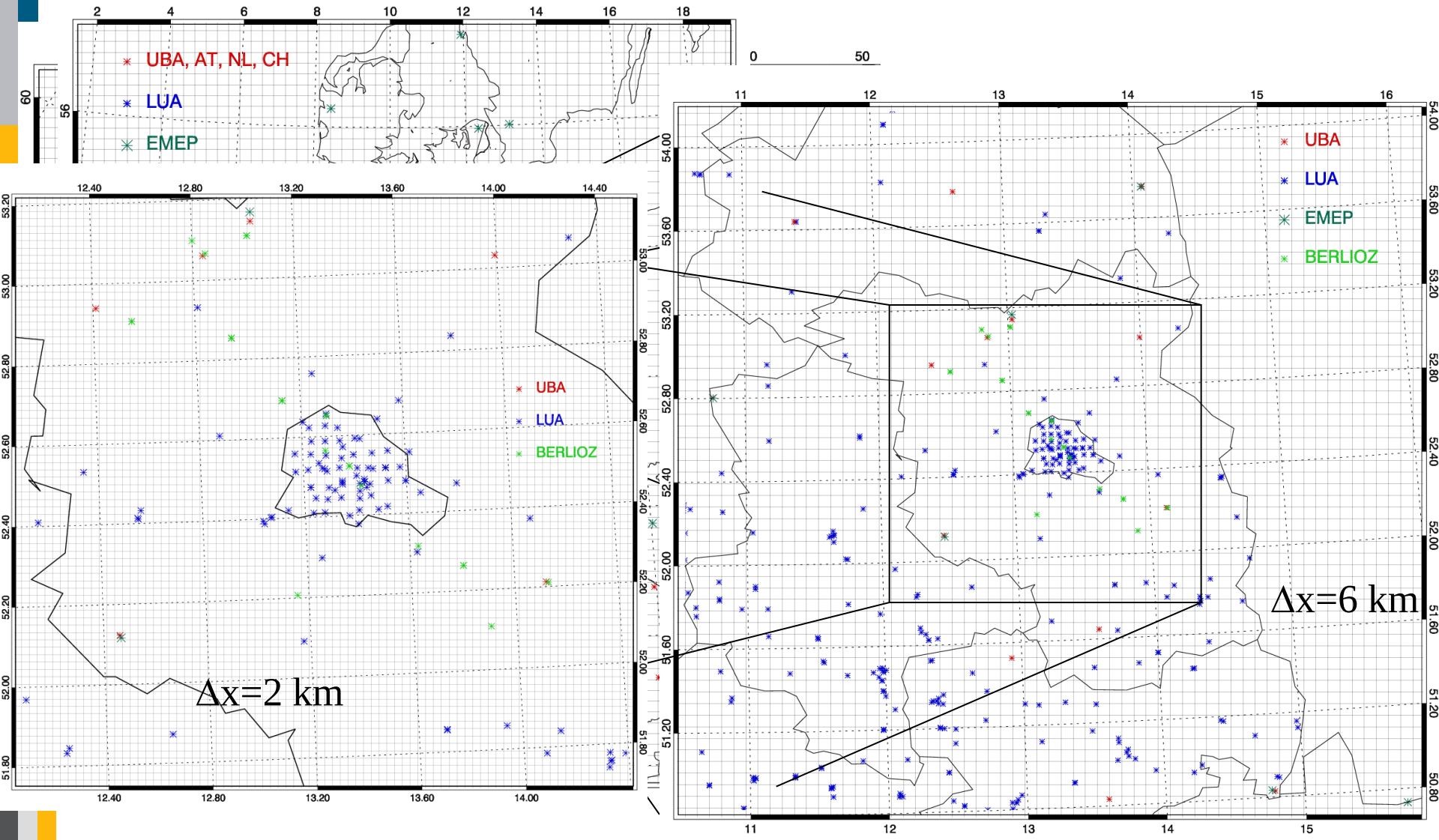

## polar orbiting satellites



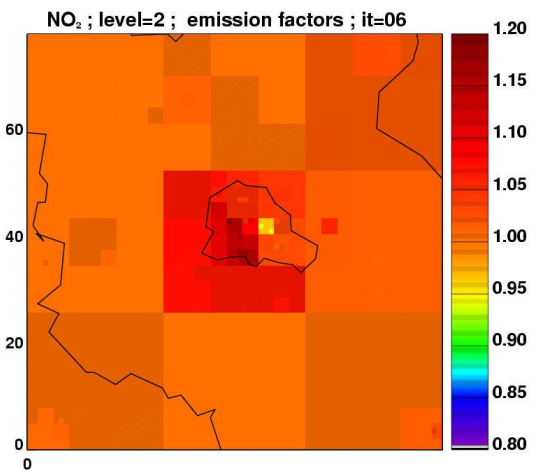

## geostationary satellites

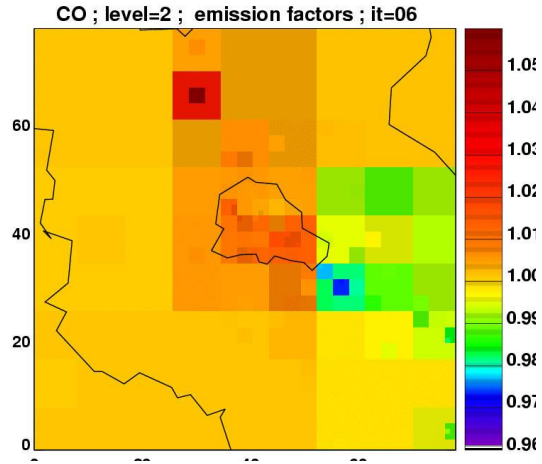


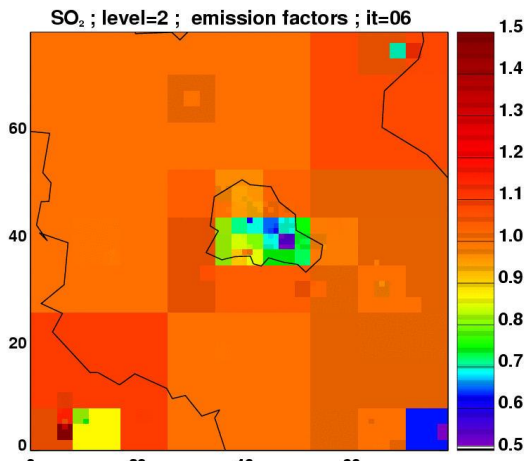
# Which is the requested resolution?
# BERLIOZ grid designs and observational sites



# Emission source estimates by inverse modelling
# Optimised emission factors

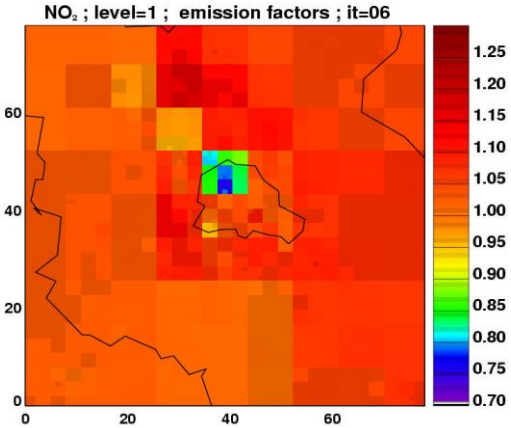


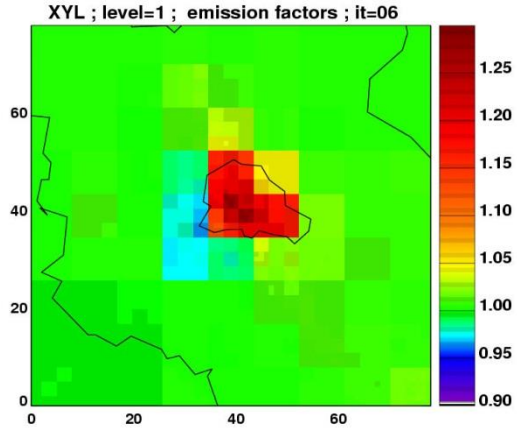



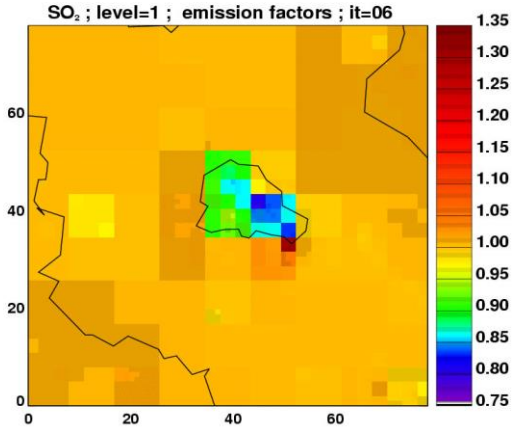




**$NO_2$** **xylene (bottom), CO (top)** **$SO_2$**

height layer ~32-~70m




surface

# Institute for Energy und Climate Research Troposphere (IEK-8)

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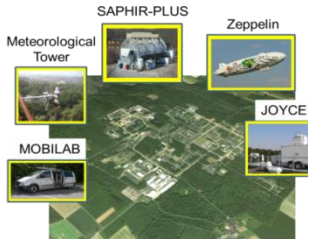
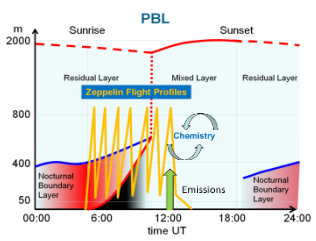
- Role of chemistry and physics in climate variability and change
- Interaction between air quality and climate change
- Leadership in international projects, coordination with universities and institutions
- Facilitating technology transfer

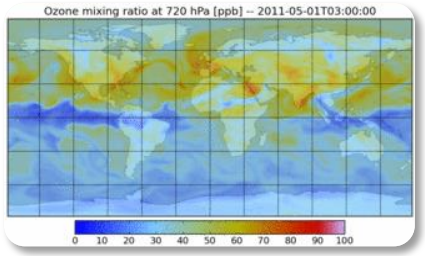
| Observation | Simulation / Prozess Understanding | Modell |
|---|---|---|

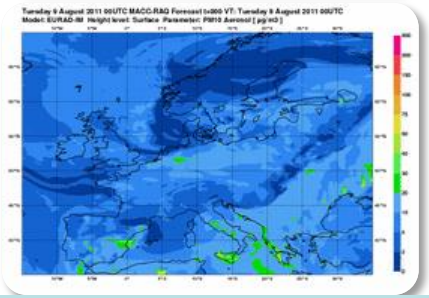








Innovation and scientific basis for societal and political decisions: energy options, mitigation- and adaption strategies


Thank you
by Glynn Gorick