Chapter 3

Measurements and Modeling of Air Pollution

Quiz

1. Causes of slowdown and resumption of CH_4 growth
2. Project the future changes in biomass burning emissions under human influences and climate change
3. Given the wind fields and NO_2 columns, estimate the lifetime of NOx
4. Given CO and/or NOx emissions, estimate emissions of other species such as CO_2 and N_2O
5. Causes of horizontal distribution in sulfur emissions from oceans
6. Why does deposition of N and S resemble their emissions

Measurements of Chemical Constituents

Studies of Earth system, including AQ, are based on measurements & modeling

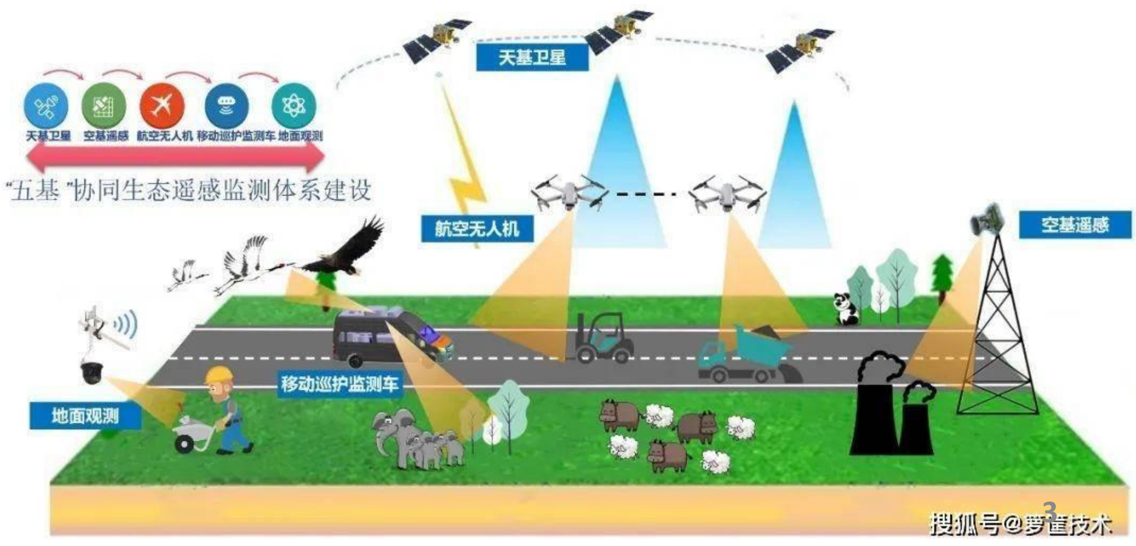
- **Ground, sounding, airborne, space borne**
- **Concentration, remote sensing**
- **Total, speciated**
- **Long-term, campaign**

➢ **Gaseous pollutants: Ozone, NOx, NMVOC, CO, NH_3, SO_2**

➢ **Aerosols: PM_{10}, $PM_{2.5}$, components, sizes, morphology, optical properties**

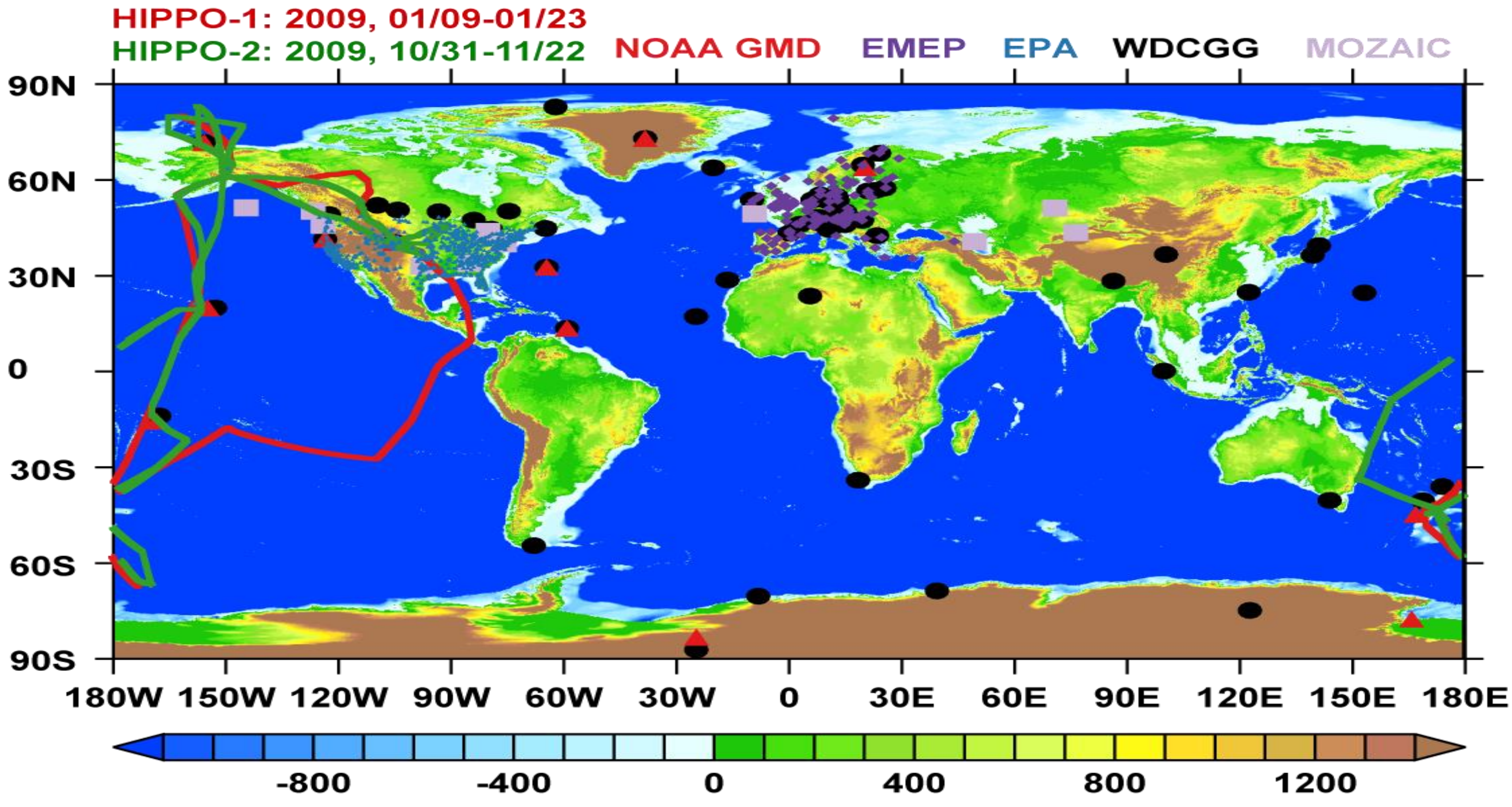
➢ **Radicals: OH, HO_2, RO_2, RO**

➢ **GHG Gases: CO_2, CH_4, N_2O**



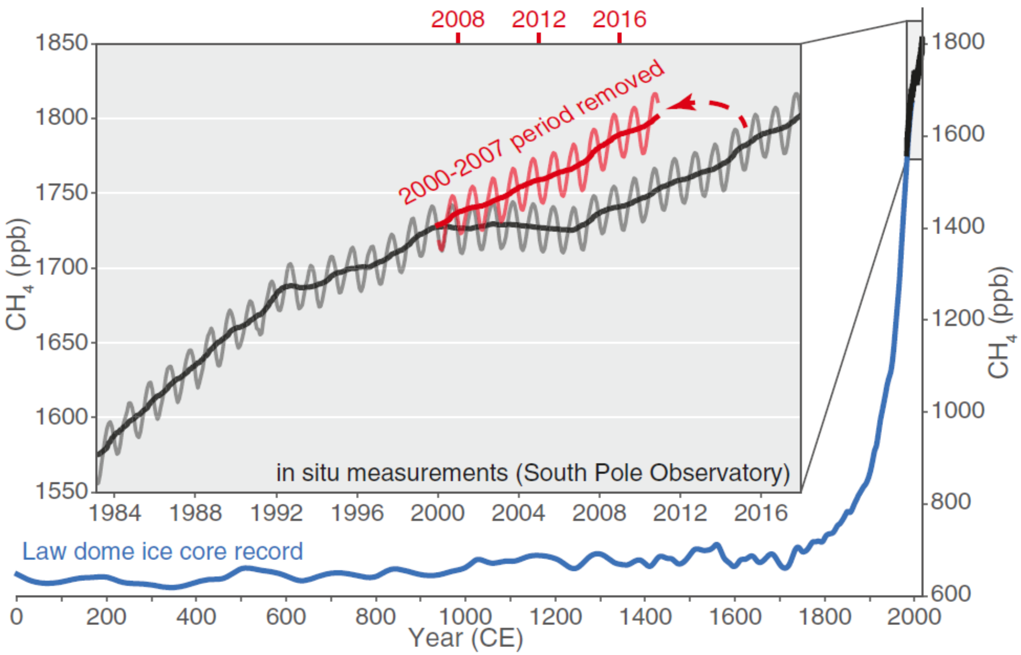
Ground Measurement Networks

# of ground sites = 1420

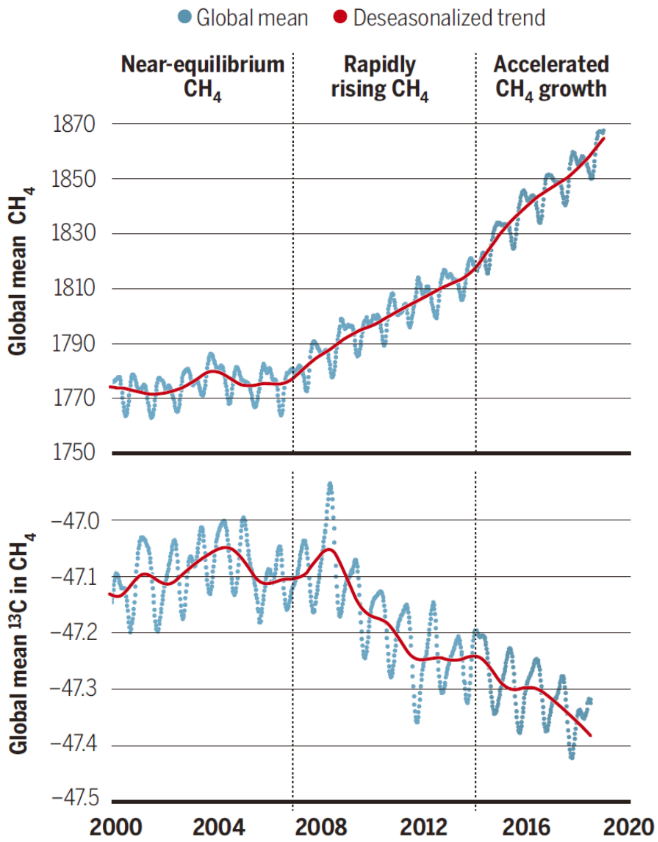


Yan et al., ACP, 2016

Measured Global CH_4 Growth



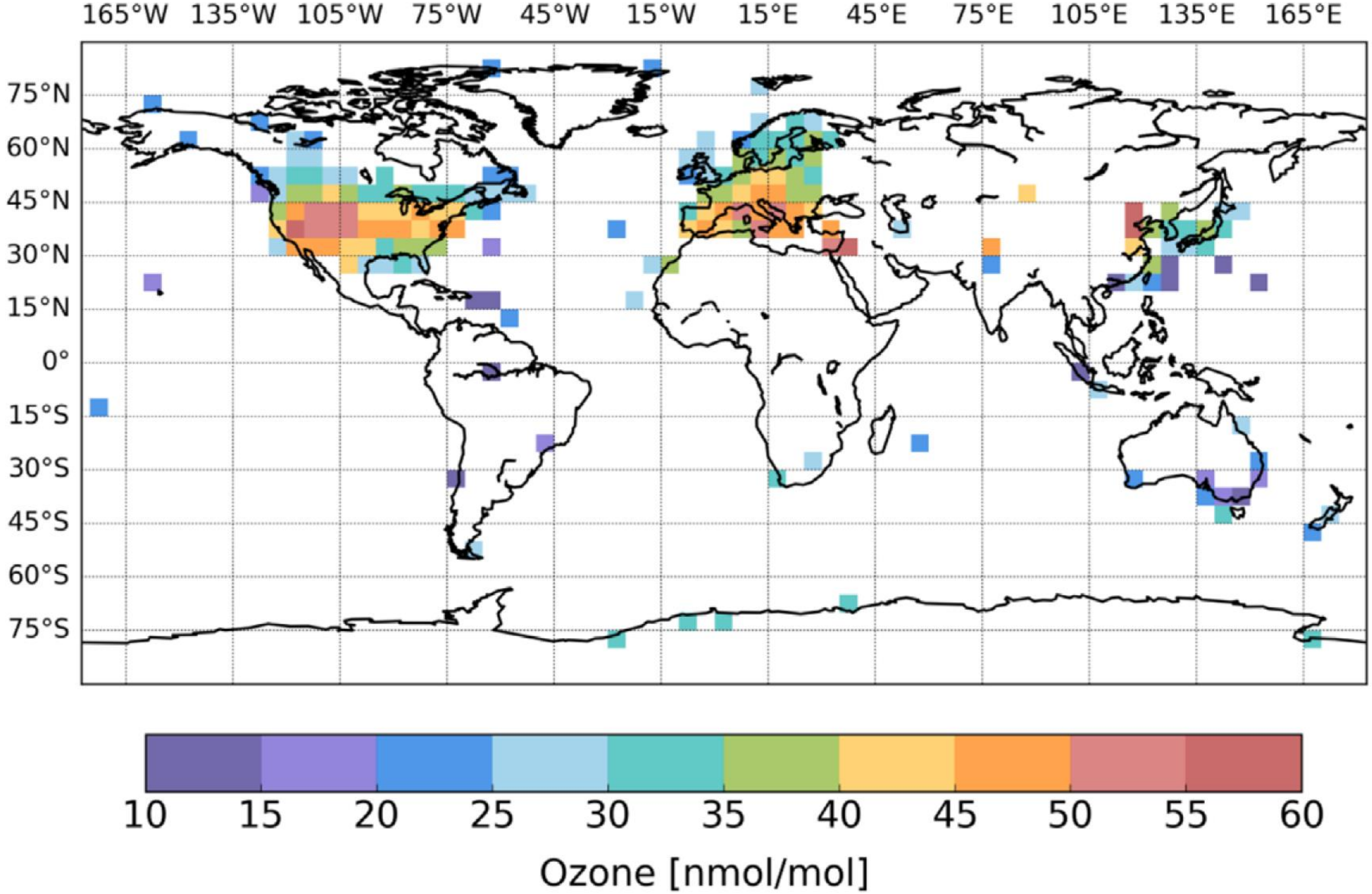
Turner et al., 2019, PNAS



Fletcher et al., 2019, Science

Global Measurements of Ozone from TOAR Project

Daytime (8-20 h LT) Mean O_3 in July 2000-2014

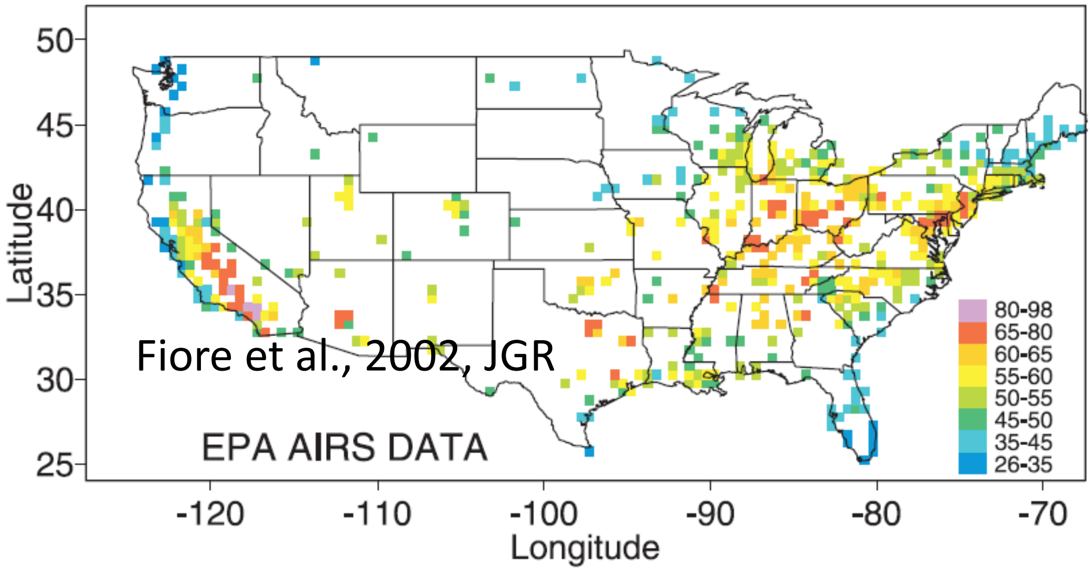


Schultz et al., 2017, Elementa

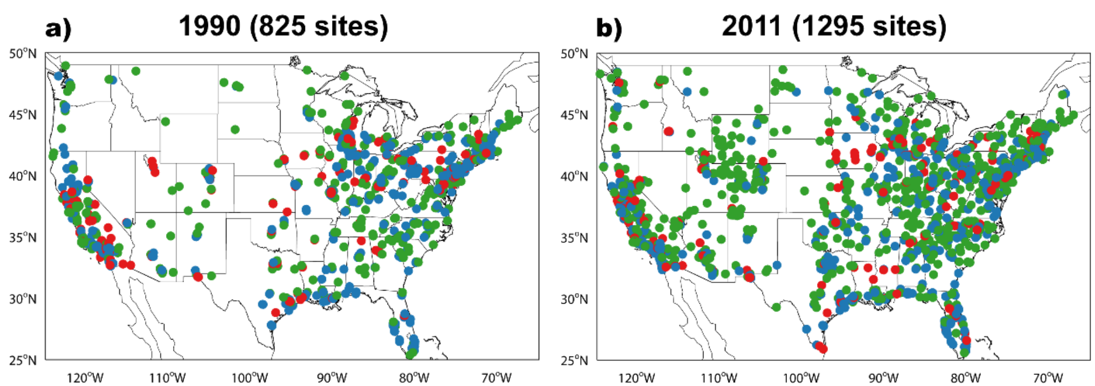
Air Quality Monitoring Network in the U.S.

- Lots of pollutants: ozone, NO_2, SO_2, CO, $PM_{2.5}$, PM components, etc.
- 800+ sites since 1990; currently more than 4000 sites

For more info: https://www.epa.gov/outdoor-air-quality-data/interactive-map-air-quality-monitors



Fiore et al., 2002, JGR



Yan et al., 2018, ACP

Air Quality Monitoring Network in China

- Before 2013: API, PM_{10}, NO_2, SO_2. Regular measurements are available in 86 cities
- Since 2013: AQI, $PM_{2.5}$, PM_{10}, O_3, NO_2, SO_2, CO. Over 300+ cities, 1500+ sites, mostly in urban/suburban locations

http://www.cnemc.cn/

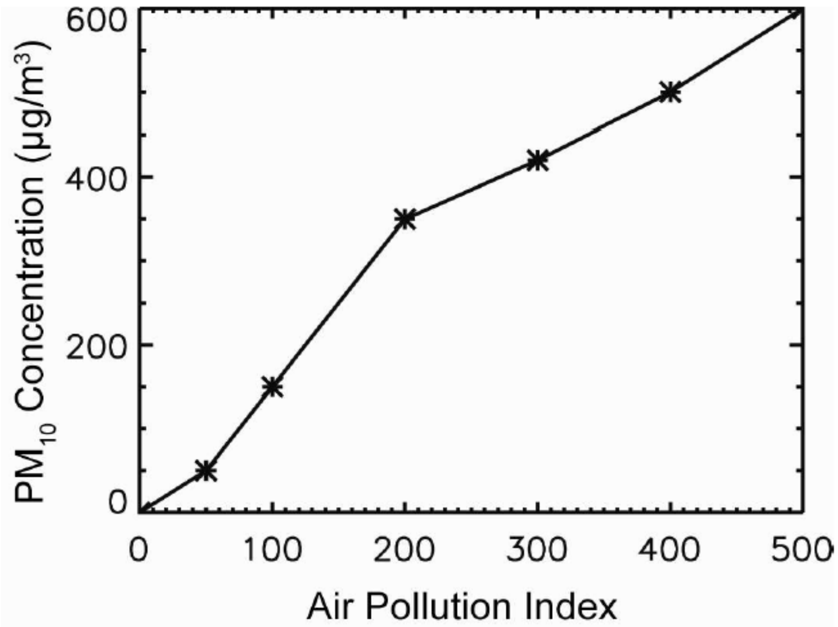
Exc. Good S.P. M.P. H.P. E.P.

https://www.aqistudy.cn/

Surface Measurements: The Chinese Case

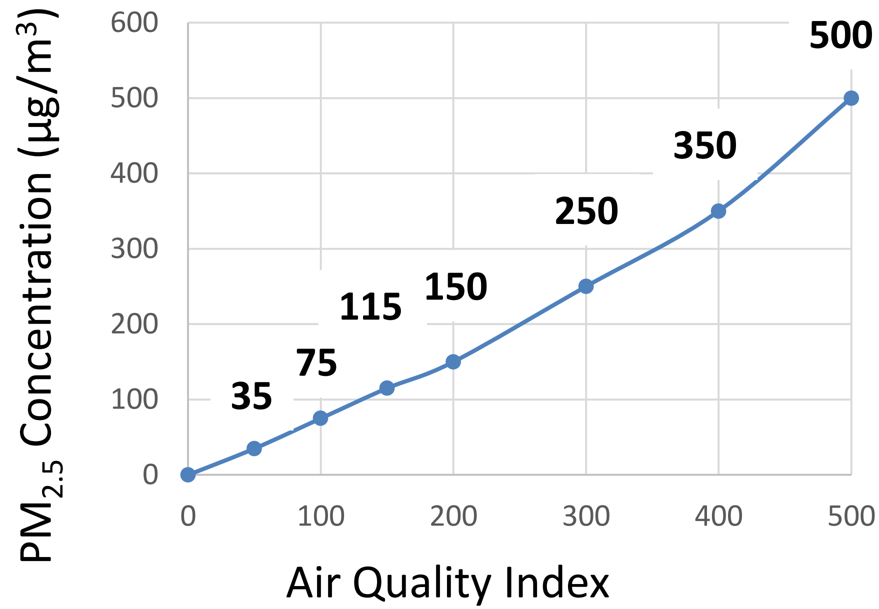
API for PM_{10}

Prior to 2013



AQI for $PM_{2.5}$

In effect since 2013



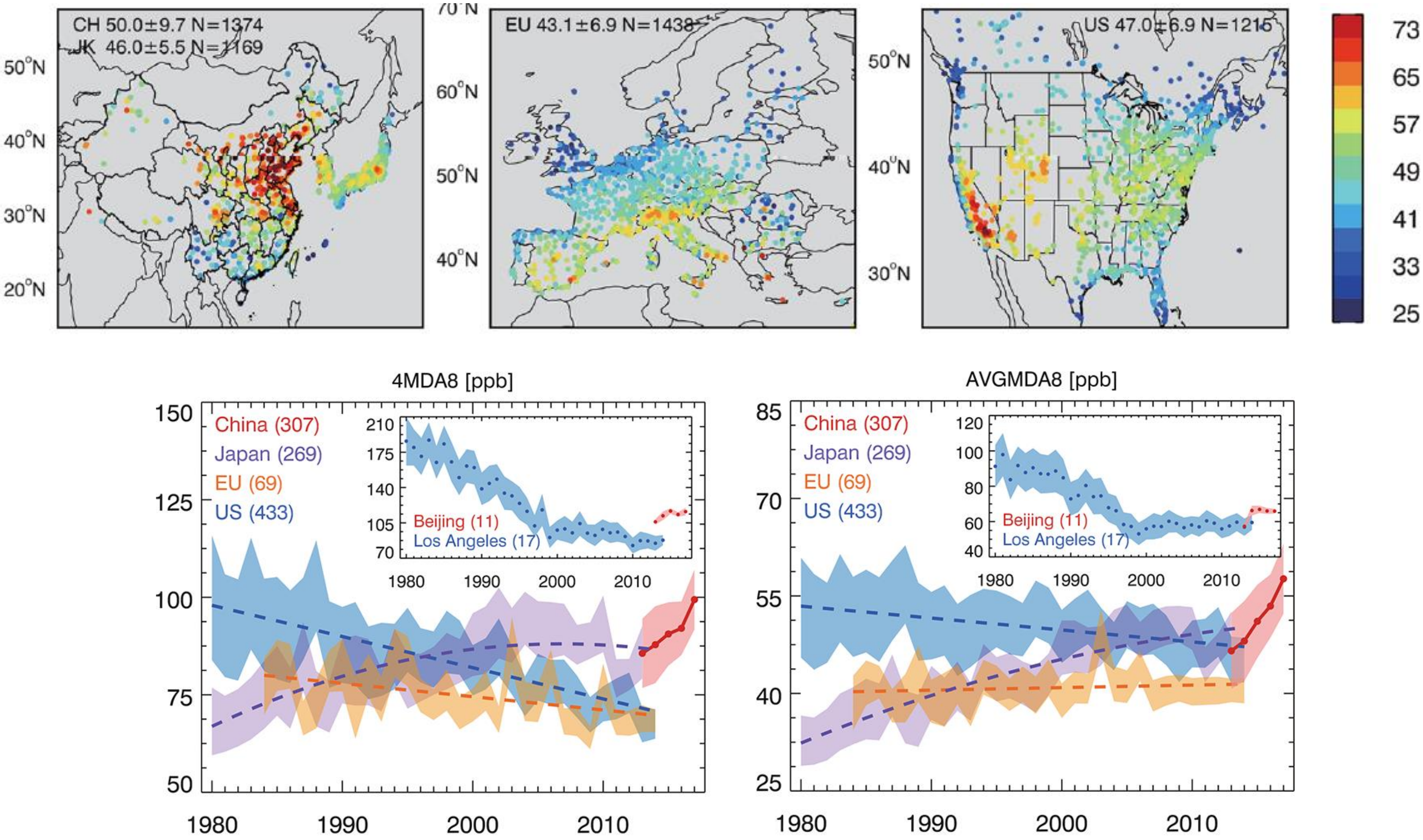
《环境空气质量标准》（GB 3095-2012）修改单

3.14 “标准状态 standard state 指温度为273 K，压力为101.325 kPa时的状态。本标准中的污染物浓度均为标准状态下的浓度”修改为：“参比状态 reference state 指大气温度为298.15 K，大气压力为1013.25 hPa时的状态。本标准中的二氧化硫、二氧化氮、一氧化碳、臭氧、氮氧化物等气态污染物浓度为参比状态下的浓度。颗粒物（粒径小于等于10 μm）、颗粒物（粒径小于等于2.5 μm）、总悬浮颗粒物及其组分铅、苯并[a]芘等浓度为监测时大气温度和压力下的浓度”。

该标准修改单自2018年9月1日起实施。

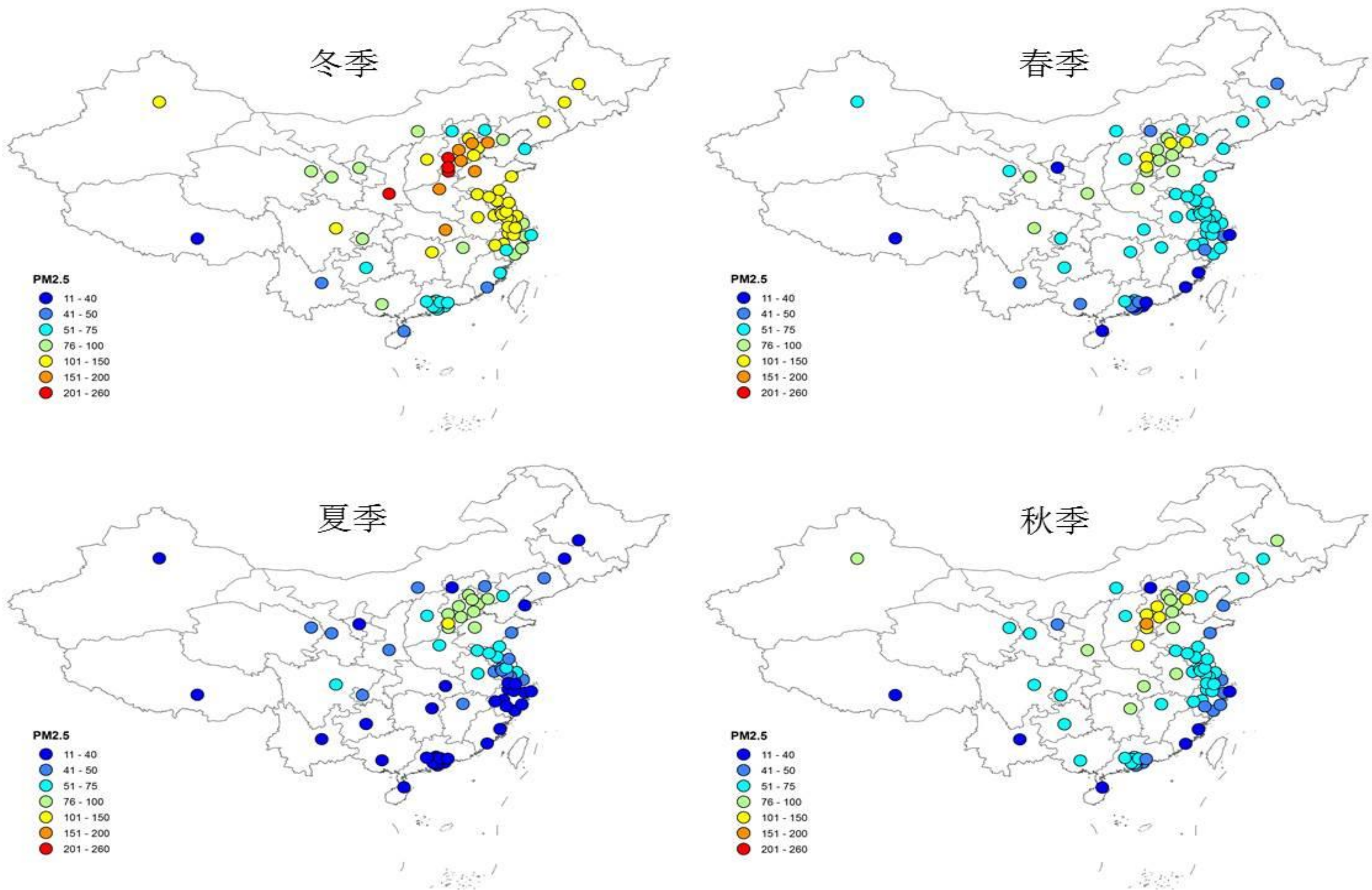
Ozone Pollution over China: Global Perspective

AVGMDA8 for April–September, 2013–2017



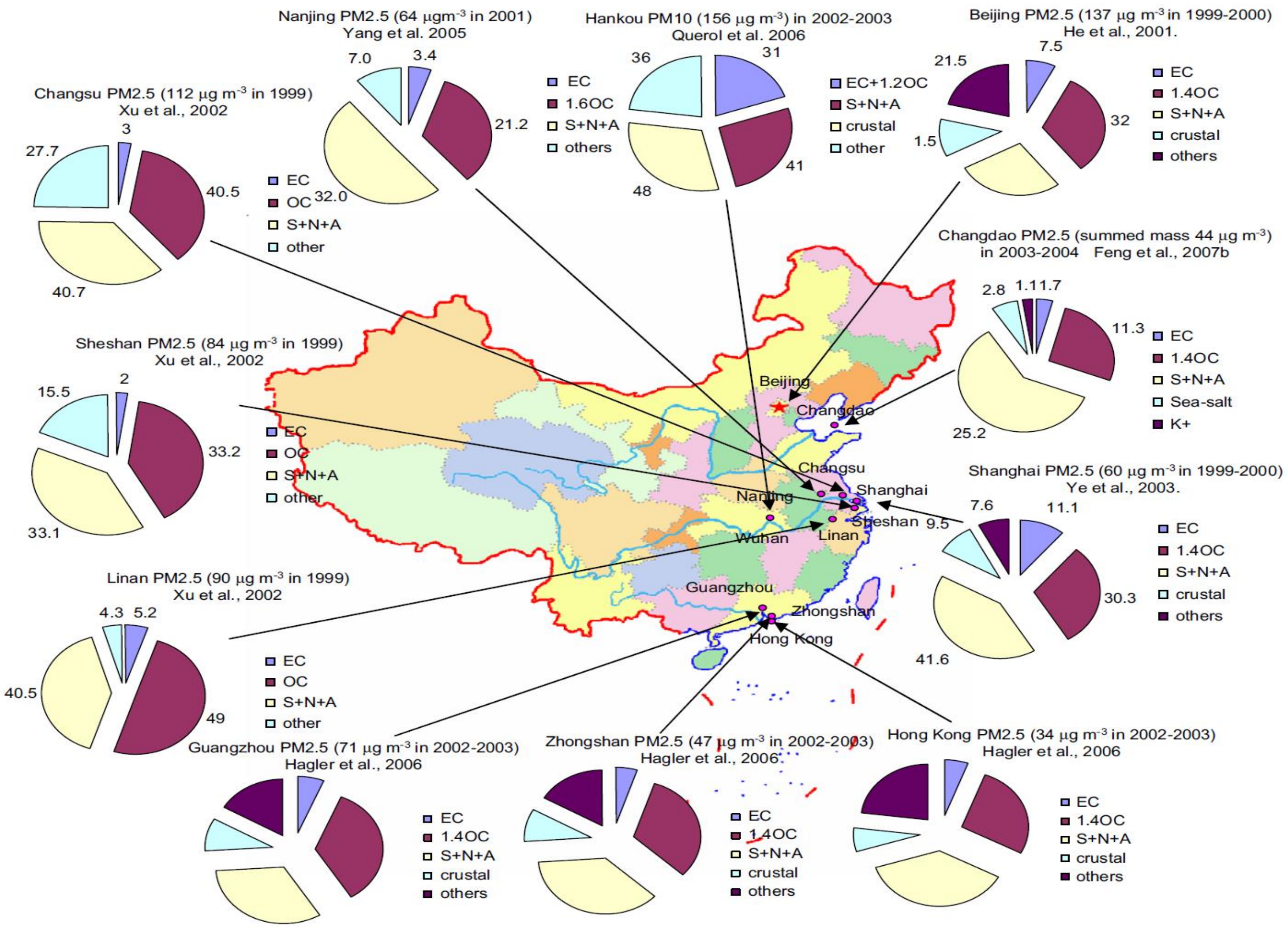
Lu et al., 2018, ESTL

Surface $PM_{2.5}$ Measurements in China



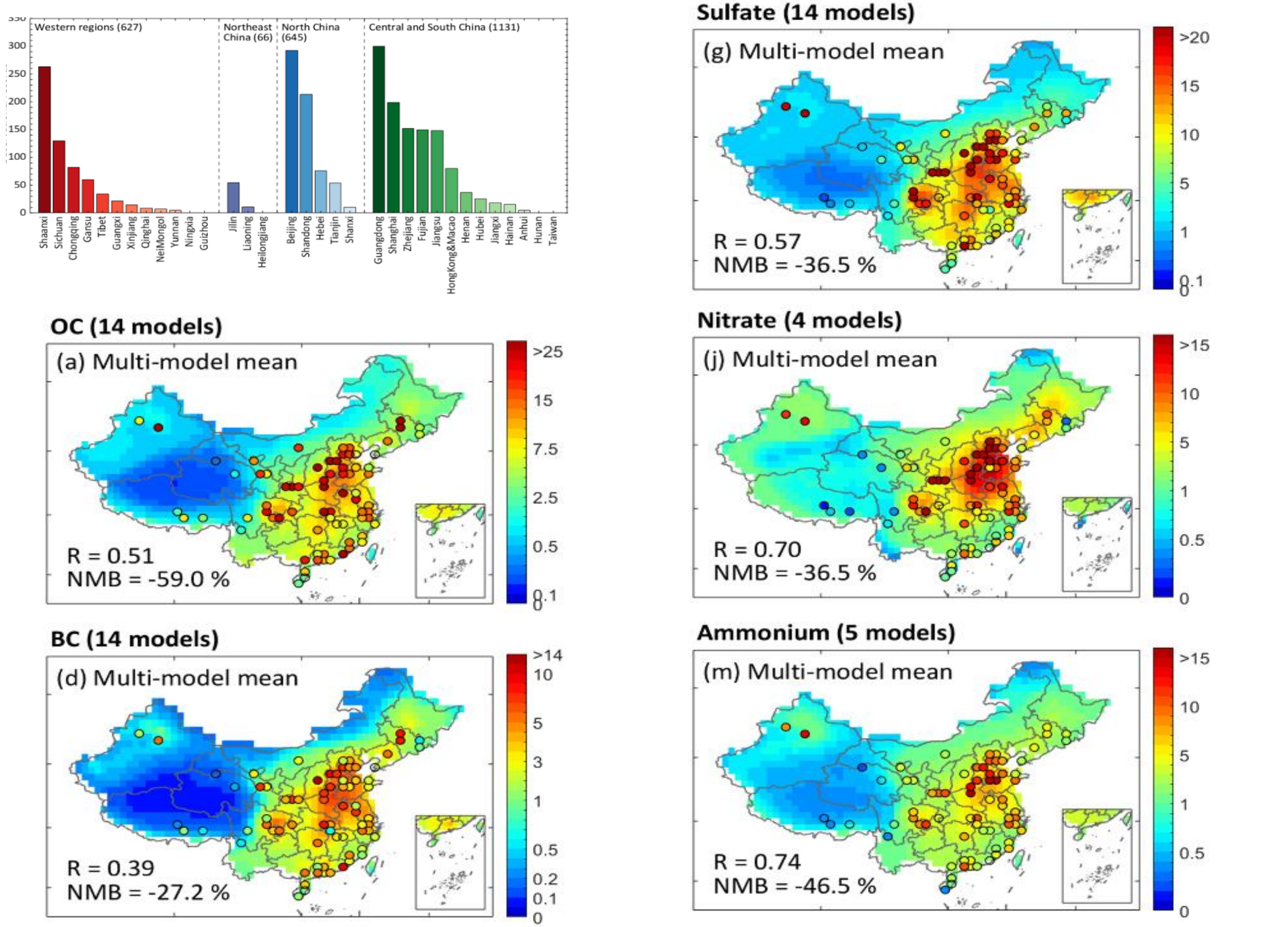
贺克斌，2014

Speciated PM Measurements in China



Fang et al., 2009

Speciated PM Measurements in China



Ren F.-X. et al., GMD, 2023

Sounding: “Big Fish” over Tibetan Plateau

第二次青藏高原综合科学考察研究
“大气成分垂直结构及其气候影响”
科考分队“系留气艇探空观测实验”

Pictures taken in Lhasa in August 2020

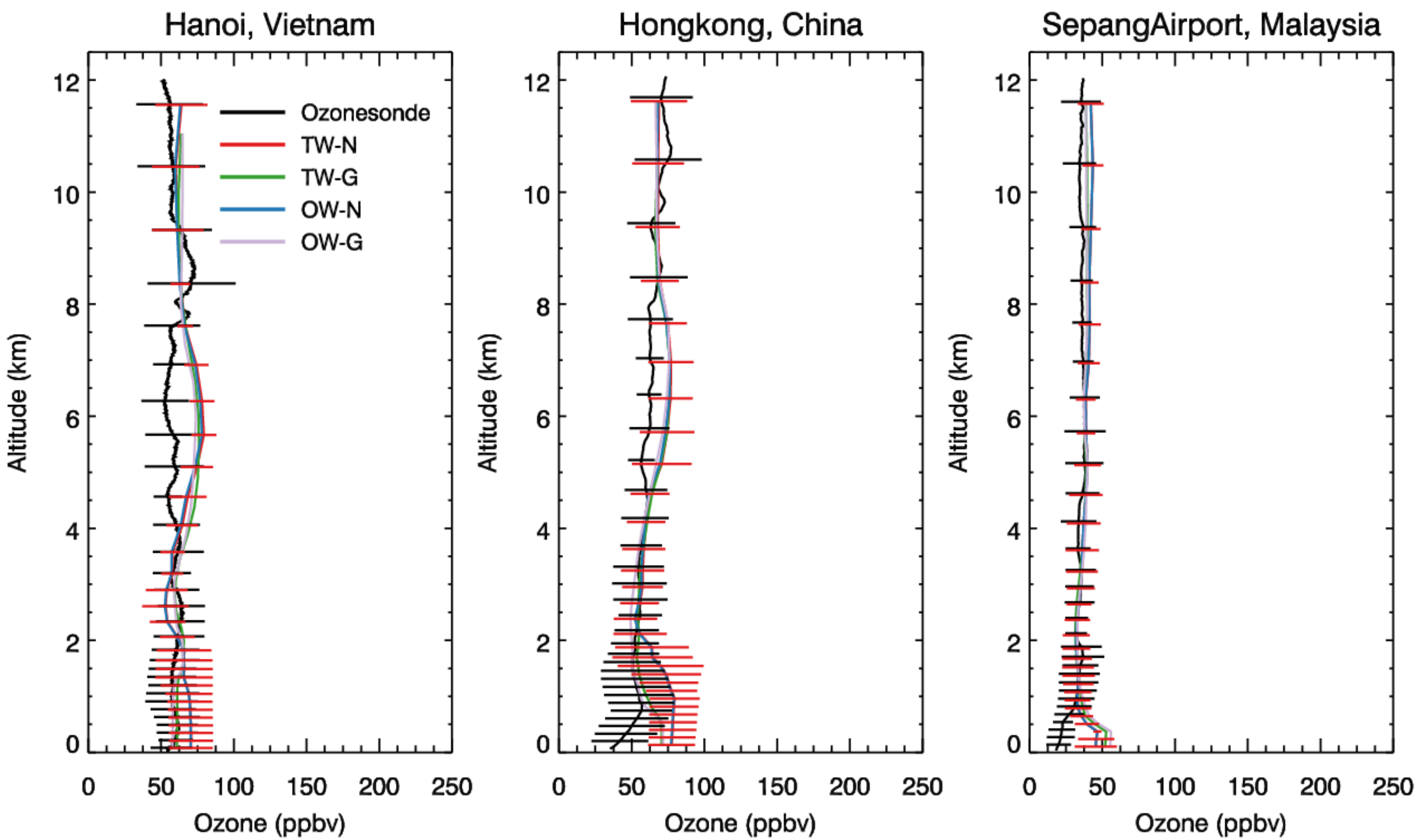
Zhaoze Deng

Guiqian Tang

WOUDC Ozonesonde Network

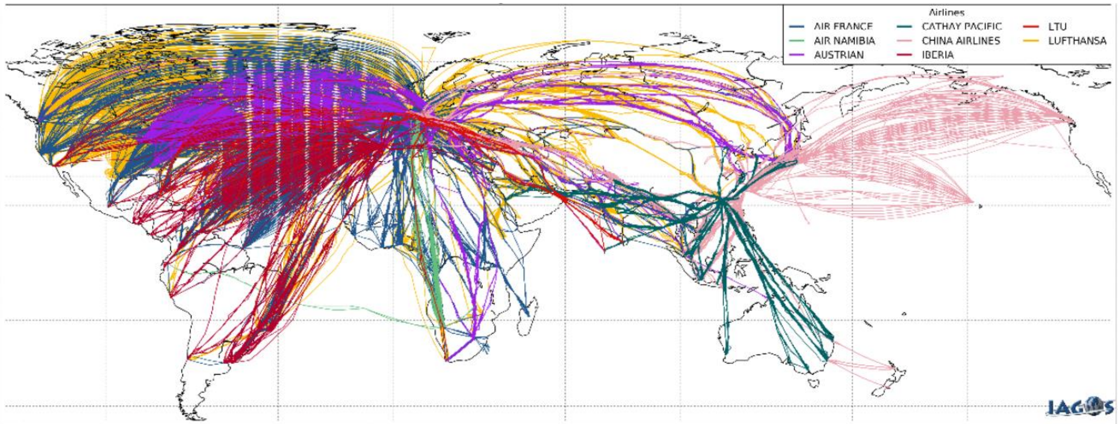
https://woudc.org/data/dataset_info.php?id=ozonesonde

WOUDC Ozonesonde Data for Model Evaluation (2008)

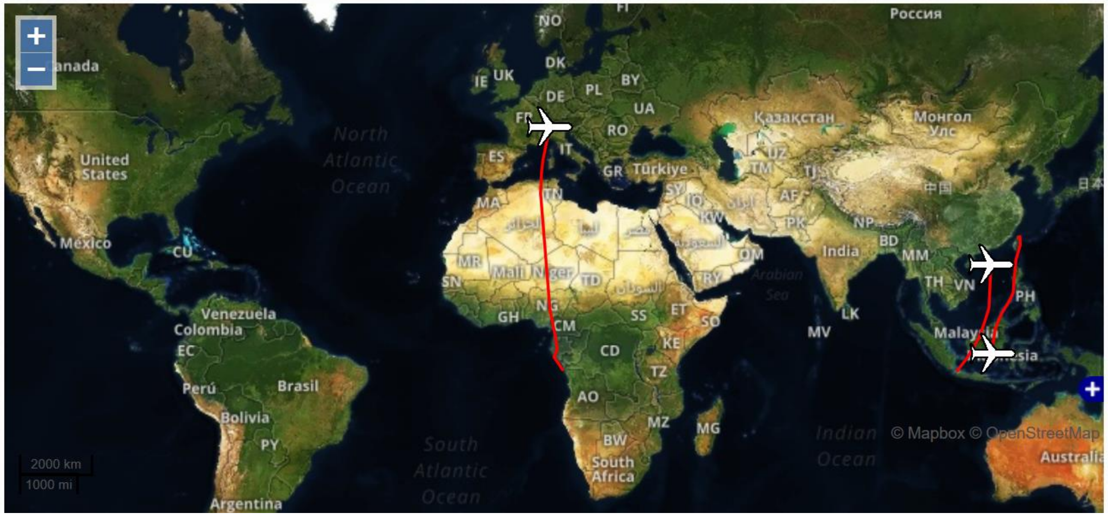


Ni, R.-J., 2018, ACP

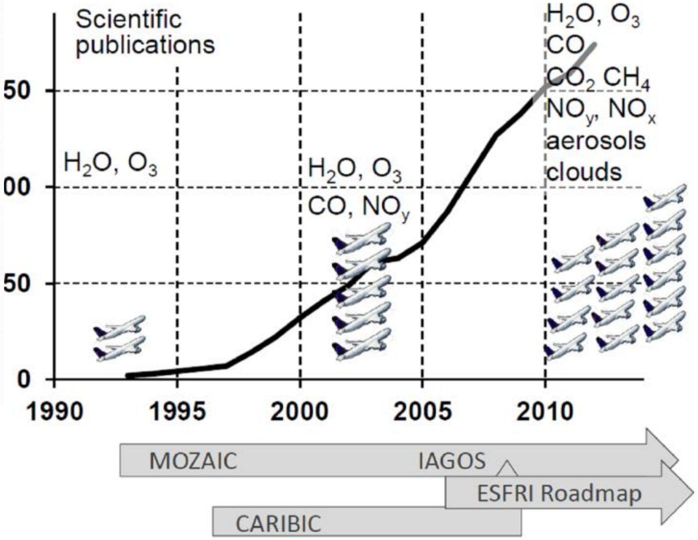
Aircraft Measurements: MOZAIC/IAGOS, CARIBIC



Map of IAGOS flights

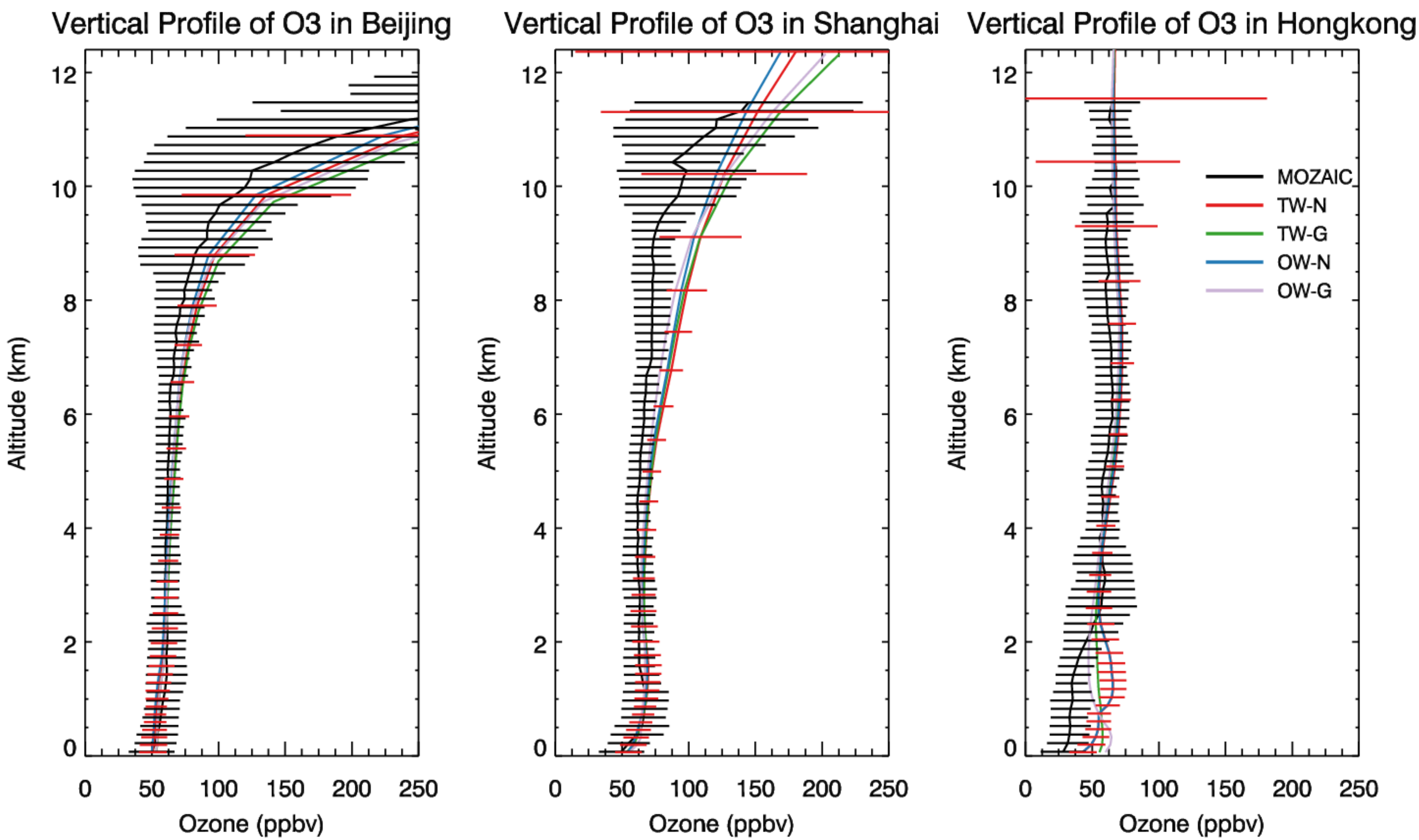


Petzold et al., 2012



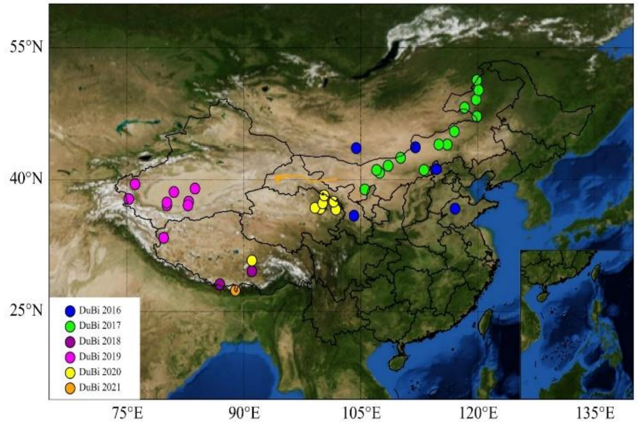
http://iagos.sedoo.fr/

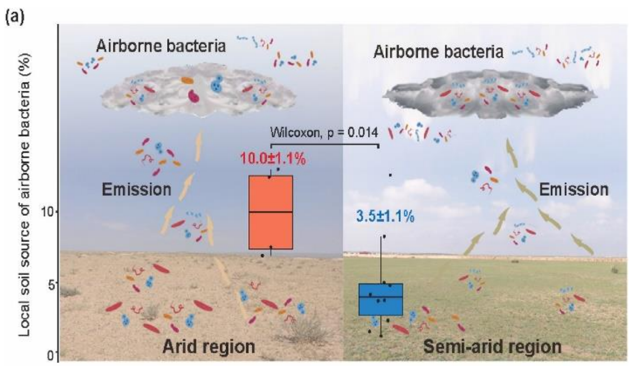
MOZAIC Ozone Data for Model Evaluation (2000-2005)

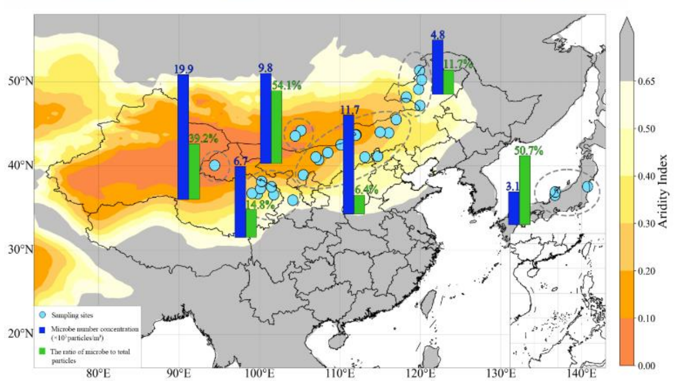


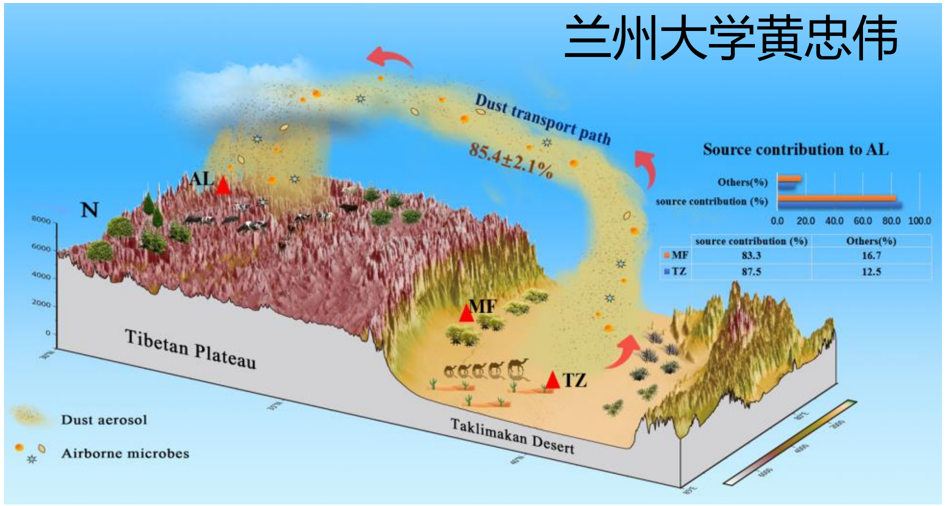
Ni, R.-J., 2018, ACP

我国生物气溶胶观测网络





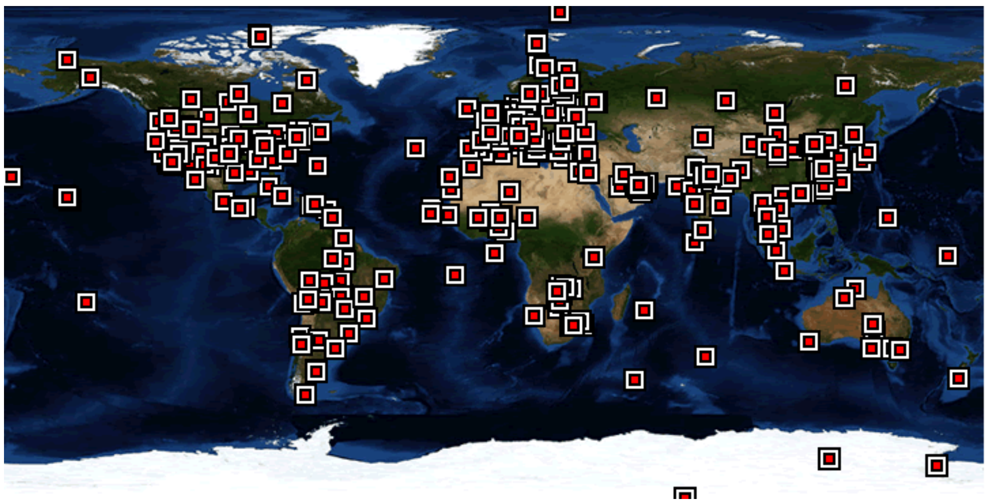




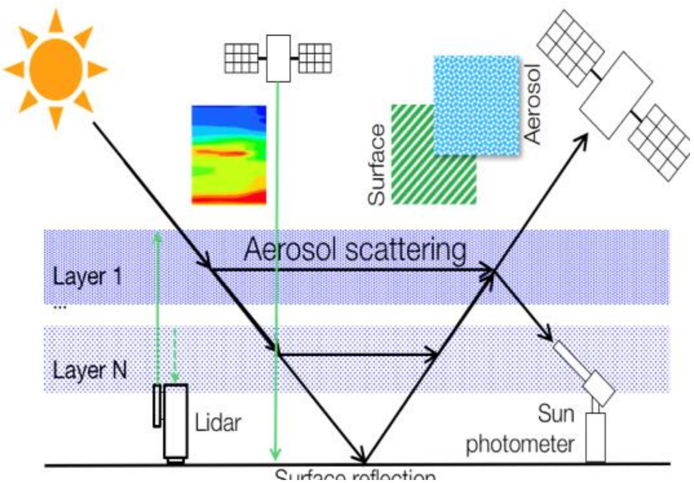
- 干旱区生物气溶胶数浓度高于半干旱区
- 半干旱区生物气溶胶在总悬浮颗粒物中占比均低于干旱区与湿润区
- 塔克拉玛干沙尘对青藏高原大气生物气溶胶贡献为85.4%，特别是增加了高原潜在病原体(16.43%)和冰核细菌(73.8%)

AERONET for Aerosol Optical Properties

- Automatic sun-tracking photometer (CIMEL 318)
- Globally consistent algorithm, including cloud screening
- Few sites in China with multi-year measurements (Beijing IAP, Xianghe, Taihu, SACOL, Hong Kong PolyU)

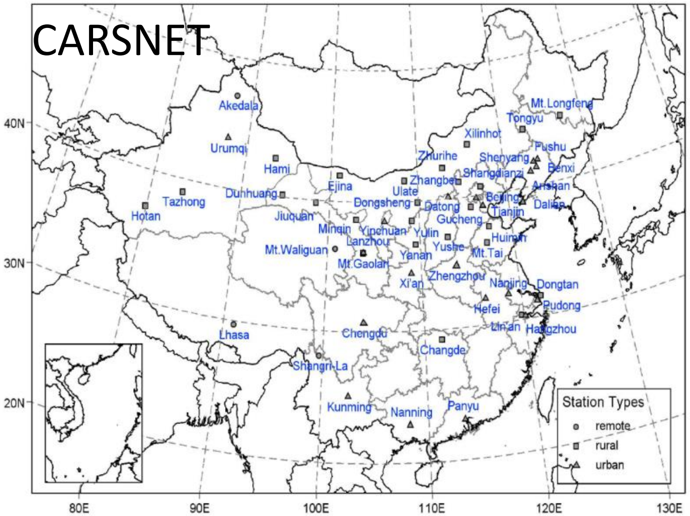


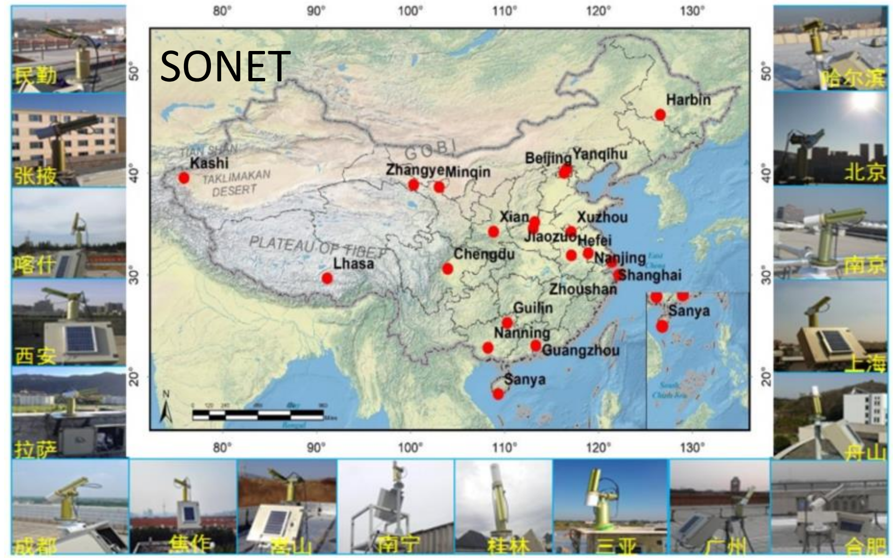
NASA

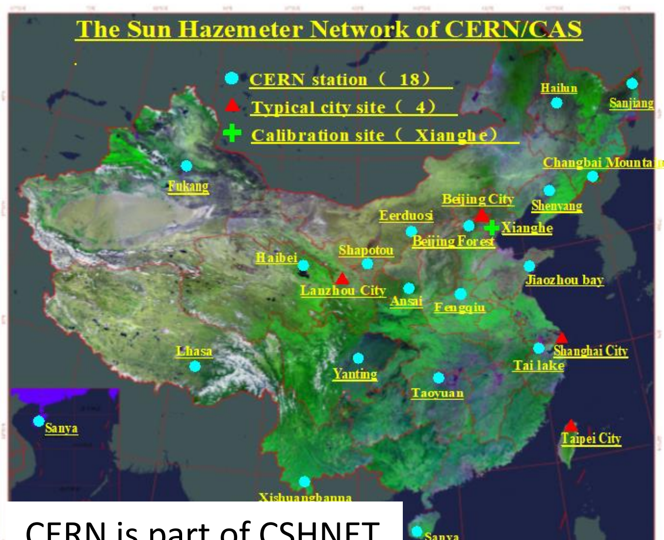


Huizheng Che

中国地基气溶胶光学观测
（AERONET、CARSNET、CSHNET、SONET等）

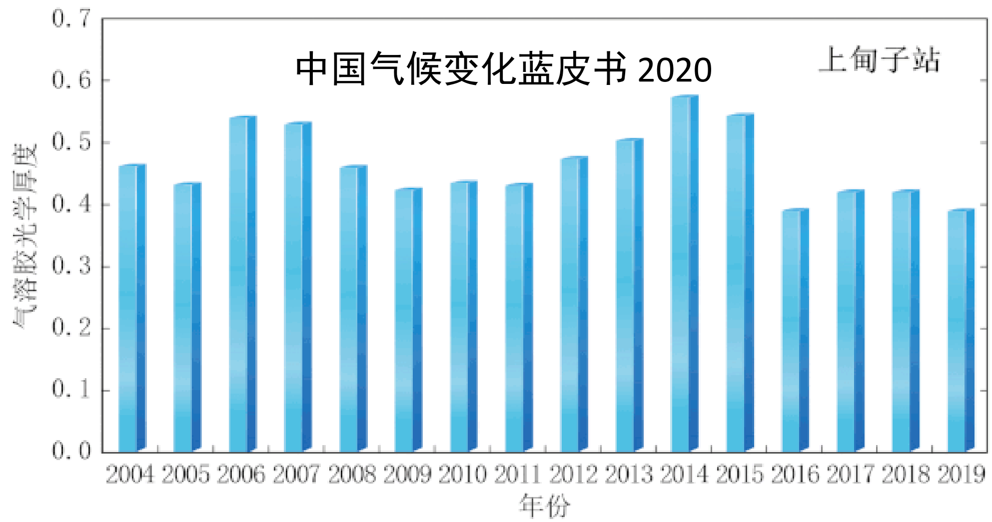






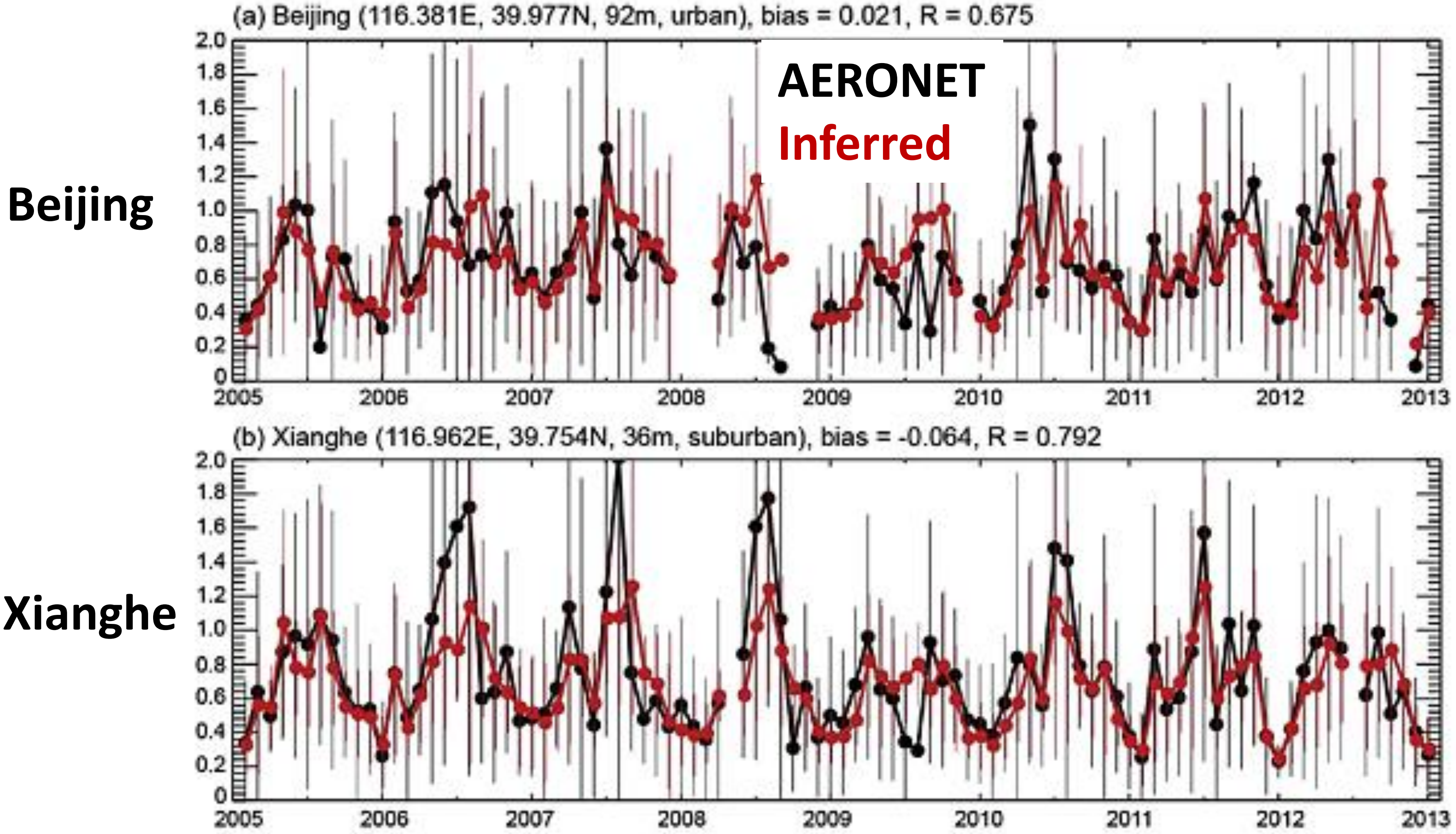
CERN is part of CSHNET

区域大气本底站观测到的AOD变化



AERONET for Data Evaluation

2005–2012 monthly time series at 550 nm



Lin et al., 2014, 2016, AE

Visibility Measurements

Manual

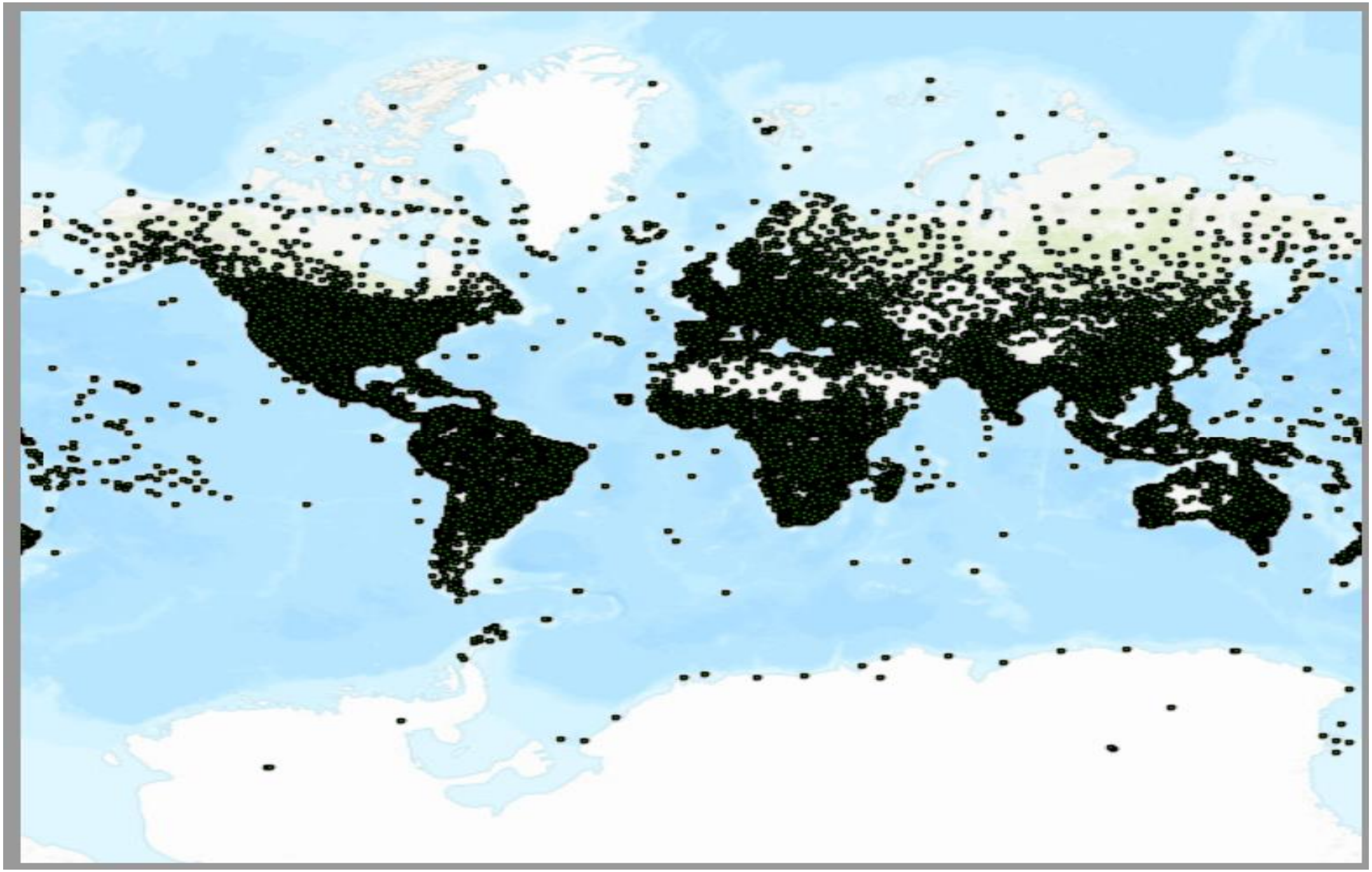
Automatic

Visibility = Coefficient / Extinction_efficiency

- Used traditionally as a meteorological indicator, but can also be employed to study (long-term) PM pollution

Surface Meteorological Measurement Stations

Also for visibility measurements



Source: WorldClim

AOD Inferred from Visibility Measurements

2005–2012 mean AOD at 550 nm for days with valid MODIS data

$$AEC = K/V$$ (Koschmieder Eq.)

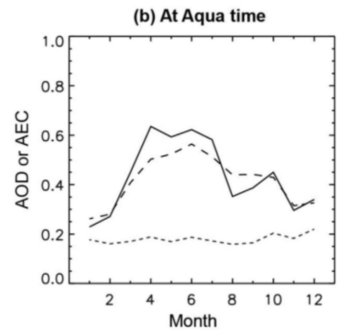
$$AEC = K/V - K/V_0$$ (Modified Koschmieder Eq.)

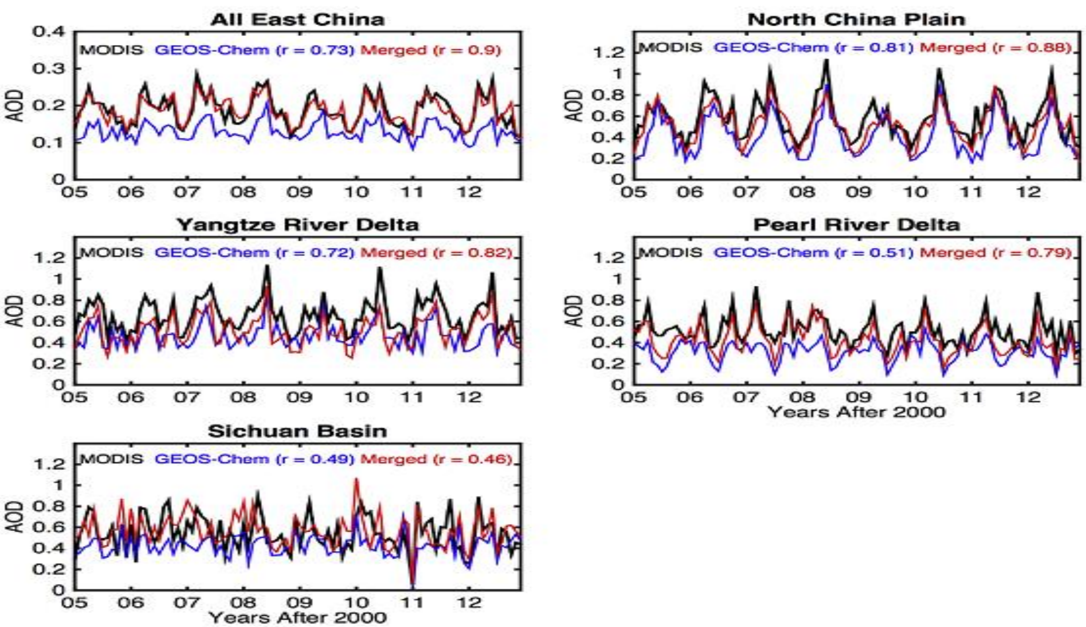
$$= K/V*(1 - V/V_0)$$

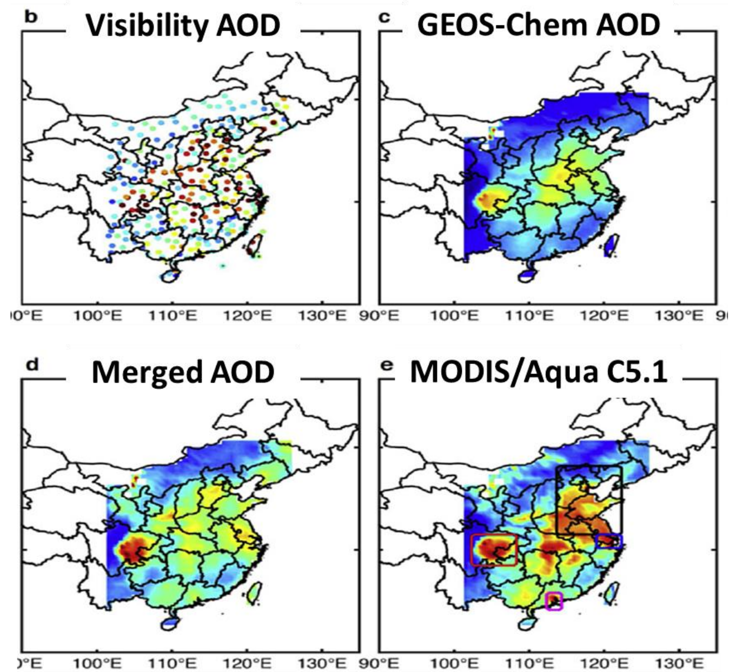
$$AOD = AEC*(AOD_m/AEC_m)$$

$$= K/V*(1 - V/V_0)*(AOD_m/AEC_m)$$

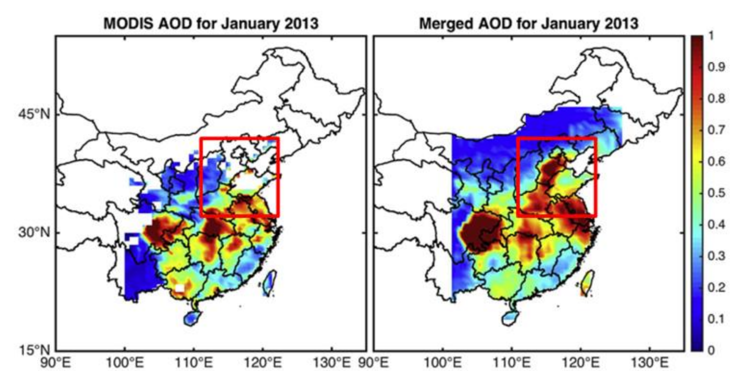
- Koschmieder Constant = 3.92
- Measured Visibility
- Visibility Offset = 70 km
- Modeled AOD
- Modeled Near-surface Extinction Coefficient





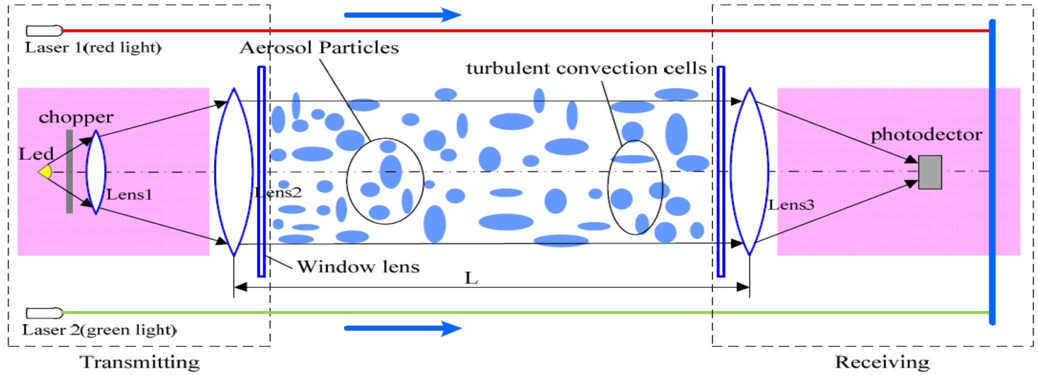


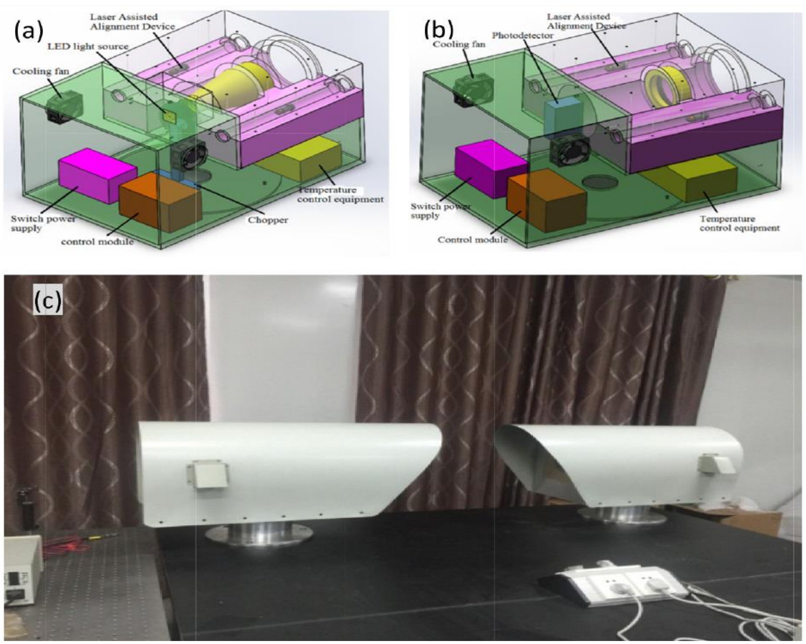
Lin et al., 2014, 2016, AE

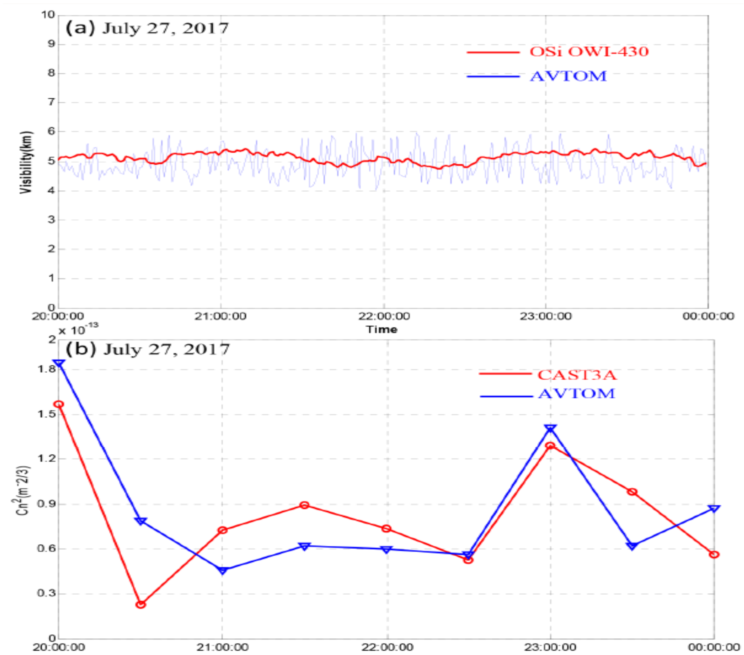


Instrument for Aerosol-Turbulence-Optical Interaction

中大韩永

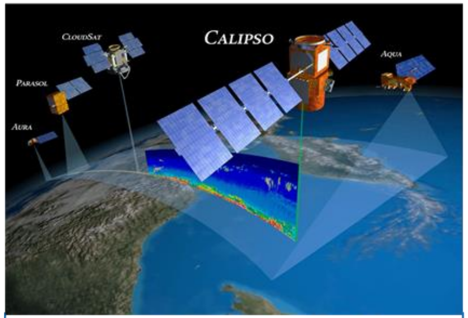




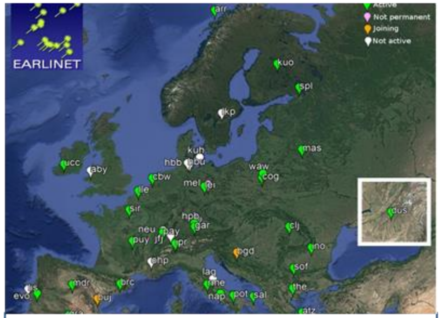


大气激光雷达

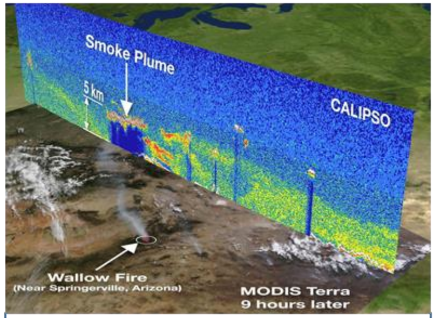
激光雷达：探测激光与气溶胶、气体分子等粒子相互作用的回波信号（强度、偏振态、光学频率）



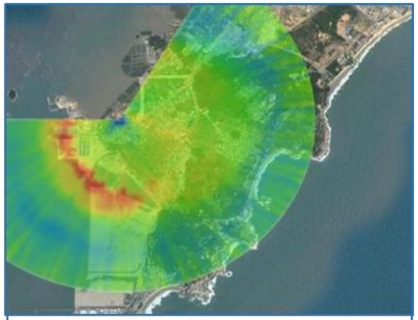
NASA星载激光雷达



欧洲激光雷达观测网



气溶胶时空演变探测



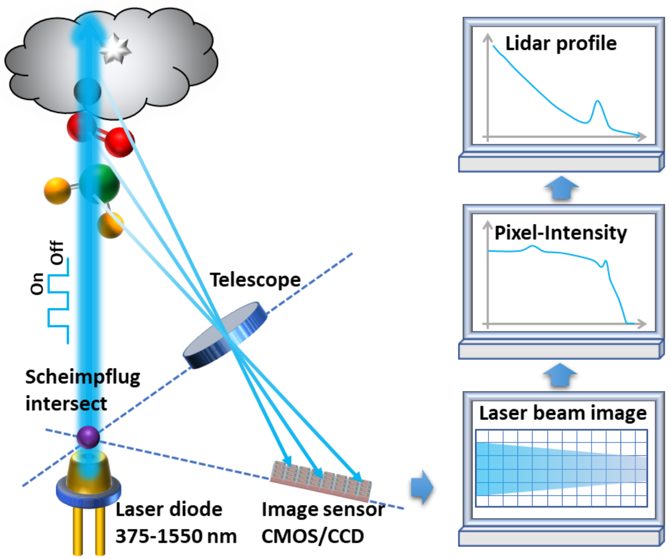
大气污染源扫描探测

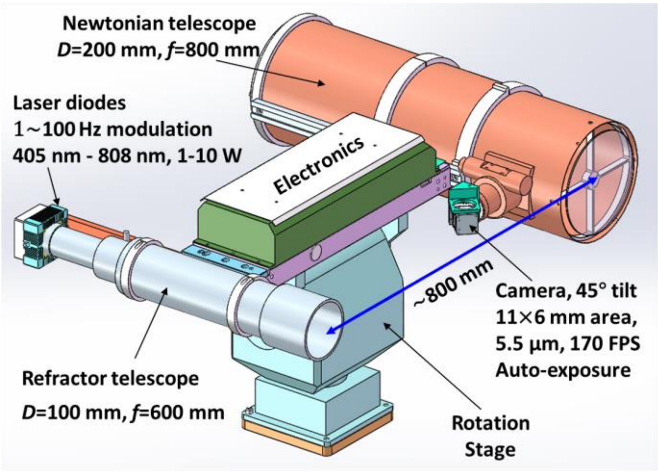
- **地基激光雷达：** 欧美日等发达国家已建立区域性的大气激光雷达观测网络，如欧洲EARLINET，美国MPLNET，日本AD-NET；中国也已初步建成激光雷达观测网络
- **星载激光雷达：** 美国NASA早在2006年即发射CALIPSO偏振大气激光雷达卫星，欧洲即将发射激光雷达卫星（ALADIN）；2022，中国发射全球首颗搭载高光谱分辨率激光雷达卫星（ACDL）

来源：梅亮

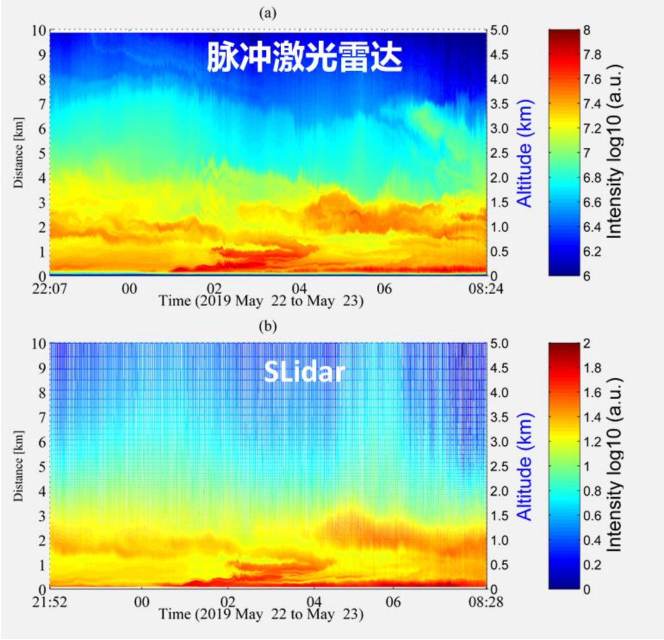
沙式激光雷达

大连理工大学梅亮





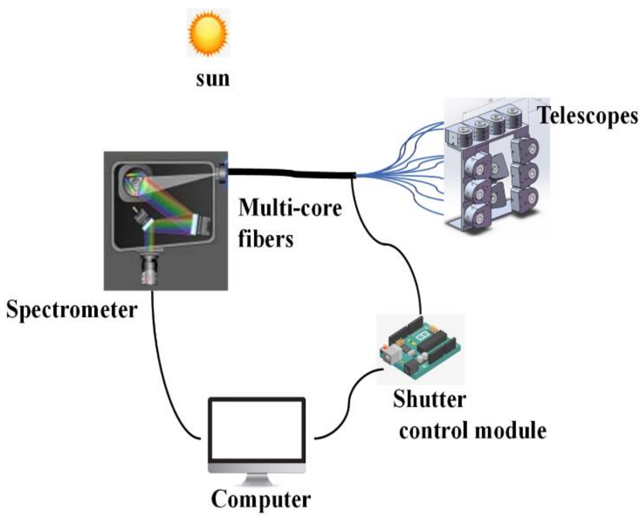
30° 仰角测量激光雷达信号

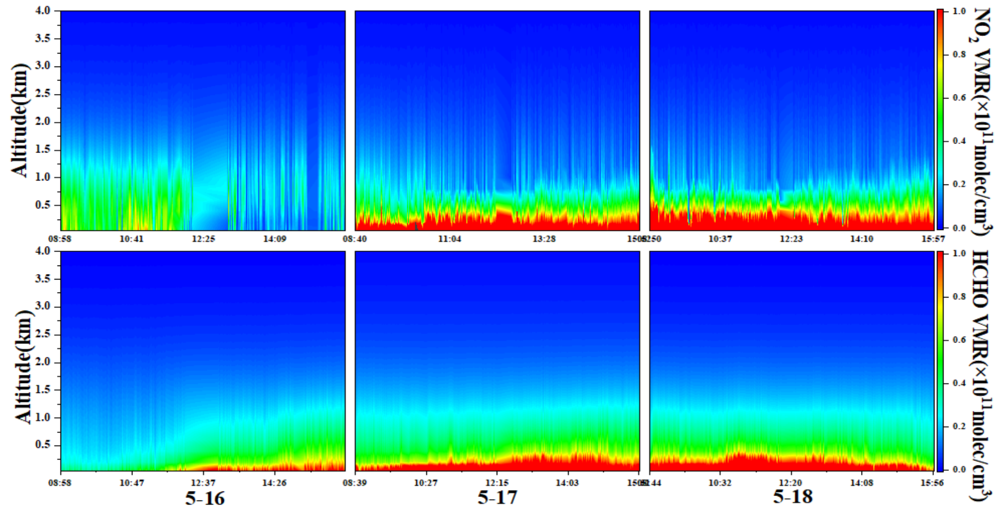


FS MAX-DOAS 高时间分辨率的同步多轴系统

多仰角同步观测取代电机顺序扫描以提高采集时间分辨率

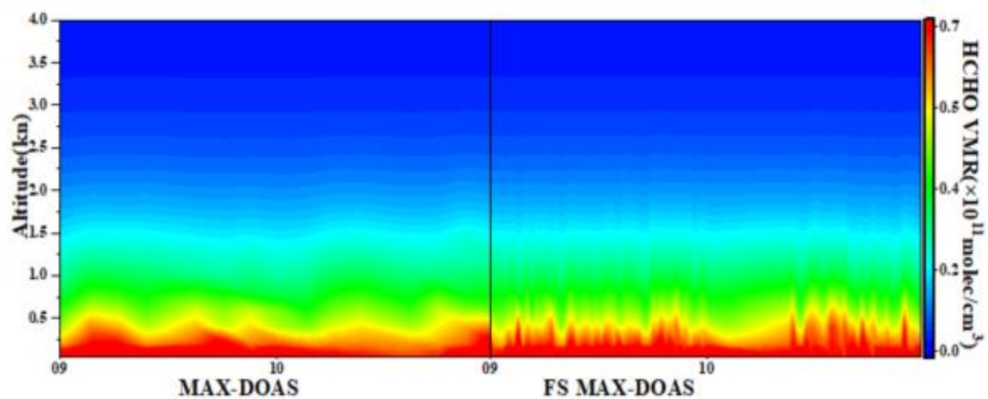
安光所李昂





气体	柱浓度探测限
NO_2	1.67×10^{15} molec./cm^2
SO_2	2.89×10^{15} molec./cm^2
HCHO	1.01×10^{16} molec./cm^2

时间分辨率：≤1min



Satellite Measurements

Sputnik 1: Oct 4, 1957

Sputnik 2: Nov 3, 1957

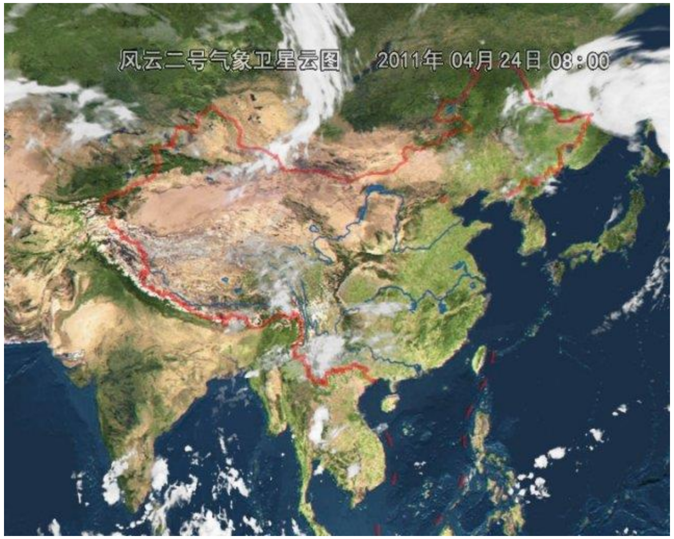
⋮

Early weather sat.: 1950s-1960s

⋮

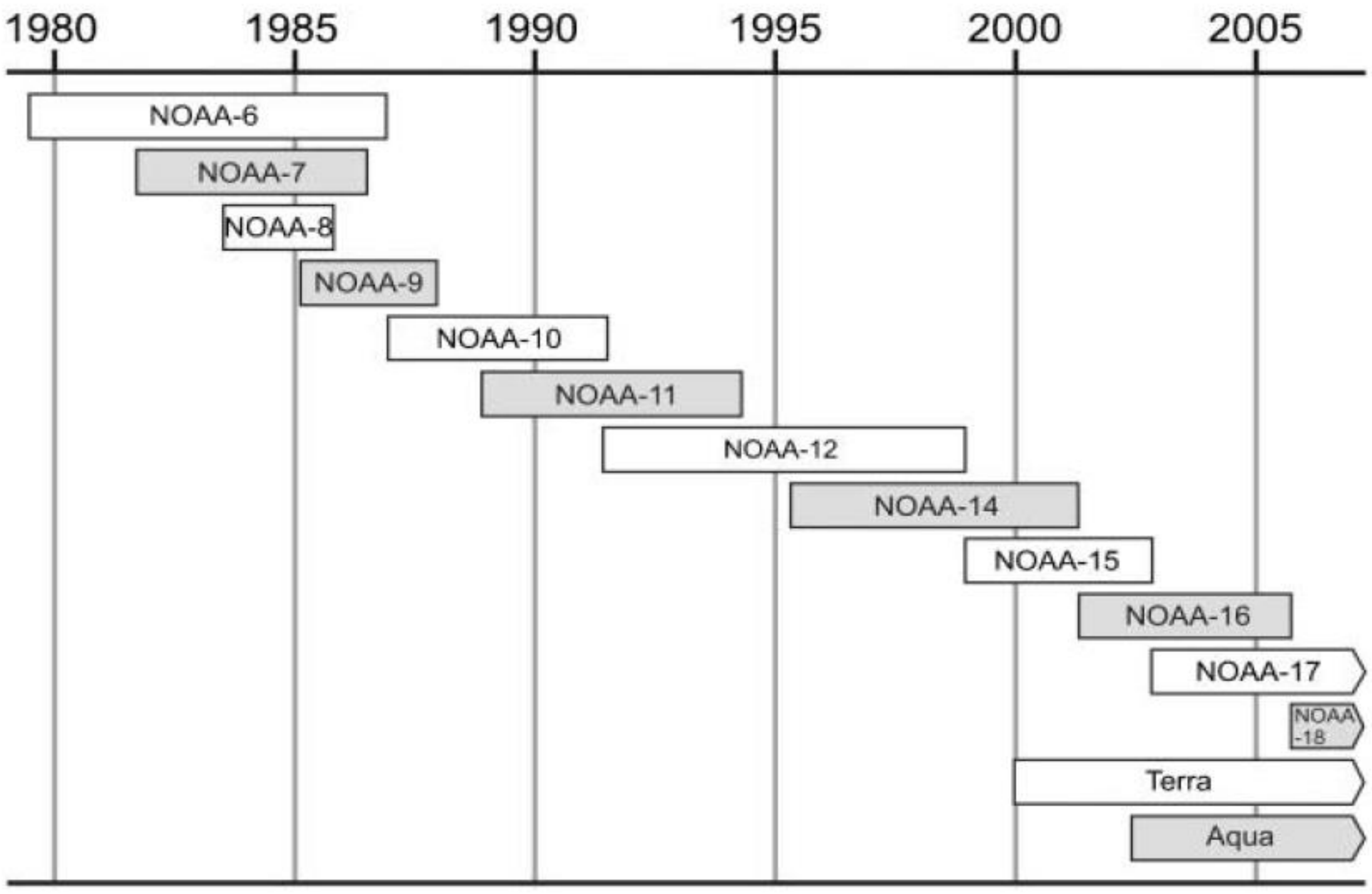
Modern weather satellites: 1970s-

- Polar orbiting satellites
- Geostationary satellites

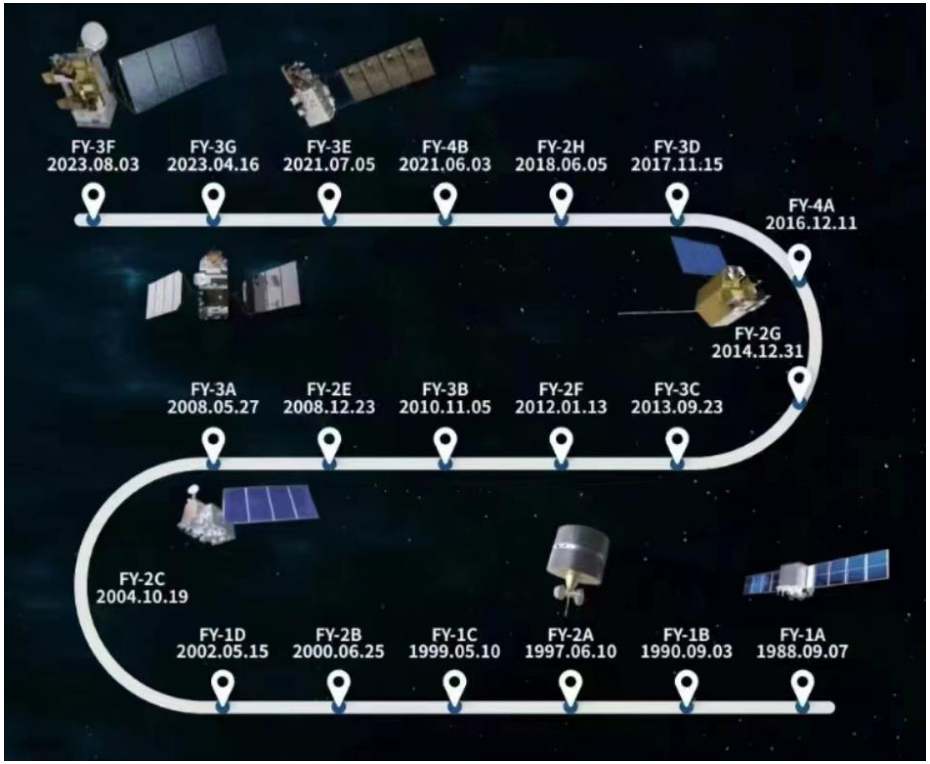


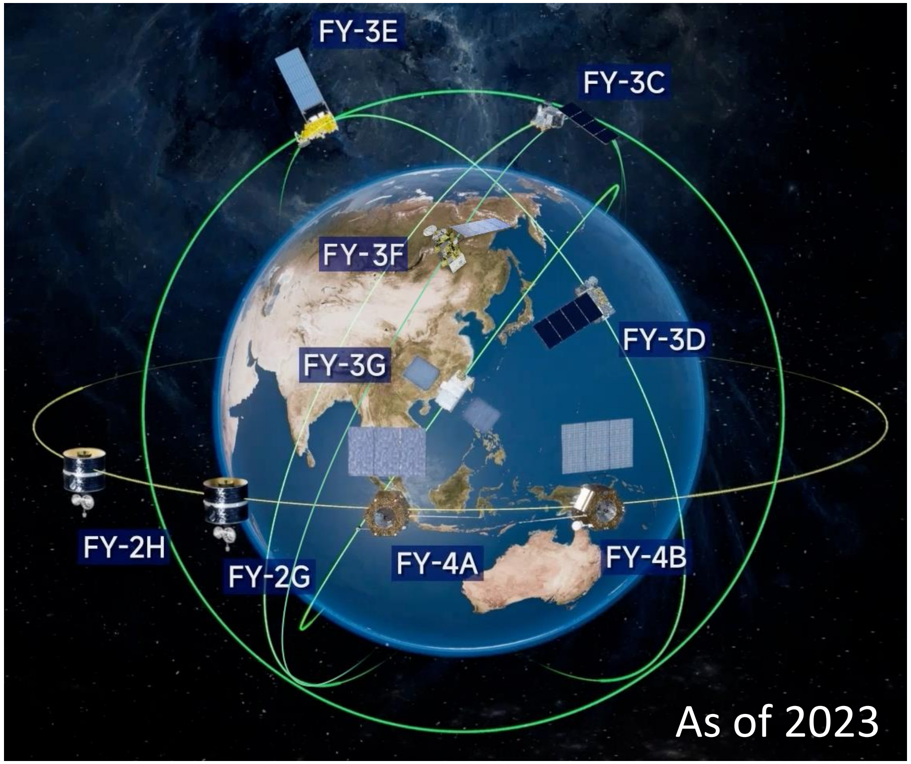

GEOS-1; Oct 25, 1975

Satellite Meteorological Measurements Also Provide Information to Infer Aerosols



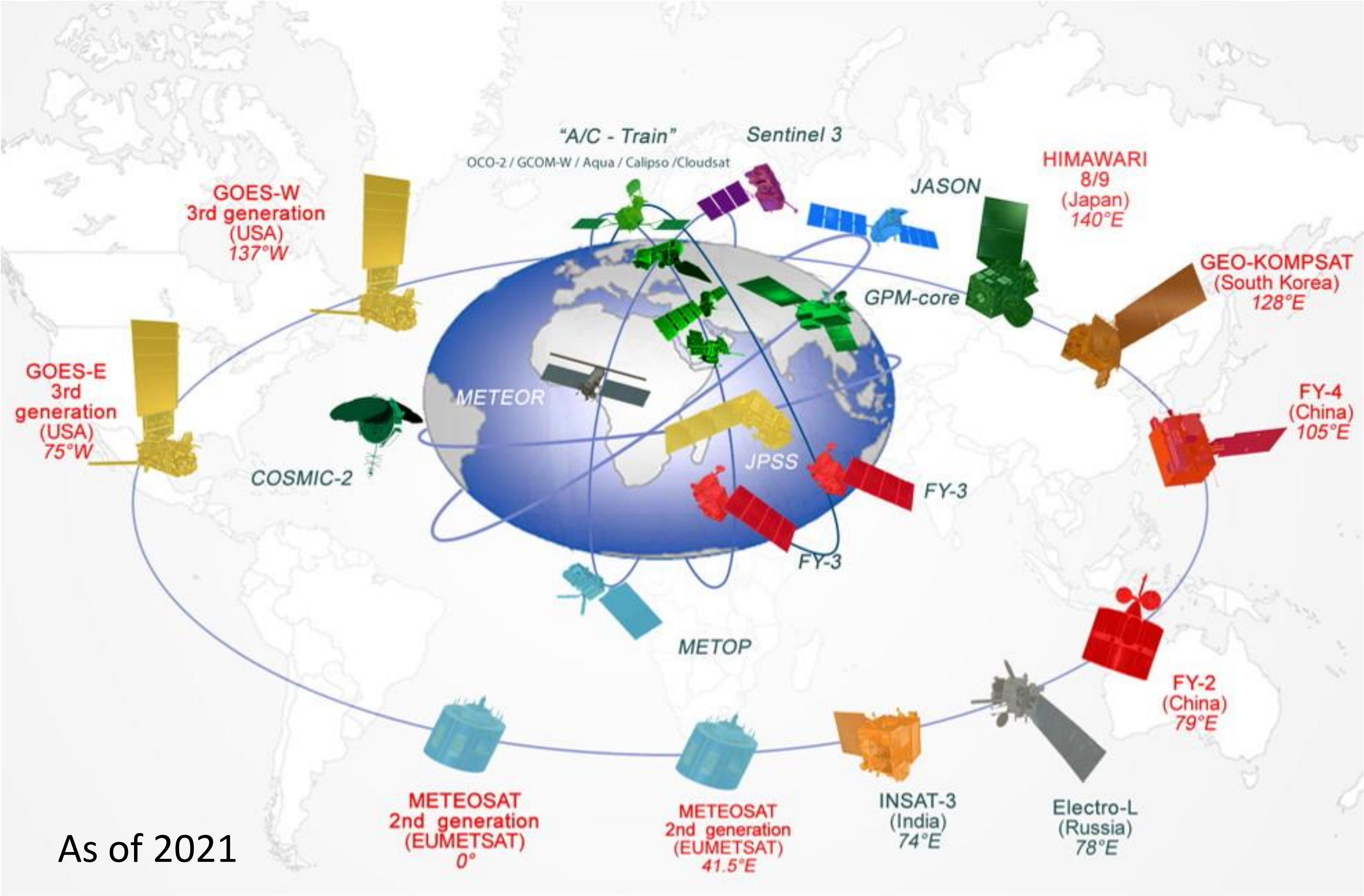
China’s Operational Weather Satellites





Source: http://www.nsmc.org.cn/nsmc/cn/satellite/index.html

Global Operational Weather Satellites



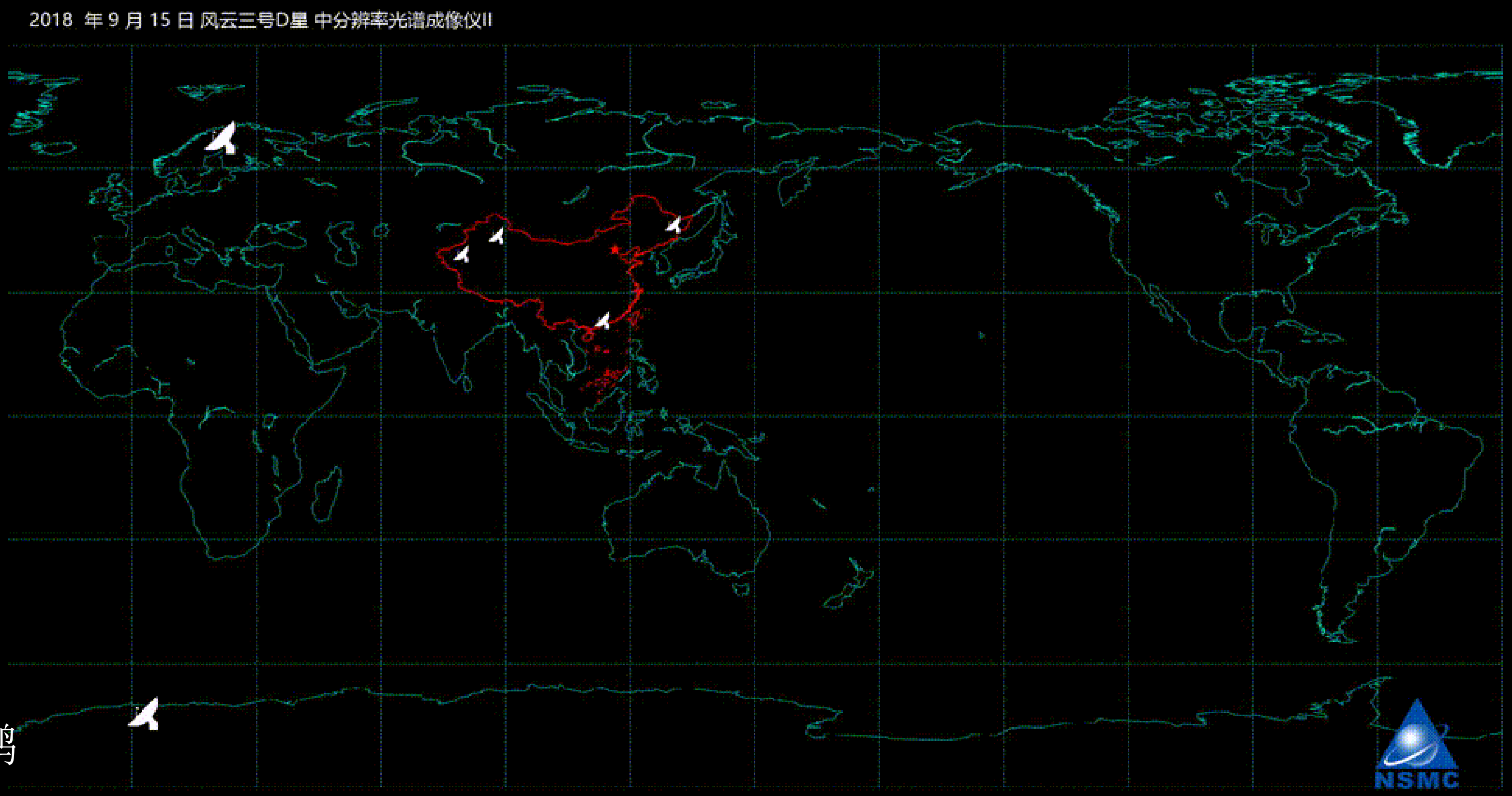
Source: http://www.nsmc.org.cn/nsmc/cn/satellite/index.html

Polar Orbiting Satellite: FY-3

极轨气象卫星

观测特点：

1. 在约800公里轨道高度绕地球南北极飞行，每12小时无缝隙覆盖全球
2. 搭载多种遥感仪器，获取大气和地球环境综合探测信息



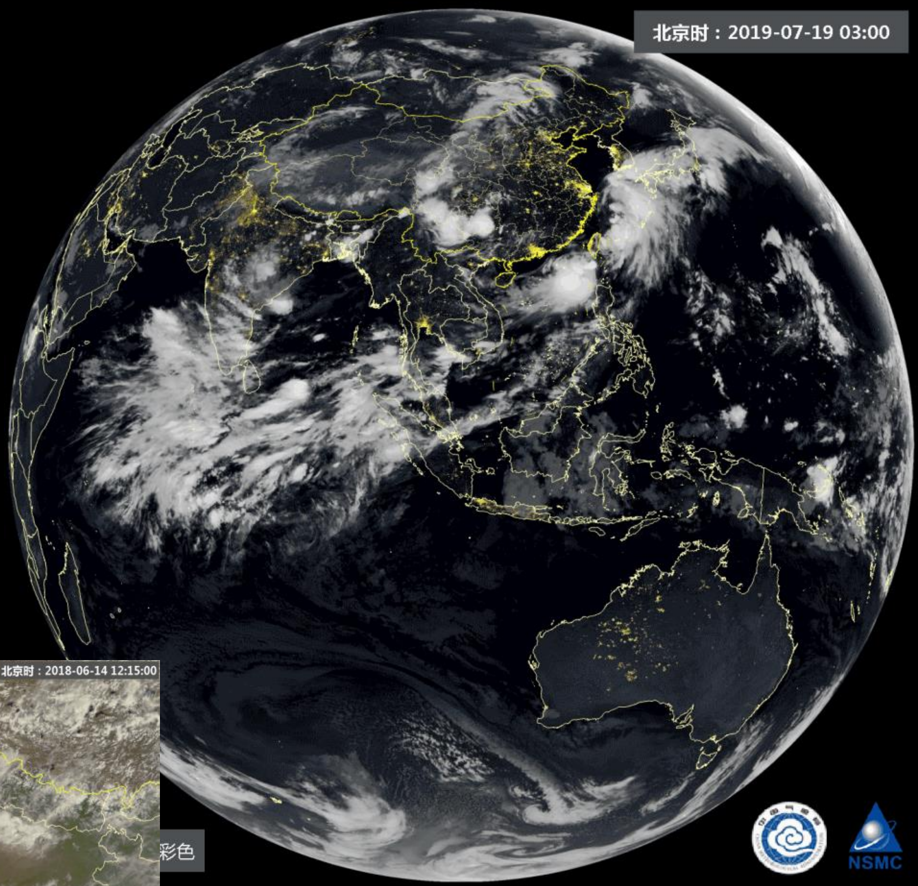
张鹏

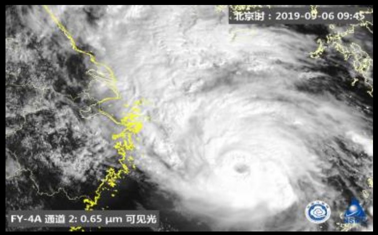
Geostationary Satellite: FY-4A

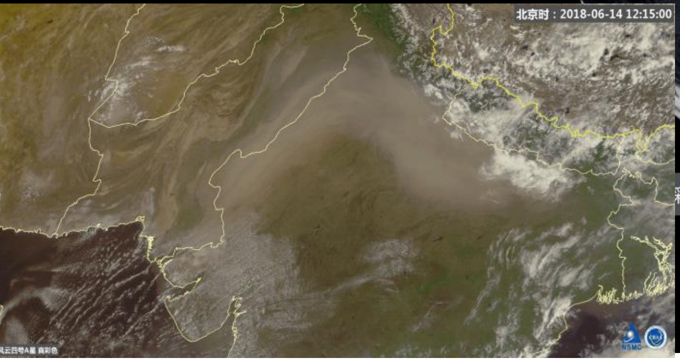
静止气象卫星

气象卫星作用和优势：

1. 全球全天候无缝隙观测，实现对地球大气和环境综合探测
2. 局地高频次观测，实现对自然灾害和环境事件的动态观测







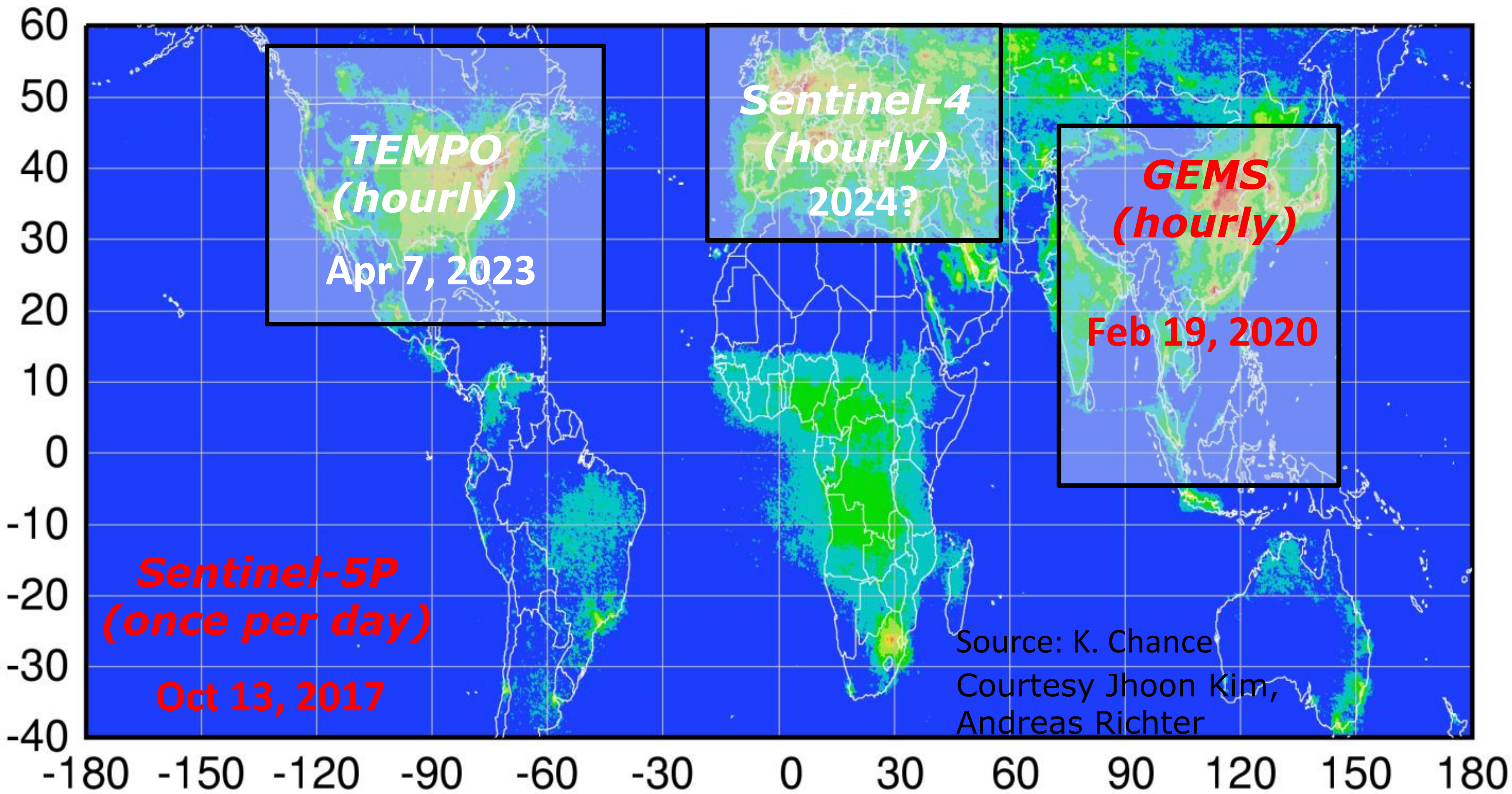
彩色

观测特点：

1. 轨道高度约35800公里，与地球自转同步，观测区域相对固定
2. 可每15分钟获取地球全圆盘图像；每5分钟对中国区域进行高频扫描。

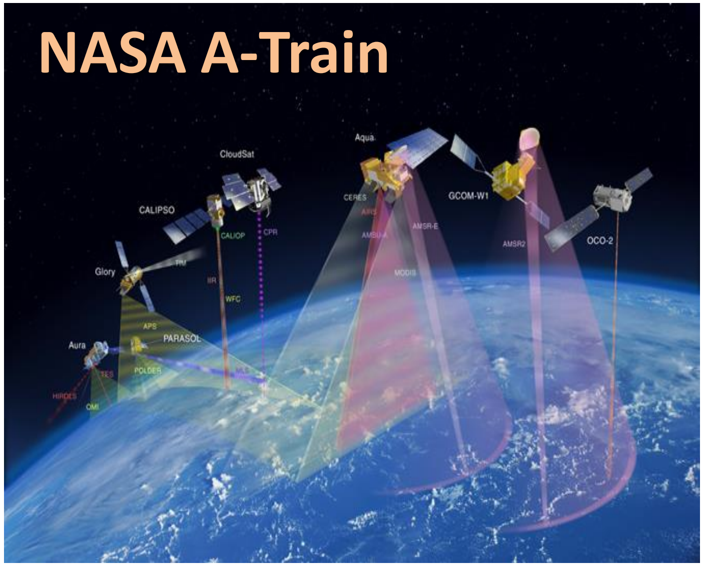
张鹏

High-Resolution Geostationary and Polar Orbiting Satellite Measurements of NO_2 and Other Tracers



NO_2 sensors: GOME, SCIAMACHY, OMI, GOME-2A/B, OMPS, TROPOMI, GEMS…

Modern Satellite Remote Sensing of Air Pollutants

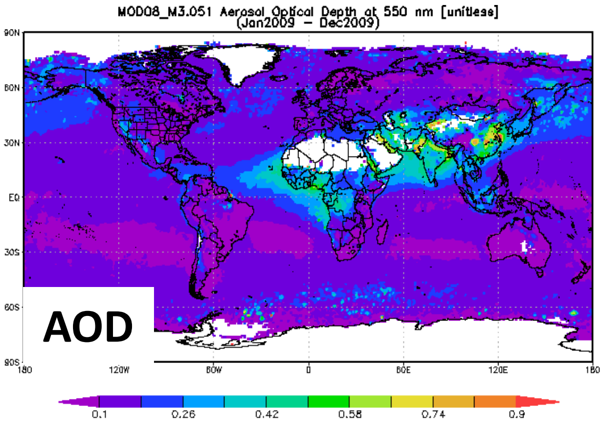


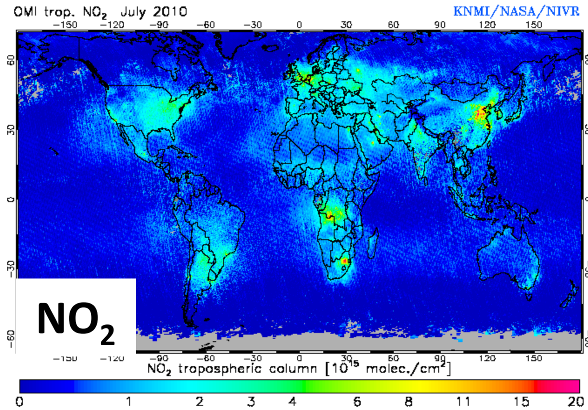
Advantages:

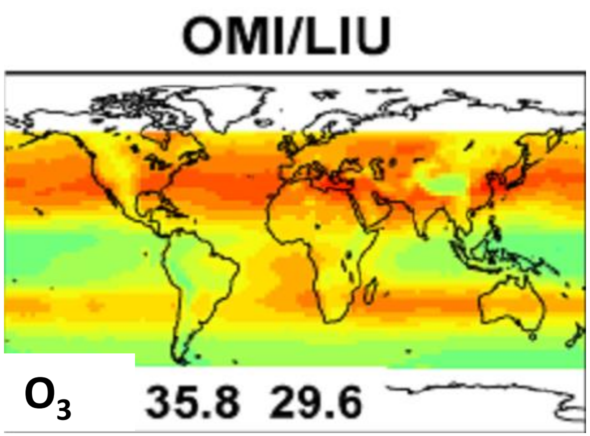
- Near real-time
- Multiple species
- Excellent spatial coverage
- Long-term data
- High resolution data
- Easily accessible & verifiable

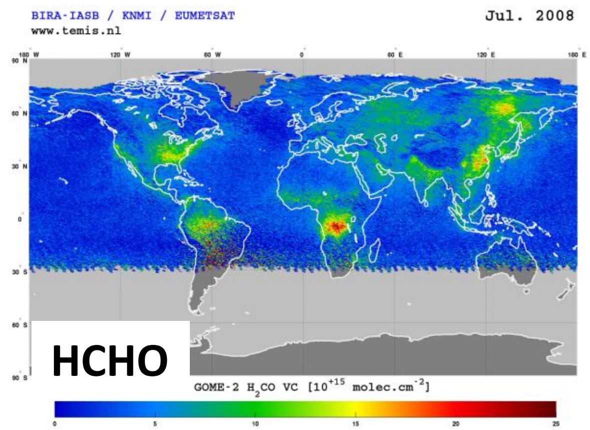
- ➢ Aerosols: MODIS, MISR, CALIOP, FY
- • O_3: OMI, TES, AIRS, MLS, FY
- • CO: TES, MOPITT, IASI, FY
- • NH_3: TES, IASI, CrIS, FY
- • ISOP: CrIS
- ✓ NO_2: TROPOMI, OMI, GEMS, FY
- ✓ SO_2: OMI, TROPOMI, GEMS, FY
- ✓ HCHO: OMI, TROPOMI, GEMS

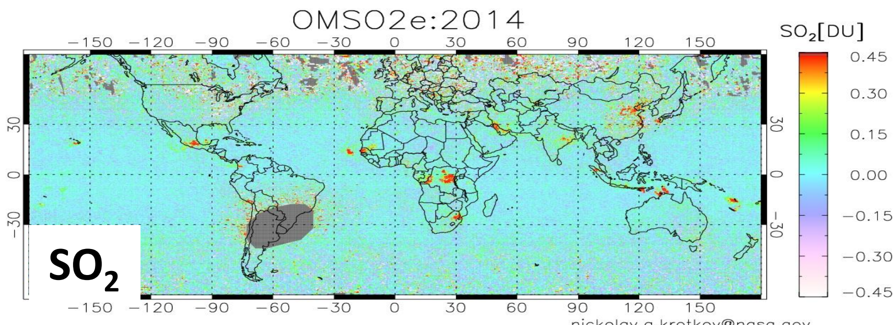
Satellite Measurements of Global Air Pollution







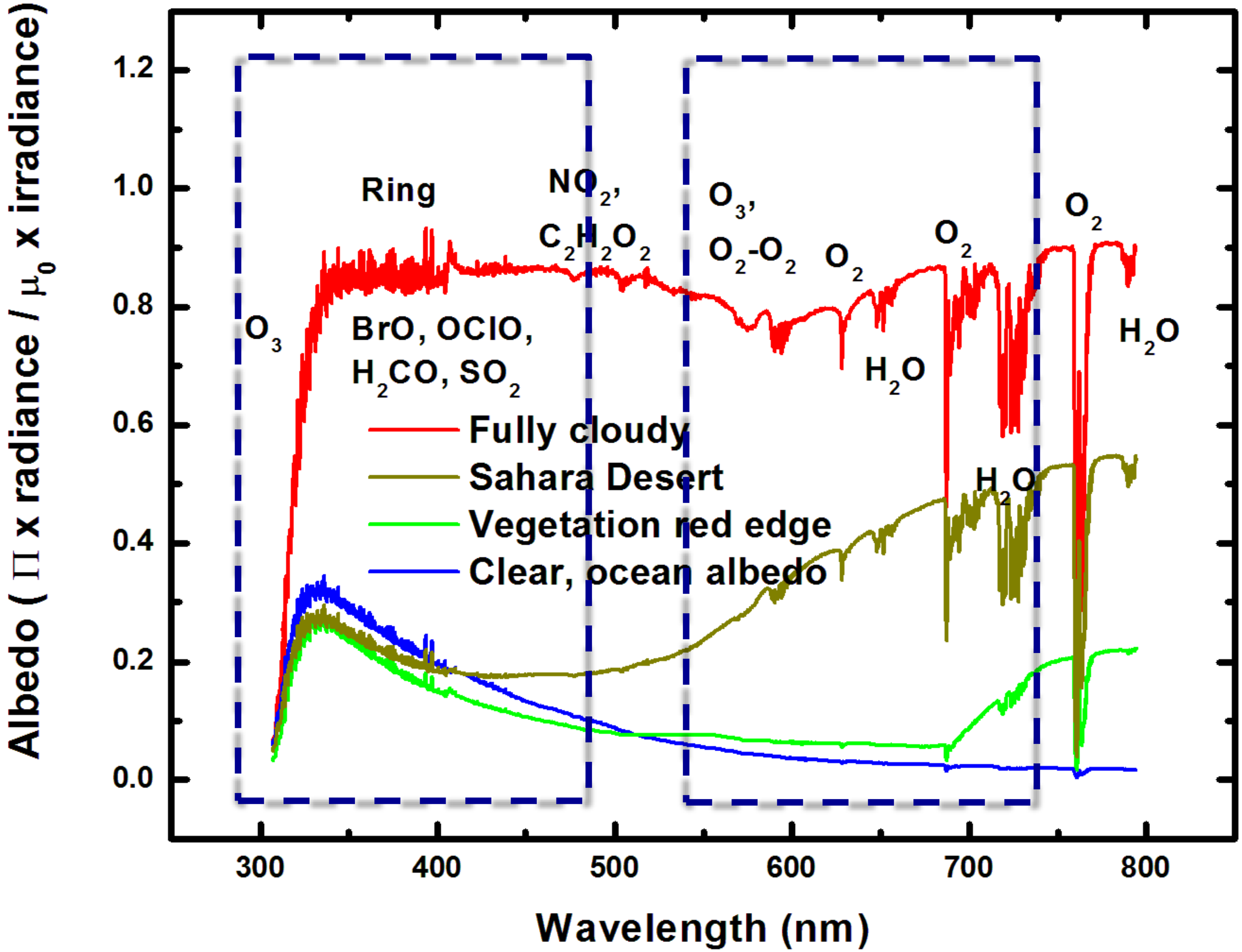




Satellite data applications:

- **High-resolution monitoring & forecast**
- **Local-regional-global scale pollution & transport**
- **Trends and variability**
- **Emission constraint**
- **Impacts assessment**

Reflectance Spectra at VIS-NI (from ESA GOME-1)

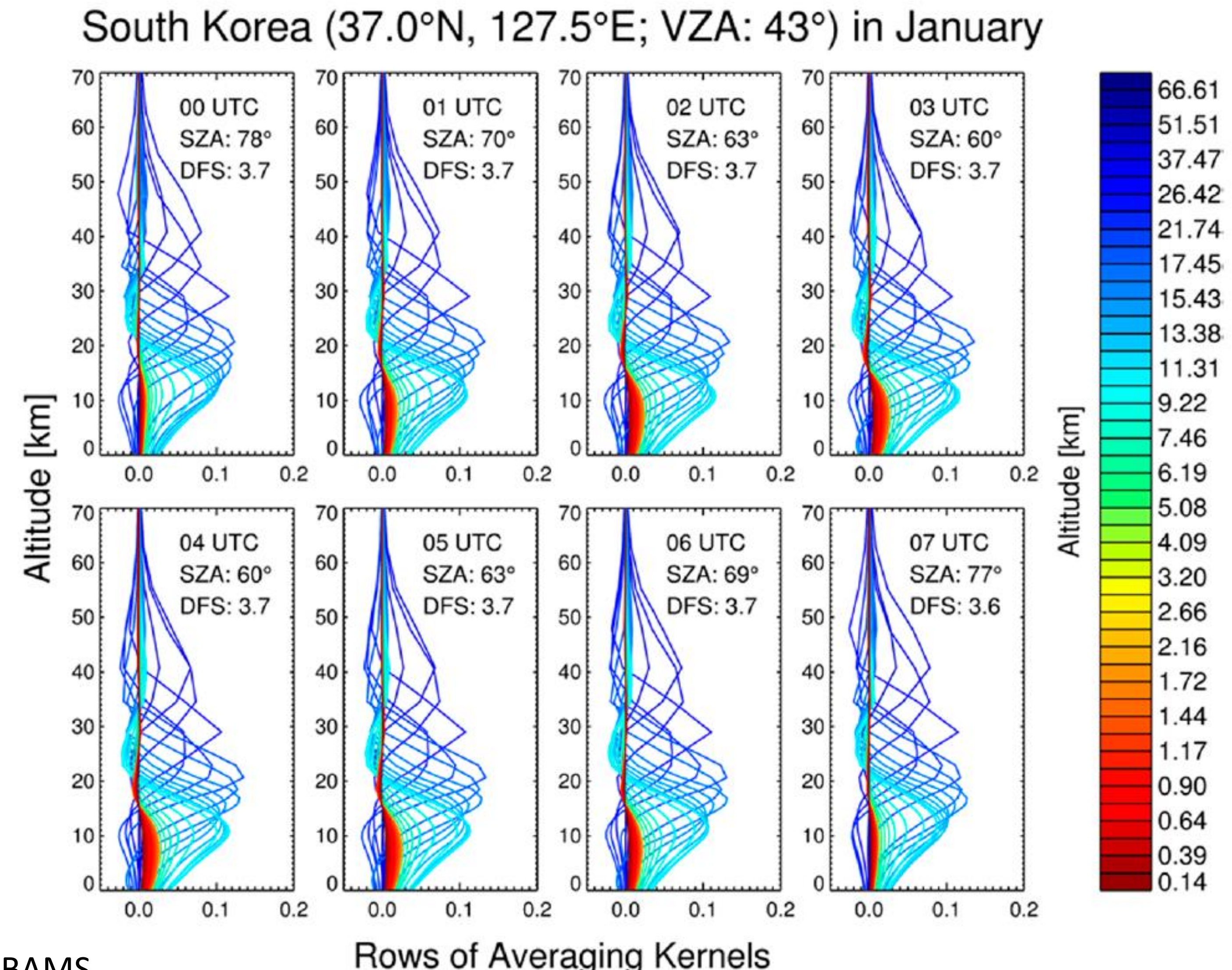


Adopted from Kelly Chance

Averaging Kernel and Air Mass Factor

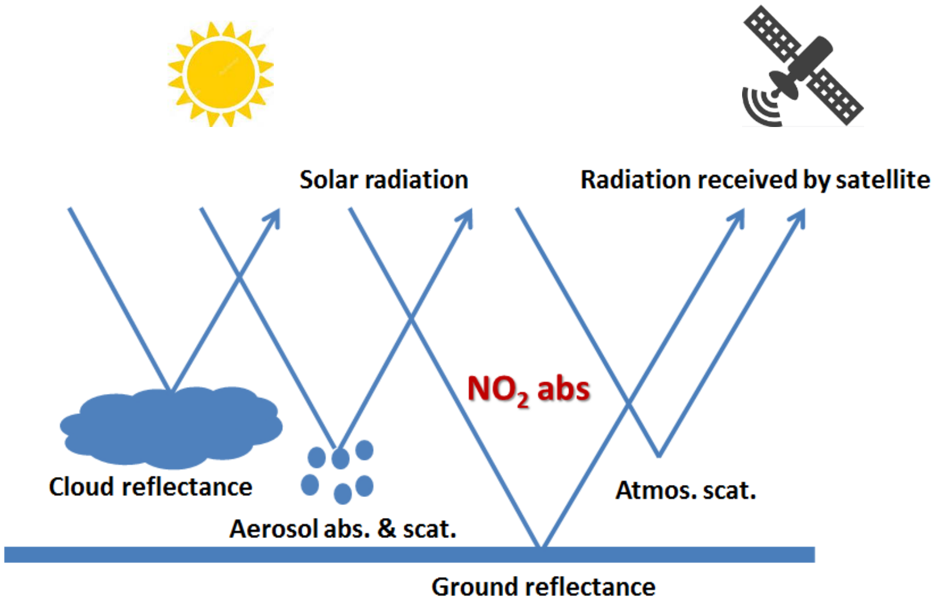
$$\mathbf{A} = \frac{\partial \hat{\boldsymbol{x}}}{\partial \boldsymbol{x}}$$

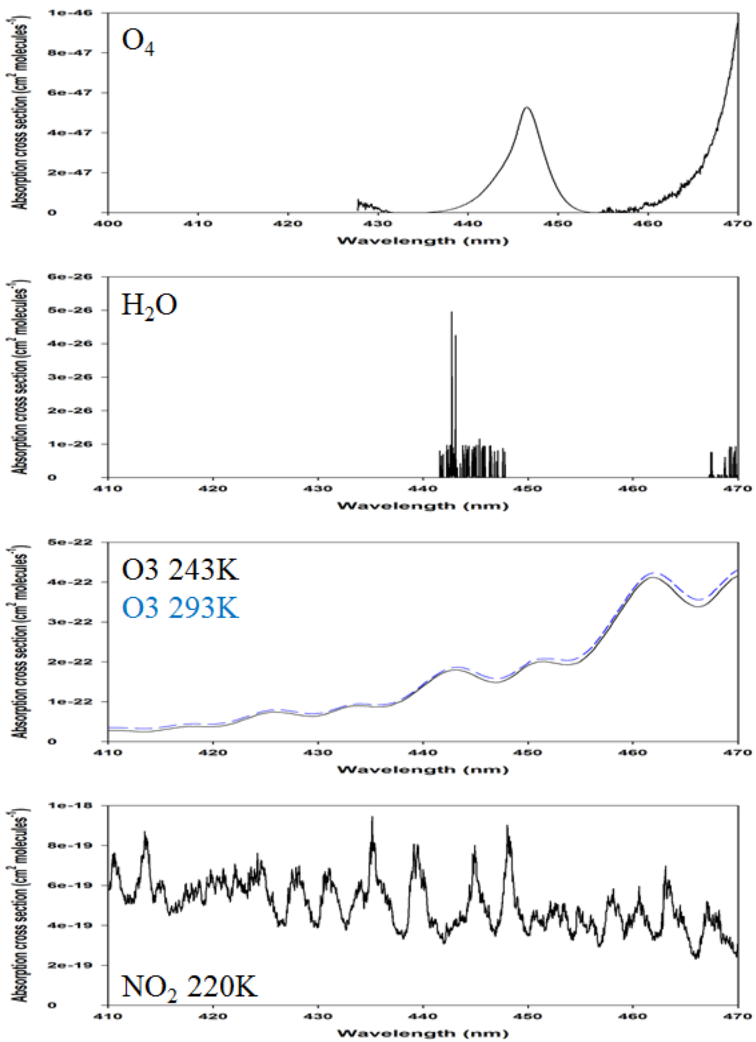
For O_3



Kim et al., 2020, BAMS

DOAS Approach to Retrieving NO_2, SO_2, HCHO, CHOCHO from Satellite Remote Sensing





$$I(\lambda) = I_0(\lambda)e^{-\sum_i \sigma_i(\lambda)N_{s,i} + \sum_j a_j \lambda^j}$$

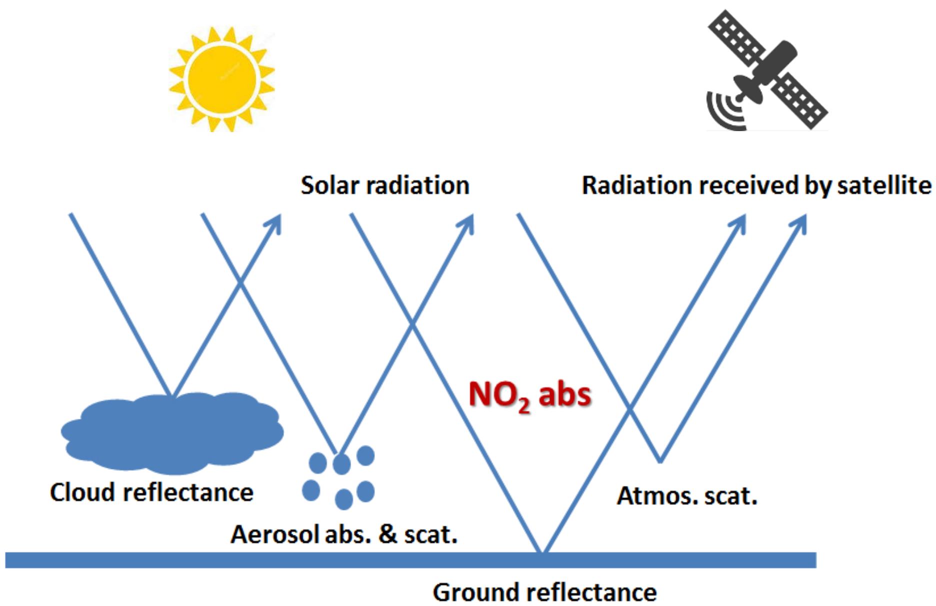
DOAS

$$\ln\left(\frac{I(\lambda)}{I_0(\lambda)}\right) = -\sum_i \sigma_i(\lambda)N_{s,i} + \sum_j a_j \lambda^j$$

Retrieving NO_2 from Satellite Remote Sensing

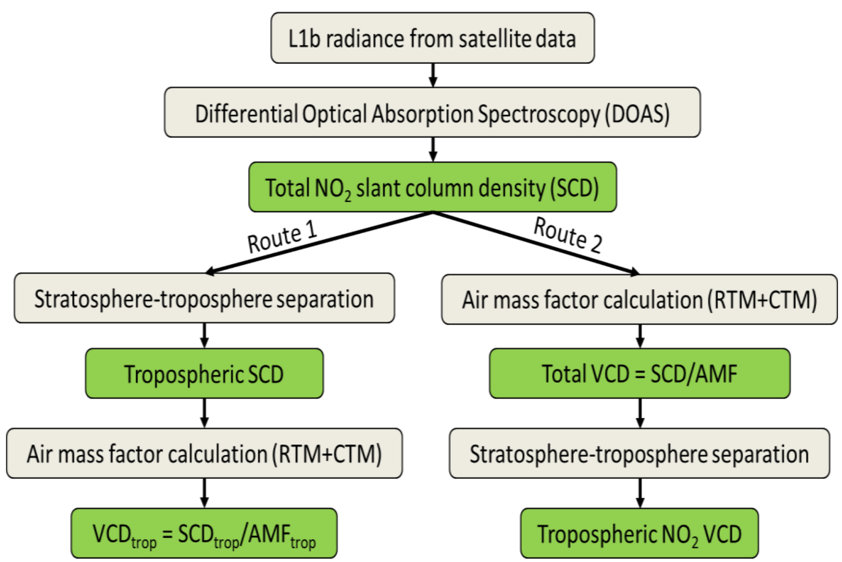
DOAS method to derive total SCD:

$$I(\lambda) = I_0(\lambda) e^{-\sum_i \sigma_i(\lambda) S_i + \sum_j a_j \lambda^j}$$



From total SCD to tropospheric VCD:

$$\Omega_t = \frac{S_t}{M_t} = \frac{S - S_s}{M_t}$$

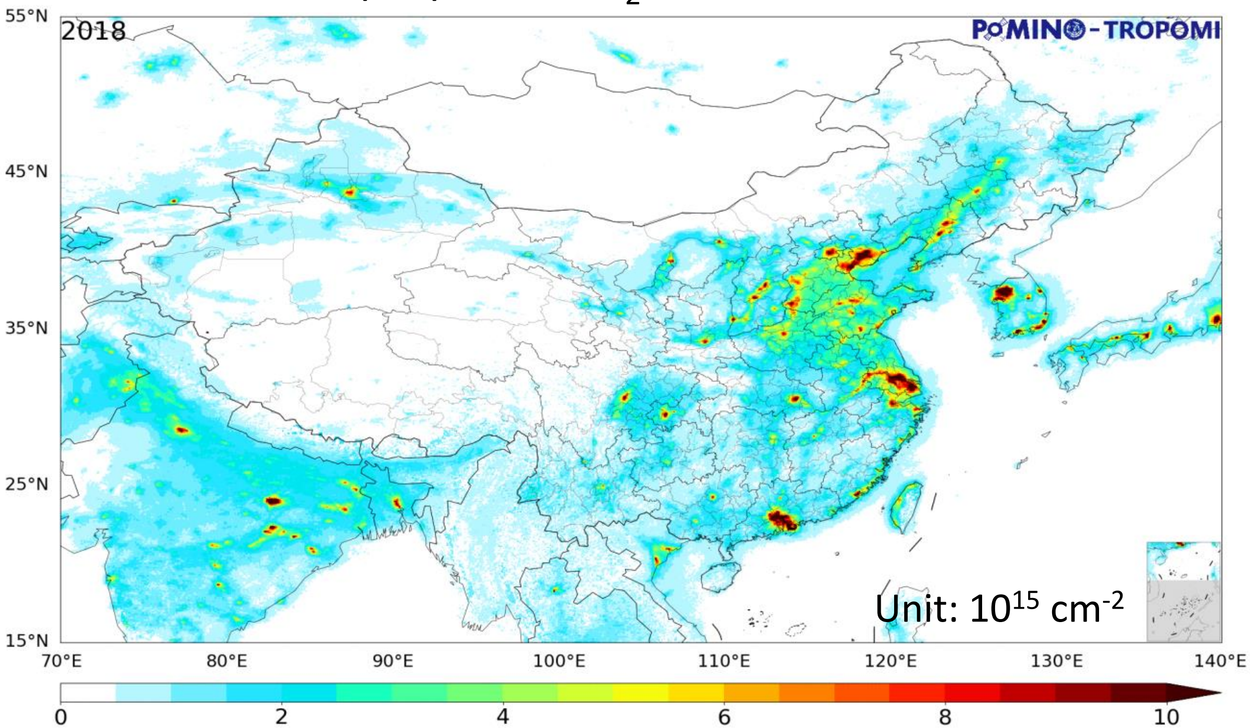


POMINO NO_2 VCD Products for OMI, TROPOMI & GEMS

http://www.pku-atmos-acm.org/acmProduct.php

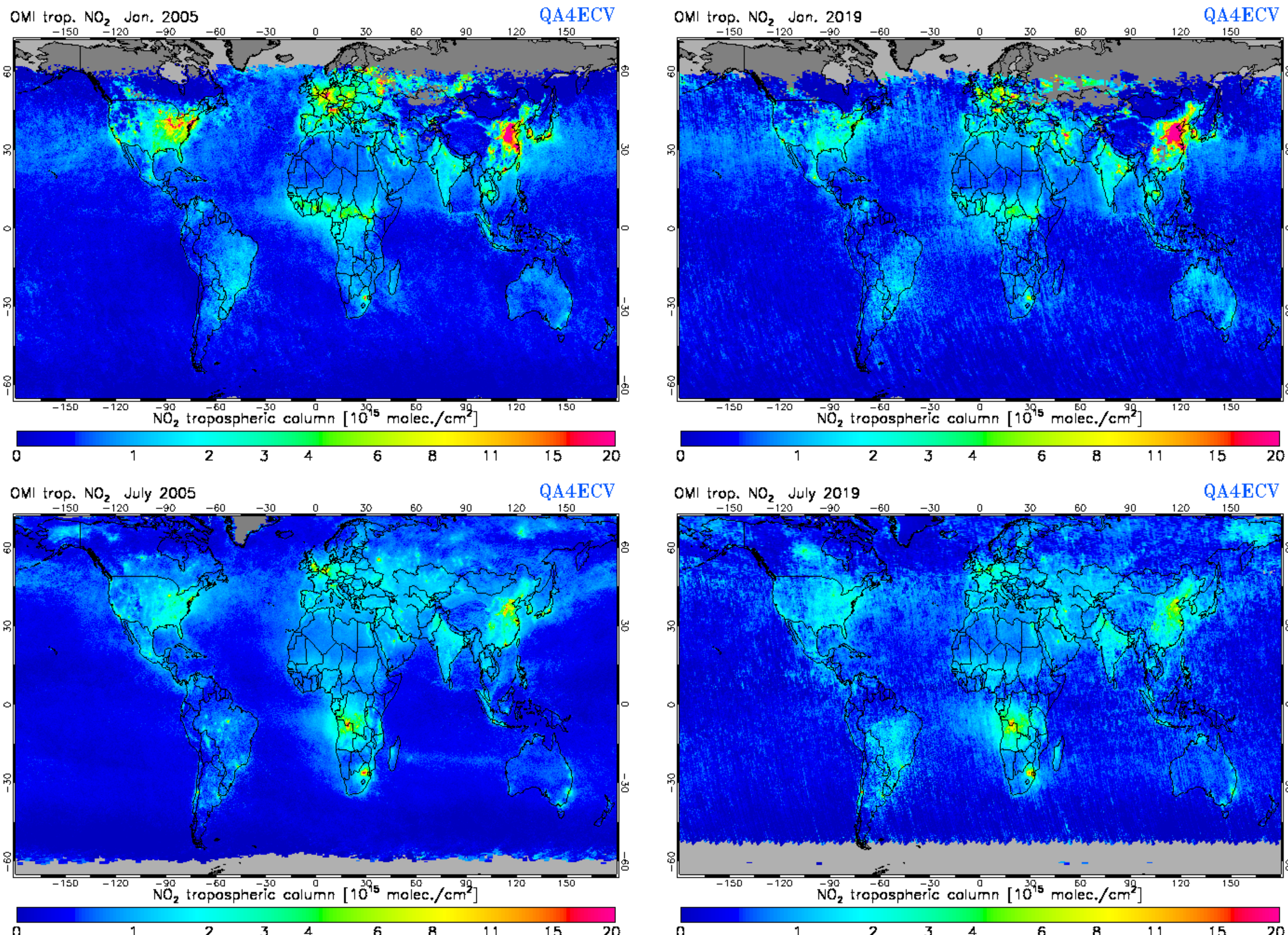
All Level-2 and Level-3 data are freely available (2004-present)

5 km-res Tropospheric NO_2 VCDs in JJA 2018–2022



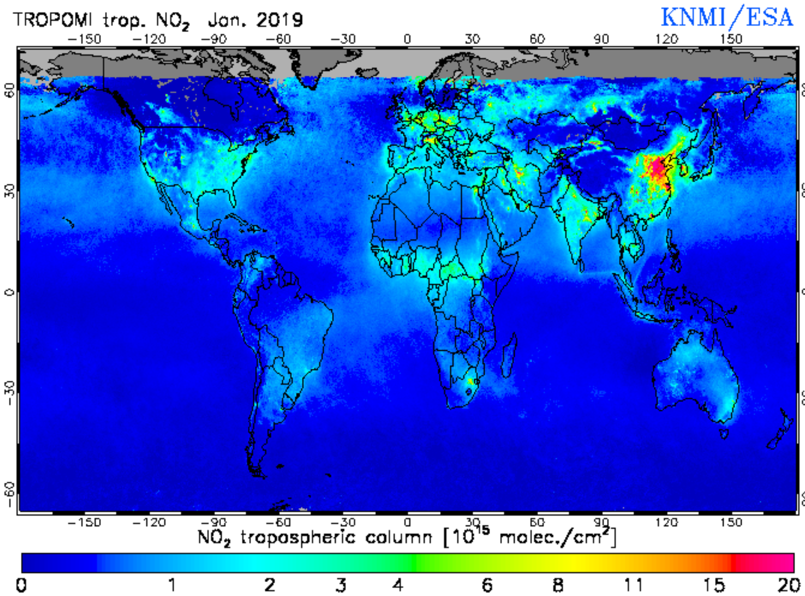
Lin et al., ACP, 2014
Lin et al., ACP, 2015
Liu et al., AMT, 2019
Liu et al., AMT, 2020
Zhang et al., NRSB, 2022
Zhang et al., AMT, 2023
Zhang et al., AMT, 2025

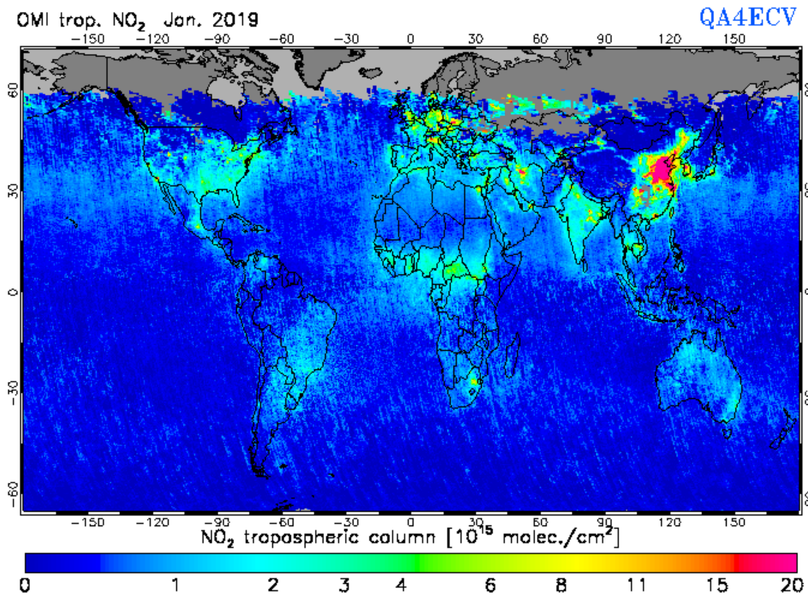
OMI-Retrieved Tropospheric NO_2 Column: 2005-2019

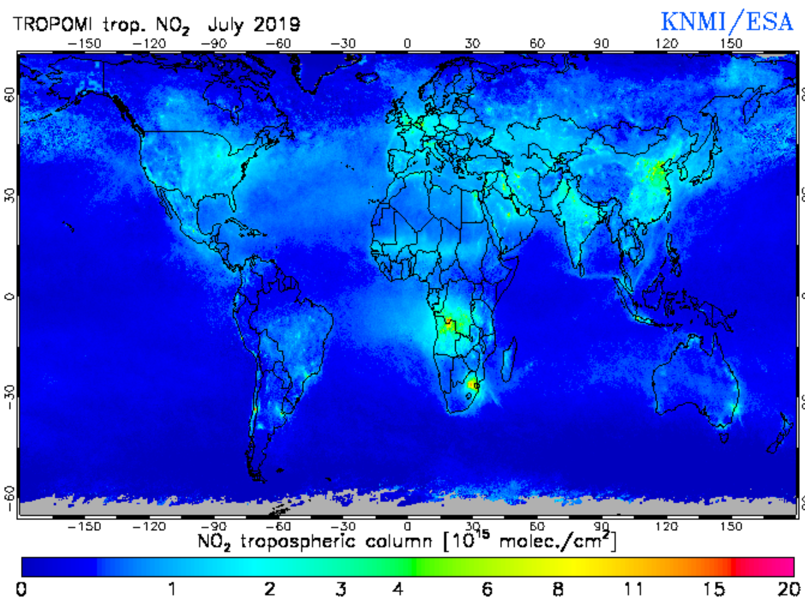


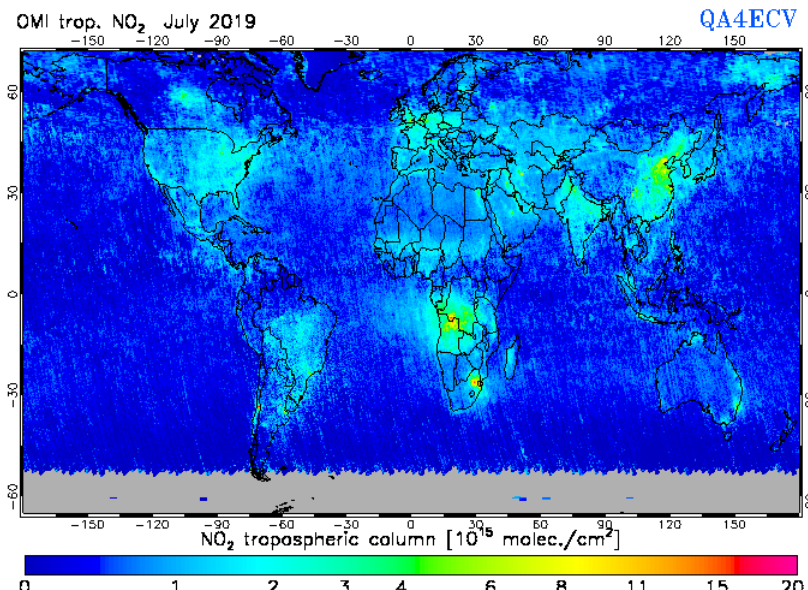
www.temis.nl

Tropospheric NO_2 Column: OMI versus TROPOMI





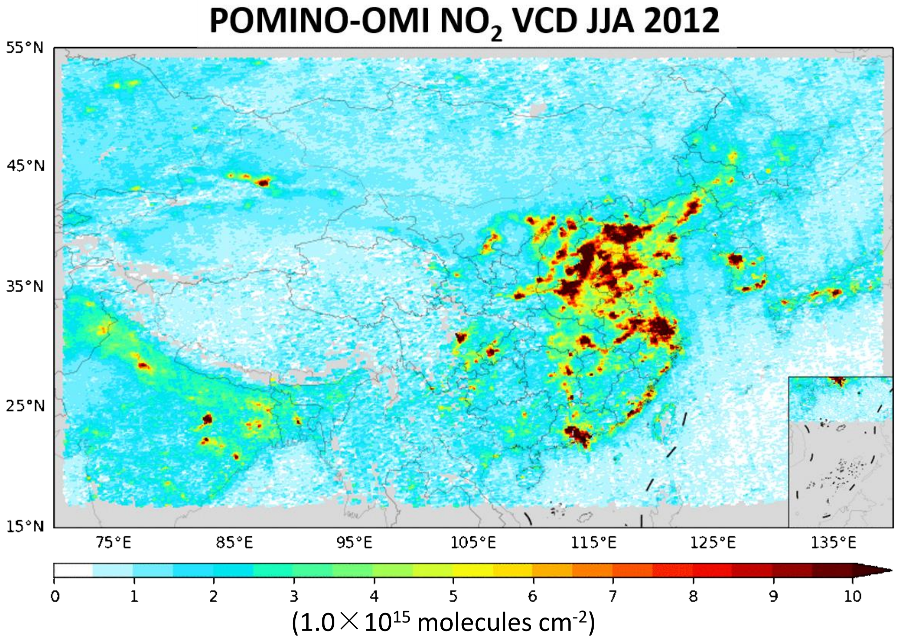




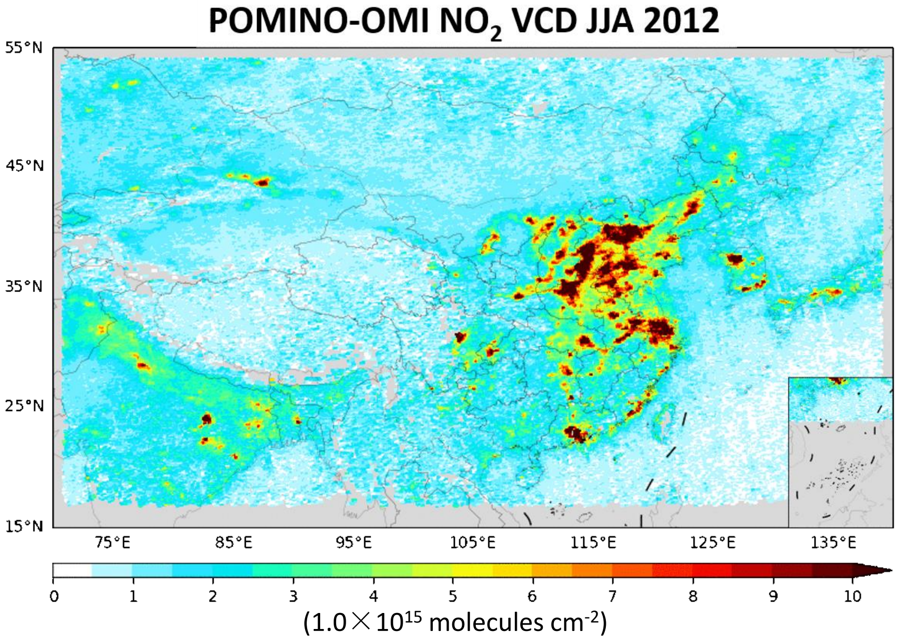
www.temis.nl

De-striping OMI NO_2 VCDs based on Empirical Distribution

Before de-striping



After de-striping

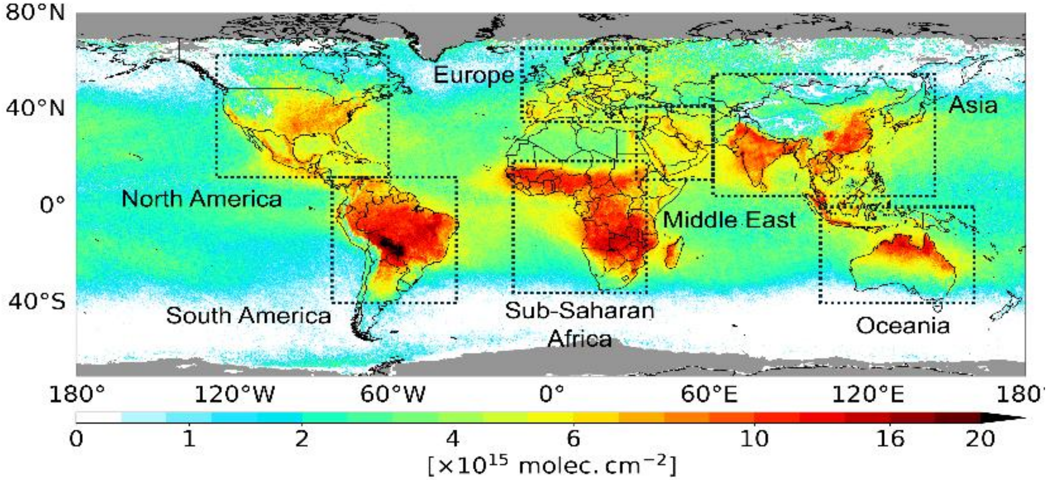


Kong et al., submitted

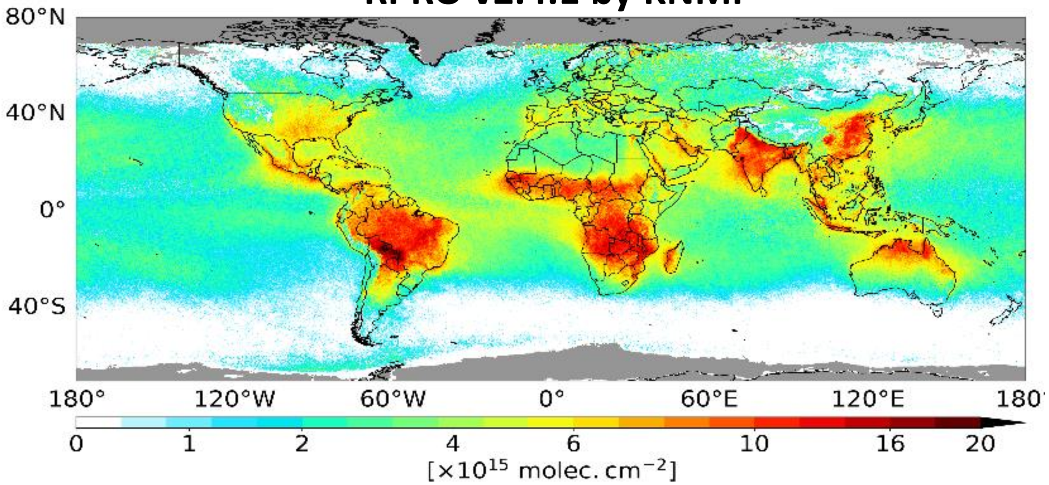
Global TROPOMI HCHO VCDs

Tropospheric HCHO VCDs (April, July, October 2021, and January 2022)

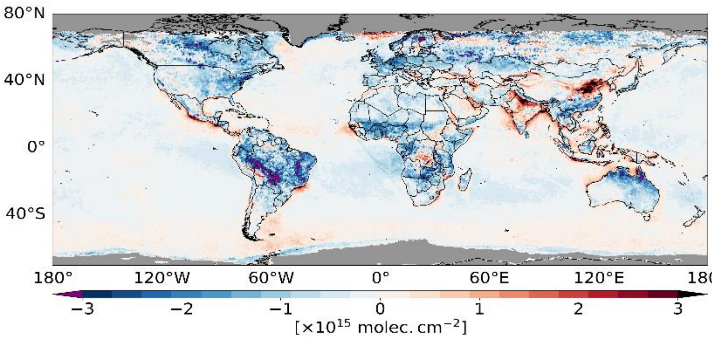
POMINO



RPRO v2.4.1 by KNMI

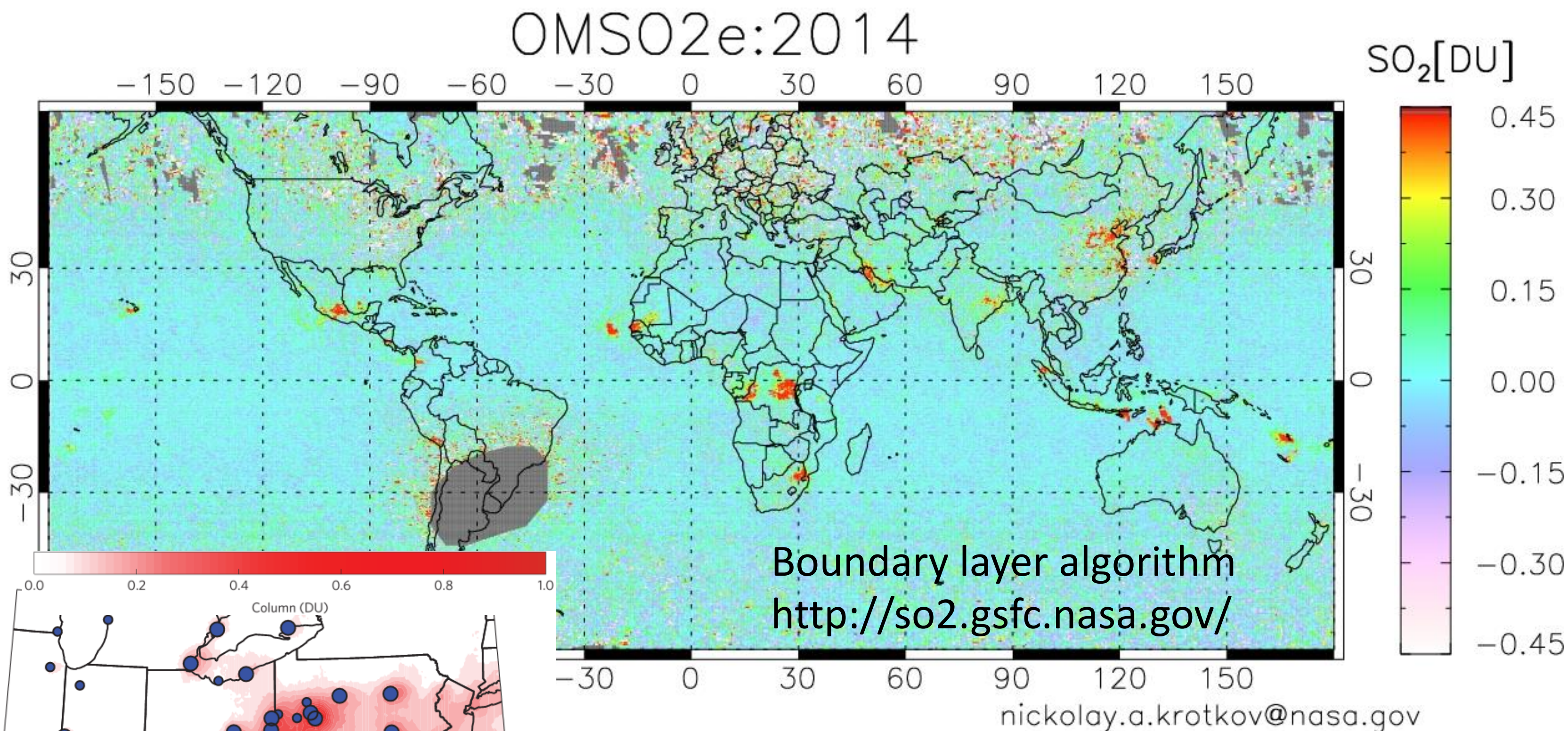


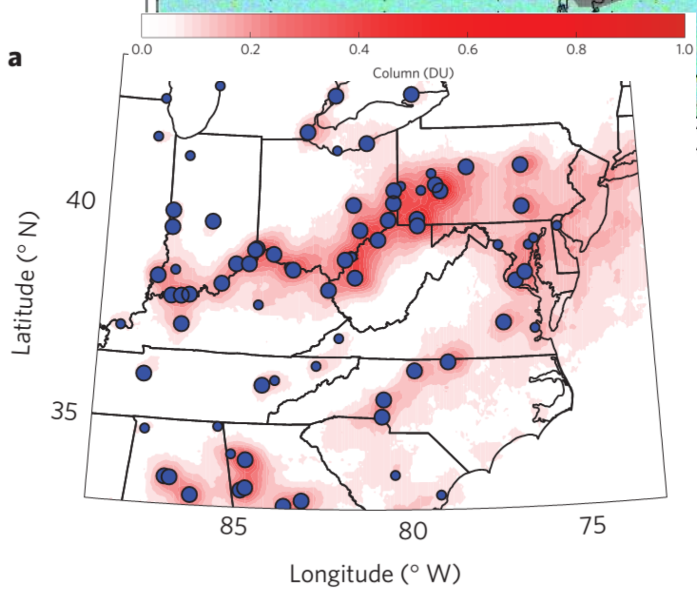
RPRO minus POMINO



Zhang et al., AMT, 2025

OMI-retrieved VCDs of Tropospheric SO_2

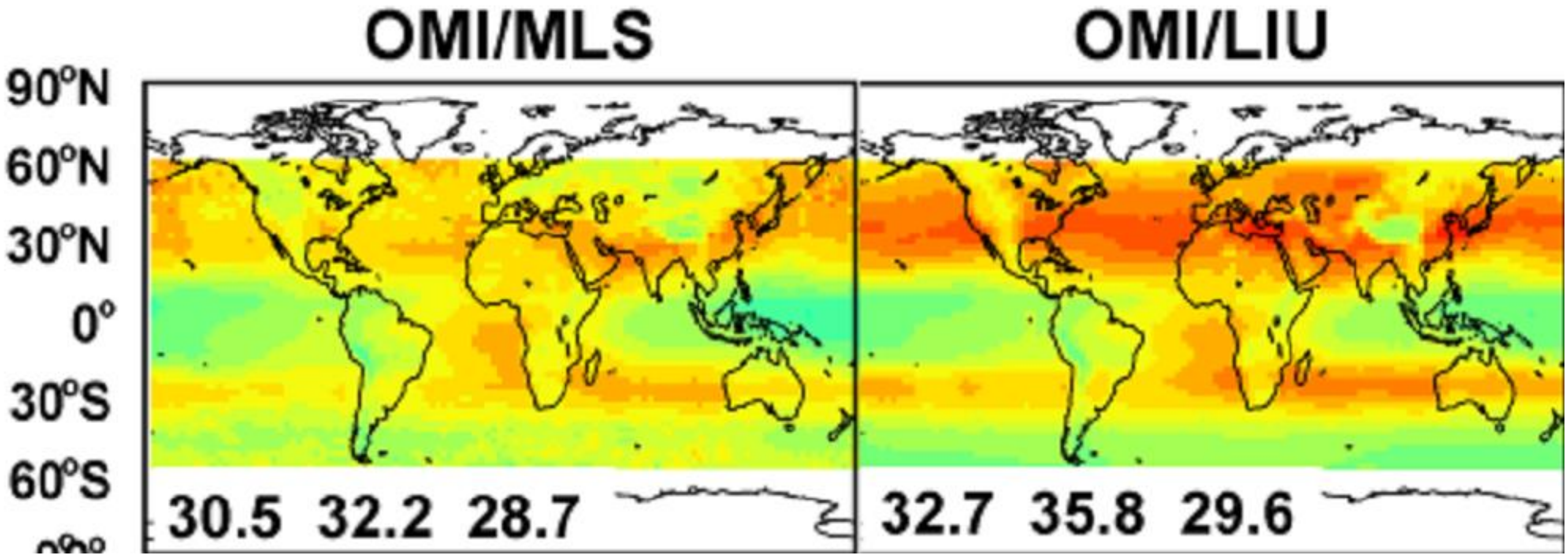




Mclinden et al., 2016, Nature Geoscience

OMI-retrieved VCDs of Tropospheric Ozone

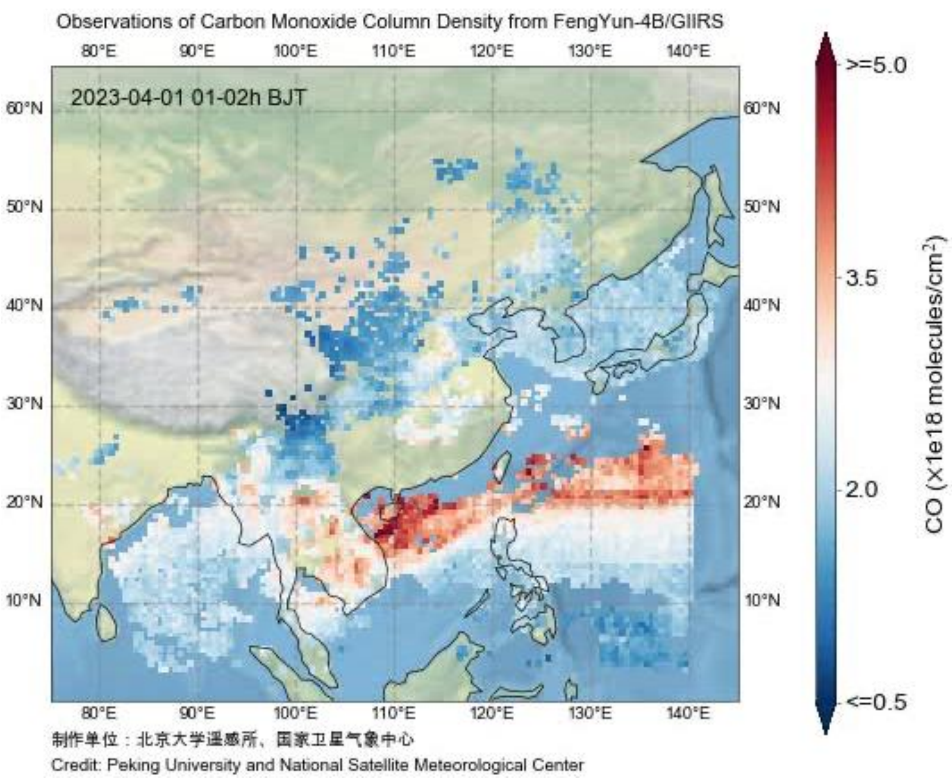
Annual mean in 2009 (DU)



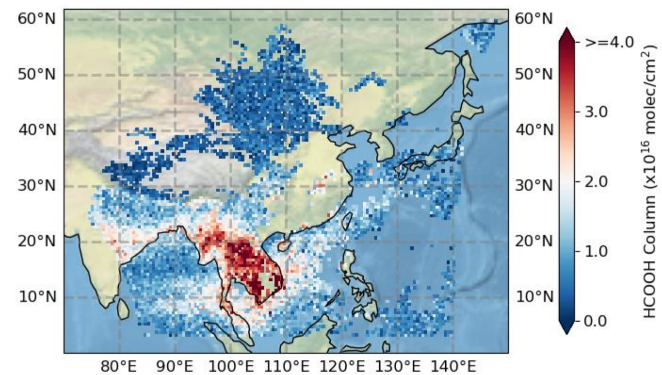
Yan et al., 2016

FY-4B/GIIRS 干涉式大气垂直探测仪

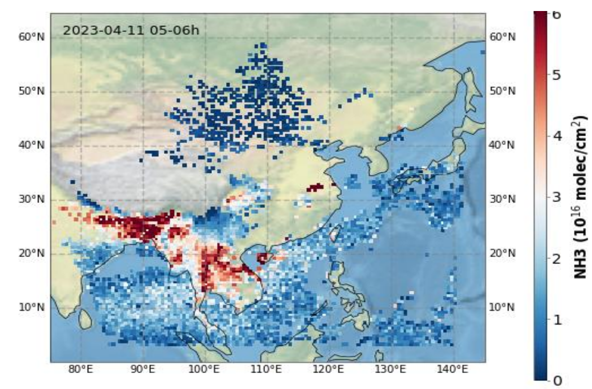
(a) 一氧化碳



(b) 甲酸



(c) 氨气



Zeng AMT 2023a,b; Zeng 2024 JGR-Atmosphere

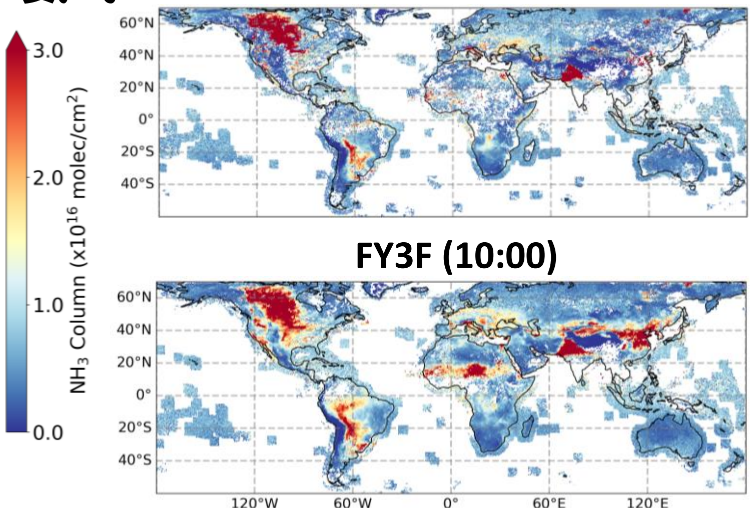
曾招城@北大遥感所

FY-3E/F HIRAS 红外高光谱大气垂直探测仪

氨气

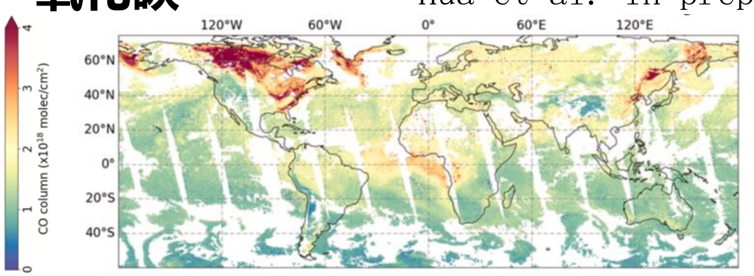
FY3E (05:30)

FY3F (10:00)

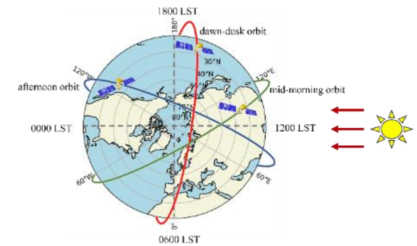


一氧化碳

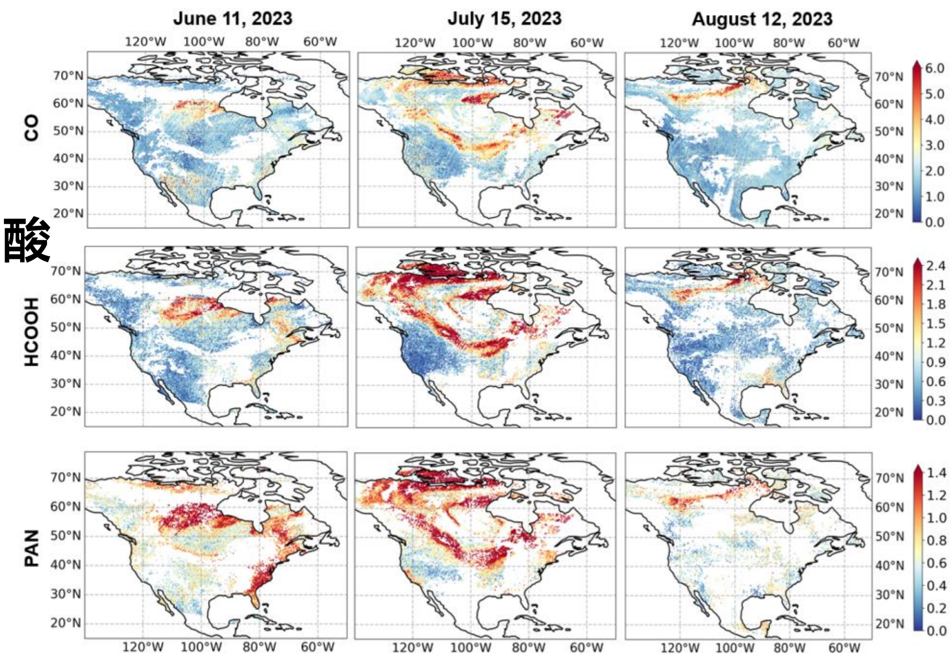
Hua et al. in prep.



Zeng et al. 2025 JQSRT



甲酸

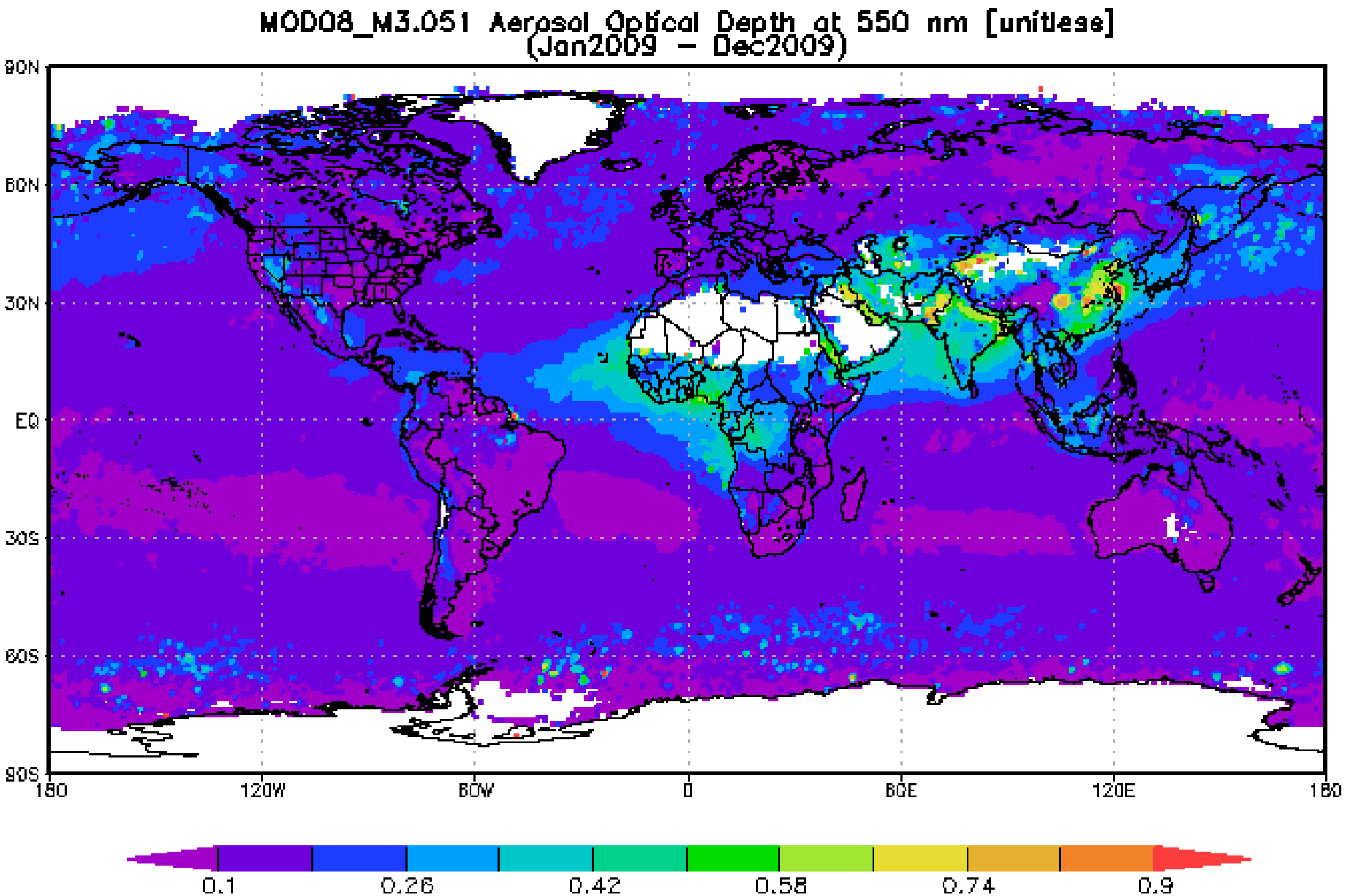


过氧乙酰硝酸酯

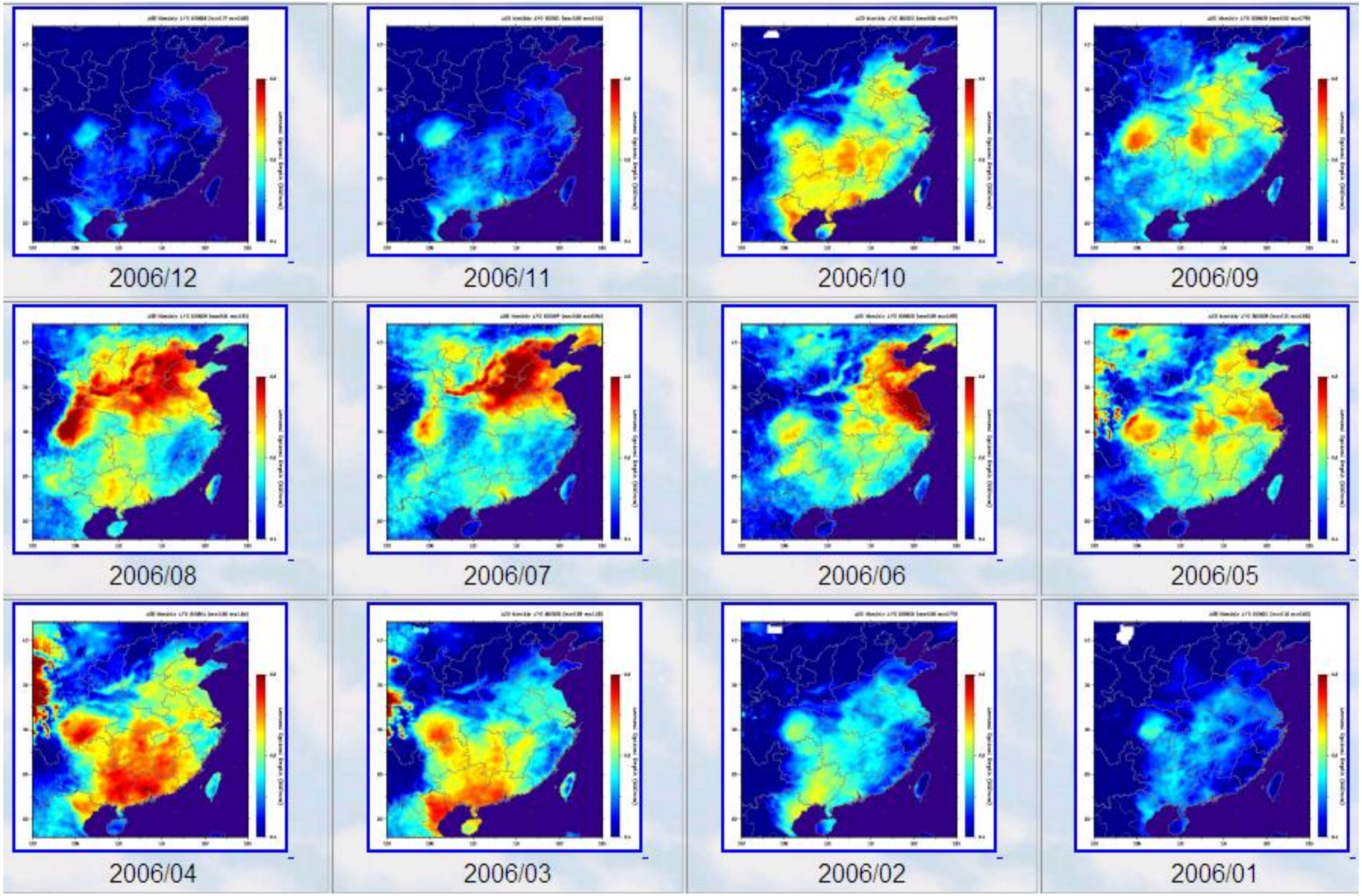
Hua et al. RSE, in revision

曾招城@北大遥感所

MODIS AOD in 2009

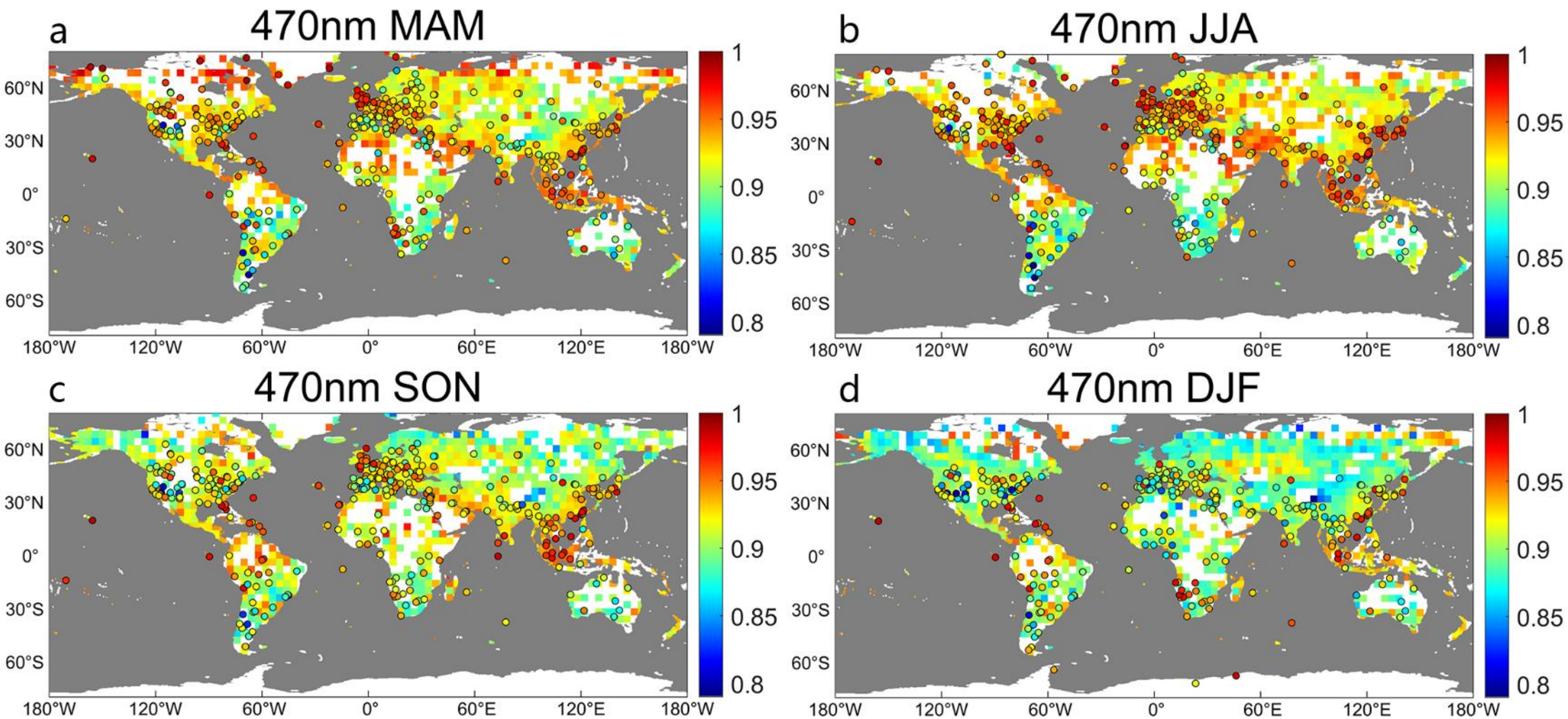


MODIS Monthly AOD at Kilometer Resolution



Li et al., 2003

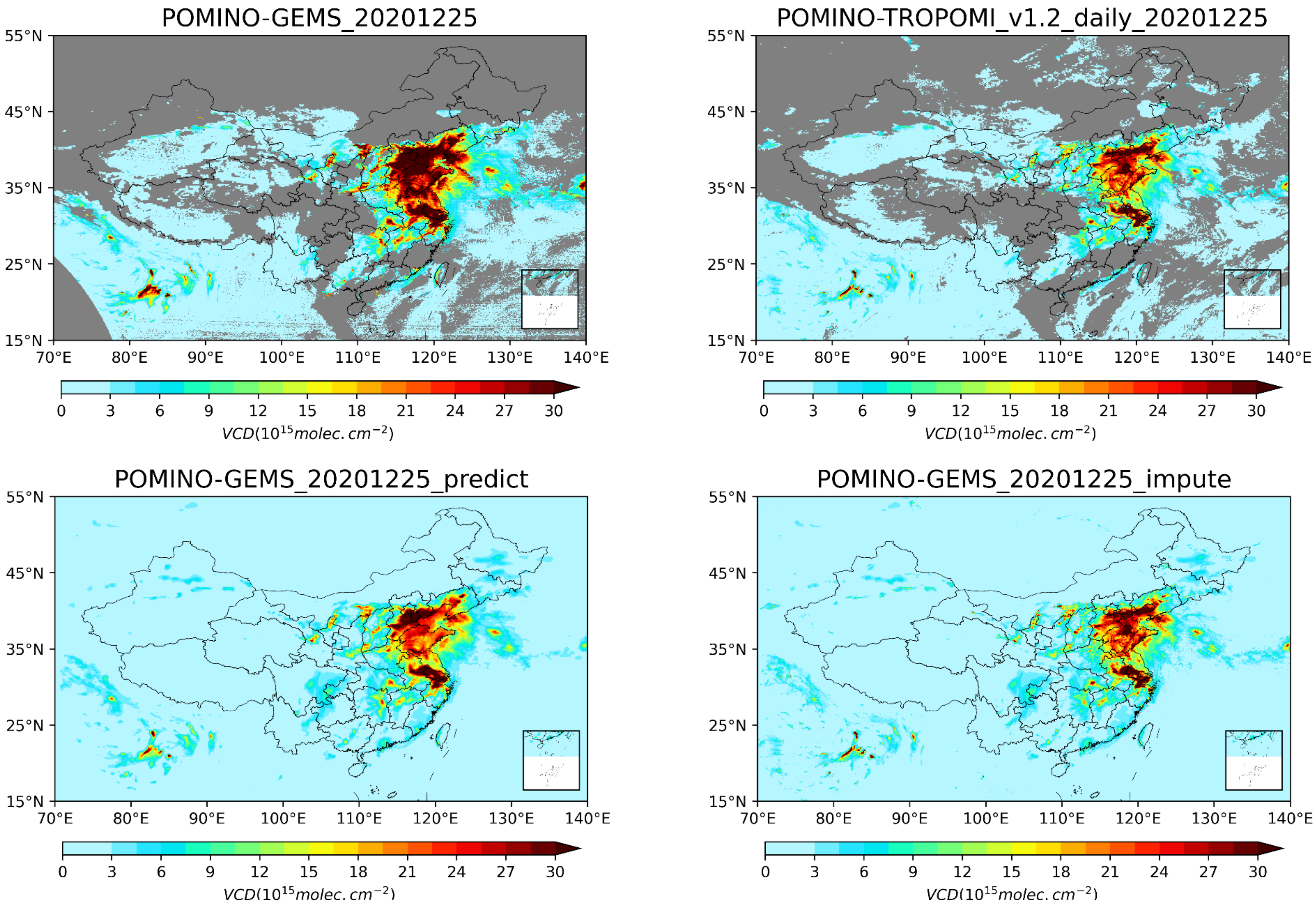
MODIS-VIS Single Scattering Albedo Retrieval



Jing Li

Gap Filling for Satellite Data: NO_2

GEMS + GEOS-CF + UNet → TROPOMI



Wang et al., in prep

云知道——大气环境遥感数据平台

大气环境遥感服务

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林金泰	秦凯	毛飞跃	朱雷	沈路	张羽中	朱丽叶	白开旭

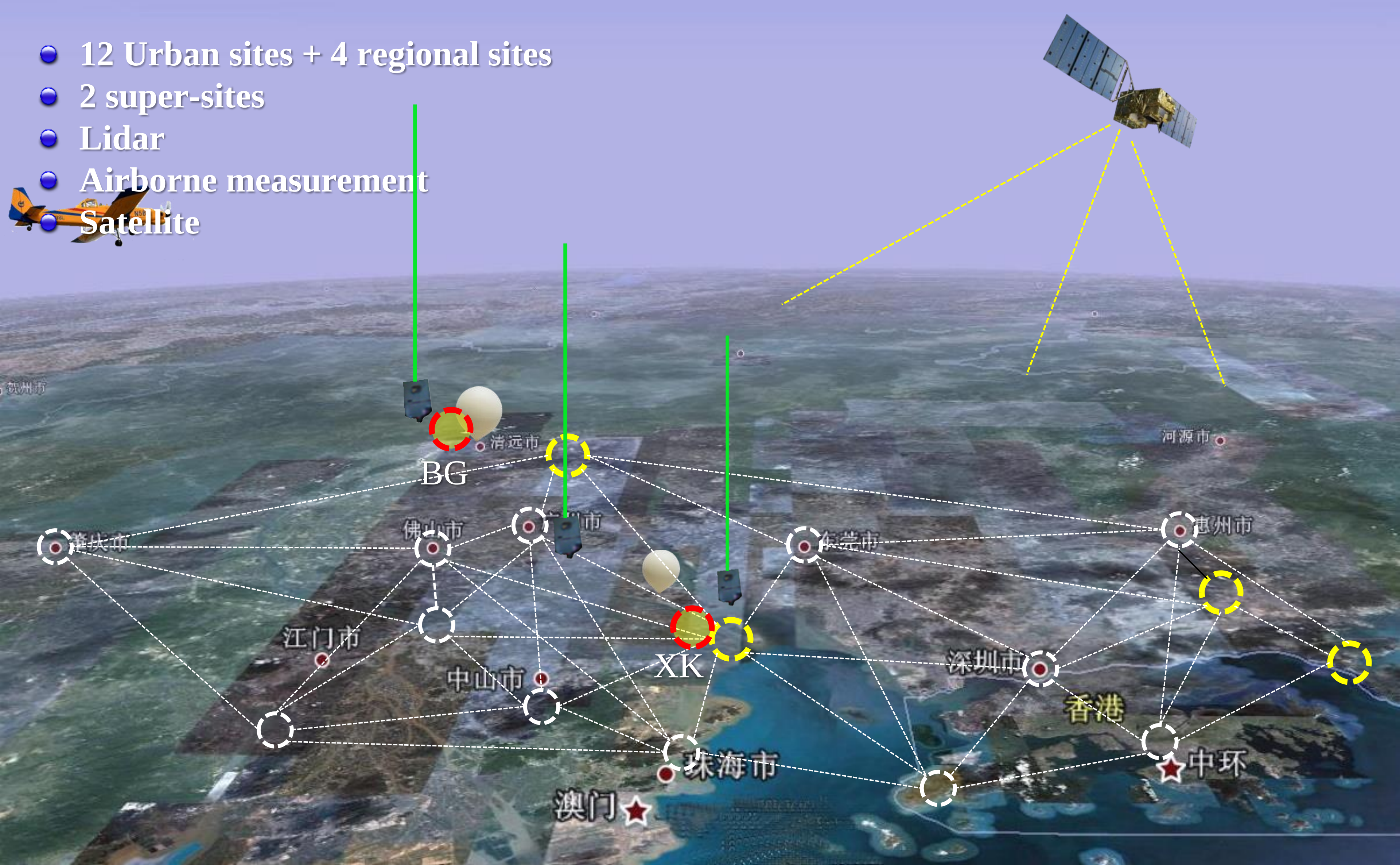
Field Campaign

- **Measurement campaigns: intensive measurements of targets (e.g., pollutants) in a short period (weeks to months), employing a variety of instruments.**
- **TRACE-P**
- **ICARTT**
- **INTEX-B**
- **ARCTAS**
- **PRIDE-PRD**
- **CAREBEIJING**
- **……**

✓ **Aircraft measurements are used in these campaigns**

PRIDE-PRD 2004, 2006, 2008

- 12 Urban sites + 4 regional sites
- 2 super-sites
- Lidar
- Airborne measurement
- Satellite

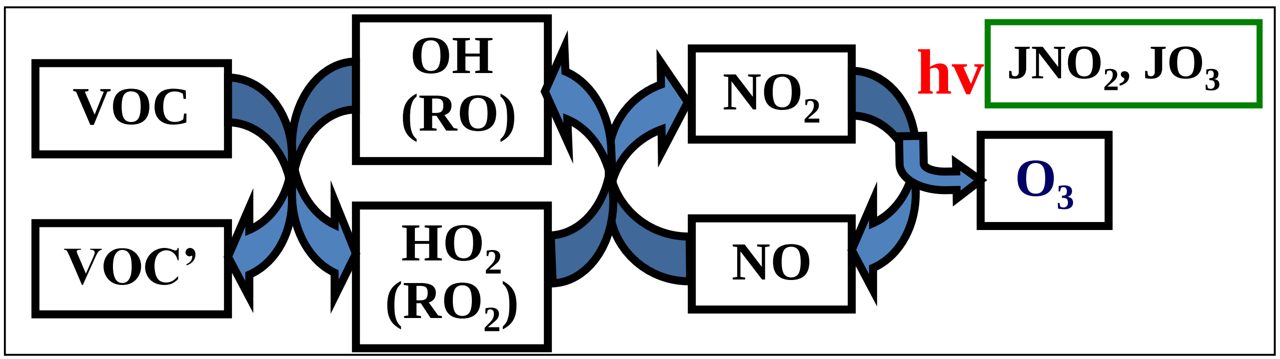


Field Campaign Measurement Parameters

Gases:

- O_3, NOx, NOy, CO, SO_2
- H_2O_2, ROx VOCs,
- HNO_2, HNO_3, HCl, NH_3
- OVOCs, OH, H_2SO_4

Process:
radicals
photolysis rates

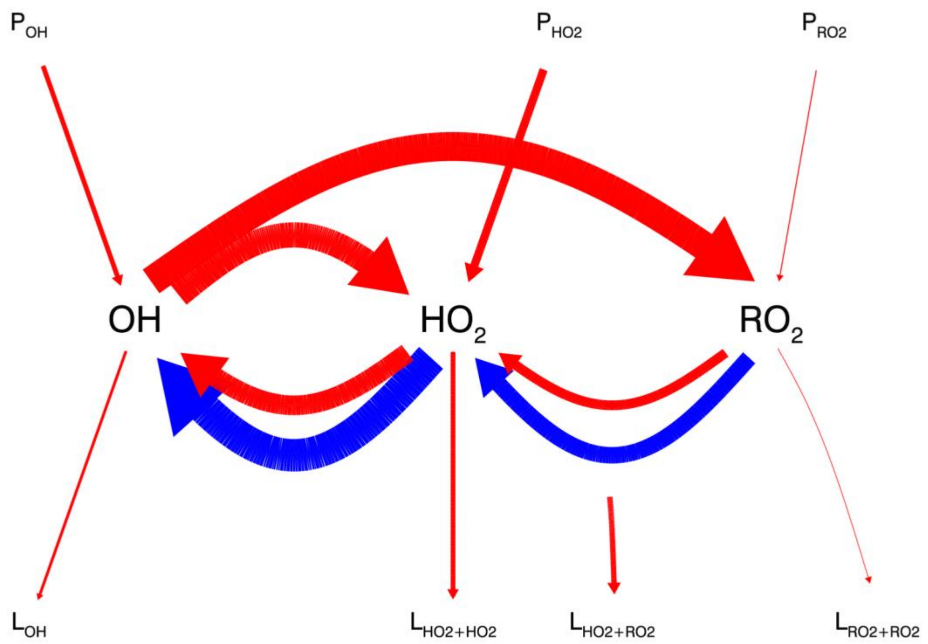


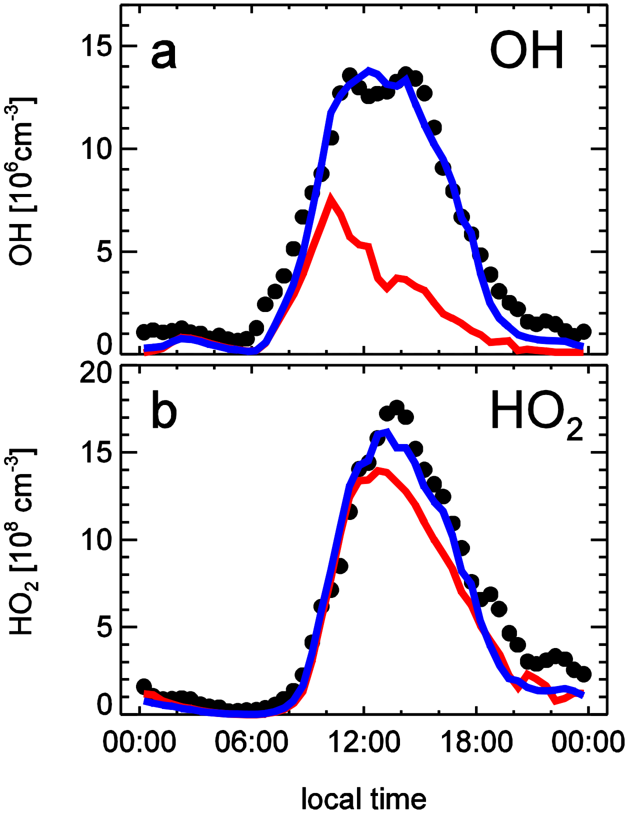
Particles:
Size distribution
Optical property
Chemical comp.

- Trace elements, ions, OC/EC, POM, WSOC
- SO_4^{2-}, NO_3^-, NH_4^+, Cl-
- Na^+, K^+, Ca^{2+}, Mg^{2+}
- PM, Number distribution (0.01-10 um)
- Light scattering, Light absorption

Unknown OH Recycle Mechanism Inferred from Campaign

Low NOx, high ISOP situation





Hofzumahaus et al. "Amplified Trace Gas Removal in the Troposphere." Science 324(5935): 1702-1704.

Numerical Models in Atmospheric Research

- Type
  - Statistical model, AI model, physical model
  - Dynamic, process-based, parameterization
- Purpose
  - Meteorological, climate, ocean, sea ice, chemical transport, …, Earth system
- Dimension
  - Box model, 1-D, 2-D, 3-D
- Domain (scale)
  - Global, regional, urban, nested
- Proceeding
  - Forward, backward (back-trajectory), adjoint

Primitive Equations for Large-scale Motions

Meteorological and climate models are based on these equations

Hypsometric equation (hydrostatic)
$$\frac{\partial \Phi}{\partial p} = -\frac{RT}{p} \qquad d\Phi = g dz$$

Horizontal equation of motion
$$\frac{d\boldsymbol{V}(u,v)}{dt} = -\nabla\Phi - f\boldsymbol{k} \times \boldsymbol{V} + \boldsymbol{F}$$

Continuity equation
$$\frac{\partial \omega}{\partial p} = -\nabla \cdot \boldsymbol{V} \qquad \omega = \frac{dp}{dt}$$

Thermodynamic energy equation
$$\frac{dT}{dt} = \frac{\kappa T}{p}\omega + \frac{J}{c_p} \qquad \kappa = R/c_p$$

Bottom boundary condition
$$\frac{\partial p_s}{\partial t} = -(\boldsymbol{V} \cdot \nabla p\,)_s - \left(w\frac{\partial p}{\partial z}\right)_s - \int_0^{p_s} (\nabla \cdot \boldsymbol{V}) dp$$

Five unknowns
$$\mathbf{V}(u, v), \omega, \Phi, T$$

Wallace and Hobbs, 2006

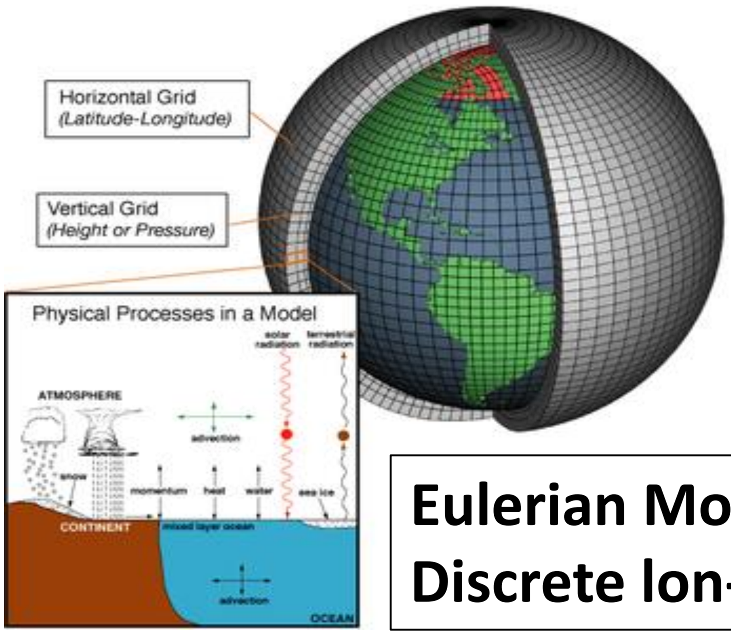
J and $\boldsymbol{F}$ need to be parameterized

Atmospheric Chemical Transport Modeling

Emis Dep Transport & Mixing Chemistry

$$\frac{\partial C}{\partial t} = E - D - \nabla \cdot C\boldsymbol{V} - \nabla \cdot \overline{C'\boldsymbol{V}'} + (P - L)$$

Grid-resolved Unresolved

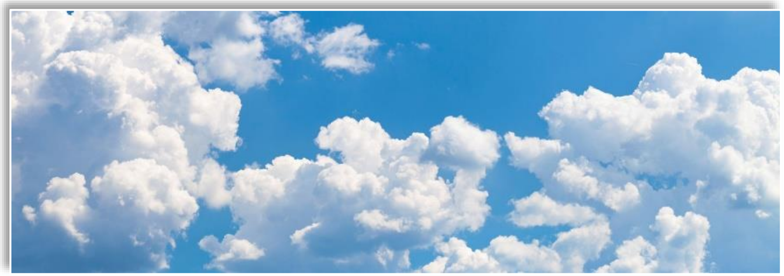


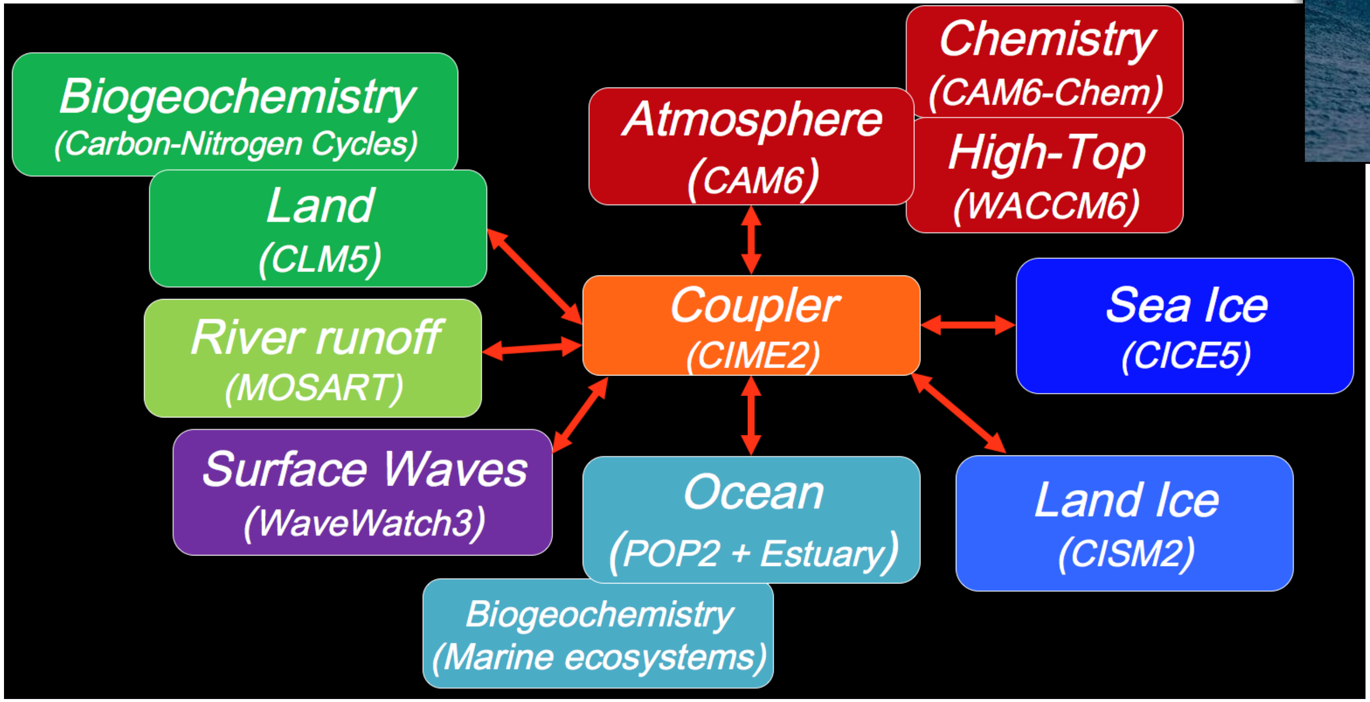
**Eulerian Model:
Discrete lon-lat grid**

Atmospheric chemical transport models:

– Simulating spatiotemporal variations of trace species after they or their precursors are emitted into the atmosphere

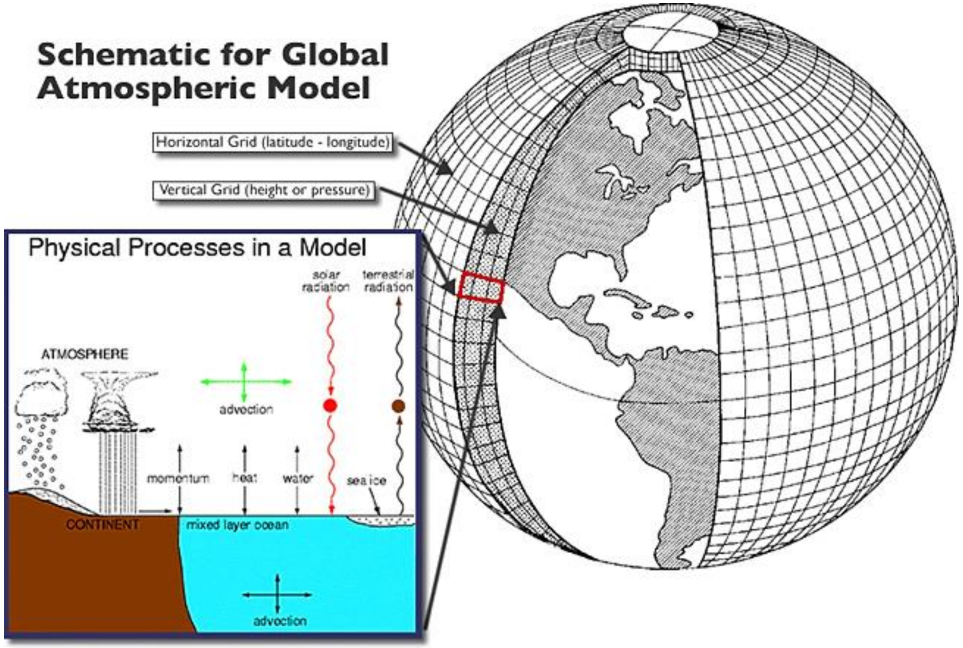
Chemistry in Earth System Models





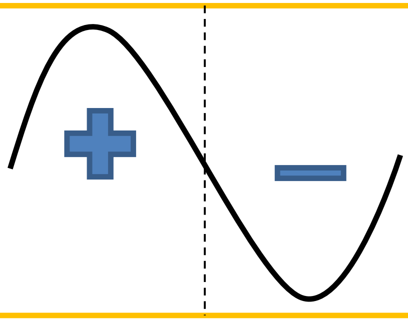
J.-F. Lamarque

Numerical Modeling of Atmosphere



Initial conditions → Governing equations / Parameterizations / Numerical dissipation / Boundary conditions ? → Evolution of atmosphere

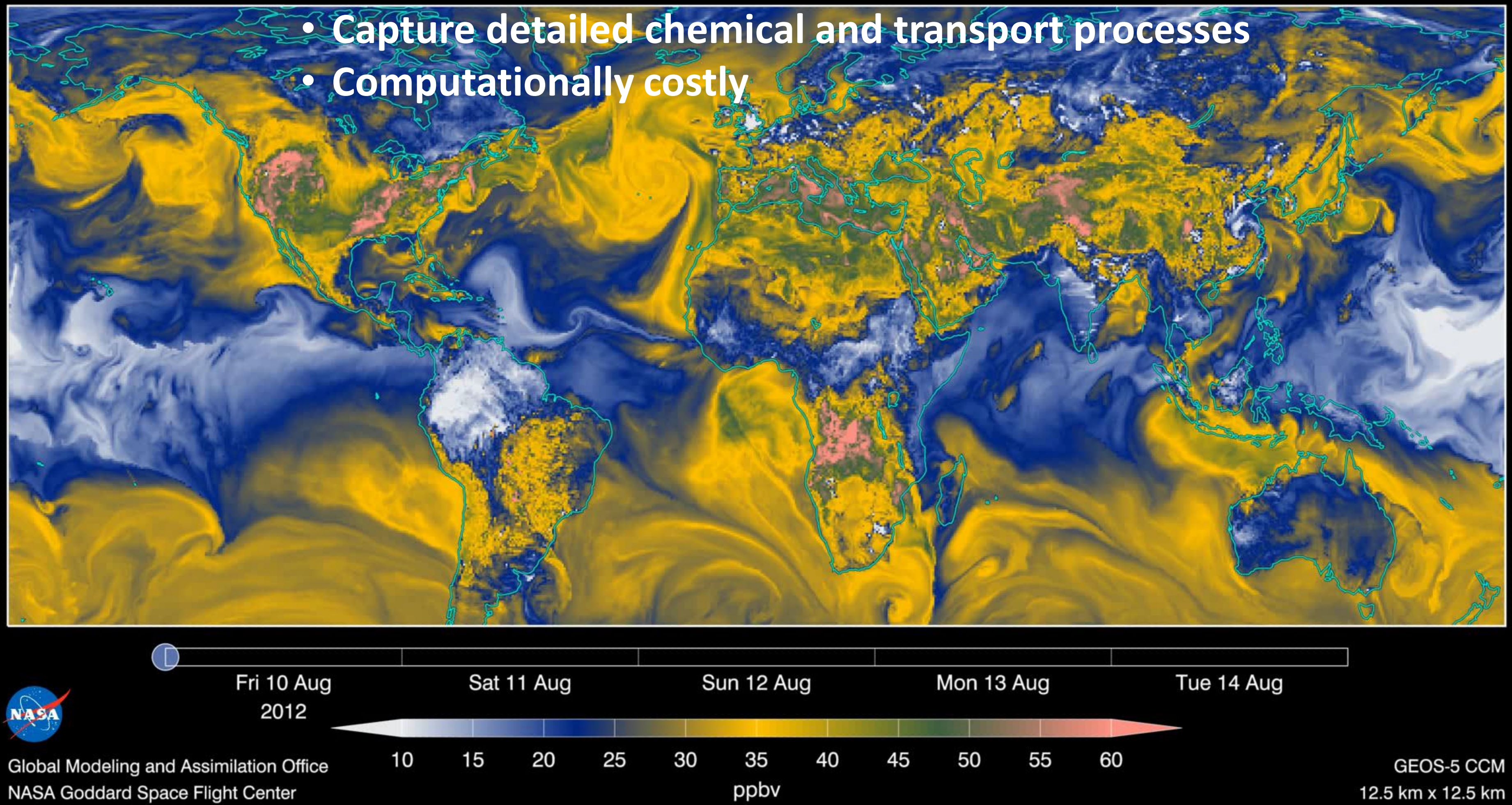
Resolution
&
Parameterization



Global High-Resolution Simulation of Surface Ozone

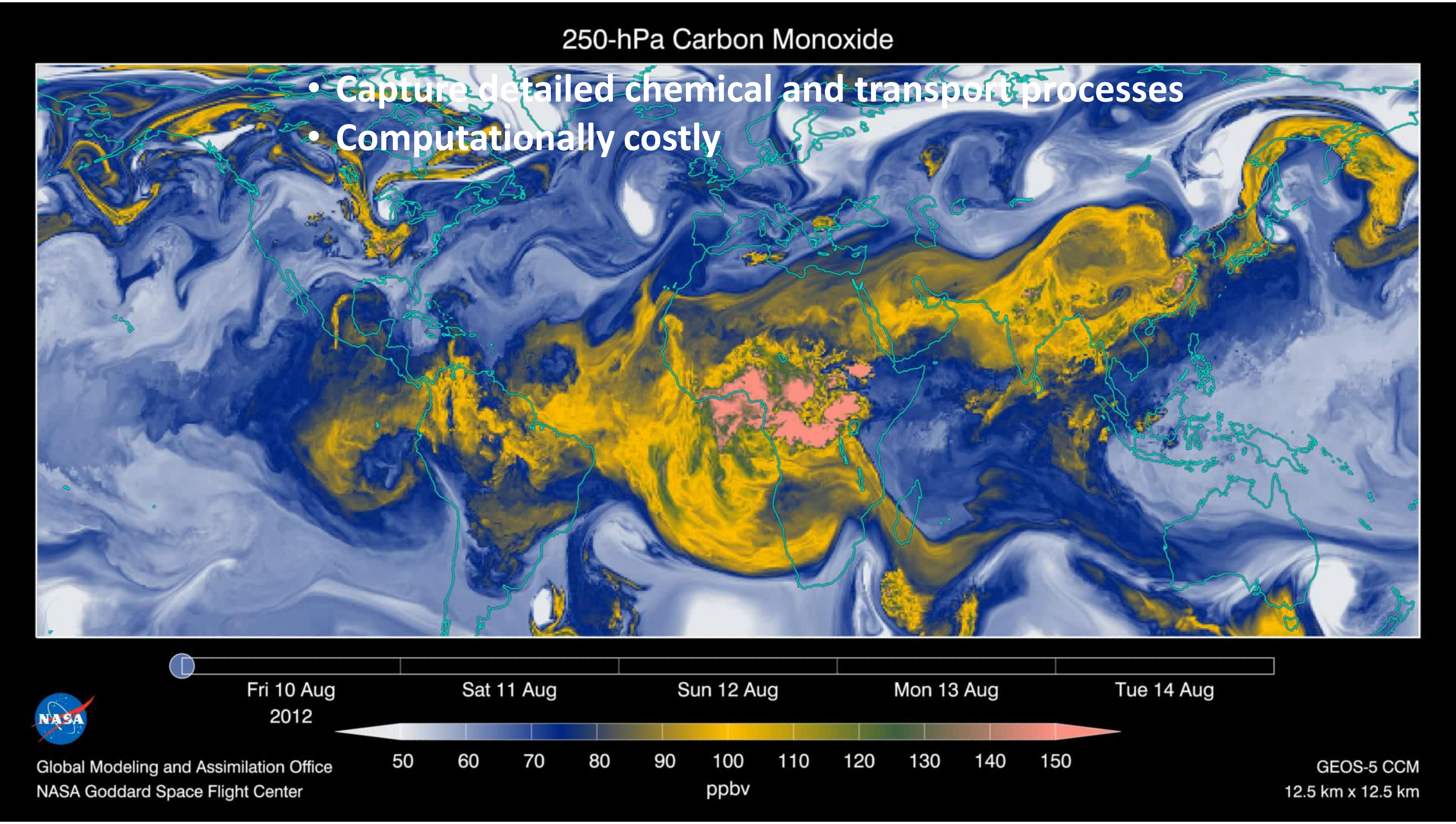
Surface ozone simulation at 12.5 km x 12.5 km

- Capture detailed chemical and transport processes
- Computationally costly

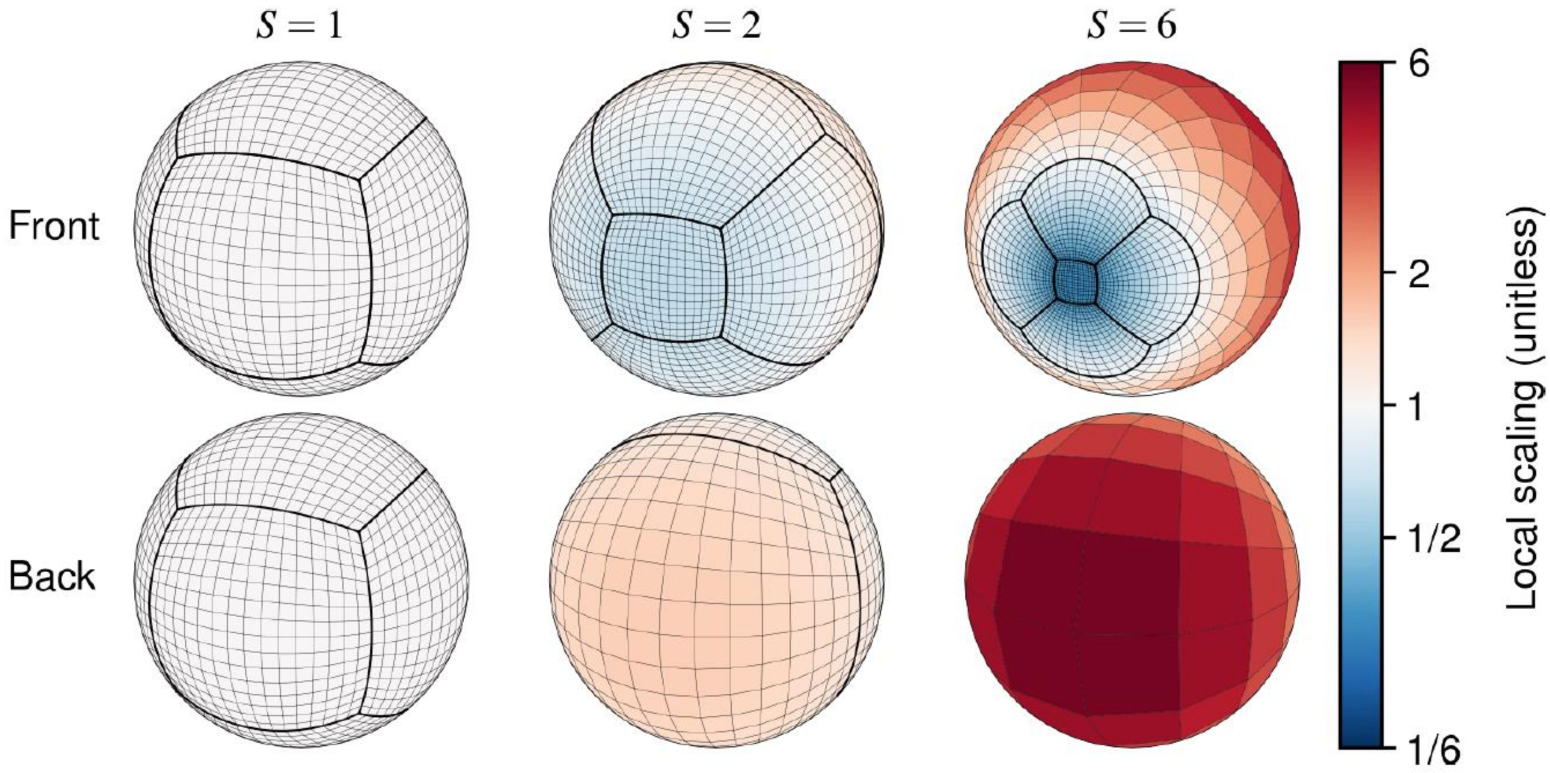


Global High-Resolution Simulation of Tropospheric CO

- Capture detailed chemical and transport processes
- Computationally costly



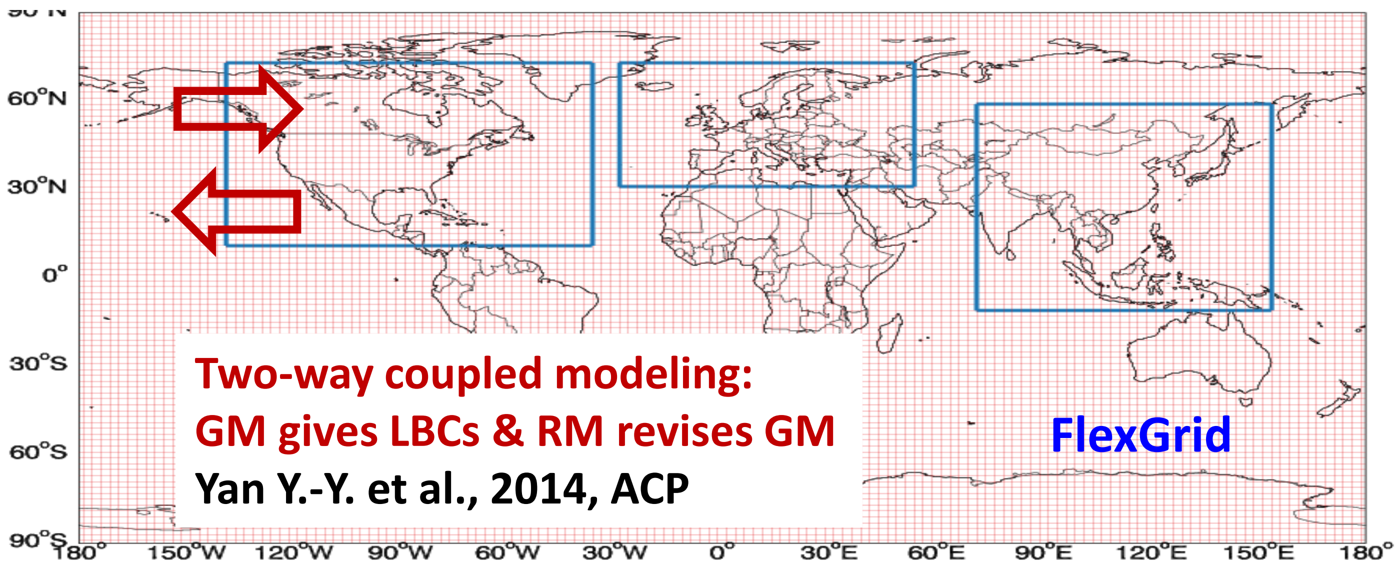
Stretched Grid Modeling for Single Targeted Domain



Bindle et al., GMD, 2021

Global versus Regional Models

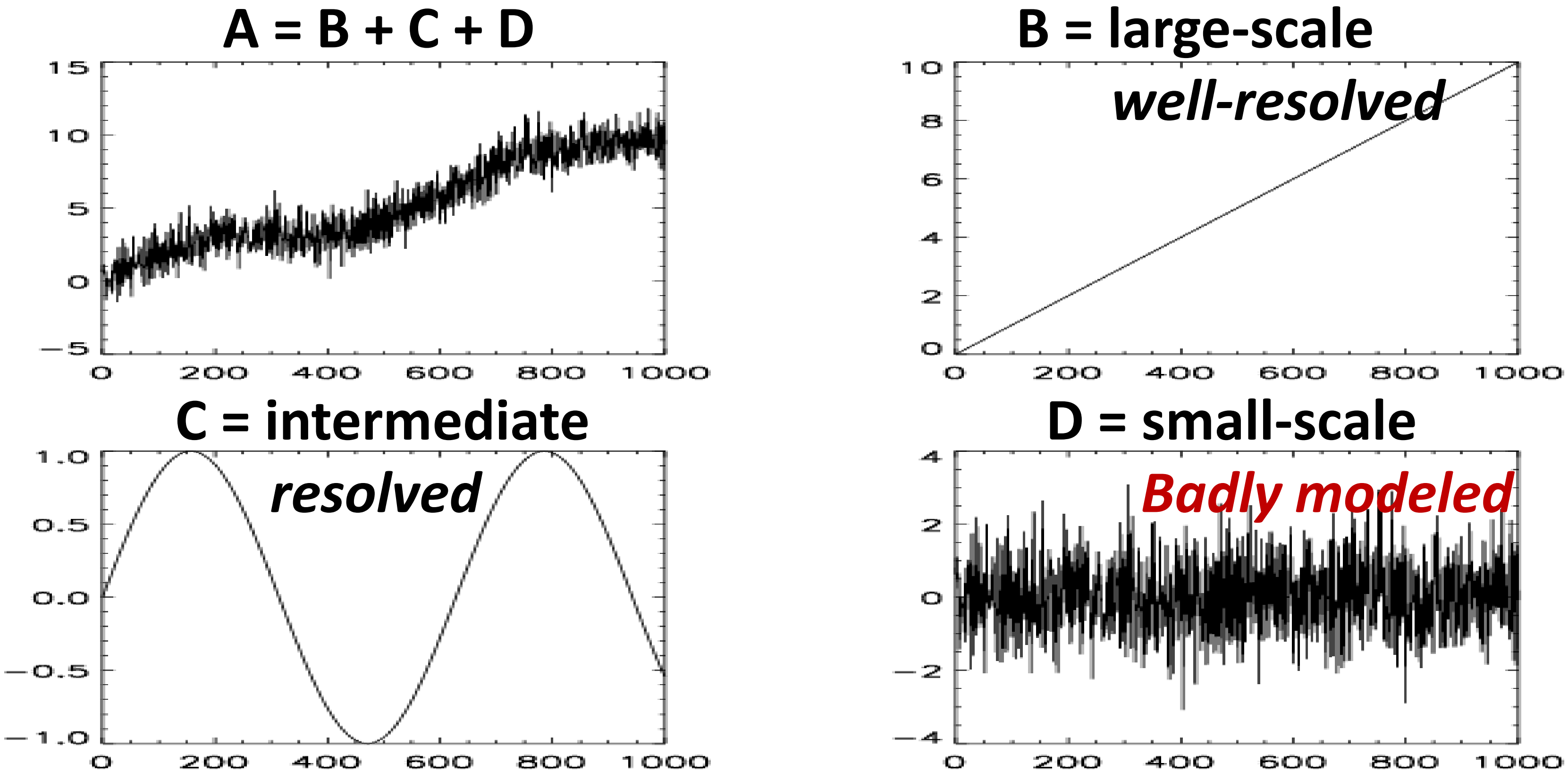
Global Models	Regional Models
▪ Covers the globe – Good for global studies – No LBCs are necessary ▪ Low-resolution (≥ 100 km) – Sim. or no small-scale processes ▪ Example: GEOS-Chem, AM3	▪ Covers a region – Need LBCs from global models via nesting ▪ High-resolution (~ 10 km) – Resolve small-scale processes ▪ Example: CMAQ, WRF-Chem



Two-way coupled modeling:
GM gives LBCs & RM revises GM
Yan Y.-Y. et al., 2014, ACP

Models Often Miss or Misrepresent Small-scale Processes

- Atmospheric chemical & physical processes have multiple scales
- Models often misrepresent scales smaller than 2 x grid size
  - Critical, because small-scale processes affect large-scale ones
  - Affect both distribution and total mass of trace species



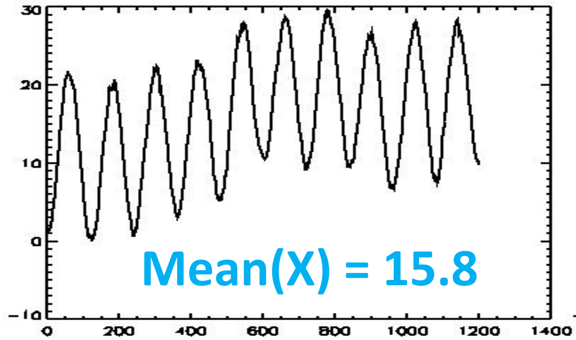
A Simple Case

How Small Scales Affect Large Scales

$X_0 = 1$

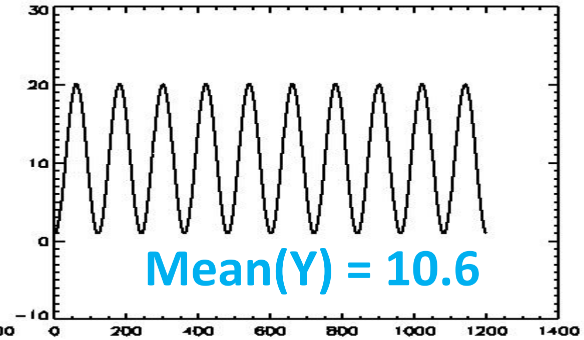
$X_{t+1} = X_t + 0.5*\sin(t/P) + Xr$

$Xr = N(0, 0.2)$; $P = 120$

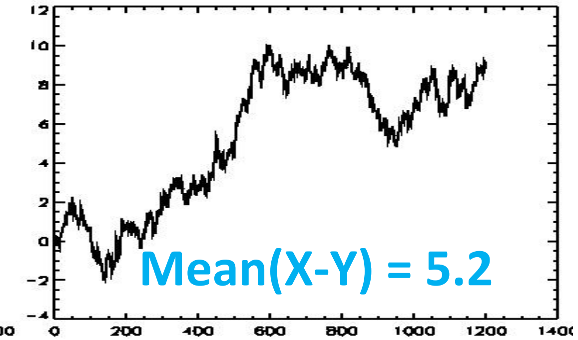


$Y_0 = 1$

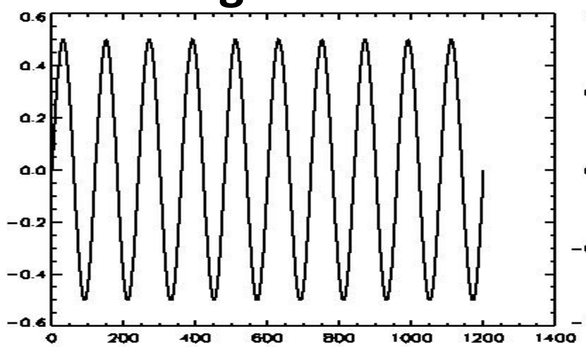
$Y_{t+1} = Y_t + 0.5*\sin(t/P)$



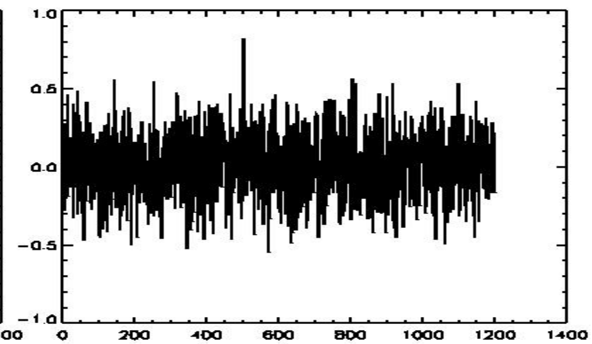
$X_t - Y_t$



0.5*sin(t/P)
larger scale



Xr = N(0,0.2)
smaller scale



Limited by Resolution

Models Often Miss or Misrepresent Small-scale Processes

- Un-even terrain
- Small-scale meteorology
- Variability in land use, vegetation, etc.
- Small-scale horizontal & vertical transport
- Small-scale variability in chemistry & emissions

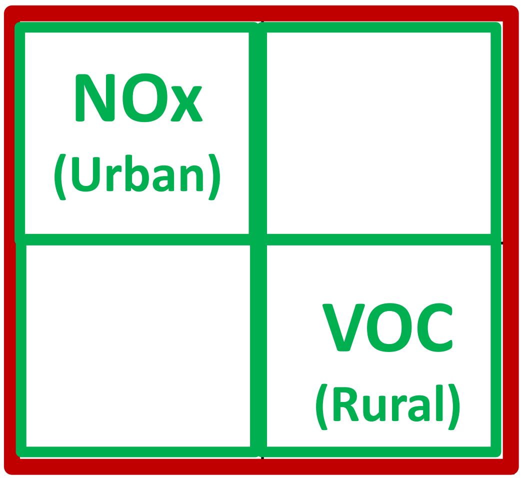
model reality

$$\bar{A} \cdot \bar{B} - \overline{A \cdot B} = -\overline{A' \cdot B'} = -r_{AB} \cdot \sigma_A \cdot \sigma_B$$

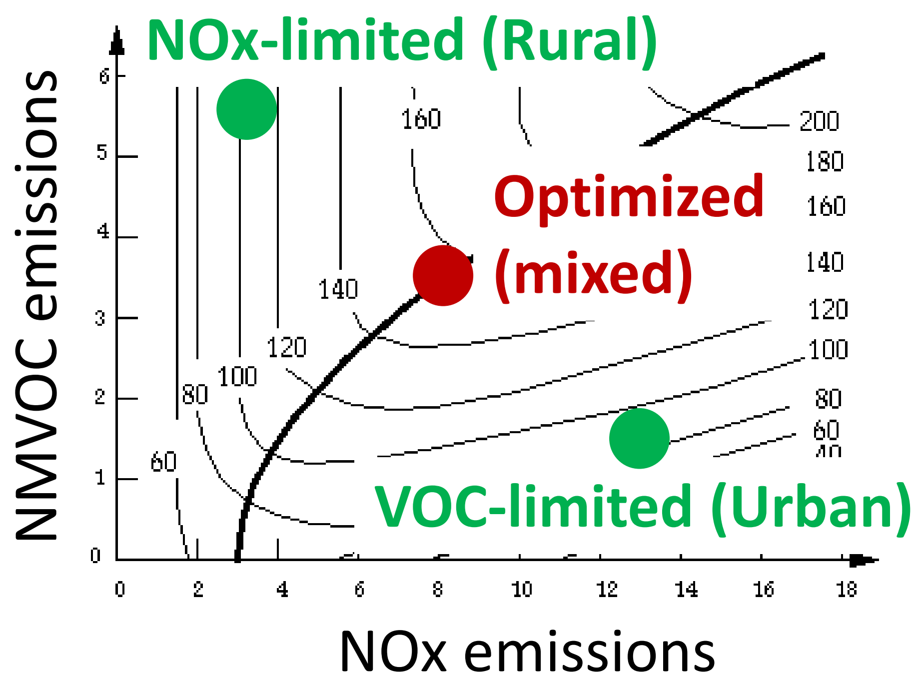
- $r_{AB} < 0$: Model has an overestimation
- $r_{AB} > 0$: Model has an underestimation

Coarse Models Tend to Overestimate Ozone Production

1 coarse gridcell = 4 fine gridcells



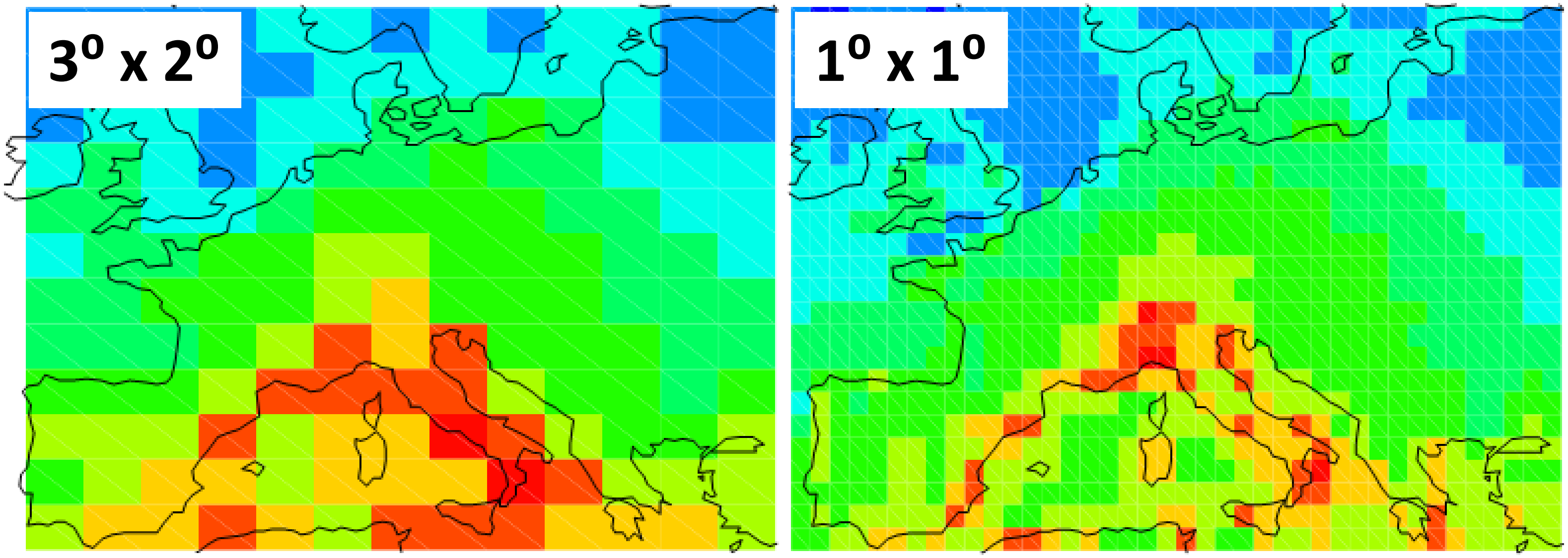
O_3 Production Rate

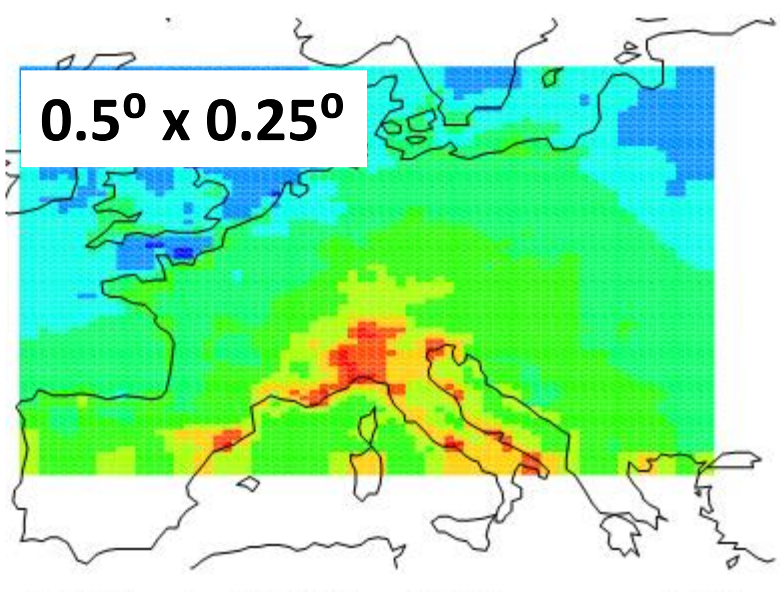


Sillman et al., 1990

Finer Resolution Leads to Less Ozone

Surface Ozone over Europe in June 2006 at 12:00 UTC





Huijnen et al., 2010

2-way Coupling Improves Tropospheric Simulation by Reducing Modeled Oxidative Capability

	Global Model	Two-way Model	'Observation'
OH (10^5 cm^{-3})	11.8	11.2 (– 5% *)	10.4 – 10.9
O_3 (DU)	34.5	31.5 (– 8.7%)	31.1 ± 3 (OMI/MLS)
O_3 (Tg)	384	348 (– 9.5% #)	
NOx (TgN)	0.169	0.176 (+ 4.1%)	
CO (Tg)	359	398 (+ 10.8% &)	
MCF lifetime (yr)	5.58	5.87 (+ 5.2%)	6.0 – 6.3
CH_4 lifetime (yr)	9.63	10.12 (+ 5.1%)	10.2 – 11.2
NMVOC (TgC)	10.1	10.2	

* Greater than its interannual variability (2.3%)

\# Greater than the change from 2000 to 2100 under RCP6.0

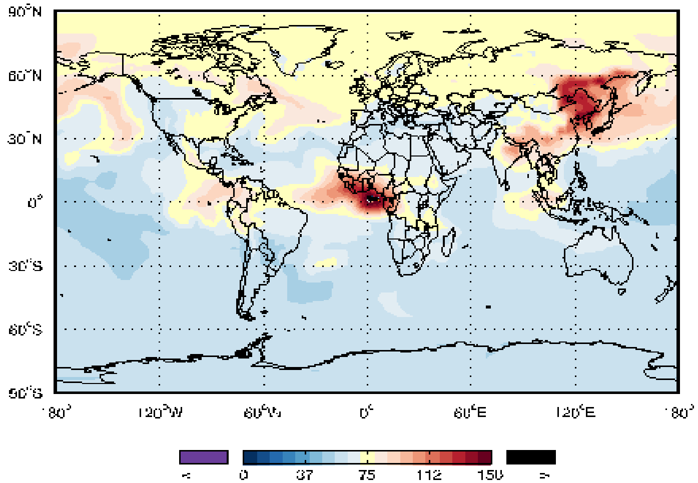
& Equivalent to a 25% increase in global CO emissions

Yan Y.-Y. et al., ACP, 2014, 2016

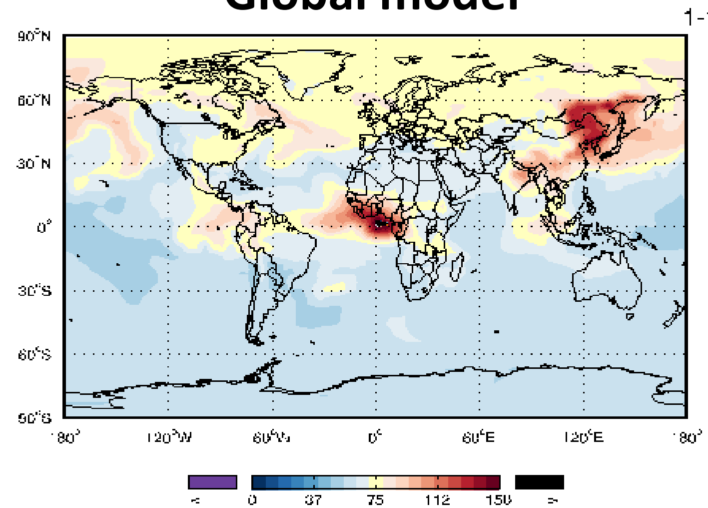
2-way Coupling Better Simulates Tropospheric CO

CO at 6.5 km altitude. 2008/07/01 – 2008/08/15

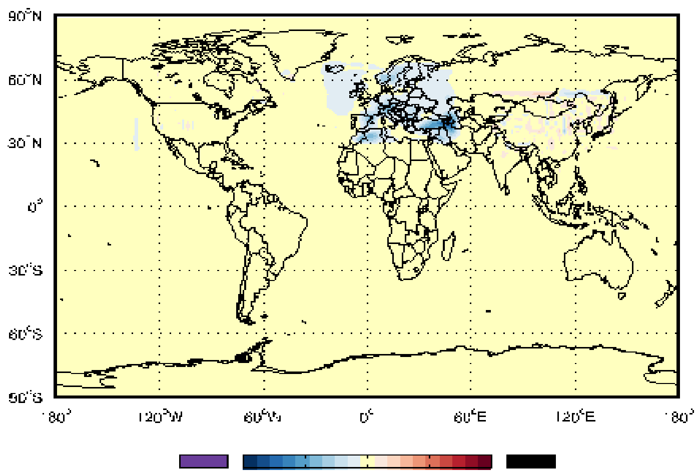
Two-way model



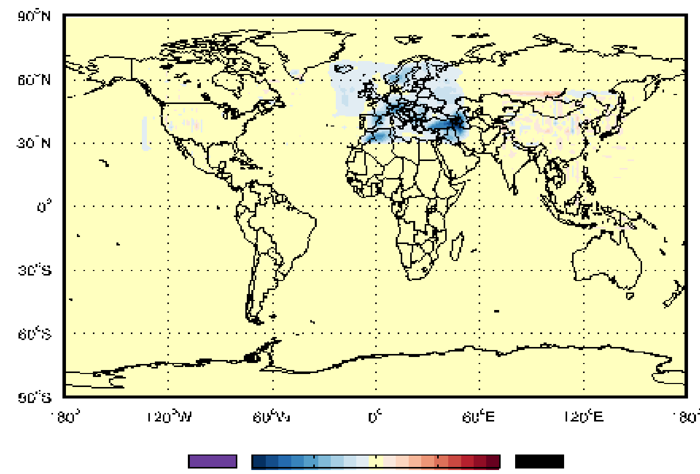
Global model



Two-way minus Global



Relative difference



Yan Y.-Y. et al., ACP, 2014, 2016

Modeling of Atmospheric Transport and Source Attribution

Data-based

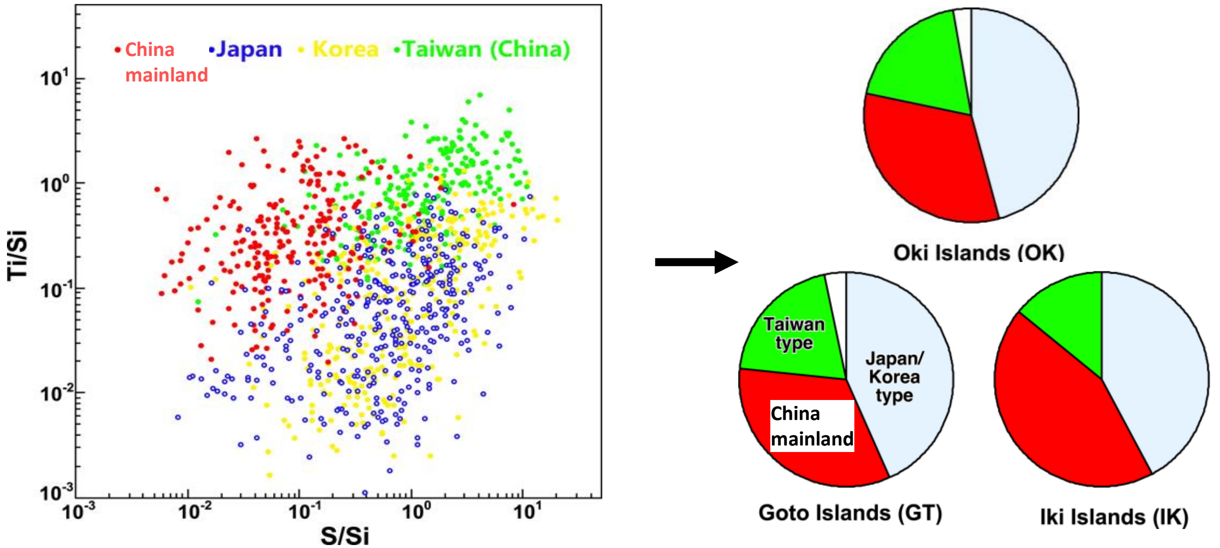
- **Traditional observation-based methods (PMF, CMB)**
  - Simplified treatments of chem & transport; short-distance attribution
  - Difficult to represent nonlinear (chemical) processes, or chem-met interactions
- **AI models**
  - Fast and low costs (in prediction); derivatives are easily calculated
  - Lack physical mechanisms and explainability; causality is unclear or lacking

Physics-based

- ✓ **Backward trajectory models**
  - Lagrangian approach to track the flow backwards; relatively fast and low cost
  - Substantial limitations in chemistry and mixing
- ✓ **Chemical transport models (CTMs)**
  - Forward approach with zero-out simulations, tagged approach, etc.
  - Account for different processes, but are resource-costly
- ✓ **Assimilation (Adjoint models, EnKF)**
  - (Local) linearization of CTMs; powerful for attribution to each LOCATION
  - Slowest, and still cannot fully address the nonlinearity issue
- ➢ **Combination of physics-based and data-based methods**

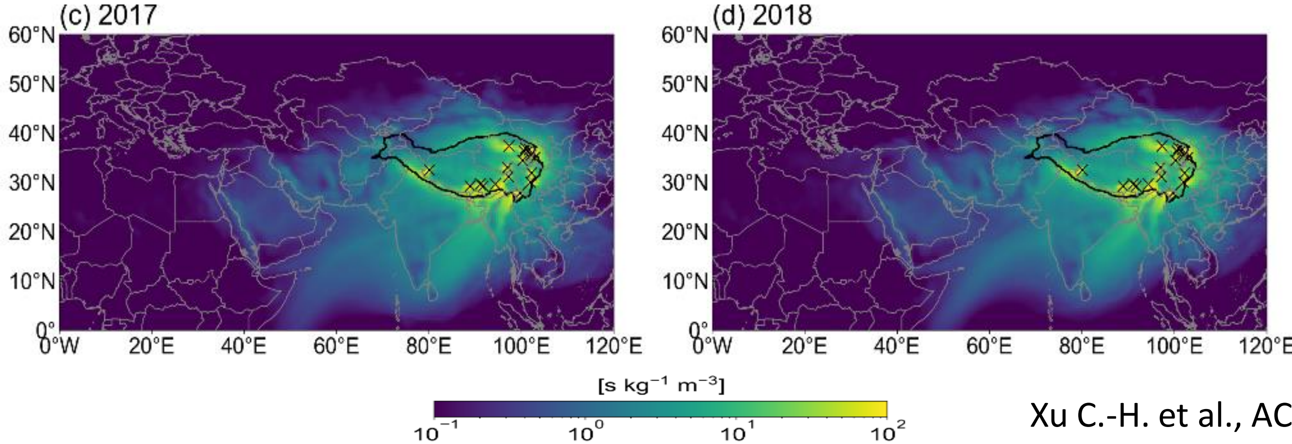
Observation-based versus Back Trajectory

Observation-based attribution of source regions for spheroidal carbonaceous particles



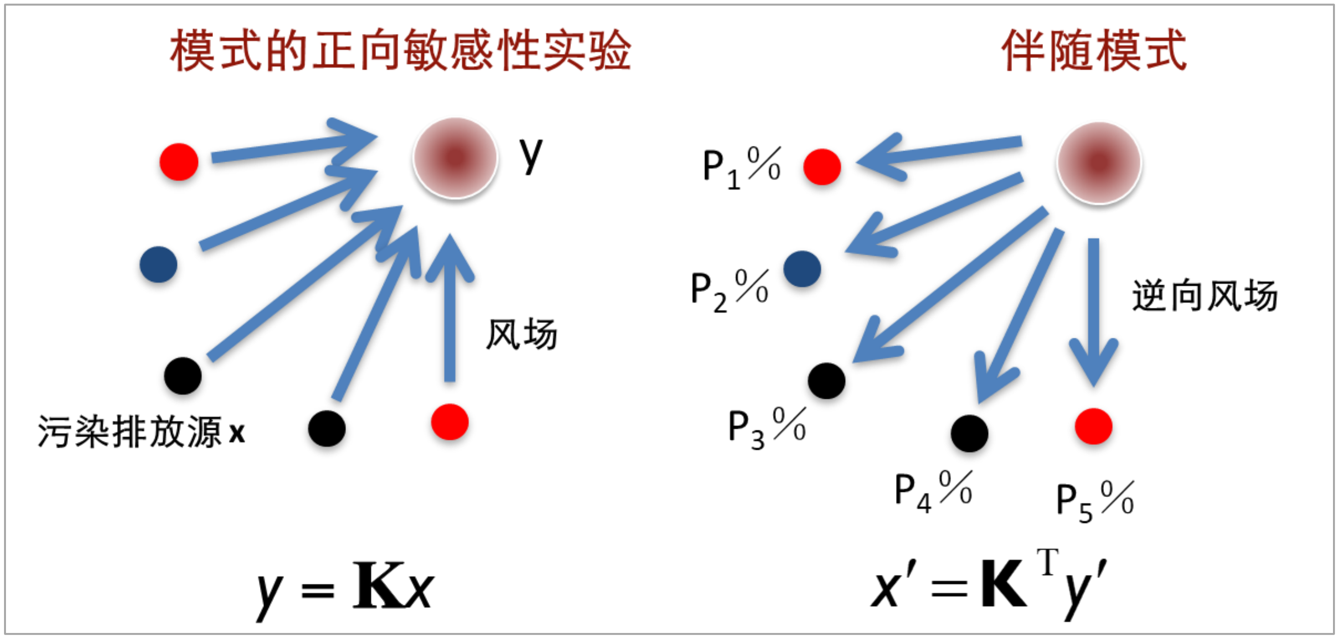
Jun et al., 2014

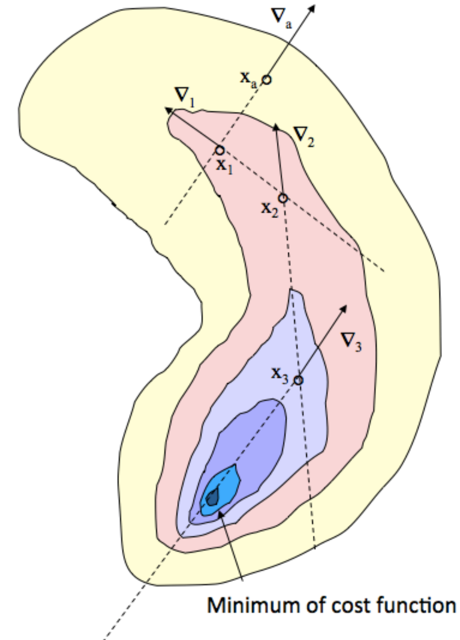
Back trajectory for source attribution



Xu C.-H. et al., ACP, in review

Adjoint Modeling





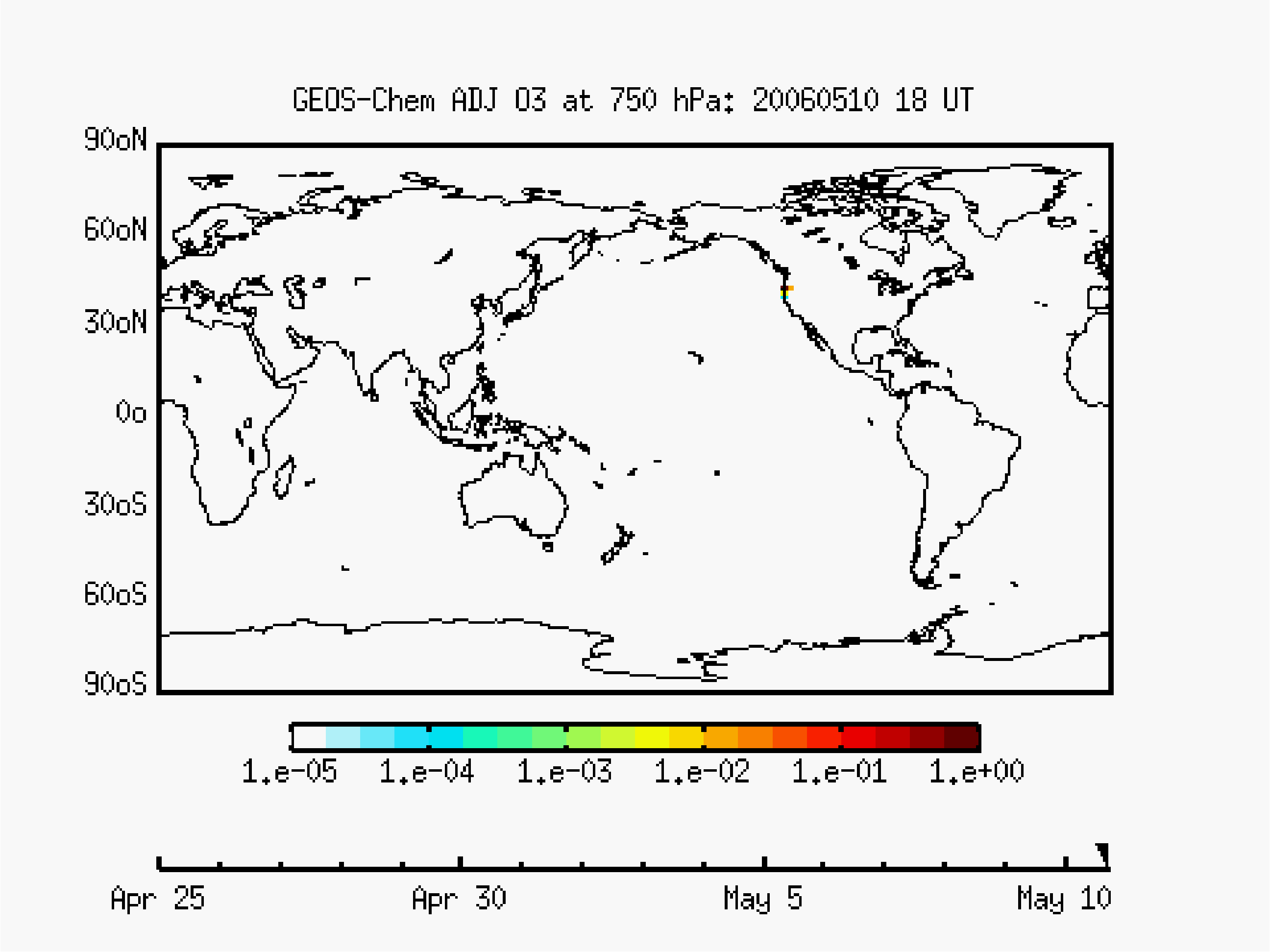
Numerically solve

$$\nabla_{\mathbf{x}} J(\mathbf{x}) = 2\mathbf{S}_{\mathbf{a}}^{-1}(\mathbf{x} - \mathbf{x}_{\mathbf{a}}) + 2\mathbf{K}^{T}\mathbf{S}_{e}^{-1}(\mathbf{K}\mathbf{x} - \mathbf{y})$$
$$= 0$$

Source: Lin Zhang

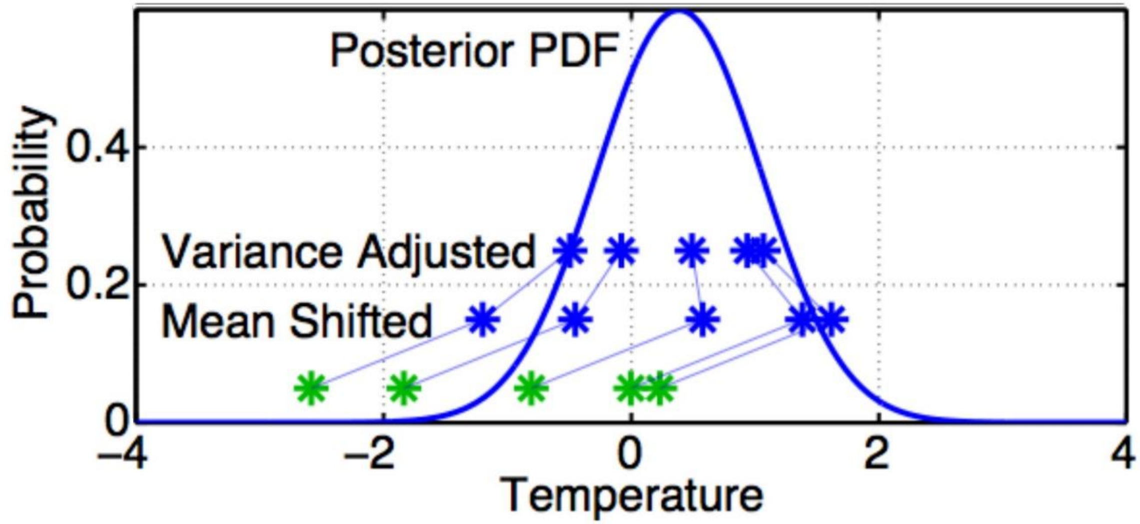
GEOS-Chem Adjoint

Sensitivity of ozone concentration at Mt Bachelor on May 10, 2006 at 18 UT to ozone fields at earlier time steps (April 25 - May 10, 2006)



Zhang et al., 2009

Ensemble Kalman Filter (EnKF)



建立扰动参数集合:

$X^b = x^b - \overline{x^b}$

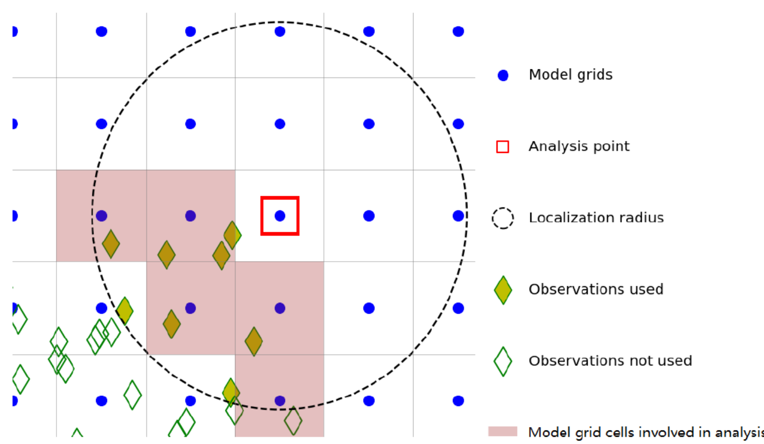
转换至观测空间:

$y^b = H(x^b); Y^b = y^b - \overline{y^b}$

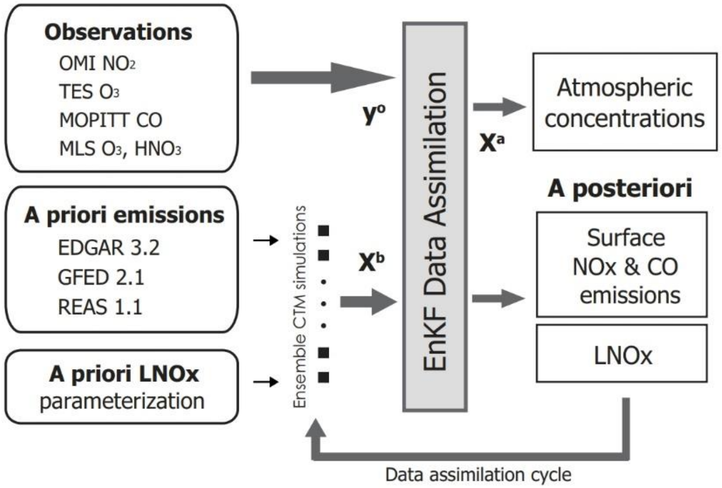
生成分析值:

$\bar{x}^a = \bar{x}^b + X^b P (Y^b)^T R^{-1} (y^o - \overline{y^b})$

局域化处理（LETKF）

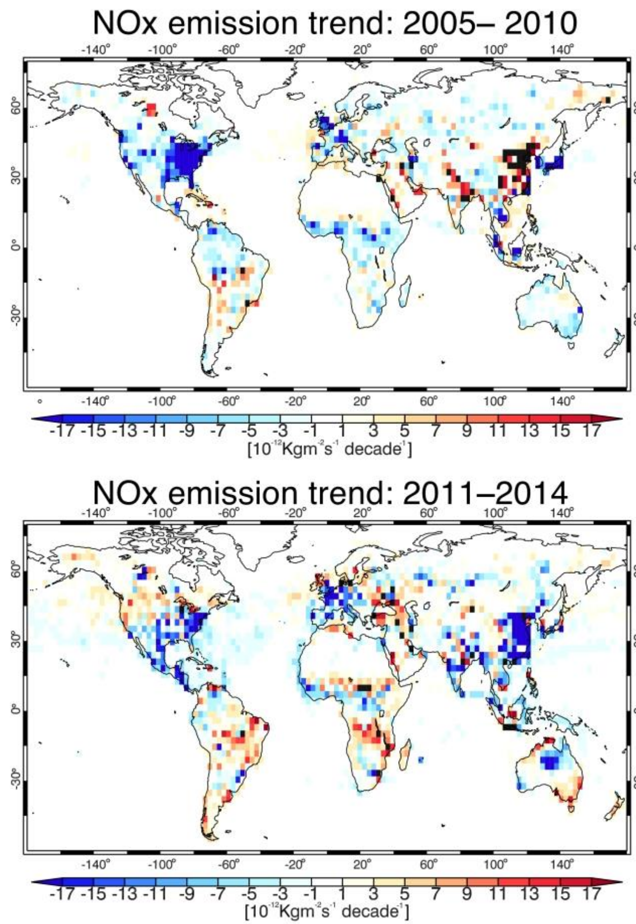


EnKF for NOx Emission Inversion



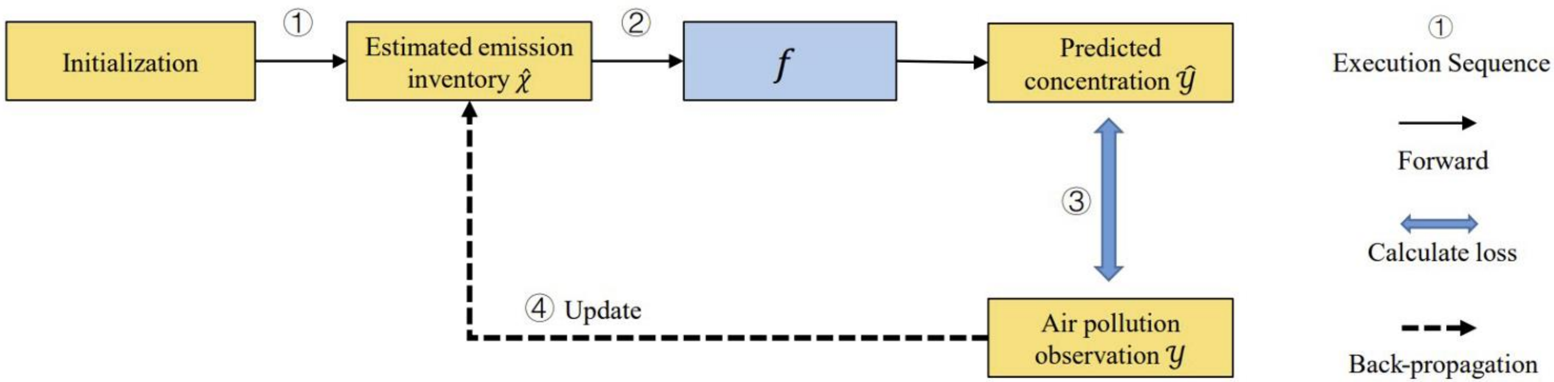
Miyazaki et al., ACP, 2012

- # of ensemble members: 32
- Localization distance: 450km

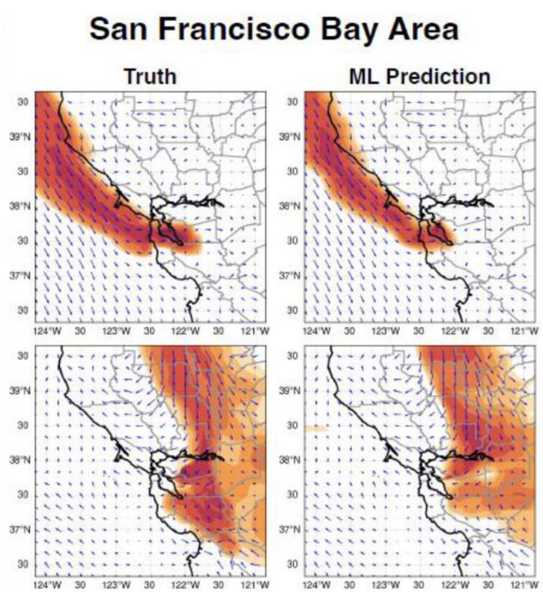


Miyazaki et al., ACP, 2017

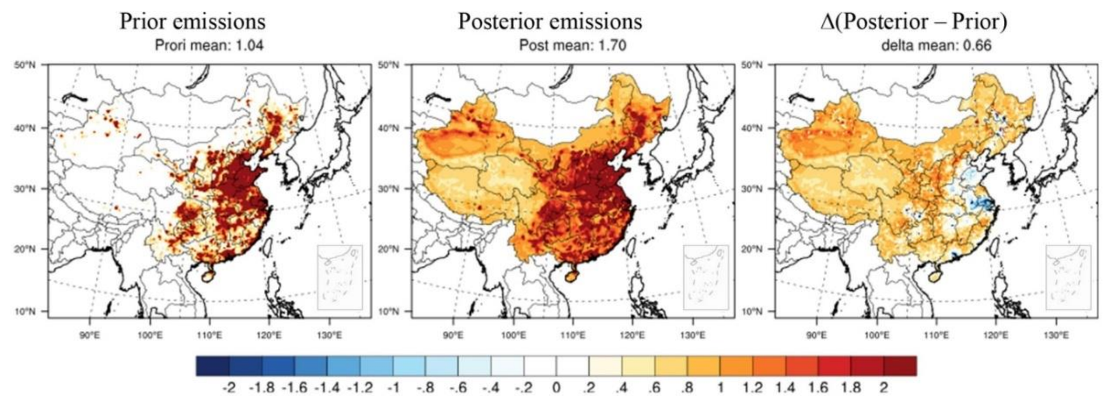
Physics-Guided Artificial Intelligence for Emission Inversion



Trained by trajectory models
He et al., GMD, 2025



Trained by CTMs
Xing et al., EST, 2022

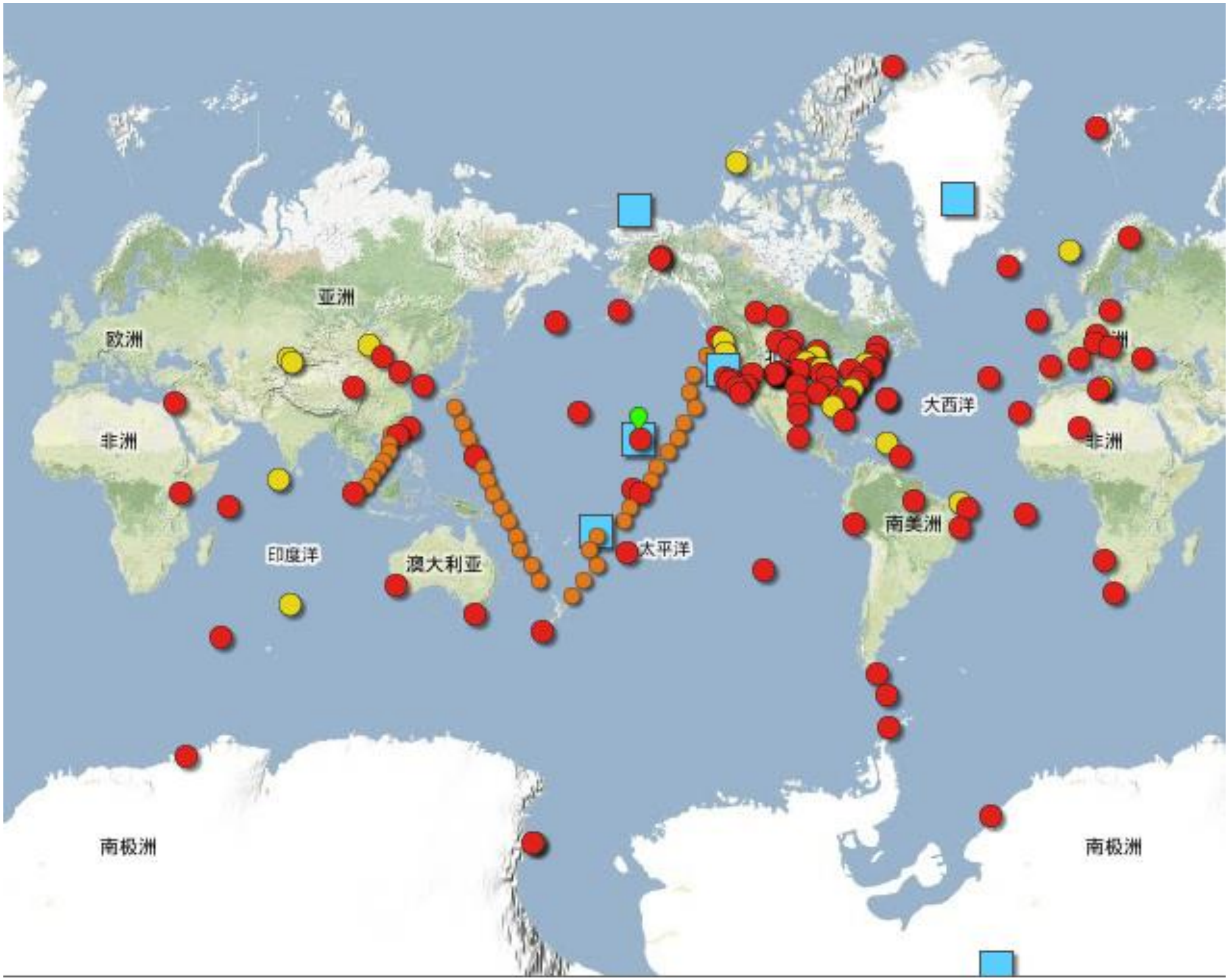


(a) Spatial distribution (unit: mol/s, annual averages)

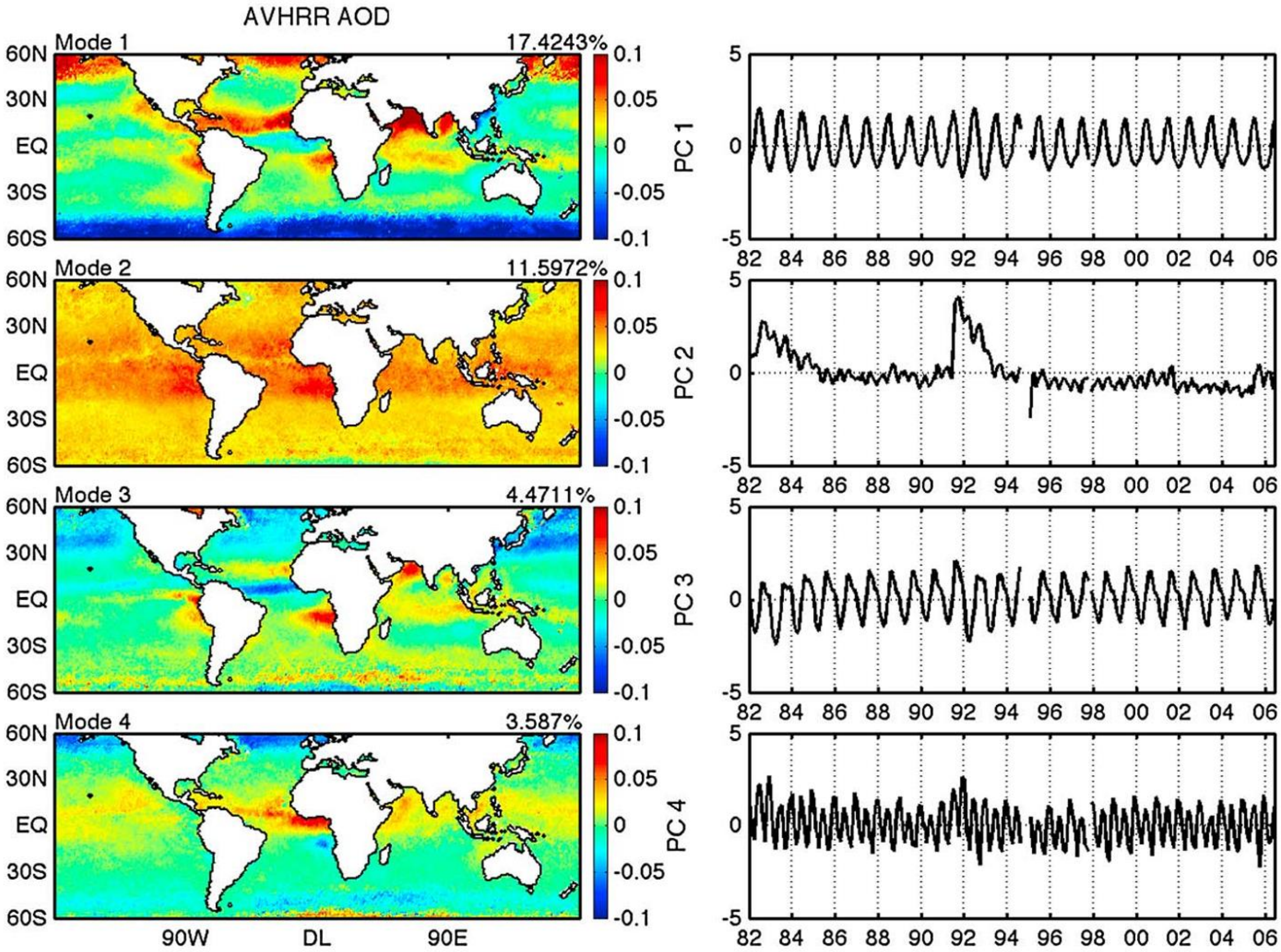
Quiz

- What are the challenges of measurements in China? How can we conquer these challenges? What should be the priority?
- Can pollution measurements also benefit studies of greenhouse gases? If so, how?
- To what extent can we retrieve vertical profiles of NO_2 based on satellite remote sensing? What are the bottleneck in theory and technology?
- Can we retrieve multiple species from satellite remote sensing using a (single) generalized algorithm? Why?
- For a horizontal resolution of 200 km, what is the smallest scale a model can resolve? Discuss wrt chemistry and dynamics (e.g., winds), individually.

Global Monitoring Division Network



AVHRR AOD @ 550 nm: 1982-2006



Li et al., 2014, JGR

AOD @ 380 nm from Nimbus-7 TOMS: 1979-1991

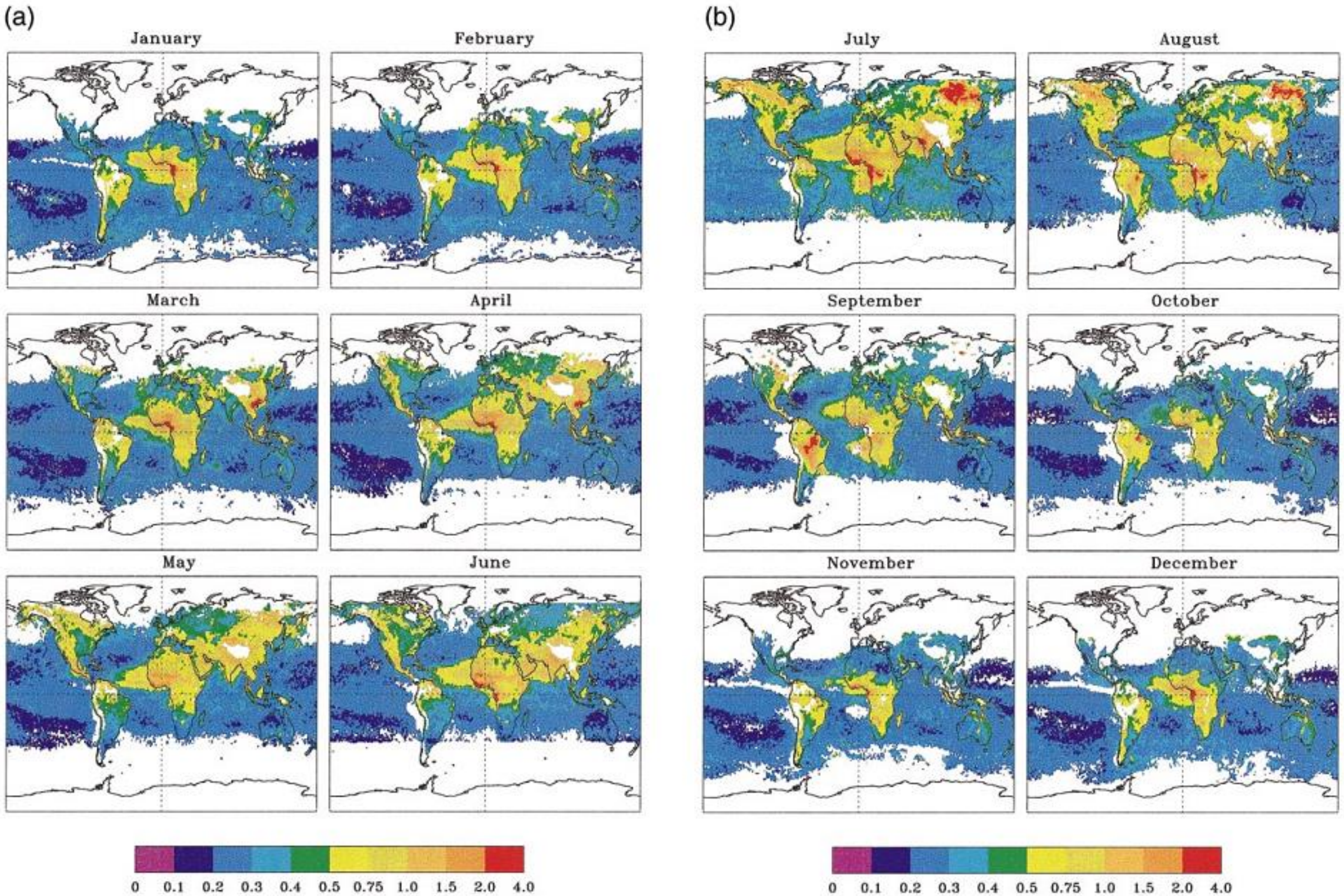
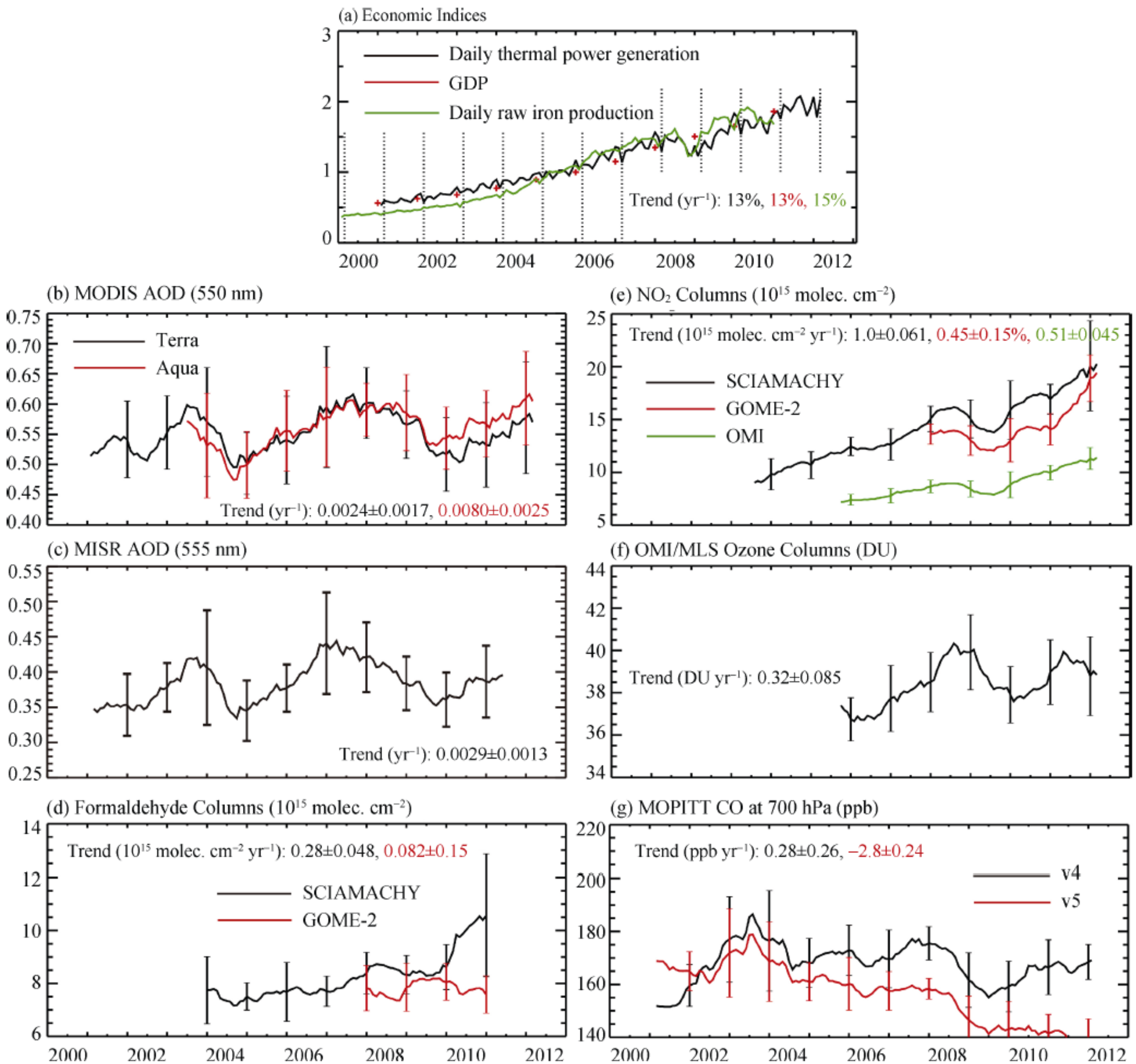


FIG. 4. Long-term (1979–91) global monthly average aerosol optical depth derived from *Nimbus-7*-TOMS observations.

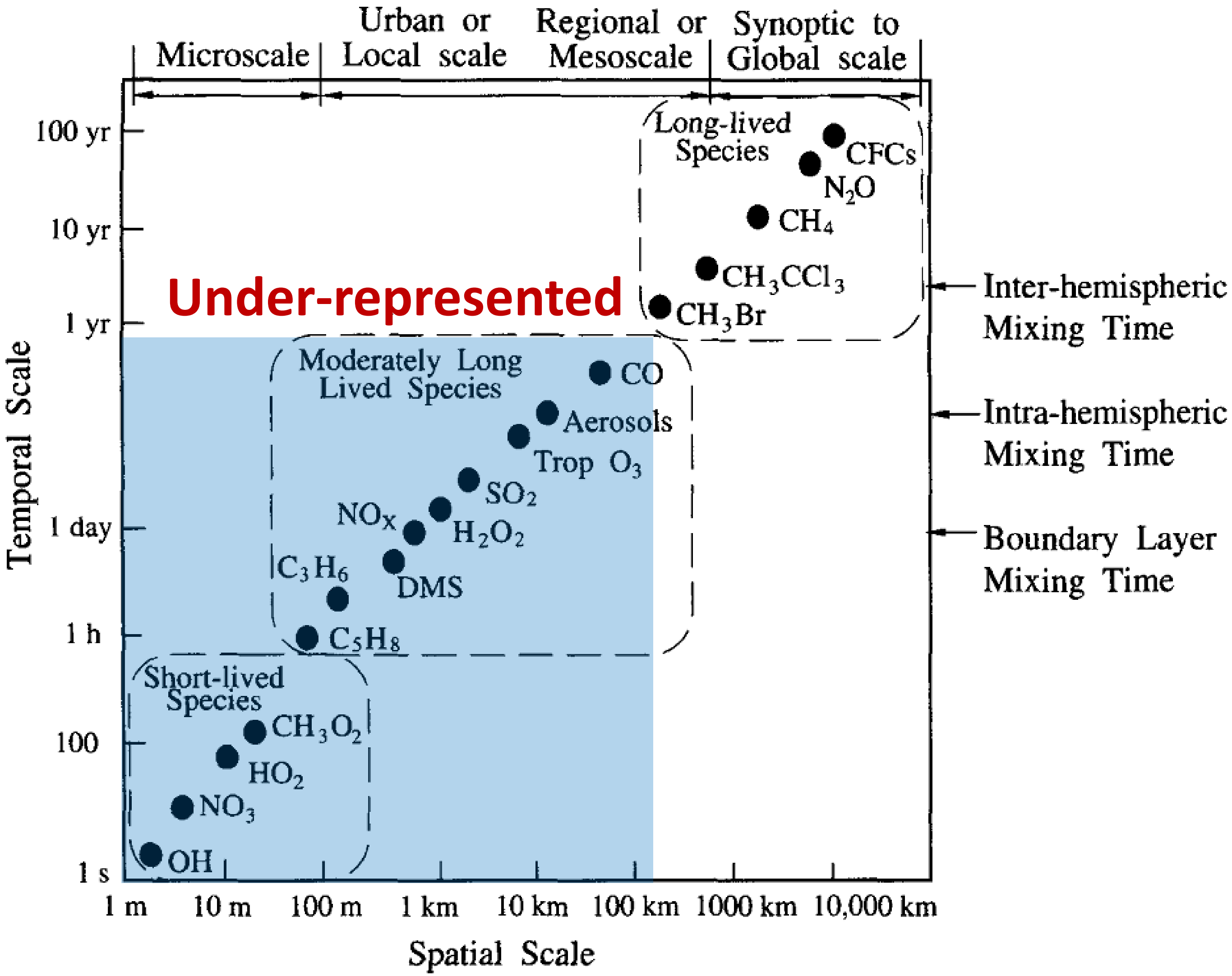
Torres et al., 2002, JAS

Satellite Observed Pollution Trends and Variability over China during 2000-2012



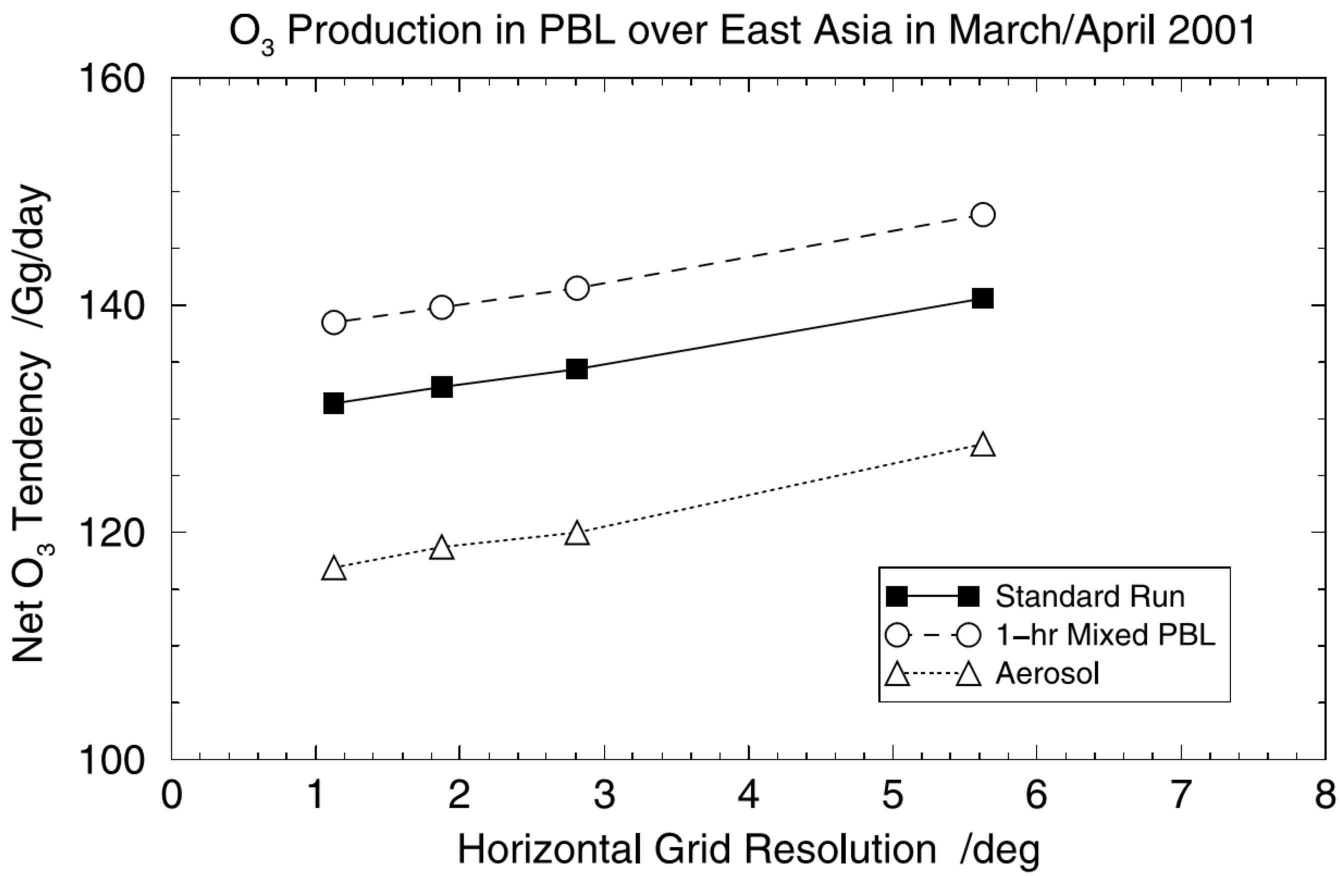
Lin et al., 2013, AOSL

Coarse Models Under-represent Small Scales



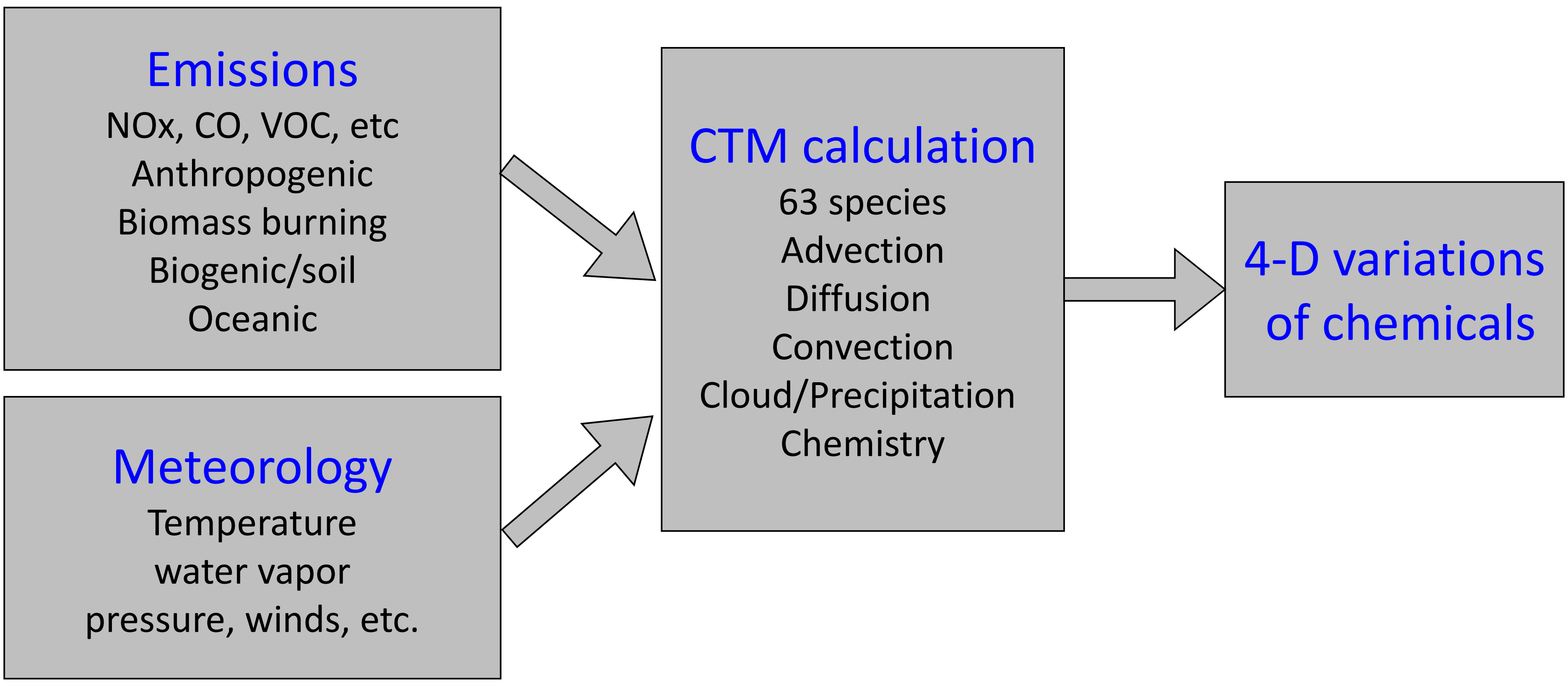
Seinfeld and Pandis, 2006

Resolution-dependent Net Ozone Production

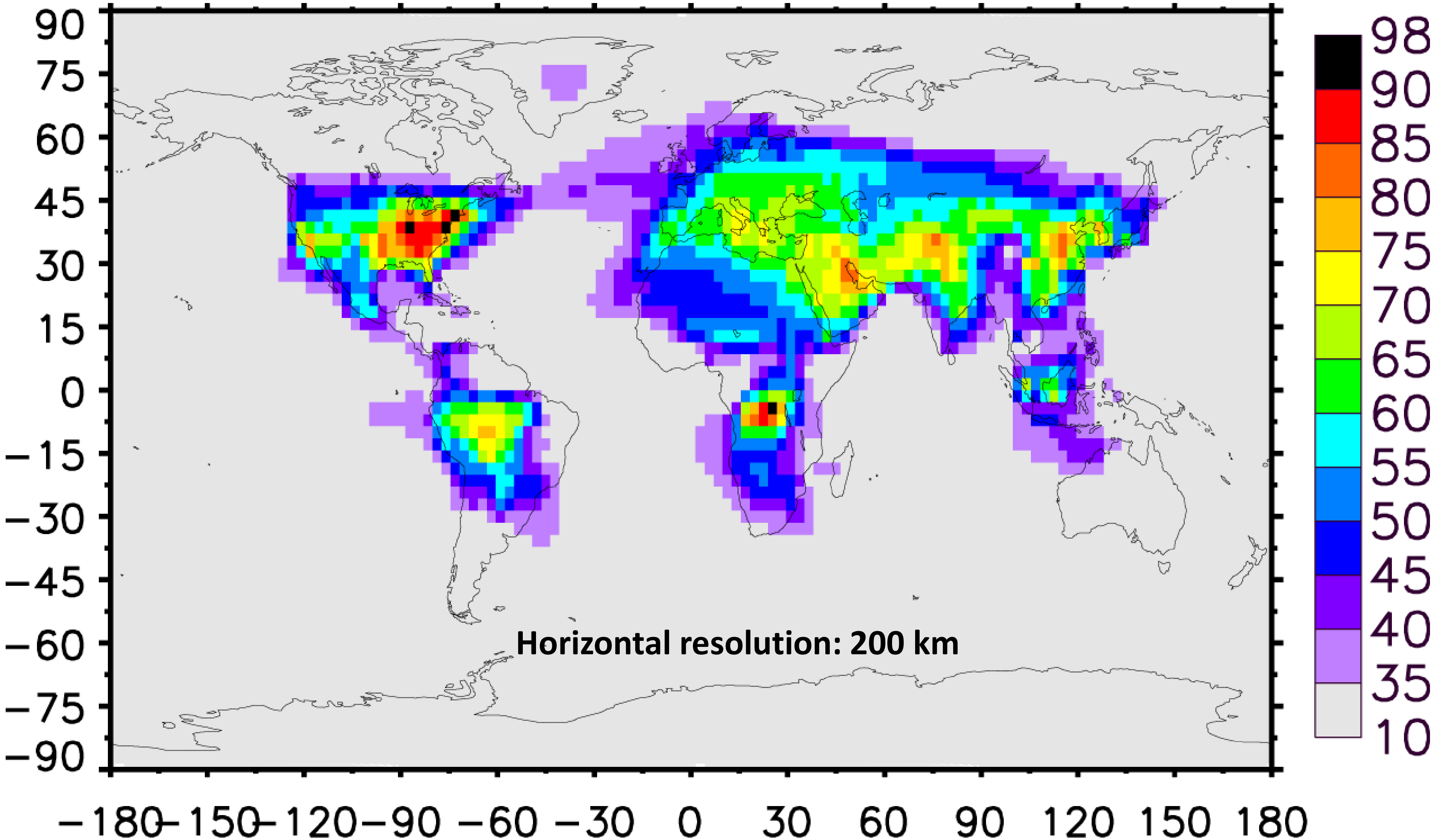


Wild an Prather, 2006

Atmospheric Chemical Transport Model



MOZART-Simulated Near-Surface Ozone in 1990s JJA



From Radiance (L1b) to Tropospheric NO_2 VCD (L2)

$$VCD_{trop} = \frac{SCD - SCD_{strat}}{AMF_{trop}}$$

S1: Total slant column density (SCD)

S2: Tropospheric SCD = SCD – SCD_{strat}

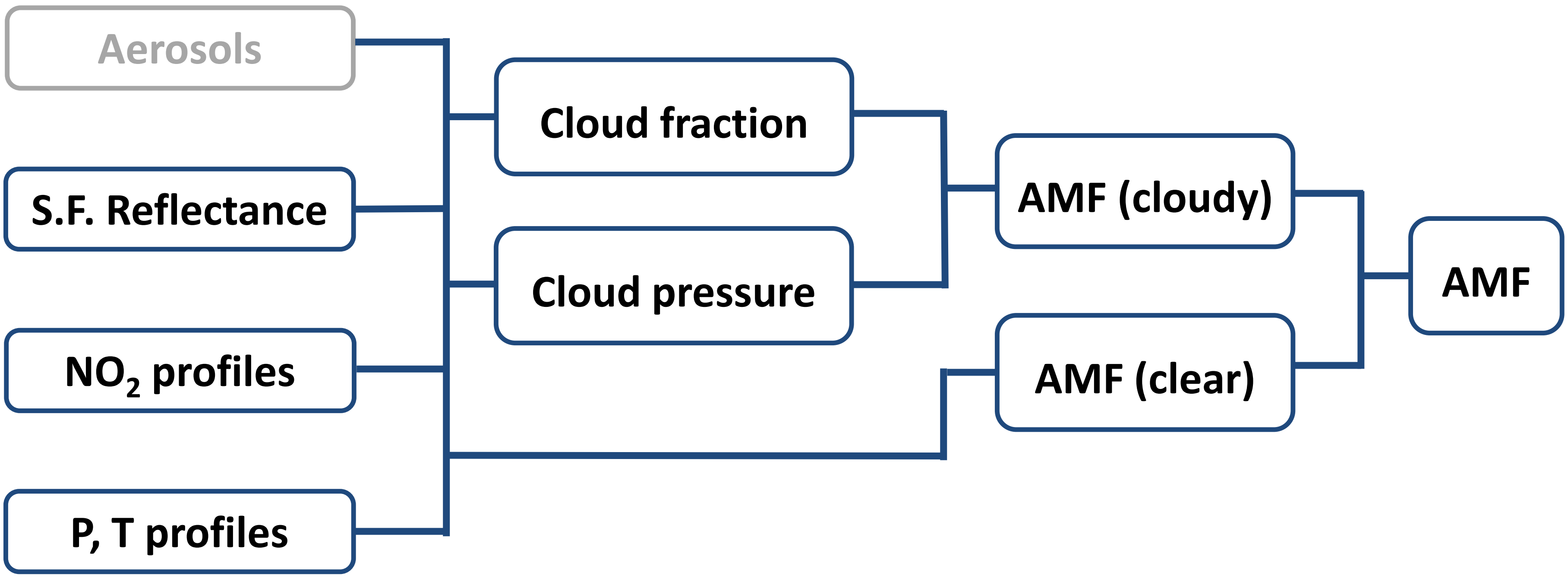
S3: Tropospheric air mass factor (AMF_{trop})

For polluted cases:

Error = ~5%

Error = ~5-10%

Error = ~30-60%

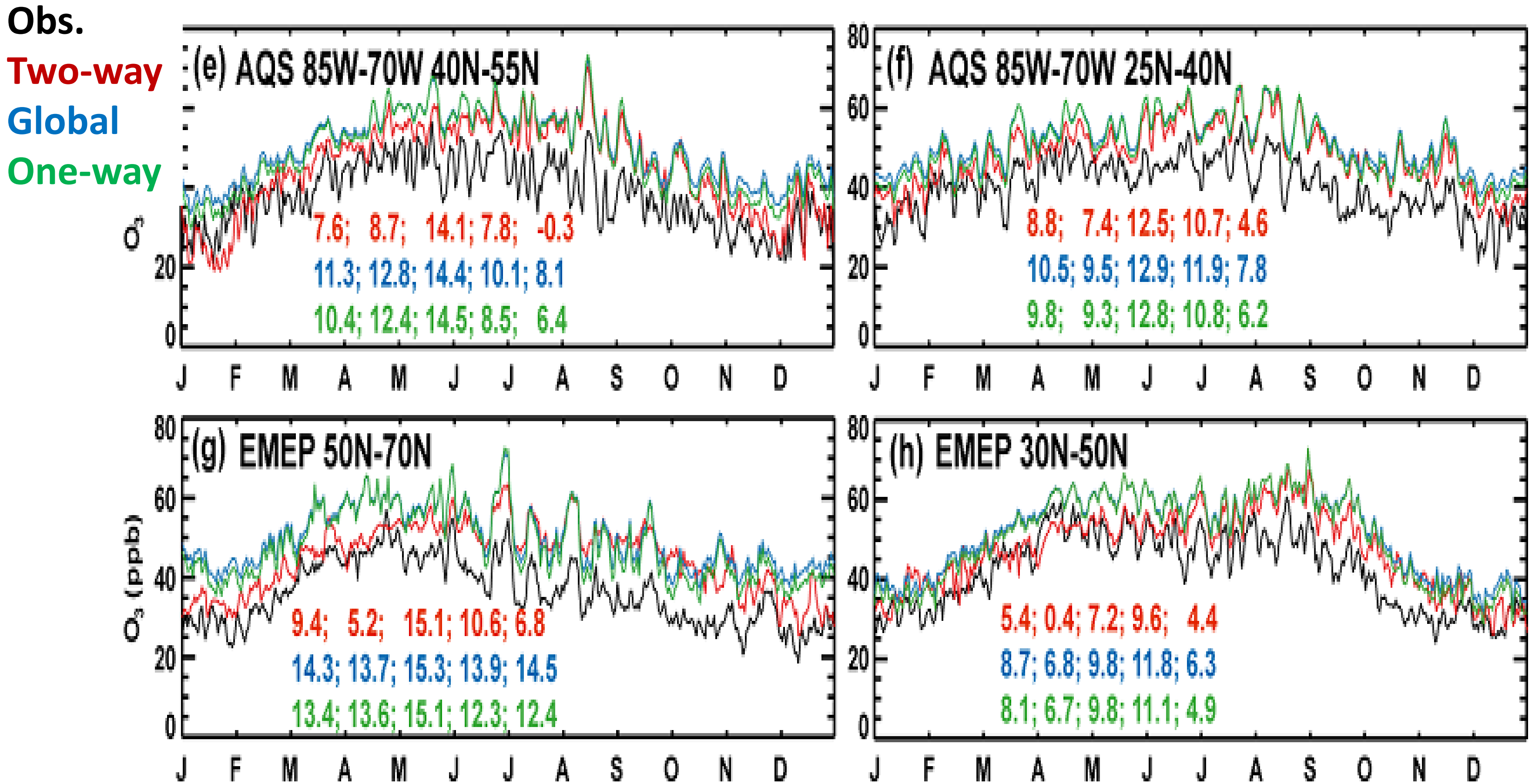


$$M = wM_{cld} + (1 - w)M_{clr} \qquad w = \frac{f_{cld}I_{cld}}{R} = \frac{f_{cld}I_{cld}}{f_{cld}I_{cld} + (1 - f_{cld})I_{clr}}$$

2-way Model Better Simulates Surface O_3

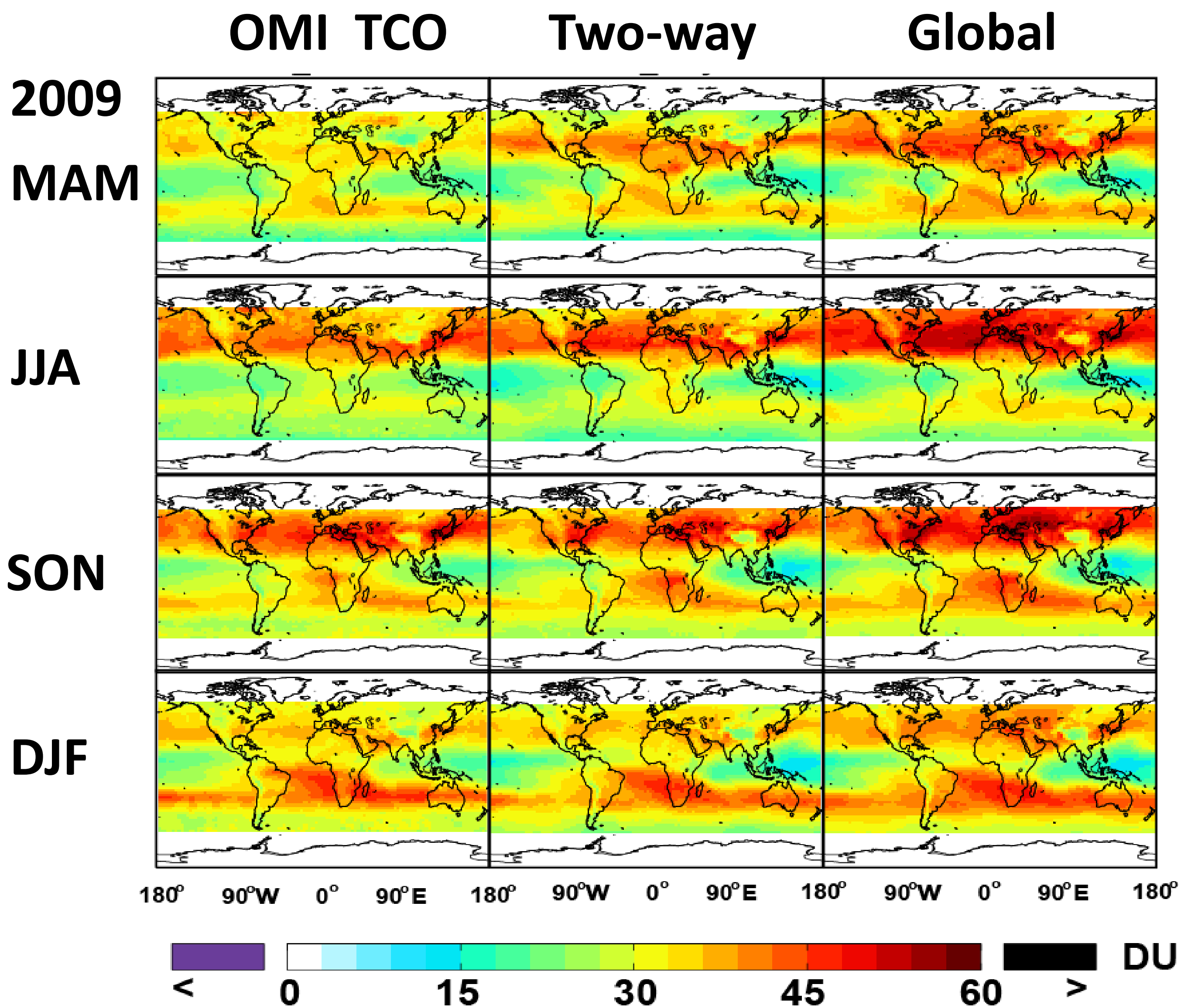
Comparisons with AQS and EMEP observations:

- **Improvement is most significant in cold season**
- **Improvement from 1-way to 2-way is 1-7 times that from global to 1-way**



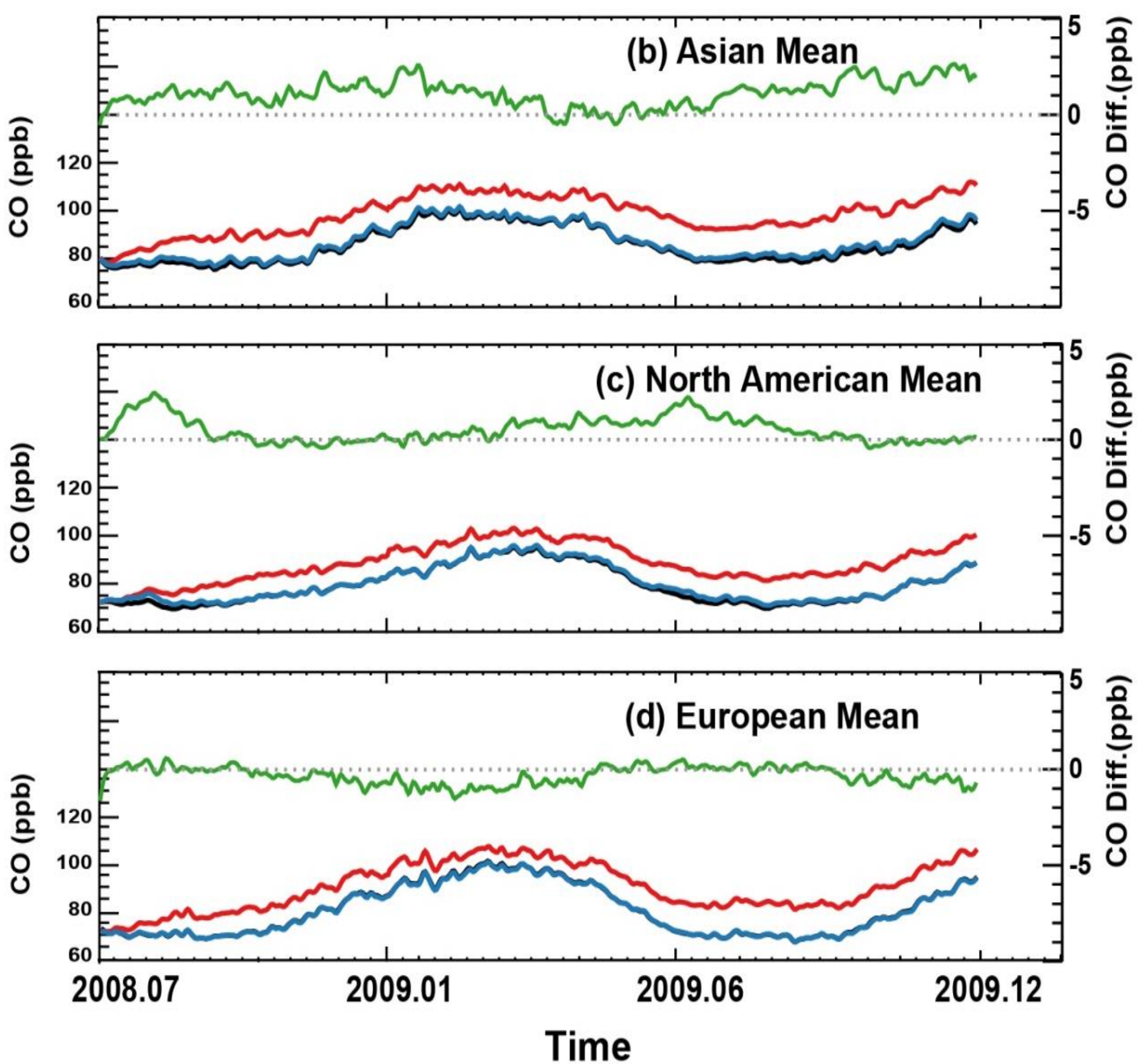
Yan Y.-Y. et al., ACP, 2014, 2016

2-way Model Better Simulates Tropospheric O_3



Yan Y.-Y. et al., 2016 ACP

2-way Coupling Better Simulates Tropospheric CO



Global model

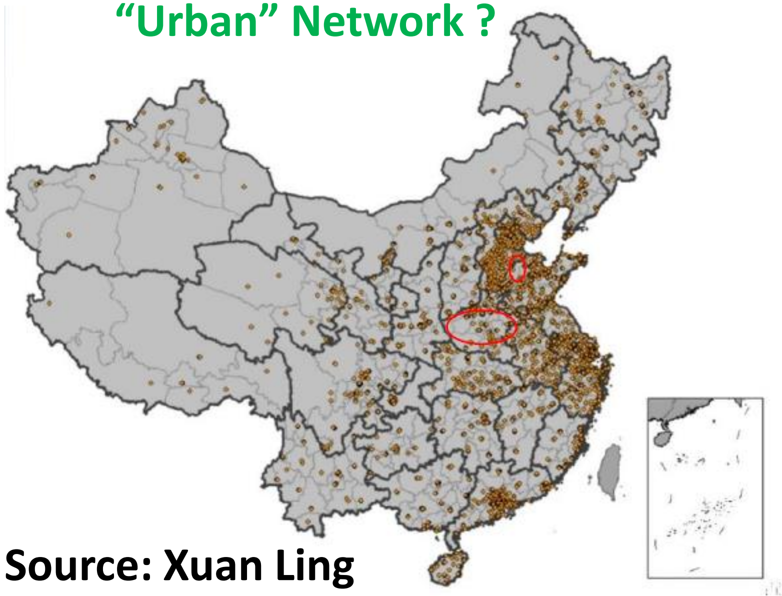
Two-way coupled model

One-way nested model

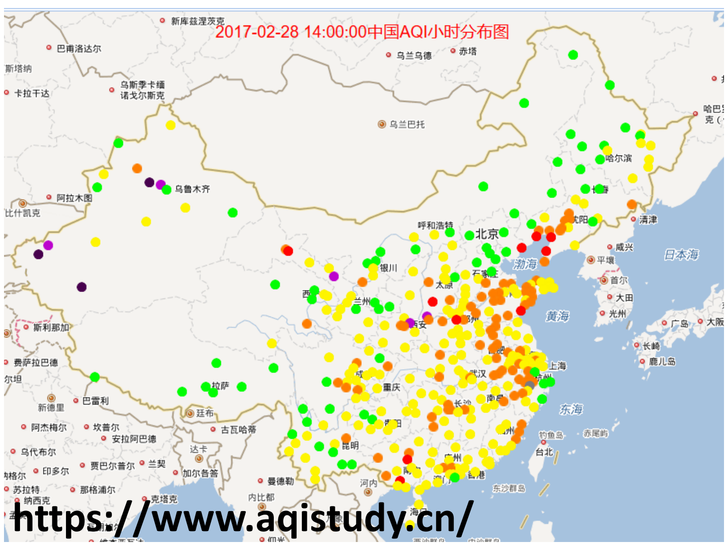
One-way nested model minus Global model

Air Quality Monitoring Network in China

"Urban" Network ?



Source: Xuan Ling



https://www.aqistudy.cn/

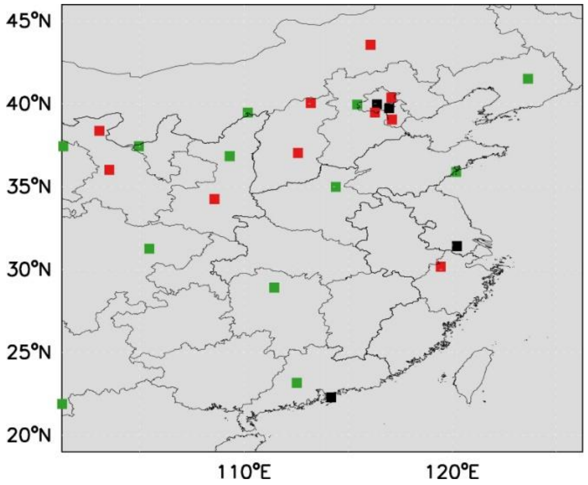
Measurements are limited by:

- Lack of historical data
- Lack of representativeness
- Lack of profile and column data
- Data verifiability and accessibility

What we want:

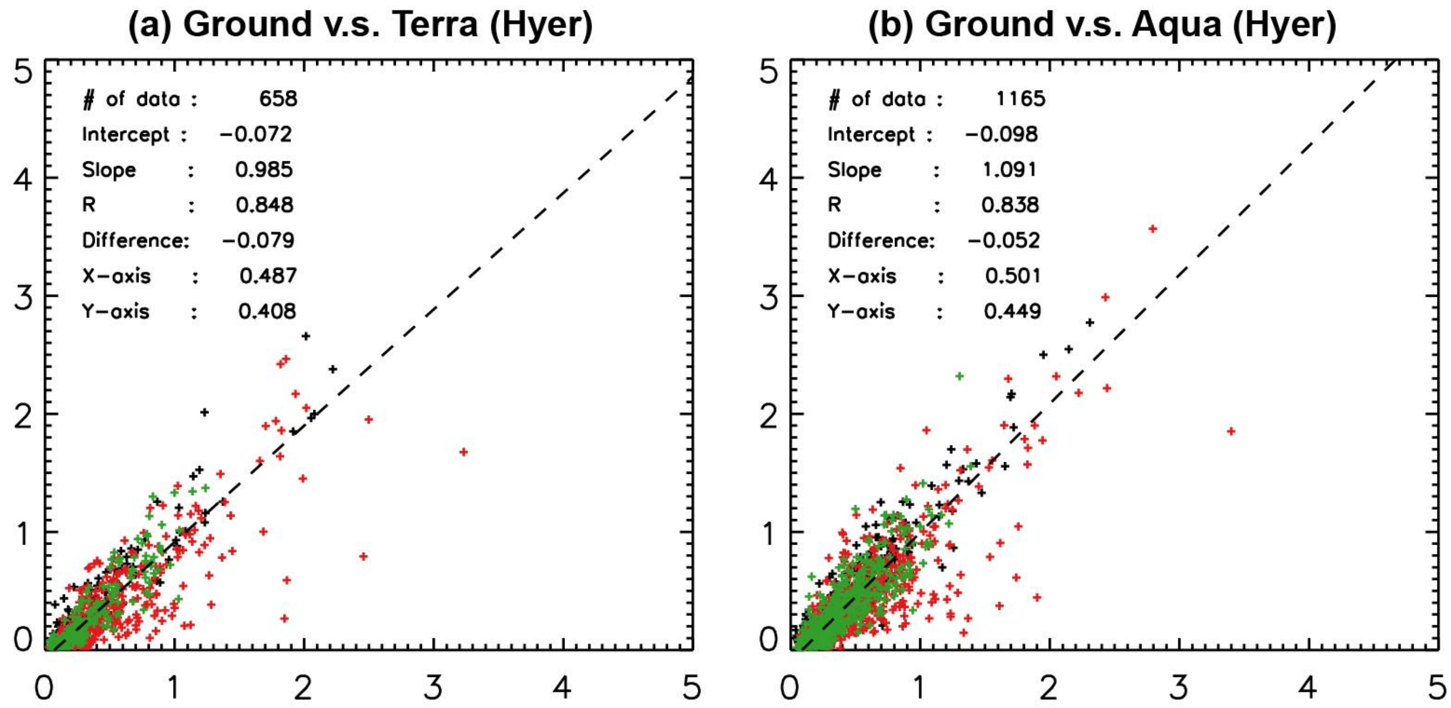
- Long-term data
- Good geographical coverage
- High spatiotemporal resolution
- Vertical and surface data
- Easily verifiable and accessible

Chinese Networks for Aerosol Properties



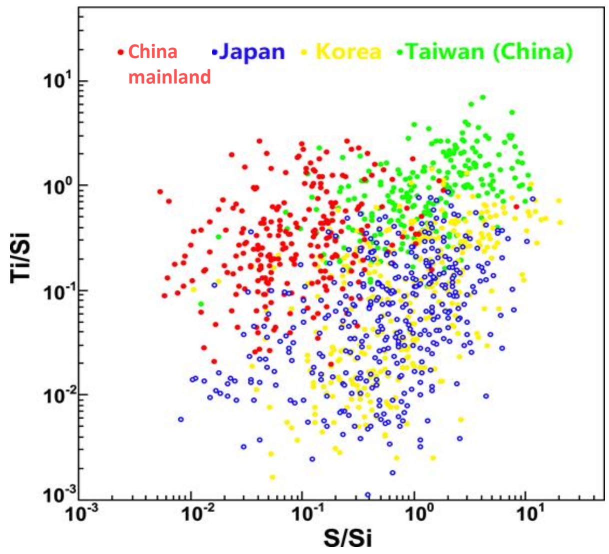
AERONET
CARSNET
CSHNET

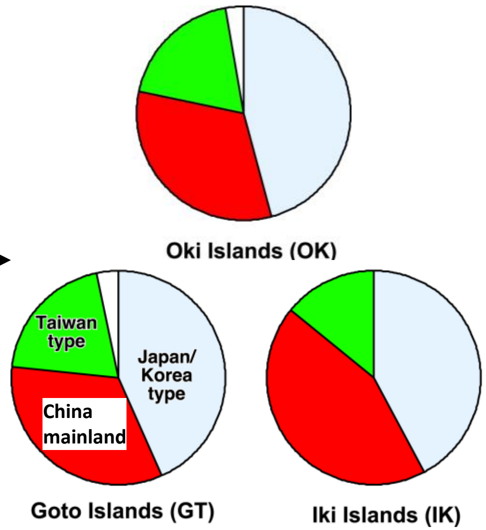
Lin et al., 2014 AE



Observation-based versus Back Trajectory

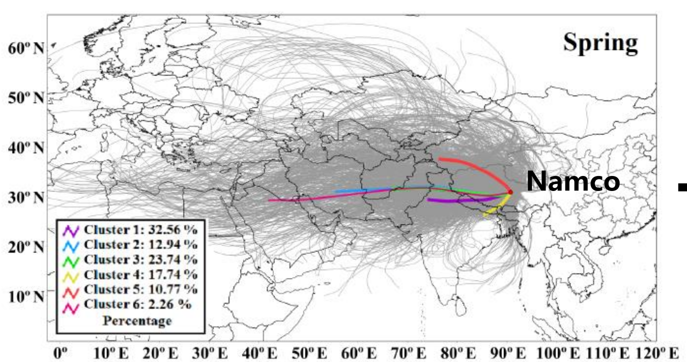
Observation-based attribution of source regions for spheroidal carbonaceous particles

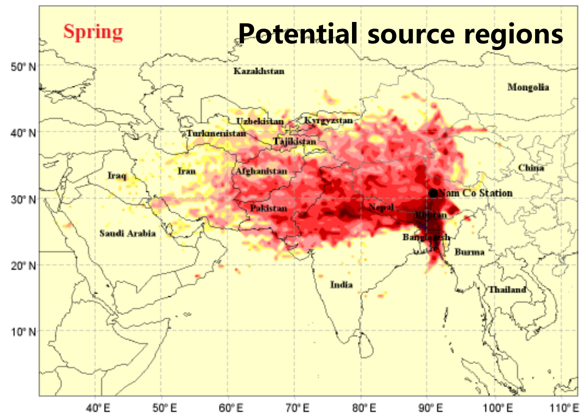




Jun et al. 2014

Back trajectory for source attribution





Yin et al. 2017