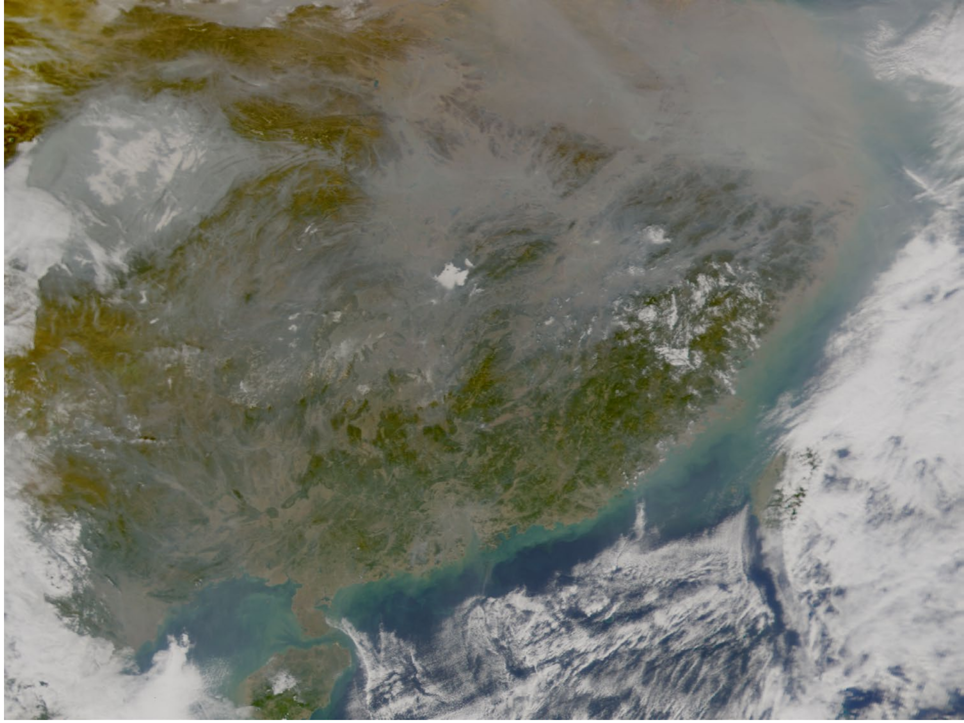
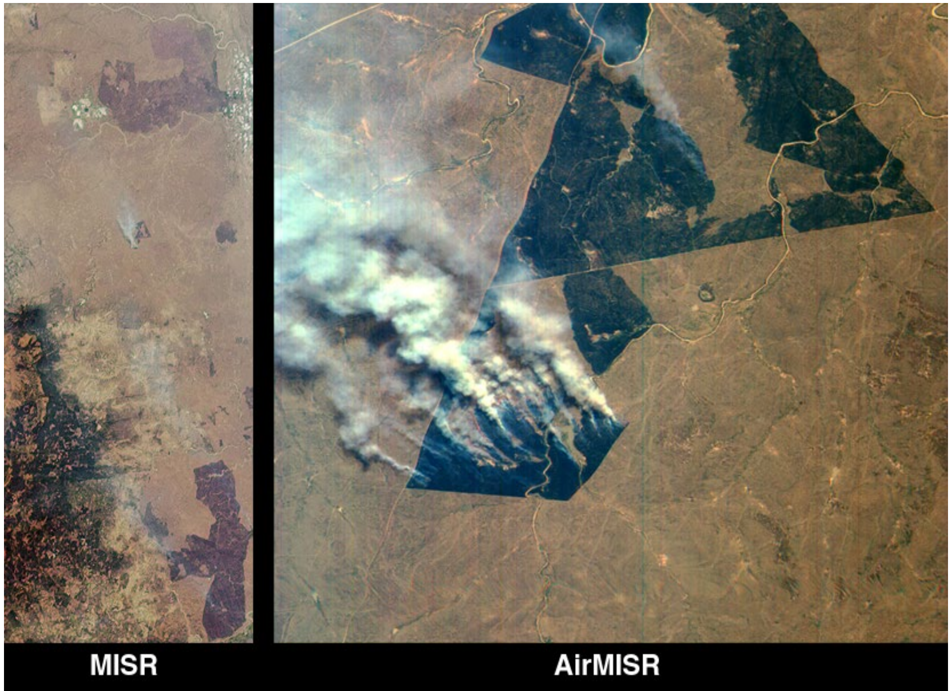
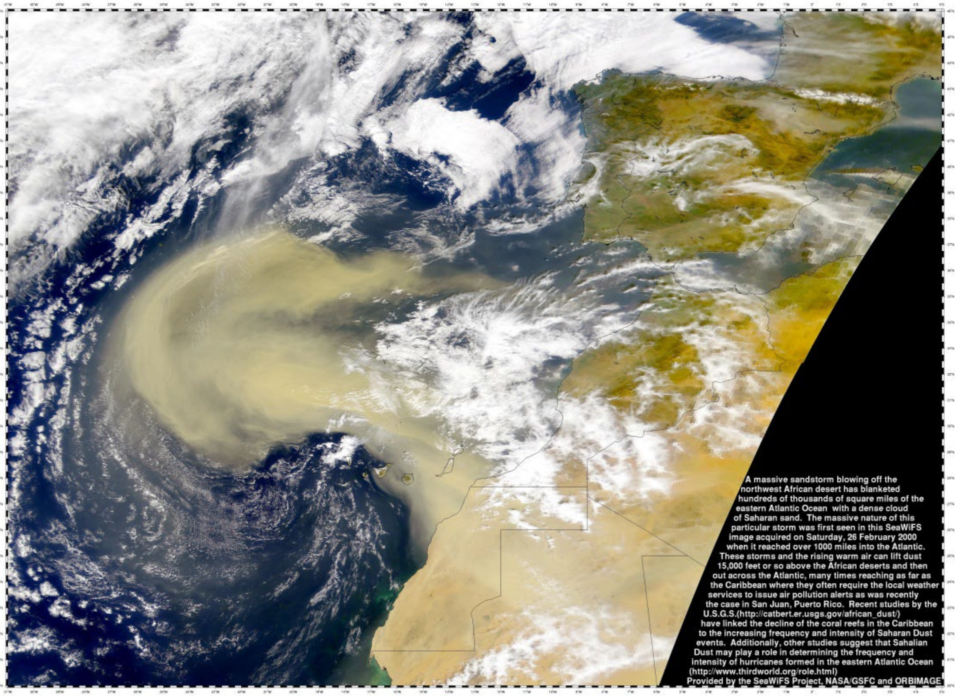
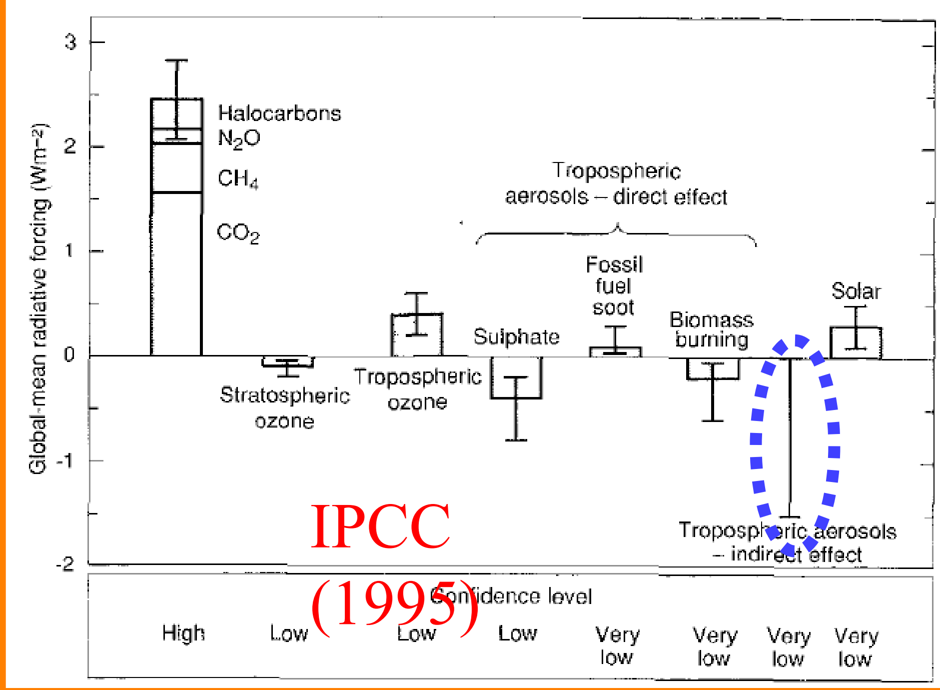
Lecture 23. Aerosol modeling and comparisons with observations

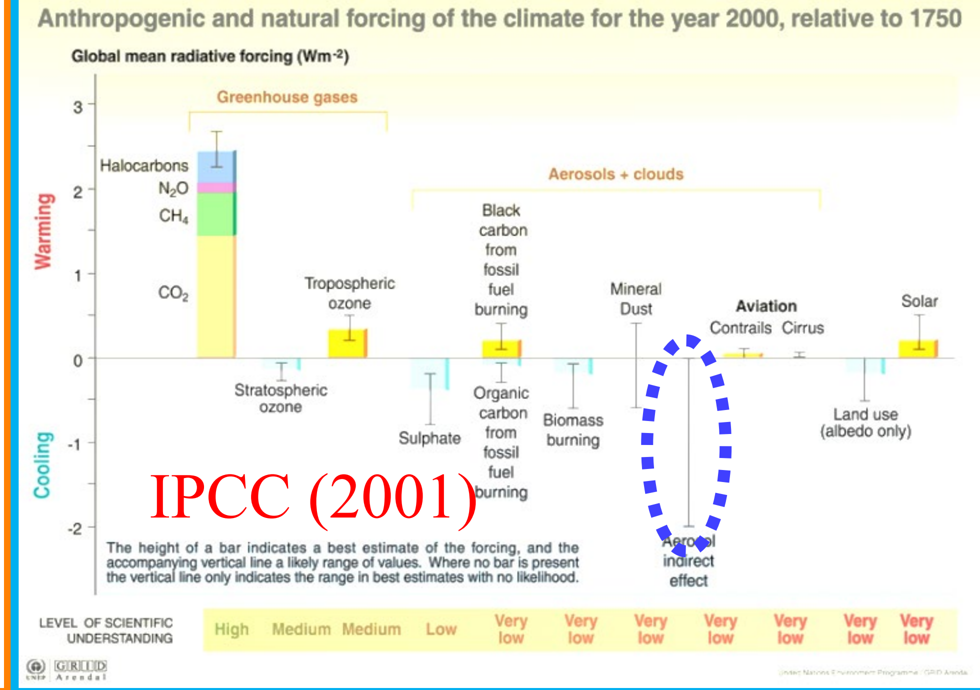




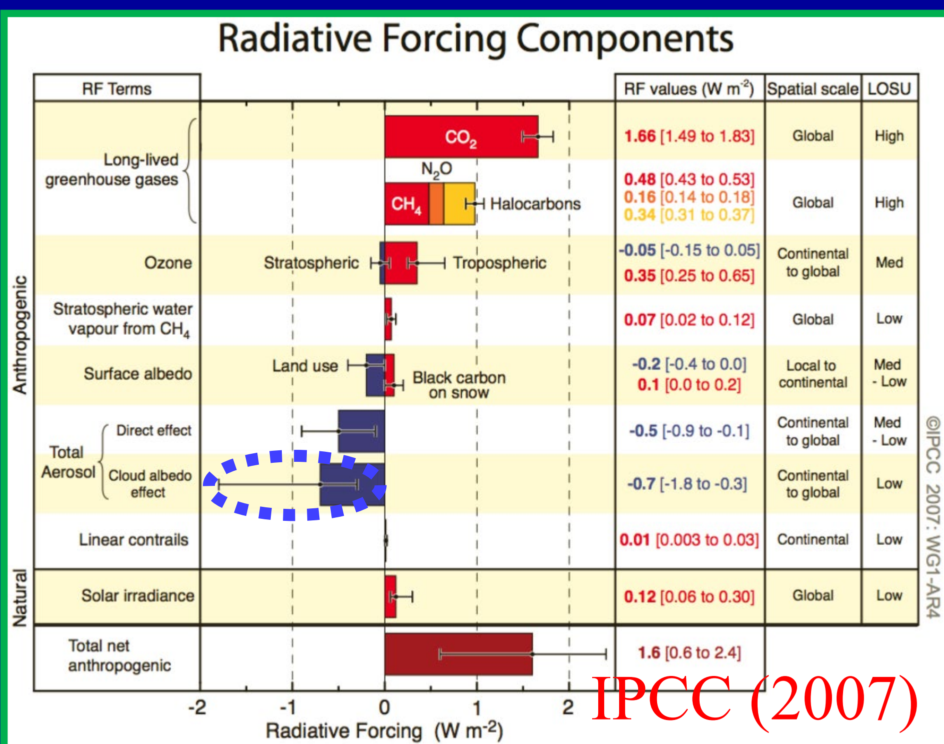




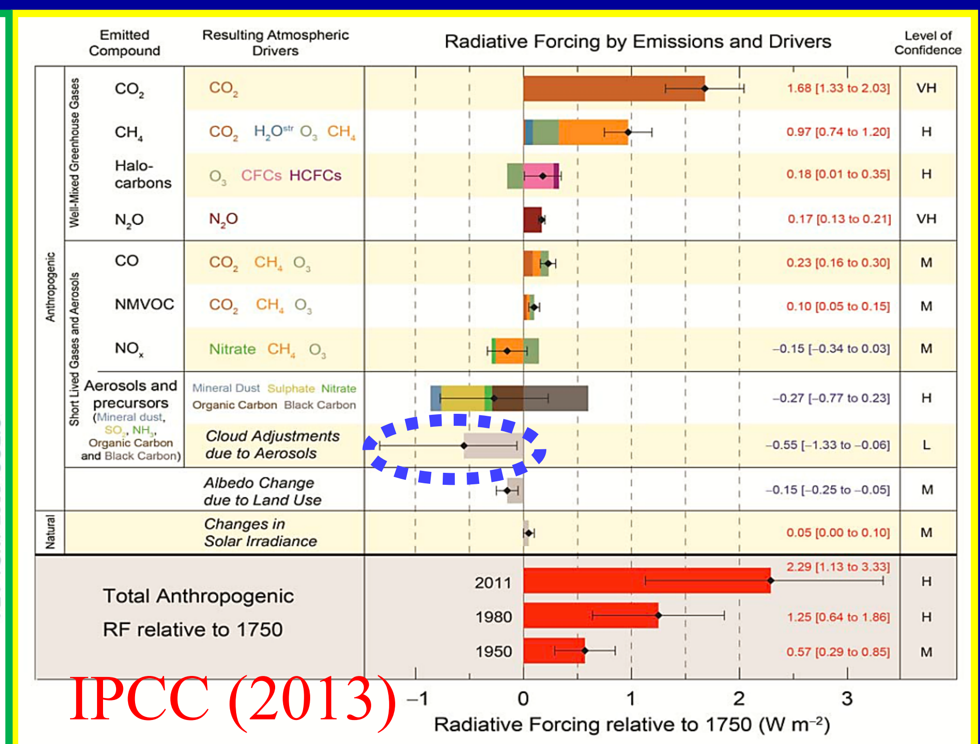
Global-mean radiative forcing (Wm−2)
3
2
1
0
-1
-2
Halocarbons
N2O
CH4
CO2
Tropospheric aerosols – direct effect
Fossil fuel soot
Solar
Sulphate
Biomass burning
Stratospheric ozone
Tropospheric ozone
Tropospheric aerosols – indirect effect
IPCC (1995)
Confidence level
High
Low
Low
Low
Very low
Very low
Very low
Very low



Anthropogenic and natural forcing of the climate for the year 2000, relative to 1750
Global mean radiative forcing (Wm-2)
Warming
Cooling
3
2
1
0
-1
-2
Greenhouse gases
Aerosols + clouds
Halocarbons
N2O
CH4
CO2
Tropospheric ozone
Stratospheric ozone
Black carbon from fossil fuel burning
Organic carbon from fossil fuel burning
Sulphate
Biomass burning
Mineral Dust
Aerosol indirect effect
Aviation
Contrails
Cirrus
Land use (albedo only)
Solar
IPCC (2001)
The height of a bar indicates a best estimate of the forcing, and the accompanying vertical line a likely range of values. Where no bar is present the vertical line only indicates the range in best estimates with no likelihood.
LEVEL OF SCIENTIFIC UNDERSTANDING
High
Medium
Medium
Low
Very low
Very low
Very low
Very low
Very low
Very low
Very low
GRID Arendal



Radiative Forcing Components
RF Terms
RF values (W m-2)
Spatial scale
LOSU
Anthropogenic
Long-lived greenhouse gases
CO2
1.66 [1.49 to 1.83]
Global
High
N2O
CH4
Halocarbons
0.48 [0.43 to 0.53]
0.16 [0.14 to 0.18]
0.34 [0.31 to 0.37]
Global
High
Ozone
Stratospheric
Tropospheric
-0.05 [-0.15 to 0.05]
0.35 [0.25 to 0.65]
Continental to global
Med
Stratospheric water vapour from CH4
0.07 [0.02 to 0.12]
Global
Low
Surface albedo
Land use
Black carbon on snow
-0.2 [-0.4 to 0.0]
0.1 [0.0 to 0.2]
Local to continental
Med - Low
Total Aerosol
Direct effect
-0.5 [-0.9 to -0.1]
Continental to global
Med - Low
Cloud albedo effect
-0.7 [-1.8 to -0.3]
Continental to global
Low
Linear contrails
0.01 [0.003 to 0.03]
Continental
Low
Natural
Solar irradiance
0.12 [0.06 to 0.30]
Global
Low
Total net anthropogenic
1.6 [0.6 to 2.4]
-2
-1
0
1
2
Radiative Forcing (W m-2)
©IPCC 2007: WG1-AR4
IPCC (2007)



Emitted Compound
Resulting Atmospheric Drivers
Radiative Forcing by Emissions and Drivers
Level of Confidence
Anthropogenic
Well-Mixed Greenhouse Gases
CO2
CO2
1.68 [1.33 to 2.03]
VH
CH4
CO2 H2Ostr O3 CH4
0.97 [0.74 to 1.20]
H
Halo-carbons
O3 CFCs HCFCs
0.18 [0.01 to 0.35]
H
N2O
N2O
0.17 [0.13 to 0.21]
VH
Short Lived Gases and Aerosols
CO
CO2 CH4 O3
0.23 [0.16 to 0.30]
M
NMVOC
CO2 CH4 O3
0.10 [0.05 to 0.15]
M
NOx
Nitrate CH4 O3
−0.15 [−0.34 to 0.03]
M
Aerosols and precursors (Mineral dust, SO2, NH3, Organic Carbon and Black Carbon)
Mineral Dust Sulphate Nitrate Organic Carbon Black Carbon
−0.27 [−0.77 to 0.23]
H
Cloud Adjustments due to Aerosols
−0.55 [−1.33 to −0.06]
L
Albedo Change due to Land Use
−0.15 [−0.25 to −0.05]
M
Natural
Changes in Solar Irradiance
0.05 [0.00 to 0.10]
M
Total Anthropogenic RF relative to 1750
2011
2.29 [1.13 to 3.33]
H
1980
1.25 [0.64 to 1.86]
H
1950
0.57 [0.29 to 0.85]
M
−1
0
1
2
3
Radiative Forcing relative to 1750 (W m−2)
IPCC (2013)

IPCC, Climate Change 2021: The Physical Science Basis

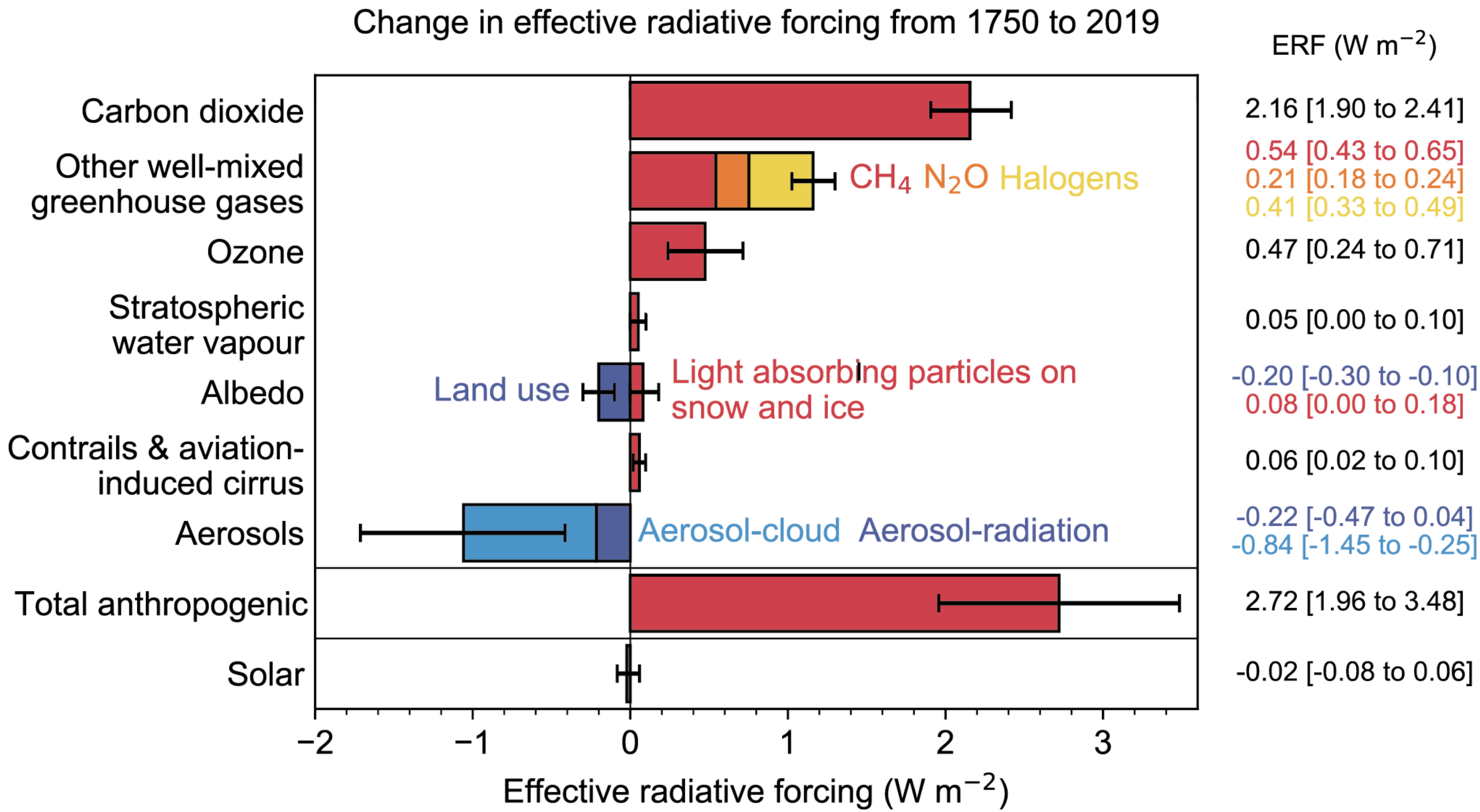
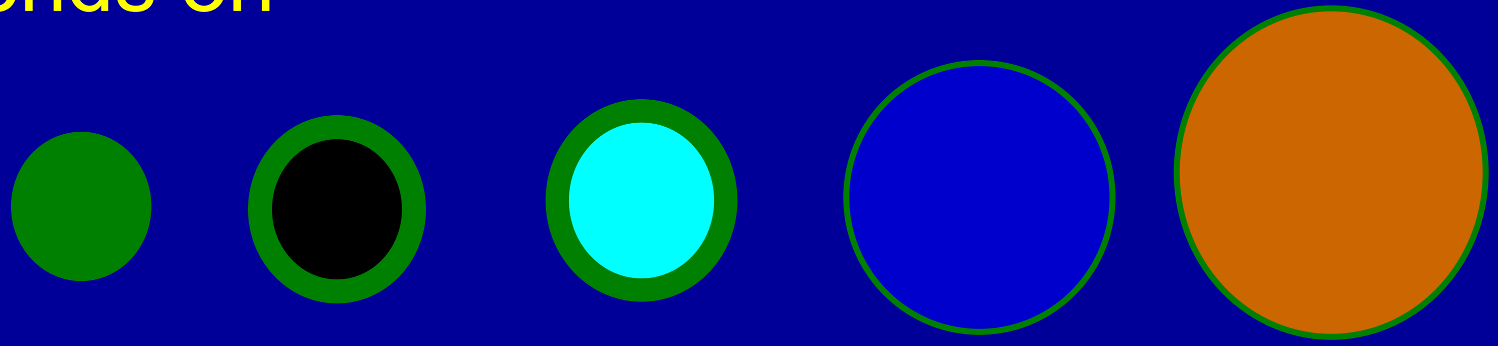


Figure 7.6 | Change in effective radiative forcing (ERF) from 1750 to 2019 by contributing forcing agents (carbon dioxide, other well-mixed greenhouse gases (WMGHGs), ozone, stratospheric water vapour, surface albedo, contrails and aviation-induced cirrus, aerosols, anthropogenic total, and solar).

Aerosol climatic and environmental impacts

depends on



Concentrations,

Sizes,

Compositions,

Mixing States

Emission, Deposition,

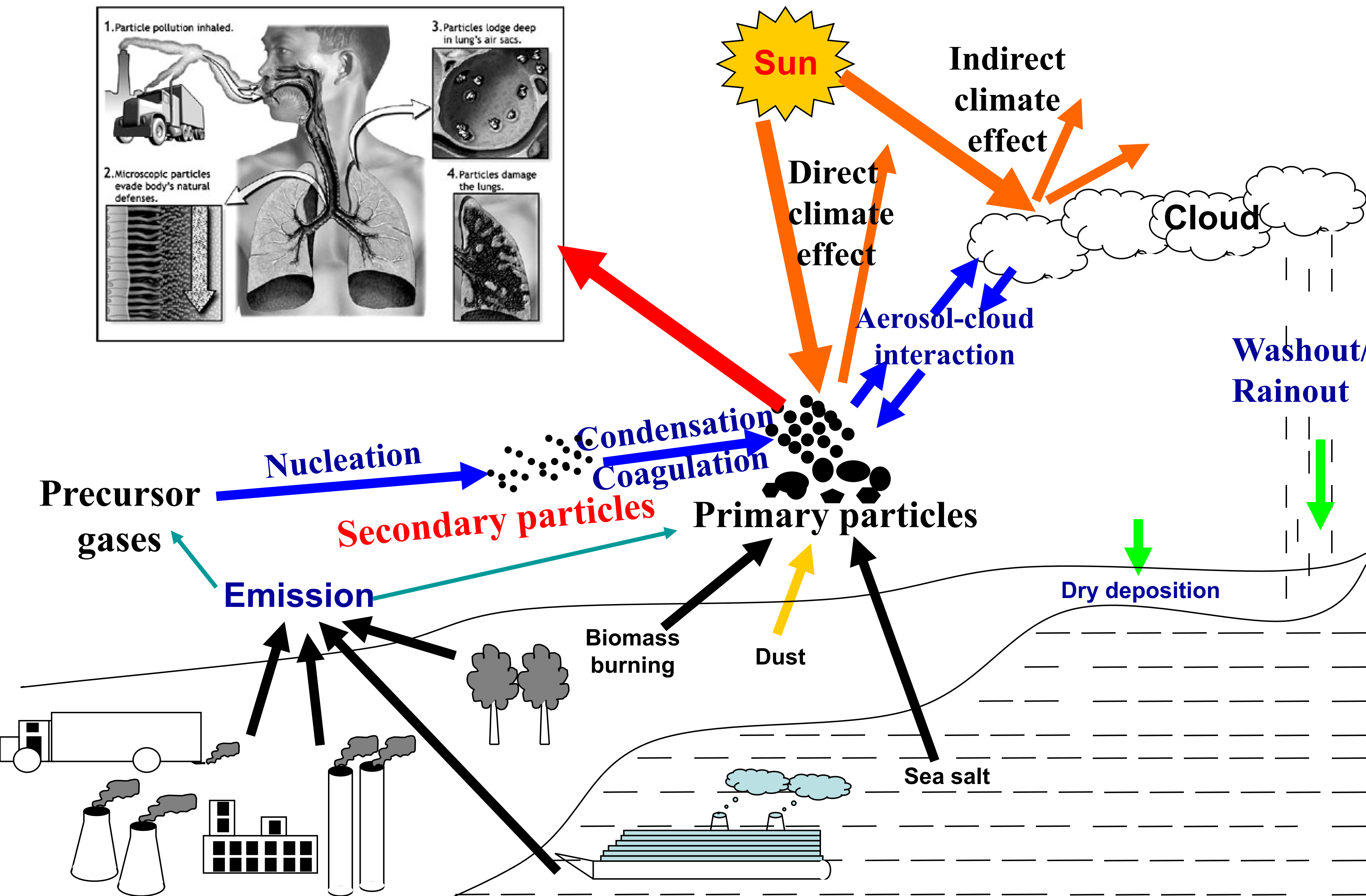
Nucleation, Growth,

Coagulation,
Scavenging,

Aqueous Chemistry

which have large spatial and temporal variations.

Physical processes controlling aerosol properties



$$\frac{\partial n(v,t)}{\partial t} = \frac{1}{2}\int_0^v K(v-q,q)n(v-q,t)n(q,t)\,dq$$
$$- n(v,t)\int_0^\infty K(q,v)n(q,t)\,dq - \frac{\partial}{\partial v}[I(v)n(v,t)]$$
$$+ J_0(v)\delta(v-v_0) + S(v) - R(v)$$

TABLE 12.6 Properties of Coagulation, Condensation, and Nucleation

Process	Number Concentration	Volume Concentration
Coagulation	Decreases	No change
Condensation	No change	Increases
Nucleation	Increases	Increases
Coagulation and condensation	Decreases	Increases

Approaches to modeling aerosols

Sizes:

1. Bulk
2. Modal
3. Sectional

Mixing states:

1. External
2. Internal
3. Semi-external

Yu, 1998, Ph.D Dissertation, Advisor: Prof. R. Turco

*"**A Study of the Formation and Evolution of Aerosols and Contrails in Aircraft Wakes**: Development, Validation & Application of an Advanced Particle Microphysics (**APM**) Model"*

Two versions of APM model:

1. **A comprehensive APM box model** for detailed particle microphysics studies

Atmos. Chem. Phys., 18, 17451–17474, 2018
https://doi.org/10.5194/acp-18-17451-2018

Atmospheric Chemistry and Physics
Open Access
EGU

H_2SO_4–H_2O–NH_3 ternary ion-mediated nucleation (TIMN): kinetic-based model and comparison with CLOUD measurements

Fangqun Yu[1], Alexey B. Nadykto[1,2,3], Jason Herb[1], Gan Luo[1], Kirill M. Nazarenko[2], and Lyudmila A. Uvarova[2,3]

Environmental Science & Technology
Open Access

pubs.acs.org/est
Article

Revisiting Contrail Ice Formation: Impact of Primary Soot Particle Sizes and Contribution of Volatile Particles

Fangqun Yu,* Bernd Kärcher, and Bruce E. Anderson

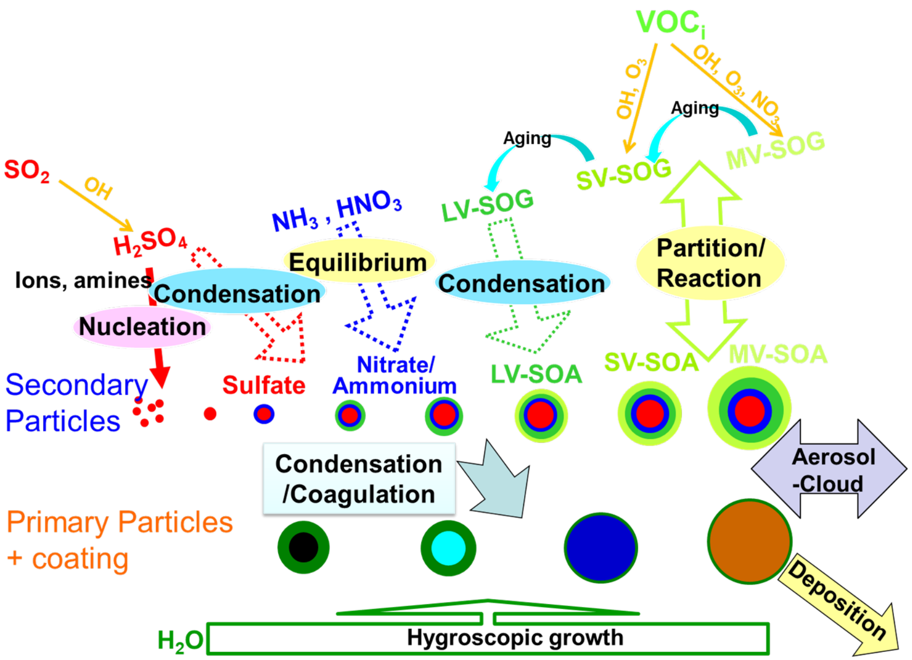
Cite This: *Environ. Sci. Technol.* 2024, 58, 17650–17660
Read Online

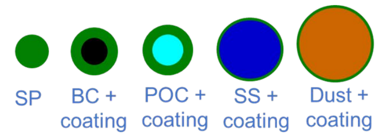
2. A **simplified and computationally efficient APM** for integrating with 3-D global and regional models

- → **GEOS-Chem** (Yu and Luo, ACP, 2009)
- → **WRF-Chem** (Luo and Yu, ACP, 2011)
- → **NAQPMS** (Chen et al., SOLA, 2017)
- → **IAP-AACM** (Chen et al., ACP, 2021)
- → **CESM2-WACCM** (Williamson et al., Nature, 2019; Yu et al., under review, 2025)
- → **WRF-CMAQ** (Mao et al., JGR, 2025)
- → **E3SMv3** (Luo et al., to be submitted, 2025)

Advanced Particle Microphysics (APM) for 3-D Models

- APM considers particle nucleation, condensation, coagulation, equilibrium/partition, and deposition processes.
- APM includes 40 size-bins for secondary particle,15 size-bins for OC and BC, 20 size-bins for sea salt, and 15 size-bins for dust.





Secondary particles (SP) : **40** bins
(composed of SO4, NO3, NH4, SOA)

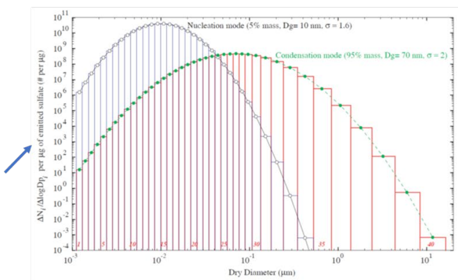
Sea salt particles: 20 bins

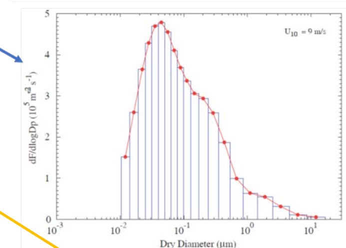
Dust: 15 bins

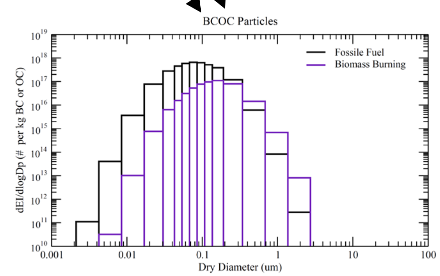
BC: 15 bins

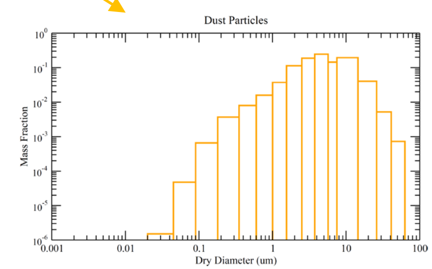
Primary OC: 15 bins

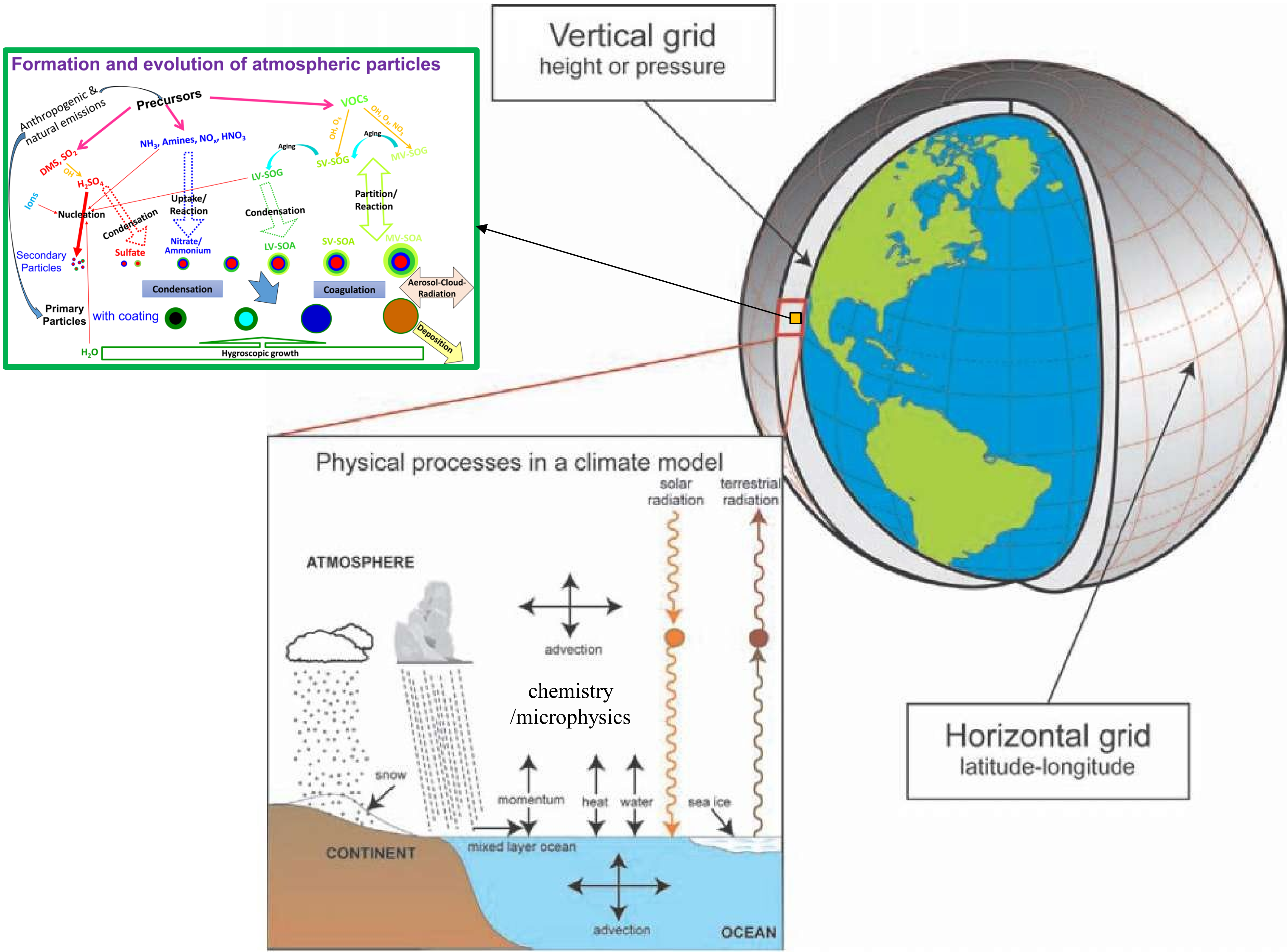
Coating of primary particles by secondary species tracked.











Formation and evolution of atmospheric particles
Anthropogenic & natural emissions
Precursors
VOCs
NH3, Amines, NOx, HNO3
DMS, SO2
OH
H2SO4
Ions
Nucleation
Condensation
Uptake/ Reaction
Nitrate/ Ammonium
Sulfate
Secondary Particles
LV-SOG
SV-SOG
MV-SOG
Aging
Partition/ Reaction
LV-SOA
SV-SOA
MV-SOA
Condensation
Coagulation
Aerosol-Cloud-Radiation
Primary Particles
with coating
Deposition
H2O
Hygroscopic growth
Vertical grid
height or pressure
Horizontal grid
latitude-longitude
Physical processes in a climate model
solar radiation
terrestrial radiation
ATMOSPHERE
advection
chemistry /microphysics
snow
momentum
heat
water
sea ice
mixed layer ocean
CONTINENT
advection
OCEAN

Key features of APM

Binary and Ternary Ion-Mediated Nucleation (IMN) and other Nucleation Schemes (Yu and Turco, GRL1997, GRL 2000, JGR 2001, ACP 2008, 2011; Yu, JCP 2005, ACP 2006, JGR 2010; Yu et al., 2017, 2018)

Equilibrium uptake of NH_3, HNO_3, and H_2O: ISORROPIA II (Fountoukis and Nenes, ACP, 2007)

SOA formation: Extended 2-product method which considers successive oxidation aging and kinetic condensation (Yu, ACP, 2011)

Mixing state: Semi-externally mixed that tracks the amount of secondary species coated on primary particles (Yu and Luo, ACP, 2009; Yu et al., ACP, 2011)

Validation: Computationally efficient and simulations validated by a large number field measurements (Yu and Luo, 2009, 2010; Yu, 2010; Luo and Yu, 2011a, b; Yu et al., 2011, 2012; Ma et al., 2012a, b)

GEOS-Chem-APM

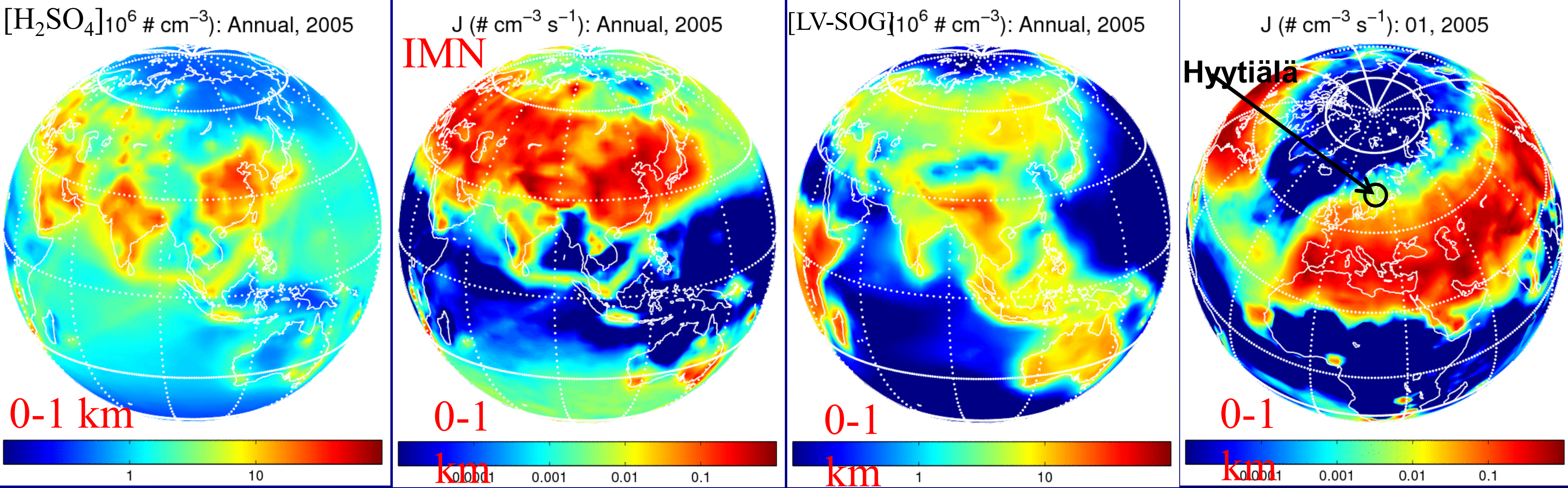
GEOS-Chem-APM (Yu and Luo, 2009)

- ✓ Full chemistry (NOx, SOx, VOCs, etc.)
- ✓ Full size-resolved microphysics
- ✓ Offline assimilated meteorology
- ✓ Suitable for studies of processes and global long-term simulations

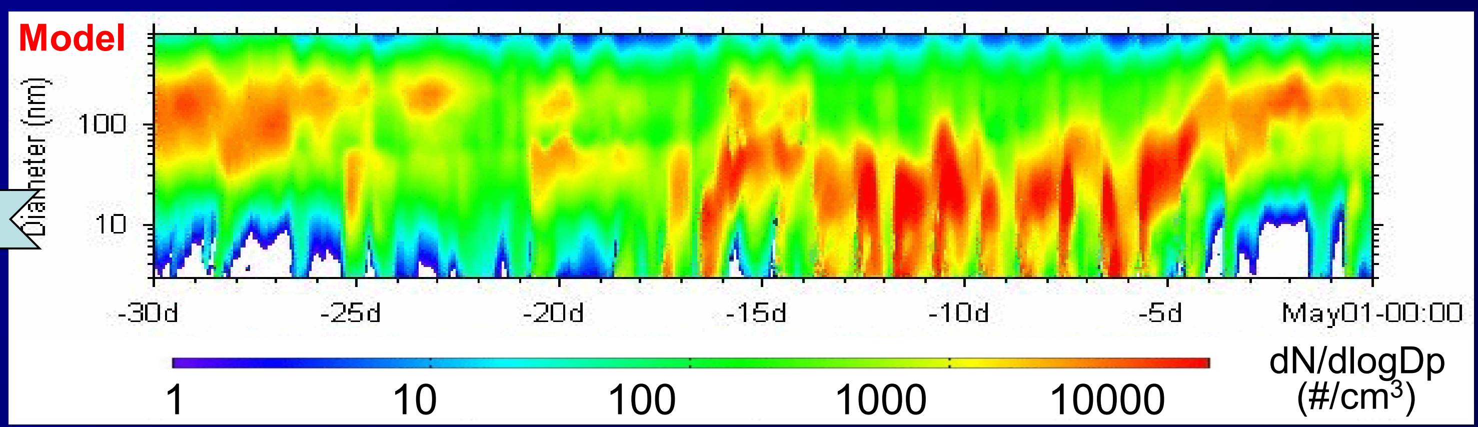
Computing cost (24-core workstation)

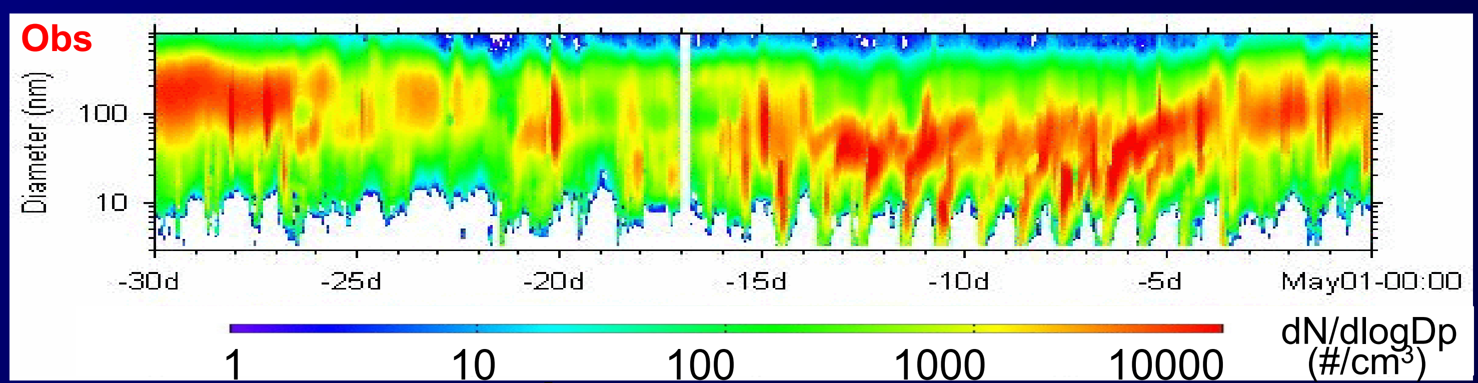
GEOS-Chem (2^ox2.5^o , 47 layers, **1 yr**)

Original model	With APM
59 tracers	59+88= 147 tracers
~ 5 day	**~ 11** days

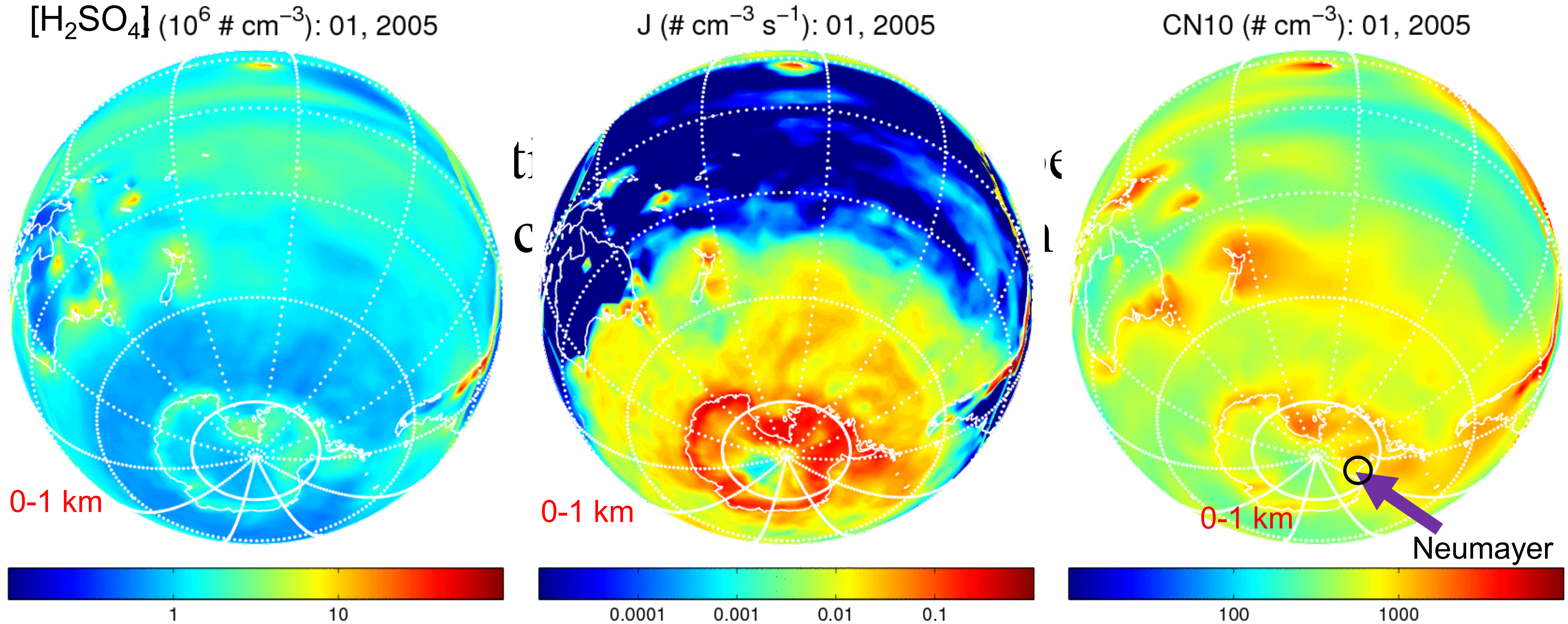


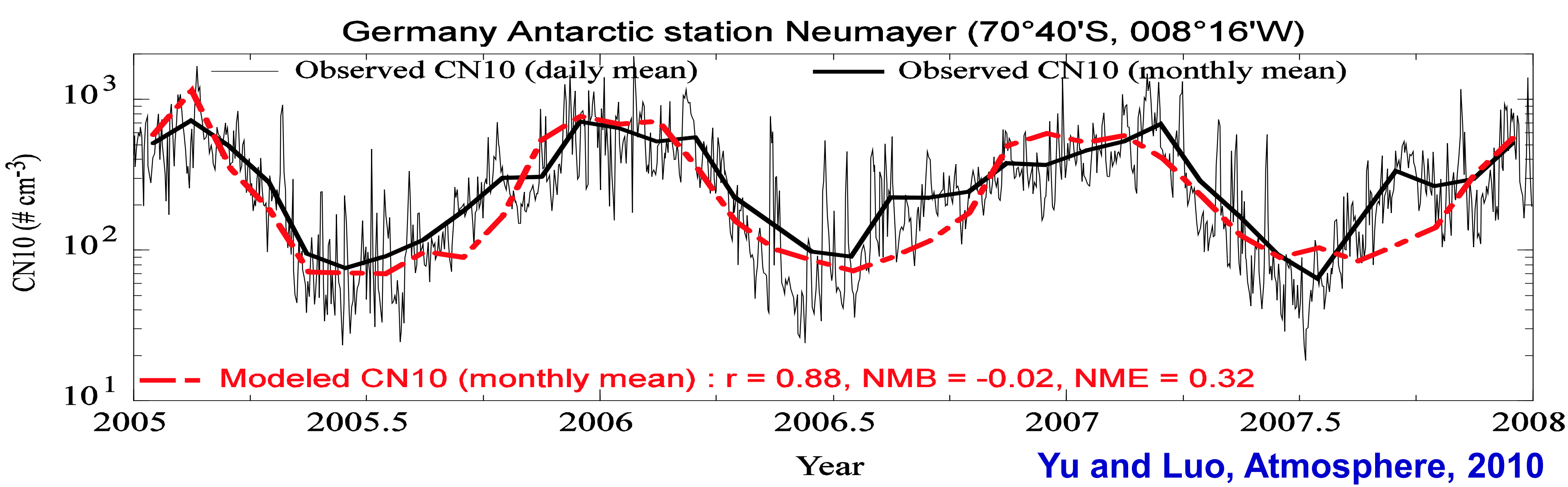
CN
CCN/IN
Ext Coef.
AOD





Data acknowledgements: Prof Markku Kulmala, CREATE and EUSSAR data base.

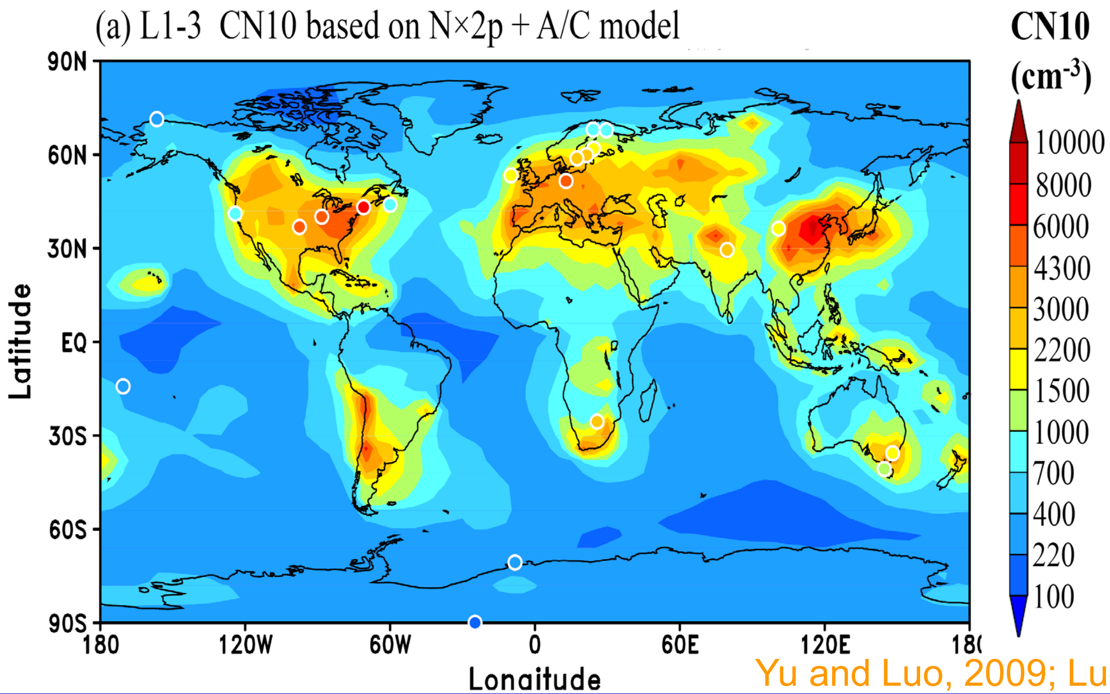


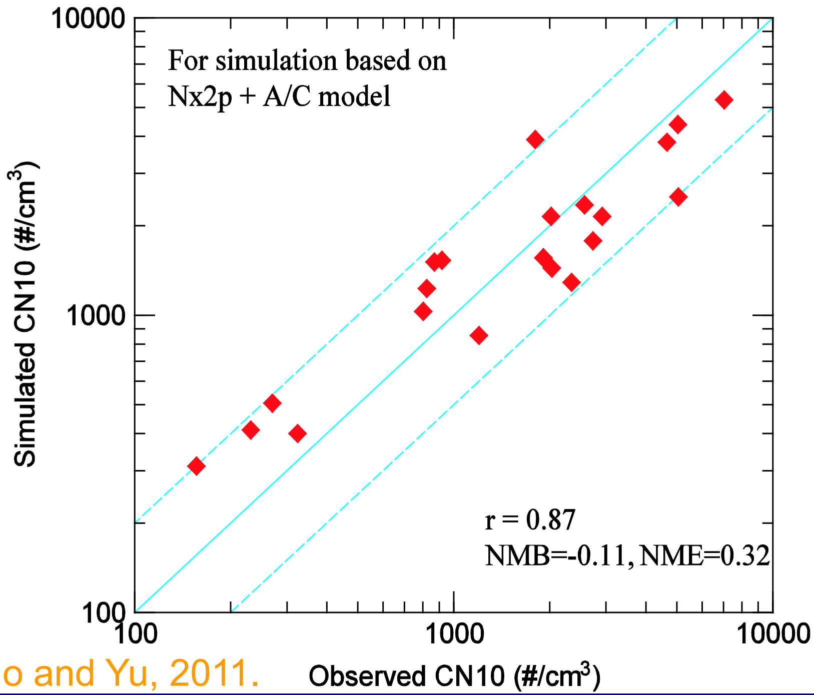


Yu and Luo, Atmosphere, 2010

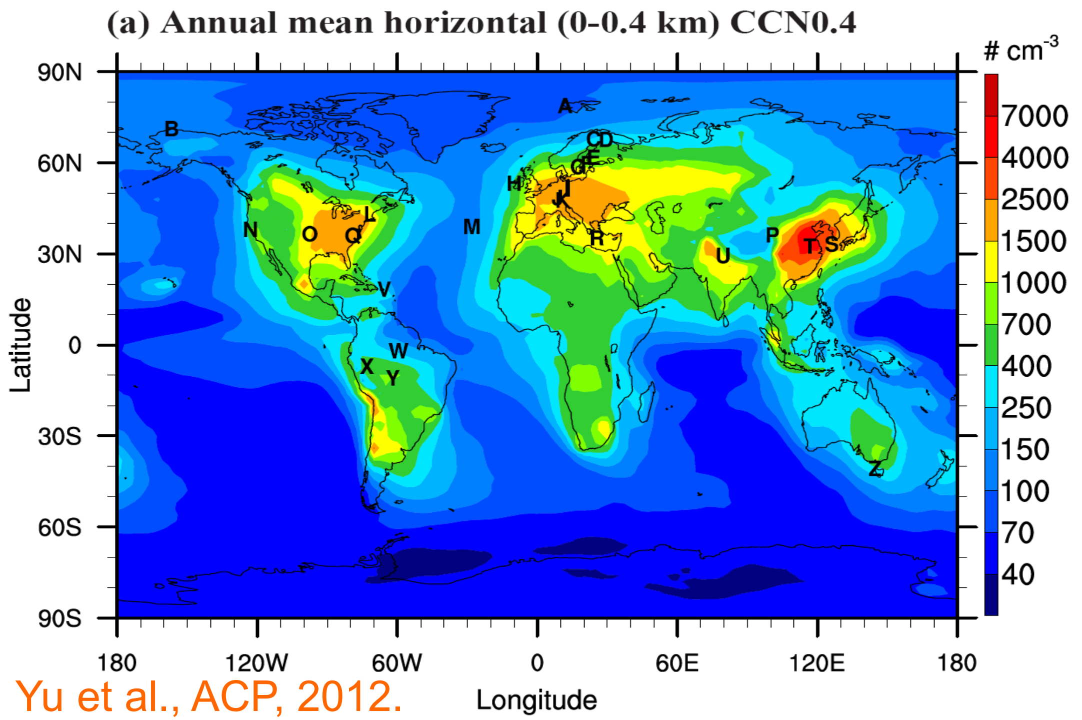
data references: König-Langlo et al. (1998), Weller and Lampert (2008)

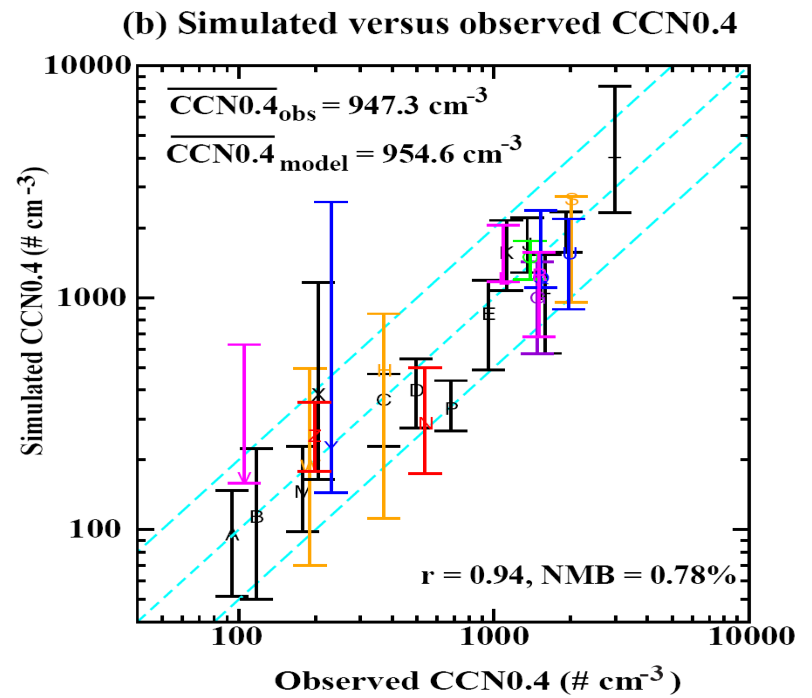
Modeling results are for surface layer



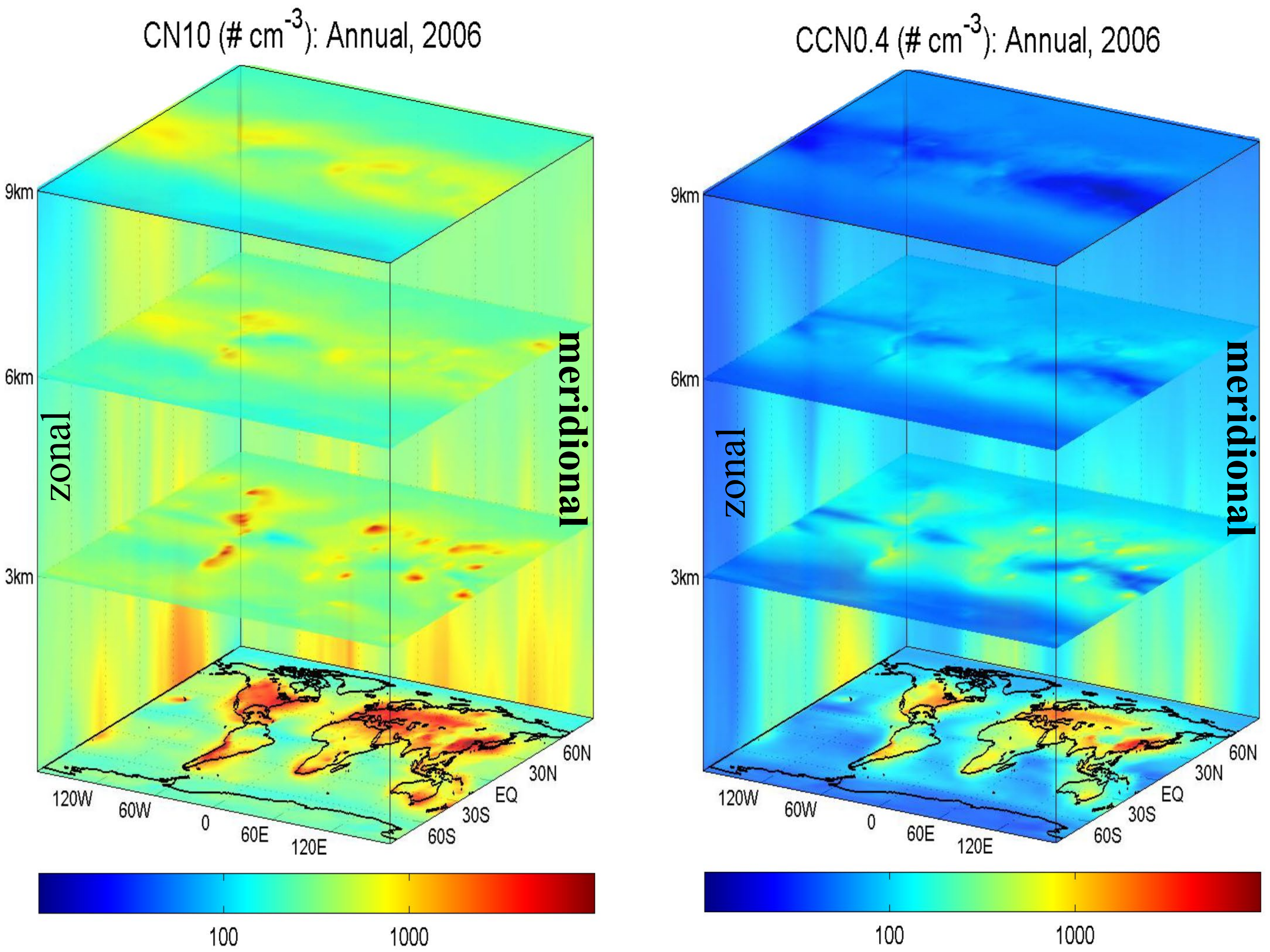


Yu and Luo, 2009; Luo and Yu, 2011.



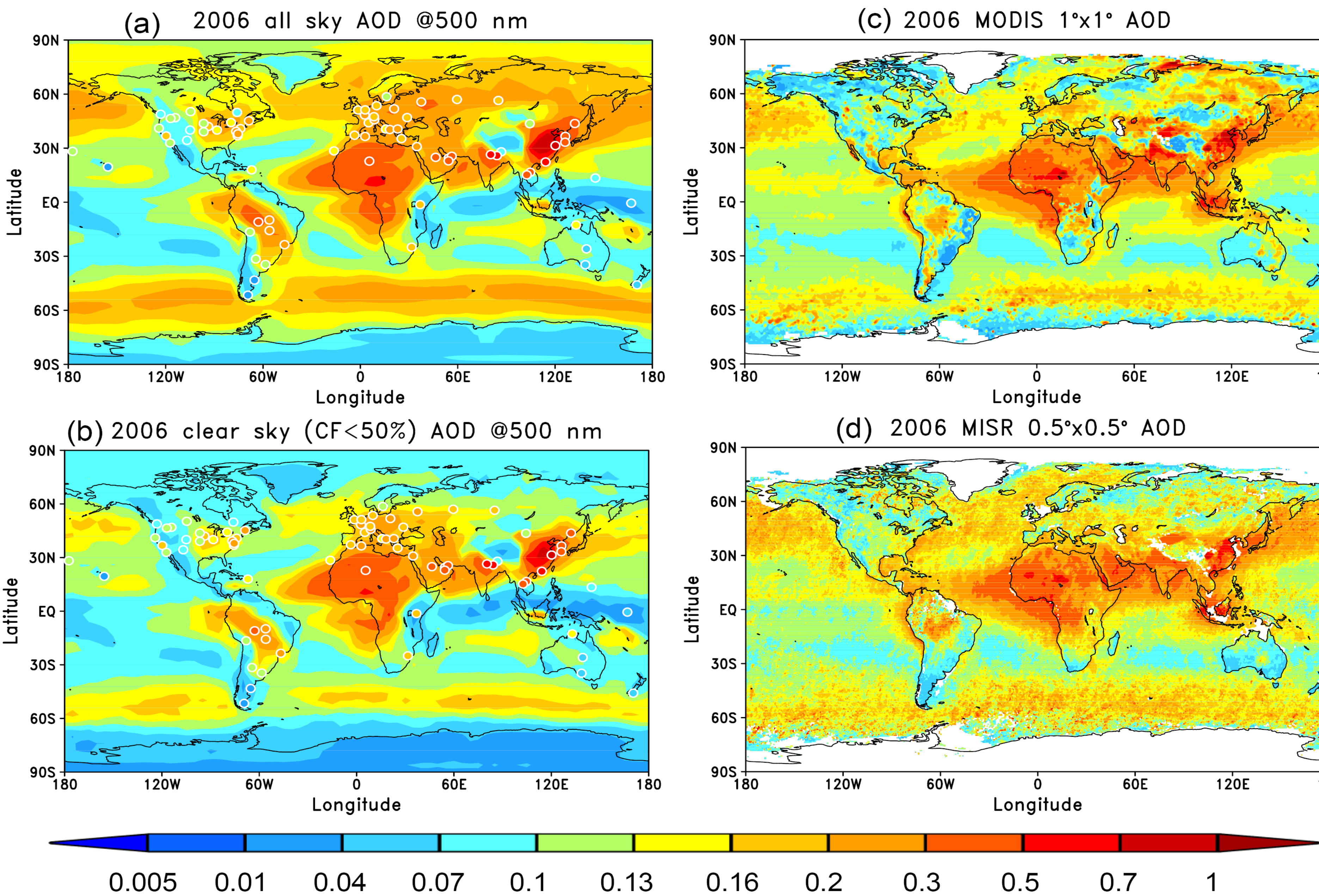


Yu et al., ACP, 2012.

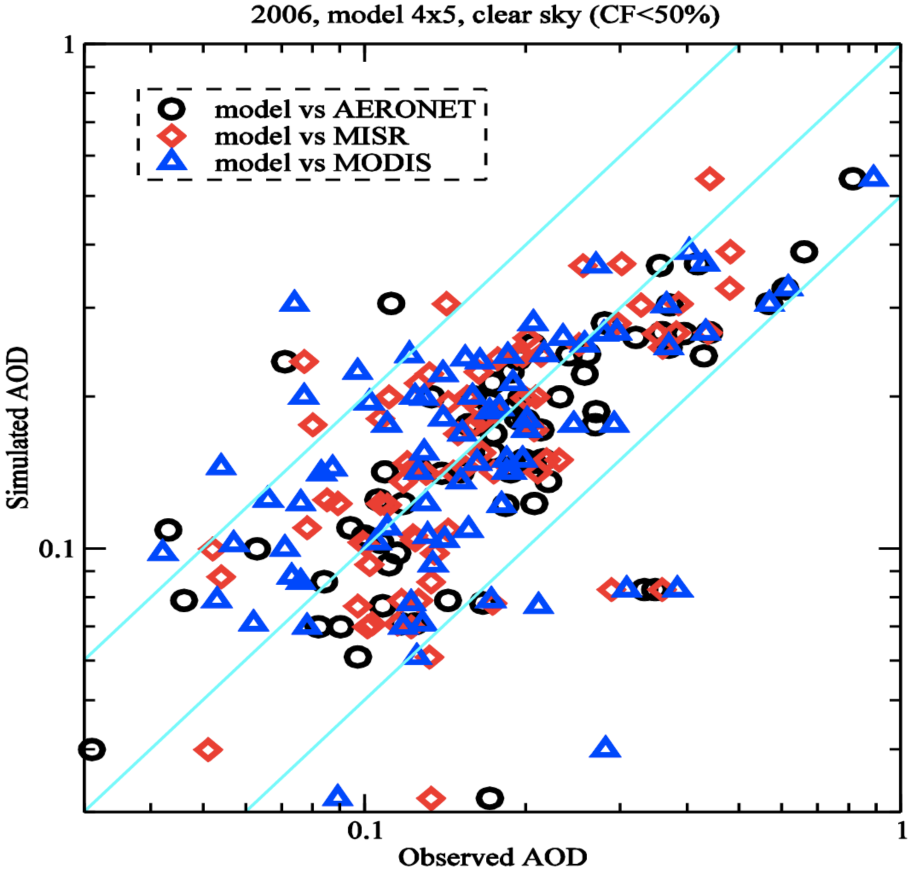


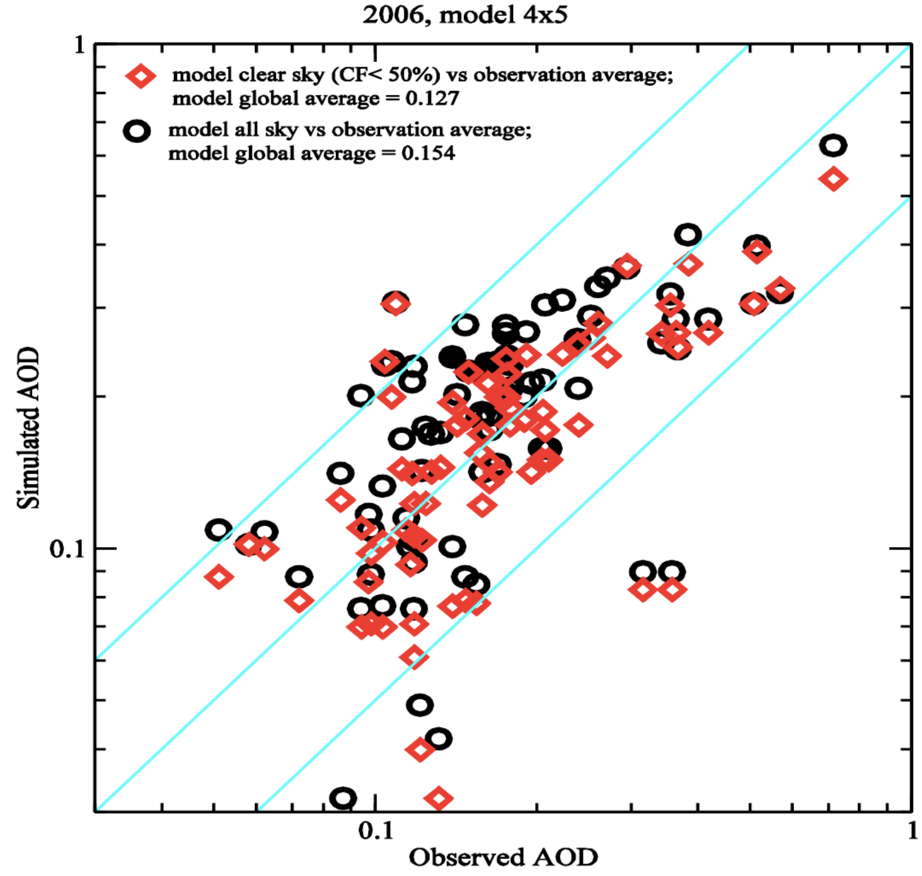
CN10 (# cm^-3): Annual, 2006
9km
6km
3km
zonal
meridional
120W
60W
0
60E
120E
60S
30S
EQ
30N
60N
100
1000
CCN0.4 (# cm^-3): Annual, 2006
9km
6km
3km
zonal
meridional
120W
60W
0
60E
120E
60S
30S
EQ
30N
60N
100
1000

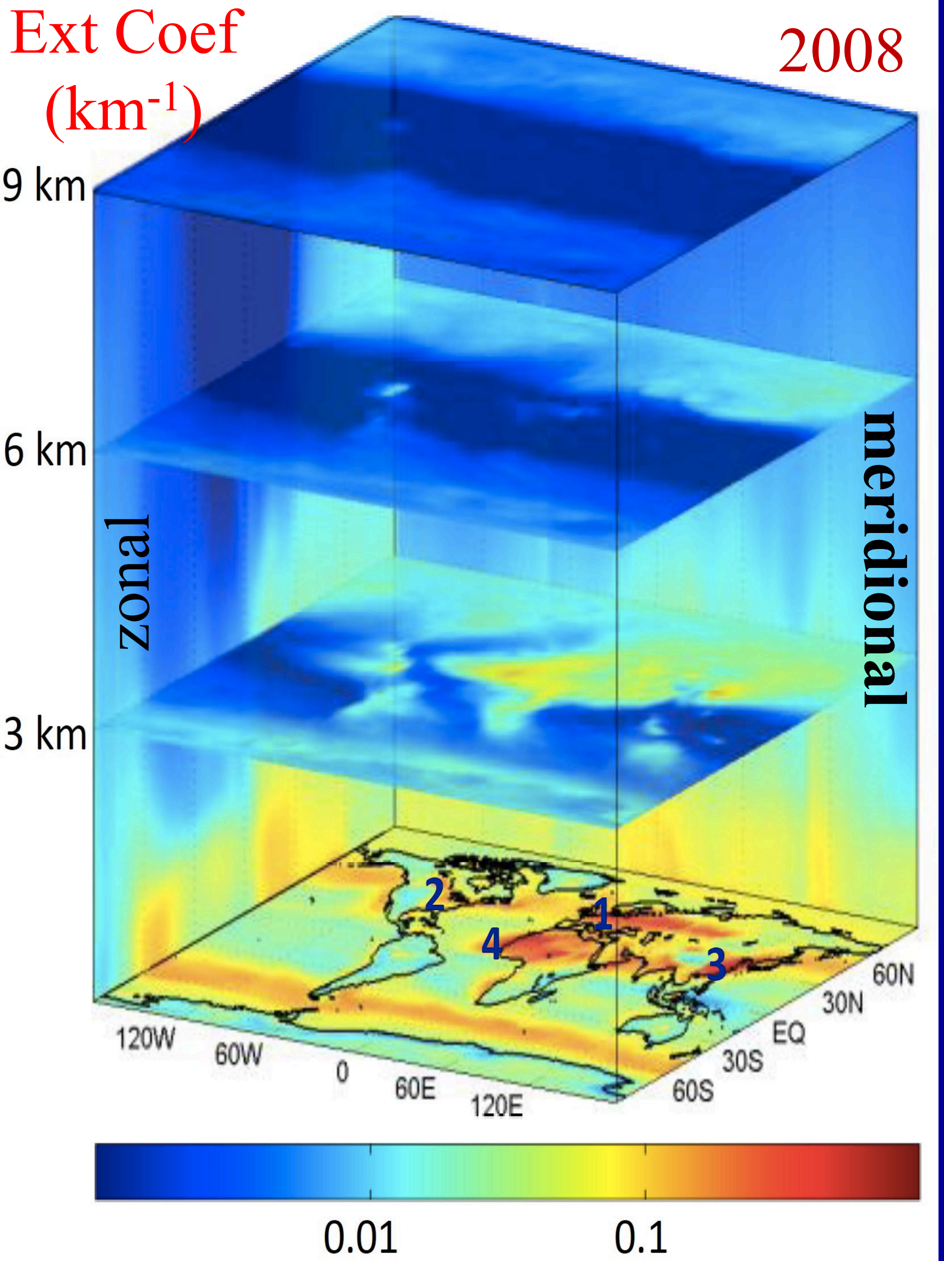
Comparison with AOD measurements



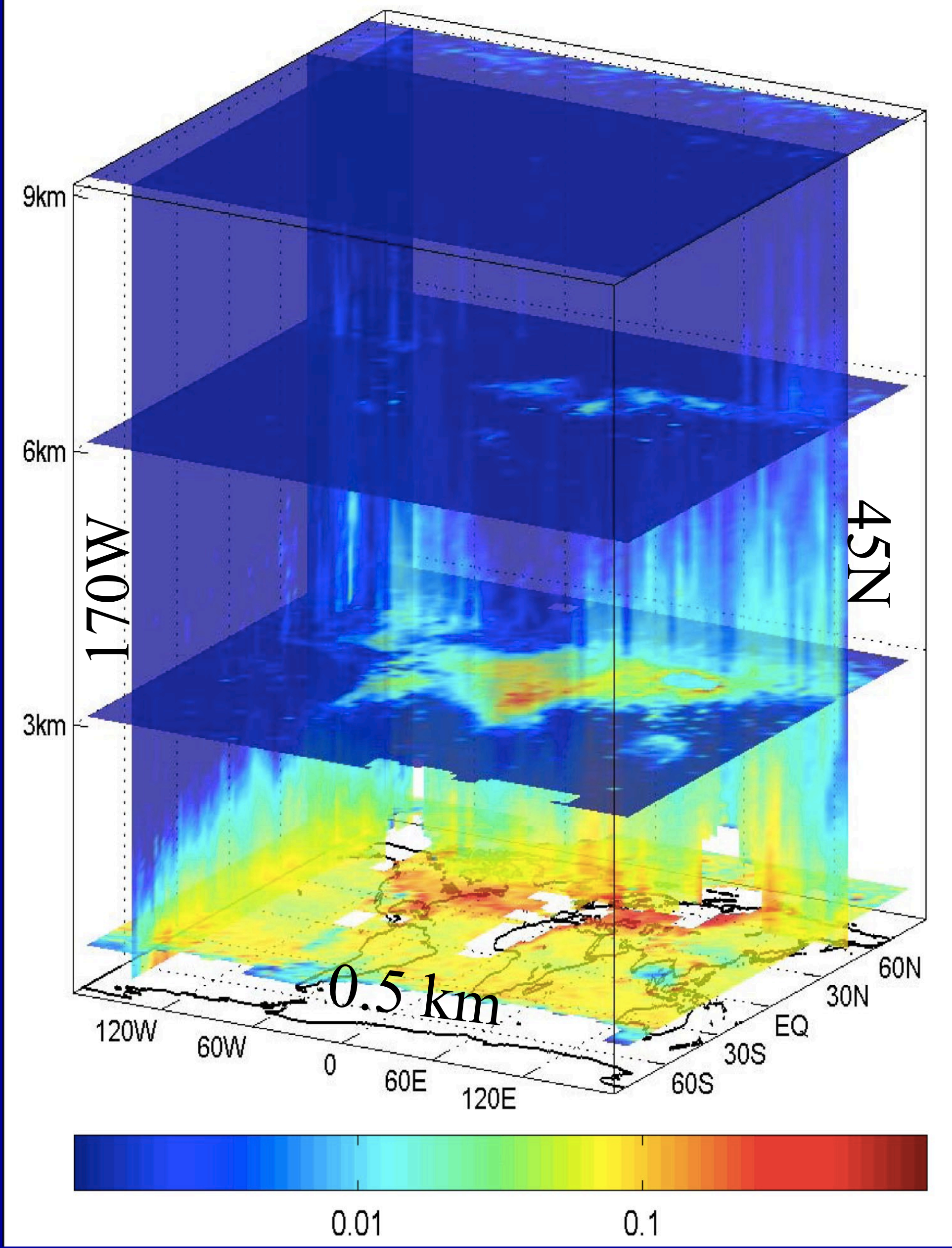
Comparison with AOD measurements



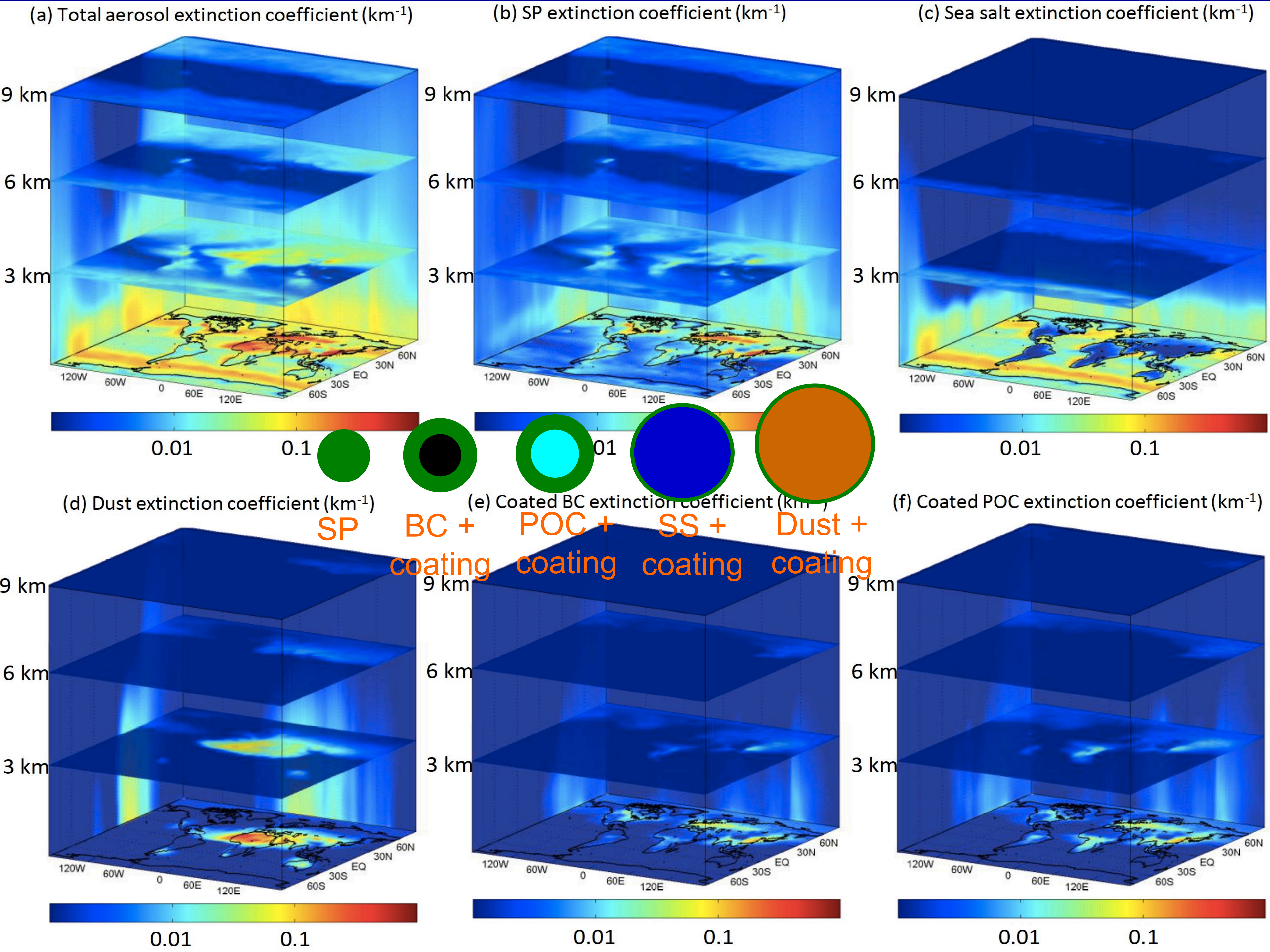




Model: All sky, annual average
Vertical sigma coordinate



CALIOP: night time all sky, annual,
Vertical asl coordinate



(a) Total aerosol extinction coefficient (km-1)
(b) SP extinction coefficient (km-1)
(c) Sea salt extinction coefficient (km-1)
(d) Dust extinction coefficient (km-1)
(e) Coated BC extinction coefficient (km-1)
(f) Coated POC extinction coefficient (km-1)
9 km
6 km
3 km
120W
60W
0
60E
120E
60S
30S
EQ
30N
60N
0.01
0.1
SP
BC + coating
POC + coating
SS + coating
Dust + coating

Ma and Yu, 2014

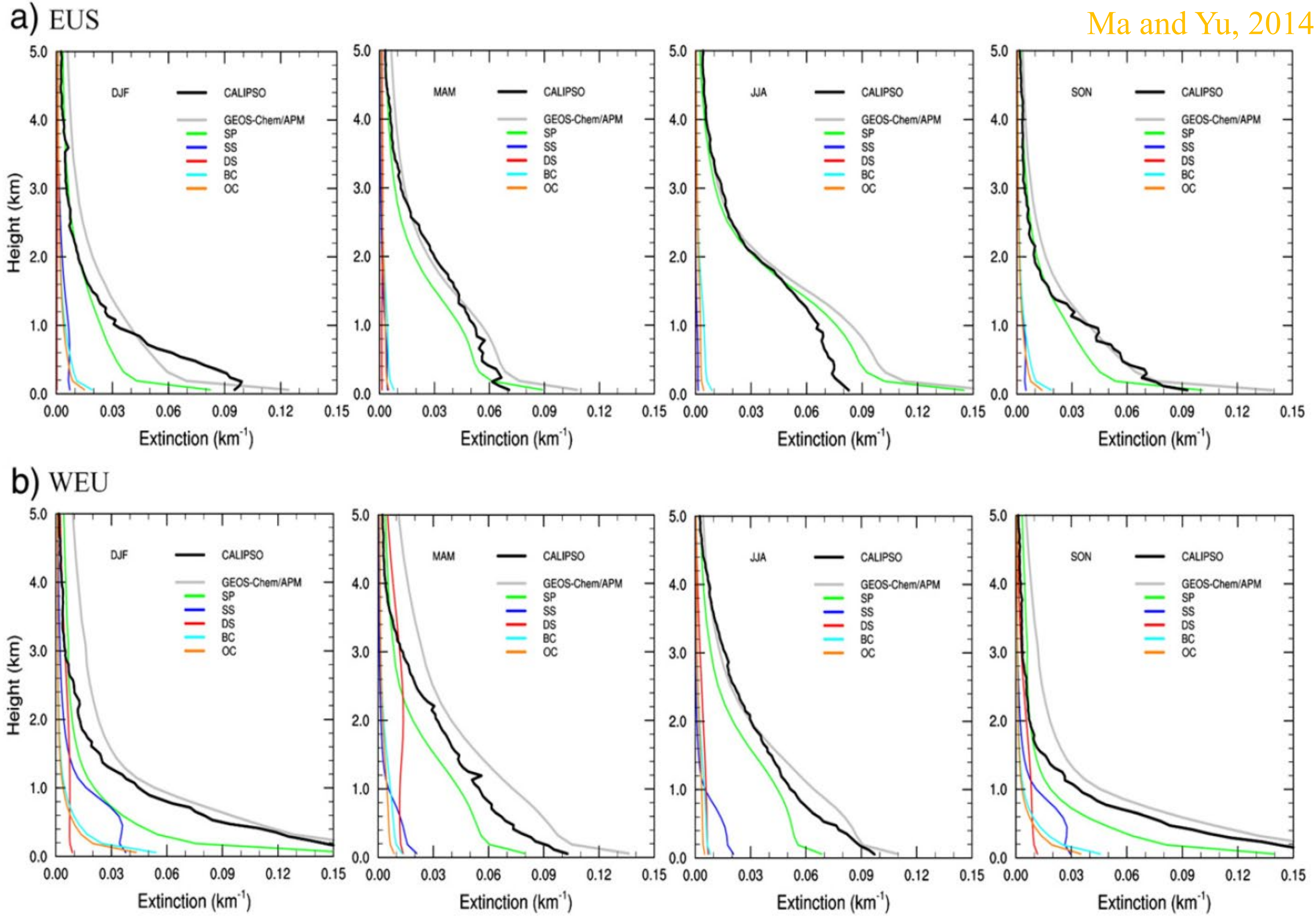
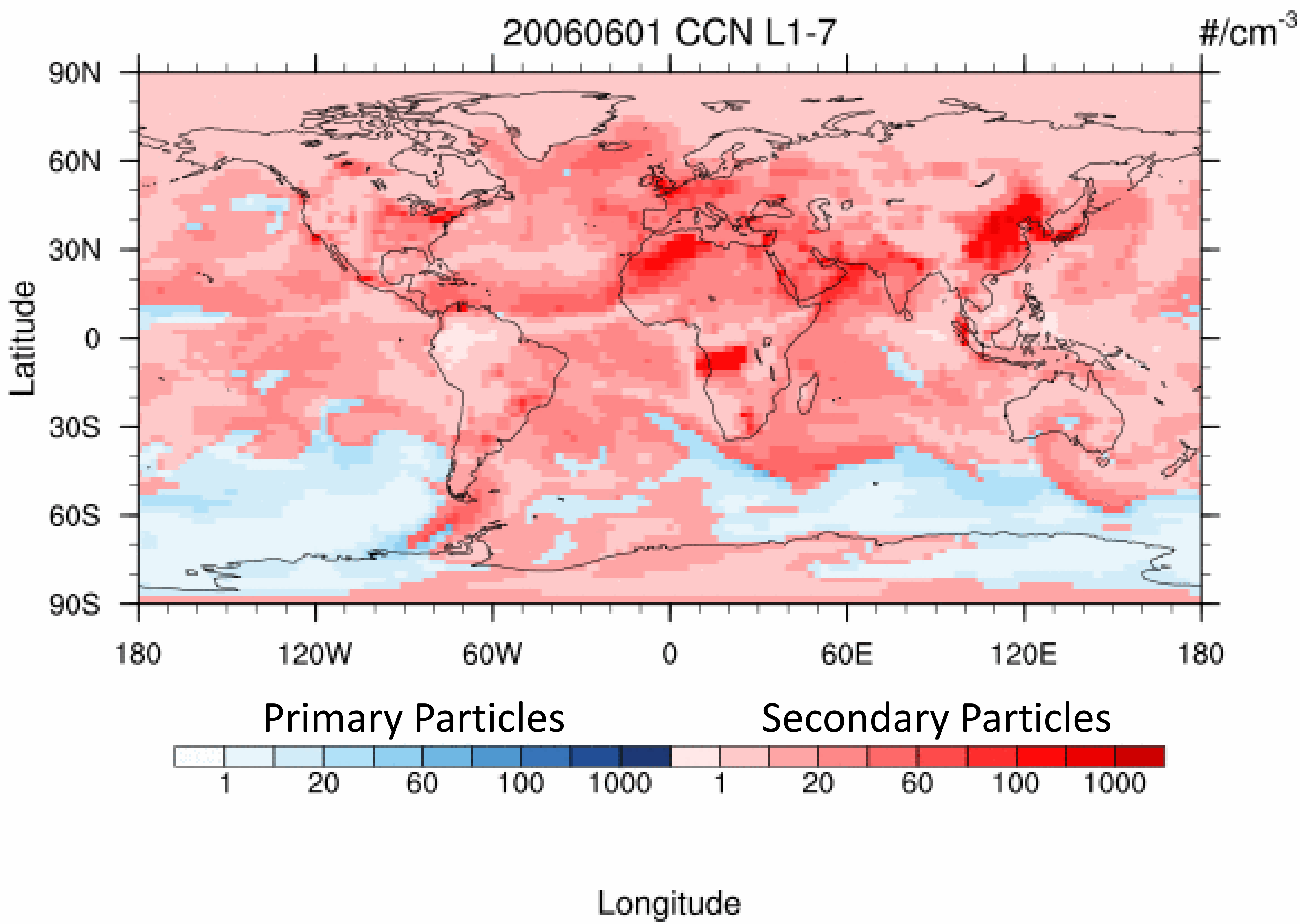
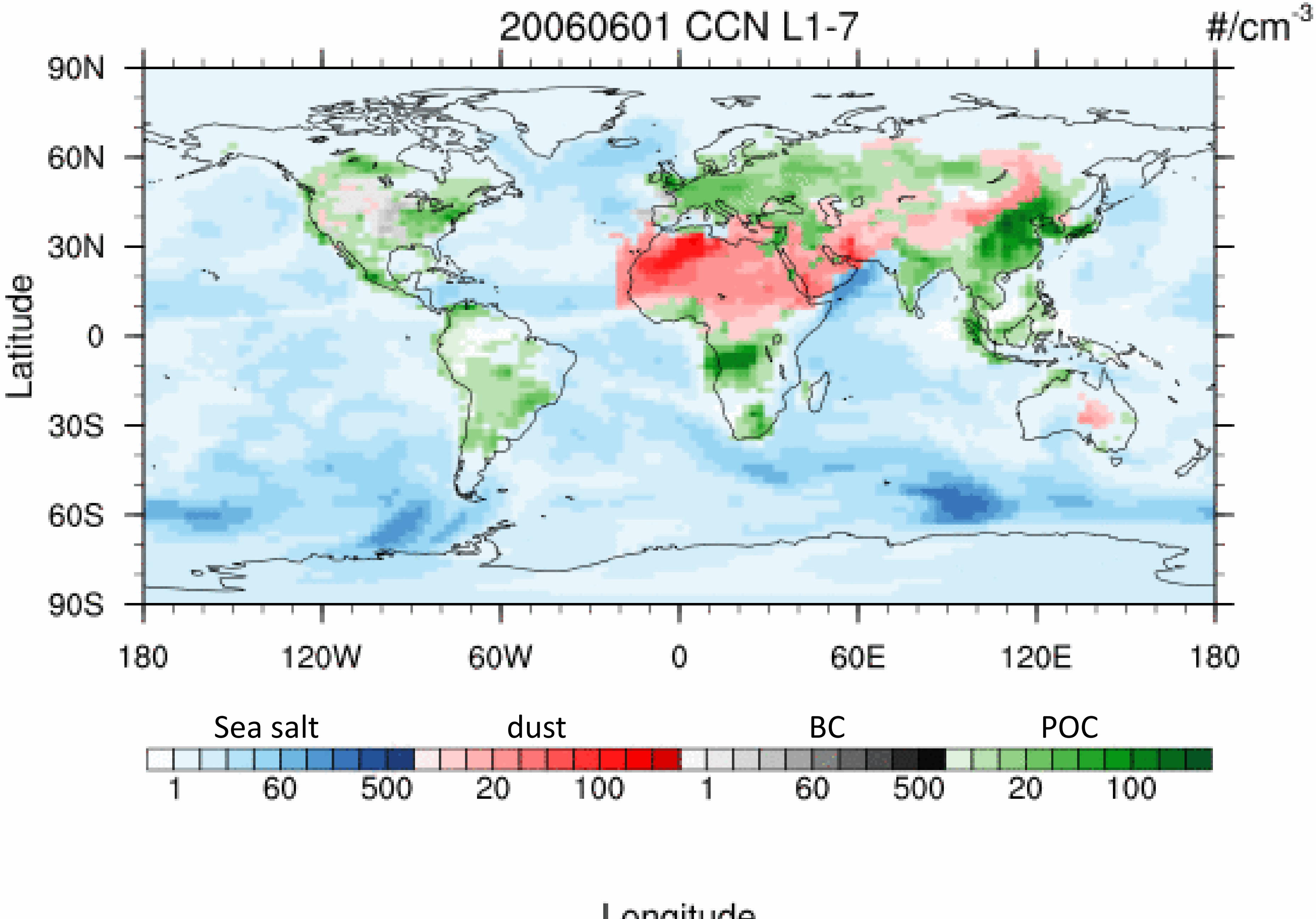


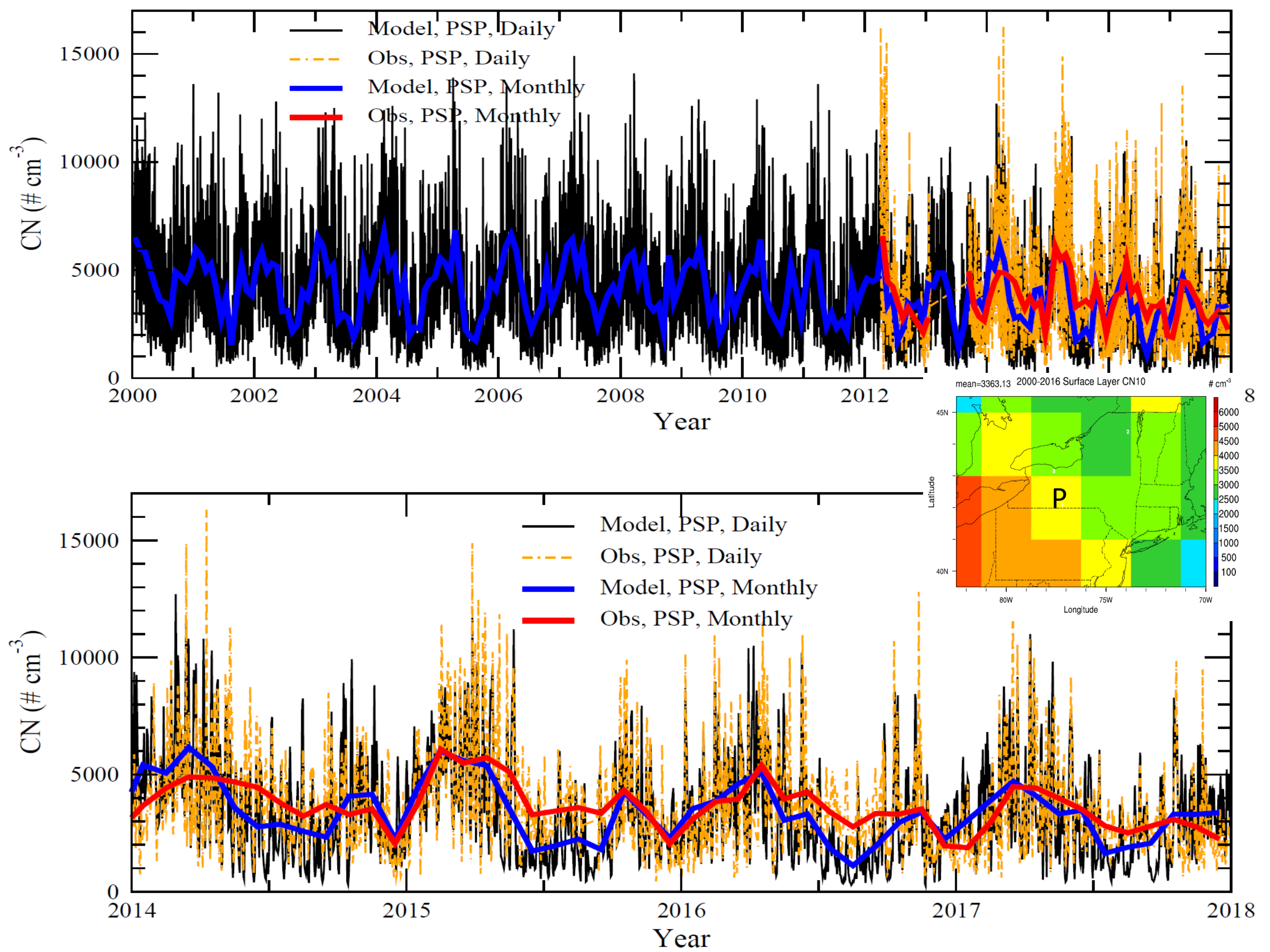
Fig. 5. Seasonal mean (DJF, MAM, JJA, and SON) extinction profiles from all aerosols and each species simulated from the GEOS-Chem/APM model, along with CALIPSO observations, over EUS (a) and WEU (b).



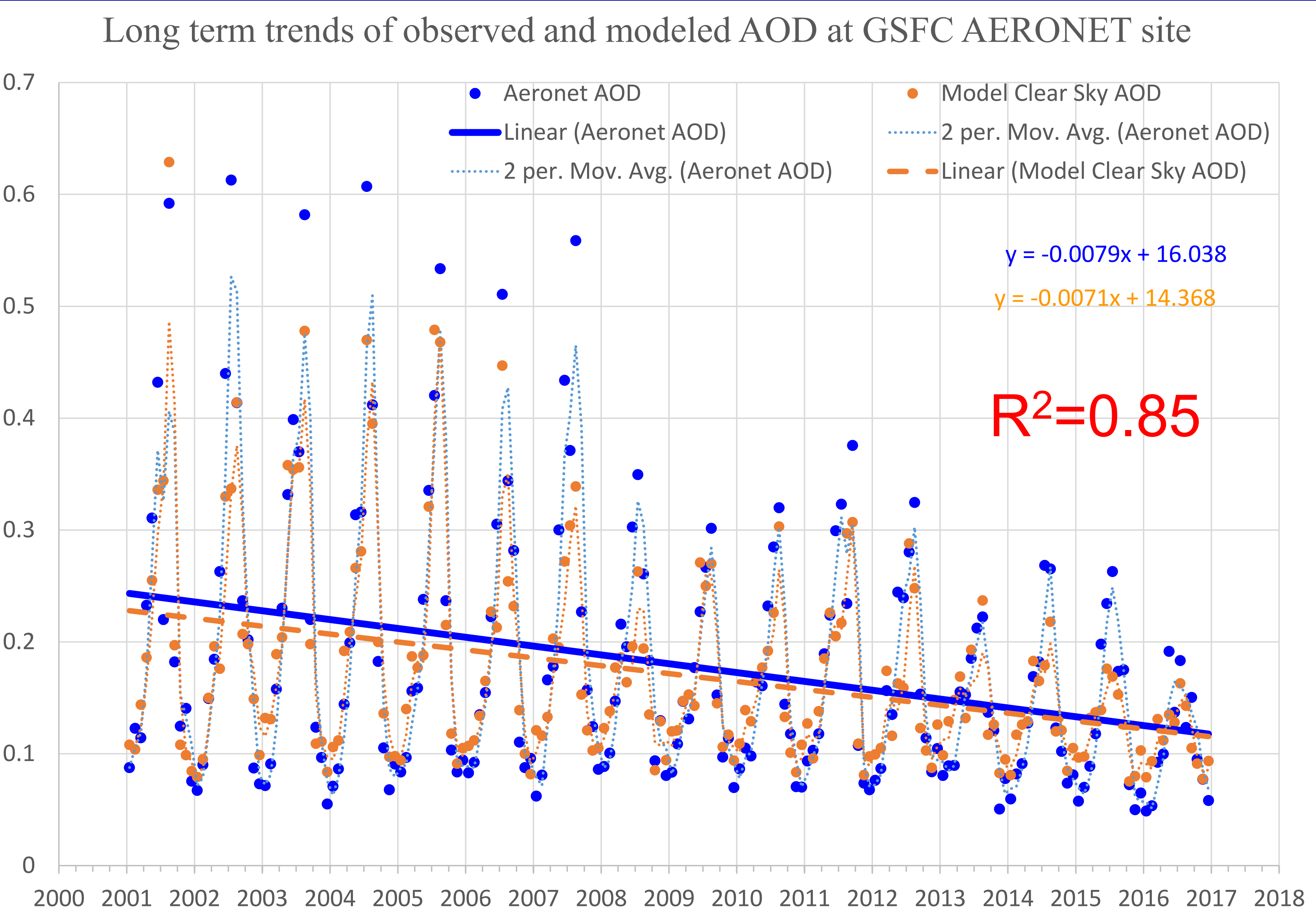
20060601 CCN L1-7
#/cm^-3
90N
60N
30N
0
30S
60S
90S
Latitude
180
120W
60W
0
60E
120E
180
Primary Particles
Secondary Particles
1
20
60
100
1000
1
20
60
100
1000
Longitude



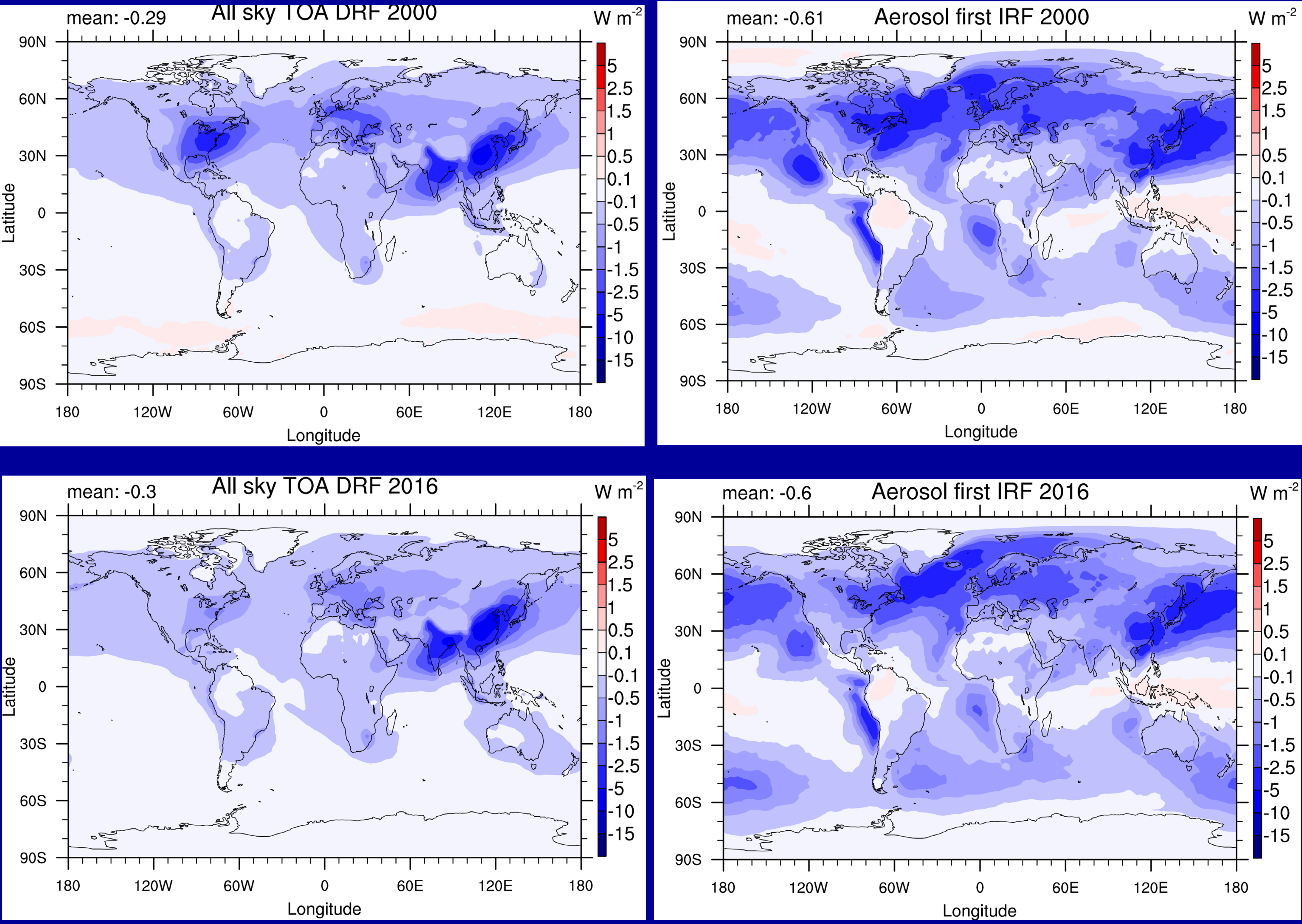
20060601 CCN L1-7
#/cm-3
90N
60N
30N
0
30S
60S
90S
Latitude
180
120W
60W
0
60E
120E
180
Sea salt
dust
BC
POC
1
60
500
20
100
1
60
500
20
100
Longitude



Model, PSP, Daily
Obs, PSP, Daily
Model, PSP, Monthly
Obs, PSP, Monthly
CN (# cm^-3)
0
5000
10000
15000
2000
2002
2004
2006
2008
2010
2012
Year
mean=3363.13
2000-2016 Surface Layer CN10
cm^-3
6000
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
100
45N
40N
Latitude
80W
75W
70W
Longitude
P
Model, PSP, Daily
Obs, PSP, Daily
Model, PSP, Monthly
Obs, PSP, Monthly
CN (# cm^-3)
0
5000
10000
15000
2014
2015
2016
2017
2018
Year



Long term trends of observed and modeled AOD at GSFC AERONET site
Aeronet AOD
Model Clear Sky AOD
Linear (Aeronet AOD)
2 per. Mov. Avg. (Aeronet AOD)
2 per. Mov. Avg. (Aeronet AOD)
Linear (Model Clear Sky AOD)
y = -0.0079x + 16.038
y = -0.0071x + 14.368
R2=0.85
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
2000
2001
2002
2003
2004
2005
2006
2007
2008
2009
2010
2011
2012
2013
2014
2015
2016
2017
2018


mean: -0.29
All sky TOA DRF 2000
W m-2
mean: -0.61
Aerosol first IRF 2000
W m-2
mean: -0.3
All sky TOA DRF 2016
W m-2
mean: -0.6
Aerosol first IRF 2016
W m-2
90N 60N 30N 0 30S 60S 90S
Latitude
180 120W 60W 0 60E 120E 180
Longitude
5 2.5 1.5 1 0.5 0.1 -0.1 -0.5 -1 -1.5 -2.5 -5 -10 -15

WRF-Chem-APM

WRF-Chem-APM simulations

Time periods: April 5-21, 2009; May 5 – 21, 2012

Horizontal resolution: 27km x 27 km

# of grid boxes: 180 X 126 X 30

Computing cost (Intel Xeon, 28 cores):

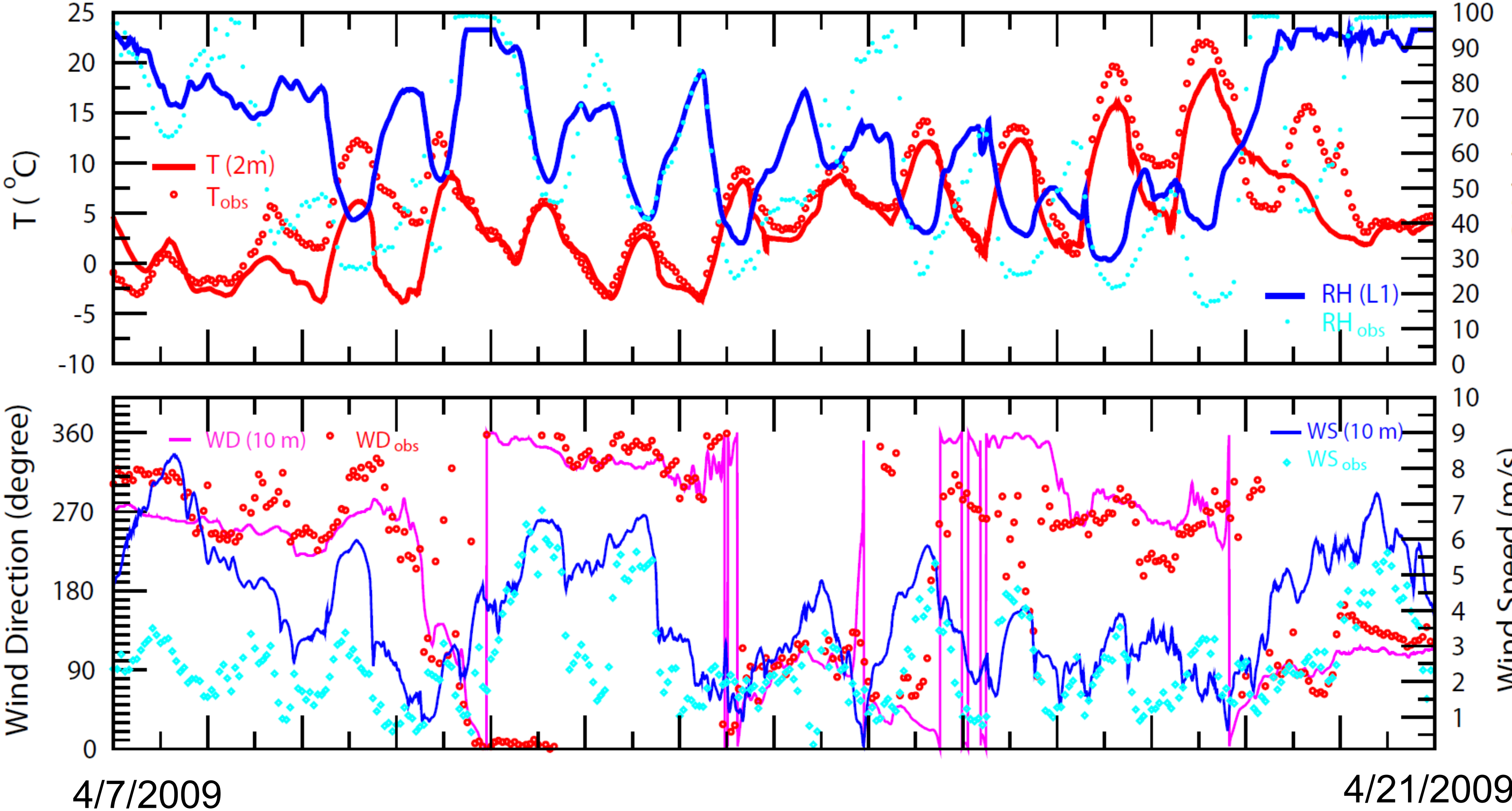
1 hour of wall clock for **1-day** simulation

Nucleation schemes:

Baseline: Ion-mediated nucleation (Yu, 2010)

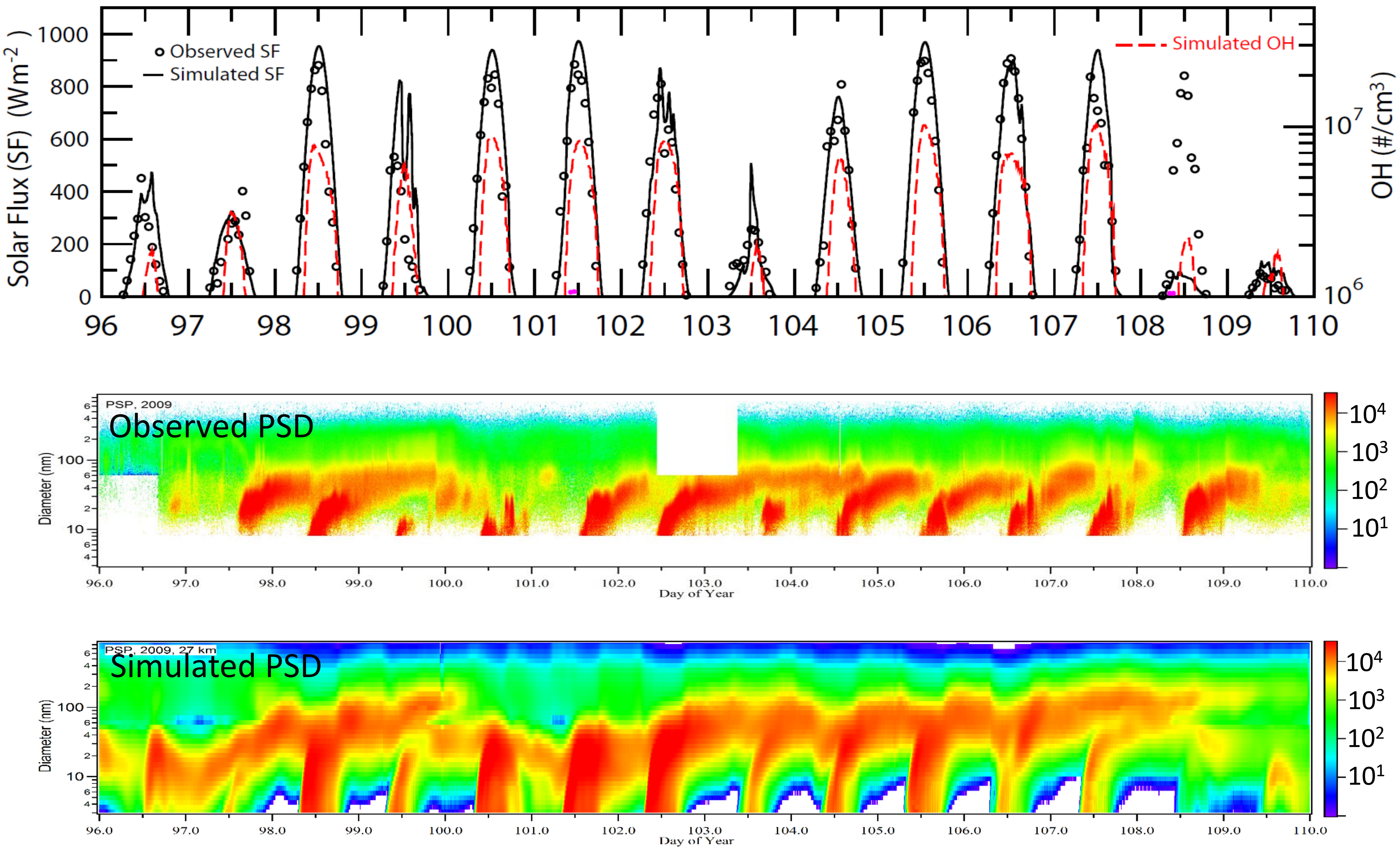
Sensitivity study: Organics-mediated nucleation (Riccobono et al., 2014)

Comparison of simulated T, RH, Wind direction, and wind speed with observations: Overall reasonable



April 7-21, 2009

Model captures 10 out 11 strong NPF events

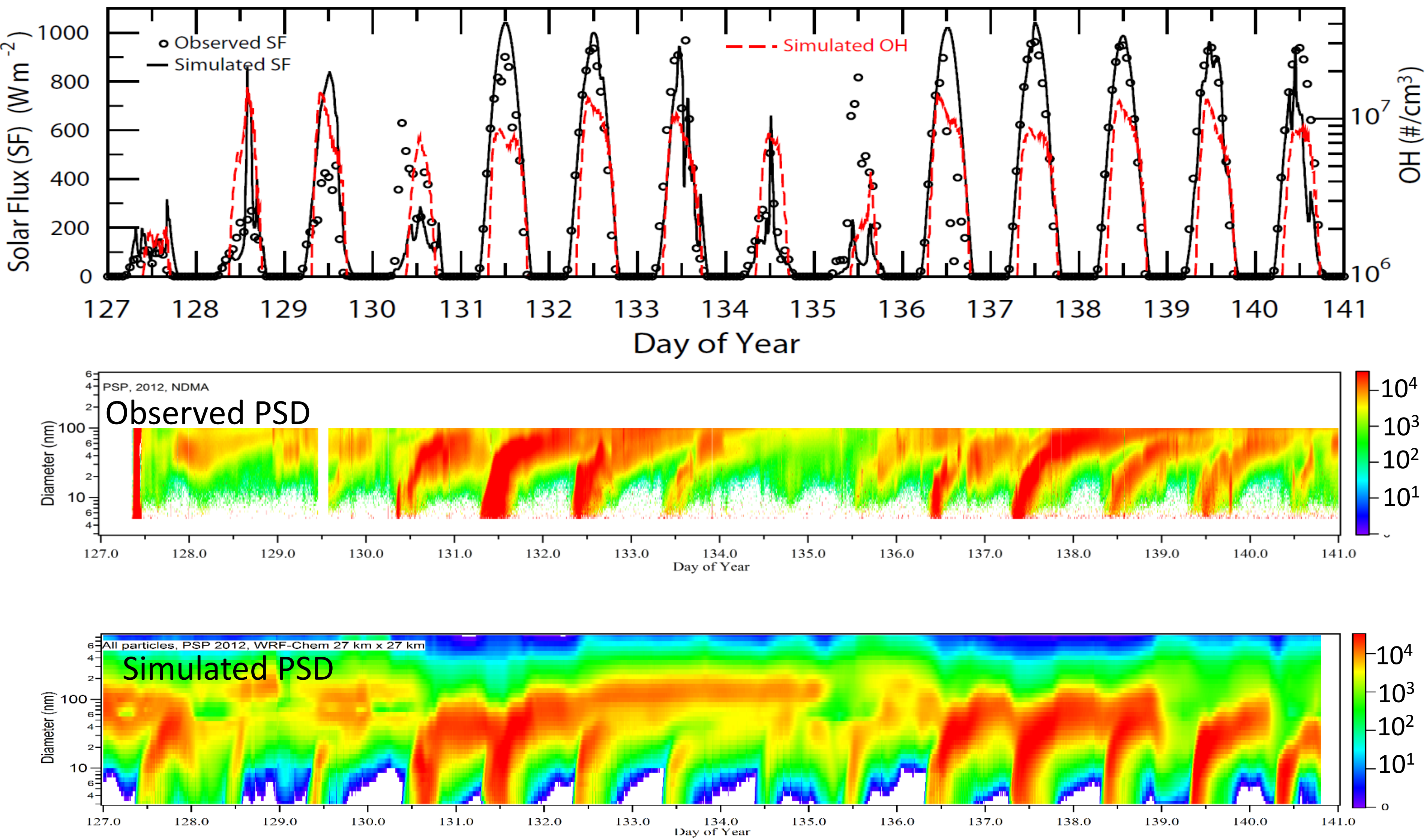


4/7/2009

4/21/2009

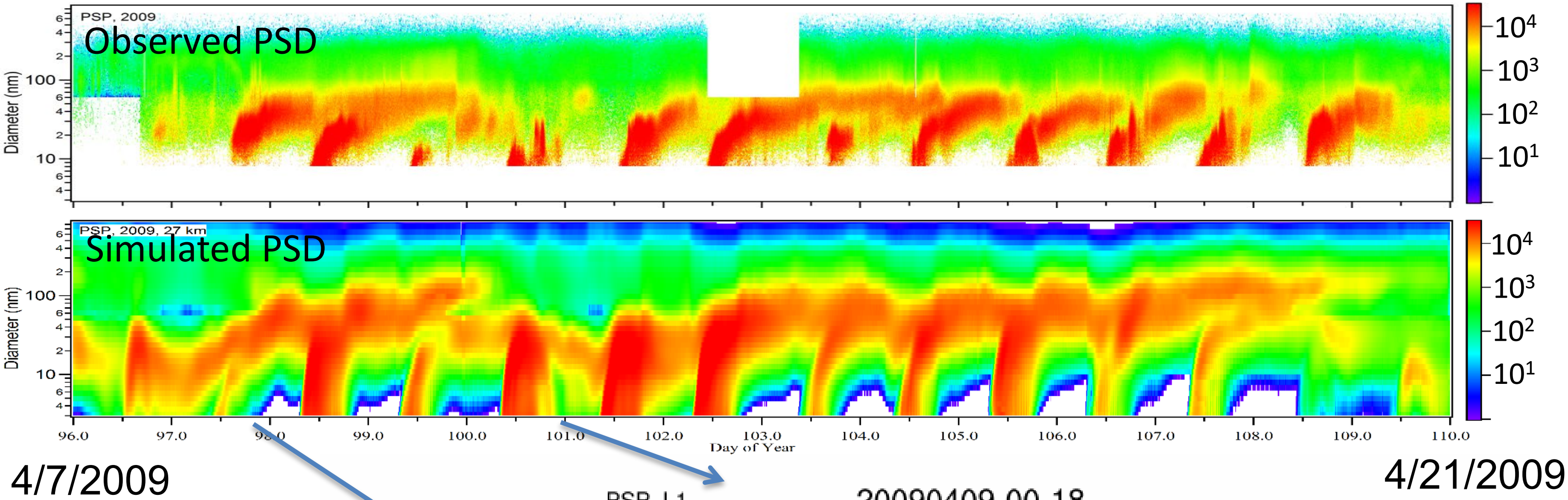
May 7-21, 2012

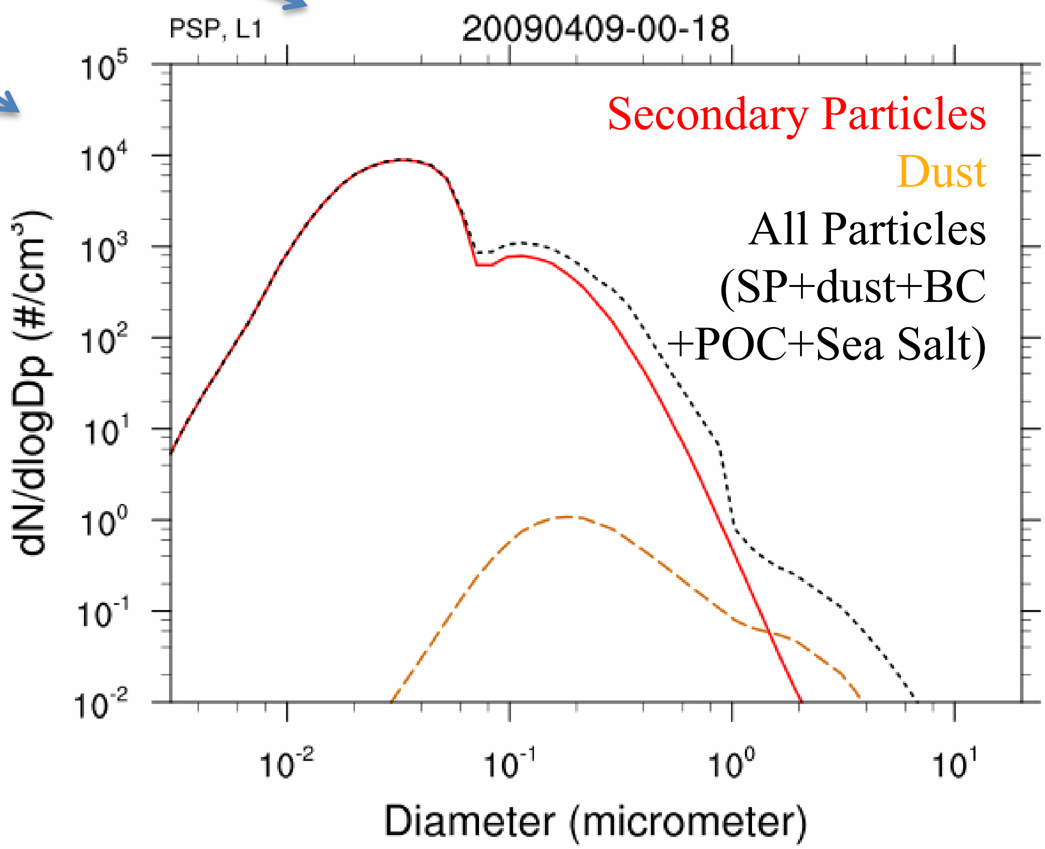
Model captures 7 out 7 strong NPF events



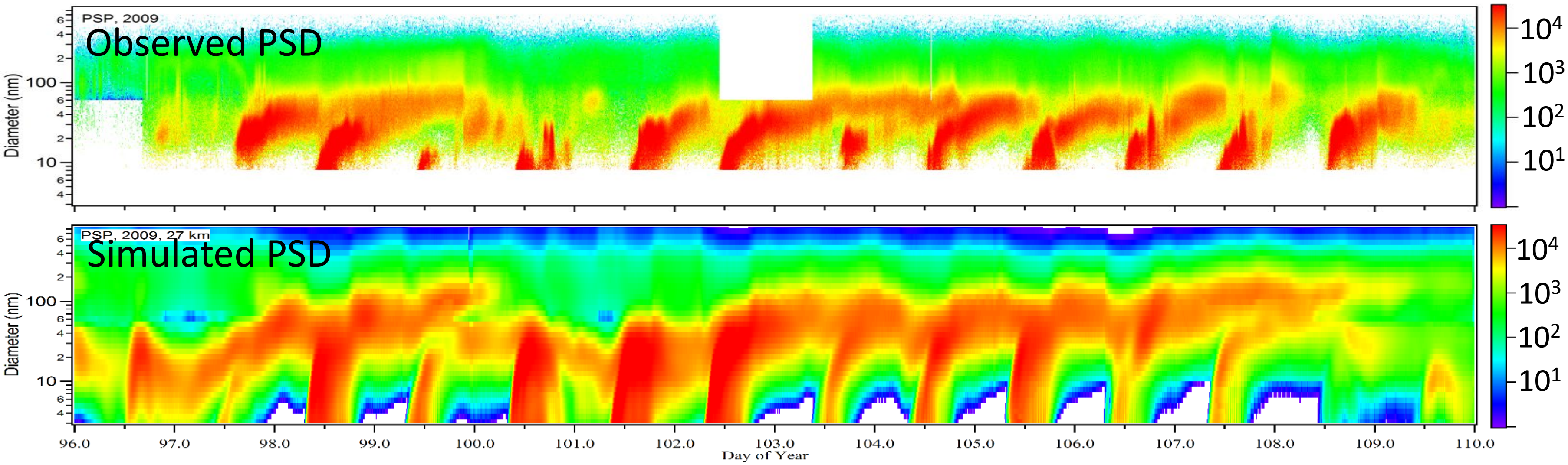
5/7/2012

5/21/2012





Particle formation and growth and contribution to CCN



4/7/2009 4/21/2009