GEOS-5 Nature Runs and Observation Simulations for the Atmospheric Composition Geostationary Constellation

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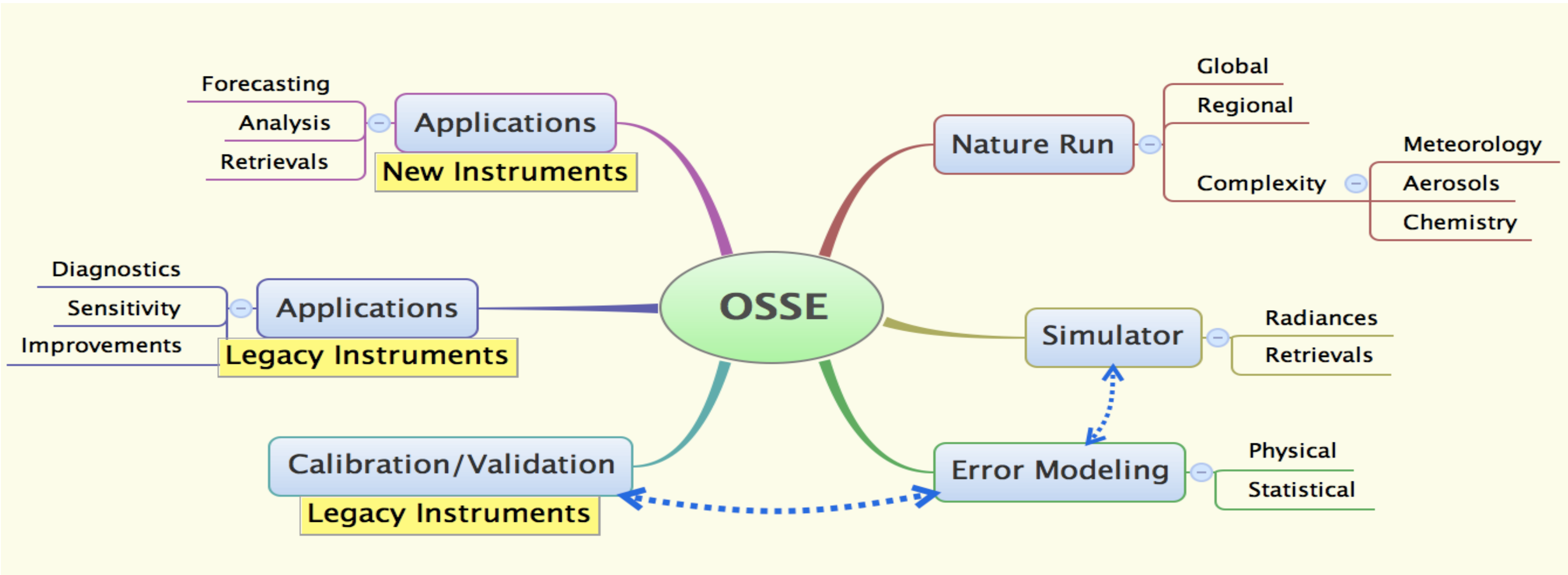
Michael Long, Lu Hu, Daniel Jacob (Harvard University) and the GEOS-Chem Development Team
Shobha Kondragunta and Pubu Ciren (NOAA /NESDIS/STARR)

13th Meeting of the
Atmospheric Composition Virtual Constellation
Paris, France, June 27-29, 2017

Outline

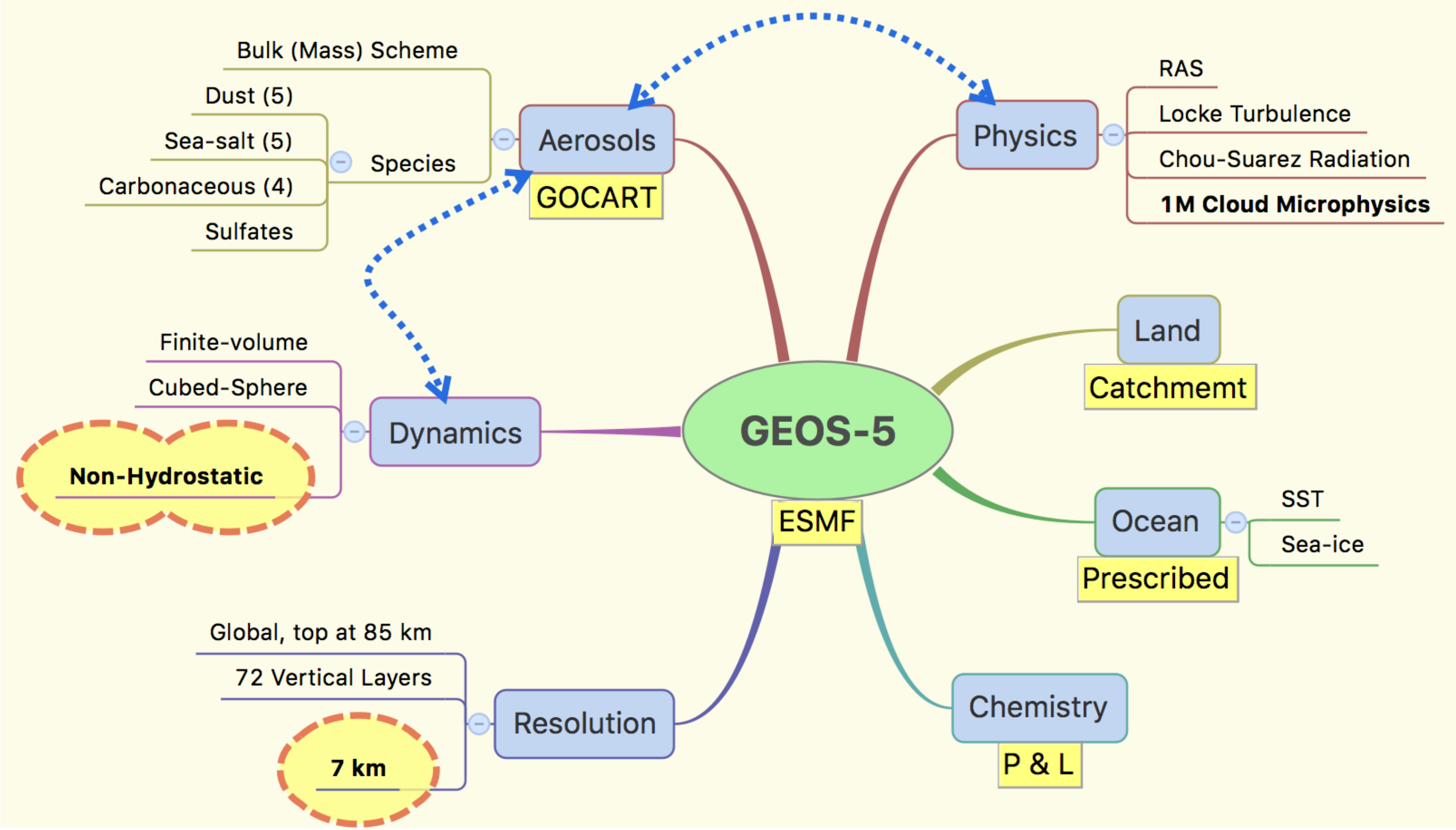
- GEOS-5 Nature Runs
  - 7 km GEOS-5 Nature Run (G5NR)
  - 12 km GEOS-5 Nature Run with Full Chemistry
- Observation simulators for Geo constellation
  - Instruments: TEMPO, GEMS, SENTINEL-4, GOES-R
  - Vector RT optimizations
  - Retrieval simulators: UV & GOES-R synergism

Elements of an OSSE System

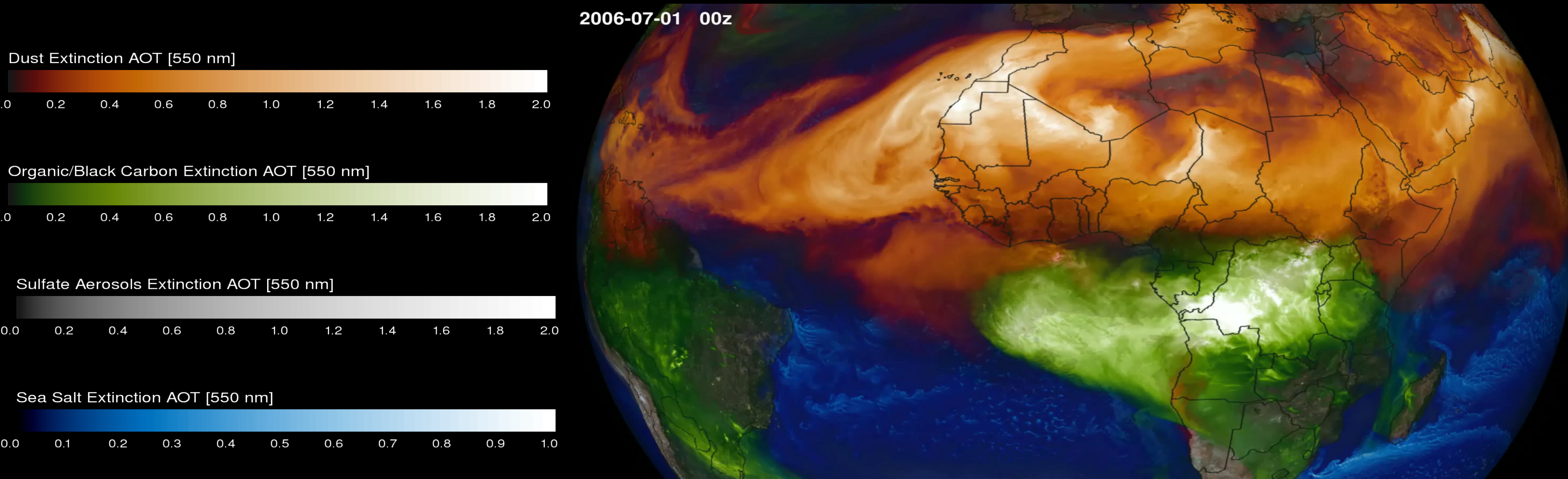


Nature Runs

G5NR Configuration

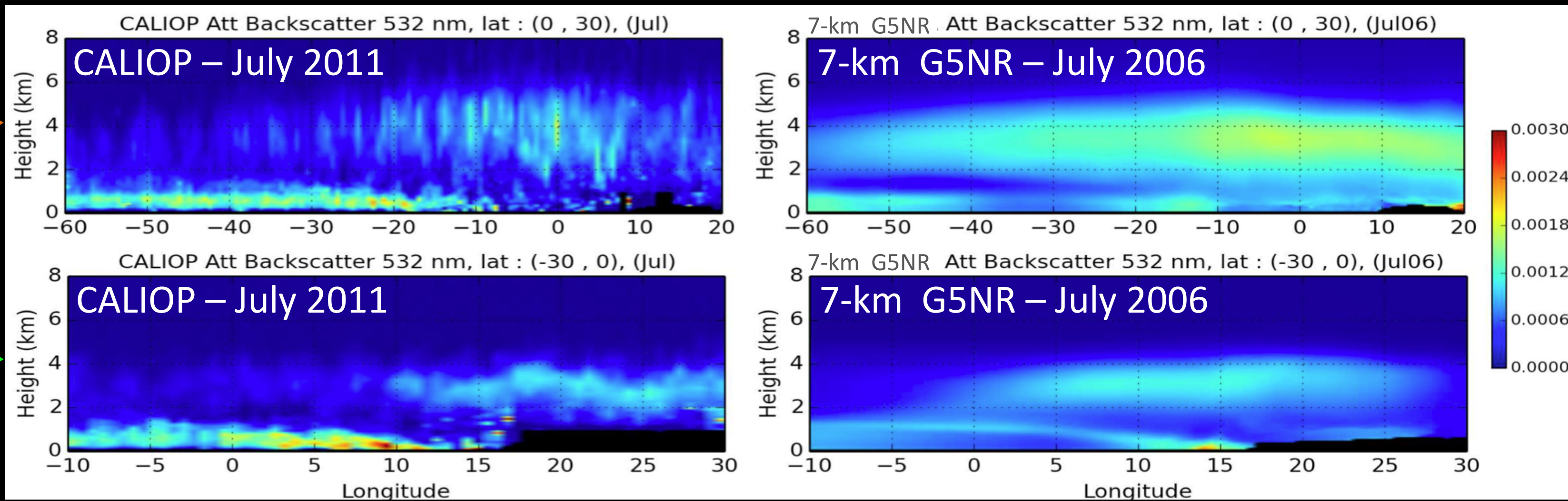


Aerosols

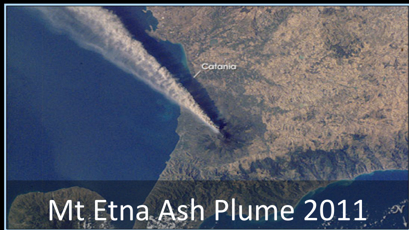


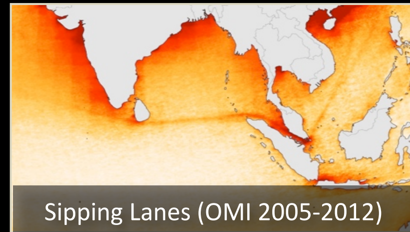
North African Dust

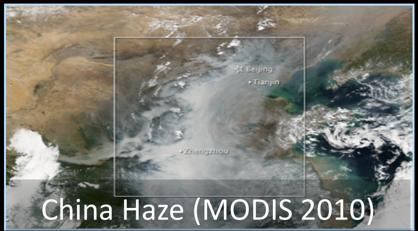
South African Fires

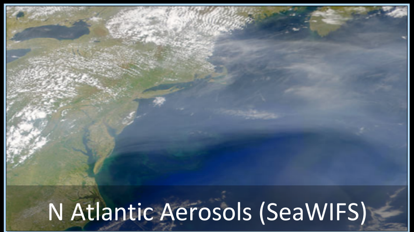


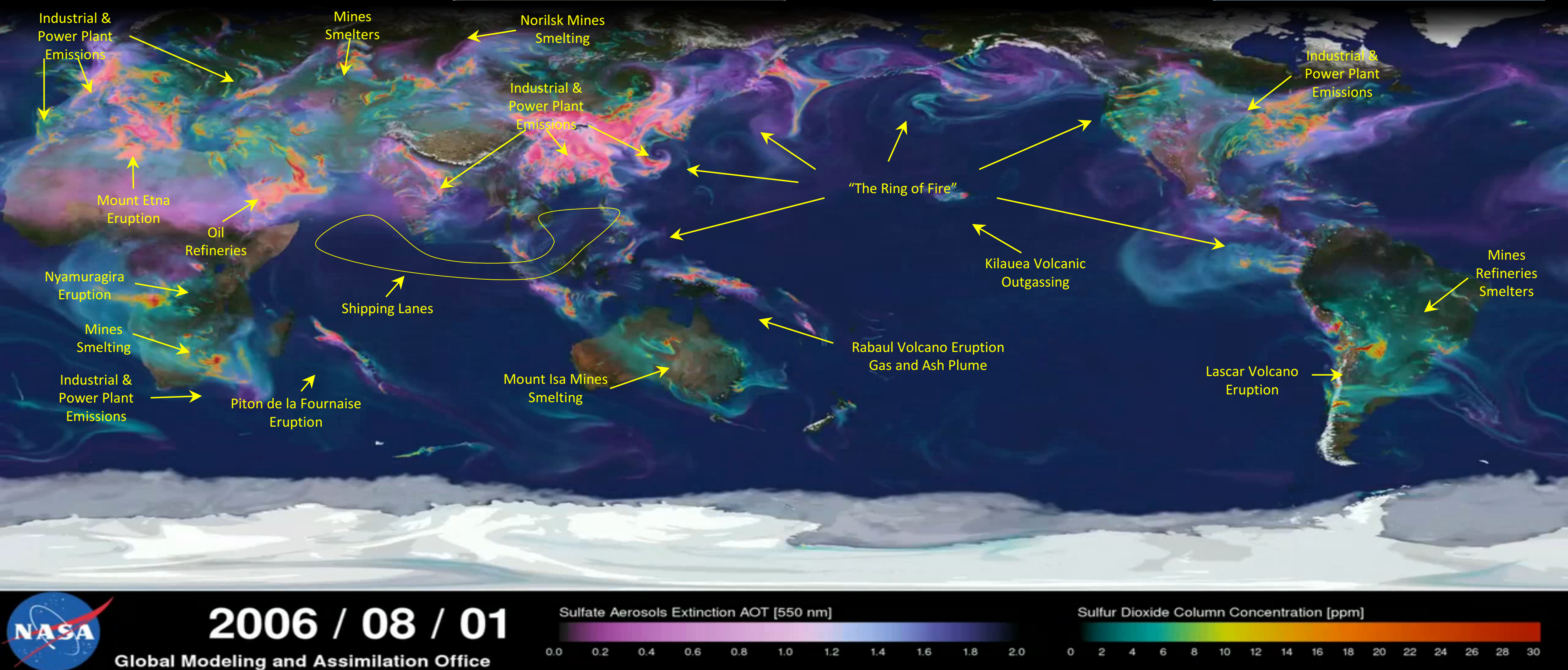
Sulfate and Sulfur Dioxide











G5NR Aerosol Validation

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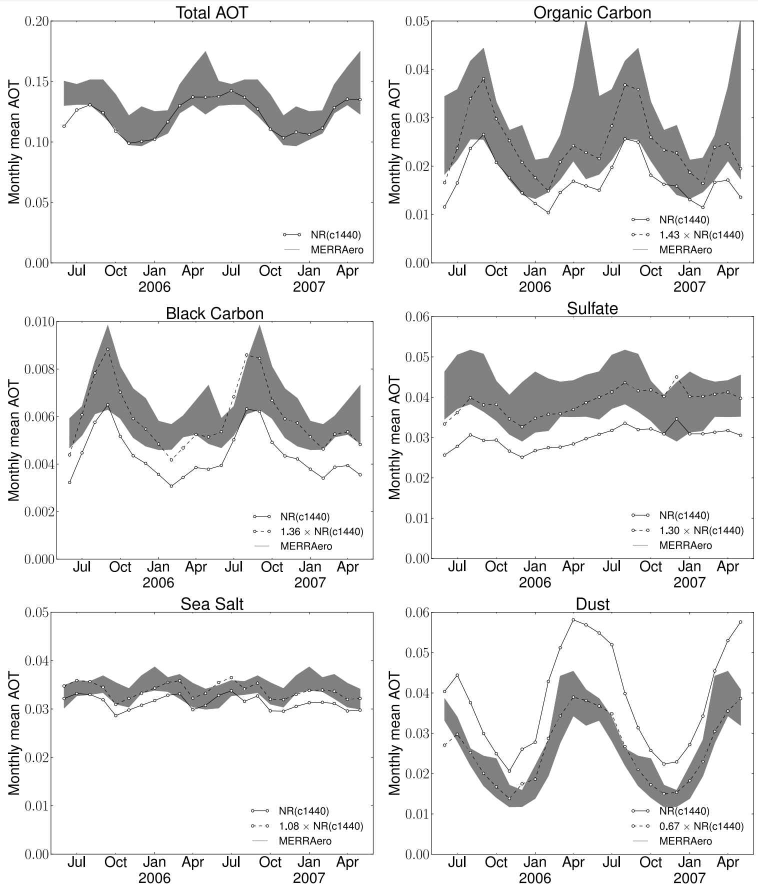
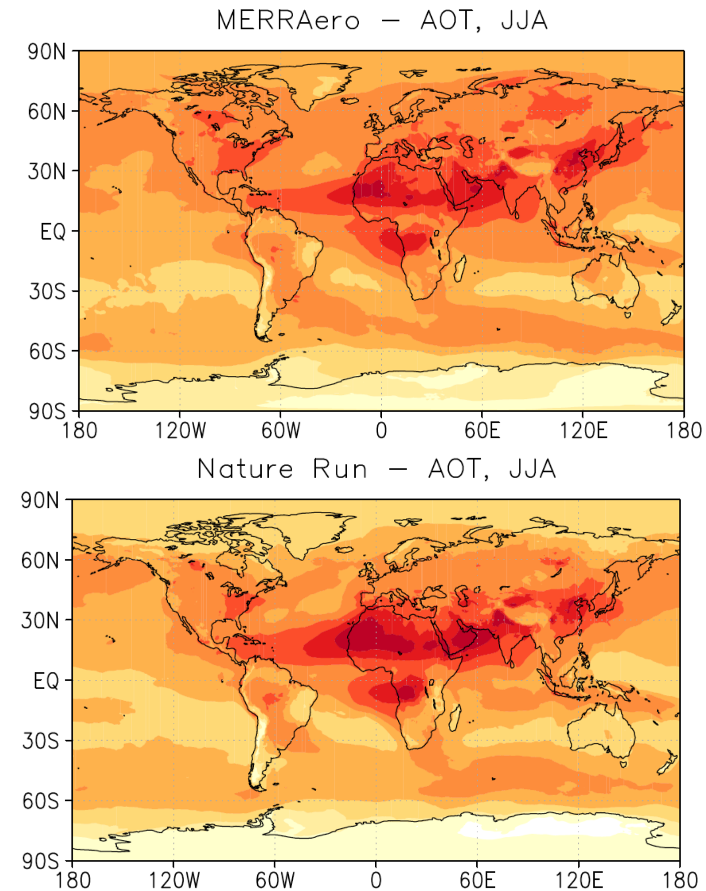
Randal D. Koster, Editor

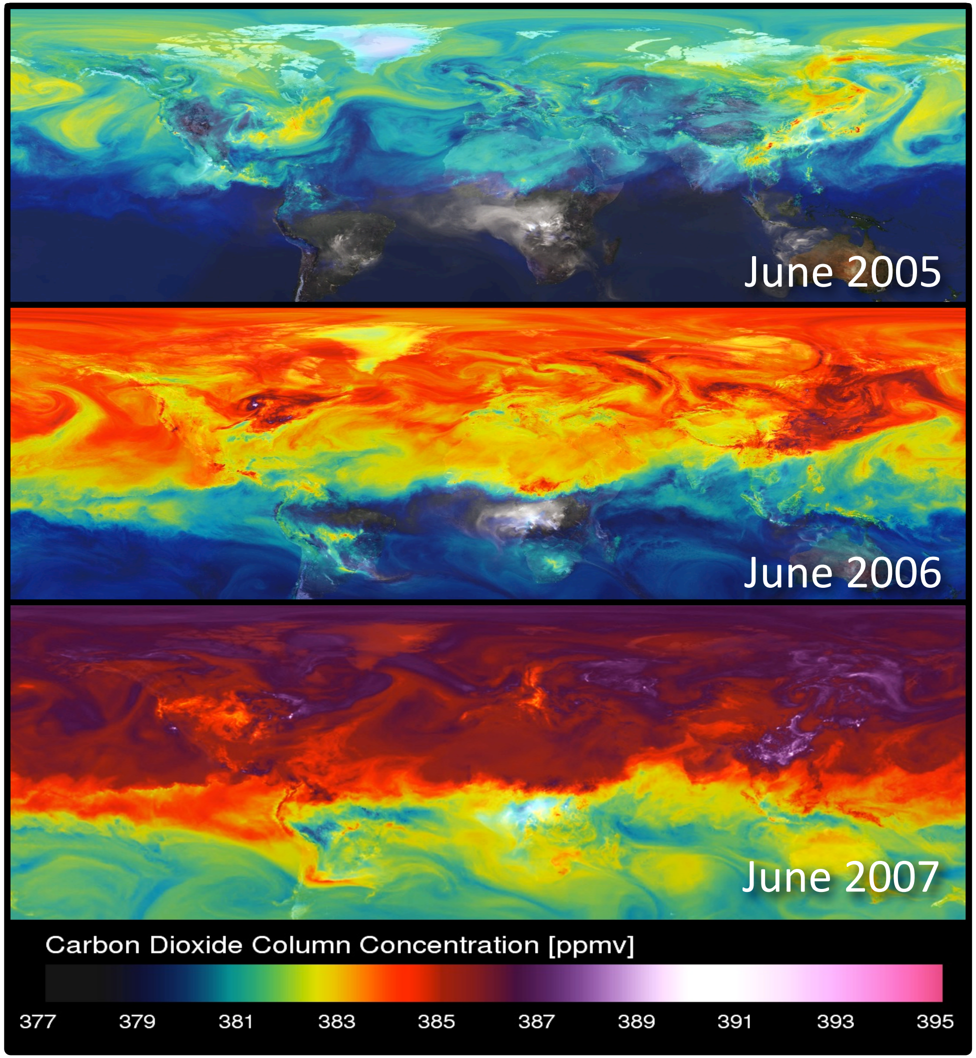
Evaluation of the 7-km GEOS-5 Nature Run

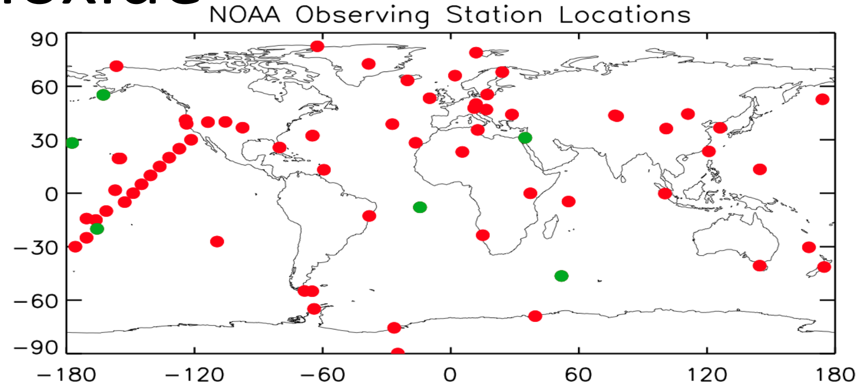
Ronald Gelaro, William M. Putman, Steven Pawson, Clara Draper, Andrea Molod, Peter M. Norris, Lesley Ott, Nikki Privé, Oreste Reale, Deepthi Achuthavarier, Michael Bosilovich, Virginie Buchard, Winston Chao, Lawrence Coy, Richard Cullather, Arlindo da Silva, Anton Darmenov, Ronald M. Errico, Marangelly Fuentes, Min-Jeong Kim, Randal Koster, Will McCarty, Jyothi Nattala, Gary Partyka, Siegfried Schubert, Guillaume Vernieres, Yuri Vikhliaev, and Krzysztof Wargan



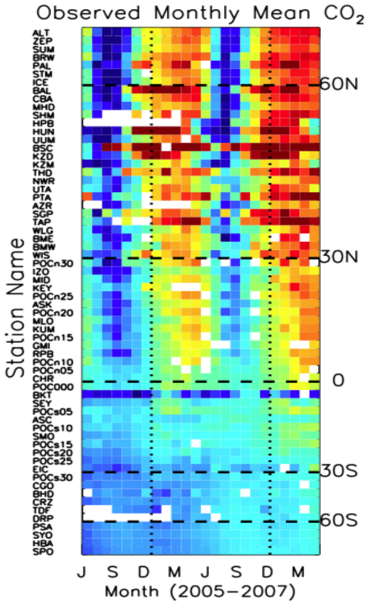


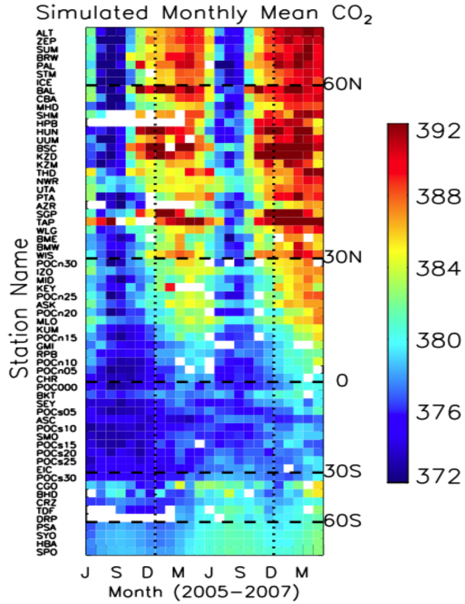
Carbon Dioxide





Monthly mean CO_2 (ppmv) at NOAA surface sites (above) for the 2005-2007 period





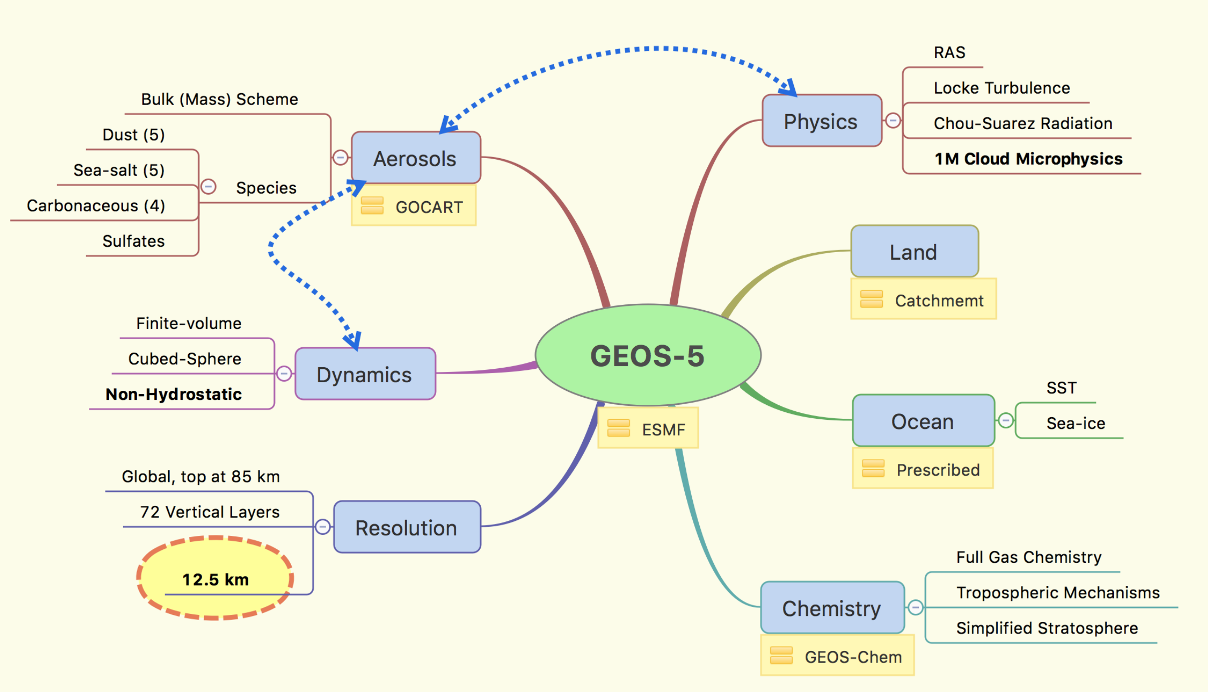
G5NR Summary

- Clouds and Radiation / Precipitation
  - Generally good
  - Too cloudy (drizzly) in subsidence regions
  - Tendency to produce double ITCZ
- Waves and Cyclones
  - Weak MJO (but several waves of eastward propagation observed)
  - Excellent tropical cyclone activity, structure and intensity
  - Northern hemisphere DJF extratropical activity slightly over active
  - Realistic mesoscale structure and regional impacts
- Aerosols and Carbon Species
  - Local fidelity of emissions and global transport
  - Representative climatology and seasonal trends

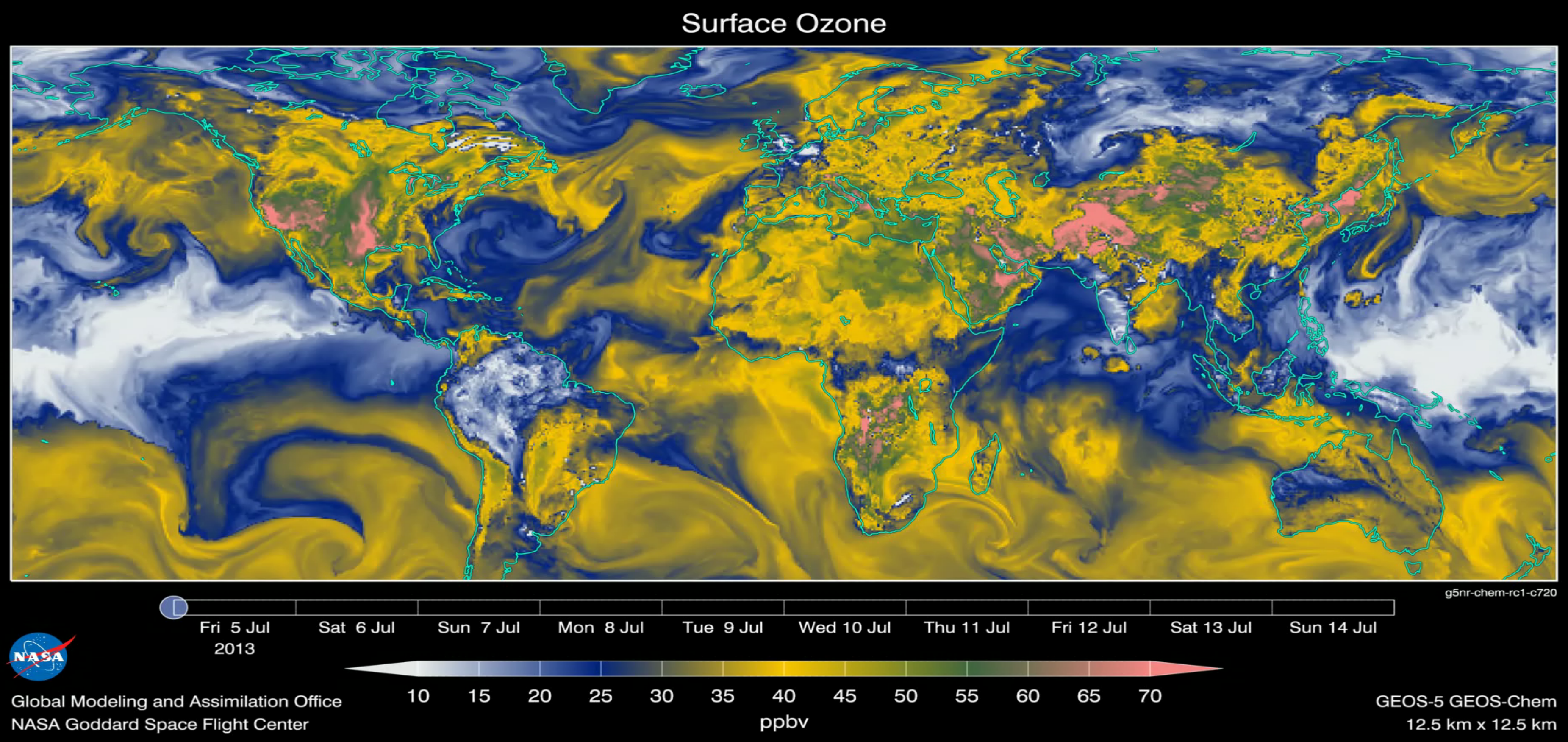
G5NR-Chem

GEOS-5 Nature Run with Full Gas Chemistry

- Period: July 2013-June 2014, May-June 2016
- Validation: **SEAC4RS, KORUS-AQ**
- Chemical mechanisms from GEOS-Chem, simplified statrosphere
- Meteorology constrained by MERRA-2 downscaling
- Hourly output of 3D *retrievable gases*
- Documentation in prep:
  - File Spec
  - Model Configuration
  - Evaluation Tech Memo

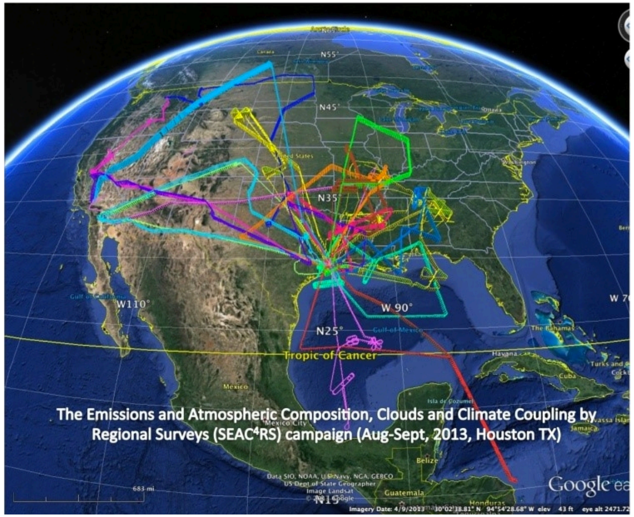


Surface Ozone

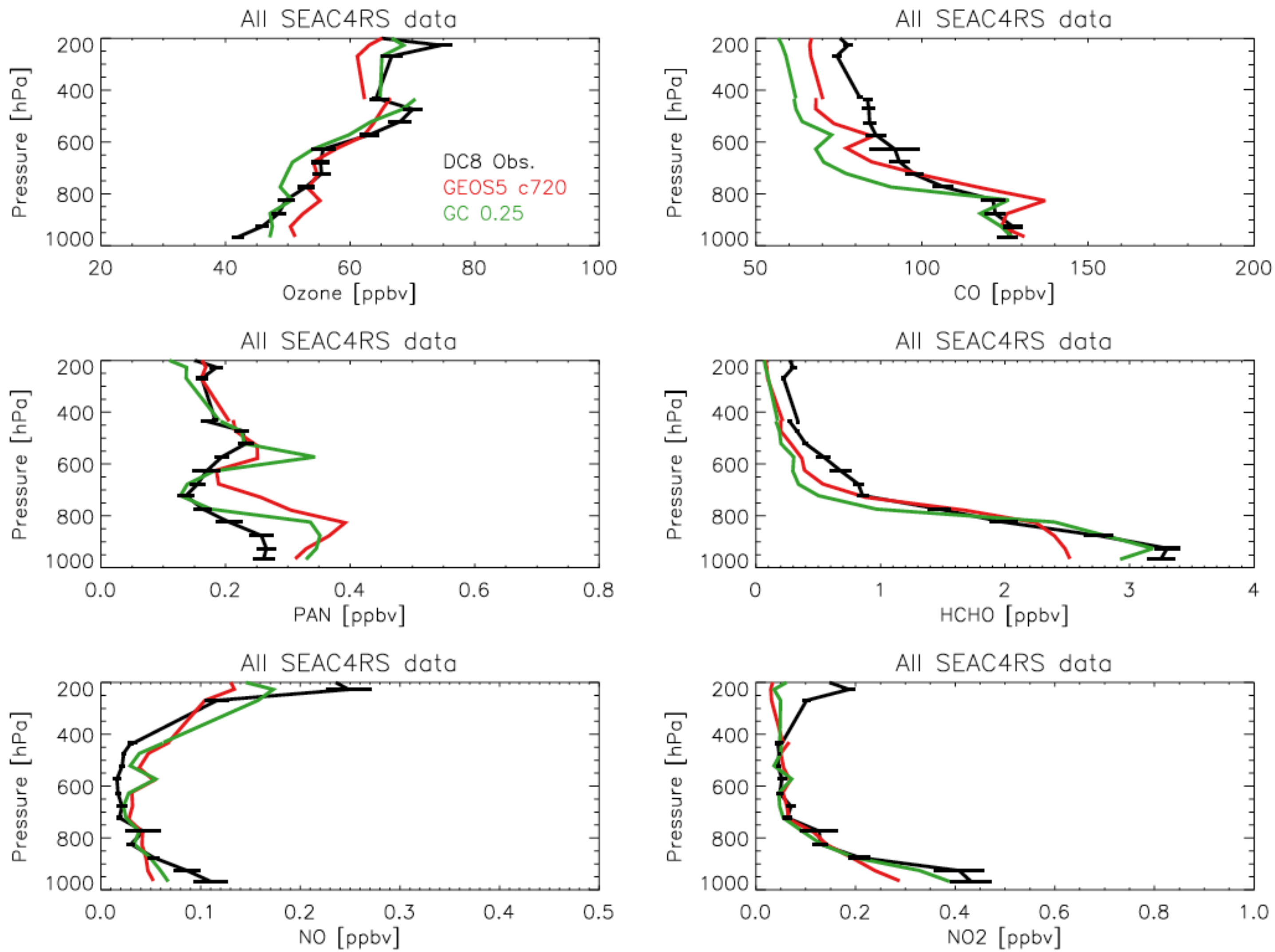


G5NR-Chem Validation during the SEAC^{4}RS Field Campaign

- SEAC^{4}RS field campaign over the U.S.
  - Detailed chemical species during August-September 2013
- The worldwide network of ozonesondes (WOUDC and NOAA ESRL-GMD)
  - Global ozone vertical distribution
- OMI satellite data
  - Global mid-tropospheric ozone distribution
- Benchmark against GEOS-Chem CTM
  - Emission
  - Chemical species

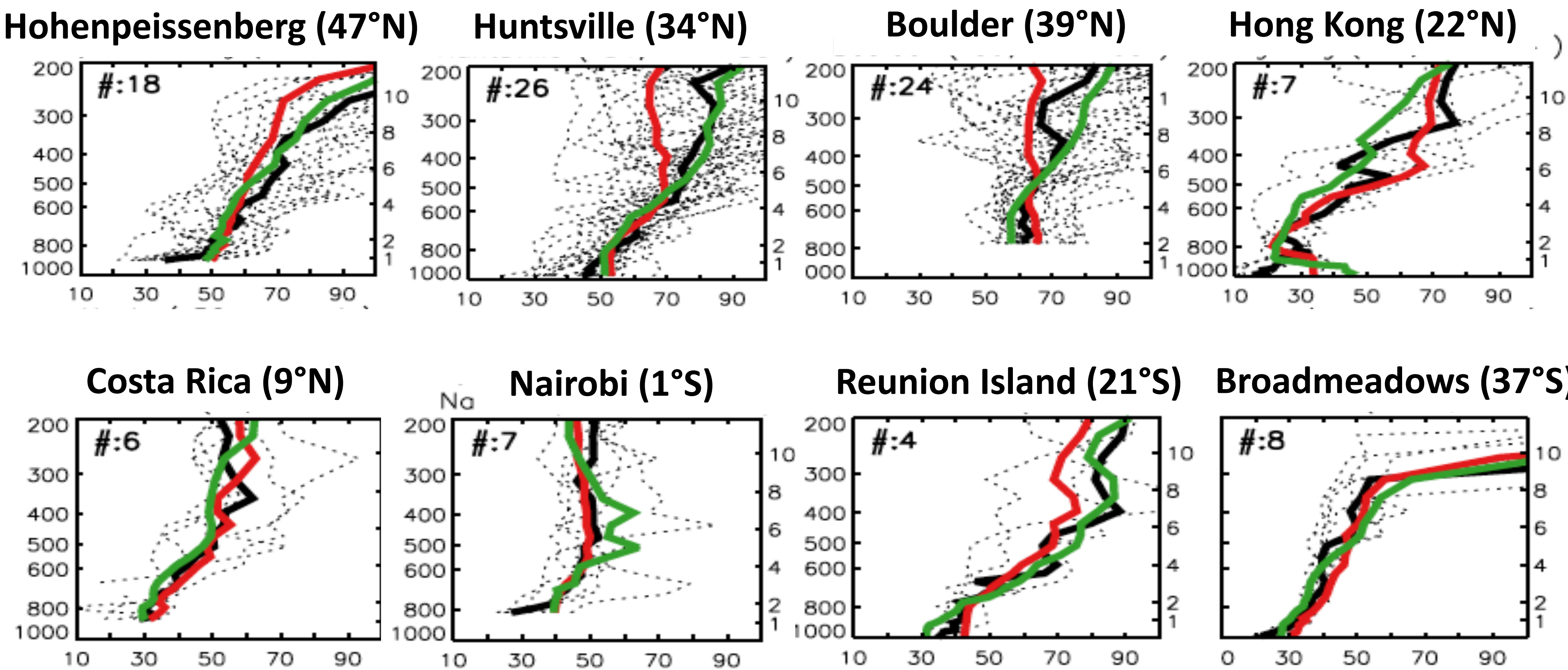


DC-8 Observations G5NR-Chem GEOS-ChemCTM ~25km

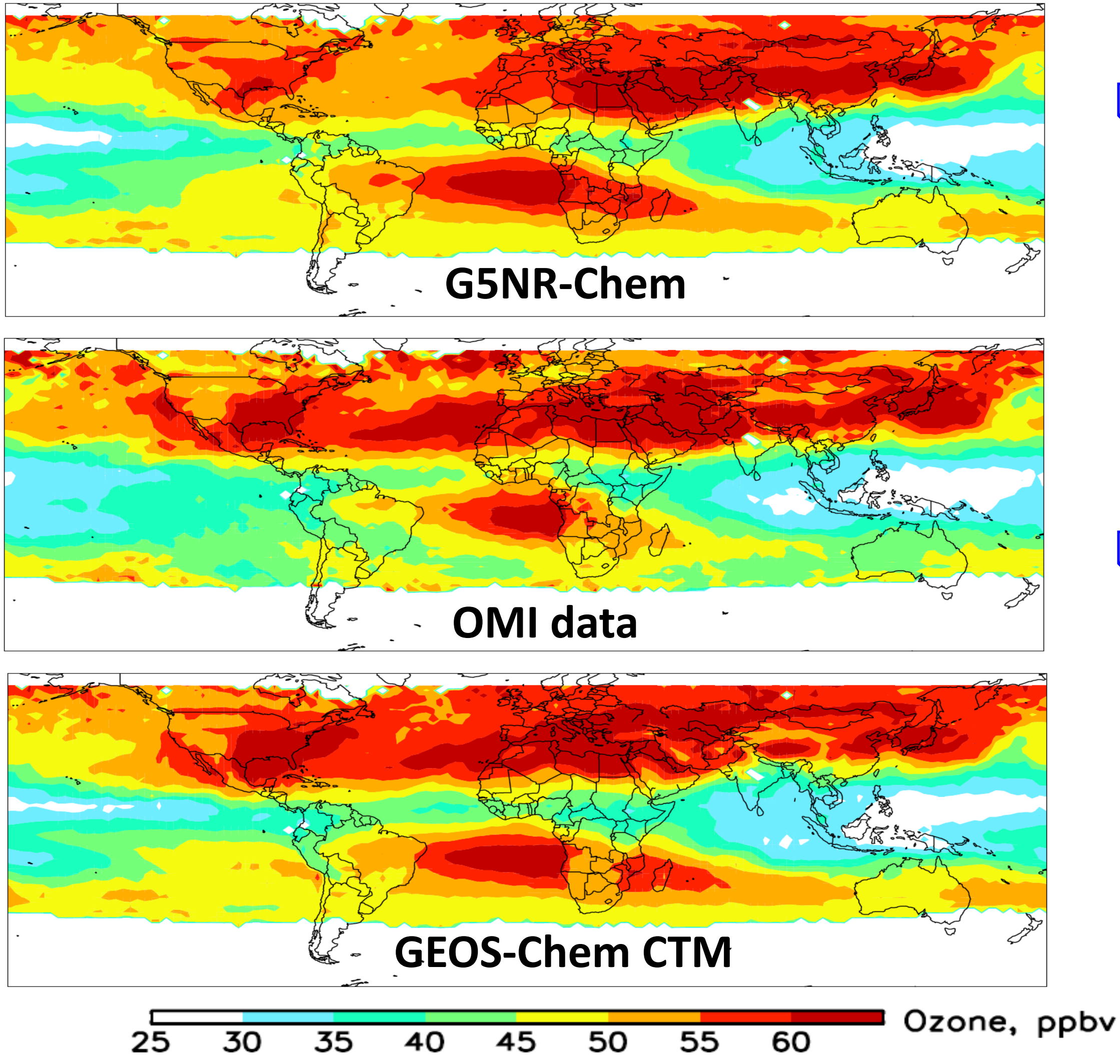


Comparison to Worldwide Network of Ozonesondes

Black: Ozonesonde **Red: GEOS5-Nature Run ~12km** **Green: GEOS-Chem ~200km**



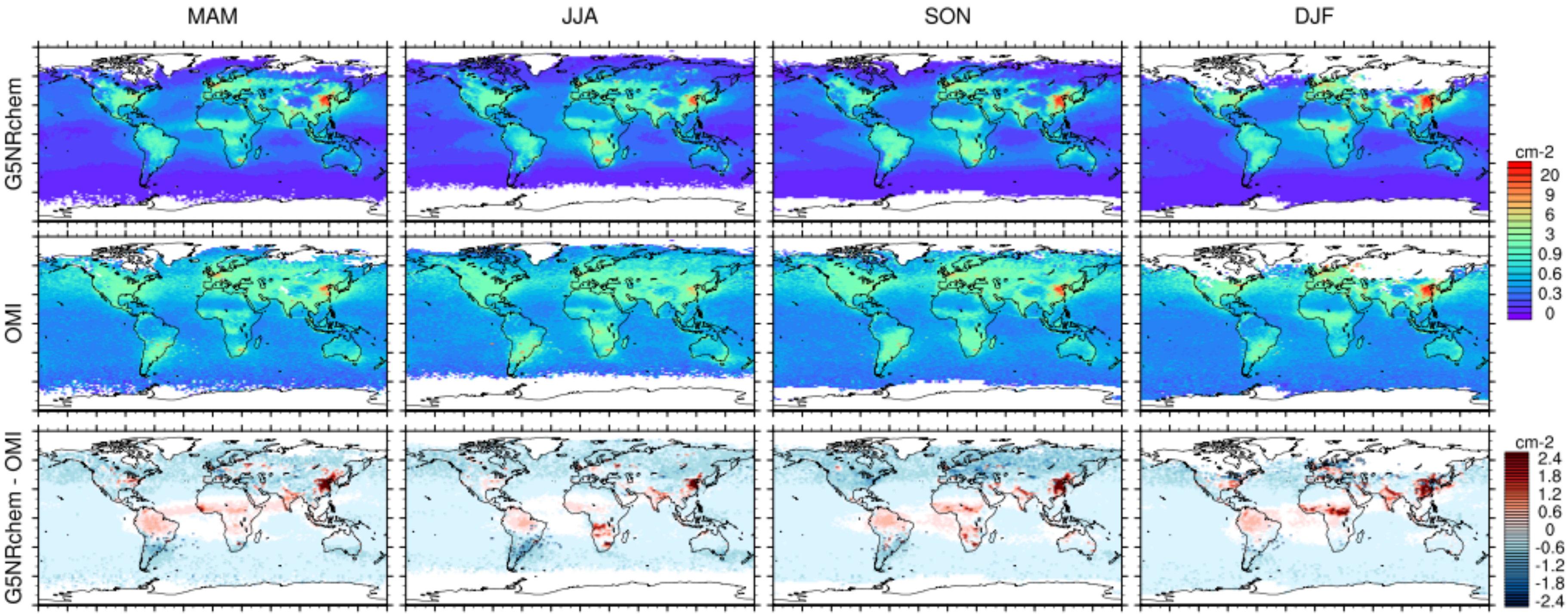
Global comparison to OMI ozone data at 700-400 hPa for August 2013



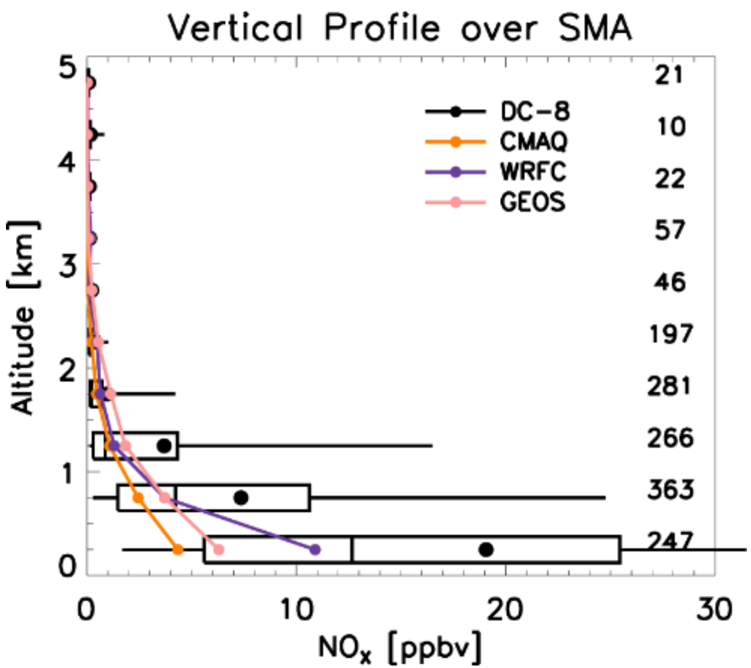
- OMI data have been
  - a) adjusted to a single fixed a priori
  - b) corrected for a global bias relative to ozonesondes
- Model data have been
  - a) sampled along the OMI tracks
  - b) smoothed by OMI averaging kernels

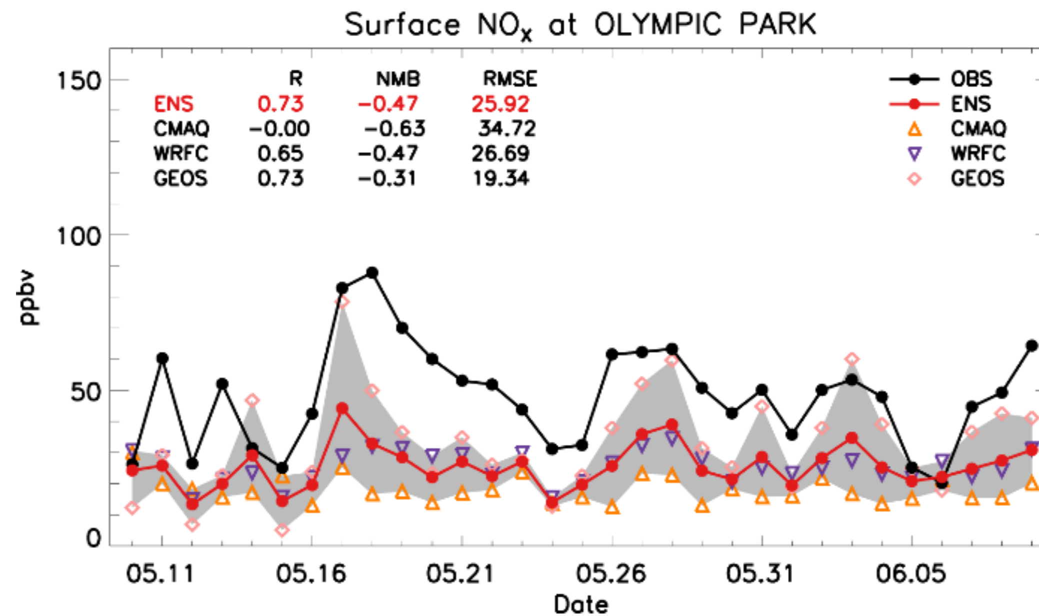
OMI ozone data from Xiong Liu (CFA, Harvard-Smithsonian)

OMI NO2 Comparison: 2013



Preliminary Finding: The magnitudes of NOx emissions and key reactive VOCs (e.g. toluene) are underestimated in the current inventory for SMA





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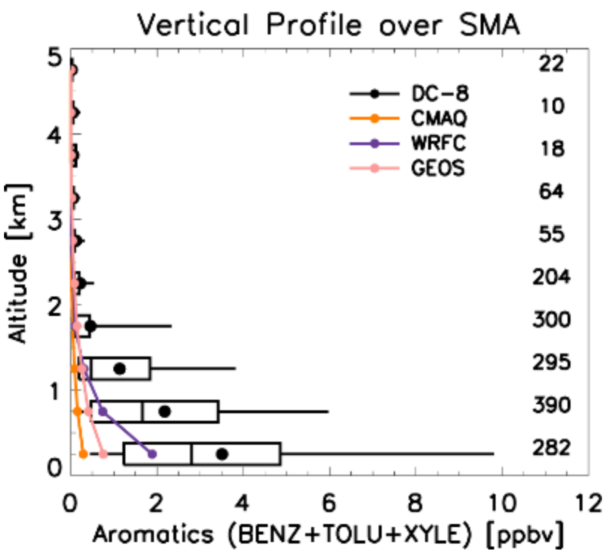
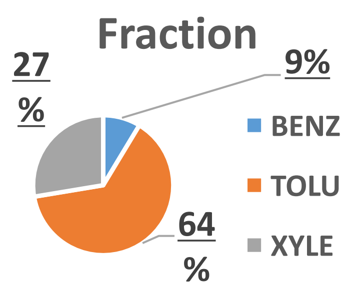
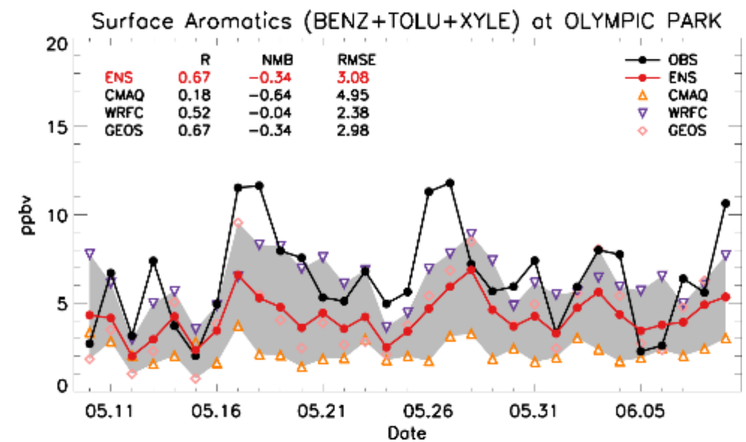
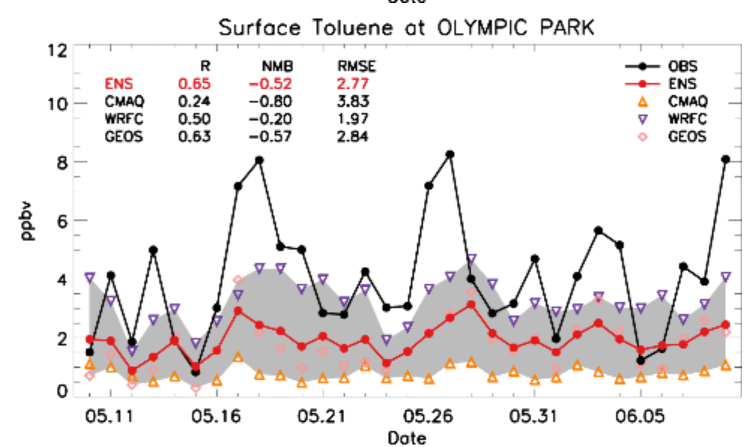








G5NR-Chem Summary

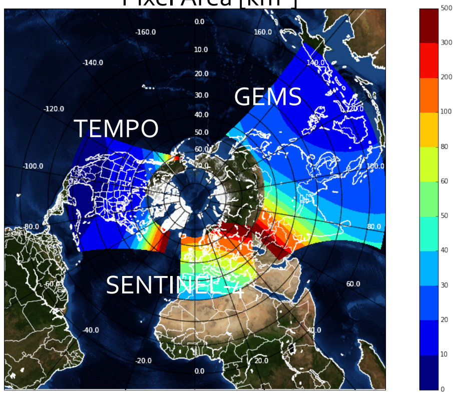
- G5NR-Chem is broadly consistent with SEAC4RS field observations, ozonesondes, and OMI satellite data
- Compared to the GEOS-Chem CTM, G5NR-Chem tends to show better CO simulation in the free troposphere
- Unlike the GEOS-Chem CTM, G5NR-Chem tends to underestimate free tropospheric ozone in the mid-latitudes
  - likely reflecting differences in parameterization of lightning NOx locations
- Validation for the full year in progress

Observation Simulators

Geostationary Constellation: TEMPO+GOES-R, GEMS and SENTINEL-4

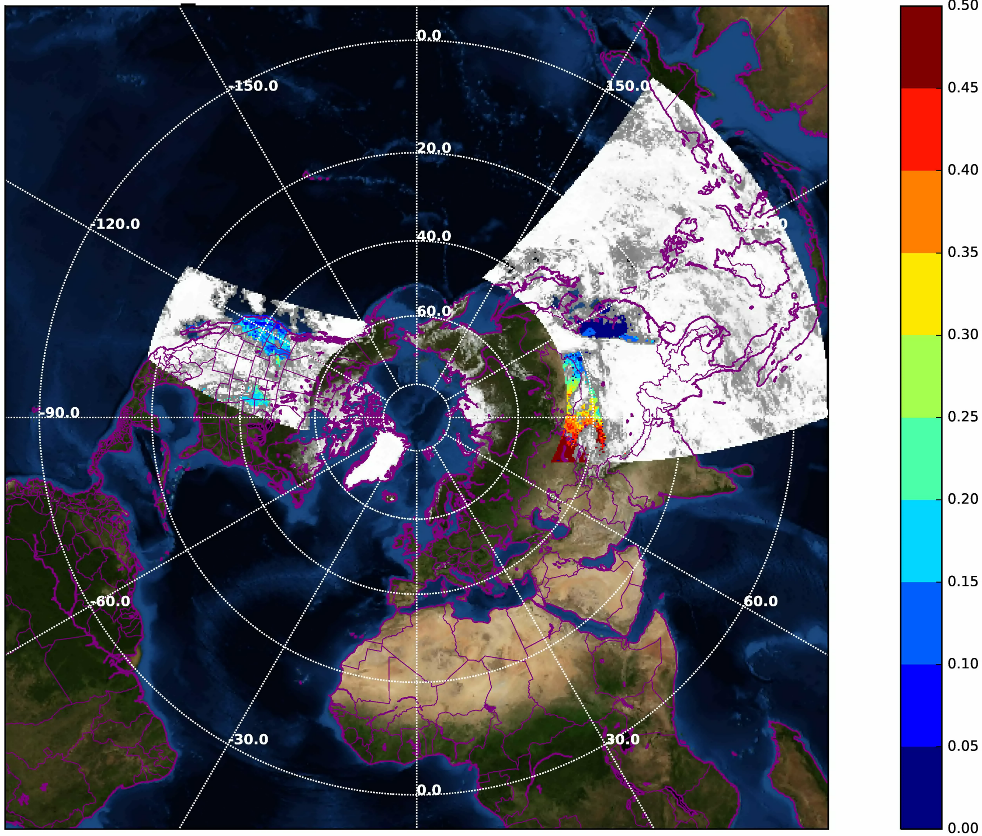
- TOA Reflectance for 6 aerosol relevant channels
- 354, 388, 412, 470, 550, and 670 nm
- Radiative Transfer Model: VLIDORT
- Surface
- MAIAC BRDF Kernels
- Atmosphere
  - GEOS-5 Nature Run with GOCART aerosols

Pixel Area [km²]



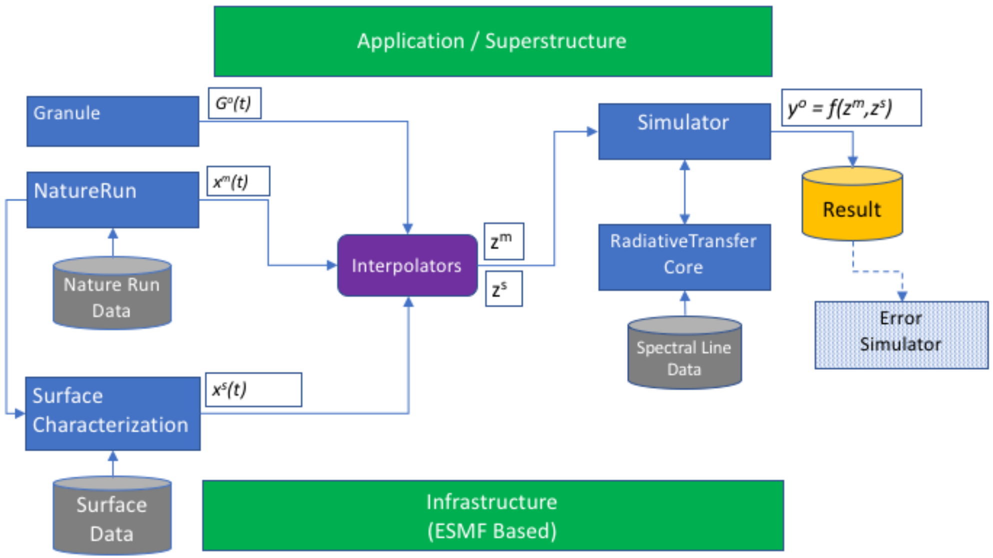
Download TEMPO, GEMS, SENTINEL-4, and GOES-R synthetic data from http://g5nr.nccs.nasa.gov/data/OBS

TOA_REFLECTANCE 20060727 00z 550nm



FORSE

- Framework for Observation of Radiances: Simulation and Experimentation
- Collaboration between Goddard, JPL and UW/CIMSS, NOAA
- Focus on Aerosols, Cloud,Trace Gases
- Target: future hyperspectral atmospheric composition sensors: UV, VIS, NIR, TIR



TEMPO/GOES-R Synergism

Thanks to: Shobha Kondagrunta & Pubu Ciren (NOAA/NESDIS/STAR)

TEMPO Aerosol Retrievals

TEMPO

- No cloud camera
- No short-wave Infrared channel (2.1 μm)
  - Cannot adapt MODIS aerosol algorithms
- Science team plan is to adapt OMI aerosol algorithm

TEMPO/GOES-R Synergy

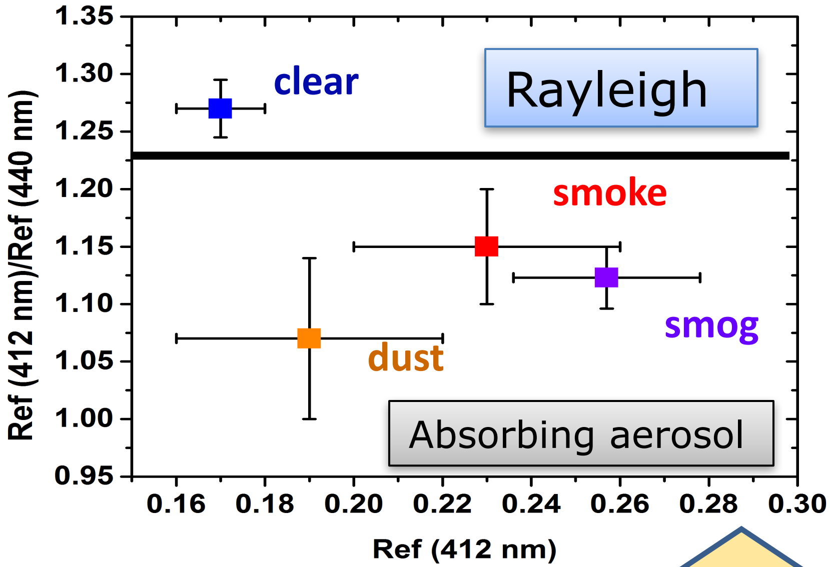
- Can GOES-R ABI cloud mask be used by TEMPO?
  - Remapped to TEMPO grid
- Can GOES-R ABI 2.25 μm be combined with TEMPO visible bands?
  - Derive AOD using MODIS aerosol algorithms (MAIAC or dark target)
  - Use AOD in OMI aerosol algorithm to get aerosol height

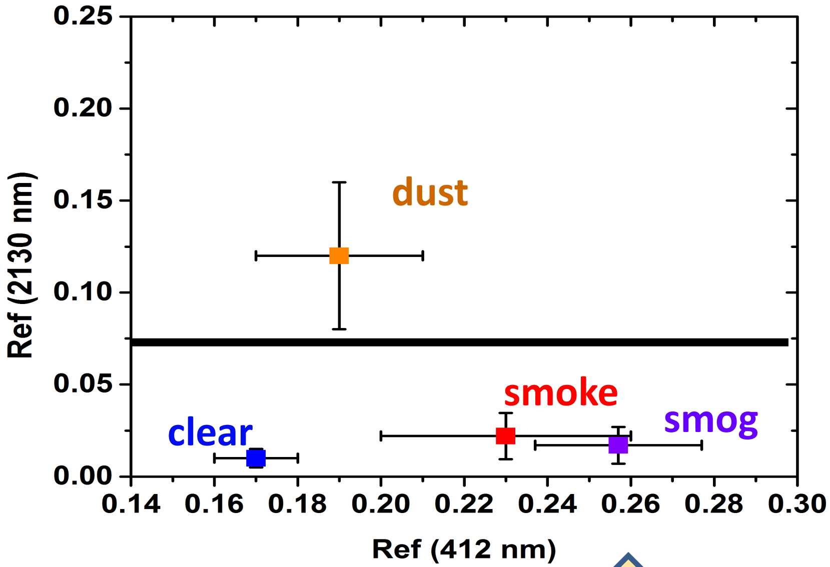
In this study we tested a simple aerosol detection algorithm (developed for SNPP VIIRS) to test the TEMPO/GOES-R synergy

TEMPO/GOES-R Synergy Experiments

- **G5NR generated synthetic radiances for about 22 cases**
  - Hourly, 7-km nature run for; smoke cases for July 27 and August 7, 2006 used in this study
  - Simulated radiances for GOES-R and TEMPO footprints using VLIDORT
  - Aerosol optical properties from OPAC data base
- **JPSS Enterprise Processing System (EPS) *Aerosol Detection* algorithm was applied to the synthetic radiances**
  - EPS aerosol detection algorithm detects the presence of absorbing aerosols, by using the fact that absorbing aerosol reduces the contrast between two neighboring wavelengths in deep-blue region, due to their strong wavelength-dependent absorption.
  - EPS aerosol detection algorithm further separates smoke from dust by using the observations at short-wave IR, such as 2.25um.

Aerosol Detection Algorithm (1)





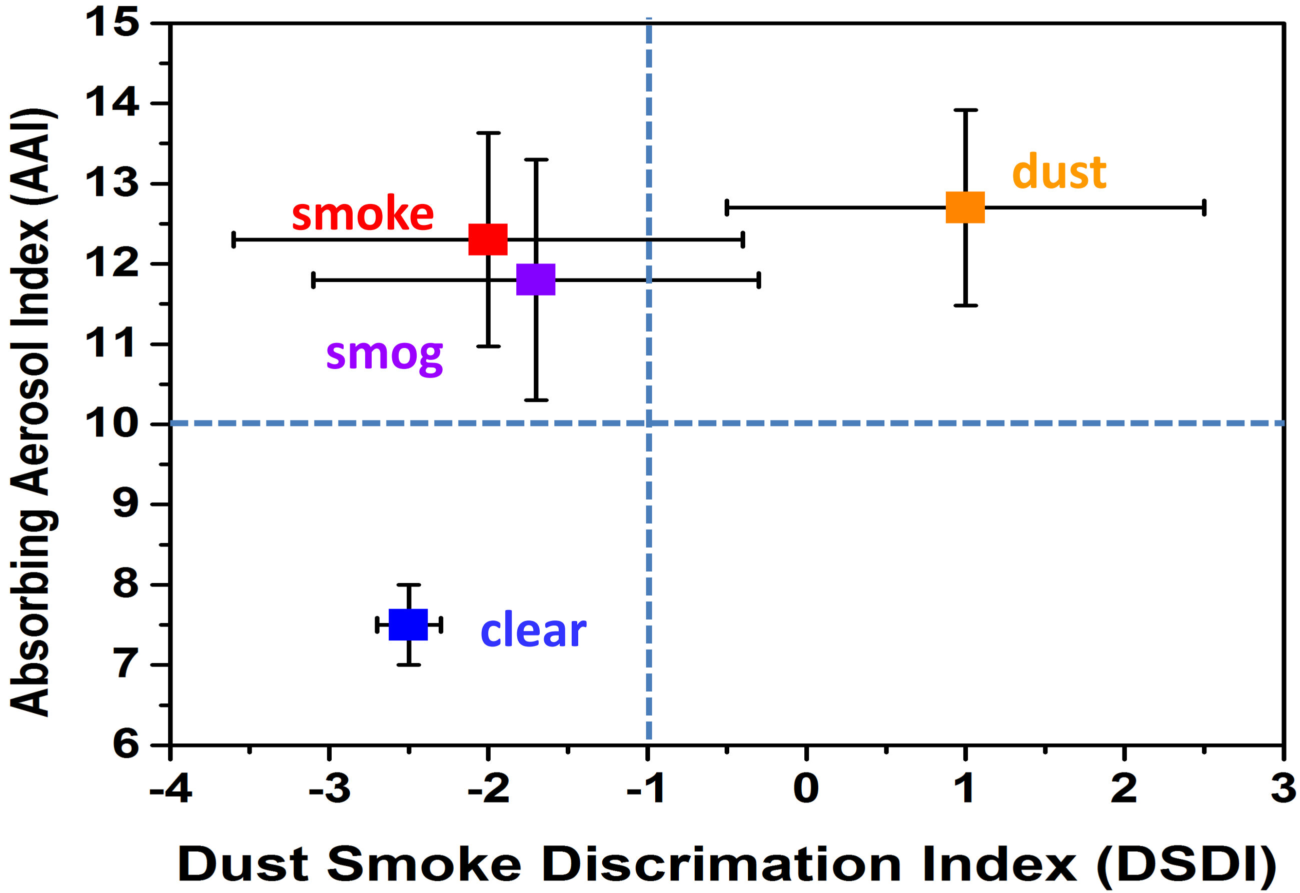
Absorbing Aerosol Index

$AAI = -100[\log_{10}(R_{412}/R_{440}) - \log_{10}(R'_{412}/R'_{440})]$

Dust Smoke Discrimination Index

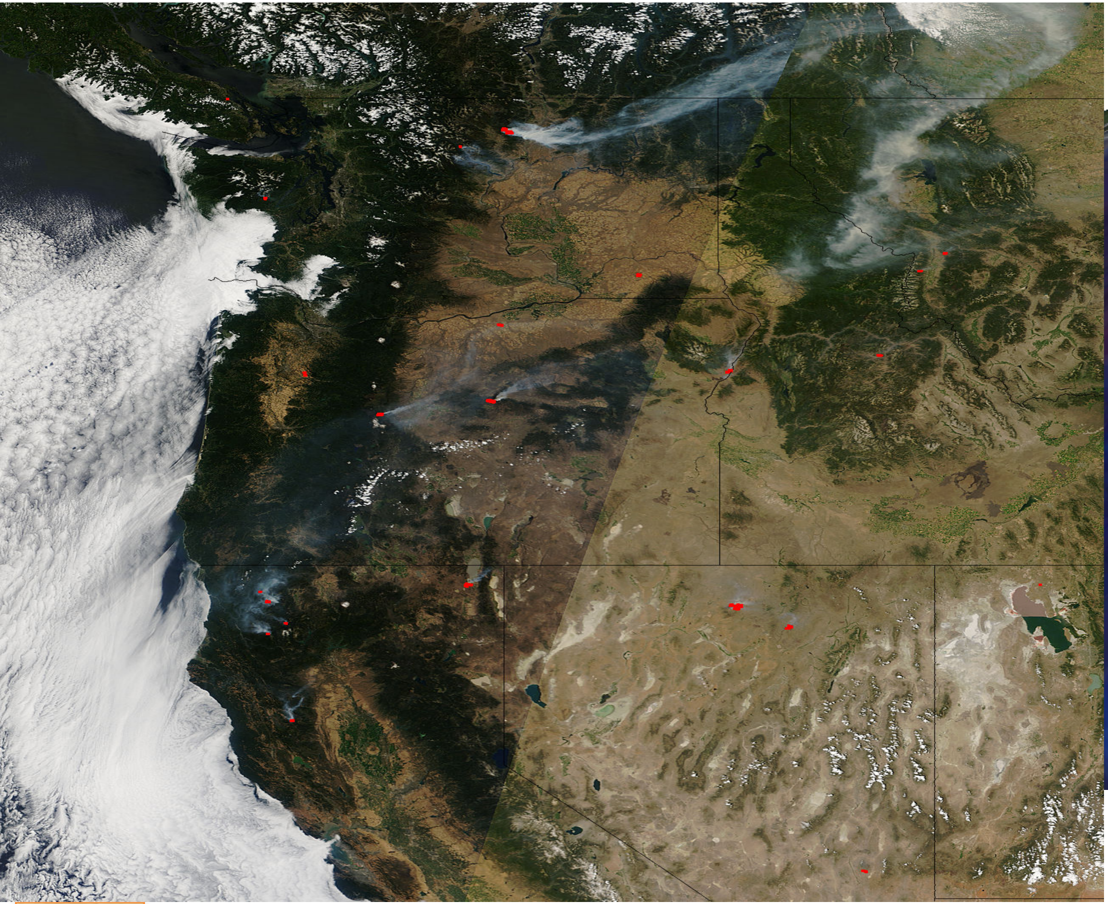
$DSDI = -10[\log_{10}(R_{412}/R_{2250})$

Aerosol Detection Algorithm (2)

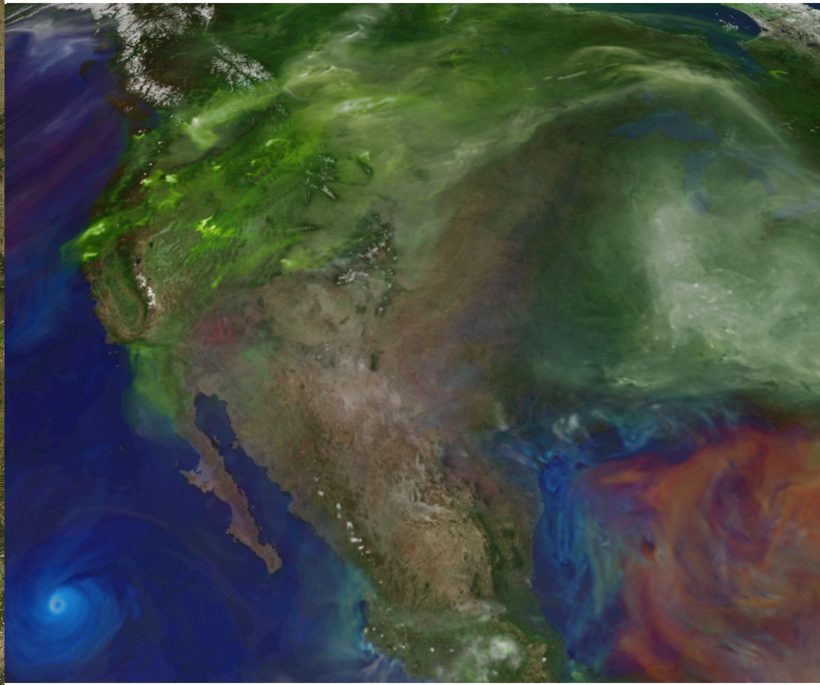


Case Study 1: July 27, 2006

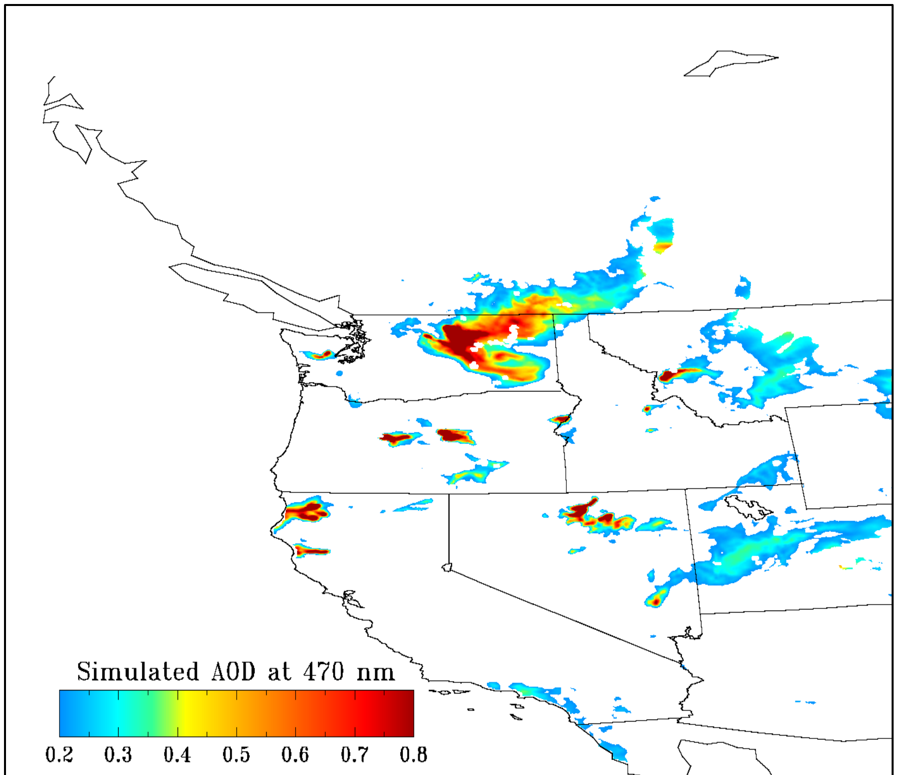
MODIS (Terra) RGB with hotspots

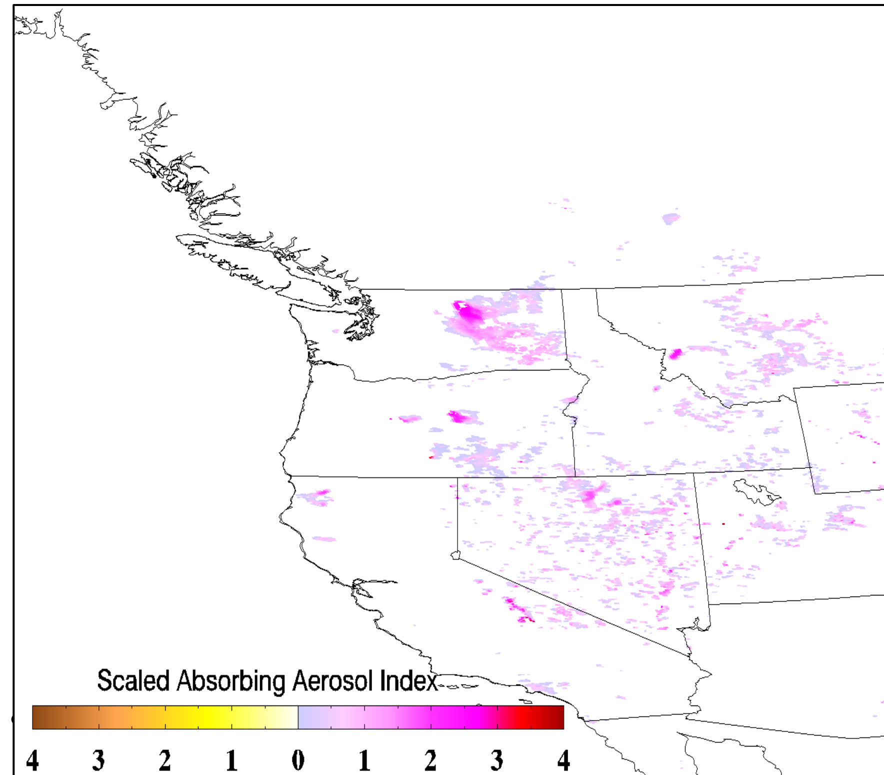


Aerosol Inputs to Nature Run



UTC: 14:00





Dust **Smoke**

Key Findings

- Successful testing of VIIRS aerosol detection algorithm with GOES-R and TEMPO synthetic radiances
- Results indicate that with some loss of diurnal capability, aerosols can be detected and identified
- GOES-R ABI 2.25 μm channel is a viable complement to TEMPO's UV-VIS channels

Future Work

- Optimize aerosol detection retrieval and study a dust episode
- Apply VIIRS aerosol optical depth (AOD) algorithm

TEMPO UV Aerosol Retrieval

Thanks to: Santiago Gasso, Omar Torres, Pete Colarco

Carry out a full retrieval for one TEMPO scan using synthetic radiances generated by GEOS-5

- G5NR Radiances 354, 388 and CO
- TEMPO Viewing Geometry
- OMAERUV Surface albedo database

Radiances, Geometry, CO

- OMI aerosol algorithm OMAERUV 1.6.2

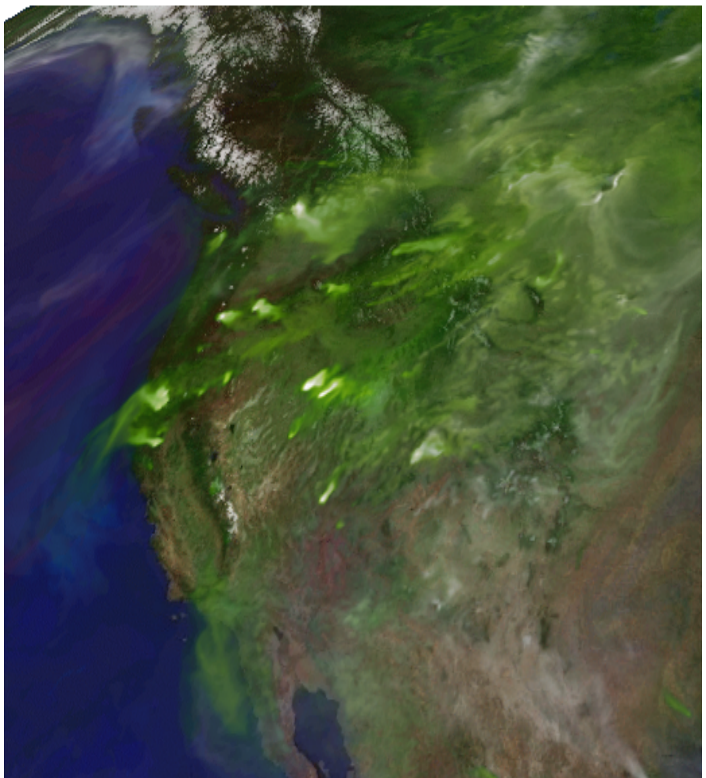
Ground Truth
AOD388
SSA388

Retrieved
AOD388
SSA388

Compare
GEOS-5 vs OMAERUV
AOD and SSA

GEOS-5 scene: Smoke in the West US

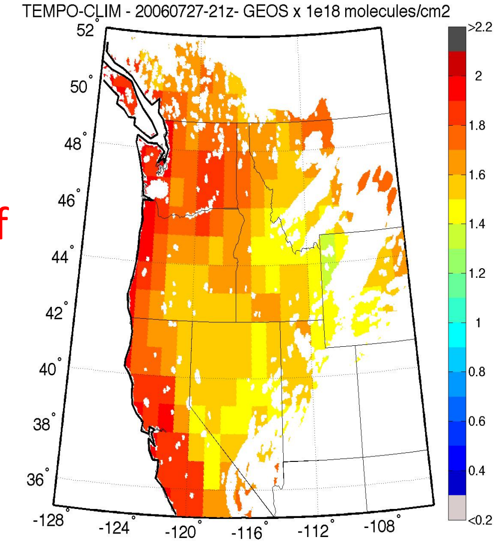
Fires for July/27/2007 – 21UTC



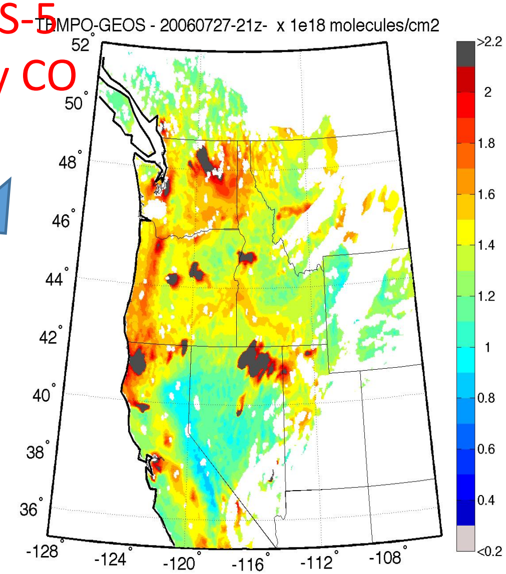
Right from the initial comparisons it became apparent that the OMI algorithm needed a better proxy for smoke. The OMI CO climatology was not adequate.

In the subsequent comparisons all OMI retrievals ingested the CO from GEOS-5.

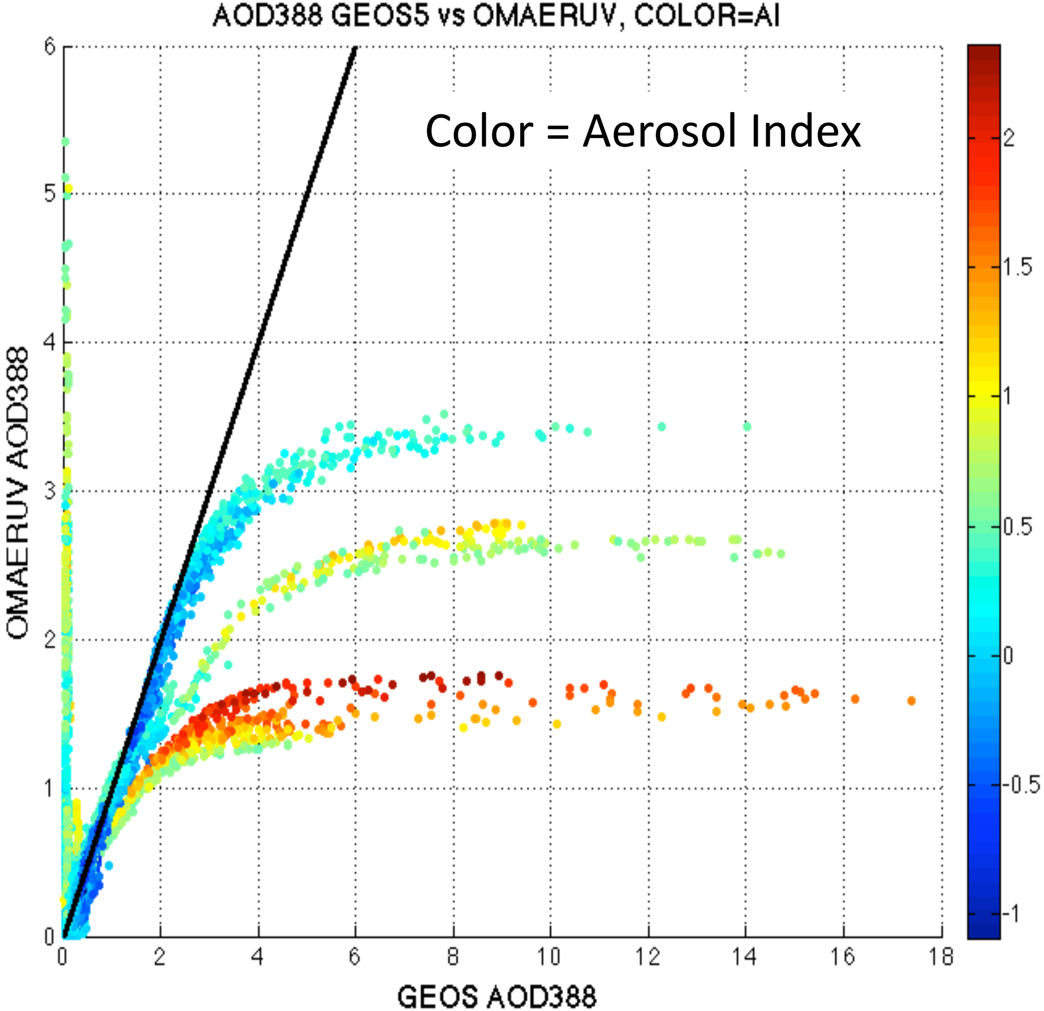
OMI Monthly Climatology of CO



GEOS-5 Daily CO



G5NR vs OAMERUV AOD388



- Saturation of OMAERUV retrievals
- Some GEOS-5 AODs seem too high

G5NR vs OAMERUV AOD388

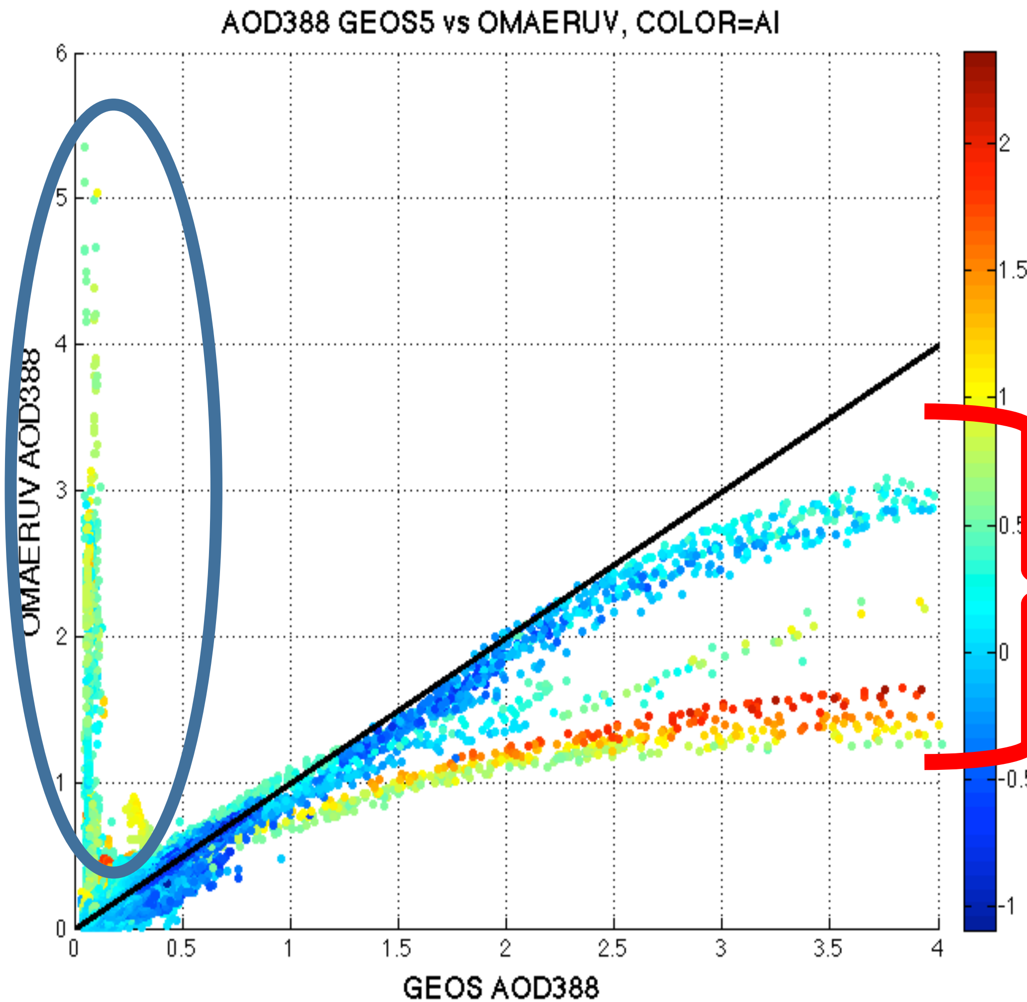
Why?

Cloud contamination?

There are no clouds in the GEOS-5 simulation

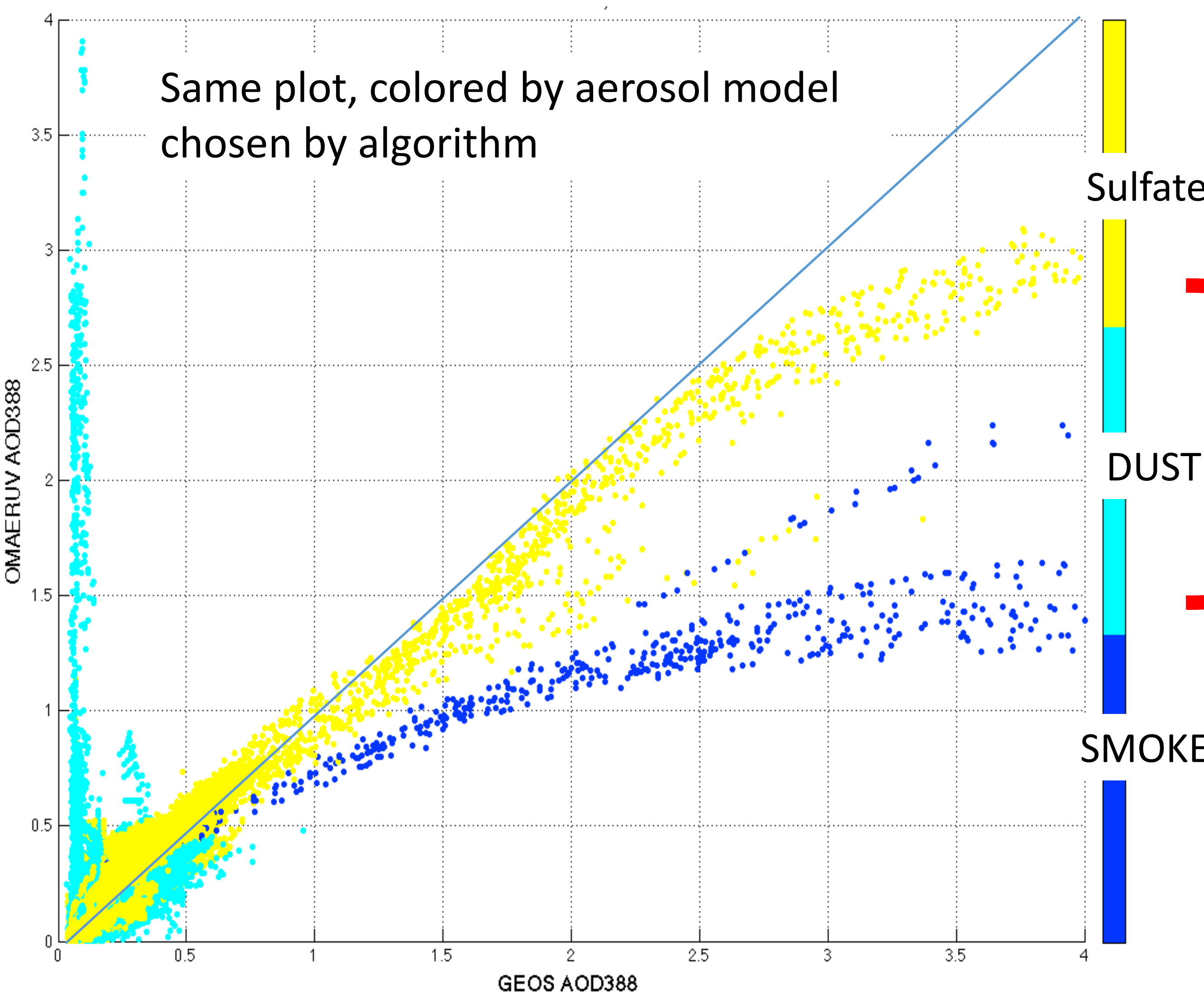
Surface?

Both GEOS5 and OMAERUV use the same database



Why?

Let's focus on the source of the differences at higher AODS

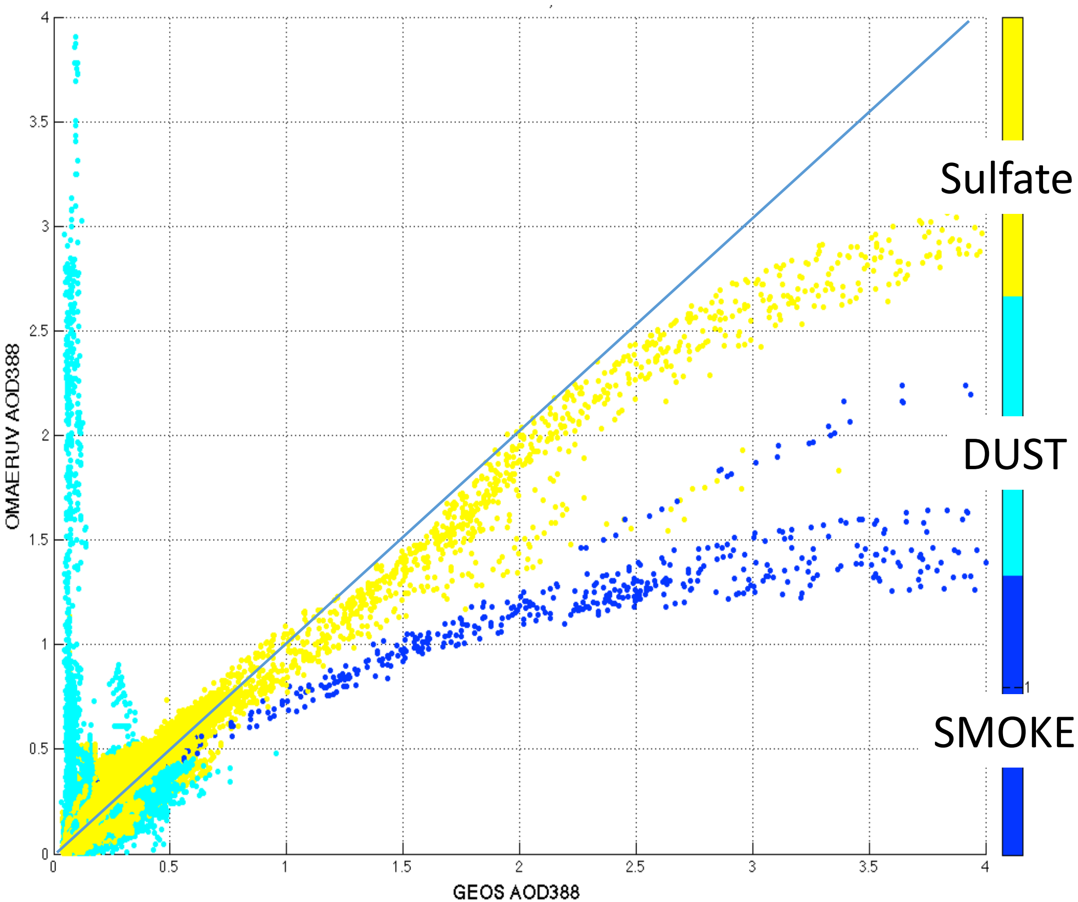


Why the algorithm choses different aerosol models?

and

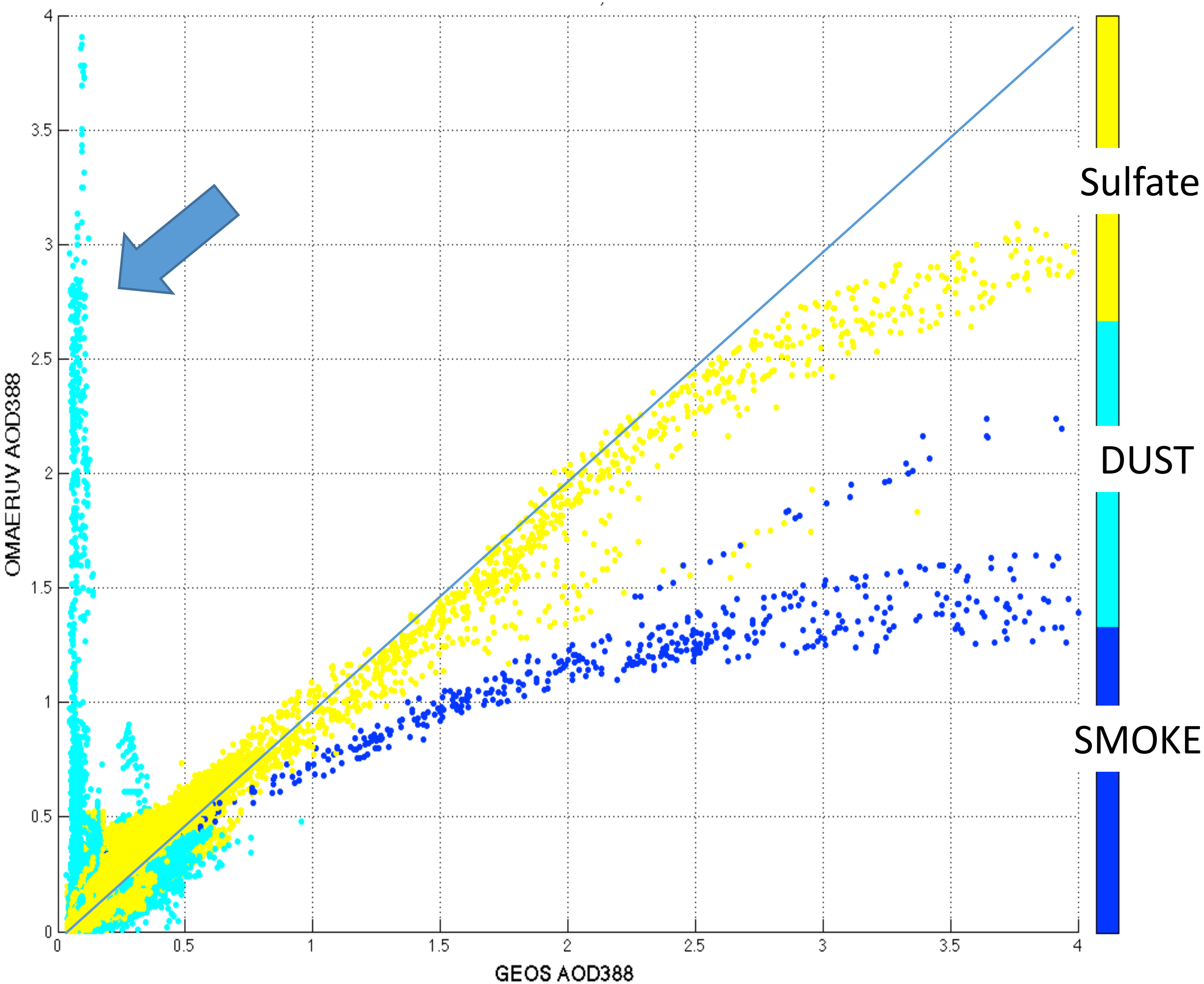
What in the aerosol models causes the different AODs?

So, why OMI SULFATE AODs agree better with GEOS-5?



- OMI SULFATE models have less absorption and low AAE than its SMOKE models.
- OMI SULFATE models resemble more the optical properties of GEOS-5 models.

Let focus in the cases with LOW GEOS-5 AODs...



- Only in dust!
- Only in cases of low aerosol loading
- The source of this discrepancy is traced to the processing of the surface albedo database

TEMPO UV Aerosols: Summary

- This retrieval OSSE exercise exposes the challenges of under-determined UV aerosol algorithms
  - Are NR/retrieval inconsistencies representative of such discrepancies in reality?
- OMI-like aerosol retrievals for TEMPO will need additional information to differentiate smoke from dust

Summary

NATURE RUNS

- The Current GEOS-5 Nature Run (G5NR) includes
  - Meteorology
  - Aerosols
  - Carbon Species
- A new nature run including full gas chemistry based on Harvard's GEOS-Chem mechanisms has been produced

OSSE APPLICATIONS

- Synthetic UV-VIS radiances have been simulated for a constellation of GEO satellites:
  - TEMPO, GEMS, GOES-R, SENTINEL-4
  - Working WITH JPL on efficient RT approaches for full spectra (2000 channels, PCA)
- Other AC OSSE activities:
  - GEO-CAPE aerosol retrievals
  - Lidar/polarimeter joint retrievals
  - Aerosol above cloud algorithms
  - Aerosol emission inversions

Data Availability

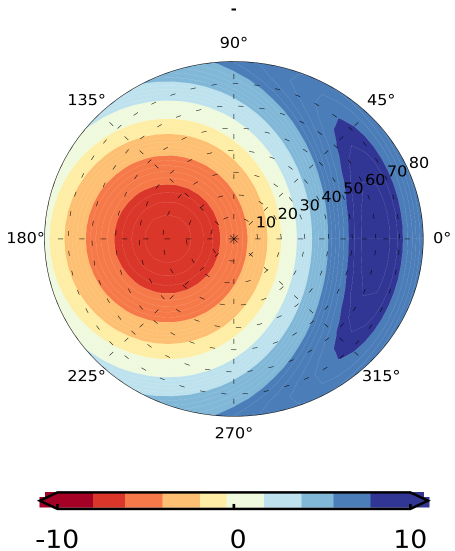
- G5NR Portal:
  - https://gmao.gsfc.nasa.gov/global_mesoscale/7km-G5NR/
- G5NR-Chem Data:
  - https://portal.nccs.nasa.gov/datashare/G5NR-Chem/Heracles/12.5km/DATA/
- G5NR-Chem OPeNDAP:
  - https://opendap.nccs.nasa.gov/dods/OSSE/G5NR-Chem/Heracles/12.5km

Backup Slides

Computational Challenges

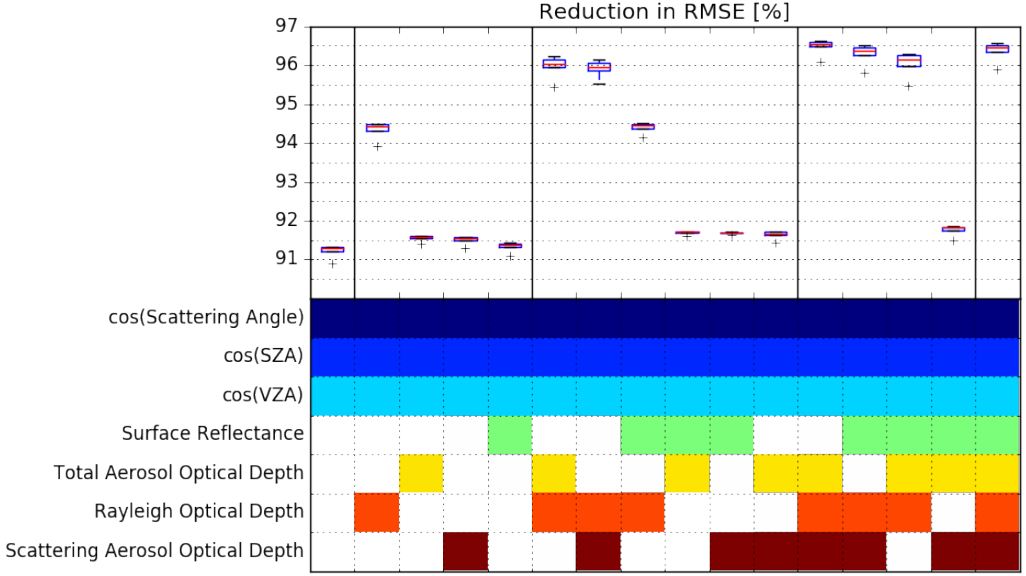
- Radiative transfer calculations for high spatial resolution, hyper-spectral sensors is extremely expensive
- *Vector* calculations that are critical in the UV are 6-8 times more expensive than *scalar calculations*

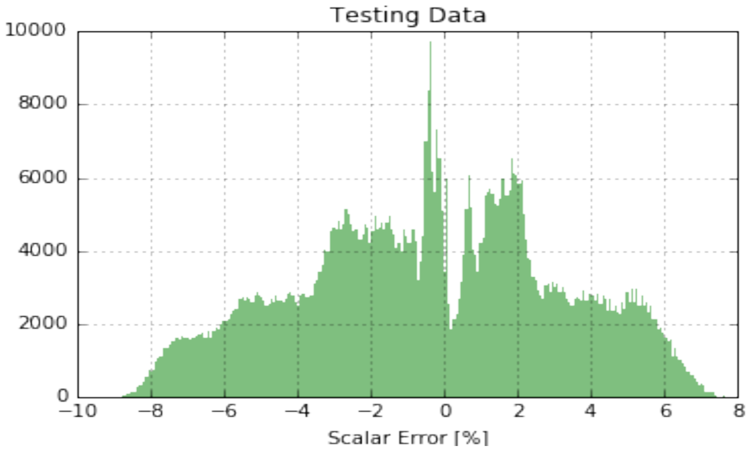
Rayleigh Slab [400 nm]

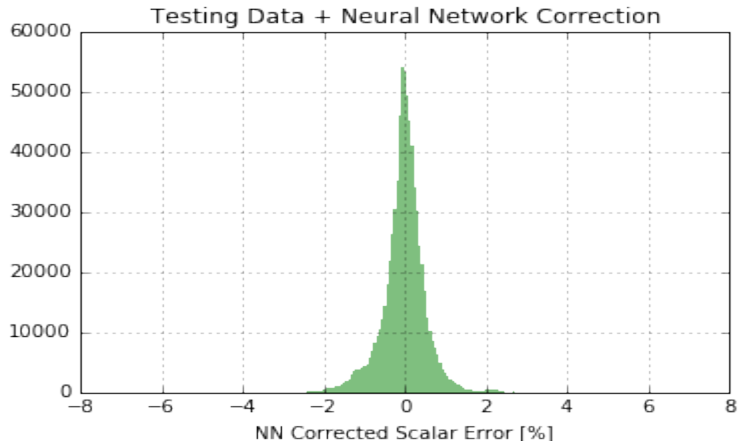


Scalar Error [%]

Neural Net Correction [354 nm]







O.S.S.E.

- Observing System
- Simulation
- Experiment

Model-based OSSE

A framework for numerical experimentation in which *observables* are simulated from fields generated by an earth system model, including a *parameterized* description of the *observational error* characteristics.

Simulations are performed in support of an experimental goal.

Goddard
SPACE FLIGHT CENTER

The Validation Imperative

- As with any simulation, OSSE results apply to new instruments only to the degree they have been validated with existing legacy instruments.
- OSSE credibility is first determined by carefully comparing a variety of statistics that can be computed in both the real and OSSE simulated contexts.

OSSEs need to be validated as a *System*.

Observation Error
at Instrument Footprint

Measurement equation:

$$y = f(z^t) + \epsilon$$

where

y	measurement
z^t	true state at instrument footprint
f	observation operator
ϵ	observation error w.r.t. z^t (detector noise)

Radiance Error Modeling

Radiance errors (detector noise) ϵ are defined as

$$y = f(z^t, b^t) + \epsilon$$

where

y	radiance measurement
f	forward function (radiative transfer function)
z^t	true state ($z^t = Hw^t$)
b^t	true forward model parameters (e.g., spectral line data, calibration parameters)
ϵ	detector noise + error of representativeness

The real physics of the radiative transfer is often too complex or its details unknown. In practice, a forward model (F) is used

$$f(z^t, b^t, b'^t) = F(z^t, b^t) + \delta f(z^t, b^t, b'^t)$$

Retrieval Error Analysis

Ignoring the transfer function bias for the prior states, the retrieval error reads:

$$\begin{aligned}\epsilon^r &\equiv z - Hw^t \\ &= (I-A)\epsilon^p + D_y F_b \epsilon_b + D_y \delta f + D_y \epsilon\end{aligned}$$

where $\epsilon^p = z^p - z^t = H(w^p - w^t)$, etc., and

A	averaging kernel ($= D_y F_z$)
$(I-A)\epsilon^p$	smoothing error (prior error)
$D_y F_b \epsilon_b$	forward model parameter error
$D_y \delta f$	forward model error
$D_y \epsilon$	instrument + representativeness error

Error of Representativeness

Let x^t be the true state in model grid point space:

$$z^t = \mathcal{I}(x^t) + \epsilon'$$

where

$$\begin{array}{ll} \mathcal{I} & \textit{remapping}\ \text{operator} \\ \epsilon' & \text{representativeness error} \end{array}$$

In OSSE studies the Nature Run is assumed to provide the ground truth, but it does so in grid-point space: x^t

$$\begin{aligned} y &= f(\mathcal{I}(x^t) + \epsilon') + \epsilon \\ &= h(x^t) + \epsilon + F_z\epsilon' + .. \end{aligned}$$

It is critical to account for error of representativeness errors when simulating observables with a footprint much smaller than the Nature Run resolution.

Retrieval Error Modeling

- Retrievals are produced as result of a nonlinear estimation,
$$z = D(y, b, z^p) = D(F(z^t, b^t) + \delta f + \epsilon, b, z^p)$$
where z^p is a background state (prior) used in the retrieval.

- In order to obtain a basic understanding we linearize this equation around a known state, say the prior z^p
$$\begin{aligned} z - z^p \quad = \quad & [D(F(z^p, b), b, z^p) - z^p] \\ & + D_y F_z (z^t - z^p) \\ & + D_y F_b (b^t - b) \\ & + D_y \epsilon \end{aligned}$$
where $T(z^p, b) = D(F(z^p, b), b, z^p)$ is the so-called Transfer Function.

- The term in brackets is the transfer function bias and should be small for any reasonable retrieval,
$$T(z^p, b) = D(F(z^p, b), b) \approx z^p$$
i.e., the retrieval should return the first guess when noiseless data consistent with it is input.

Retrieval Error Mechanisms

- Averaging Kernel. The retrieved state is a smoothed version of the true state with smoothing functions given by the rows of A

  $$z = Az^t + (I - A)z^p + ...$$

  Those details of the true state which are smoothed out by the retrieval must be provided by the first guess z^p. Notice that A is state dependent.

- Model parameter errors are usually associated with biases. If retrieval is too sensitive to a parameter then it should be retrieved as well (state augmentation).

- Model error. Hard to evaluate. If correct physics is known then it can be modeled (e.g., approximations introduced for computational efficiency.)

- Instrument error. Usually the easiest to evaluate. It can have a strong dependence on the state through D_y, although the detector noise ϵ is usually assumed stationary and state independent in clear sky. Cloud clearing introduces additional complications. However, error of representativeness is often state dependent.

Simulating Retrievals

FROM RADIANCES

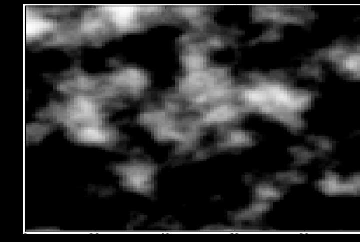
- Synthetic retrievals
  - Simulate radiances by radiative transfer
  - Model radiance errors
  - Apply retrieval code

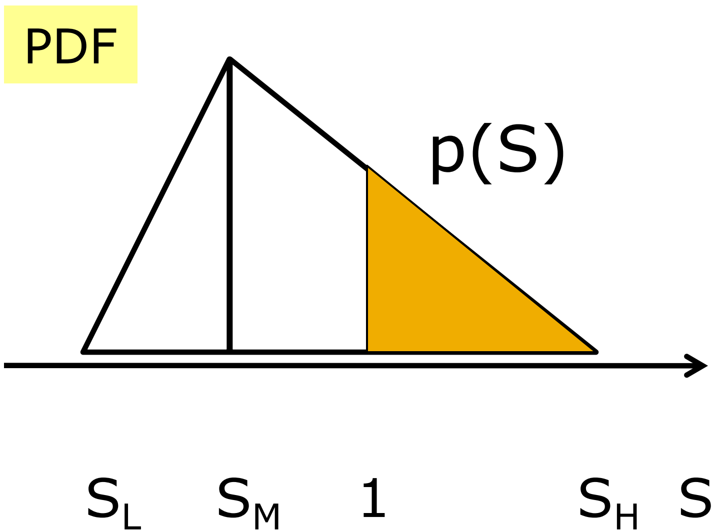
BY MODEL SAMPLING

- Sample and perturb
  - Interpolate geophysical to obs location
  - Model retrieval errors
  - Done.

While interpolating a model simulated geophysical quantity to observation location is much more straightforward than performing a full RT calculation, modeling retrieval errors is far more complex than modeling radiance errors.

Clouds & Sub-grid Variability





$S = (q_v + q_L + q_I) / q_S(T)$

Norris and da Silva, 2016

- PDF-based cloud parameterizations provide very useful information about sub-grid variability
- Given a PDF of total water one can generate sub-columns consistent with that PDF
- Observation simulators can account for representativeness error by operating on these sub-columns

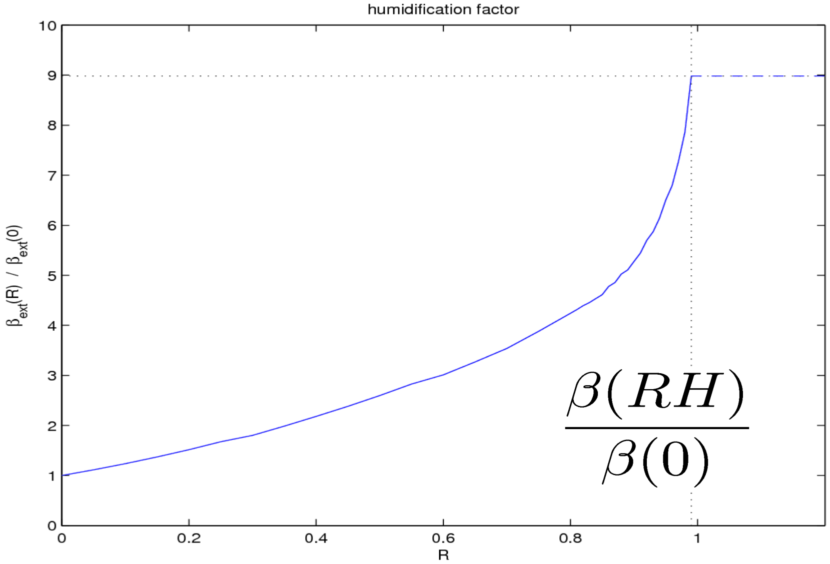
Hygroscopic Aerosols

GOCART prognosticate aerosol dry mass mixing ratio q_{dry}, with humidification effects being included diagnostically prior to computing optical depth

$$\tau = \beta(RH;p) \cdot q_{\mathrm{dry}} \cdot \rho_a \delta z$$

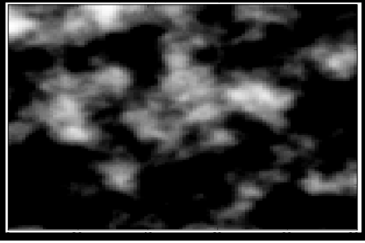
The normalized mass extinction efficiency

$$\hat{\beta} = \frac{\beta(RH)}{\beta(0)} \sim 1 - 10$$



$\hat{\beta}$ saturates at 99%

PDF-based Humidification



Recall that aerosol satellite retrievals are only available under *clear sky* conditions:

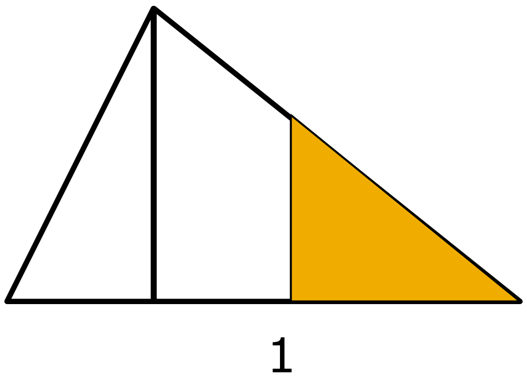
$$\tau_{\text{clear}} = \beta_{\text{clear}}(RH) \cdot q_{\text{dry}} \cdot \rho_a \delta z$$

PDF-based cloud schemes as in GEOS-5 can be used to estimate the mean humidification effect on a GCM gridbox

$$\begin{aligned} <\hat{\beta}> &= \int_0^\infty p(S)\hat{\beta}(S)dS \\ &= \int_0^1 p(S)\hat{\beta}(S)dS + \int_1^\infty p(S)\hat{\beta}(S)dS \\ &= (1-f)\cdot <\hat{\beta}>_{\text{clear}} + f\cdot <\hat{\beta}>_{\text{cloudy}} \end{aligned}$$

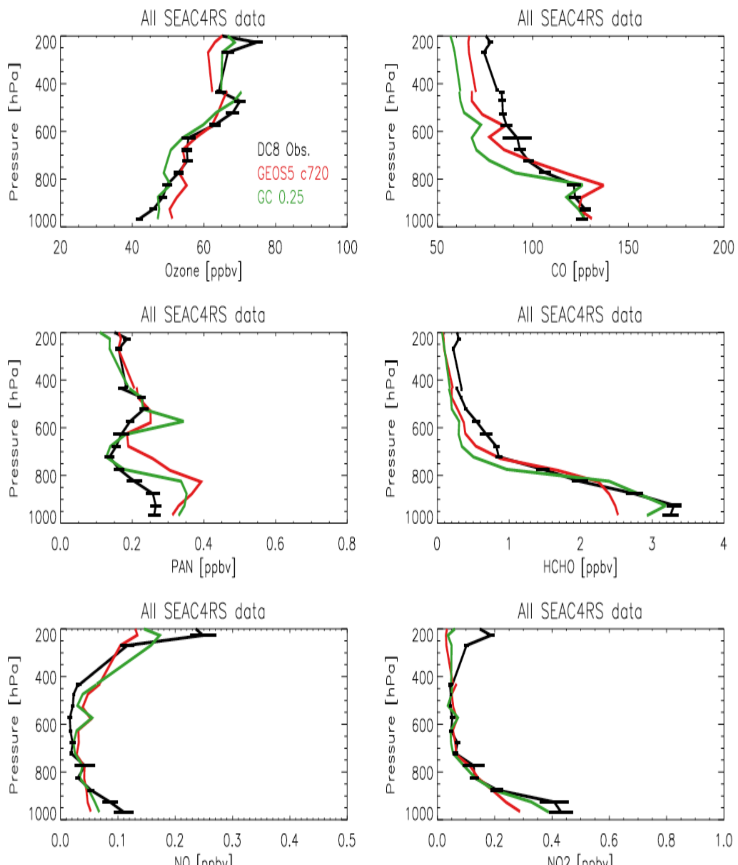
where the *cloud fraction* f is given by

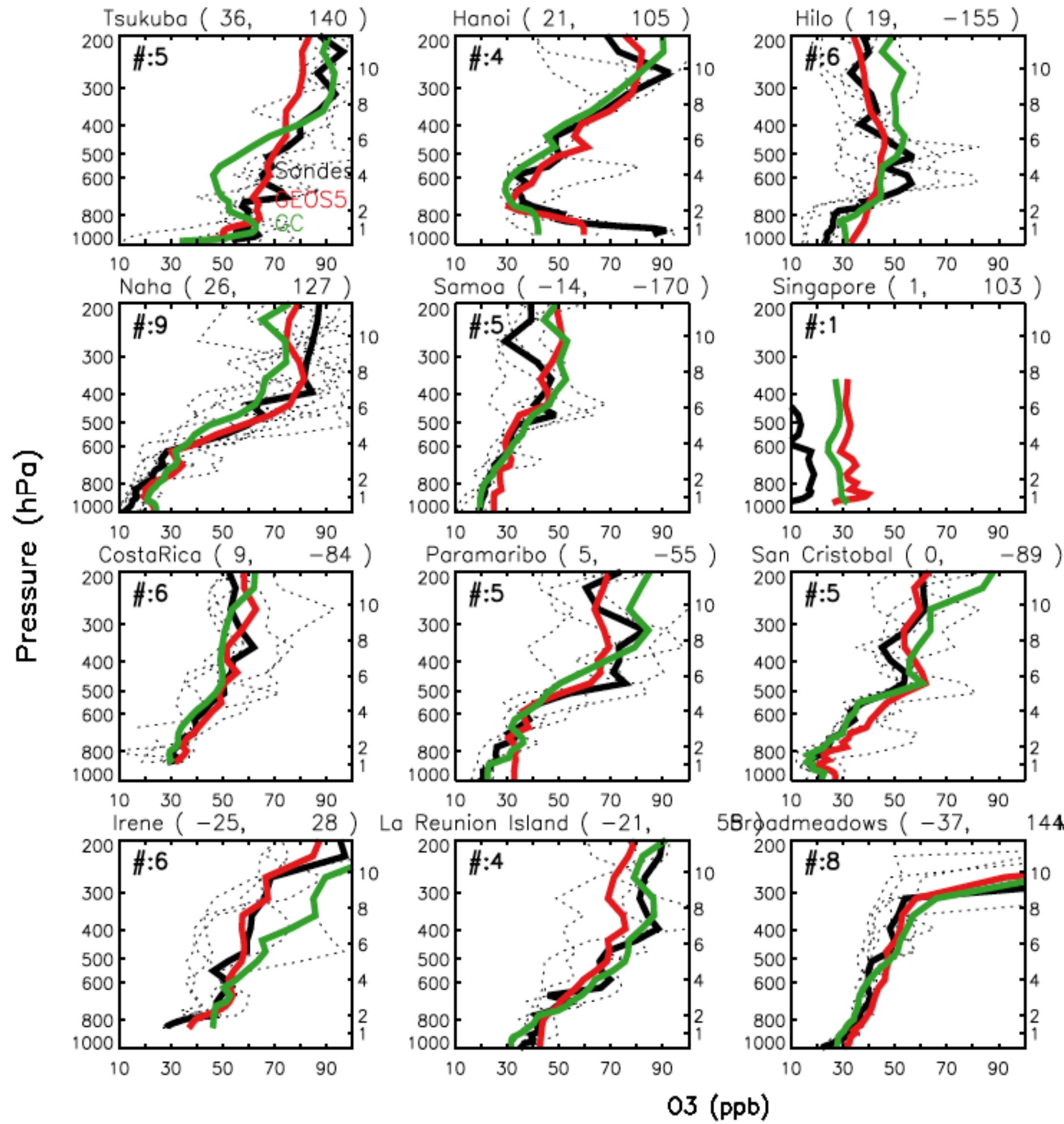
$$f = \int_1^\infty p(S)ds$$



A PDF of water vapor + condensate is provided in each gridbox

G5NR-Chem Validation

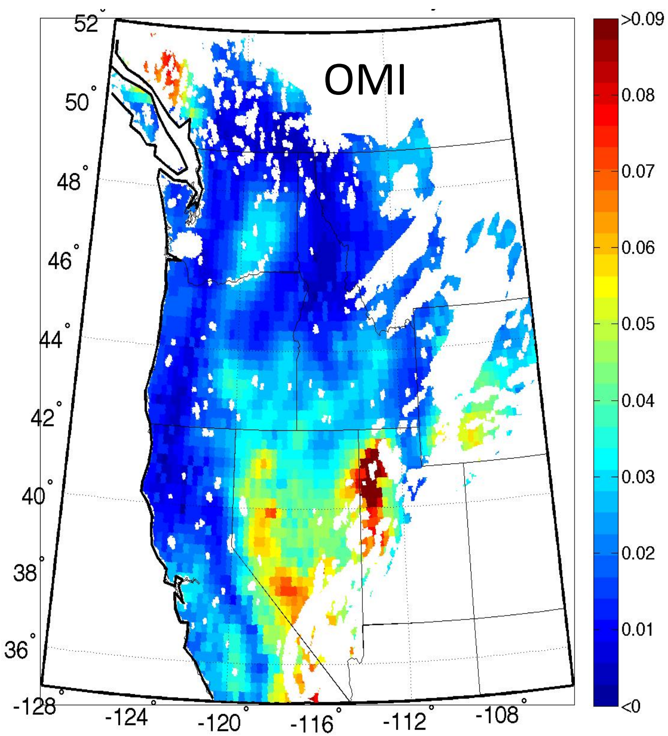


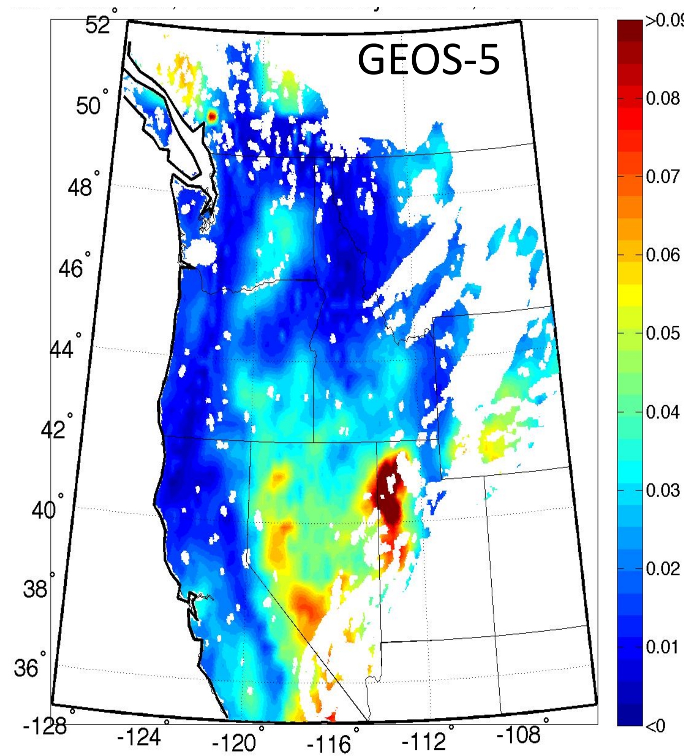


Surface albedos in OMI and GEOS-5

Both OMI and GEOS-5 extract the surface albedo from the same common database. However, they look different

Output Surface Albedo used in the retrieval



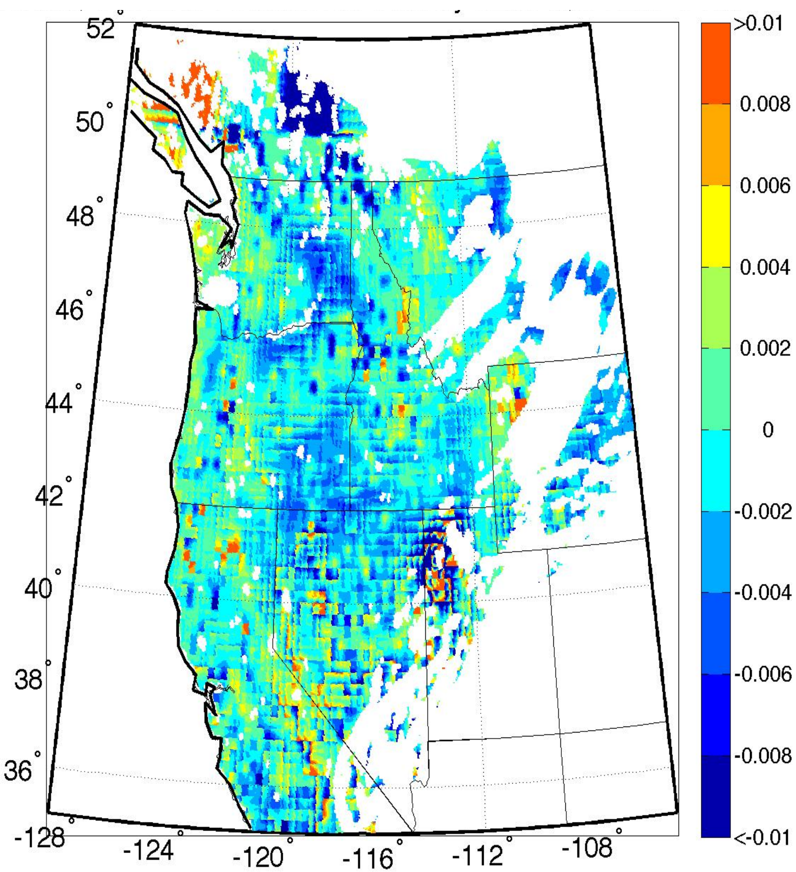


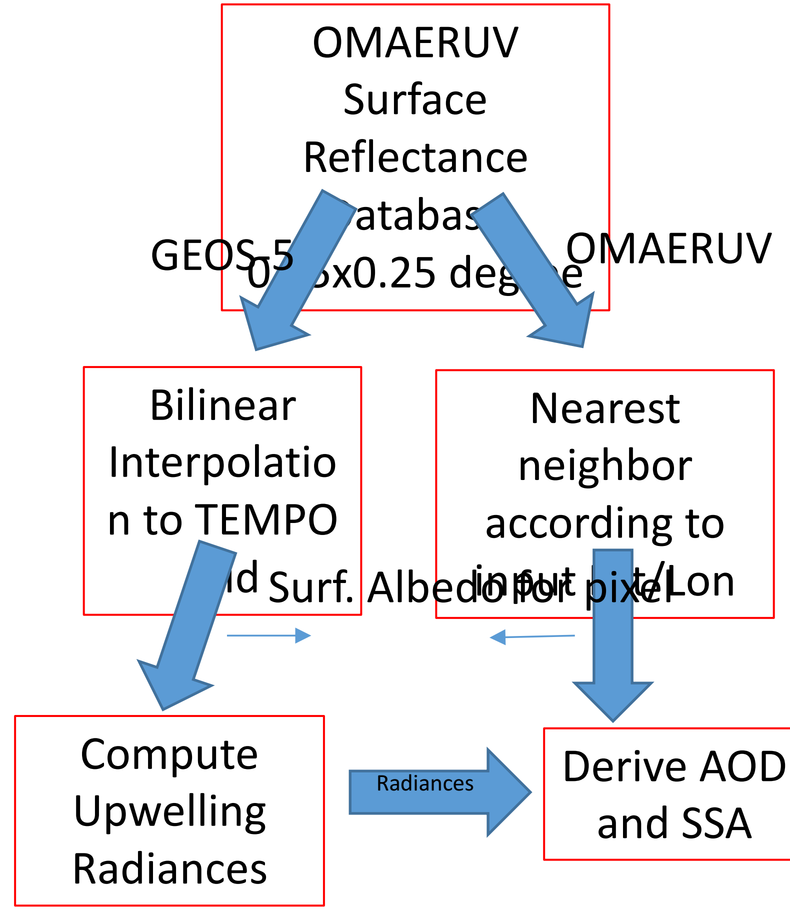
Albedo used by GEOS5 to compute the TOA radiances provided to OMI algorithm

General Patterns are the same but both maps are not the same.

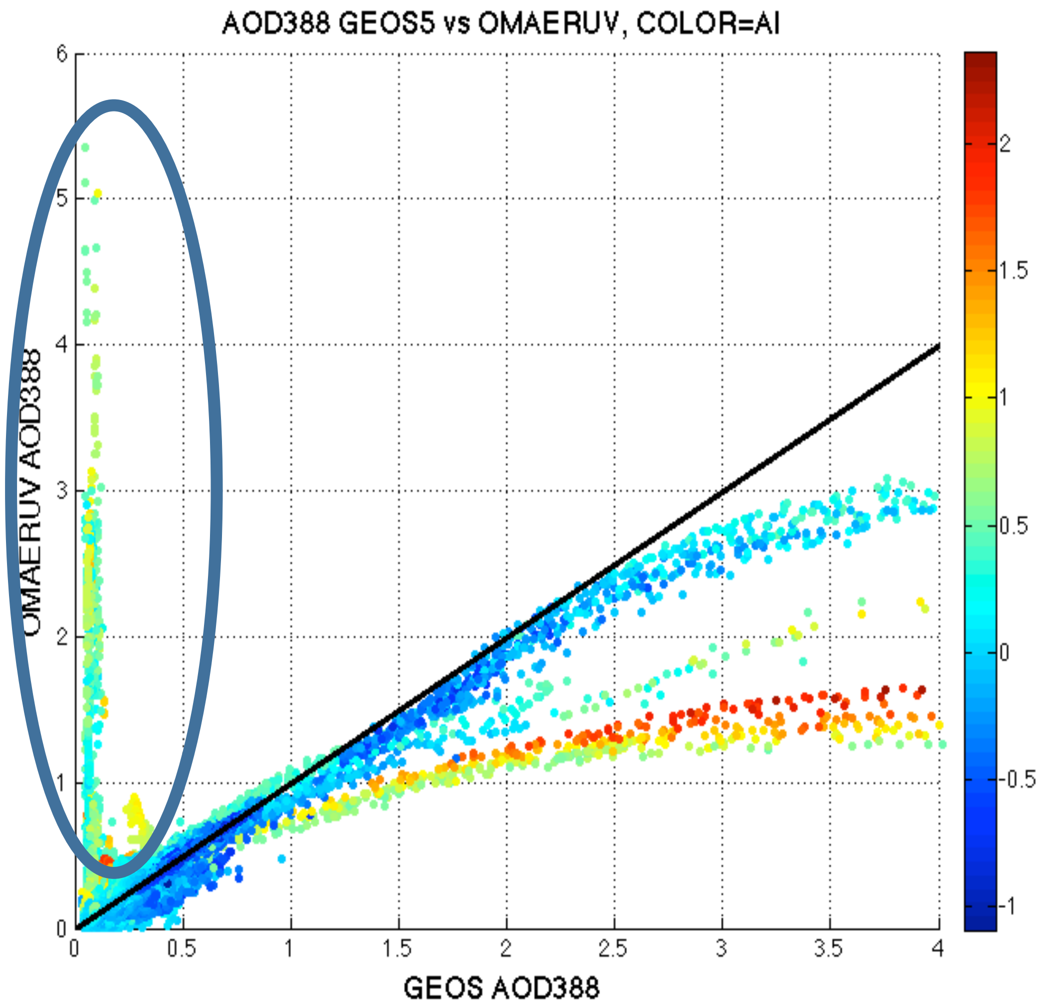
The difference in Surface albedos originates on the interpolation approaches

OMAERUVx minus GEOS 5 Surface Reflectance at 388nm





So , why the high AODs ?



- The GEOS-5 Radiances were generated with surface reflectances inconsistent with those used by OMI algorithm
- Before carrying out the aerosol retrievals, OMI algorithm subtracts the surface contribution from the total radiance.
- The small differences between the two surfaces become apparent at low aerosol loadings.