Jet Propulsion Laboratory
California Institute of Technology

Utility of Multispectral Measurements to Improve Atmospheric Composition Retrievals

Vijay Natraj

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Acknowledgements

- JPL: Susan Kulawik, Annmarie Eldering, Thomas Kurosu, Stan Sander, Kevin Bowman, John Worden, Ming Luo, Dejian Fu
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- GSFC: Ken Pickering
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- AMES: Bob Chatfield
- RT Solutions: Rob Spurr

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Outline

- GEO-CAPE and atmospheric composition
- Multispectral retrieval concept
- Tools and analysis for ozone
- Future work
- Observation System Simulation Experiments
- Beyond atmospheric composition

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Introduction to GEO-CAPE

- GEOstationary Coastal and Air Pollution Events
- Recommended by NRC Earth Science Decadal Survey (2007) as Tier-II mission
- Objectives
  - Identify human versus natural sources of aerosols and ozone precursors
  - Track air pollution transport
  - Understand short-term dynamics of coastal ecosystems in response to riverine and atmospheric inputs, human activity and climate change

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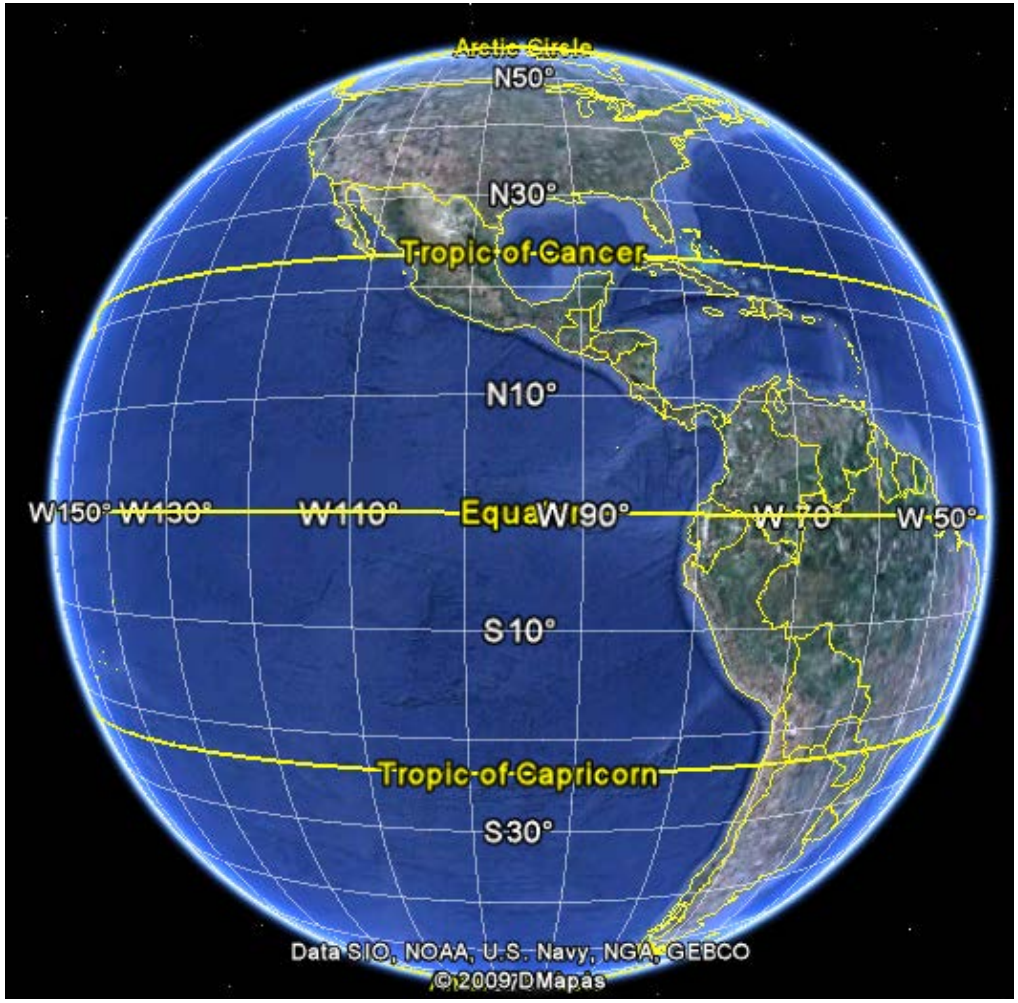
Proposed Viewing Domain



- Orbit centered at 100° W
- Footprint: 4 km (gases), 1 km (aerosols) at 40° N
- Higher spatial resolution for aerosols to avoid cloud contamination
- Observe North America land and coastline with hourly resolution
- Observe North Pacific, North Atlantic, and South/Central America with daily resolution

Daniel Jacob, Harvard

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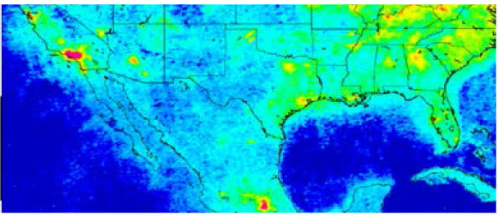
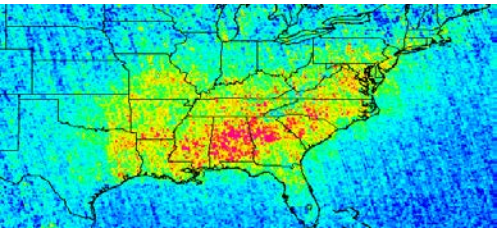
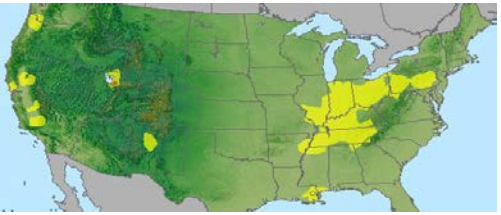
Science Questions



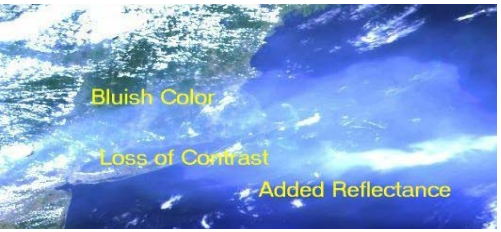
1. What are the emissions of gases and aerosols important for air quality and what are the processes controlling these emissions?



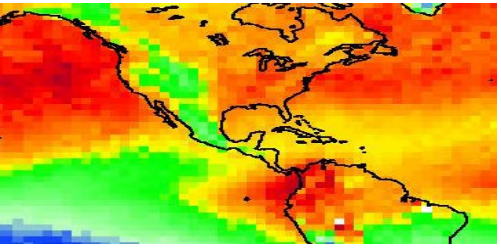
2. How do atmospheric transport, chemical evolution, and deposition determine tropospheric composition over scales ranging from urban to continental?



3. How can we improve air quality forecast and assessment models?



4. How do changes in air quality drive climate forcing on a continental scale?



5. How does intercontinental transport affect air quality?

Daniel Jacob, Harvard

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Improvement to Existing Measurements

- High temporal resolution measurements capture changes in pollutant distributions due to changing photochemistry, emissions and meteorology
- High spatial resolution measurements access city scale with continuous full coverage of North America
- Exploitation of multispectral observations improve information content in the vertical profile
- Measurements complementary to observations from ground-based, suborbital, LEO and other GEO satellite platforms

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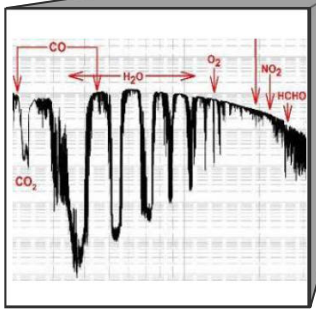
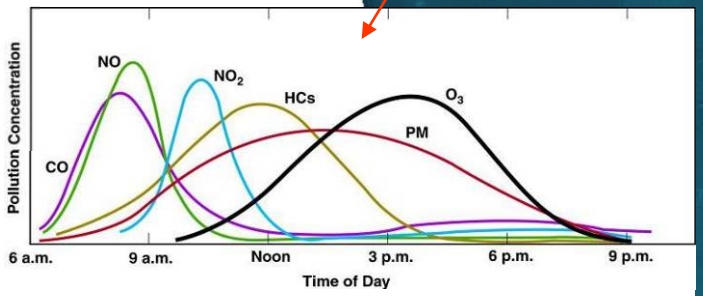
Geostationary Orbit for Hourly Sampling

500 km x 500 km scene is imaged onto a 128x128 pixel focal plane array which provides a 4x4 km size pixel at nadir and records spectra in every pixel for 60 seconds per scene



Spectra in every pixel captures rapidly evolving tropospheric chemistry



Rapidly evolving chemistry in the boundary layer

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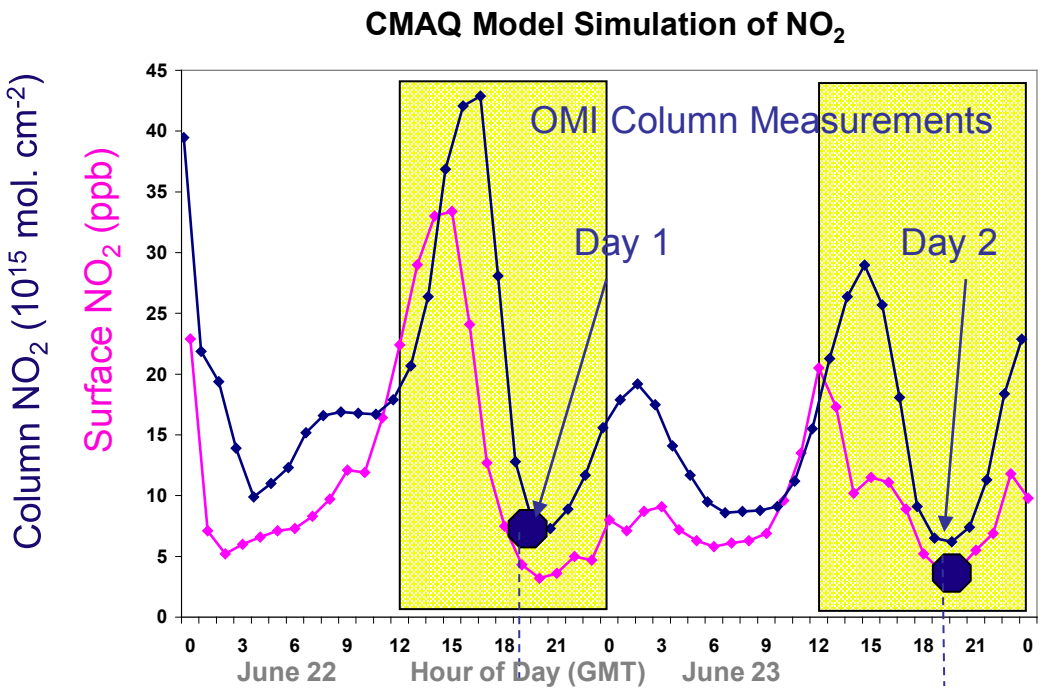
Diurnal Cycle



- High temporal resolution measurements required to capture critical diurnal variability in photochemical and boundary layer processes necessary for understanding regional pollution formation

- Measurements provided once per day provide relatively little information that can be used to examine how well AQ models perform

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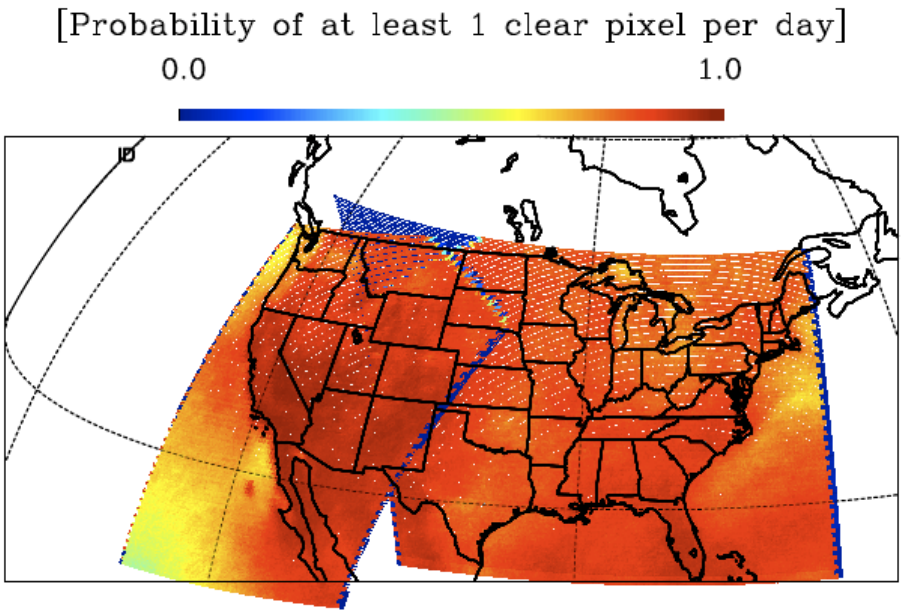
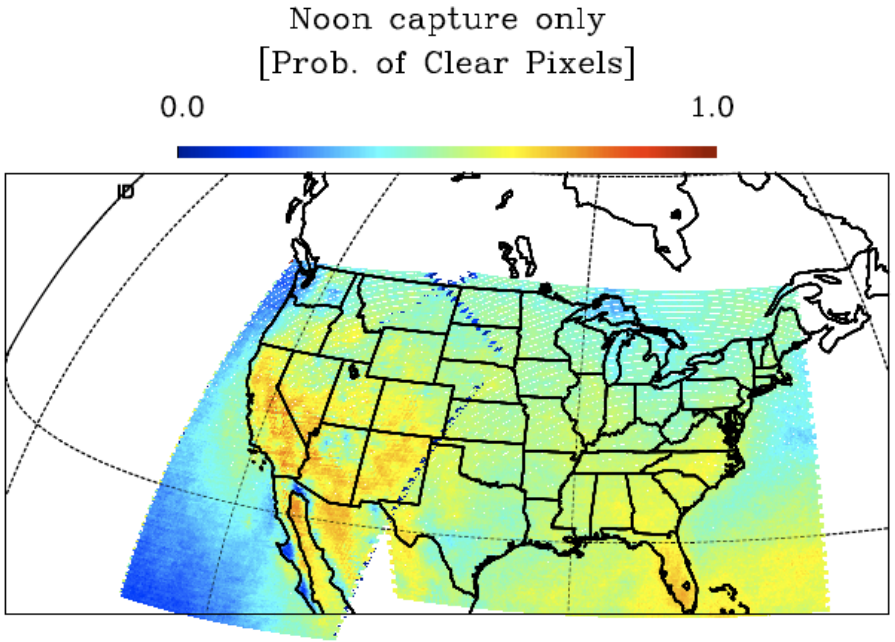
Probability of Observing Clear Sky Scenes

Geostationary (hourly observation)



Low-elevation orbit (daily observation)



J. Moisan, NASA/GSFC

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Improvement to Existing Measurements

- High temporal resolution measurements capture changes in pollutant distributions due to changing photochemistry, emissions and meteorology
- High spatial resolution measurements enable study of city to regional scale processes in North America
- Exploitation of multispectral observations improve information content in the vertical profile
- Measurements complementary to observations from ground-based, suborbital, LEO and other GEO satellite platforms

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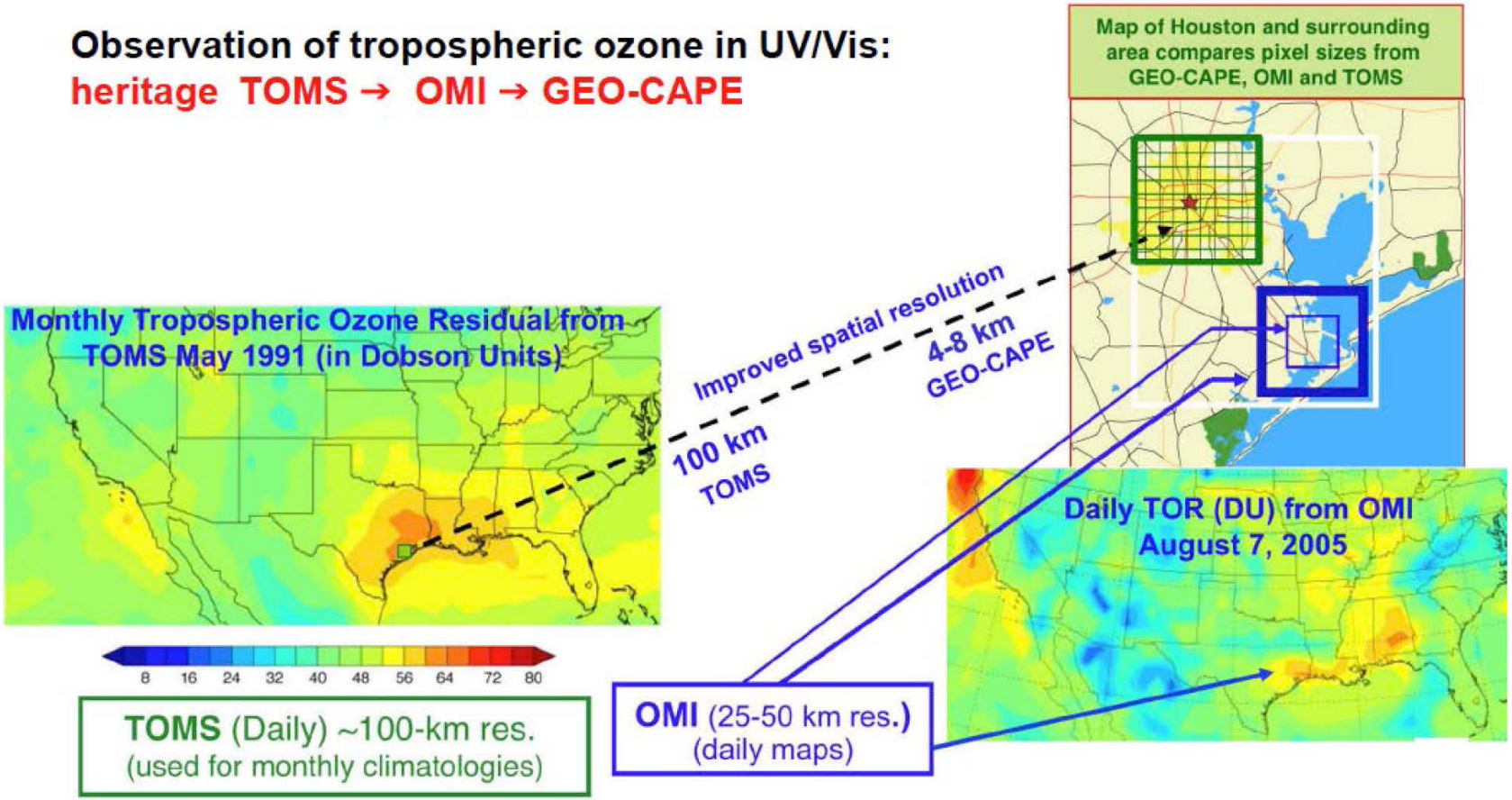
City Scale Analysis

Observation of tropospheric ozone in UV/Vis:
heritage TOMS → OMI → GEO-CAPE



Daniel Jacob, Harvard

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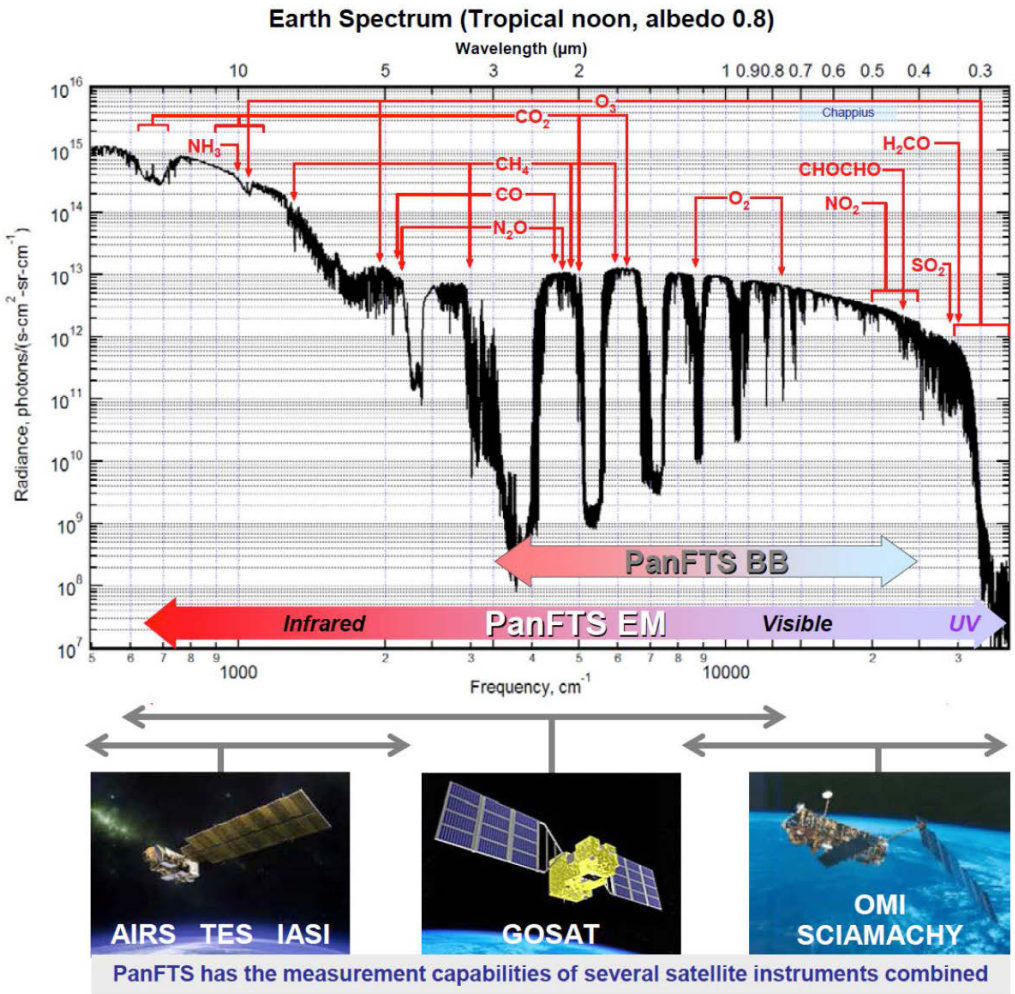
Why Multispectral?



Stan Sander, JPL

Wide spectral coverage and high spectral resolution enables retrieval of multiple chemical families of atmospheric species (O_2, O_3, O_4; H_2O, HDO; NO_2, NH_3, N_2O; CO, CO_2, CH_4, HCHO, CHOCHO, CH_3OH; SO_2, BrO)

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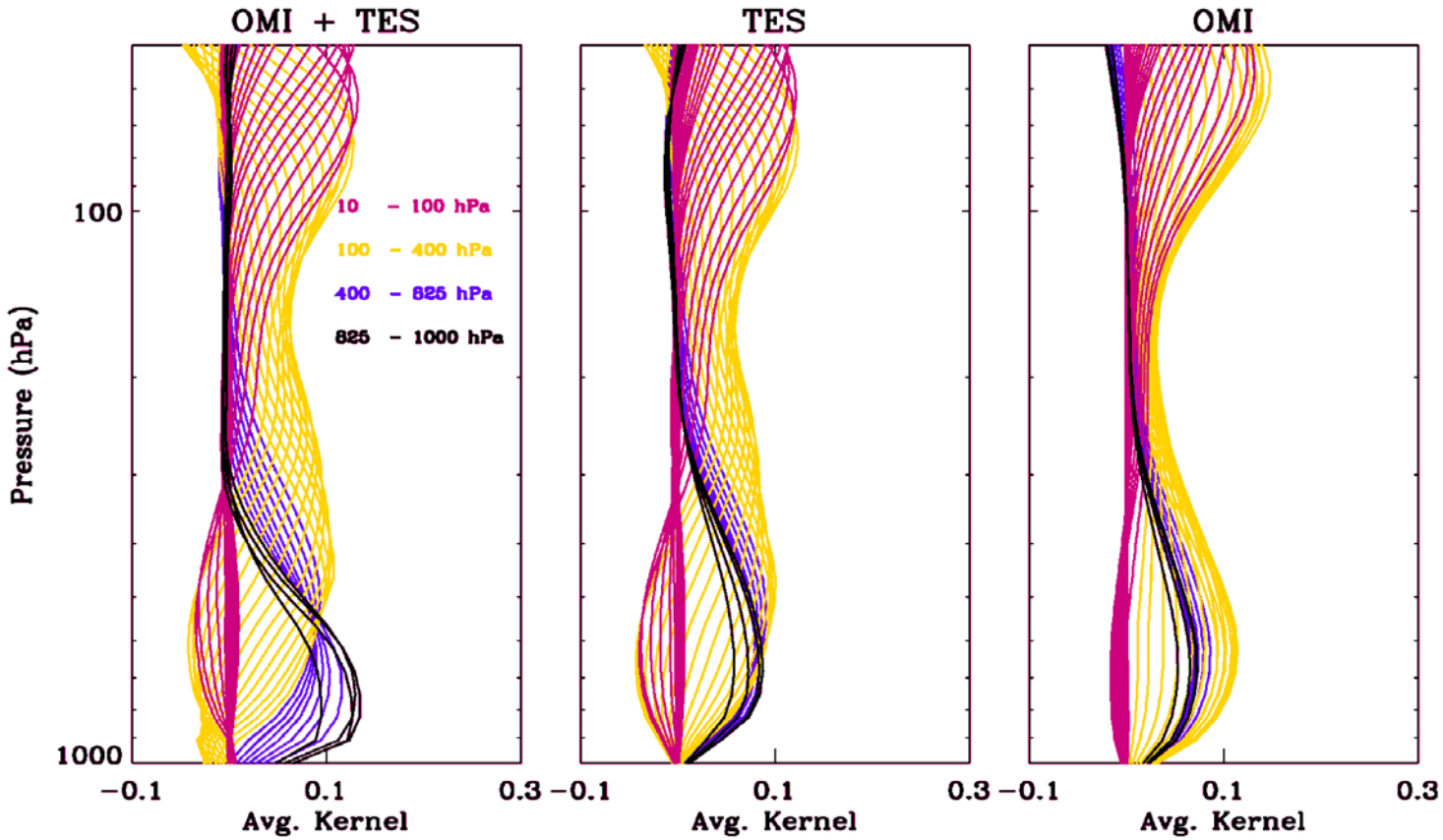
UV + TIR Measurements of Ozone



J. Worden et al. [GRL 2007]

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GEO-CAPE Measurement Requirements

O3	Hourly, SZA<70	9×10^{18}	0-2 km: 10 ppbv 2km–tropopause: 15 ppbv Stratosphere: 5%	Observe O3 with two pieces of information in the troposphere with sensitivity to the lowest 2 km for surface AQ; also transport, climate forcing
CO	Hourly, day and night	2×10^{18}	0-2 km: 20ppbv 2km–tropopause: 20 ppbv	Track anthropogenic and biomass burning plumes; observe CO with two pieces of information in the vertical with sensitivity to the lowest 2 km in daylight
AOD	Hourly, SZA<70	0.1 – 1	0.05	Observe total aerosol; aerosol sources and transport; climate forcing
NO2	Hourly, SZA<70	6×10^{15}	1×10^{15}	Distinguish background from enhanced/ polluted scenes; atmospheric chemistry

Spectral region : ***A to H***		Typical use
UV, Vis, TIR	O3	Provide multispectral retrieval information in daylight
SWIR, MWIR	CO	
UV	SO2, HCHO	Retrieve gas species from their atmospheric spectral signatures (typical)
SWIR,TIR	CH4	
TIR	NH3	
Vis	AOD, NO2, CHOCHO	Obtain spectral-dependence of AOD for particle size and type information

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Multispectral Retrievals of Ozone

- Rationale: Measurement requirements for GEO-CAPE go beyond current demonstrated capability

- Focus: Assess sensitivity (to amounts and vertical distribution) of trace gas retrievals to wavelength set used
  - Can needed vertical sensitivity be achieved with new combinations of wavelengths?

- Method: Radiative transfer simulations and Jacobian analysis (focus on ozone)

- Results published in Natraj *et al.* (2011), Atmos. Environ., 45, 7151-7165.

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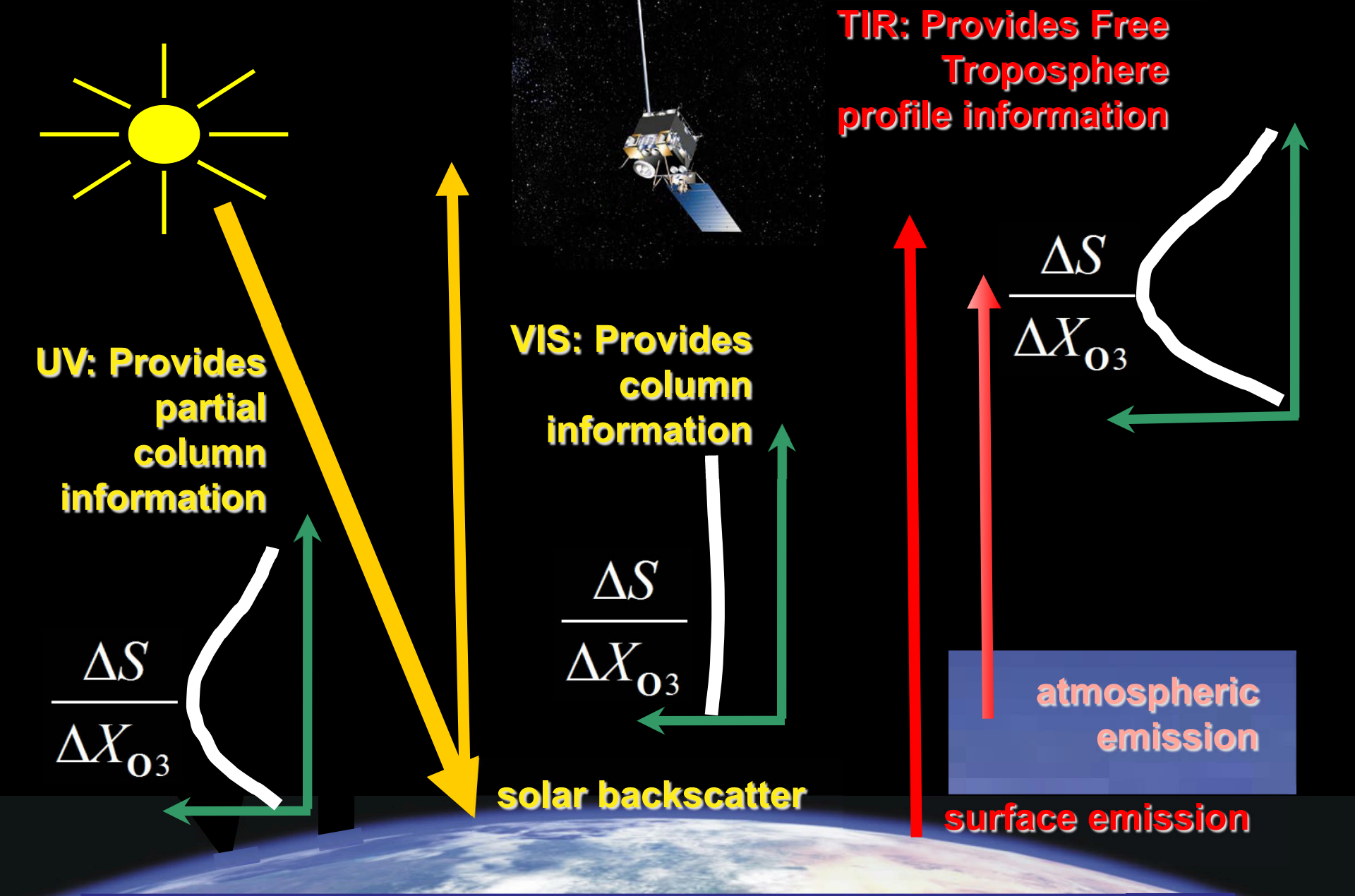
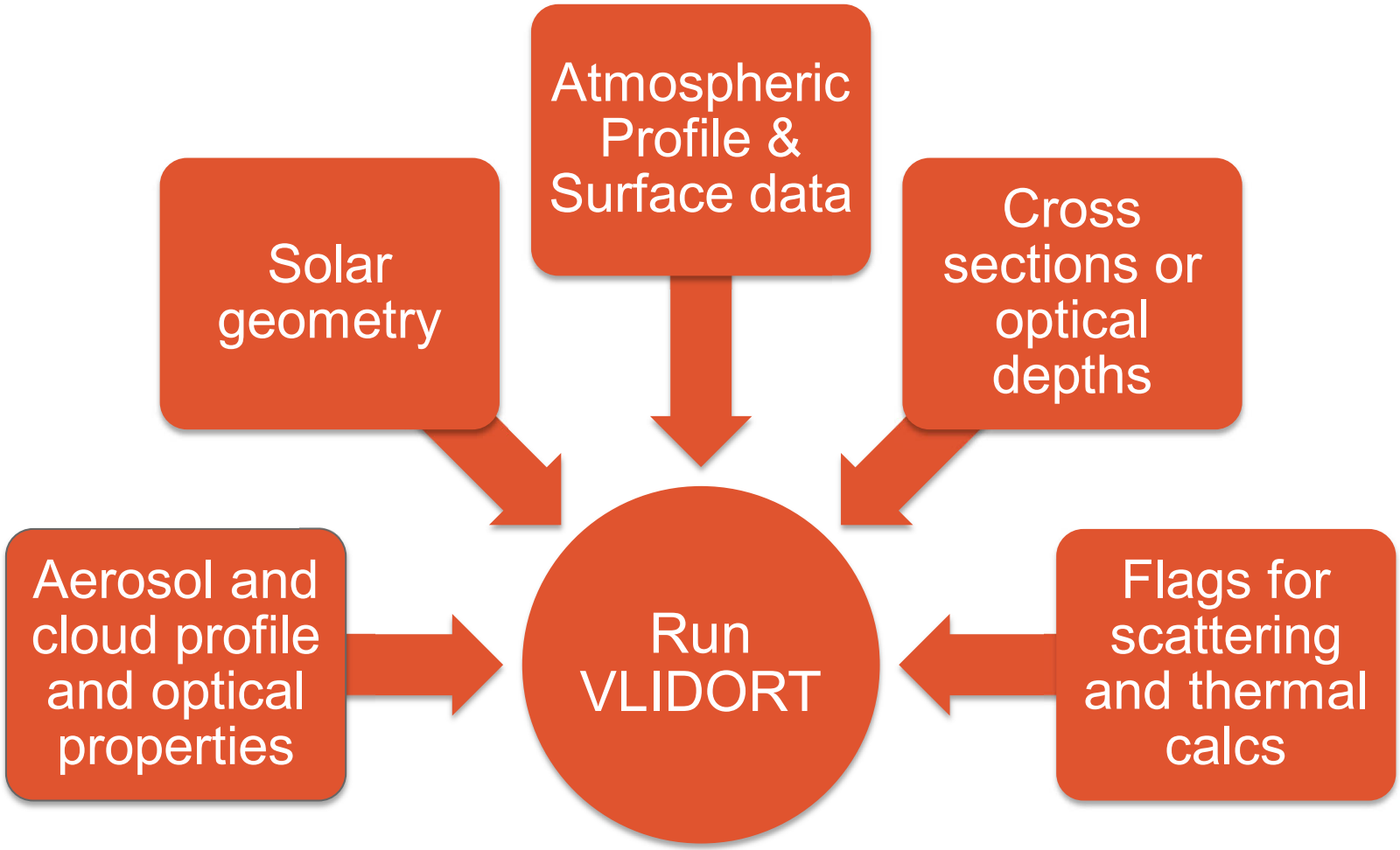


O_3 Multi-Spectral Remote Sensing

Image: NASA

RT Tool: VLIDORT



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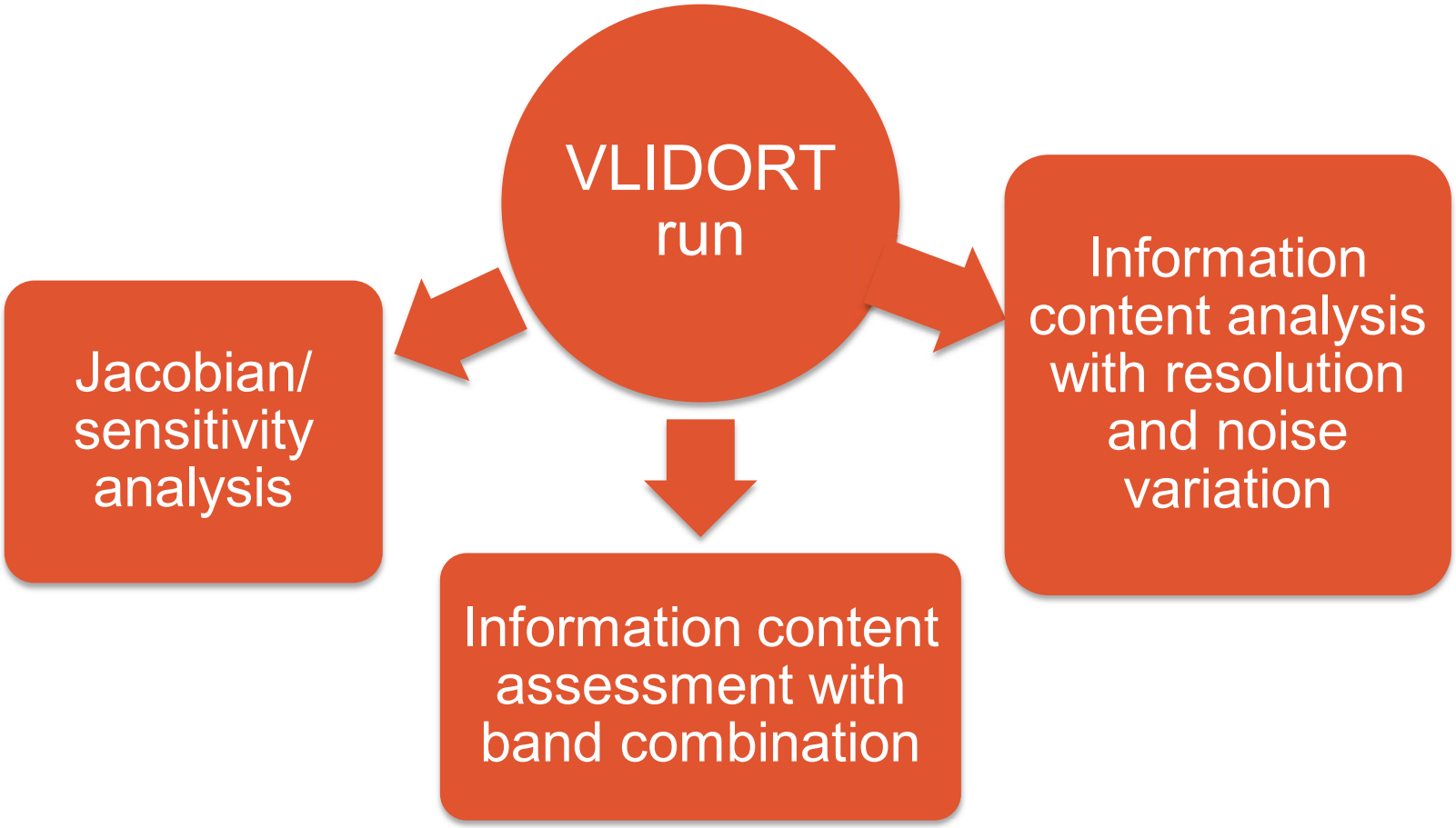
Error Analysis



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Spectral Regions

	UV/UVQ	VIS	MIR	TIR
Wavelength	290-340 nm	560-620 nm	3035-3055cm^{-1} 2780-2833cm^{-1}	980-1070 cm^{-1}
Spectral Resolution	0.4 nm	0.4 nm	0.18 cm^{-1}	0.1 cm^{-1}
Spectral Interval	0.1 nm	0.1 nm	0.0275 cm^{-1}	0.06 cm^{-1}
Signal to Noise Ratio	3 times of OMI	3 times of OMI	TIMS group 6×6 km^2 10s	3 times of TES

UVQ denotes polarized radiation

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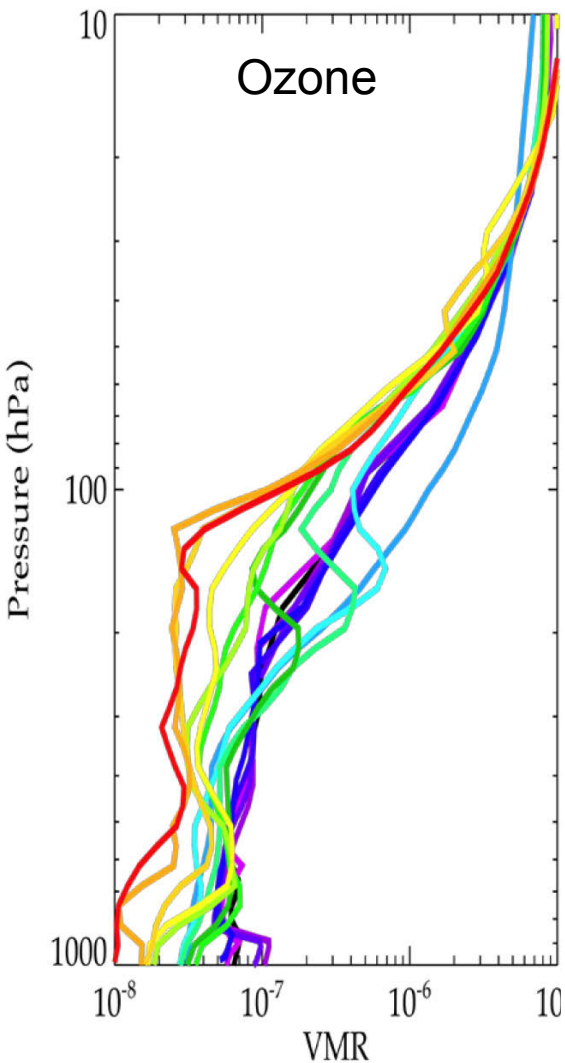
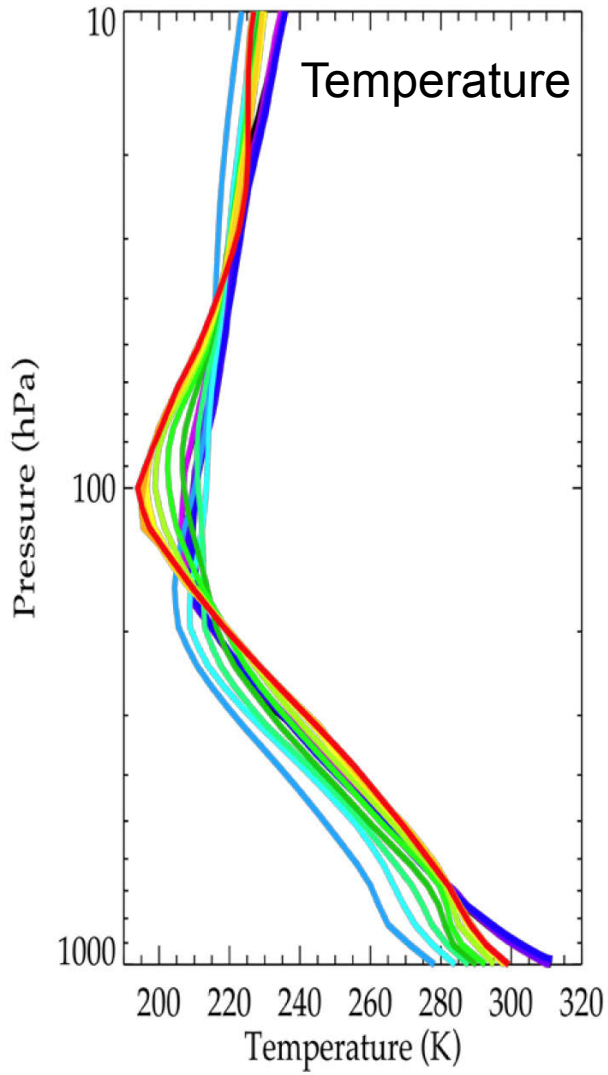
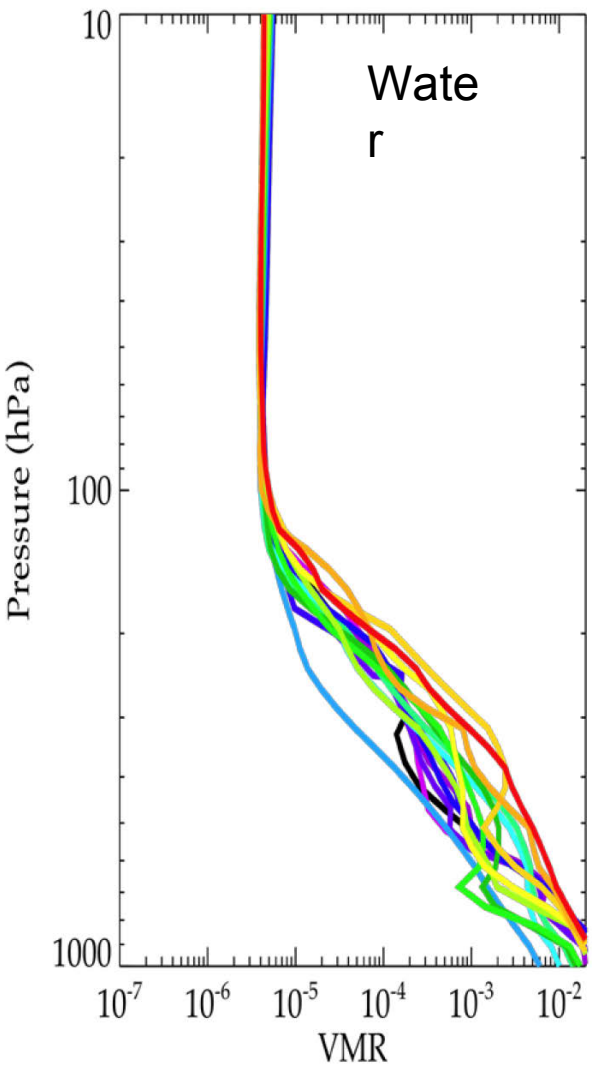
Profile Characteristics



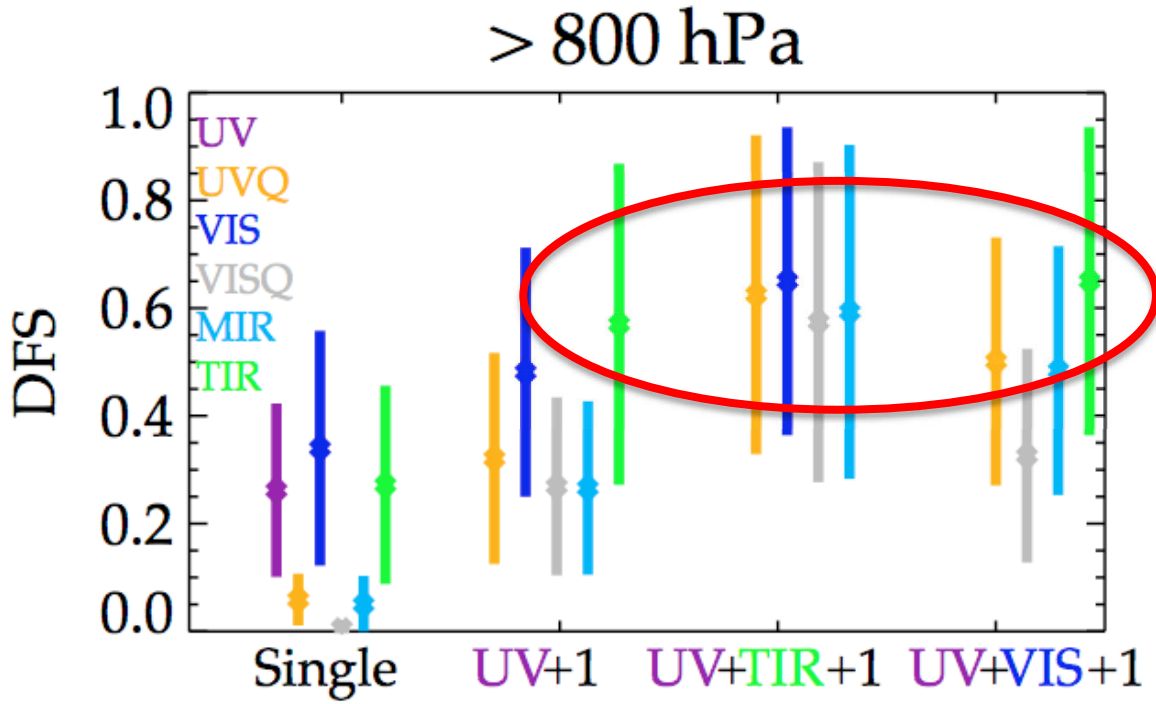




Degrees of Freedom for Signal

Clearly, there is a group that provides an improvement of sensitivity in the lowest layers

Note: use of Lambertian surface may underestimate power of polarized measurements.



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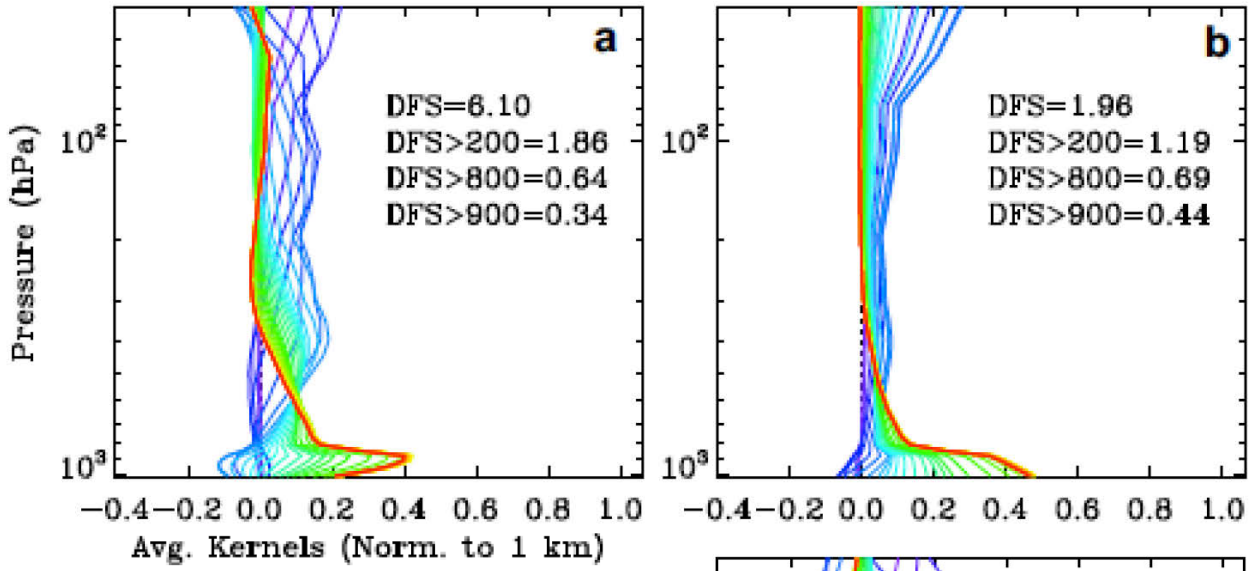
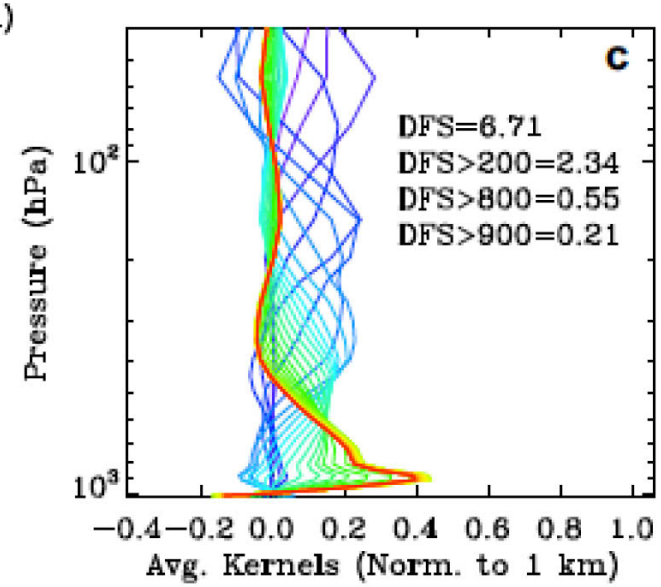
High Sensitivity Scenario (Single Band)

UV

VIS



Polluted atmosphere with an enhanced ozone layer of 80-100 ppbv below 900 hPa



TIR

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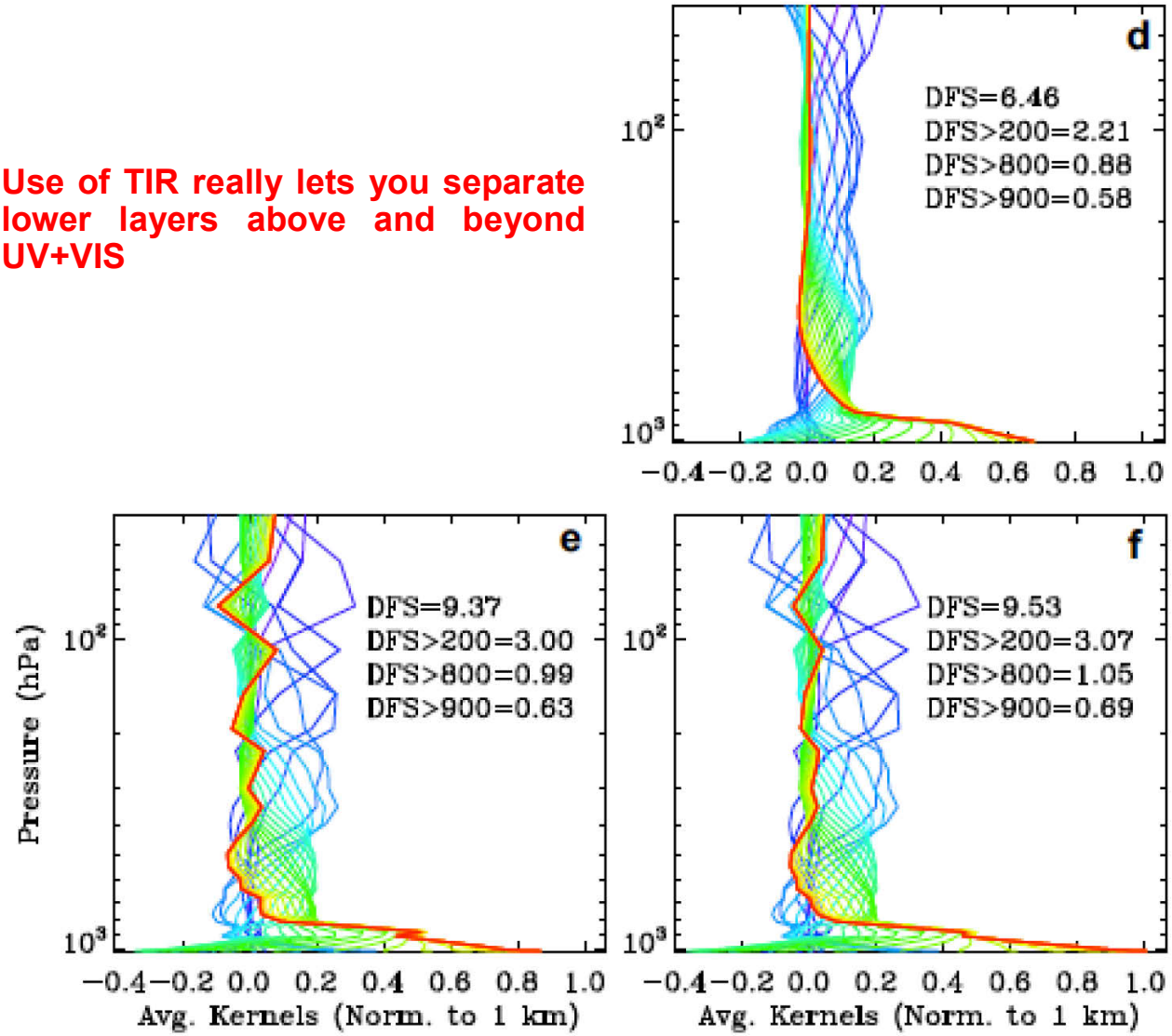
High Sensitivity Scenario (Joint Bands)

UV+VIS

Use of TIR really lets you separate lower layers above and beyond UV+VIS



UV+TIR

UV+VIS+TIR

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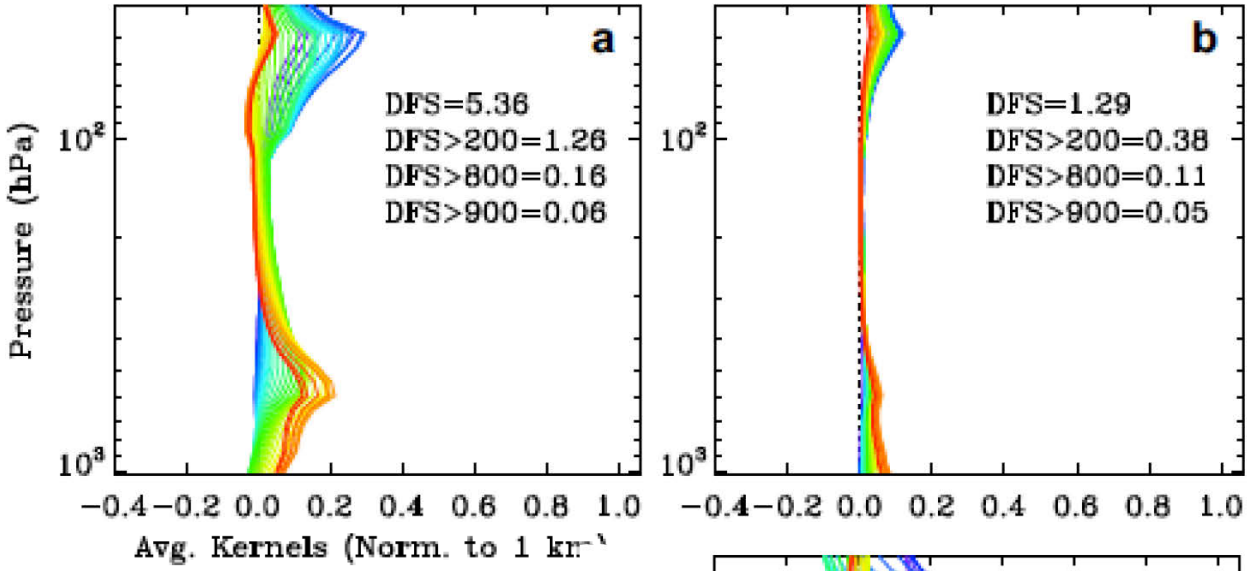
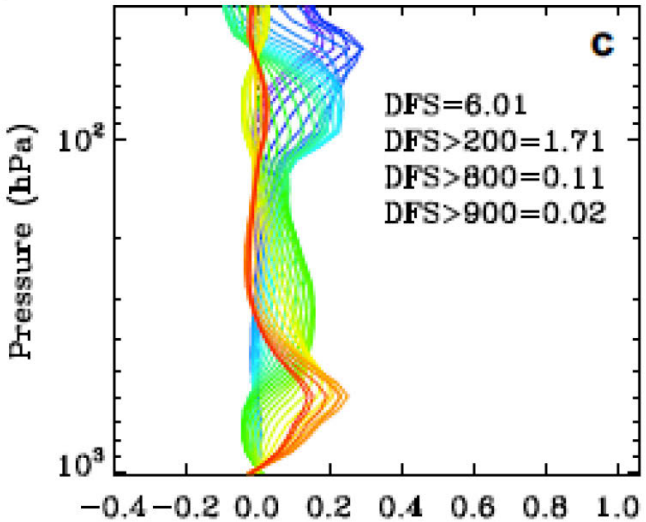
Low Sensitivity Scenario (Single Band)

UV

VIS



Clean atmosphere, high SZA, low temperature and thermal contrast



TIR

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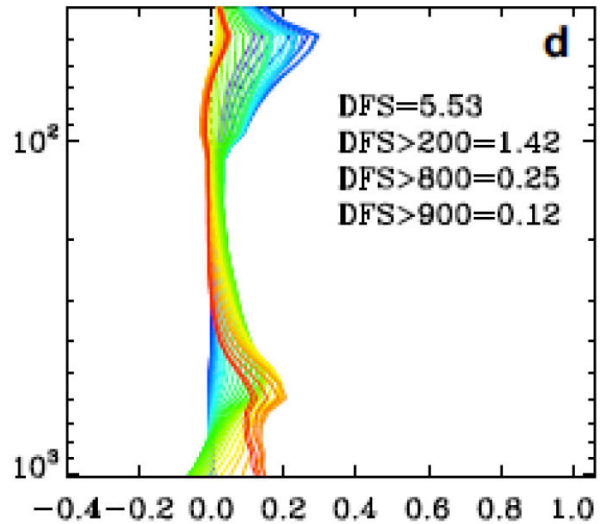
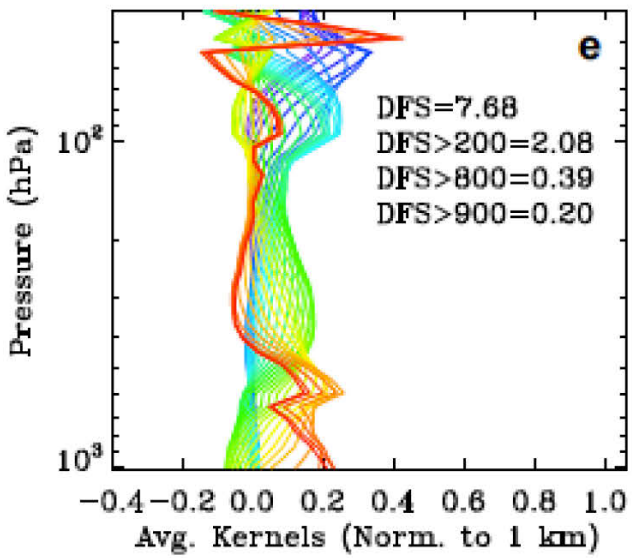
Low Sensitivity Scenario (Joint Bands)

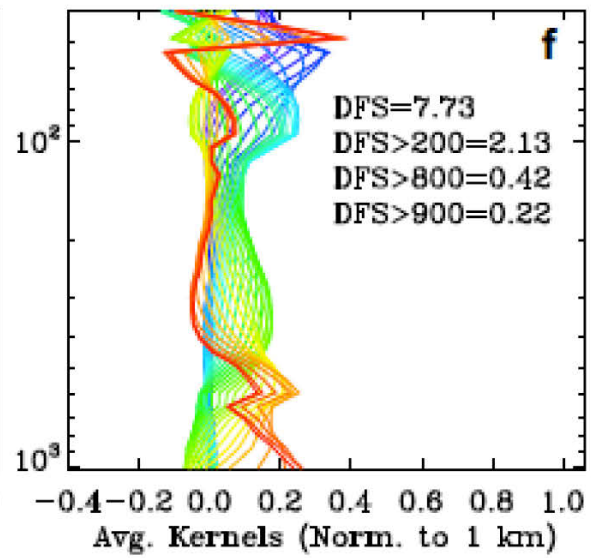
UV+VIS

Less dramatic change, but there is increased sensitivity in lower layers



UV+TIR





UV+VIS+TIR

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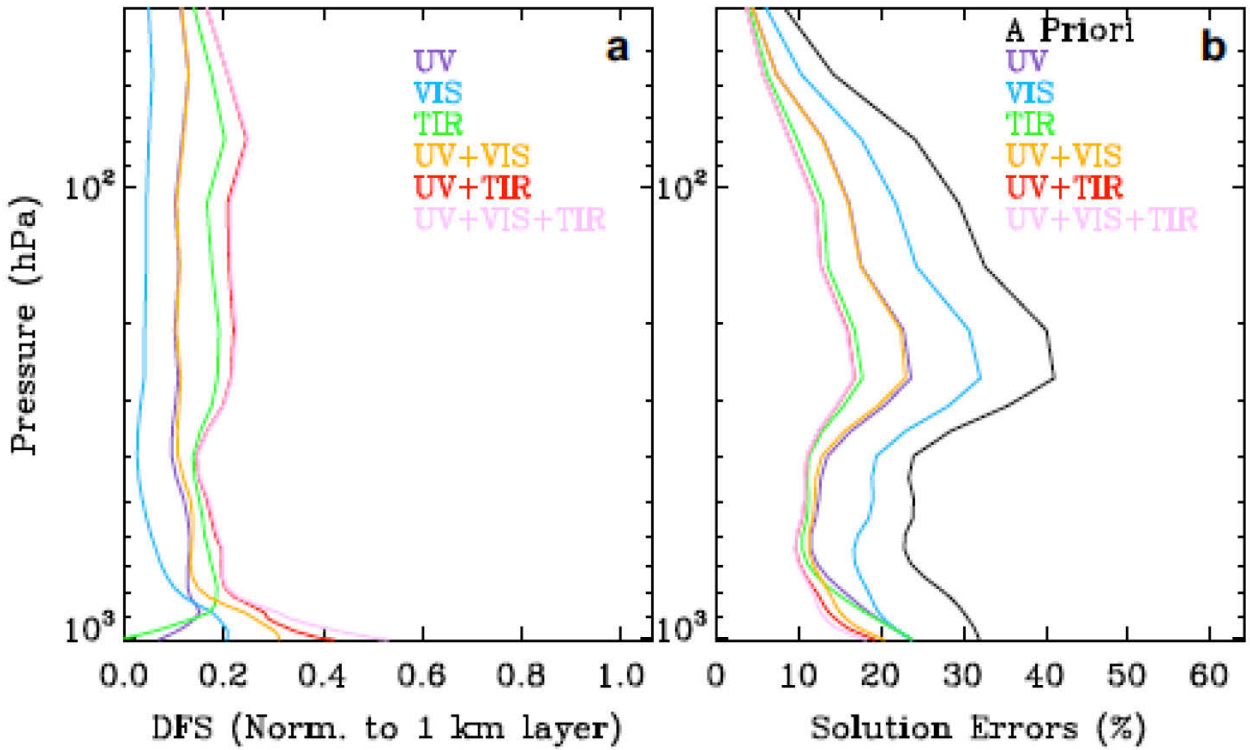
DFS and Solution Errors



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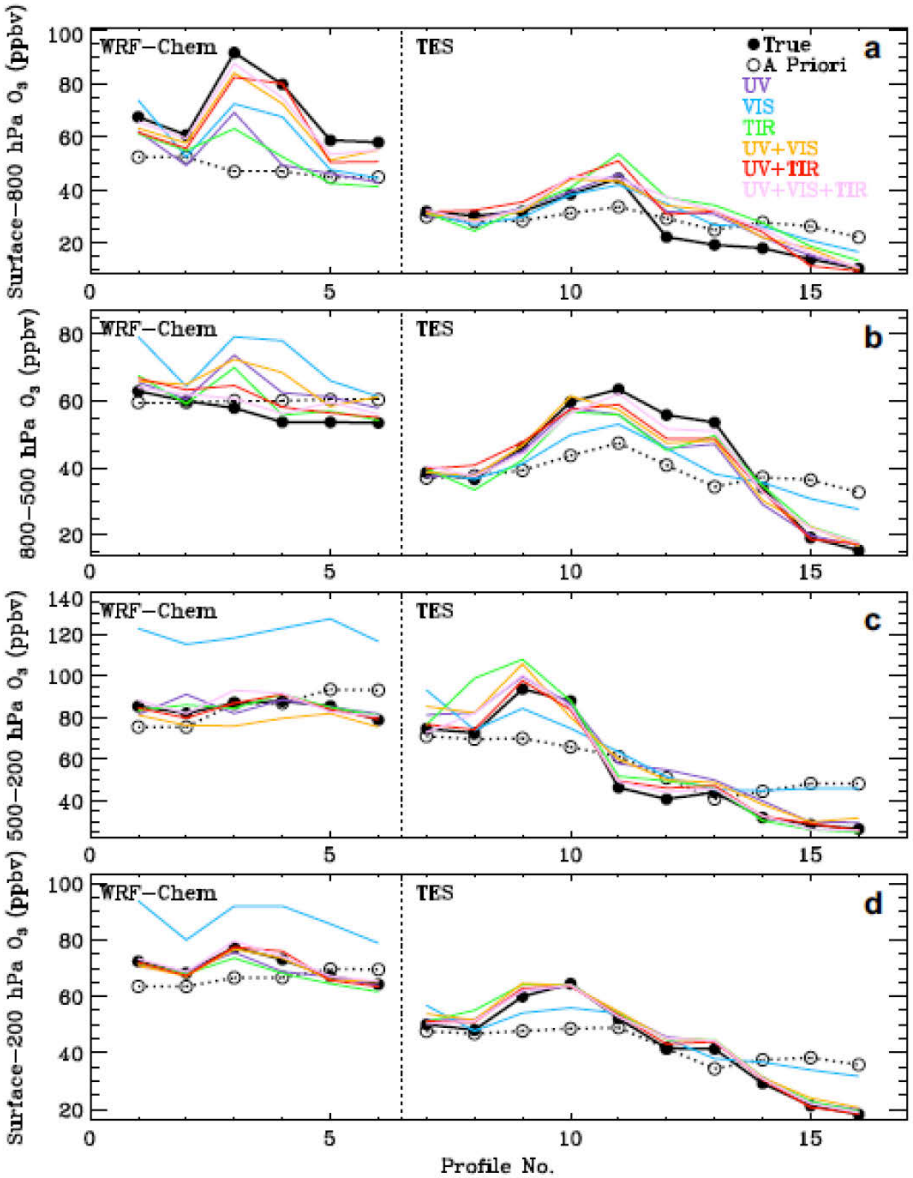
Ozone Retrievals



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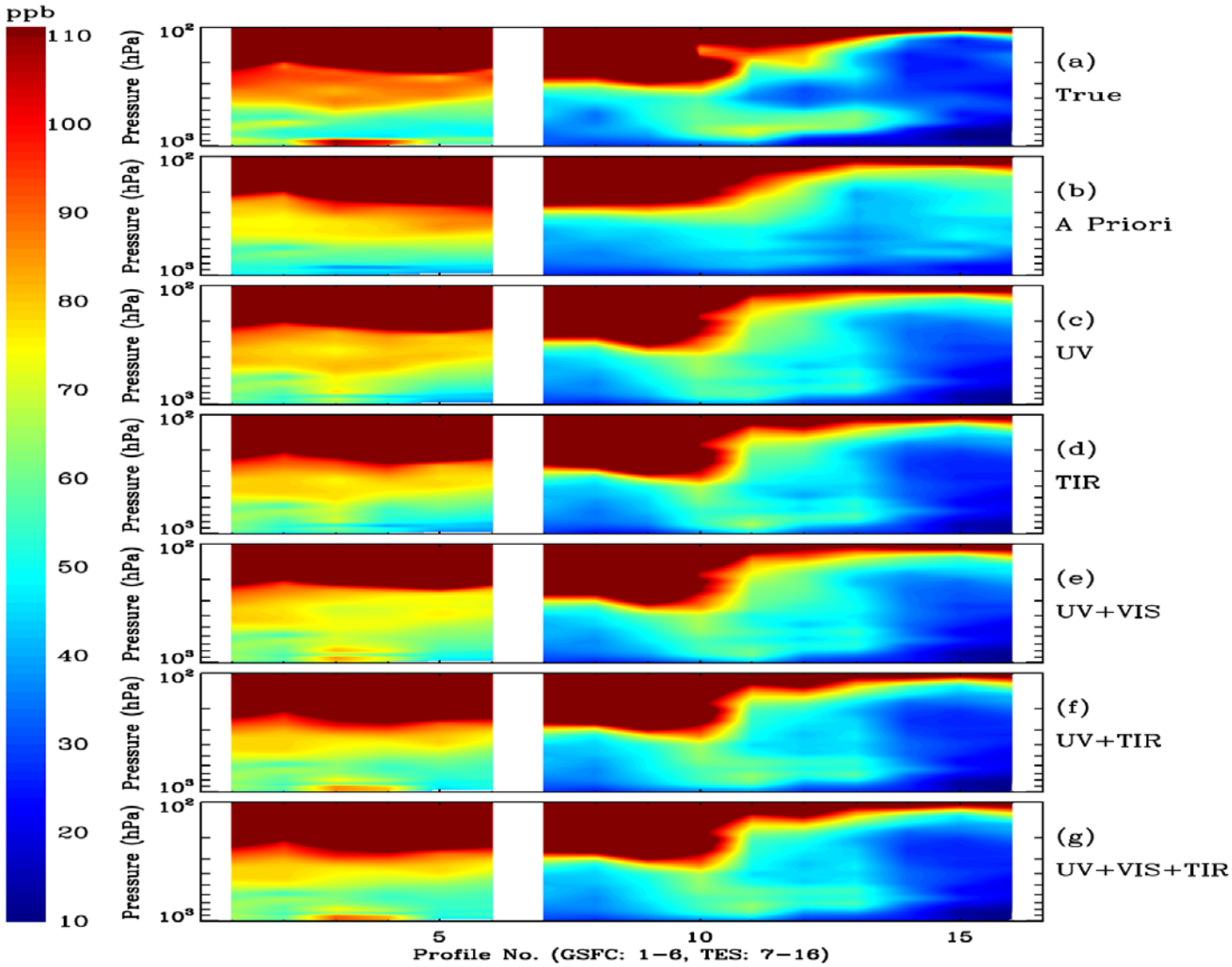
Another Perspective



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Other Issues

- Effects of spectral resolution, sampling interval and SNR
- Polarization and surface model
- Spectroscopy and calibration consistency
- Aerosols and clouds
- Realistic profiles and single scattering properties

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DFS for Varying Spectral Resolution and SNR

Trade-off runs		Total	>200 hPa	>800 hPa	>900 hPa
Twice better spectral resolution	UV	5.93	1.41	0.26	0.11
	VIS	1.69	0.79	0.34	0.19
	TIR	6.95	2.06	0.29	0.10
	UV + VIS	6.26	1.72	0.48	0.27
	UV + TIR	9.17	2.53	0.58	0.32
	UV + VIS + TIR	9.30	2.63	0.66	0.38
Twice worse spectral resolution	UV	5.79	1.36	0.25	0.11
	VIS	1.69	0.79	0.34	0.19
	TIR	5.93	1.85	0.24	0.08
	UV + VIS	6.13	1.68	0.47	0.27
	UV + TIR	8.38	2.36	0.54	0.29
	UV + VIS + TIR	8.54	2.48	0.63	0.37
Four times worse spectral resolution	UV	5.55	1.27	0.24	0.10
	VIS	1.69	0.79	0.34	0.19
	TIR	5.55	1.72	0.21	0.06
	UV + VIS	5.91	1.61	0.47	0.27
	UV + TIR	8.08	2.27	0.51	0.28
	UV + VIS + TIR	8.26	2.41	0.61	0.35
Half SNR	UV	5.12	1.16	0.19	0.08
	VIS	1.38	0.54	0.22	0.12
	TIR	5.37	1.67	0.20	0.06
	UV + VIS	5.35	1.37	0.34	0.19
	UV + TIR	7.49	2.08	0.43	0.23
	UV + VIS + TIR	7.58	2.15	0.49	0.27
Double SNR	UV	6.66	1.65	0.33	0.15
	VIS	2.04	1.06	0.45	0.25
	TIR	7.65	2.28	0.37	0.15
	UV + VIS	7.12	2.05	0.62	0.37
	UV + TIR	10.14	2.83	0.70	0.41
	UV + VIS + TIR	10.33	2.97	0.81	0.49

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DFS for Different Surface Models

Surface Model		Total	>200 hPa	>800 hPa	>900 hPa
Lambertian	UV	5.89	1.39	0.26	0.12
	UVQ	4.64	0.76	0.05	0.01
	UVPOL	2.26	0.99	0.18	0.08
	UV + UVQ	6.54	1.63	0.32	0.16
Ocean BPDF (same viewing geometry)	UV	5.92	1.42	0.27	0.13
	UVQ	4.79	0.90	0.12	0.05
	UV + UVQ	6.62	1.77	0.42	0.23
Ocean BPDF (sun glint)	UV	6.18	1.54	0.37	0.19
	UVQ	5.13	1.08	0.27	0.14
	UV + UVQ	6.93	1.91	0.52	0.30

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Spectroscopy and Calibration Consistency

- Discrepancy between UV and TIR spectroscopic parameters
- Laboratory intercomparisons show TIR-UV differences of 5.5%
- Intercomparisons of ground-based measurements show 4.5% differences
- Satellite retrievals also show high bias for TIR compared to UV
- HITRAN should address this; if not FM corrections may be necessary
- Radiometric calibration consistency among different spectral regions

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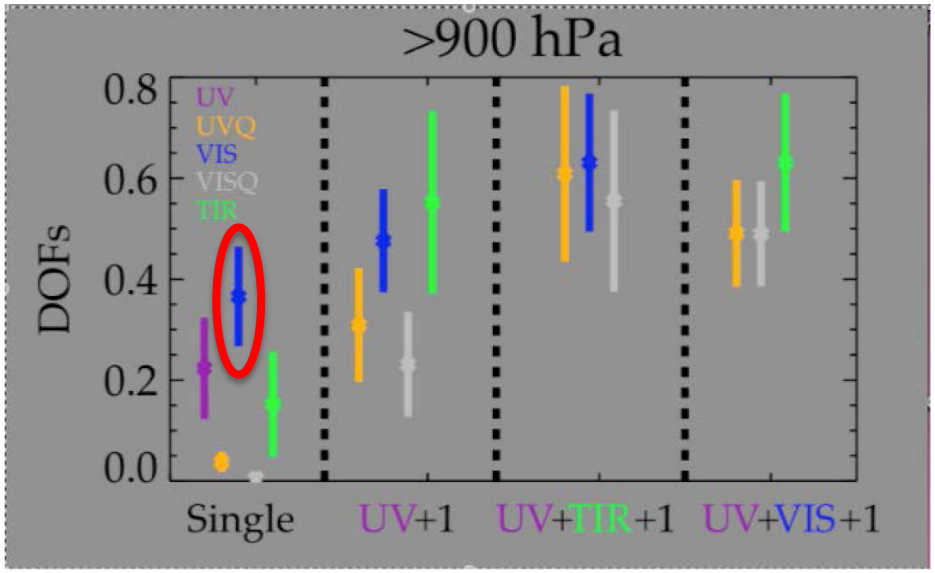
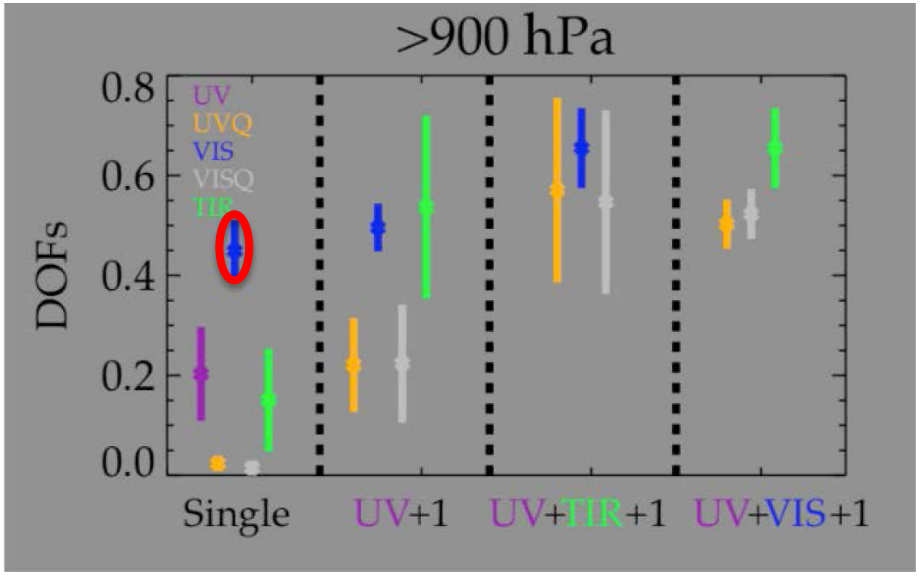
Aerosols: First Results

Clear Sky



Aerosols



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Conclusions

- Multi-spectral retrievals (UV+VIS, UV+TIR, UV+VIS+TIR) improve sensitivity to the variability in near-surface O_3 by a factor of ~2-3 over those from UV or TIR alone.
- Multi-spectral retrievals provide the largest benefit when there is enhanced O_3 near the surface.
- Combining all 3 wavelengths (UV+VIS+TIR) provides the greatest sensitivity below 900 hPa, with a 36% improvement over UV+VIS and a 16% improvement over UV+TIR.
- The impacts of clouds and aerosols are being assessed.

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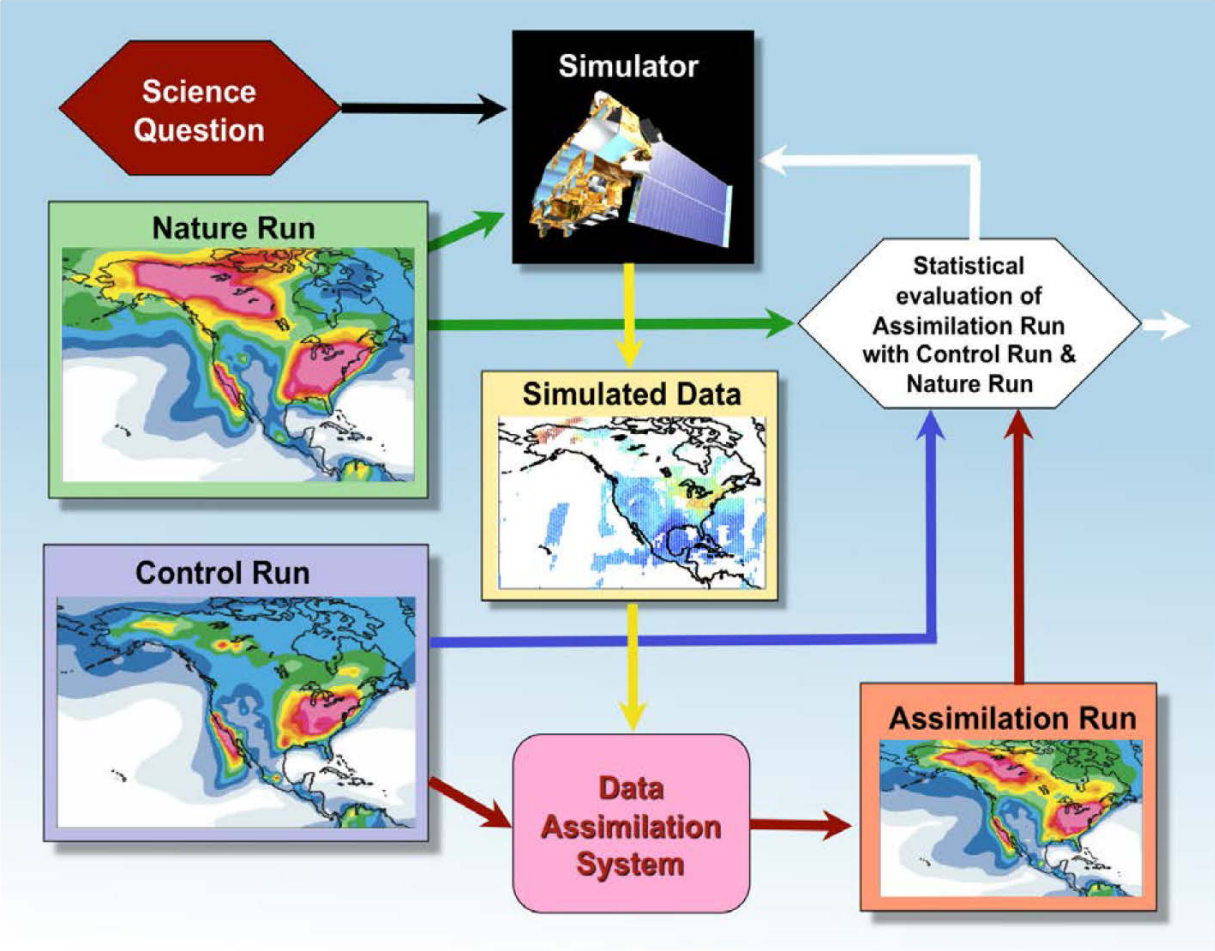
Observation System Simulation Experiments

Observation System Simulation Experiments (OSSEs) provide a practical way to map science requirements through measurement requirements onto instrument requirements.



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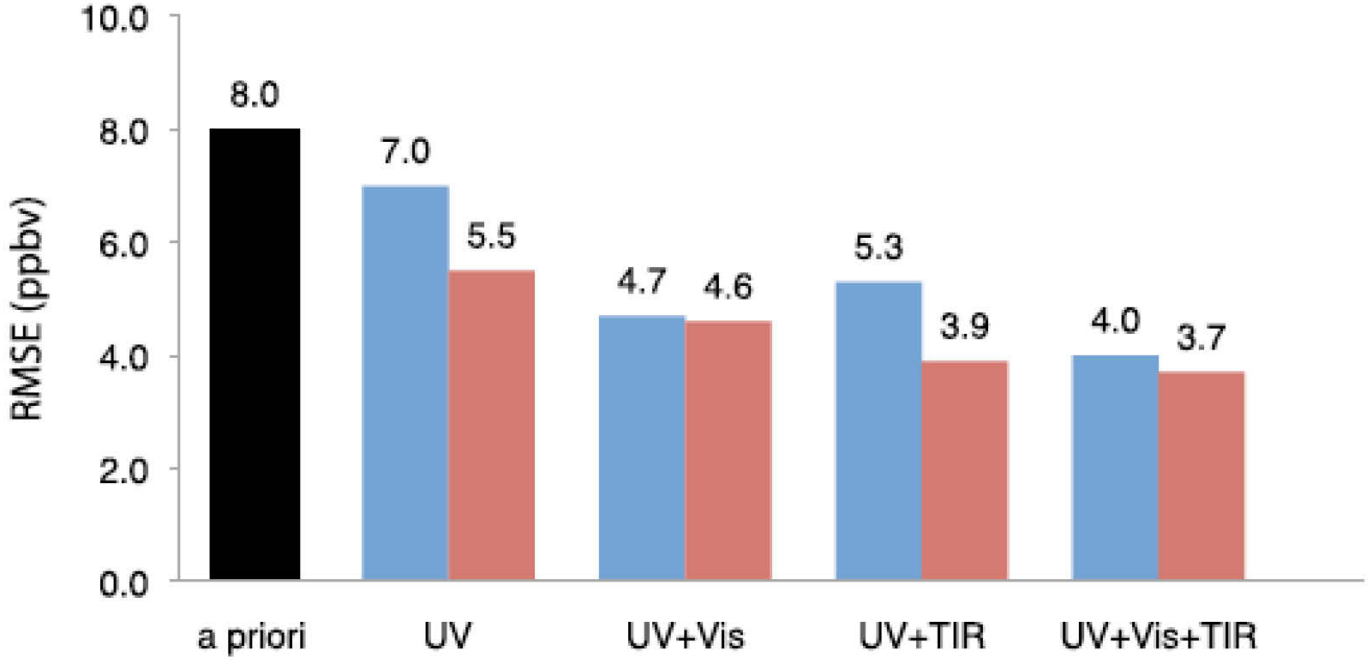
Preliminary OSSE Results

Root-mean-square error (RMSE) of data assimilation system for daily maximum 8-h average (MDA8) surface ozone before (*a priori*) and after assimilation of synthetic GEO-CAPE data



Zoogman et al. [Atmos. Environ. 2011]

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Improvement to Existing Measurements

- High temporal resolution measurements capture changes in pollutant distributions due to changing photochemistry, emissions and meteorology
- High spatial resolution measurements access city scale with continuous full coverage of North America
- Exploitation of multispectral observations improve information content in the vertical profile
- Measurements complementary to observations from ground-based, suborbital, LEO and other GEO satellite platforms

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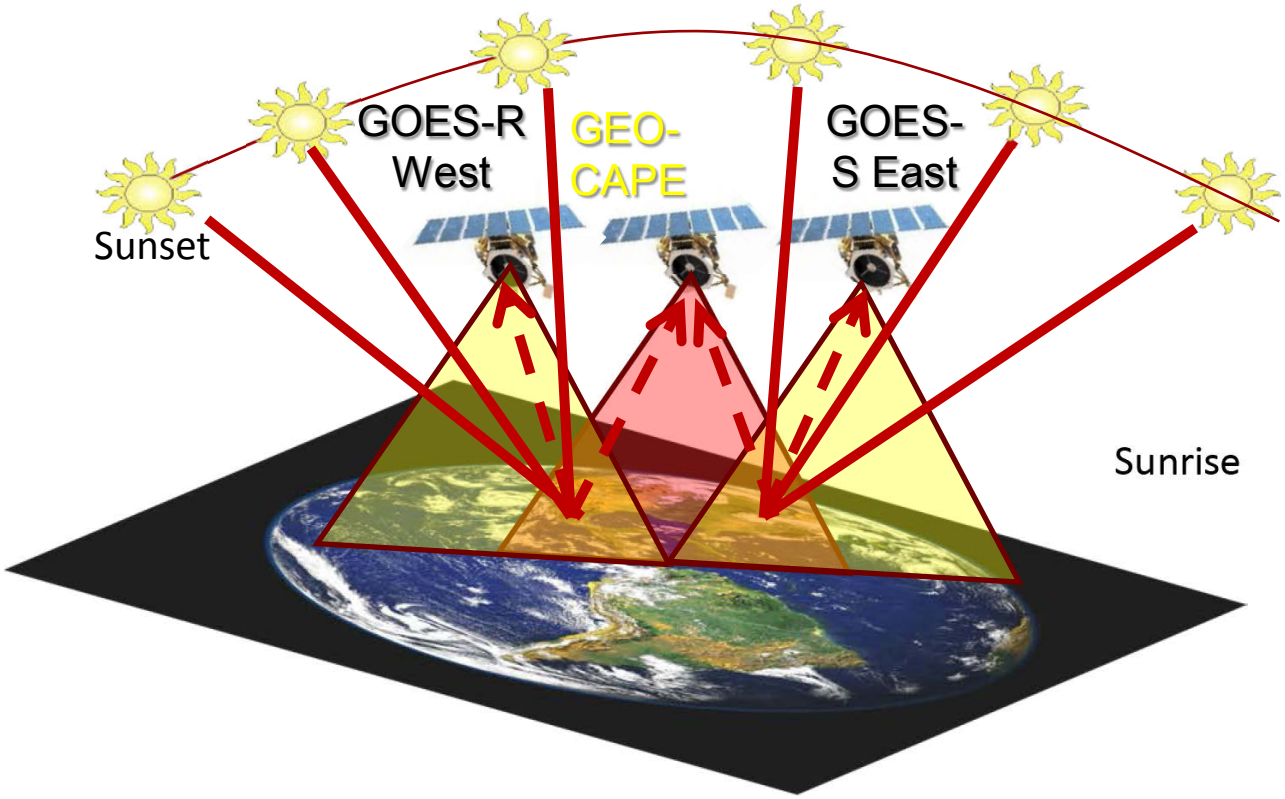
GEO-CAPE and GOES-R/S Synergy

Joint retrieval from observations collected from dual viewing angles and multiple scattering angles to characterize particle shape and derive aerosol plume speed and stereo height



Jun Wang, U. Nebraska-Lincoln

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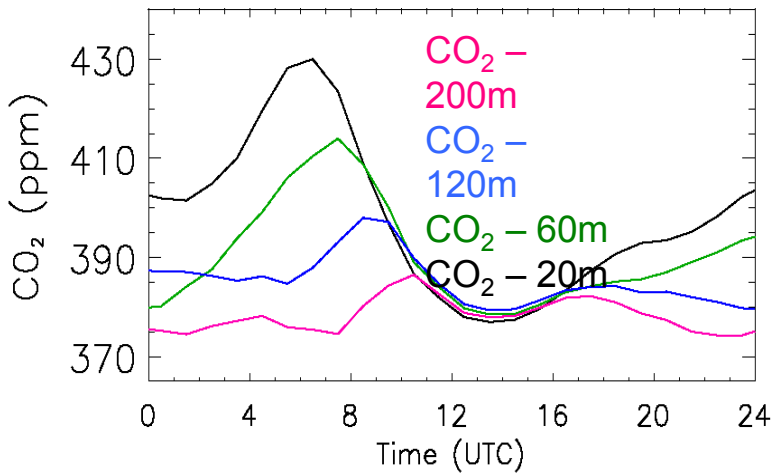
Another Application: Diurnal Profiling of CO_2

Pino et al. (2010)

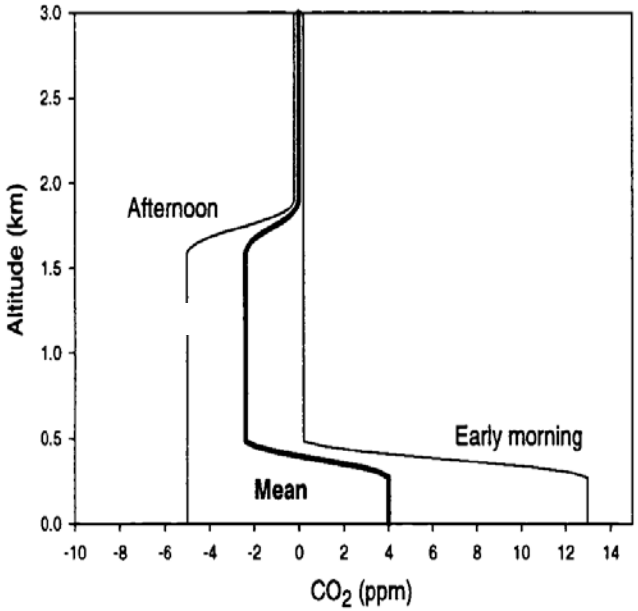


The diurnal cycle of CO_2 reflects emissions, uptake by the biosphere, and atmospheric mixing

DAYTIME
- **Plants take up CO_2**
- **Turbulence mixes the PBL**
- **Low CO_2 throughout PBL**

NIGHTTIME
- **Little turbulent mixing**
- **Plants are respiring**
- **High CO_2 near the surface**

Stephens et al. (2000)



Surface measurements cannot distinguish between changes in BL CO_2 due to vertical transport and sources/sinks.

Profile measurement at a single time cannot identify diurnal changes in vertical transport.

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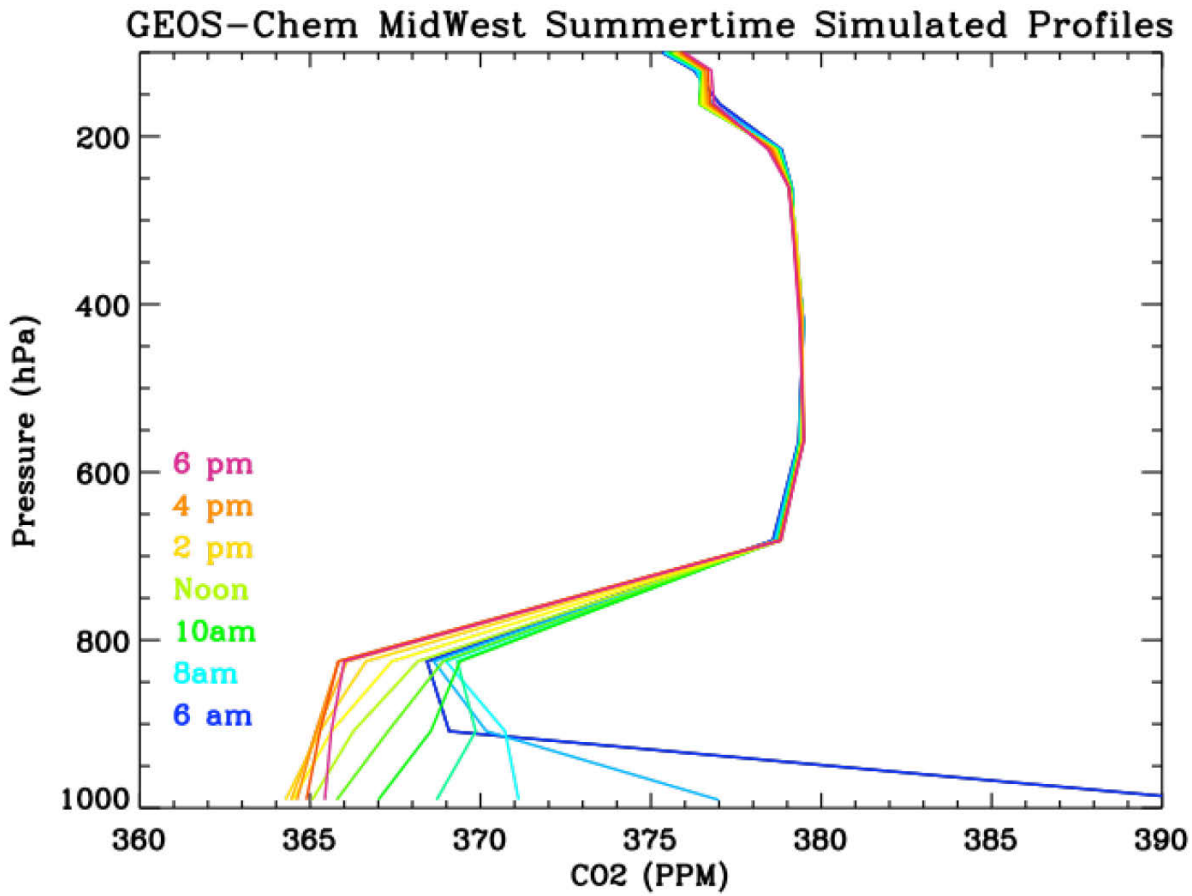
Analysis of Expected Sensitivity for CO_2



Randy Kawa, GSFC

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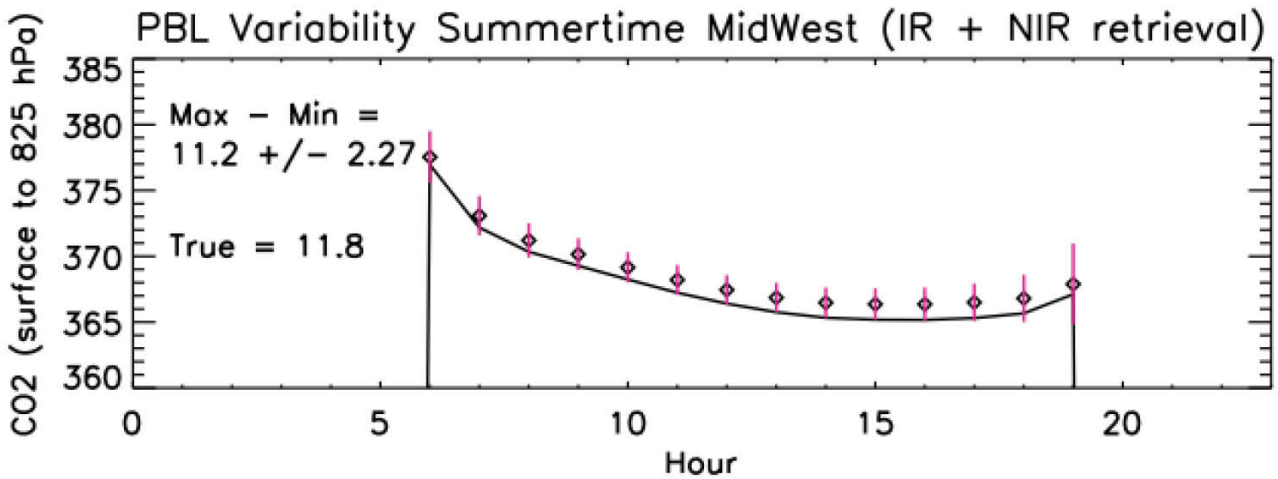
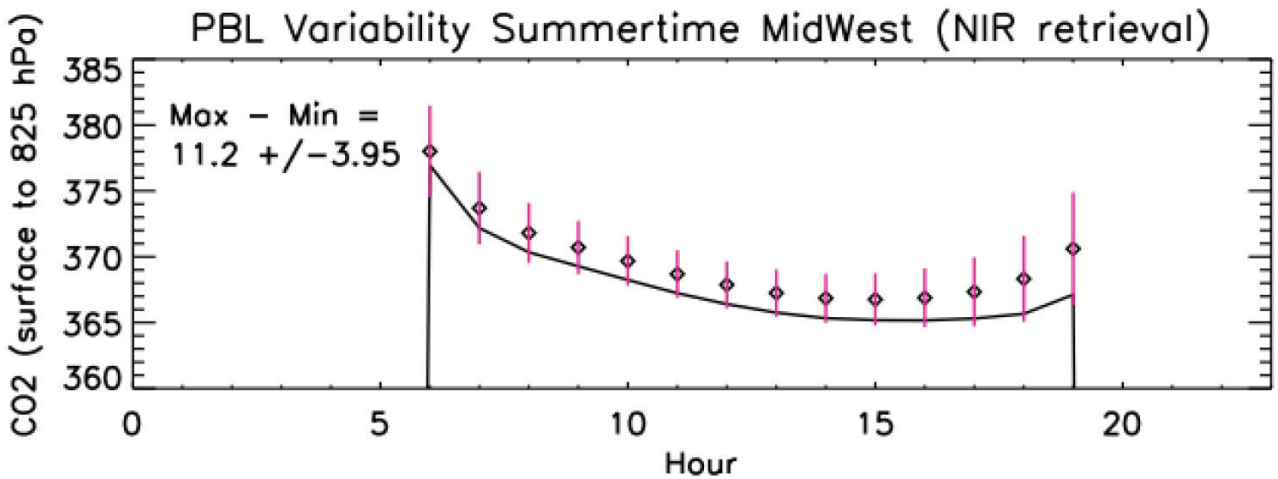
Characterizing PBL Variability





Combined NIR and IR can correctly characterize the PBL variability

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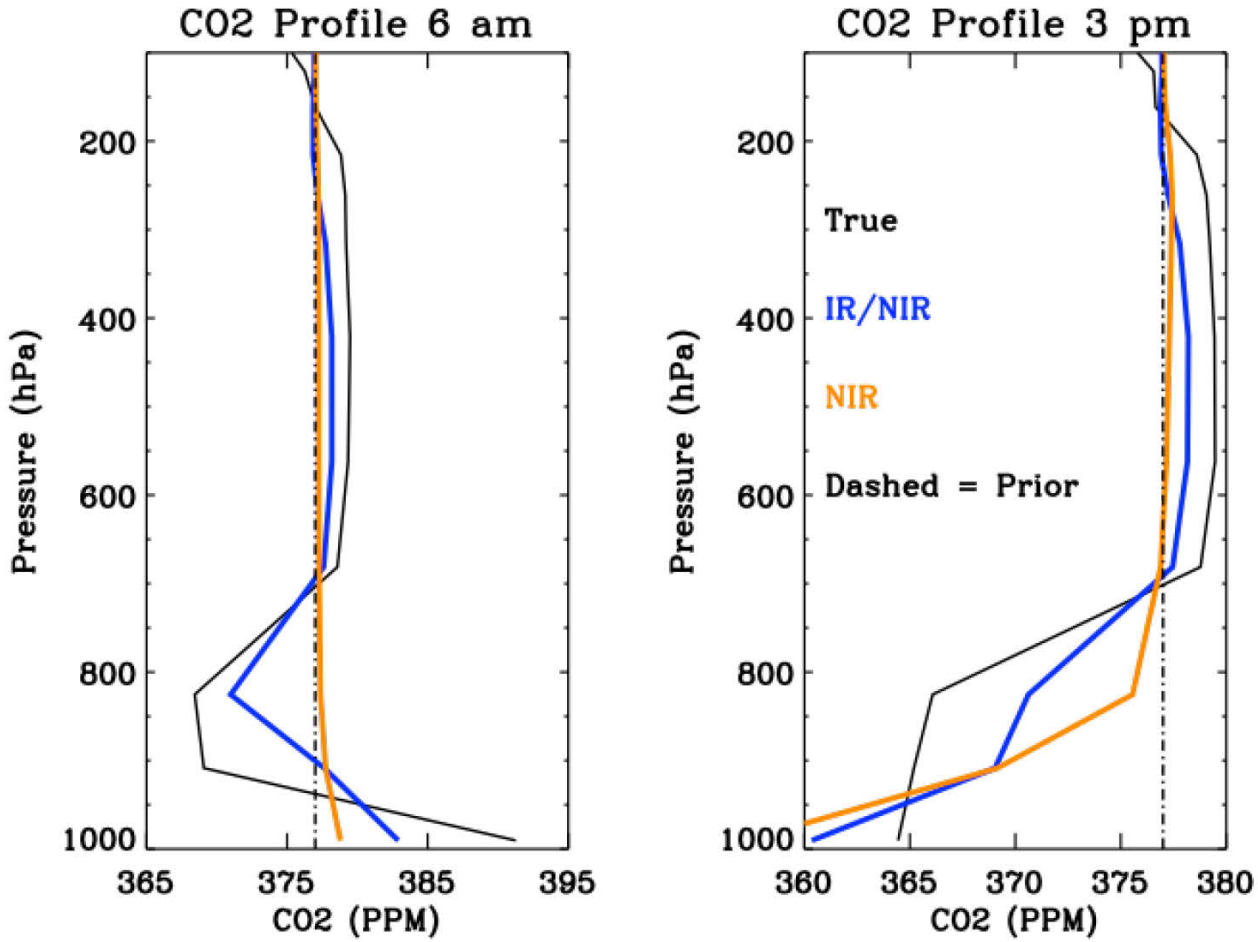
CO_2 Profiling with Combined Wavelengths



Combined wavelengths provide improved capability to measure vertical structure

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Conclusions

- Our understanding of sources and sinks of CO_2 is limited by the number of observations, as well as uncertainty in vertical transport.
- Geostationary satellites could be used to make hourly observations.
- Multispectral retrievals improve the vertical sensitivity for CO_2 with discrimination of the free troposphere and boundary layer.
- A viable instrument design – GeoFTS – has been developed for this goal.
- Advancements are being made in the instrument technology and retrieval framework.

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Backup Slides

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Science Traceability Matrix

Mission Objectives	Measurement Requirements	Mission Requirements	Instrument Requirements	Mission Concept	Ancillary Requirements
Quantify spatial and temporal emissions of ozone and aerosol precursors	NO_2 and HCHO tropospheric partial column, CO with sensitivity in the boundary layer (BL)	Cover US and adjoining regions Simultaneous constituent measurements Continuous daytime coverage	High spatial resolution (5 km) to resolve source locations and sample between clouds; high precision detection (SNR>1000:1) CO measurement in reflected sunlight	Instruments in geo orbit continuously scan populous North America coast-to-coast. UV/Visible spectrometer measures O_3, NO_2, HCHO, SO_2, and aerosol column density; plus CO, O_3 detectors for BL and free trop	Surface in situ and remote sensing monitoring network; in situ aircraft and balloon mmts; stratospheric O_3, NO_2, and dynamics Inverse models for source inference.
Measure distributions of O_3, aerosol, and precursors at high spatial and temporal resolution over the US and surrounding regions.	O_3 partial column; O_3 with sensitivity in PBL; aerosol optical depth Measure diurnal changes of constituents	Map sunlit earth at near-nadir Hourly sampling frequency in polluted regions View upwind and downwind of the continent Day/night CO and O_3 sampling	Spectrally resolved, high-SNR reflected UV/Vis radiances O_3 measurement in thermal emission bands (and/or reflected sunlight) CO measurement in thermal emission bands	Ability to stare at target region from geo enables high-resolution ground sampling at high SNR. Hourly or better sampling frequency during daytime for UV/Vis, and during day and night for free-troposphere CO and O_3.	GOES T, H_2O profiles, surface, and upper-air weather observations; accurate, detailed meteorological analyses 3-D global chemistry-transport model integrations Process-oriented research field campaigns
Track transport of aerosol and gases into, across, and out of NA; including large episodic releases from environmental disasters	CO in mid-troposphere; O_3, NO_2 tropospheric partial columns; aerosol optical depth, SO_2 column density				
Characterize regional air quality for model evaluation, assessment, and forecasting.	O_3, NO_2, HCHO, CO partial columns; O_3 with sensitivity in PBL; aerosol optical depth	Accommodate large data collection and retrieval rates; 2-5 yr mission lifetime	Continental field of regard; hourly temporal resolution in polluted regions	High-resolution, frequent sampling maximizes lower troposphere data in presence of clouds	Data assimilation methodology; Regional mesoscale chemistry-transport modeling

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Aerosols: Profiles and Properties

- 5 aerosol types: black carbon, organic carbon, coarse seasalt, fine seasalt, sulfate
- AOD profiles at 300 nm, 400nm, 600 nm and 999 nm (Courtesy: Ken Pickering)
- MODIS total column AOD at 550 nm (Courtesy: Omar Torres)
- RH profiles (Courtesy: Melanie Follette-Cook)
- Single scattering properties

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