Assessing Information Content of CLARREO Measurements to Size-Dependent Dust Emissions: An OSSE Study

Xiaoguang (Richard) Xu
Jun Wang
Yi Wang
University of Nebraska-Lincoln, now in The University of Iowa

Daven Henze
Li Zhang
University of Colorado-Boulder

CGRER SDT Meeting at National Institute of Aerospace
Nov 29 – Dec 1, 2016

Image acquired on September 23, 2011 from MODIS
Outline

• Introduction and research objectives
• The design of observing system simulation experiments (OSSEs)
• Synthetic CLARREO observations
• Information content of synthetic CLARREO RS and IR spectra to size-dependent dust optical depths
• CLARREO OSSEs on size-resolved dust emissions
• Conclusion and future efforts
How are dust emissions modeled?

Inputs: Wind speed, friction velocity \((u_*)\), soil texture and moisture, Land surface properties

Ideal threshold wind friction \(v\):
\[
u_* = f(D_0, \rho_p)
\]

Threshold wind friction affected by drag partition and moisture inhabitation:
\[
u_* (q, z_0, m) = u_* \times f(q) \times f(z_0, m)
\]

Horizontal saltation flux:
\[
Q_s(u_*; u_*) = \begin{cases} 
\frac{C_k \rho_a}{g} u_*^3 \left(1 - \frac{u_*}{u_t}\right) \left(1 + \frac{u_*}{u_t}\right)^2, & \text{if } u_* > u_t \\
0, & \text{if } u_* \leq u_t
\end{cases}
\]

Dust emissions are distributed among different particle size bins with a pre-described function

Vertical entrainment flux:
\[
F_{d,j} = T_0 f_{bare} S \alpha Q_s \sum_{i=1} M_{i,j}
\]
- \(f_{bare}\) Fraction of bare soil
- \(S\) Soil “erodibility” (GOCART)
- \(\alpha\) Sand blasting efficiency factor (Fixed)
- \(M_{i,j}\) Mass fraction of dust bin \(j\) from parent soil mode \(i\)

Zender et al [2003]
Iversen and White [1982]
Marticorena and Bergametti [1995]
Fairlie et al [2007]
Diversity of dust emissions & uncertainty of dust radiative forcing

Global dust emission inter-comparison in AeroCom

Adopted from Huneeus et al.[2011]

The sign of anthropogenic dust forcing is still unknown.
Spectral signature of dust absorption and scattering in both RS reflectance and IR radiance

**Left:** SW reflectances for various dust loadings (DOD: dust optical depth at 0.55 μm)
**Right:** IR brightness temperatures for various dust loadings.
(rg = 0.5 μm, Hpeak = 2.0 km; Mid-latitude summer over ocean surface)
Previous efforts used MODIS visible reflectance to constrain dust emissions

- Dust emission estimates were constrained by MODIS visible radiances
- Top-down emission estimates produced improved simulations of aerosol optical depths (versus AERONET) and PM concentrations (versus PM$_{10}$ measurements)

Wang, Xu, et al., 2012, GRL
Xu, Wang, et al., 2013, JGR

Spectrally resolved measurements span an additional dimension that contain spectrally-dependent dust absorption and scattering, and therefore could be used to detect the change of dust size-dependent emissions.
## Current and future hyperspectral measurements from satellites

<table>
<thead>
<tr>
<th>Type</th>
<th>Satellite sensor</th>
<th>Spatial resolution (km)</th>
<th>Spectral range</th>
<th>Spectral resolution</th>
<th>Radiometric accuracy</th>
<th>Available for</th>
</tr>
</thead>
<tbody>
<tr>
<td>RS</td>
<td>GOME</td>
<td>40 × 320</td>
<td>240 – 790 nm</td>
<td>0.2 – 0.4 nm</td>
<td>2% – 5%</td>
<td>1996 – 2011</td>
</tr>
<tr>
<td></td>
<td>GOME-2</td>
<td>40 × 80</td>
<td>240 – 790 nm</td>
<td>0.2 – 0.4 nm</td>
<td>2% – 5%</td>
<td>2006 – present</td>
</tr>
<tr>
<td></td>
<td>SCIAMACHY</td>
<td>32 × 215</td>
<td>240 – 2380 nm</td>
<td>0.24 – 1.48 nm</td>
<td>2% – 4%</td>
<td>2002 – 2012</td>
</tr>
<tr>
<td></td>
<td>TRUTHS</td>
<td>0.04</td>
<td>320 – 2450 nm</td>
<td>5 – 10 nm</td>
<td>0.3%</td>
<td>Undetermined</td>
</tr>
<tr>
<td></td>
<td>CLARREO and CPE</td>
<td>0.5</td>
<td>320 – 2300 nm</td>
<td>8 nm</td>
<td>0.3%</td>
<td>2020 (CPF)</td>
</tr>
<tr>
<td>IR</td>
<td>AIRS</td>
<td>50 (3×3 13.5)</td>
<td>645 – 2700 cm⁻¹</td>
<td>0.5 – 2.0 cm⁻¹</td>
<td>0.5 K</td>
<td>2002 – present</td>
</tr>
<tr>
<td></td>
<td>IASI</td>
<td>50 (2×2 12.0)</td>
<td>645 – 2760 cm⁻¹</td>
<td>0.25 cm⁻¹</td>
<td>0.5 K</td>
<td>2006 – present</td>
</tr>
<tr>
<td></td>
<td>CrIS</td>
<td>50 (3×3 13.0)</td>
<td>645 – 2700 cm⁻¹</td>
<td>0.6 cm⁻¹</td>
<td>0.2 – 0.3 K</td>
<td>2011 – present</td>
</tr>
<tr>
<td></td>
<td>CLARREO</td>
<td>25</td>
<td>200 – 2000 cm⁻¹</td>
<td>0.5 cm⁻¹</td>
<td>0.065 K</td>
<td>Undetermined</td>
</tr>
</tbody>
</table>

Xu et al. 2016, submitted
Introduction to OSSE (Observation System Simulation Experiment)

An OSSE is a modeling experiment used to evaluate the impact of new observing systems on operational forecasts when actual observational data is not available.

- A long free model run is used as the “truth” - the Nature Run (NR)
- The Nature Run fields are used to back out “synthetic observations” from the new observing systems.
- Suitable errors are added to the synthetic observations
- The synthetic observations are assimilated into a different operational model (DA)
- Forecasts are made with the second model and compared with the Nature Run to quantify improvements due to the new observing system

Adopted from Privé and Errico, 2015, JCSDA Summer Colloquium
Specific objectives

• Develop a simulator to generate the synthetic hyperspectral RS reflectance and IR radiance (integrating global chemistry model, radiative transfer, and satellite emulator)

• Perform OSSEs to identify the size-resolved dust spectral signature in the CLARREO hyperspectral measurements.

• Assess the ability of using these information (signature) to diagnose the emission changes of mineral dust: What are the advantages of CLARREO measurements (combined RS and IR spectrally-resolved radiances) for determining size-resolved dust emissions?
Flowchart of the OSSE design

**Forward modeling**
- **Dust Emissions:**
  - Spatial-resolved
  - Size-resolved
  - Monthly scale
- **Nature Run:**
  - T, P, H2O, cloud
  - Trace gases
  - Aerosols

**Synthetic CLARREO Data**
- IR radiance spectra
- RS reflectance spectra
- Analytic Jacobians to DOD

**Observation Operator:**
- CLARREO emulator
- UNL-VRTM radiative transfer

**Analysis:**
- Dust emissions
- Dust loadings
- CLARREO spectra

**4D-Var Inverse Modeling**
- GEOS-Chem
- Adjoint-based

**Information & Uncertainty**
- Optimal estimation
- DOD posterior error
- DFS & averaging kernel

**Validation**

**Adjoint analysis**

\[
\frac{\partial \text{spectra}}{\partial \text{emissions}} = \frac{\partial \text{AODs}}{\partial \text{emissions}} \times \frac{\partial \text{spectra}}{\partial \text{AODs}}
\]
OSSE Nature run: NOAA/ESRL FIM-Chem Model

- Global Flow-following finite-volume Icosahedra Model coupled with the GOCART aerosol modules.
- Icosahedral grid: mostly hexagons except for 12 pentagons.
- Dust scheme: the Air Force Weather Agency (AFWA).
- Performed on 240-km grids, and re-gridded into 1° X 1° grids.
- 64 vertical layers of the isentropic-sigma hybrid vertical coordinate
OSSE assimilation model: GEOS-Chem adjoint

GEOS-Chem:
- GEOS-5 2°X 2.5° meteorology
- 47 vertical layers.
- Dust scheme: DEAD

GEOS-Chem Adjoint:
- Adjoint-based 4D-Var
Dust Sizes in FIM-Chem and GEOS-Chem

<table>
<thead>
<tr>
<th>radii</th>
<th>FIM-Chem</th>
<th>GEOS-Chem</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1– 1.0 μm</td>
<td>DST1</td>
<td>DST1</td>
</tr>
<tr>
<td>r-eff=0.7</td>
<td>11.35</td>
<td>12.2</td>
</tr>
<tr>
<td>1.0–1.8 μm</td>
<td>DST2</td>
<td>DST2</td>
</tr>
<tr>
<td>r-eff=1.5</td>
<td>11.35</td>
<td>25.3</td>
</tr>
<tr>
<td>1.8–3.0 μm</td>
<td>DST3</td>
<td>DST3</td>
</tr>
<tr>
<td>r-eff=2.5</td>
<td>23.30</td>
<td>32.3</td>
</tr>
<tr>
<td>3.0–6.0 μm</td>
<td>DST4</td>
<td>DST4</td>
</tr>
<tr>
<td>r-eff=4.0</td>
<td>54.00</td>
<td>30.2</td>
</tr>
<tr>
<td>6.0–10.0 μm</td>
<td>DST5</td>
<td>DST5</td>
</tr>
<tr>
<td>r-eff=8.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The largest size bin is not used for consistency.

Mass contributions of each size bin:

<table>
<thead>
<tr>
<th></th>
<th>Bin 1 (%)</th>
<th>Bin 2</th>
<th>Bin 3</th>
<th>Bin 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>GEOS-Chem</td>
<td>12.2</td>
<td>25.3</td>
<td>32.3</td>
<td>30.2</td>
</tr>
<tr>
<td>FIM-Chem</td>
<td>11.35</td>
<td>11.35</td>
<td>23.30</td>
<td>54.00</td>
</tr>
</tbody>
</table>

For optical calculation:

- 0.1–0.18 μm: 3.3%
- 0.18–0.3 μm: 6.9%
- 0.3–0.6 μm: 23.9%
- 0.6–1.0 μm: 65.9%
UNified & Linearized Vector Radiative Transfer Model (UNL-VRTM)

UNL-VRTM can calculate Jacobians of any Stokes vector with respect to any aerosol parameters, a powerful tool to assess of the information content of remote sensing observations.

Spurr, R., J. Wang, et al., 2012
Wang, J., X. Xu, et al., 2014
Xu and Wang, 2015
CLARREO emulator: Simulation of one-month orbits

Spatial sampling: 25-km footprint for both IR and IS spectra scanned every 200 km.
Spectral sampling: 4 nm for RS and 1 cm⁻¹ for IR
Spectral resolution: 8 nm for RS and 0.5 cm⁻¹ for IR
Synthetic CLARREO data based on FIM-Chem nature run
Jacobians of synthetic CLARREO spectra to DOD of each size bin

Jacobians of RS reflectance spectra

Jacobians of IR reflectance spectra
Jacobians of synthetic CLARREO spectra to DOD of each size bin

(a) Avg. Jacobians of RS reflectance spectra

(b) Avg. Jacobians of IR reflectance spectra
We assume $S_a = \text{diag}([0.2, 0.15, 0.1, 0.05]) \pm 50\%$; BT error is 0.4 K and reflectance error is $0.03 \pm 5\%$, both including instrument noises and model errors; observation error correlation coefficients are 0.33–0.95 for pair-wise channels.
DFS for Determining Dust Optical Depth (DOD) of each Size Bin

- The RS spectra are most sensitive to dust AOD of 1\textsuperscript{st} size class, and the sensitivity decreases as bin size increases;
- The IR spectra are most sensitive to dust AOD the 3\textsuperscript{rd} size bin least sensitive to the 1\textsuperscript{st} size bin.
- Combining IR and RS spectra allows DFS for AOD in each size bin to be close to 1; information content for fully characterizing particle size is nearly 100%.
Characterization of DOD errors

DOD errors are estimated by the Bayesian theory:

\[ \hat{S}_\tau^{-1} = K^T S_\rho^{-1} K + S_{a,\tau}^{-1} \]

Three observation scenario:
- Infrared radiance (IR) spectra only
- Reflected-solar reflectance (RS) only
- RS + IR
OSSEs: One-month 4D-Var data assimilation
### Fitting of DOD “observations”

<table>
<thead>
<tr>
<th></th>
<th>DOD</th>
<th></th>
<th></th>
<th>DOD fittings before and after inversions</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>DST1</td>
<td>nature run</td>
<td>prior</td>
<td>prior run</td>
<td>IR-only</td>
<td>RS-only</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DST2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DST3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DST4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
## Inversion of dust emissions

### Nature Run vs Prior vs IR-only vs RS-only vs IR + RS

<table>
<thead>
<tr>
<th></th>
<th>Nature Run</th>
<th>Prior</th>
<th>IR-only</th>
<th>RS-only</th>
<th>IR + RS</th>
</tr>
</thead>
<tbody>
<tr>
<td>DST1</td>
<td><img src="image1" alt="Map" /></td>
<td><img src="image2" alt="Map" /></td>
<td><img src="image3" alt="Map" /></td>
<td><img src="image4" alt="Map" /></td>
<td><img src="image5" alt="Map" /></td>
</tr>
<tr>
<td>DST2</td>
<td><img src="image6" alt="Map" /></td>
<td><img src="image7" alt="Map" /></td>
<td><img src="image8" alt="Map" /></td>
<td><img src="image9" alt="Map" /></td>
<td><img src="image10" alt="Map" /></td>
</tr>
<tr>
<td>DST3</td>
<td><img src="image11" alt="Map" /></td>
<td><img src="image12" alt="Map" /></td>
<td><img src="image13" alt="Map" /></td>
<td><img src="image14" alt="Map" /></td>
<td><img src="image15" alt="Map" /></td>
</tr>
<tr>
<td>DST4</td>
<td><img src="image16" alt="Map" /></td>
<td><img src="image17" alt="Map" /></td>
<td><img src="image18" alt="Map" /></td>
<td><img src="image19" alt="Map" /></td>
<td><img src="image20" alt="Map" /></td>
</tr>
</tbody>
</table>

- **DST**
  - DST1
  - DST2
  - DST3
  - DST4

- **Colors**
  - White: < 0.01 (g/m²)
  - Light Blue: 0.01 - 0.10 (g/m²)
  - Light Yellow: 0.10 - 1.00 (g/m²)
  - Yellow: 1.00 - 10.00 (g/m²)
  - Red: > 10.00 (g/m²)
Spectral fittings

IR brightness temperature (BT, in Kelvin)

RS reflectance spectra
- nature run
- priori
- IR-only inversion
- RS-only inversion
- IR + RS inversion

Difference of GEOS-Chem RS reflectance spectra from nature run

Difference of GEOS-Chem IR BT spectra from nature run (transmittance > 85%)
Constrained dust emissions versus “truth”

- The combination of IR and RS measurements provides best constraints for size-resolved dust emissions.
Conclusions

- The RS spectra are most sensitive to dust AOD of 1\textsuperscript{st} size class, and the sensitivity decreases as bin size increases; Therefore, RS spectra yields better emission estimates for the 1\textsuperscript{st} size bin.
- The IR spectra are most sensitive to dust AOD the 3\textsuperscript{rd} size bin least sensitive to the 1\textsuperscript{st} size bin. Emissions of the 3\textsuperscript{rd} size bin are well constrained by IR spectra.
- Combining IR and RS spectra allows DFS for AOD in each size bin to be close to 1; information content for fully characterizing particle size is nearly 100\%. Such combination allows a better characterization of dust emissions for most size classes.
Future efforts

- Test the framework showed in this study with real data (SCIAMACHY, ARIS, and IASI)
- Explore the potential use of RS spectra to detect the change of water clouds (cloud droplet sizes) and anthropogenic emissions (we have showed this with MODIS data).
- Long-term study: What is the magnitude of the spectral signals arising from the dust aerosol forcing and does this exceed the natural variability of the climate system?
Back-up slides begin here!
Long-term research goals

• Identify the spectral fingerprint of mineral dust in the space-based shortwave and infrared measurements (from CLAERRO)

• Evaluate the information content of these measurements regarding to dust loadings, properties, and sources in the climate time scales.

Questions to answer: (1) What is the magnitude of the spectral signals arising from the dust aerosol forcing and does this exceed the natural variability of the climate system? (2) How can changes in reflectance/radiance spectra be ascribed to changes in the dust loadings, properties, and emissions?
Assimilation of DOD is equivalent to the assimilation of radiances

To assimilate DOD:

\[ J = \frac{1}{2} [\tau_o - \tau_m]^T \hat{S}_\tau^{-1} [\tau_o - \tau_m] + \frac{1}{2} \gamma [\mathbf{p} - \mathbf{p}_a]^T S_a^{-1} [\mathbf{p} - \mathbf{p}_a] \]

\[ \hat{S}_\tau^{-1} = K^T S_{\rho}^{-1} K + S_{a,\tau}^{-1} \]

DOD observation errors are estimated from spectral radiances

Replace \( S_\tau \) in the cost function:

\[ J = \frac{1}{2} [K(\tau_o - \tau_m)]^T S_{\rho}^{-1} [K(\tau_o - \tau_m)] + \frac{1}{2} \gamma [\mathbf{p} - \mathbf{p}_a]^T S_a^{-1} [\mathbf{p} - \mathbf{p}_a] \]

\[ \rho_o = K \tau_o; \rho_m = K \tau_m \]

In our OSSEs, same aerosol optical properties are assumed for both forward and inverse modeling.

\[ J = \frac{1}{2} [\rho_o - \rho_m]^T S_{\rho}^{-1} [\rho_o - \rho_m] + \frac{1}{2} \gamma [\mathbf{p} - \mathbf{p}_a]^T S_a^{-1} [\mathbf{p} - \mathbf{p}_a] \]

= To assimilate radiances

\( \tau_o \): observed DOD
\( \tau_m \): modeled DOD
\( S_\tau \): DOD error covariance
\( \rho_o \): observed radiances
\( \rho_m \): modeled radiances
\( K \): Jacobian of radiance wrt DOD
\( S_{\rho} \): radiance obs. error covariance
\( S_{a,\tau} \): DOD a priori error covariance
## Current and future hyperspectral measurements from satellites

<table>
<thead>
<tr>
<th>Instruments</th>
<th>Spatial</th>
<th>Spectral range</th>
<th>Spectral resolution</th>
<th>Available for</th>
</tr>
</thead>
<tbody>
<tr>
<td>GOME-1 on ERS-2</td>
<td>40x320 km²</td>
<td>240–790 nm</td>
<td>0.2–0.4 nm</td>
<td>1996 – 2011</td>
</tr>
<tr>
<td>GOME-2 on Metop-A/B</td>
<td>40x80 km²</td>
<td>240–790 nm</td>
<td>0.26-0.51 nm</td>
<td>2006 – present</td>
</tr>
<tr>
<td>SCIAMACHY/ENVISAT</td>
<td>32 x 215 km²</td>
<td>240–2380 nm</td>
<td>0.24–1.48 nm</td>
<td>2002 – 2012</td>
</tr>
<tr>
<td>AIRS on Aqua</td>
<td>50 (3x3 13.5-km)</td>
<td>645–2700 cm⁻¹</td>
<td>1200-resolving</td>
<td>2002 – present</td>
</tr>
<tr>
<td>IASI on Metop-A/B</td>
<td>50 (2x2 12.0-km)</td>
<td>645–2760 cm⁻¹</td>
<td>0.25 cm⁻¹</td>
<td>2006 – present</td>
</tr>
<tr>
<td>CrIS on Suomi-NPP</td>
<td>50 (3x3 13.0-km)</td>
<td>645–2700 cm⁻¹</td>
<td>0.6 cm⁻¹</td>
<td>2011 – present</td>
</tr>
<tr>
<td>CLARREO (SW/IR spectrometers)</td>
<td>0.5-km SW</td>
<td>320–2300 nm</td>
<td>8 nm</td>
<td>Pathfinder (2020)</td>
</tr>
<tr>
<td></td>
<td>25-km IR</td>
<td>200–2000 cm⁻¹</td>
<td>0.5 cm⁻¹</td>
<td>Full mission 2020+?</td>
</tr>
</tbody>
</table>
## CLARREO: Climate Absolute Radiance and Refractivity Observatory

### Science Instruments

<table>
<thead>
<tr>
<th>IR spectrometer</th>
<th>RS spectrometer</th>
<th>GNSS radio occultation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Systematic error &lt;0.06 K (k = 2)</td>
<td>Systematic error &lt;0.3% (k = 2) of Earth mean reflectance</td>
<td>Systematic error &lt;0.06% refractivity (k = 2) for 5–20 km</td>
</tr>
<tr>
<td>200–2000 cm⁻¹ spectral coverage</td>
<td>320–2300-nm spectral coverage</td>
<td>GPS and Galileo GNSS frequencies</td>
</tr>
<tr>
<td>0.5 cm⁻¹ unapodized spectral resolution</td>
<td>4-nm spectral samples; 8-nm resolution</td>
<td>5–20-km altitude range refractivity</td>
</tr>
<tr>
<td>NEDT &lt; 10 K for 200–600 cm⁻¹, and &gt;1600 cm⁻¹, all others &lt;2 K</td>
<td>S/N &gt; 33 for 0.3 scene reflectance, at a solar zenith angle of 75°. S/N &gt; 25 for λ &lt; 900 nm</td>
<td>&gt;1000 occultations per day to control sampling noise</td>
</tr>
<tr>
<td>25–100-km nadir FOV</td>
<td>0.5-km nadir FOVs for a 100-km-wide swath</td>
<td></td>
</tr>
</tbody>
</table>

Wielicki et al. 2013
Dust optical properties in IR

Shortwave refractive index adopted from Patterson et al., 1977, and IR refractive index from Di Biagio et al., 2014. Lognormal size distribution for each bin.

Dust size bin (um):
- DST1: 0.1 – 1 (reff = 0.7)
- DST2: 1 – 1.8 (reff = 1.5)
- DST3: 1.8 – 3 (reff = 2.5)
- DST4: 3 – 6 (reff = 4.0)
Dust optical properties in solar spectrum

![Graph showing extinction efficiency and single scattering albedo for different dust samples across various wavelengths.](image-url)

- **Extinction Efficiency**
  - DST1: Blue line
  - DST3: Red line
  - DST2: Green line
  - DST4: Cyan line

- **Single Scattering Albedo**
  - DST1: Blue line
  - DST3: Red line
  - DST2: Green line
  - DST4: Cyan line

Wavelength (µm)
Synthetic CLARREO dust optical depths based on FIM-Chem

Dust Optical Depth (0.55 μm)

DST1

DST2

DST3

DST4

Dust Optical Depth (11 μm)

DST1

DST2

DST3

DST4
Jacobians to dust optical depths

Jacobian of 0.55-μm Reflectance to DOD

DST1

DST2

DST3

DST4

Jacobian of 11-μm BT to DOD

DST1

DST2

DST3

DST4

N/A 0.00 0.01 0.02 0.03 0.04

-0.4 -0.3 -0.2 -0.1 0.0 N/A
Simulated CLARREO SW reflectance and IR brightness temperature
Jacobians of Measurements to Optical Depth of each Size Bin