The atmospheric composition geostationary satellite constellation for air quality and climate science: Evaluating performance with Observation System Simulation Experiments (OSSEs)

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Arlindo da Silva (NASA GSFC)
• The CEOS Atmospheric Composition Constellation activity identified joint OSSEs as a way to promote collaboration between the planned and proposed geostationary Earth orbit (GEO) missions from NASA GEO-CAPE/TEMPO, ESA Sentinel 4 & KARI GEMS

• OSSEs are extensively used by the NWP community to develop and optimize contemporary meteorological satellite instruments; now increasingly used in other fields of earth observation

• OSSEs assess the impact of hypothetical observations on a model analysis/forecast/inversion and provide a means to generalize on the conclusions of limited case-studies
### Funded tropospheric chemistry missions

<table>
<thead>
<tr>
<th></th>
<th>Europe Sentinel 4</th>
<th>USA TEMPO</th>
<th>Korea GEMS</th>
<th>Europe Sentinel 5 Precursor TROPOMI</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Orbit</strong></td>
<td>Geostationary</td>
<td>Geostationary</td>
<td>Geostationary</td>
<td>Low-Earth</td>
</tr>
<tr>
<td><strong>Launch</strong></td>
<td>2019</td>
<td>~2018</td>
<td>2018</td>
<td>2015</td>
</tr>
<tr>
<td><strong>Domain</strong></td>
<td>Europe</td>
<td>North America</td>
<td>Asia-Pacific</td>
<td>Global</td>
</tr>
<tr>
<td><strong>Resolution</strong></td>
<td>8km x 8km at 40N</td>
<td>8km x 4.5km at 35N</td>
<td>7 km (56 km²) at 38N</td>
<td>7km x 7km nadir</td>
</tr>
<tr>
<td><strong>Revisit</strong></td>
<td>1 hour</td>
<td>1 hour</td>
<td>1 hour</td>
<td>1 day</td>
</tr>
<tr>
<td><strong>Payload</strong></td>
<td>UV-Vis-NIR 305-500, 750-775 nm</td>
<td>UV-Vis 290-740 nm (tbc)</td>
<td>UV-Vis 300-500 nm (tbc)</td>
<td>UV-Vis-NIR-SWIR 270-500, 675-775, 2305-2385 nm</td>
</tr>
<tr>
<td><strong>Species</strong></td>
<td>O₃, NO₂, SO₂, HCHO, AAI, AOD, height-resolved aerosol</td>
<td>O₃ sensitivity to lowest 2km, NO₂, SO₂, HCHO, CHOCHO, AOD, AAOD, AAI</td>
<td>O₃, NO₂, SO₂, HCHO, AOD</td>
<td>O₃, NO₂, SO₂, HCHO, CO, CH₄, AAI, AOD, height-resolved aerosol</td>
</tr>
</tbody>
</table>
First experiments: Build on experience assimilating Terra/MOPITT multispectral tropospheric CO observations that have sensitivity to the lower troposphere, and imagine similar capability for all the members of the GEO constellation.

Such capability proposed for GEO-CAPE over the USA with EV CHRONOS; Europe currently plans column CO measurements from IRS accompanying Sentinel 4; currently no CO plans for the Korean platform to accompany GEMS.

An OSSE to demonstrate value of a GEO constellation: What is the impact of the constellation observations for improving analysis and forecast of pollutant distributions?

Control run: Met Only assimilated

Assimilation run: Met + MOPITT
A chemical OSSE framework

Science Question: What will the new data add?

Instrument Simulator

Nature & Control Runs

Simulated Data

Statistical evaluation of Assimilation Run with Control & Nature runs

Control Run

Data Assimilation

Assimilation Run

Refine Simulator

 Simulator useful
Experimental setup

- **Nature Run (NR):** GEOS-5 0.5° Global Mesoscale Simulation for summer 2006
- **Instrument Simulator:** Computationally efficient regression algorithm based on MOPITT multispectral observations (Worden et al., 2010)
- **Control Run (CR):** CESM CAM-Chem at 1° resolution
- **Assimilation Run (AS):** DART EAKF

- Assess the ability to observe impact of emissions over each region
- Look at importance of long range transport from one region to next
- Investigate the value of the measurements from each mission individually and together
Global Mesoscale Simulation: GMAO GEOS-5 7-km high resolution CO total column 15 July 2006

Courtesy Arlindo Da Silva, NASA GSFC
CO anthropogenic emissions budget

Nature: GEOS-5 Emissions
Control: CAM-Chem Emissions

Jun Jul Aug '06

GMAO GEOS-5 NR
Anth: merge of several inventories with EDGAR (2000) as a base (EPA/NEI, CAC, BRAVO, EMEP);
fires: QFED v2.2;
biog: MEGAN

NCAR CAM-Chem CR
Anthro: MACCity;
Fires: FINN
biog: MEGAN
The Observation Simulator

1. Nature Run Model
   Required state: \( \hat{X} \)

2. The Forward Model
   Simulated signal:
   \[ y = F(x) + \varepsilon \]
   Measurement Sensitivity:
   \[ K = \frac{\partial F}{\partial x} \]

3. Retrieval Model
   A priori: \( x_a, S_a \)

4. Retrieved Products:
   \( \hat{x}, \hat{S}, A = \frac{\partial \hat{x}}{\partial x} \)

Simulated Candidate Observations

Instrument Description
Noise: \( S_e \)

Radiative Transfer
- Solar backscatter
- Surface emission
- Atmospheric emission
Observation Simulator measurement & retrieval characteristics are represented by the Averaging Kernel (AK) and retrieval error.

However, running the full Observation Simulator in the OSSE is expensive and very involved.

Previously, CO and O$_3$ OSSEs have been simplified by assuming all observations can be represented with a few AK cases and these are used to sample the Nature Run model everywhere/all day.

But AKs vary a lot....

- Depend on surface characteristics, temperatures, clouds, aerosol loadings, trace gas loadings, viewing and solar angles.

- realistic OSSEs need to account for this!
Scene-dependent retrieval near-surface information content – large differences between regions

Observation simulator: Near-surface CO concentration accounting for scene-dependent measurement sensitivity

15 July 2006, 3pm local time

Barré et al., Atm. Env., accepted, 2015
Cloud coverage varies according to region with large differences affecting effective temporal coverage.

Simulated cloud coverage

July 2006 cloud coverage ratio

Barré et al., Atm. Env., in press, 2015
**GMAO GEOS-5 Nature Run**

**Emissions:**

**Chemistry:**
Only AeroChem: Global CO and CO2 tracers; GOCART aerosols

**Resolution:**
Vertical: 72 levels (Surface - 0.01hPa), Horizontal: 0.5°(0.06°)

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**NCAR CAM-Chem Control Run**

**Emissions:**
Anth/Fires: MACCity, Biog: MEGAN

**Chemistry:**
MOZART “full” tropospheric chemistry Aerosols and chemistry (87 species + 16 bulk aerosols)

**Resolution:**
Vertical: 30 levels (Surface - 3hPa), Horizontal: 1°

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Assimilation run over Summer 2006.
Meteorological Spin-up over May. Reduced NR resolution (0.5°) used

Barré et al., Atm. Env., in prep.
The OSSE result for the difference between the Assimilation Run (AS) and Control Run (CR) for June 26, 2006, for CO concentration after the assimilation of Simulated Candidate Observations from GEO over Europe, Asia and USA.
DA impact relative to nature run (NR): Assimilating all 3 GEOs
Monthly 200 – 1000 hPa average

Next look at Skill Score

$$= 1 - \frac{\text{MSE(AR-NR)}}{\text{MSE(CR-NR)}}$$

SS < 0 degraded simulation
SS > 0 improved simulation
SS = 1 perfect simulation
DA impact relative to nature run: Assimilating individual GEOs
Monthly 200 – 1000 hPa average

Assimilating US-GEO

Assimilating EUR-GEO

Assimilating ASIA-GEO
First OSSE results

- Assimilation of the GEO constellation provides a strong constraint over anthropogenic source locations.
- Global constraint of CO is also strong in remote regions due to long range transport of assimilation increments.
- Impacts are reduced over Asia due to increased cloud coverage limiting the number of clear observations.
- Experiments are being extended with a winter case study when the CO lifetime is longer, and emissions and cloud coverage also change.

Next steps

- Expand the experiments to consider LEO (TROPOMI) measurements, AOD, tropospheric ozone and chemical correlations.
Thank You!

NCAR is sponsored by the National Science Foundation
OSSE Infrastructure: Recommendations

- OSSEs need to account for realistic atmospheric variability: Requires evaluation of NR with observations

- OSSEs require realistic variability in measurement simulations generated from NR: Requires incorporation of sensitivities due to cloud, aerosol, trace gases, surface UV-visible reflectivity, and IR emissivity

- Simulated retrievals must include realistic range of sensitivities: Requires generation of scene-dependent AKs and errors

- OSSEs for relative performance between instruments/observation strategies may provide most reliable conclusions: Difficult to predict absolute performance of future systems compared to the current capability; requires full system evaluation with the existing observing system

- NWP experience: OSSE-based decisions have international stakeholders and experiments should be developed as joint global projects; community ownership and oversight of OSSE capability is also important for maintaining credibility
GEO constellation DA increments

RMS increments at Surface June

RMS increments at Surface July

RMS increments at Surface August

RMS increments Profile June

RMS increments Profile July

RMS increments Profile August
DA impact relative to nature run (NR): Assimilating all 3 GEOs
Monthly 200 – 1000 hPa average

NR-CR

Jun

Jul

Aug

NR-AR
DA impact relative to nature run (NR): Assimilating all 3 GEOs
Monthly 200 – 1000 hPa average

Skill Score = 1 – MSE(AR-NR)/MSE(CR-NR)

SS > 0 improved simulation
SS < 0 degraded simulation
SS = 1 perfect simulation
GEO constellation DA increments

GEO-US
GEO-EU
GEO-AS

Jun
Jul
Aug

RMS profile increments

GEO-US
GEO-EU
GEO-AS

RMS surface increments

Lower troposphere CO 900hPa
• Over 35% of mean surface ozone in EPA09 comes from emissions outside EPA09
• Chinese emissions contribute to mean column ozone @ 70% of local emissions
## GEOCAPE Atmosphere Regional/Urban OSSE

<table>
<thead>
<tr>
<th>Task</th>
<th>Participants</th>
<th>Institute</th>
</tr>
</thead>
<tbody>
<tr>
<td>2. Regional Nature Run*/DA*</td>
<td>B. Pierce/A. Lenzen/T. Schaack</td>
<td>NOAA/CIMSS</td>
</tr>
<tr>
<td>3. Forward RT Modeling*</td>
<td>K. Bowman/V. Natraj/T. Kurosu</td>
<td>JPL</td>
</tr>
<tr>
<td>4. AK Regression*</td>
<td>D. Edwards/H. Worden</td>
<td>NCAR</td>
</tr>
<tr>
<td>5. Multi-Spectral Retrieval*</td>
<td>L. Iraci/S. Kulawik</td>
<td>NASA/BAERI</td>
</tr>
</tbody>
</table>

* Completed in FY13  
* Completed in FY14  
* In preparation

Extends previous GEOCAPE OSSE studies by:

- Utilizing independent modeling systems for generation of the Nature atmosphere and conducting the assimilation impact experiments
- Accounting for realistic atmospheric variability, which requires evaluation of the nature runs with respect to observations.
- Inclusion of realistic variability in the synthetic radiances, which requires incorporation of realistic surface UV and visible reflectivities, and IR emissivities.
- Inclusion of realistic sensitivities, which requires generation of averaging kernels (AK) for each retrieval for use in assimilation studies
The OSSE Components

- OSSEs are extensively used by the NWP community to develop and optimize contemporary meteorological satellite instruments.
- Now also increasingly used in other fields of earth observation.
- OSSEs assess the impact of hypothetical observations on a model analysis/forecast/inversion and provide a means to generalize on the conclusions of limited case-studies.

**OSSE components:**

- **Nature Run (NR):** Model representation of ‘truth’
- **Simulated Candidate Observations:** The Observation Simulator samples the Nature Run
- **Control Run (CR):** An alternative model representation of the atmospheric state (... this might represent current capability to provide ‘ground-truth’ or the ‘a priori’ best guess)
- **Assimilation Run (AR):** Assimilation of the Simulated Candidate Observations in the Control Run
- **Compare:** Assess impact of the Candidate Observations - Does the Assimilation Run tend to the Nature Run compared to the Control Run? If so, Candidate Observation may be useful