Adjoint-based inverse modeling of OMI HCHO to constrain isoprene emissions

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TEMPO science meeting
1 June 2017
Isoprene is a major precursor to secondary pollutants. Uncertainty in bottom-up inventories is at least a factor of 2.
HCHO-$E_{\text{ISOP}}$ Link

GEOS-Chem 1-14 August 2013:

Isoprene Emission

HCHO VCD

$E_{\text{ISOP}}$ variability drives HCHO variability--HCHO provides a top-down constraint on isoprene emissions.
Linear approximations

\[ \Omega_{\text{HCHO}} = S E_{\text{isoprene}} + B \]

Palmer et al. (2003)
The smearing problem

80% of cumulative HCHO under high-NO\(_x\)
The smearing problem

Fine resolution analysis not possible with linear approach!

Concentration

Isoprene

HCHO

OMI

<5 hr

>100 km

~5 hr

>100 km

~24 hr

>100 km

80% of cumulative HCHO under high-NO\textsubscript{x}

80% of cumulative HCHO under low-NO\textsubscript{x}
Minimize cost function $J(x)$:

$$J(x) = (x - x_A)^T S_A^{-1} (x - x_A) + (F(x) - y)^T S_0^{-1} (F(x) - y)$$

- **A priori term**
  - How different are modeled and optimized isoprene emissions?

- **Observational term**
  - How different are modeled and measured HCHO columns?

1. Retain information from bottom-up estimates
2. Error is taken into account
3. Spatial displacement of $E_{ISOP}$ and HCHO fully represented

Brasseur and Jacob (2017)
Adjoint-based approach

Let’s test this as higher resolution using best knowledge from SEAC$^4$RS!

Bauwens et al. (2016)

Systematic reduction

50%!
Lessons from SEAC^4RS

(1) Impact of resolution

(2) Confidence in our isoprene oxidation mechanism

(3) Constraints on other influential factors

(4) Correcting biased satellite retrievals

Kim et al. (2015)
Lessons from SEAC$^4$RS

(1) Impact of resolution

(2) Confidence in our isoprene oxidation mechanism

(3) Constraints on other influential factors

(4) Correcting biased satellite retrievals

Fine resolution captures isoprene/NOx segregation, and is needed to explore heterogeneity of $E_{\text{ISOP}}$
Lessons from SEAC⁴RS

(1) Impact of resolution

(2) Confidence in our isoprene oxidation mechanism

(3) Constraints on other influential factors

(4) Correcting biased satellite retrievals

GEOS-Chem is up-to-date and agrees well with observations and fully explicit mechanisms

Fisher et al. (2016); Kim et al. (2015); Marais et al., (2016); Travis et al (2016).
Lessons from SEAC$^4$RS

(1) Impact of resolution

(2) Confidence in our isoprene oxidation mechanism

(3) Constraints on other influential factors

(4) Correcting biased satellite retrievals

Exhaustive analysis of the forward model allows us to isolate the role of $E_{\text{ISOP}}$
Lessons from SEAC$^4$RS

1. Impact of resolution

2. Confidence in our isoprene oxidation mechanism

3. Constraints on other influential factors

4. Correcting biased satellite retrievals

Uniform -37% bias related to spectral fitting and scattering weights
We produce a more relevant coarse grid for calculation of $\nabla J$:

$$J(x) = (x - x_A)^T S_A^{-1} (x - x_A) + (F(x) - y)^T S_O^{-1} (F(x) - y)$$

MEGAN v2.1 100%

Slant column densities
GC SCD = GC VCD x OMI-based AMF

~70% (RRE method)
Inversion results

OMI SAO $\Omega_{\text{HCHO}}$

Prior

Posterior

$10^{16} \text{ molec cm}^{-2}$

1-14 Aug 2013

GC $\Omega_{\text{HCHO}}$

Bias

$10^{16} \text{ molec cm}^{-2}$

(%)
Inversion results

Prior

Posterior

Correction

Isoprene emissions (10^{12} \text{ atms C cm}^{-2} \text{ s}^{-1})
Comparison with SEAC4RS measurements

**HCHO (ppb)**

**ISOP (ppb)**

**MVK + MACR (ppb)**

**ISOPN (ppt)**

**IEPOX (ppt)**

**ISOPOOH (ppt)**

<table>
<thead>
<tr>
<th>Prior</th>
<th>Optimized</th>
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**GEOS-Chem Adjoint**

**SEAC^4RS Measurements**
News from the bottom-up world

Emissions $\sim 2x$ lower than expected

MEGAN

Emissions factor for high emitting species

Yu et al. (2017)

Environment


Emissions well captured
News from the bottom-up world

Pine/Oak

Oak

Pine

Yu et al. (2017)

Similar conclusions from different methods!
Improvements offered by TEMPO

Diurnal variability

- TEMPO ≈ 75 x more information than OMI
- OMI pixel ≈ GC grid
- ~10% variability

Valin et al. (2016)
Recipe for a more accurate and useful top-down isoprene emission estimate:

Bias-corrected satellite retrievals + Validated fine-resolution model and it’s adjoint + Plentiful field data

TEMPO retrievals will provide far better constraints for this sort of analysis!
Bottom-up calculations

\[ F = \gamma \varepsilon_{isop} \]

\[ \gamma = \gamma_{LAI} \cdot \gamma_{Age} \cdot \gamma_T \cdot \gamma_{PAR} \cdot \gamma_{Soil Moisture} \]

Uncertainty from:

1. Limited vegetation data
2. Choice of landcover
3. Response functions and environmental parameters

Guenther et al. (2012)
Comparison with SEAC4RS measurements

Measured

Prior

Posterior

HCHO (ppb)
Improvements offered by a ground-based network

DNPH+HPLC
- O₃, NO₂ interferences
- 24h averages reported
- Some long term record at EPA sites

Mid IR Absorption
- Online, direct detection
- Hourly averages easily achievable
- Testing underway in Keutsch lab

Monitoring network on pace to keep up with satellite developments!