High-resolution inversion of OMI HCHO columns over the Southeast US to infer isoprene emissions

Jennifer Kaiser
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Daniel J. Jacob¹, Lei Zhu¹, Katherine R. Travis¹,*, Jenny A. Fisher²,⁴, Gonzalo González Abad³, Lin Zhang⁴, Xuesong Zhang⁵, Alan Fried⁶, John D. Crounse⁷, Jason M. St. Clair⁷,**, and Armin Wisthaler⁸

¹Harvard University | ²University of Wollongong | ³Harvard–Smithsonian CfA | ⁴Peking University | ⁵University of Toronto | ⁶UC Boulder | ⁷Caltech | ⁸University of Innsbruck and University of Oslo | *now at MIT | **now at NASA Goddard & UMBC

submitted to ACP
Can we use satellite HCHO to constrain isoprene emissions?

Isoprene Emissions = $\varepsilon_{\text{isop}} \times \gamma_{\text{LAI}} \times \gamma_{\text{Age}} \times \gamma_T \times \gamma_{\text{PAR}}$

MEGAN v2.1
isoprene base emission factors

Guenther et al., GMD, 2012.
Can we use satellite HCHO to constrain isoprene emissions?
SEAC4RS gave new insight on the HCHO-isoprene relationship

(1) Constrained isoprene oxidation mechanism

(2) Revealed the need for high resolution

(3) Validated satellite retrievals

Chan Miller et al., ACP, 2017.

GEOS-Chem agrees with explicit mechanisms and observations.

Wolfe et al., ACP, 2016; Marvin et al., Atmos. Environ., 2017.
SEAC$^4$RS gave new insight on the HCHO-isoprene relationship

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Isoprene emission factor $0.25^\circ \times 0.3125^\circ$

Fine resolution segregates isoprene and NO$_x$ emissions

Yu et al., *ACP*, 2016.
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NO$_x$ emissions (log scale)  
0.25° × 0.3125°

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Zhu et al., ACP, 2016.
Satellite HCHO provides top-down constraint on $E_{\text{ISOP}}$

MEGAN isoprene emissions

Aug/Sept 2013

$10^{12}$ atom C cm$^{-2}$ s$^{-1}$

GEOS-Chem HCHO column

Forward model

$0.25^\circ \times 0.3125^\circ$

OMI HCHO column

Inverse analysis

$10^{16}$ molecules cm$^{-2}$
Adjoint-based inversion to infer isoprene emission

Minimize cost function $J(x)$:

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

Prior term

$$(x - x_A)^T S_A^{-1} (x - x_A)$$

Observational term

$$(F(x) - y)^T S_0^{-1} (F(x) - y)$$

Scaling Factors

- GEOS-Chem column: 0.85
- OMI column: 100%

Instrument uncertainty
MEGAN isoprene emissions are biased high by 40%.

Scaling factors are robust to differences in error specifications.
Optimized emissions remove positive bias in HCHO columns
SEAC⁴RS observations can test optimized emissions
Optimized emissions produce better agreement with SEAC4RS

- **Isoprene**
  - MEGAN: 2.64
  - Optimized: 0.84

- **HCHO**
  - Optimized: 0.88

- **ISOPOOH**
  - Optimized: 0.96

- **MVK + MACR**
  - Optimized: 0.81

- **ISOPN**
  - Optimized: 0.66

**Legend**
- GEOS-Chem (ppb)
- Observations (ppb)
Right NO\textsubscript{x} key to inversion

![Graph showing simulated vs observed NO\textsubscript{x} and HCHO concentrations. The x-axis represents observed HCHO (ppb), and the y-axis represents GEOS-Chem HCHO (ppb). The simulated/observed NO\textsubscript{x} (dimensionless) is shown on the color scale. The 1:1 line indicates perfect agreement. Points below the line indicate underestimation, and points above the line indicate overestimation. Red points indicate overestimation of NO\textsubscript{x} and HCHO, while blue points indicate underestimation of NO\textsubscript{x} and HCHO.]

1:1

Simulated/Observed NO\textsubscript{x} (dimensionless)

Observed HCHO (ppb)

GEOS-Chem HCHO (ppb)

Overestimate NO\textsubscript{x}
Overestimate HCHO

Underestimate NO\textsubscript{x}
Underestimate HCHO
Evaluate the bottom-up emissions on an eco-system level

Optimized emissions

Ozarks: 46 reduction%
- Dense mixed pine-oak forest
- Vertical heterogeneity in canopy structure?

Edwards Plateau: factor of 3 reduction
- Oak/Juniper woodlands
- Fraction of forest cover varies widely in landcover maps
Lower isoprene emissions influences modeled air quality

Isoprene OC half of what is shown in previous work.

Isoprene explains part of the 8 ppb overestimate of surface O$_3$.

(Travis et al., ACP, 2017)

Shifting OA sources

- Anthropogenic: 28%
- Isoprene: 42%
- Monoterpenes: 20%
- Fires: 11%

Kim et al., ACP, 2015.

Reduction in surface O$_3$

Map showing isoprene emissions and surface O$_3$ levels.

13:00-17:00 L.T.

ppb
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Conclusions

1. We demonstrate the capability of a high resolution adjoint-based inverse analysis to infer isoprene emissions at ecosystem-relevant scales.

2. MEGAN is biased high by 40% across the southeast US.

3. Accurate NO\(_x\) fields are crucial in inversions of HCHO to infer isoprene emissions.

4. Reducing isoprene emissions lowers modeled O\(_3\); suggests other sources may play a greater role in OA.

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