Refining Ammonia Emissions Estimates with Observations during CalNex

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Unique Conditions

Topography conducive to trapping air

Favorable meteorology for farming

Abundant agricultural activity
Previous Work

Investigating ammonium nitrate sources & controls in the South Coast Air Basin

Russell & Cass, 1986
Clear Differences

Russell & Cass, 1986
CalNex 2010

May - June
NOAA . CIRES
Georgia Tech

vacuum ultraviolet fluorescence instrument: CO

chemical ionization mass spectrometry: NH₃, HNO₃

compact time of flight aerosol mass spectrometer: NH₄⁺, NO₃⁻

Nowak et al., 2012 (GRL)
CalNex 2010
March - July
NASA + AER, Inc.

Tropospheric Emissions Spectrometer (TES)

NH$_3$ tropospheric representative volume mixing ratio (RVMR)

K. Cary-Pereira; Shephard et al., 2011 (ACP)
TES Special Observations

March - July

CalNEX Step & Stare Obs

K. Cary-Pereira; Shephard et al., 2011 (ACP)
TES Special Observations

May - June

NASA

AER, Inc.

K. Cary-Pereira; Shephard et al., 2011 (ACP)
CalNex 2010

May - June

NSF

CalTech & Univ. of Colorado

Image: Google
CalNex 2010

May - June
NSF, NASA, NOAA
Georgia Tech + CalTech
Univ. of Colorado + AER, Inc.

Satellite Observations

Airborne Measurements

Ground-based Measurements
GEOS-Chem Adjoint

Initial $\text{NH}_3$ Concentration

$\text{NH}_4$ Concentration

0  5 10 16 21 27 (ppbv)

0  1.4  2.7  4.1  5.4  6.8 ($\mu g \text{ m}^3$)
GEOS-Chem Adjoint + ANISORROPIA

Checking Functionality

\[
\frac{\partial (\text{Nitrate})}{\partial (\text{NH}_3, \text{an})}
\]

- 2\textsuperscript{nd} Order
- 1\textsuperscript{st} Positive
- 1\textsuperscript{st} Negative

\[m = 0.995, \quad R^2 = 0.812\]
GEOS-Chem Adjoint
Assimilation Approach

- **a priori emissions estimates**
- determine differences between observations *(TES, IMPROVE)* & modeled *(GEOS-Chem)* concentrations
- **new emissions estimates & sensitivities**
- assess whether *agreement* between observations & modeled concentrations suffice
- minimize the cost function by modifying specified parameters *(emissions)* with L-BFGS algorithm
Next Steps

• Complete integration of TES observation operator

• Perform assimilation of TES observations to adjust emissions rates over continental U.S.

• Evaluate new modeled concentrations against in situ observations
Satellite Observations

Tropospheric Emissions Spectrometer

NH₃ Retrieval
Satellite Observations

Tropospheric Emissions Spectrometer

$NH_3$ Retrieval

Global Swaths
Transects over Bakersfield
{ CalNex Step & Stare }

Shepard et al., ACP (2011)
GEOS-Chem Adjoint

Initial NH$_3$ Concentration

Henze et al., ACP (2007)
GEOS-Chem Adjoint + ANISORROPIA

Capps et al., ACP (2012)
GEOS-Chem v. TES NH$_3$
GEOS-Chem v. TES NH$_3$
GEOS-Chem v. TES NH$_3$
Next Steps

- **a priori emissions estimates**
  - determine differences between observations & modeled (GEOS-Chem)

- **new emissions estimates & sensitivities**
  - assess whether agreement between observations & modeled concentrations suffice

- **minimize the cost function by modifying specified parameters (emissions) with L-BFGS algorithm**
California Nexus

Research at the Nexus of Air Quality and Climate Change

(NOAA, NASA, CalTech, Georgia Tech, CIRES)