

# GEOS-Chem Adjoint Model and the Data Assimilation Working Group

IGC6  
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Daven K. Henze, CU Boulder, Adjoint Model Scientist

Kevin W. Bowman, JPL, Data Assimilation WG Co-Chair

Dylan B. A. Jones, U Toronto, Data Assimilation WG Co-Chair

with contributions from the entire group\*

\* ~50 registered adjoint users at more than 20 institutions



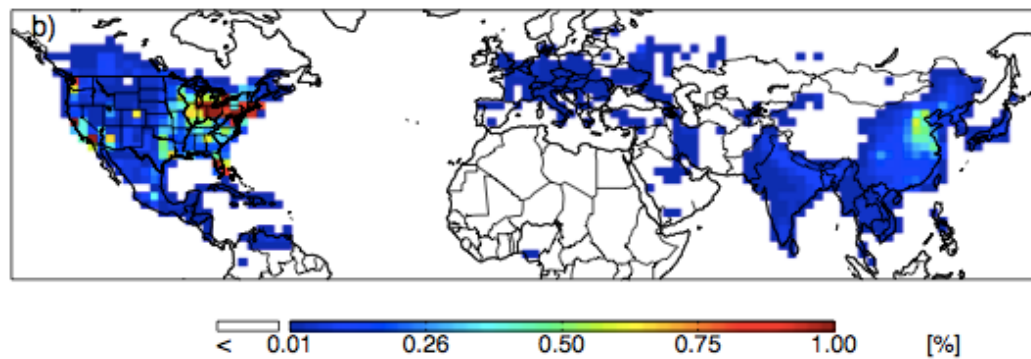
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## Sensitivity analysis



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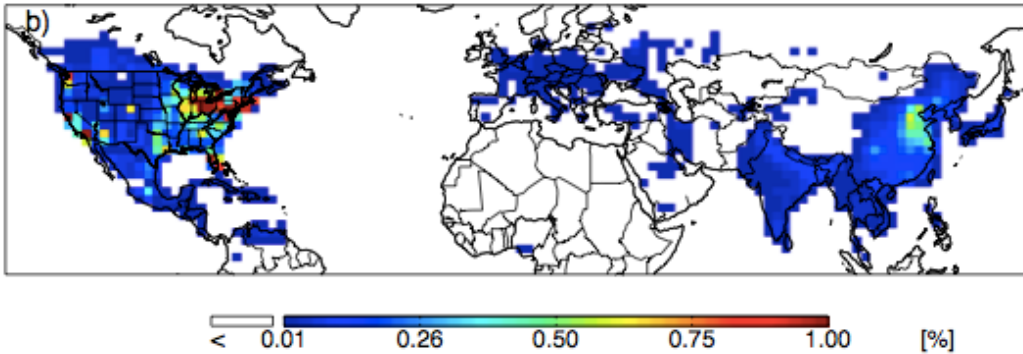
Adjoint calculates how sources of CO emissions anywhere in the world impact this response.

Katerya Lapina, CU Boulder

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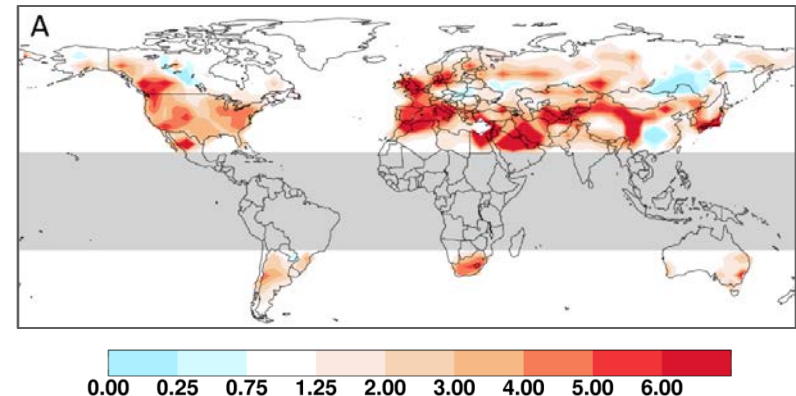
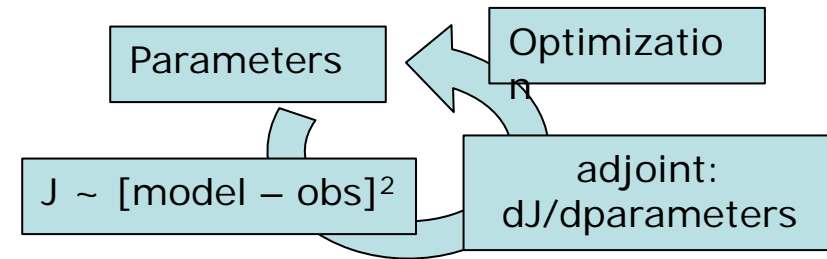


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Inverse modeling / 4D-Var



top-down CH<sub>3</sub>OH emissions using TES  
Kelly Wells, UM

# Adjoint model: current features

Standardized code: v34i, maintained / distributed via GIT

Code base: v8-02-01 with relevant fixes / updates up to v9-01-03

Meteorology: GEOS-3, GEOS-4, GEOS-5

Simulations : full chem; offline CO, O<sub>x</sub>, CO<sub>2</sub>, CH<sub>4</sub>, BC, Dust

Resolution : 4x5, 2x2.5, 0.5 x 0.667

Sensitivities : emissions, initial conditions, rate constants,  
stratospheric prod/loss rates

Processes: all main forward model process *excluding*:

- non-local pbl mixing scheme
- aerosol microphysics, online heterogeneous chemistry

Species: forward full chemistry model species *excluding*:

- SOA, SO<sub>4</sub>s, NITs, Br

see [GC adjoint wiki page](#) and [Trello board](#) for details

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## Overview

BETA RELEASE

- Previous version: [GEOS-Chem\\_Adjoint\\_v33](#)

New: benchmarking procedures

## What's new in this version

GEOS-Chem Adjoint v34 contains the following major updates and improvements.

Feature	Type	Submitted by	Committed by	Version	Status
<a href="#">Building Process Updated</a>	Adjoint Update	Daven Henze (CU Boulder), Yanko Davila (CU Boulder)	Yanko Davila (CU Boulder)	v34	Approved 14 Nov 2012
<a href="#">Add support for GFED3 Emissions</a>	Forward Model Update	Melissa Payer (Harvard)	Yanko Davila (CU Boulder)	v34	Approved 14 Nov 2012
<a href="#">Checkpoint files creation updated</a>	Adjoint Update	Daven Henze (CU Boulder), Yanko Davila (CU Boulder)	Yanko Davila (CU Boulder)	v34	Approved 14 Nov 2012

see GC adjoint wiki page and Trello board for details

# (FROM IGC5)

Developments: rank by priority (high, med, low) and assign point people or groups

Model development	Development group	Priority level	Readiness	Difficulty
Off-diagonal error covariance matrix	JPL	high	med	low
Inverse Hessian	Tang (Purdue), JPL	high	med	low
Methane	Wecht (Harvard), Tang (Purdue)	high	high	low
CH4 obs operators: SCIA, AIRS, TES	Harvard / Purdue	med	med	low
generalized DOAS obs operator	Bousserez (Dal)	high	high	low
generalized TES obs operator	Lee (JPL)	med	med	med
full chemistry nested	Zhe Jiang (UT)	highest	low	med
CO/CO2	Jones (UT), Bowman (JPL)	high	low	med
BC offline adjoint	Yuhao Mao, Qinbin Li (UCLA)	high	low	low
heterogeneous chemistry (RDAER)	Henze (CU Boulder)	med	med	low
GISS tracer advection adjoint	Henze (CU Boulder)	low	low	low
GCAP convection	Henze (CU Boulder)	low	low	med
Column addition				
Sensitivity				
Dust	Xu (ONL), Park (SNU), Li (UCLA)	high	med	low
Satellite obs operator sensitivity	Bowman, Lee (JPL)	med	med	low
Generic surface obs operator	Jones (UT)	med	med	low
Output rxn rate sensitivities	Paulot (Caltech/Harvard)	med	med	low
Joint initial condition & emissions opt	?	high	low	low
ISORROPIA adjoint	Shannon Capps (Georgia Tech)	med	med	med
Scaling factor "hooks" in forward model work w/Bob and emissions group		high	low	low

Many high priority items implemented in the last two years.

# Recent and current applications: Inverse modeling

## Aerosol and aerosol precursor emissions:

- Carbonaceous PM using IMPROVE (Mao, UCLA; Egan-Pimblett, Dalhousie)
- Asia BC with OMI AAOD (Zhang, CU Boulder)
- Aerosols with MODIS (Xu, Wang, UNL)
- Aerosols with POLDER (Meland, CU Boulder/CUD)
- NH<sub>3</sub> using TES (Zhu, CU Boulder; Capps, US EPA)
- NH<sub>3</sub> using wet deposition (Paulot, Harvard)

## Greenhouse gases:

- CH<sub>4</sub> (Wecht, Turner, Harvard; Tan, Purdue)
- CO<sub>2</sub> from GOSAT (Liu, Lee, JPL; Deng, UT; Zhu, Purdue; Shim, KEI)

## Reactive gas-phase species

- CO from MOPITT (Jiang, UT) and BORTAS (Parrington, Edinburgh)
- CH<sub>3</sub>OH from TES (Wells, UMN)



# Recent and current applications: Sensitivity analysis

## Climate / chemistry:

- Radiative forcing (Henze, Lacey, CU Boulder; Bowman, JPL)
- Arctic O<sub>3</sub> and NO<sub>y</sub> (Walker, UT) and Antarctic nitrate (Lee, CU Boulder)
- CCN (Karydis, GIT)
- Adjoint of ISORROPIA aerosol thermodynamics (Capps, GIT/US EPA)

## Satellite design and analysis

- GEOCAPE (Lee, JPL; Henze, CU Boulder; Wecht, Harvard)
- XCO<sub>2</sub> sensitivity analysis (Liu, JPL)
- Column constraints (Turner, Harvard; Padmanabhan, Dalhousie)

## Emissions mitigation strategies

- PM<sub>2.5</sub> in Asia (Kharol, Dalhousie)
- O<sub>3</sub> W126 vegetative exposure (Lapina, CU Boulder)
- PM<sub>2.5</sub> and O<sub>3</sub> health impacts (Lee, Dalhousie; Henze, CUB; Koo, MIT)
- N deposition (Henze, CU Boulder; Paulot, Harvard)



## Research Highlights: Source attribution of PM<sub>2.5</sub> related mortality

What is the health-related benefit for reducing a ton of emissions, and how does this vary by location?



# Recent and current applications

## Theory

- Weak constraint 4D-Var (Keller, UT)
- Inverse Hessian (Bousserez, CU Boulder)

## Other Data Assimilation activities

- 3D-Var assimilation of ozone from TES and MLS (Lee, Neu JPL)
- 3D-Var assimilation of CO<sub>2</sub> from TES and GOSAT (Lee)
- EnKF CO<sub>2</sub> flux estimates (Denning, CSU; Palmer, Univ Edinburgh)

## Software Engineering

- pyEnsemble Manager (Perkins, UW)
- Multi-mission observation operator M2O2 (Lee, JPL)
- full-time adjoint model code support (Yanko Davila, CU Boulder)

# New: code tracking with GitLab

<http://adjoint.colorado.edu:8080>

The screenshot displays a GitLab commit page for the repository 'ncadi\_std'. The commit hash is 'c335c1fd3', dated '19 Apr, 2018'. The commit message is: '! here we aren't assuming that TS\_CHEM is necessarily 1 hr'.

The code diff shows changes to a file, with lines 3333-3346 highlighted in red. The code includes a conditional block for 'LKGNHAYR' and a calculation for 'FACT'.

```
3333 3311 ! here we aren't assuming that TS_CHEM is necessarily 1 hr
3334 3312 NTSCHEM = NSPAN / ( GET_TS_CHEM() / 60D0 )
3335 3313
3336 - IF ( LKGNHAYR ) THEN
3337 -
3338 -     FACT = 14d-3 / TCVV(IDTNIT)
3339 -     &     * XNUMOL(IDTNIT) / DT_CHEM
3340 -     &     / NTSCHEM / 6.022D23 * 86400d0 * 365d0
3341 -     &     * 1d4
3342 -
3343 - ELSE
3344 -
3345 -     !default is molec/cm2/s
3346 -     FACT = XNUMOL(IDTNIT) / DT_CHEM
```

The discussion section shows two comments:

- Daven Henze** 21 days ago: "Shouldn't it also be possible to use LKGNHAYR for NHx deposition?"
- Fabien Paulot** 16 days ago: "but NH3 and NH4 are not in CSPEC so I think it's fine"

A 'Reply' button is visible at the bottom of the discussion.



# Future directions

- Additional adjoint model capabilities
  - Additional offline simulations ( $\text{N}_2\text{O}$ , ...)
  - more sensitivity output: convection, ...
  - more sophisticated optimization and DA analysis tools
  - further consolidation of observation operators (e.g., M2O2)
  - additional meteorology: MERRA, GCAP...
  - chemistry update when SMVGEAR is retired
- Keep an eye on grid-independent forward model development
- More connection/shared code with other assimilation methods (3D-Var and other sequential methods)
- Switch from quarterly to ~monthly WG telecons
- Adjoint Model Co-Scientist: assist with development, benchmarking, code maintenance and support



the end