Mitigating model biases and constraining North American methane emissions using weak constraint 4D-Var

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Sensitivity to Biases in North American Boundary Conditions (BCs)

Objective: can we optimize the state (CH4 concentrations) to mitigate biases in North American BCs?

Our previous inversions of Proxy and Full-Physics GOSAT CH4 retrievals using GEOS-Chem model produced large differences in the inflow to North America, due in part to differences in observational coverage.

Mean difference between CH4 concentrations at boundaries of North America in May 2010 from inversion of emissions using GOSAT Proxy and Full-Physics retrievals.
Weak Constraint 4D-Var

In weak constraint 4D-Var we account for errors in the forward model by adding corrections (forcing terms) to the modeled state, i.e., CH$_4$ concentrations ($x$), at each step:

$$ x_{n+1} = M(x_n, p) + u_n $$

$$ J(p, u) = \sum_{t=t_0}^{t_N} \frac{1}{2} (y_t - H(x_t))^T S_o^{-1} (y_t - H(x_t)) + \frac{1}{2} (p - p_a)^T S_a^{-1} (p - p_a) + \sum_{t=t_0}^{t_N} (u_t)^T Q^{-1} (u_t) $$

- **Observations contribution**
- **A priori contribution**
- **Forcing contribution**

[Holm, 2003] [Tremolet, 2006]
OSSEs to Assess State Optimization

Observing system simulation experiment (OSSE) setup

- Sample model at locations and times of Proxy retrievals to produce pseudo-observations
- Run a series of OSSEs with the forward model artificially biased relative to the truth in terms of the emissions and model transport

<table>
<thead>
<tr>
<th>Optimization period</th>
<th>February 1, 2010 – May 31, 2010</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model resolution</td>
<td>GEOS-Chem: global 4 x 5 degrees</td>
</tr>
<tr>
<td>Biased a priori</td>
<td>70% of a priori emissions</td>
</tr>
<tr>
<td>Biased initial conditions</td>
<td>Initial condition is generated by running with CONVECTION TURNED OFF EVERYWHERE and 70% of a priori emissions from July 1, 2009, to February 1, 2010.</td>
</tr>
</tbody>
</table>
| Biased transport during optimization period | Two experiments:  
1. Convection is turned on (perfect transport)  
2. Convection is off everywhere (biased transport) |
| Inversions:                | Two experiments:  
1. Weak constraint (WC) state optimization  
2. Strong constraint (SC) monthly flux optimization |
| Truth                      | CH4 state from inversion of monthly CH4 fluxes using real GOSAT Proxy retrievals from July 1, 2009 to Dec. 31, 2010 |
OSSE: mean difference between “true” and optimized BCs in May 2010

Perfect model transport during optimization period

Before inversion

WC state GOSAT

SC flux GOSAT

-40.0 – 40.0 ppb

-10.0 – 10.0 ppb
OSSE: mean difference between “true” and optimized BC in May 2010

Convection is off during optimization period

Before inversion

WC state GOSAT

SC flux GOSAT

-85.0 – 85.0 ppb

-10.0 – 10.0 ppb
OSSE: mean difference between “true” and optimized BC in May 2010
Convection is off during optimization period

A priori and a posteriori bias, [ppb]

<table>
<thead>
<tr>
<th></th>
<th>Western Boundary</th>
<th>Northern Boundary</th>
<th>Southern Boundary</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Lower trop</td>
<td>Upper trop</td>
<td>Total</td>
</tr>
<tr>
<td>A priori</td>
<td>71.1</td>
<td>64.7</td>
<td>68.1</td>
</tr>
<tr>
<td>WC (State)</td>
<td>-0.2</td>
<td>-0.8</td>
<td>-0.4</td>
</tr>
<tr>
<td>SC (Source)</td>
<td>1.0</td>
<td>5.8</td>
<td>3.3</td>
</tr>
</tbody>
</table>
Inversions of real GOSAT Proxy retrievals

Inversions Setup

- **Observations**: GOSAT UoL v5.1 Proxy retrievals
- **Model**: GEOS-Chem global 4 x 5 degrees
- **Two inversions**:
  - Strong constraint (SC) in which we optimize the monthly fluxes from July 1, 2009 to May 31, 2010
  - Weak constraint (WC) in which we optimize the state from Feb. 1, 2010 to May 31, 2010
- Both inversions have the same a priori emissions and initial conditions on Feb. 1
- **Objective**: obtain optimized Boundary Condition over North America in May 2010

<table>
<thead>
<tr>
<th></th>
<th>07/09</th>
<th>08/09</th>
<th>09/09</th>
<th>10/09</th>
<th>11/09</th>
<th>12/09</th>
<th>01/10</th>
<th>02/10</th>
<th>03/10</th>
<th>04/10</th>
<th>05/10</th>
</tr>
</thead>
<tbody>
<tr>
<td>WC</td>
<td></td>
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<tr>
<td>SC</td>
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</tbody>
</table>
Global inversion with GOSAT Proxy retrievals
Mean difference between optimized BC in May 2010

Weak constraint – Strong constraint

South at 10N
West at 140W
North at 70N

A posteriori statistics in May 2010

<table>
<thead>
<tr>
<th></th>
<th>Bias, ppb</th>
<th>Scatter, ppb</th>
<th>Correlation</th>
<th>Slope</th>
<th>R^2</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>NOAA surface flask</strong></td>
<td>7.5</td>
<td>25.2</td>
<td>0.91</td>
<td>0.96</td>
<td>0.83</td>
</tr>
<tr>
<td><strong>TCCON</strong></td>
<td>11.1</td>
<td>13.8</td>
<td>0.83</td>
<td>0.82</td>
<td>0.7</td>
</tr>
</tbody>
</table>

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</tr>
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<td><strong>TCCON</strong></td>
<td>8.7</td>
<td>10.7</td>
<td>0.91</td>
<td>0.86</td>
<td>0.82</td>
</tr>
</tbody>
</table>
Nested inversion of North American methane emissions in May 2010

<table>
<thead>
<tr>
<th>Period</th>
<th>April 22, 2010 – May 31, 2010</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>Nested GEOS-Chem, 0.5x0.67 degrees resolution</td>
</tr>
<tr>
<td>Optimization</td>
<td>Strong constraint 4D-Var flux optimization</td>
</tr>
<tr>
<td>Observation</td>
<td>GOSAT UoL v5.1 Proxy retrievals</td>
</tr>
<tr>
<td>Boundary and initial conditions</td>
<td>1. From global Strong constraint (SC) inversion 2. From global Weak constraint (WC) inversion</td>
</tr>
</tbody>
</table>

Ratio of optimized to a priori emissions in May 2010

Optimized emissions, Tg
SC vs. WC

Difference in total emissions – 0.3%

1:1
Nested inversion of North American emissions

Why inversions with WC boundary inferred higher Los Angeles emissions?

Mean difference between CH4 fields at the boundary and surface in May 2010 [before inversion]

Weak constraint – Strong constraint [+/- 10 ppb]

- Air depleted in methane is advected to the western coast of North America and reaches Los Angeles
- Inversion compensates for this effect making emissions become larger
- The rest of the continent is not affected due to blocking by mountains
- High sensitivity arises from frequent GOSAT sampling of LA with weak signal of local emissions in total column above the city
Conclusions

- Although GOSAT retrievals have limited vertical sensitivity, the OSSEs show that the weak constraint (WC) 4D-Var method is able to mitigate model biases related to transport.

- The WC (state) optimization is in closer agreement with TCCON data, whereas the SC (source) optimization better matches the surface in situ data.

- Regional inversion of Proxy data using boundary conditions from the WC (state) and SC (source) optimization produced consistent total North American emission estimates (differences of 0.3%), but regional difference in emissions (e.g. Los Angeles emissions significantly reduced with SC boundary conditions) due to discrepancies in the boundaries.

  - With better satellite coverage of North America sensitivity of inverted fluxes to biases in BCs may increase due to higher chance to sample biased background air
Can we trust our regional inversion?
Consider ideal situation

Observing system simulation experiment (OSSE) setup

<table>
<thead>
<tr>
<th>Optimization period</th>
<th>May 2010</th>
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</thead>
<tbody>
<tr>
<td>Model resolution</td>
<td>Global 4 x 5 degrees</td>
</tr>
<tr>
<td>A priori emissions</td>
<td>Same as “true” inversion</td>
</tr>
<tr>
<td>Initial conditions</td>
<td>Same as “true” inversion</td>
</tr>
<tr>
<td>Model biases</td>
<td>Perfect model</td>
</tr>
<tr>
<td>Data assimilation</td>
<td>Strong constraint 4D-Var flux inversion</td>
</tr>
<tr>
<td>Observations</td>
<td>Pseudo GOSAT Proxy total columns sampled from “true” CH4 fields with no noise added and real retrieval uncertainties</td>
</tr>
</tbody>
</table>
| “True” inversion    | Inversions of global CH4 emissions in May 2010 with real GOSAT Proxy retrievals:
  • Inferred emissions = “true” emissions
  • Updated CH4 fields = “true” CH4 fields |
| Purpose             | Obtain the original (“true”) emissions |
Ideal OSSE: results
Ratio of optimized to a priori emissions in May 2010

"Truth"

OSSE
Ideal OSSE: results
Ratio of optimized to a priori emissions in May 2010

“Truth”

Here we also include in situ pseudo observations daily at 1pm at North American surface sites
Sensitivity of inferred fluxes to biases in boundary conditions (BC)

Bias in boundary conditions taken as a difference between optimized methane fields from global PROXY and FP inversions (with a “-” sign).

Pseudo-obs: hourly total column measurements over every land gridbox

Pseudo-obs: hourly boundary layer column (ground to ~750 hPa) measurements over every land gridbox
Impact a priori emissions on atmospheric CH$_4$ in August

**SIGNAL OF CH$_4$ EMISSIONS**

- In surface measurements
- In boundary layer column (ground to ~750 hPa), SZA < 70
- In total column, SZA < 70

**Propagated BC bias as a fraction of emissions signal, August 2010**

- At the surface
- In total columns