Evaluating mass balance methods for constraining global NO$_x$ emissions

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Satellite NO$_2$ Observations Provide Top-Down Constraints on NO$_x$ Emission Inventories

- Emissions inventories have significant uncertainties
- Using satellite observations as a constraint requires inverse modeling
Improving Mass Balance Inversions with Finite Difference

- Basic mass balance: $E_{\text{top down}} = \alpha \Omega_{\text{obs}}$
- Actual relationship is more complicated
- Use finite difference to linearize the model around its *a priori* state
- Iterative mass balance proposed to reduce errors from transport
- Goal: To evaluate mass balance methods

Finite Difference Mass Balance Equations

$$\beta = \frac{\Delta E}{\Delta \Omega}$$
$$E_t = E_a \left( 1 + \frac{\Omega_{\text{obs}} - \Omega_a}{\Omega_a} \beta \right)$$
Evaluating Mass Balance Inversions using Synthetic Observations

- Synthetic observations made by making specific perturbations to NO\(_x\) emissions
- Use synthetic observations to evaluate inversion methods
- Provides a known “truth” for evaluating inversion results

• GEOS-Chem Adjoint is benchmark for evaluating mass balance methods
  • Adjoint is more rigorous, but more computationally demanding
Iterative Approach Reduces Horizontal Smearing Errors

• Transport weakens assumptions in mass balance method
• Smearing most prevalent in winter hemisphere (longer \( NO_x \) lifetime)
• Iterating the mass balance method reduces smearing
• Adjoint method best retrieves true emissions in this case
Iterative Finite Difference Mass Balance has Similar Accuracy as Adjoint for Complex Emission Perturbations

- Two weeks of hourly observations
- Iterative finite difference improves basic mass balance by ~ factor of 2
- Iteration impacts January when NO\textsubscript{x} lifetime is longer
- Finite difference impacts July when non-fossil fuel emissions contribute more to the NO\textsubscript{2} column
Iterative Finite Difference Mass Balance has Similar Accuracy as Adjoint

- Tested resolution: Consistent results at both 2°x2.5° and 4°x5° resolution
- Tested observational errors: Added Gaussian random noise, random bias values
- Tested sampling: Hourly observations, Synthetic LEO, Geostationary (hourly, day only)

Results from 4°x5° Inversion
Summary

• Iterative finite difference improves upon the basic mass balance method

• While adjoint method can better account for smearing in simplified cases, the advantage is minimal in more complex scenarios

• For more complex scenario, iterative finite difference mass balance method has same accuracy as the adjoint method

Conclusion

Iterative finite difference mass balance offers ability to estimate top-down NO$_x$ emissions in a computationally efficient manner