

Simultaneous Optimization of Global Fluxes of Methane and Carbon Dioxide using Satellite Data

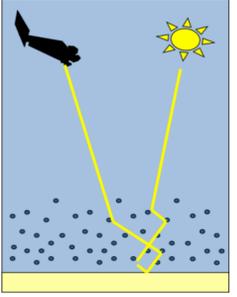
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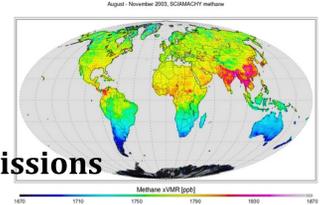
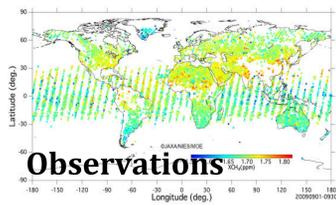
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Introduction

Inverse modeling technique is used to translate satellite and ground based observations into corresponding emissions of greenhouse gases at the Earth's surface. However, in the case of long-lived greenhouse gases, such as methane, it is a challenge for the satellites to meet the required level of accuracy. A successful method is the so-called proxy retrieval (Butz et al., 2011), which yields the ratio of the total column averaged mixing ratios of CH₄ and CO₂. In the past, this ratio has been used to study the global sources and sinks of CH₄. To account for the contribution of CO₂ to the measured CH₄/CO₂ ratio, CO₂ concentrations fields were used from a model (for example CarbonTracker). Systematic errors in satellite data, e.g. due to atmospheric scattering, affect both carbon dioxide and methane similarly. Hence, taking the ratio largely eliminates this error. It is assumed that the contribution of carbon dioxide is understood well enough to use this method for studying methane. However, with the improved measurement quality obtained using the GOSAT instrument this assumption is starting to become an important limitation (Schepers et al., 2012).



We present a new inverse modeling method (called the 'ratio' method from here on) based on the 4DVAR technique (Meirink et al., 2008). The aim is to optimize the ratio of methane and carbon dioxide, i.e. without translation to CH₄ assuming the prior values of carbon dioxide. Our approach of using proxy retrievals to optimize both methane and carbon dioxide allows us to make use of the powerful proxy retrieval approach, without biasing the inversion-derived flux estimates by imposing constraints on CO₂ derived from a model.



Method

The aim of the optimization is to minimize the cost function J , which is defined by:

$$J^b(x_o) = (x_o - x_o^b)^T B^{-1} (x_o - x_o^b)$$

$$J(x_o) = J^b(x_o) + J^o(x_o)$$

$$J^o(x_o) = \sum_{i=0} (y_i^o - H_i(x_i))^T R_i^{-1} (y_i^o - H_i(x_i))$$

B, R are the background and measurement error correlation matrices, i represents the different timesteps.

where, H is an atmospheric transport model sampled according to the measurements y and forced by the sources and sinks x .

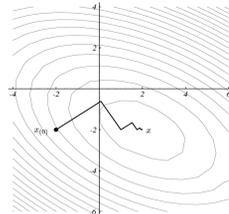
$$x = [\delta(CO_2)_1 \quad \delta(CO_2)_2 \quad \dots \quad \delta(CH_4)_1 \quad \delta(CH_4)_2 \quad \dots]$$

The state vector x is comprised of the fluxes (represented by δ in the equation) and measurements y comprises of the ratio of measurements of mixing ratio of CO₂ and CH₄.

$$y = \begin{bmatrix} [CO_2]_1 & [CO_2]_2 & \dots \\ [CH_4]_1 & [CH_4]_2 & \dots \end{bmatrix}$$

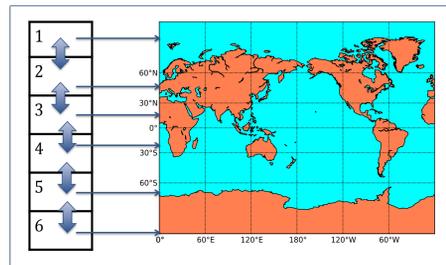
The minimization of the cost function involves iteratively calculating the gradient of the cost function to decide the direction of descent of state vector.

$$\nabla J(x_o) = 2B^{-1}(x_o - x_o^b) - 2 \sum H_i^T [y_i^o - H_i(x_o)]$$



Toy model

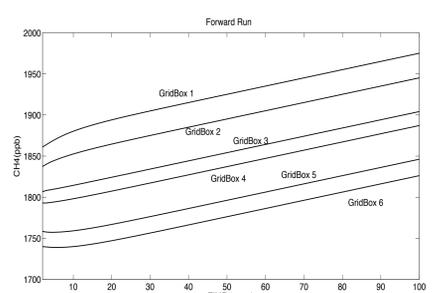
We test this method using a synthetic test setup (toy model) to check its efficiency. The Earth is divided into six grid boxes along the latitudes (three in each hemisphere). For simplicity, we assume that the model has no sinks.



The transport model is defined as follows:

$$C_f^k = C_i^k + S^k + \sum_{\text{adjacent zones}} \alpha (\Delta C)_n^k$$

C, S are the mixing ratio and fluxes respectively, in grid box k . Δ represents the difference and α is a constant.



Results of a forward model run of the toy model over 100 years. The north-south gradient reaches equilibrium after a few years of simulation.

Comparison Test Setup

We prepare a test environment setup, to test how the performance of the ratio method compares with the traditional direct optimization method in terms of efficiency and accuracy. For this test we keep all boundary conditions the same. For simplicity, The observation (R) and prior covariance matrix (B) are assumed to be diagonal matrices.

Direct Optimization

$$[CH_4]_{obs} = \frac{[CH_4]_{init}}{[CO_2]_{init}} \times [CO_2]_{obs}$$

- Linear observation operator
- Congrad subroutine is used as the optimization subroutine
- Congrad is the most efficient optimization subroutine for linear cases

Ratio Optimization

$$\frac{[CH_4]_{init}}{[CO_2]_{init}}$$

- Nonlinear observation operator
- We use m1qn3 (Gilbert et al., 2009) as our optimization subroutine instead.

The optimization subroutine takes the gradient and calculates the next value of the x along the direction of the gradient.

Adjoint coding

In applications using real data, it is not possible to store the matrices H, B and R on computer memory. This happens for two reasons:

- Matrix size (10^{11})
- Non linearity (when evaluating ratios H depends on the state x)

Therefore, instead of storing matrixes, their elements are computed when needed. The calculation of cost function gradients requires H^T , which is the adjoint of the forward model H . Our ratio method requires the following extension of the forward and adjoint model.

The Forward Model

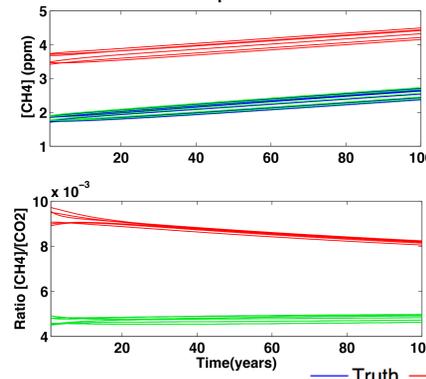
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do i=1,n
  x_ratio(i) = xch4(i)/xco2(i)
end do
```

The Adjoint Model

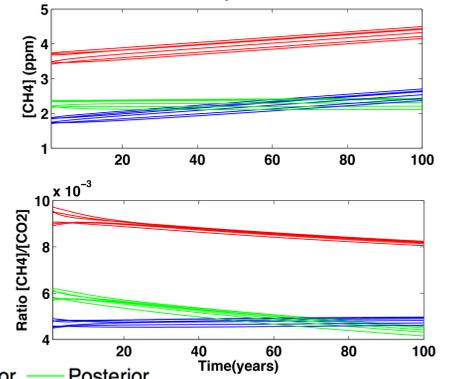
```
do i = n, 1, -1
  adj_xch4(i) = adj_xch4(i) + adj_x_ratio(i) / xco2(i)
  adj_xco2(i) = adj_xco2(i) - adj_x_ratio(i) * xch4(i) / (xco2(i)**2)
  adj_x_ratio(i) = adj_x_ratio(i)
end do
```

Results

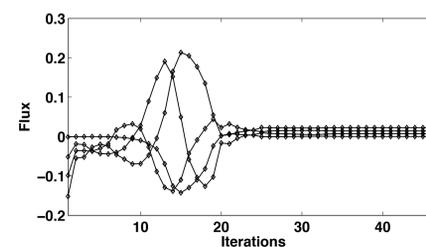
Ratio Optimization



Direct Optimization



M1qn3 can solve the non-linear optimization problem for ratio measurements of CH₄ and CO₂. The gradient method accounts for the uncertainty in CO₂, which biases the solution of the Direct approach



Solutions converge to values that are close to the 'truth' in less than 20 iterations (for gradient norm reduction in order of 10⁴)

	Ratio	Direct
Norm Flux diff (ppm)	4.329e-5	1.678e-3
Iterations performed	47	16
Gradient norm reduction	3.8 e-10	0.5299 -13

Compared to direct method, Ratio method is able to optimize the fluxes and concentrations more efficiently.

Conclusions: The test shows that Ratio method is more accurate in finding a posterior solution. It promises to be a potential tool for reducing the uncertainty in flux calculation by Atmospheric models. The next step is to implement this method on Global transport model, such as TM5.

References

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