Characterizing model errors in inverse modelling of CH_4 and CO_2 fluxes using weak constraint 4D-Var

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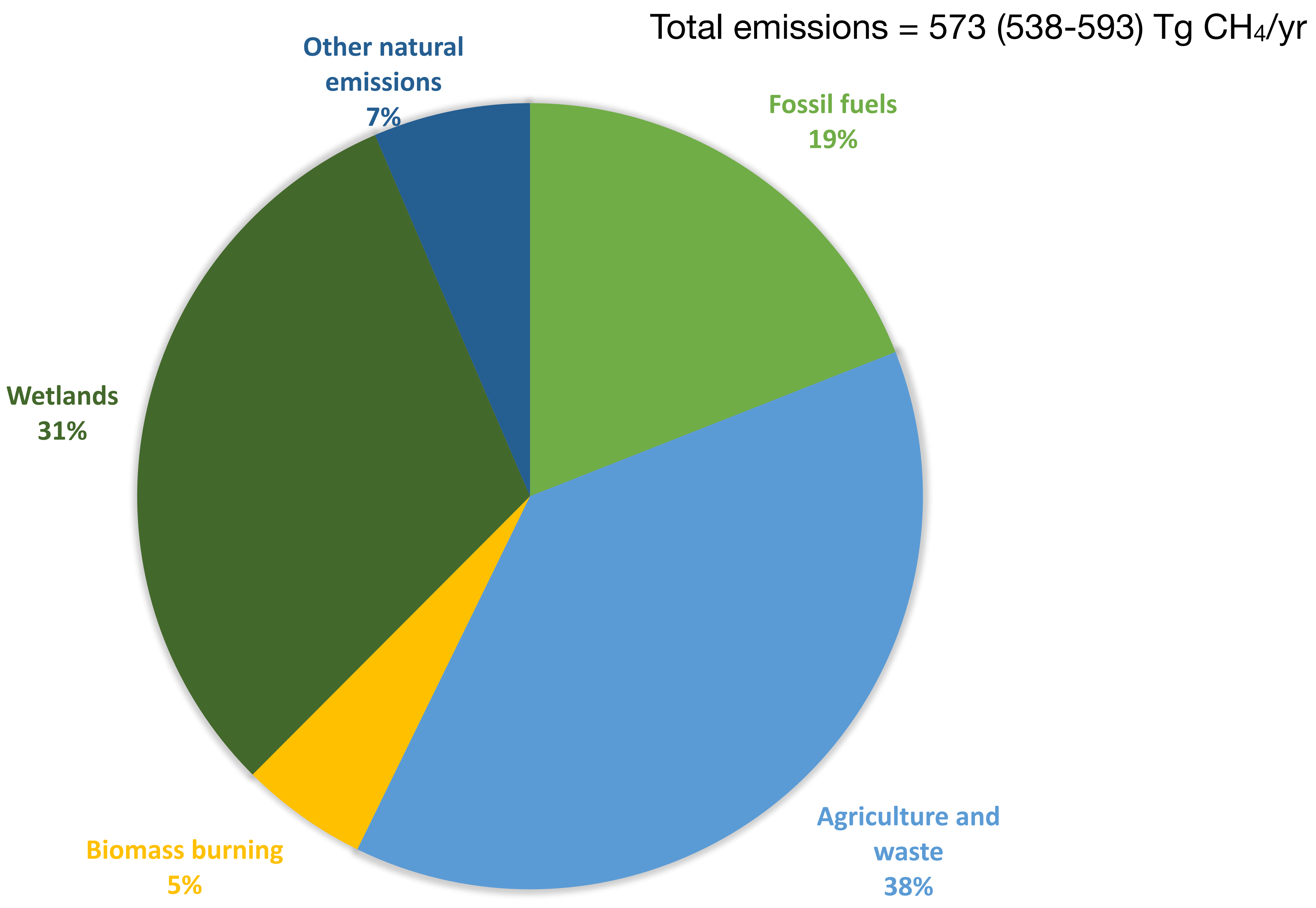
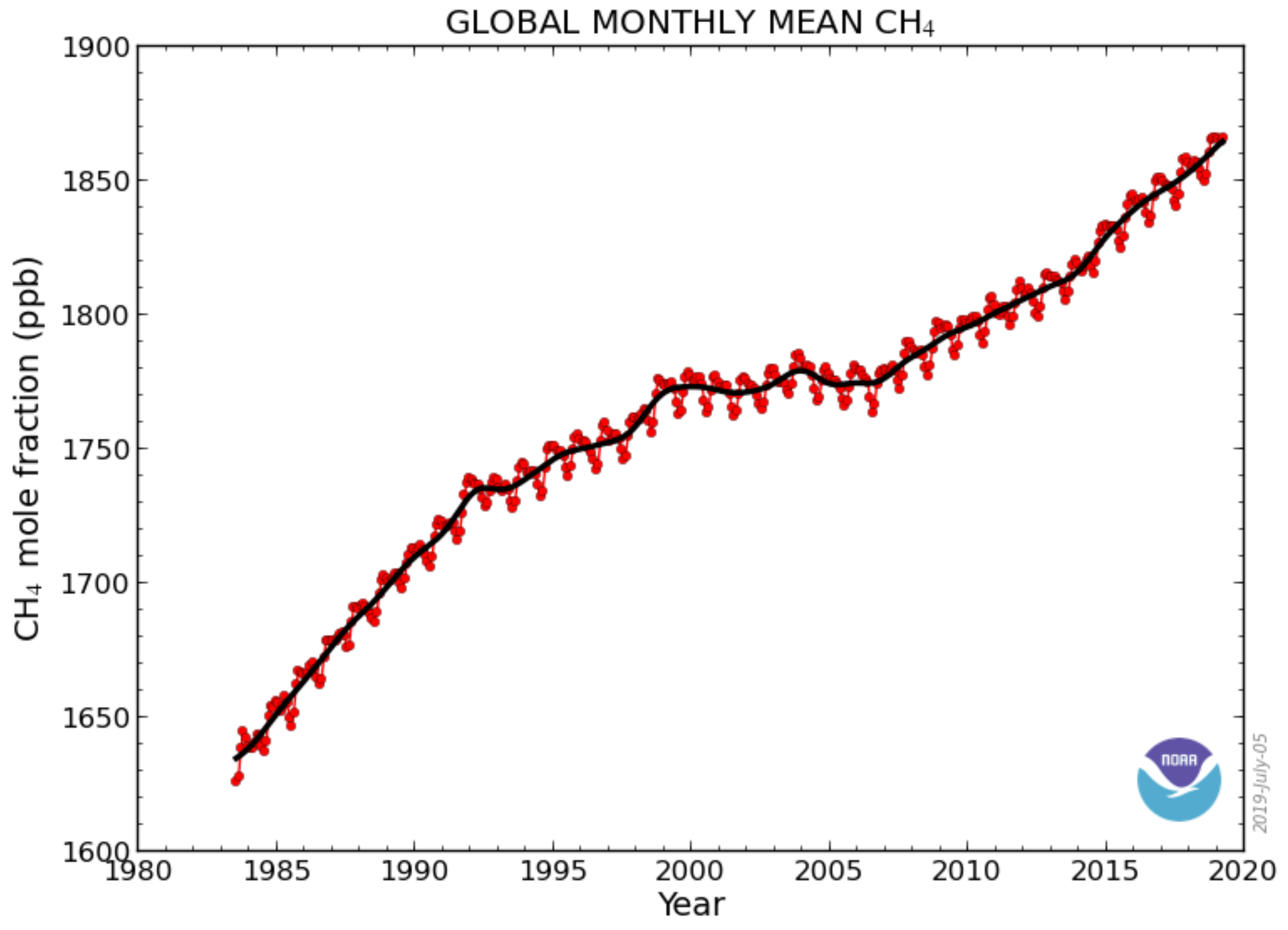
The methane budget

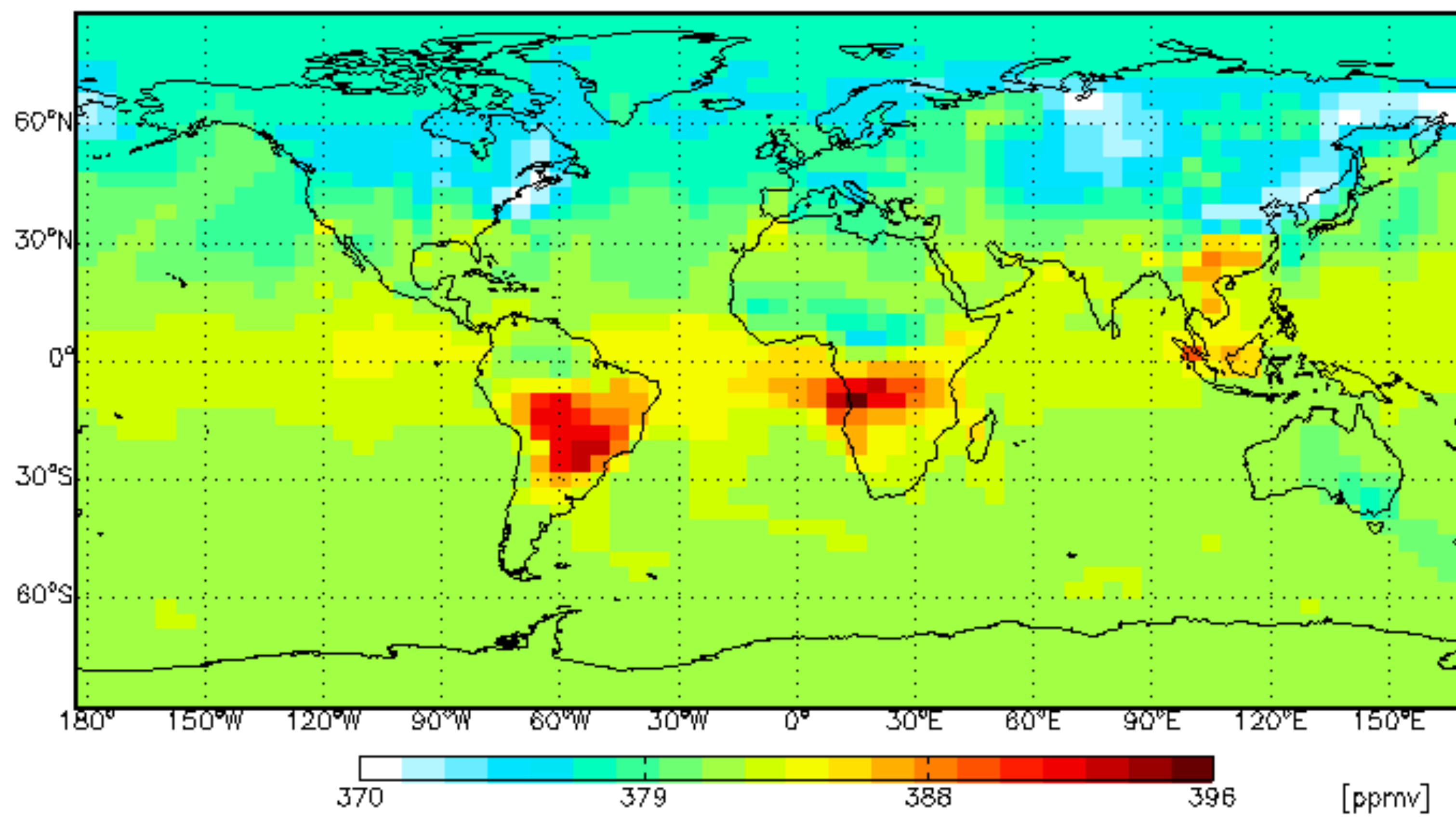




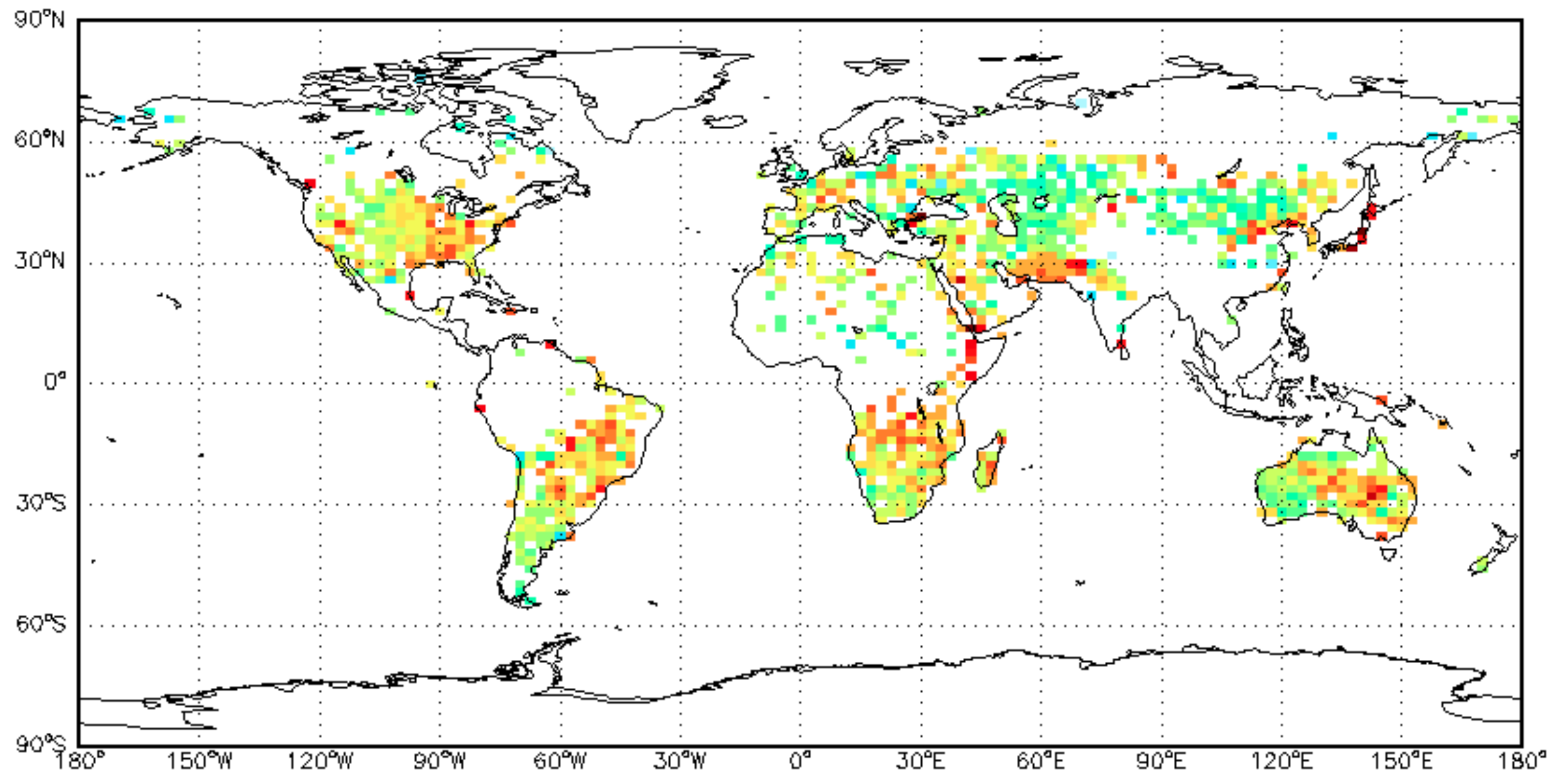
- Methane, in addition to being second most important greenhouse gas, and is a source of stratospheric water vapour and tropospheric ozone, which are also greenhouse gases.
- Anthropogenic emissions account for about 60% of total emissions. Emissions from wetlands are the largest natural source of methane.
- Atmospheric concentrations of methane stabilized between 2000–2007, but the cause of the stabilization and the subsequent increase in the growth rate is uncertain.

Inverse modeling of fluxes

Modeled CO_2 ($\mathbf{x}$)

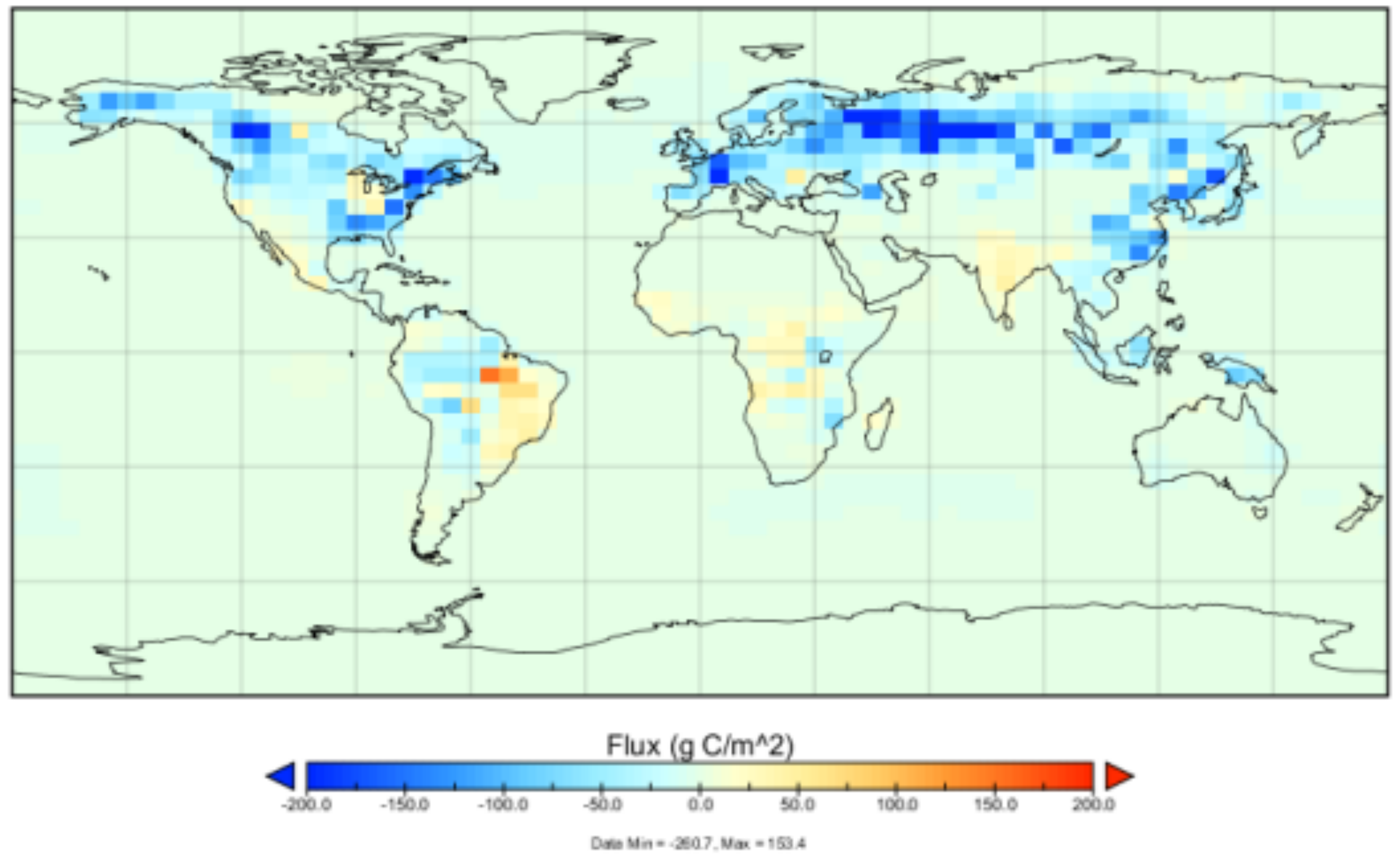


Observed CO_2 ($\mathbf{y}$)



atmospheric
model (M)

A Priori Fluxes ($\mathbf{p}^b$)



$$J(\mathbf{p}) = \frac{1}{2}[\mathbf{y} - H(M(\mathbf{x},\mathbf{p}))]^T\mathbf{R}^{-1}[\mathbf{y} - H(M(\mathbf{x},\mathbf{p}))] + \frac{1}{2}(\mathbf{p}-\mathbf{p}^b)^T\mathbf{B}_p^{-1}(\mathbf{p}-\mathbf{p}^b)$$

$$\mathbf{x}_{i+1} = M(\mathbf{x}_i, \mathbf{p})$$

$$\mathrm{B}_p = \text{A priori flux error covariance matrix}$$

$$\mathbf{p}^a = \mathbf{p}^b + (\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H} + \mathbf{B}_p^{-1})^{-1}\mathbf{H}^T\mathbf{R}^{-1}(\mathbf{y} - \mathbf{H}\mathbf{p}^b)$$

Flux estimation with strong constraint 4D-Var

For the flux estimation problem using 4D-Var, the cost function takes the form

$$J(\mathbf{x}_0, \mathbf{p}) = \frac{1}{2}\sum_{i=0}^{N}[\mathbf{y}_i - H_i(M_{i,0}(\mathbf{x}_0, \mathbf{p}))]^T \mathbf{R}^{-1}[\mathbf{y}_i - H_i(M_{i,0}(\mathbf{x}_0, \mathbf{p}))]$$
$$+ \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}^b) + \frac{1}{2}(\mathbf{p} - \mathbf{p}^b)^T \mathbf{B}_p^{-1}(\mathbf{p} - \mathbf{p}^b)$$

However, often the initial state is not optimized as part of the inversion so the form of the cost function most widely used is as follows:

$$J(\mathbf{p}) = \frac{1}{2}\sum_{i=0}^{N}[\mathbf{y}_i - H_i(M_{i,0}(\mathbf{x}_0, \mathbf{p}))]^T \mathbf{R}^{-1}[\mathbf{y}_i - H_i(M_{i,0}(\mathbf{x}_0, \mathbf{p}))]$$
$$+ \frac{1}{2}(\mathbf{p} - \mathbf{p}^b)^T \mathbf{B}_p^{-1}(\mathbf{p} - \mathbf{p}^b)$$

- Here the control variable is just the surface fluxes ($\mathbf{p}$).
- In this case, other approaches are used to obtain a suitable initial state.
- Any discrepancies in the initial state and/or the evolution of the initial state will be projected onto the estimated fluxes.

Weak constrain 4D-Var: Accounting for model errors

Model evolution: $\mathbf{x}_i = M_i(\mathbf{x}_{i-1}) + \eta_i$

Cost function:

$$
\begin{aligned}
J(\mathbf{x}) =& \frac{1}{2}\sum_{i=0}^{N}[\mathbf{y}_i - H_i(\mathbf{x}_i)]^T\mathbf{R}^{-1}[\mathbf{y}_i - H_i(\mathbf{x}_i)] \\
&+ \frac{1}{2}\sum_{i=1}^{N}[\mathbf{x}_i - M_i(\mathbf{x}_{i-1})]^T\mathbf{Q}^{-1}[\mathbf{x}_i - M_i(\mathbf{x}_{i-1})] \\
&+ \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}^b)
\end{aligned}
$$

- $\mathbf{Q}$ is the model error covariance.
- The control variable is the full 4-D state vector.

[Adapted from Trémolet (2006)]

Weak constrain 4D-Var: Accounting for model errors

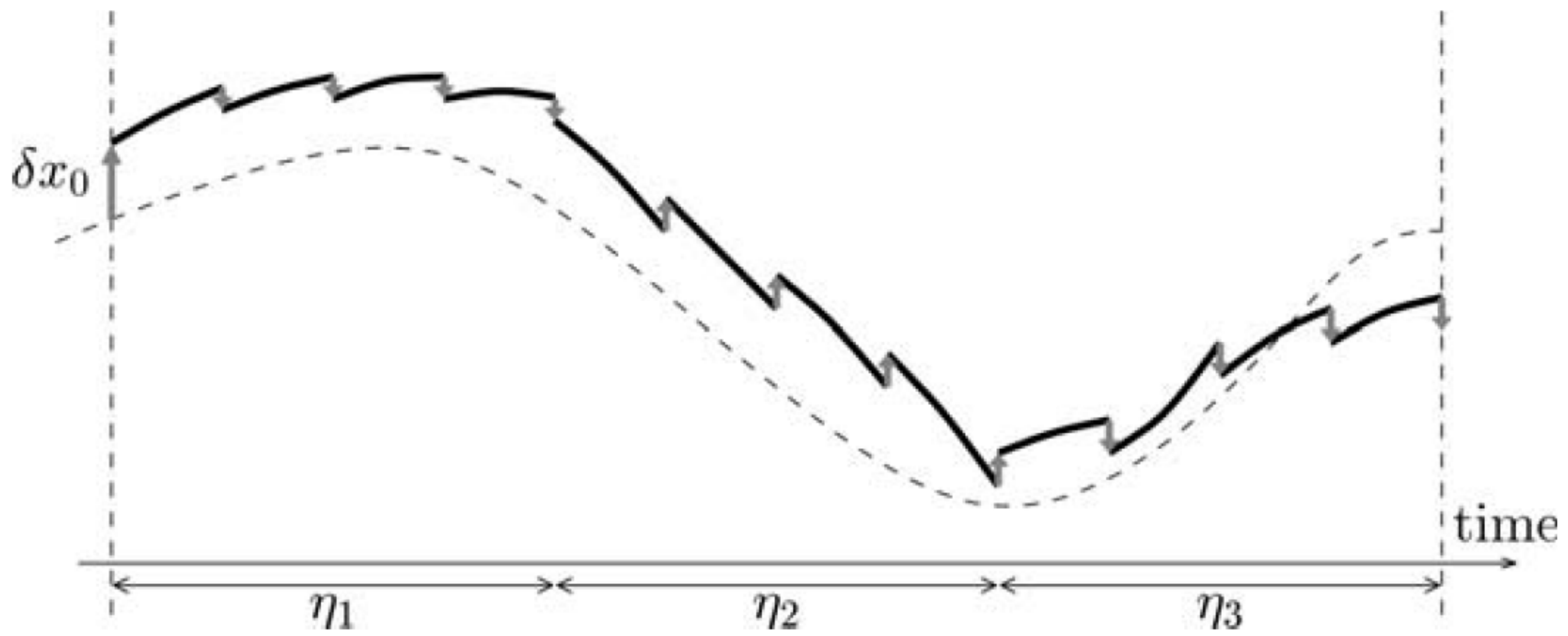
An alternative approach is to solve for the initial state ($\mathbf{x}_0$) and the model error forcing ($\boldsymbol{\eta}$).

$$\mathbf{x}_{i+1} = M_i(\mathbf{x}_i) + \eta_{i+1}$$

$$J(\mathbf{x}_0, \eta) = \frac{1}{2}\sum_{i=1}^{N}[\mathbf{y}_i - H_i(M_{i,0}(\mathbf{x}_0))]^T\mathbf{R}^{-1}[\mathbf{y}_i - H_i(M_{i,0}(\mathbf{x}_0))]$$

$$+ \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}^b) + \frac{1}{2}\sum_{i=1}^{N}\eta_i^T\mathbf{Q}_i^{-1}\eta_i$$

The model error forcing ($\boldsymbol{\eta}$) is assumed to be constant over a given interval, which can be as short as the model time step or as long as the whole assimilation window (in which case we are solving for a bias in the assimilation).



[Trémolet, 2006]

Weak constrain 4D-Var: Accounting for model errors

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A Variational Continuous Assimilation Technique

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(Manuscript received 12 January 1989, in final form 8 May 1989)

ABSTRACT

A variational assimilation technique is presented which continuously adjusts a model solution by introducing a correction term to the model equations. The technique is essentially a modification of the adjoint technique. The Variational Continuous Assimilation (VCA) technique optimizes the correction to the model equations rather than the initial conditions as is done in the adjoint technique.

The VCA-technique characteristics were examined by inserting independent analyses into a simple quasi-geostrophic model using both the VCA technique and the adjoint technique. Because the model equations do not have to be satisfied exactly in the VCA technique, some of the effects of systematic model errors can be removed from the assimilation. Thus, the VCA technique was able to consistently fit the data better than the adjoint technique. Predictions from the results from the assimilation techniques showed that the forecast from the adjoint technique's solution was consistently inferior to those from the VCA technique and those from the Geophysical Fluid Dynamics Laboratory's (GFDL's) First GARP (Global Atmospheric Research Program) Global Experiment (FGGE) IIIb analyses. As a by-product of the VCA technique, an empirical correction for the model's systematic error is produced. Application of this correction during a forecast produced substantially improved simulations.

Flux estimation with weak constraint 4D-Var

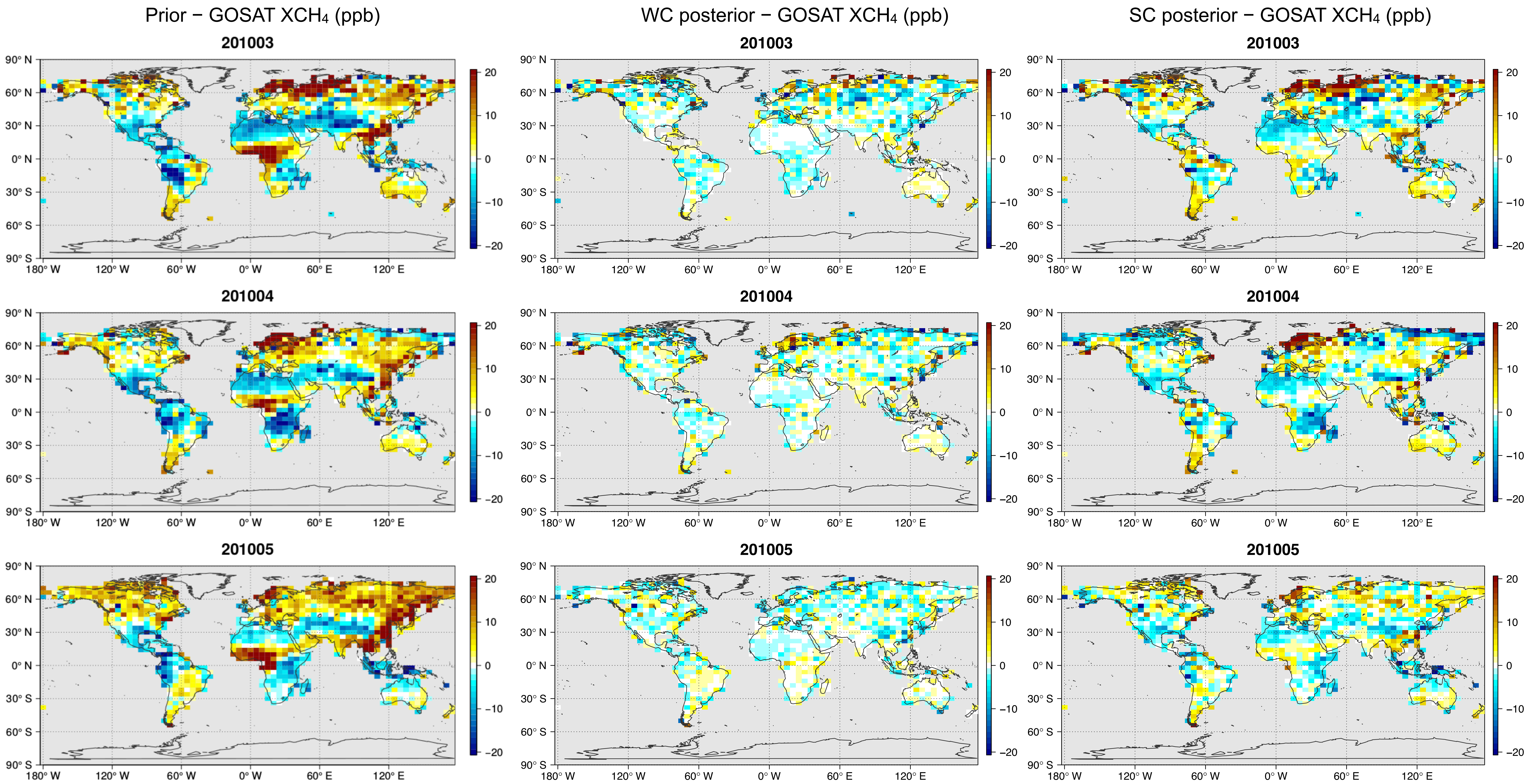
$$J(\mathbf{p},\eta) = \frac{1}{2}\sum_{i=1}^{N}[\mathbf{y}_i - H_i(M_{i,0}(\mathbf{x}_0))]^T\mathbf{R}^{-1}[\mathbf{y}_i - H_i(M_{i,0}(\mathbf{x}_0))]$$

$$+ \frac{1}{2}(\mathbf{p}-\mathbf{p}^b)^T\mathbf{B}_p^{-1}(\mathbf{p}-\mathbf{p}^b) + \frac{1}{2}\sum_{i=1}^{M}\eta_i^T\mathbf{Q}_i^{-1}\eta_i$$

- We used v35 of the GEOS-Chem adjoint model.
- GEOS-Chem was run with GEOS-5.2.0 meteorology at horizontal resolutions of 4°x5° and 2°x2.5°.
- GOSAT XCH_4 retrievals over land were assimilated from February – May 2010 to optimize the CH_4 state and emissions.
- The model was evaluated using data from the Total Carbon Column Observing Network (TCCON) and the Atmospheric Chemistry Experiment Fourier Transform Spectrometer (ACE-FTS).
- Assumptions:
  - ➡ Initial conditions $\mathbf{x}_0$ are from a previous strong constraint emission optimization using GOSAT XCH_4 data
  - ➡ Diagonal $\mathbf{Q} = q\mathbf{I}$, with $q = 50$ ppb.
  - ➡ The forcing terms were optimized every 3 days.
  - ➡ $\mathbf{B}_p$ is diagonal with a uniform emission error of 50%.
  - ➡ $\mathbf{R}$ is based on the reported GOSAT retrieval uncertainty, which was inflated to match the GOSAT scatter against TCCON observations.

Assimilation of GOSAT XCH_4 data

Differences in monthly mean CH_4 column abundances between the model and GOSAT

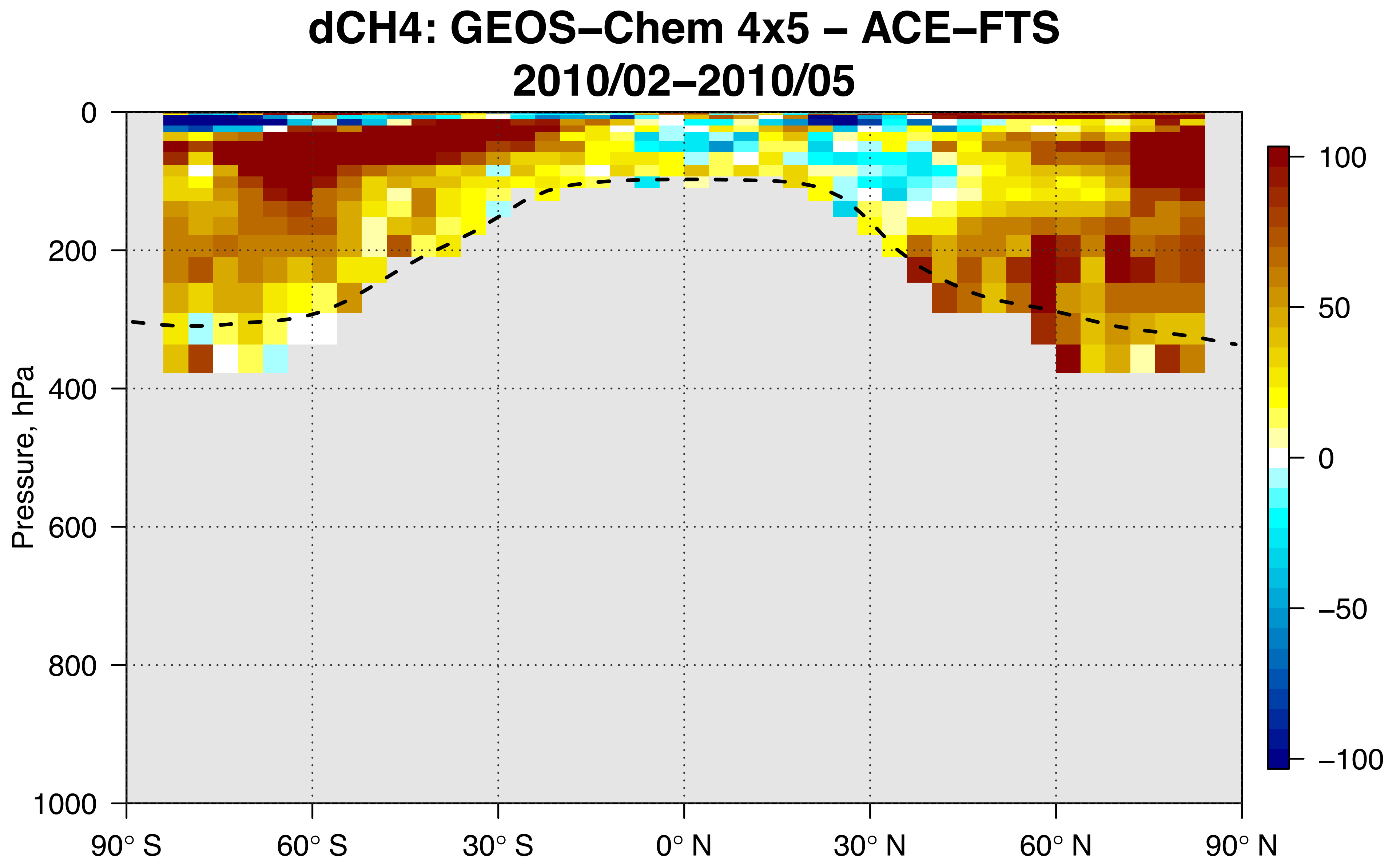


[Stanevich et al., 2021]

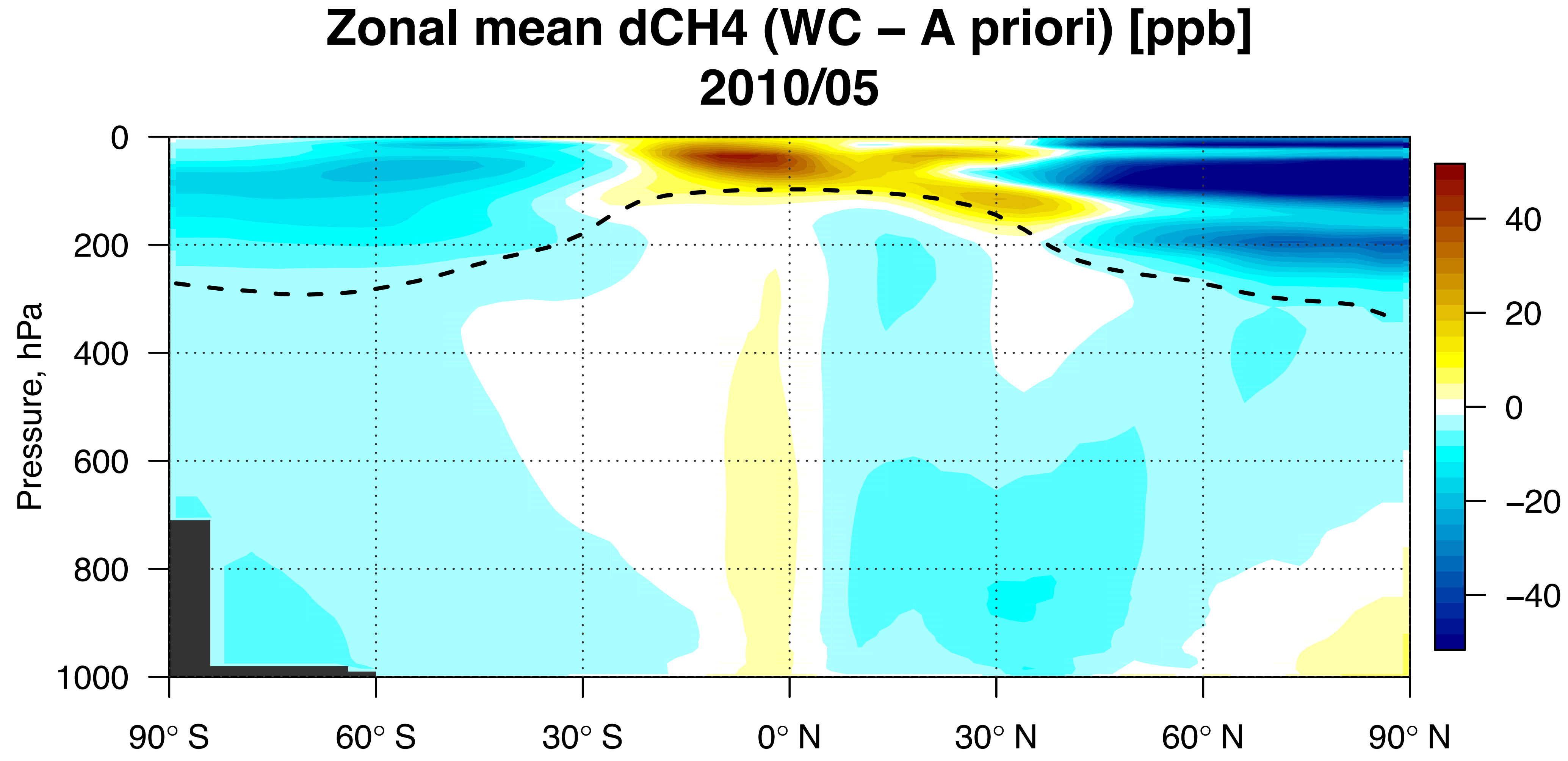
The weak constraint (WC) assimilation at 4°x5° successfully reduced the model biases relative to GOSAT, whereas there is more residual structure in the strong constraint (SC) (emission optimization) assimilation.

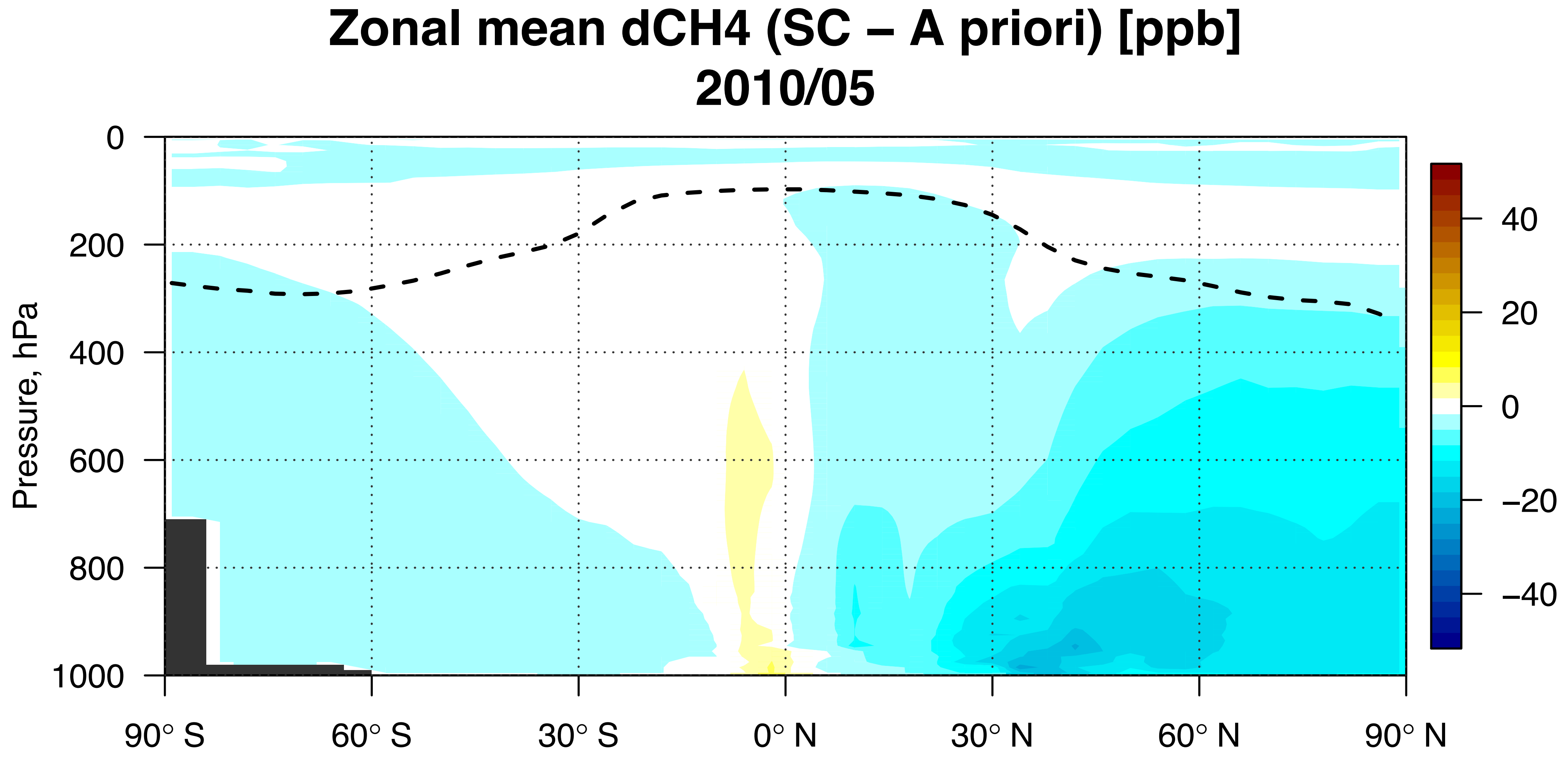
Model biases in the stratosphere

Comparison of the prior with ACE-FTS CH_4 retrievals



Differences in zonal mean CH_4 between the posterior and prior fields in May 2010





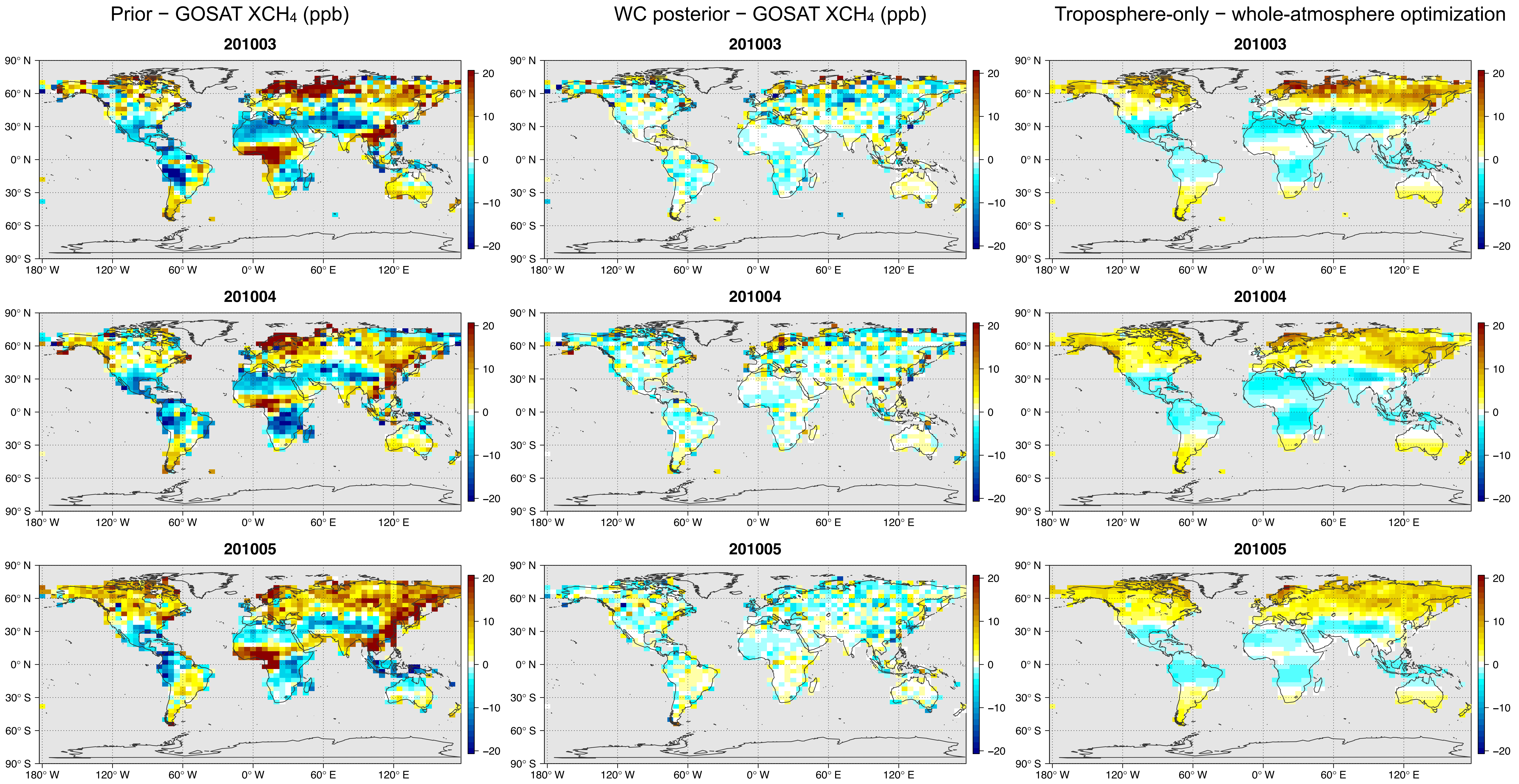
- The GEOS-Chem a priori stratosphere at 4°x5° is positively biased against ACE-FTS at middle to high latitudes and is negatively biased in the tropics.
- The WC 4D-Var corrects for the bias in the model stratosphere.
- SC 4D-Var (which can adjust only the emissions) cannot mitigate the stratospheric bias.

[Stanevich et al., 2021]

Model biases in the stratosphere

Model minus GOSAT differences

Stratospheric bias in XCH_4

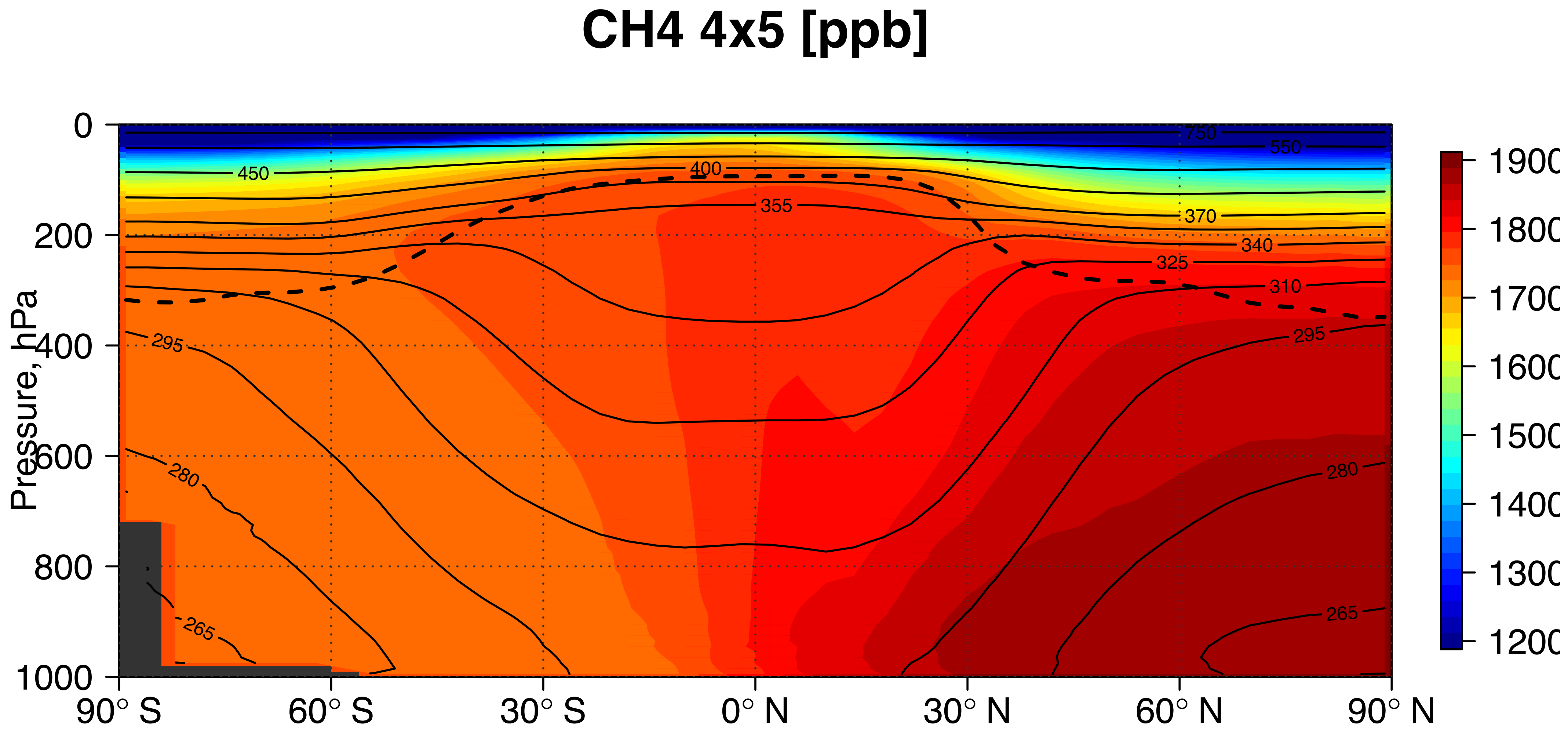


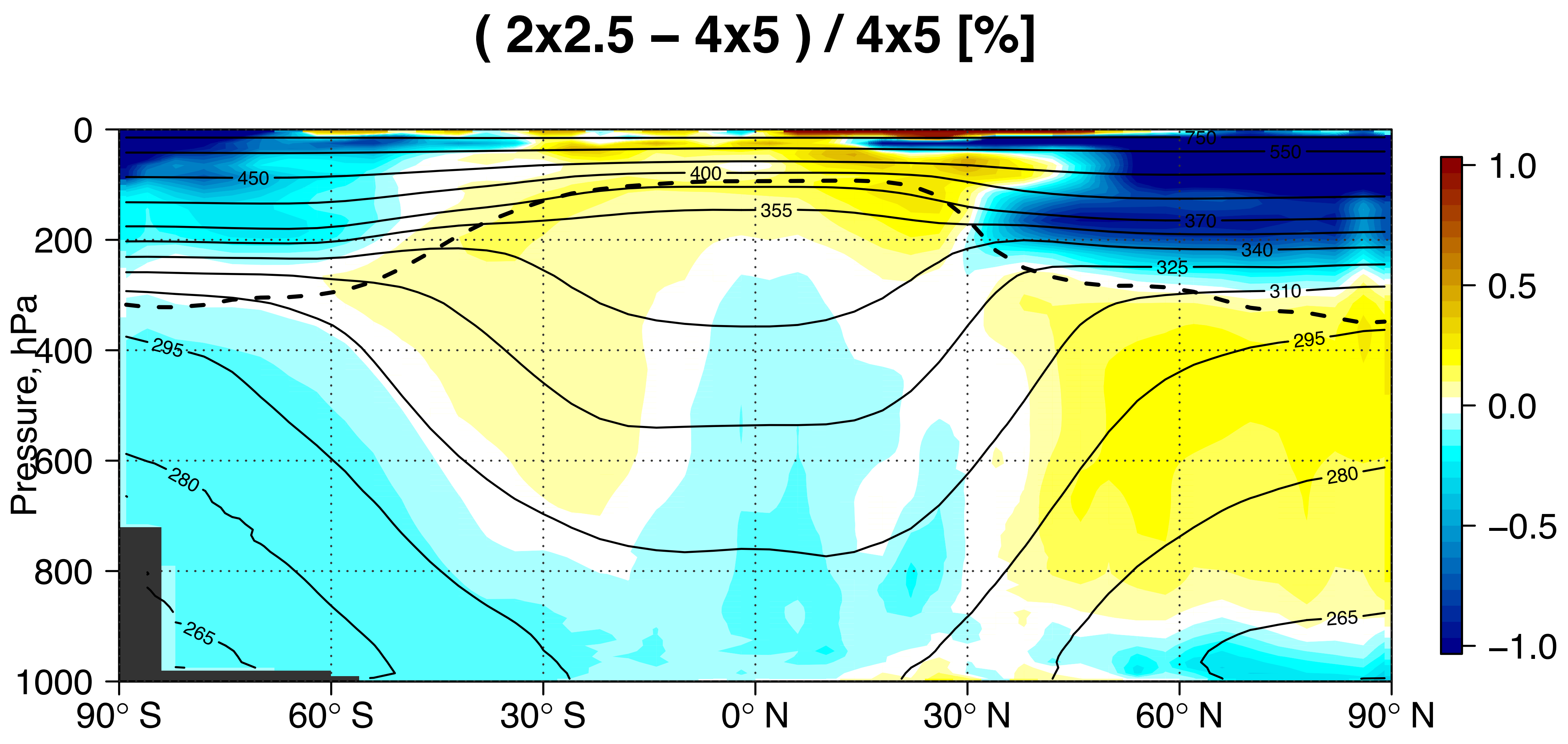
[Stanevich et al., 2021]

The latitude-dependent stratospheric bias in the column is revealed clearly in the differences between the troposphere-only state optimization and the whole-atmosphere (troposphere and stratosphere) state optimization.

Resolution-dependent model biases

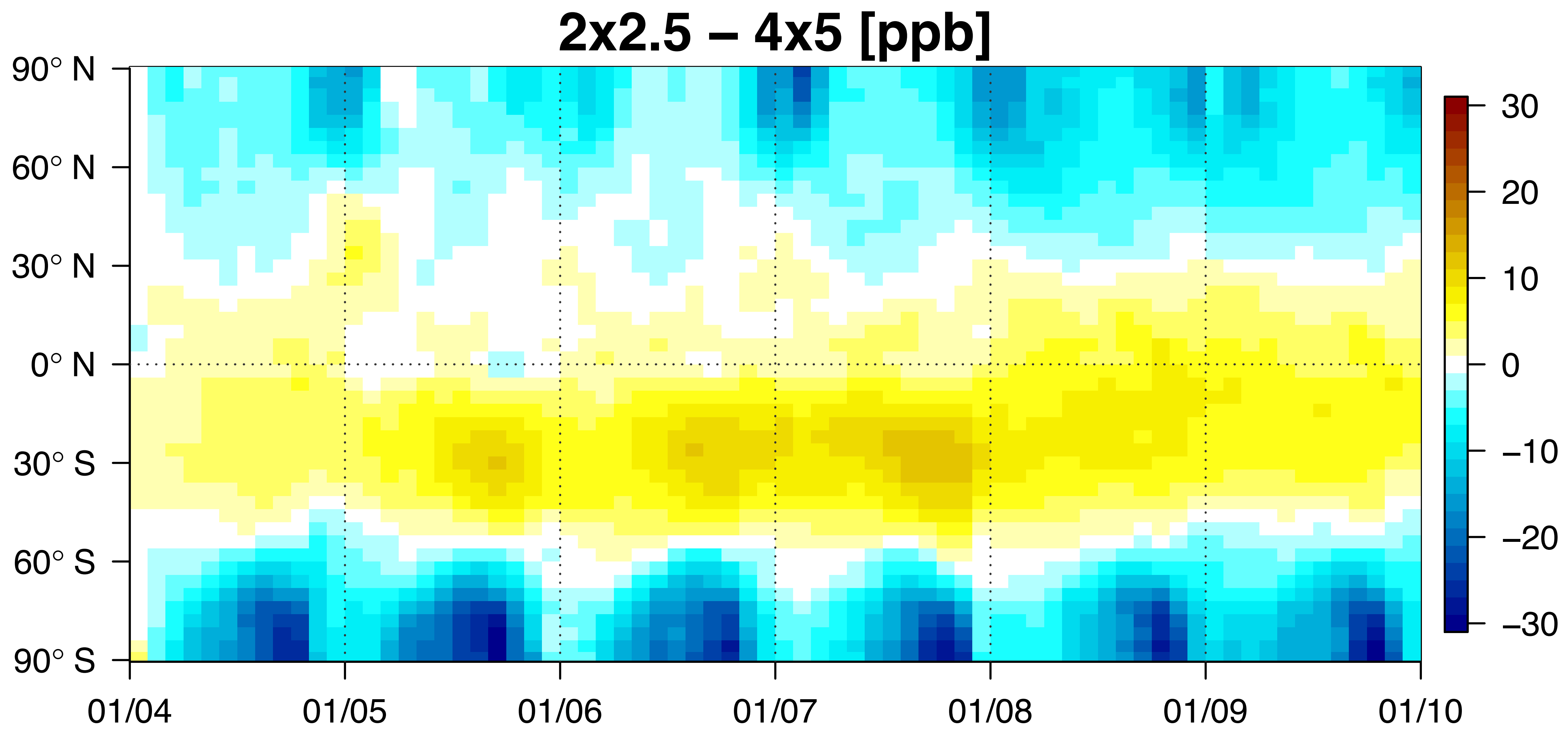
Zonal mean CH_4 in March 2010





[Stanevich et al., 2020]

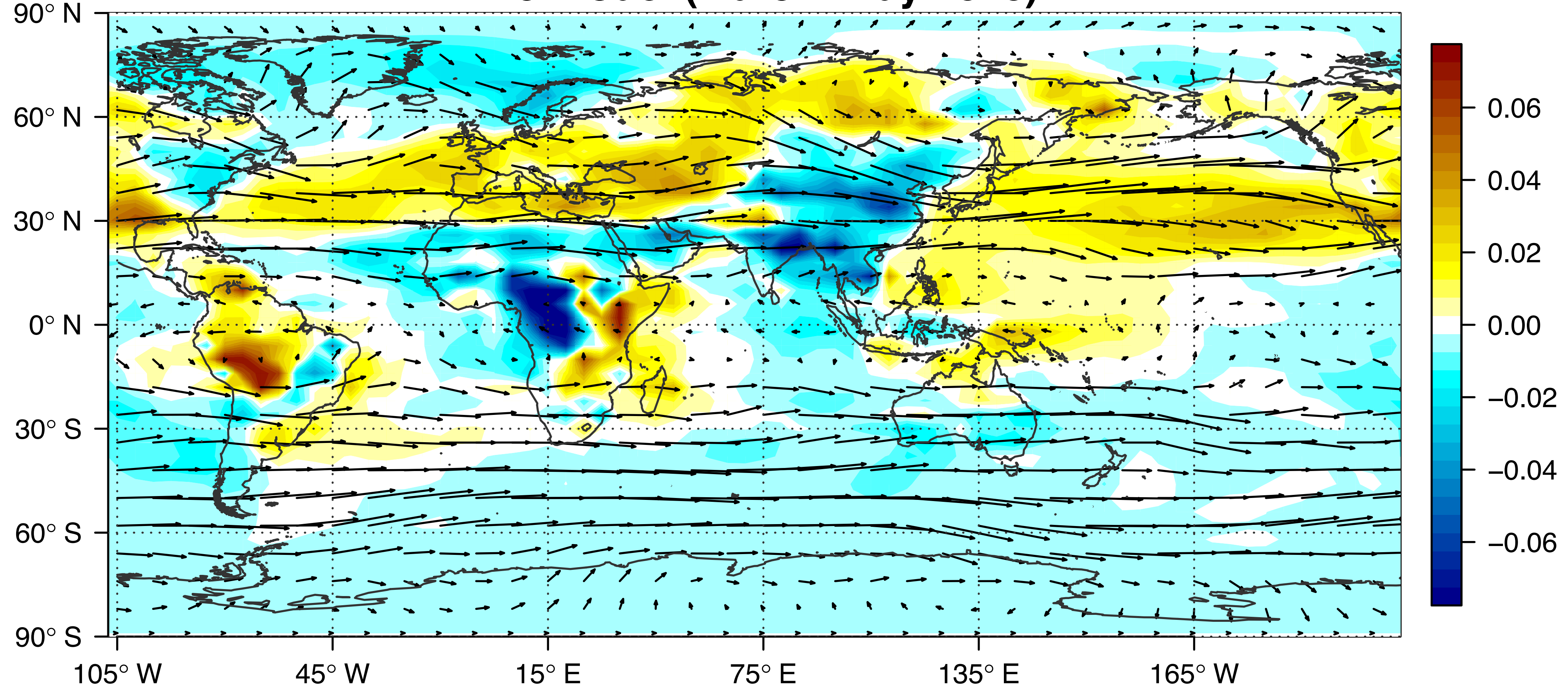
XCH_4 differences between 2°x2.5° and 4°x5° over the period 2004–2010



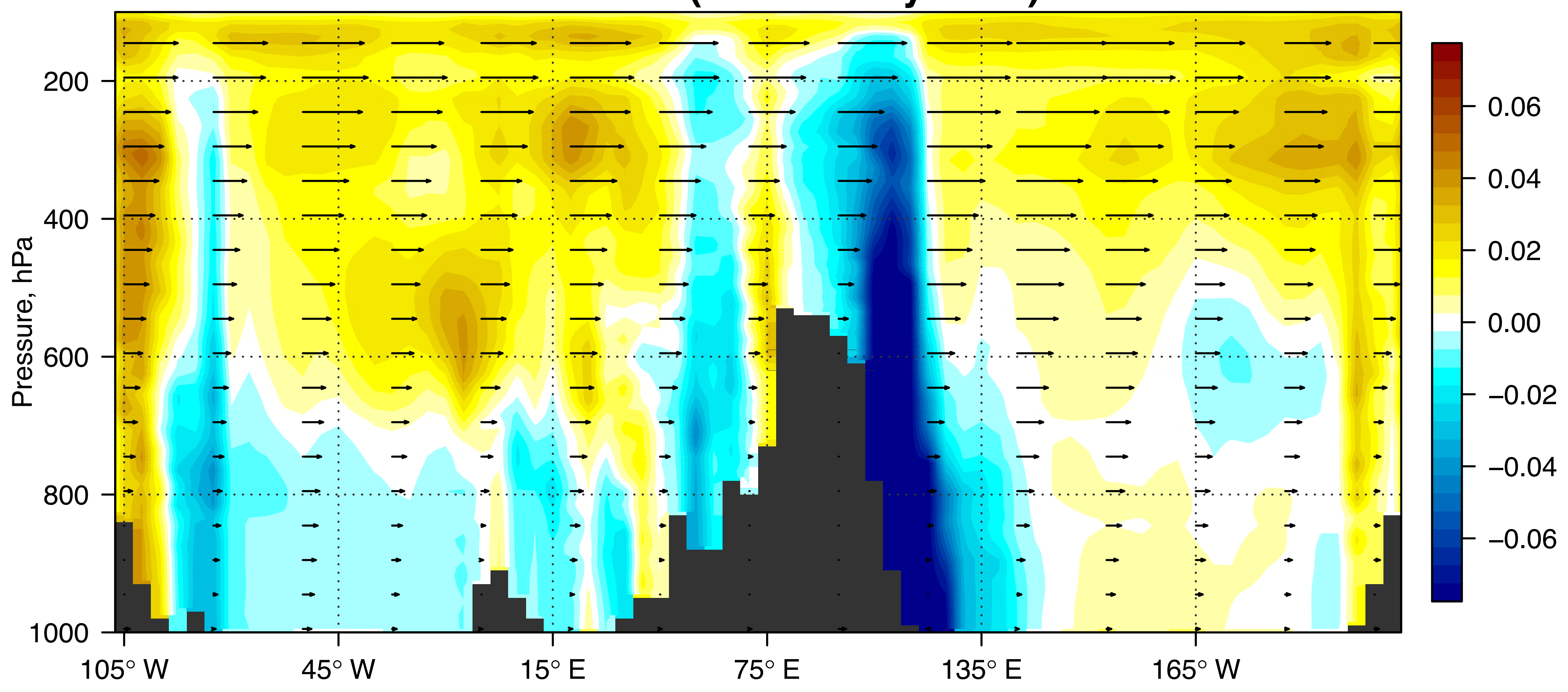
- The modelled columns at 4°x5° are positively biased relative to the 2°x2.5° simulation at middle to high latitudes, and are negatively biased in the tropics.
- At 4°x5° there is more (less) CH_4 in the extratropical (tropical) lower stratosphere than at 2°x2.5°.
- At 4°x5° there is less CH_4 in the northern extratropical free troposphere and more CH_4 in the boundary layer than at 2°x2.5°.

Mean forcing terms (state corrections) in the troposphere for March - May 2010

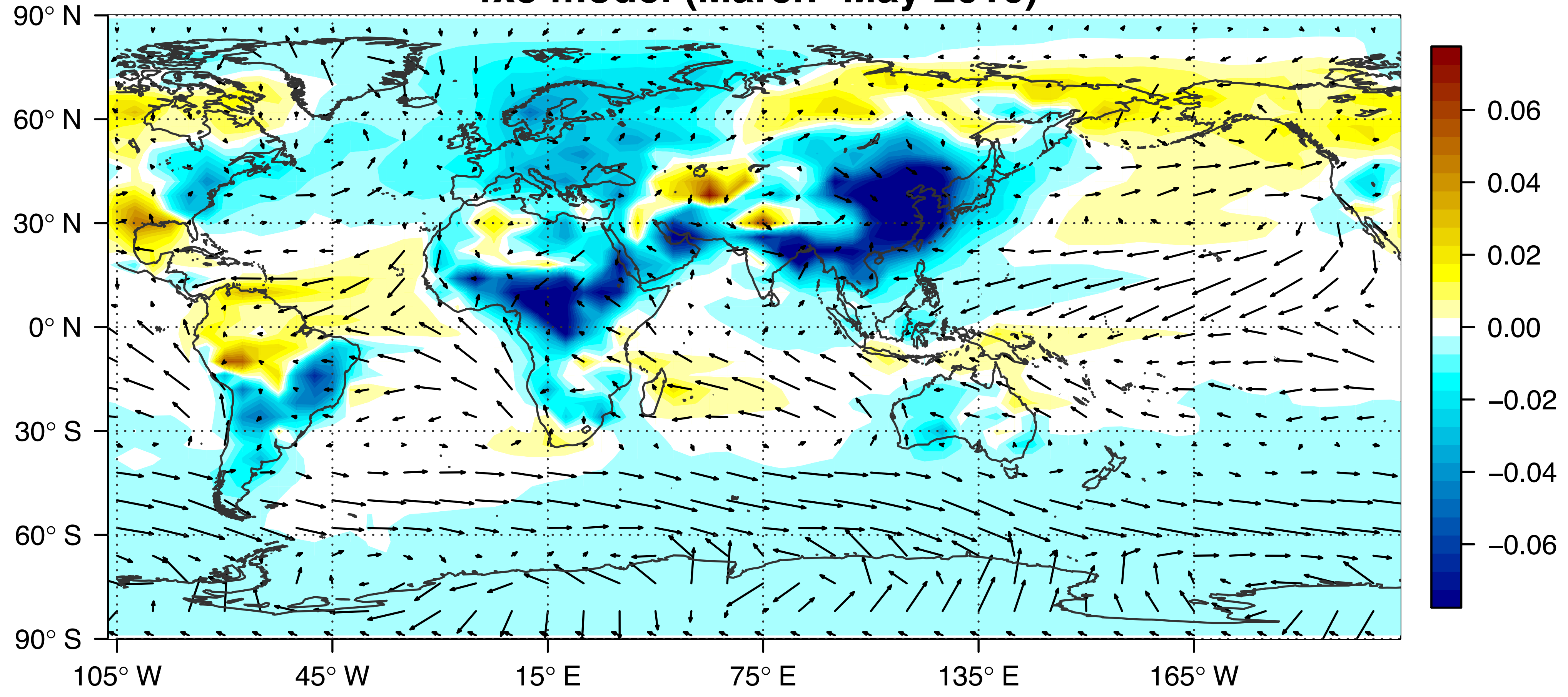
Mean CH4 forcing corrections at 300hPa [ppb]
4x5 model (March–May 2010)



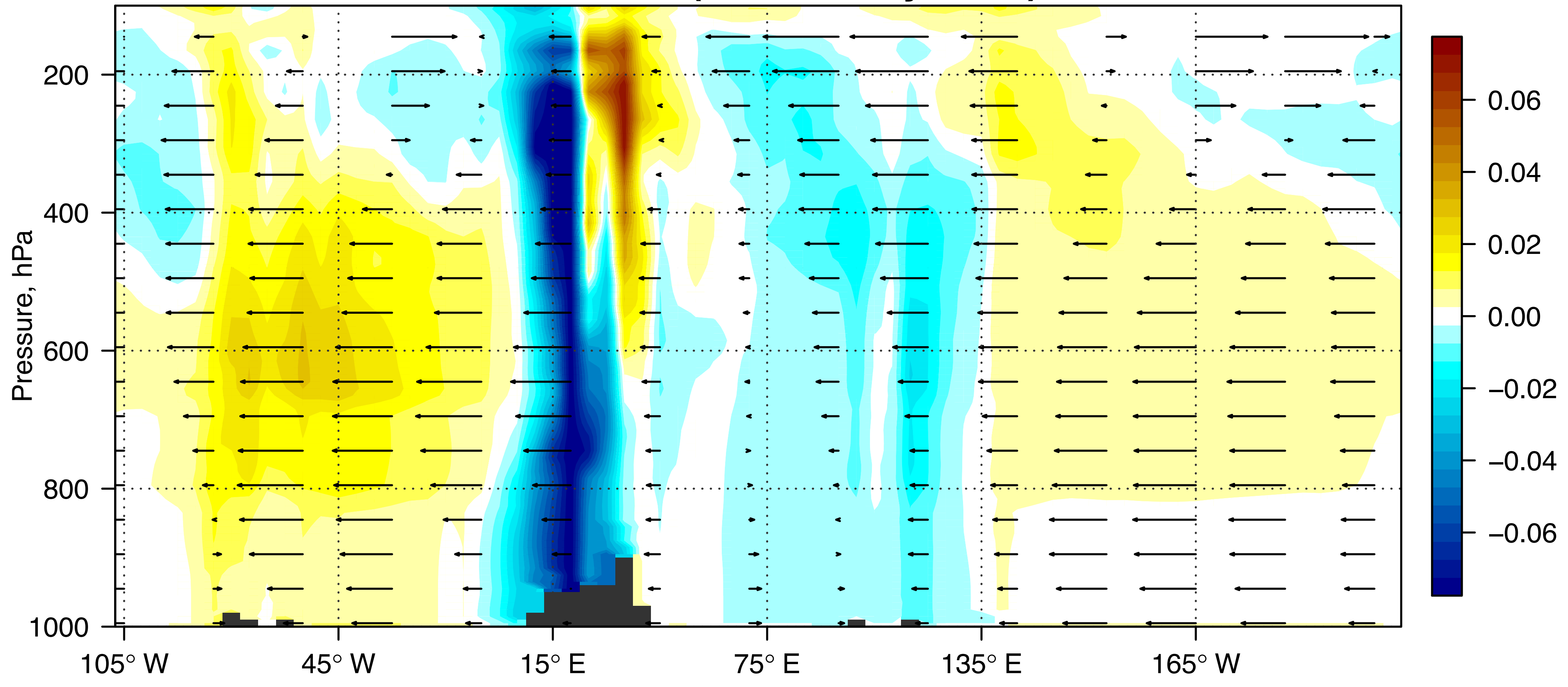
Mean CH4 forcing corrections at 34N [ppb]
4x5 model (March–May 2010)



Mean CH4 forcing corrections at the surface [ppb]
4x5 model (March–May 2010)



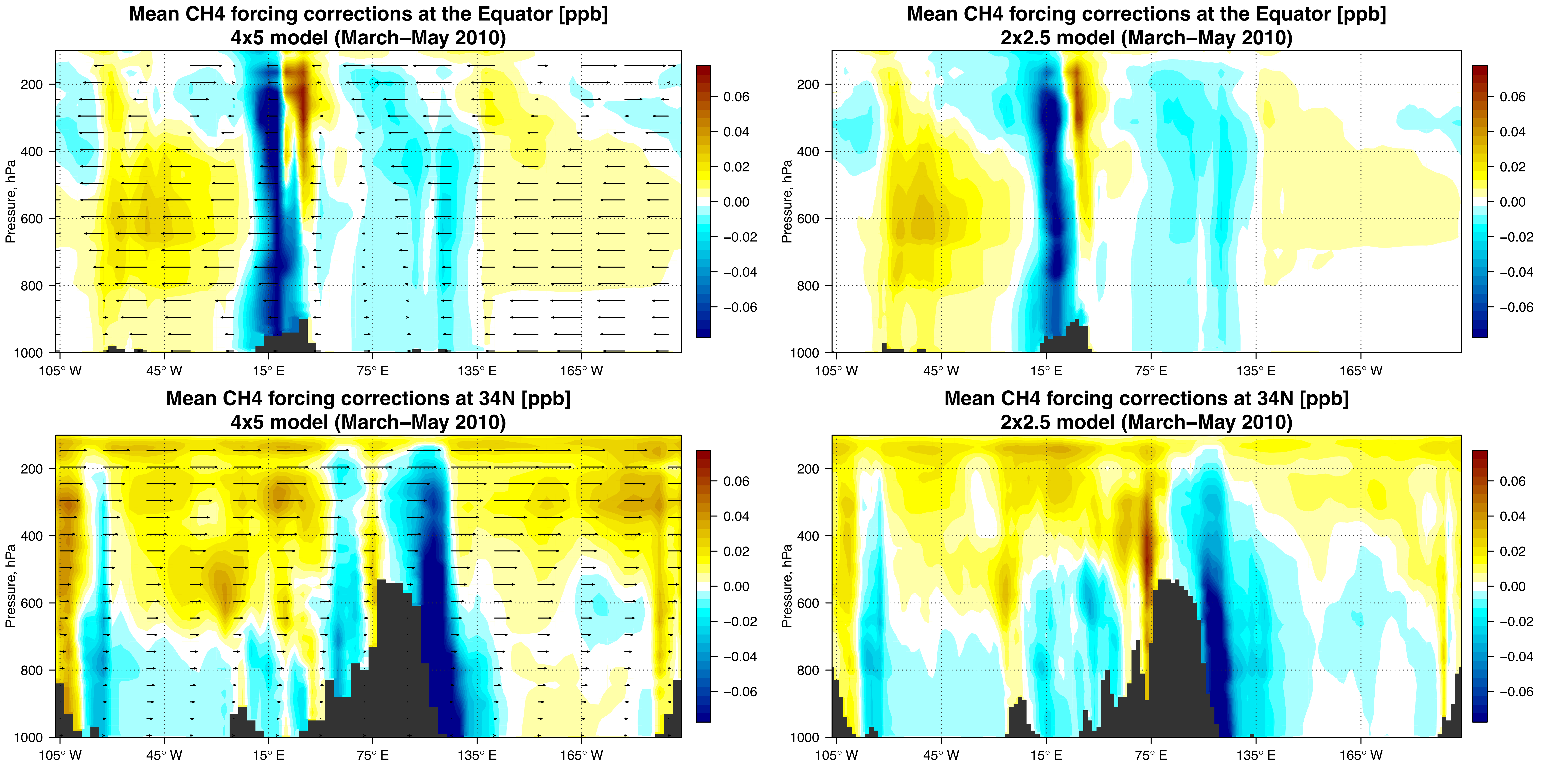
Mean CH4 forcing corrections at the Equator [ppb]
4x5 model (March–May 2010)



[Stanevich et al., 2021]

- Forcing terms reduced CH_4 in the lower troposphere over the major source regions.
- Forcing terms increased CH_4 in the free troposphere, downwind of the major continental source regions, suggesting weakened export of CH_4 in the prior model.

Tropospheric forcing at 4°x5° and 2°x2.5°



Forcing terms are smaller at 2°x2.5° than at 4°x5°, especially in the extratropics.

Evaluation of the 4°x5° weak and strong constraint assimilation with TCCON data

	Mean difference (ppb)			Standard deviation (ppb)			Correlation (R)		
	Prior	SC	WC	Prior	SC	WC	Prior	SC	WC
Sodankylä (67.37° N, 26.63° E)	30.0	25.7	13.7	18.9	19.1	12.6	0.49	0.50	0.81
Bialystok (53.23° N, 23.03° E)	11.9	7.3	5.1	9.3	10.6	8.0	0.39	0.43	0.65
Bremen (53.10° N, 8.85° E)	6.3	3.2	0.7	14.3	15.2	10.5	−0.37	−0.28	0.47
Karlsruhe (49.10° N, 8.44° E)	6.4	4.4	0.8	9.7	9.9	8.9	0.33	0.29	0.49
Orleans (47.97° N, 2.11° E)	3.9	3.5	2.5	8.9	9.6	8.3	0.31	0.30	0.51
Garmisch (47.48° N, 11.06° E)	9.9	10.0	5.7	9.0	9.7	8.4	0.46	0.56	0.65
Park Falls (45.95° N, 90.27° W)	1.9	3.6	2.3	9.7	10.6	8.5	0.37	0.47	0.65
Lamont (36.60° N, 97.486° W)	1.4	3.7	4.4	11.1	11.5	9.4	0.27	0.30	0.49
Izana (28.30° N, 16.5° W)	−5.8	−5.3	3.1	7.6	8.2	6.7	0.64	0.58	0.72
Wollongong (34.41° S, 150.88° E)	7.5	3.9	3.7	8.9	8.8	8.4	0.58	0.55	0.59
Lauder (45.04° S, 169.68° E)	9.6	9.2	5.9	5.6	5.7	5.4	0.72	0.72	0.73

[Stanevich et al., 2021]

The WC optimization improved the correlation and reduced the bias between the model and the TCCON observations.

Conclusions

- Previous work identified biases in the GEOS-Chem model at the 4°x5° resolution in the troposphere and stratosphere and the weak constraint 4D-Var assimilation was able to detect and partly reduce these biases.

- A proper specification of Q is critically needed to help distinguish between the signals from the surface emissions and the other model errors.

- Our results suggest that weak constraint 4D-Var data assimilation could be a valuable tool for diagnosing systematic model errors in inversion analyses.