

On CH₄ inversions using TROPOMI, and how to better combine different measurements (maybe...)

Santiago Parraguez Cerda

Laboratory for Modelling and Observation of the Earth System (LAMOS)

Rasmus Nüß, Nikos Daskalakis, Arjo Segers, Oliver Schneising,
Michael Buchwitz, Mihalis Vrekoussis, Maria Kanakidou

35th International TM5 Meeting
21-22 October 2024
Wageningen, The Netherlands

Overview

1. Motivation
2. Observations and measurements
3. Background
4. Simulations with adaptative factor

1. Motivation

Inverse modelling pillars



Objective

To robustly harmonize data from different sources with uneven amount of observations for inversions

...like TROPOMI and the NOAA network

WHY?

CURRENT?

PROBLEM?

APPROACH?



1. Motivation

2. Observations and measurements

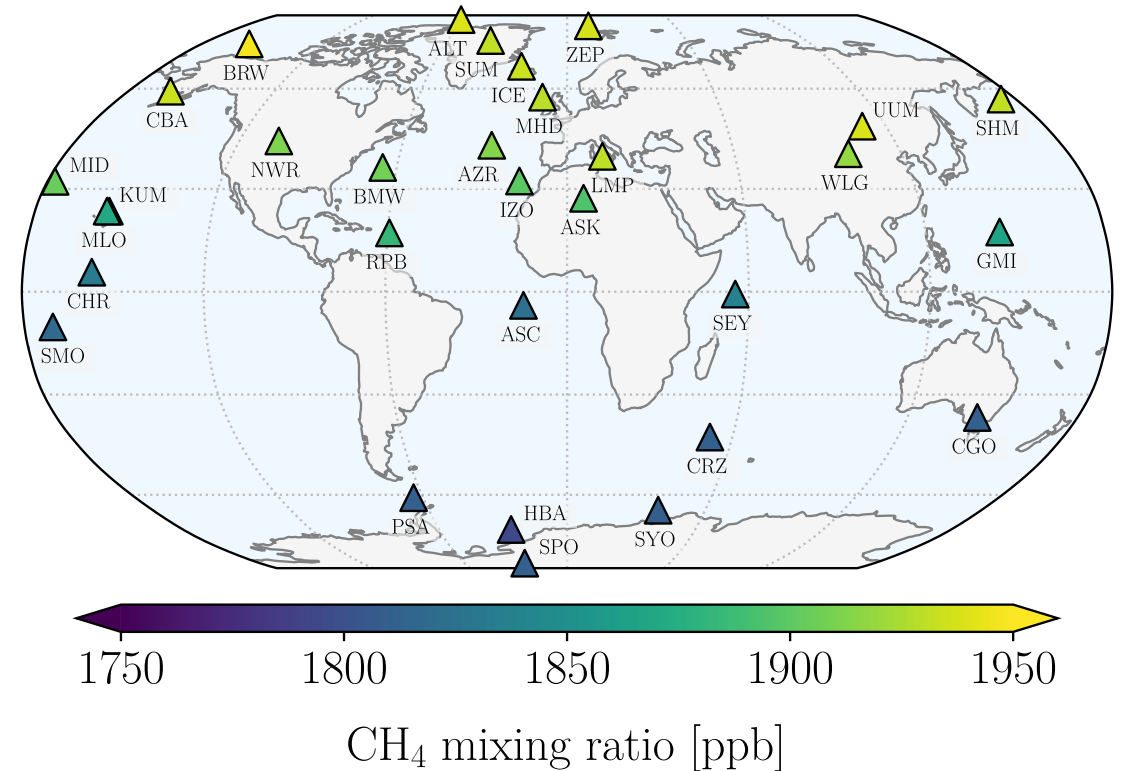
Ground measurements: NOAA

High precision, in-situ measurements

Global background network,
less affected by sources

Sparse temporal coverage

Stations mean XCH₄ for 2018



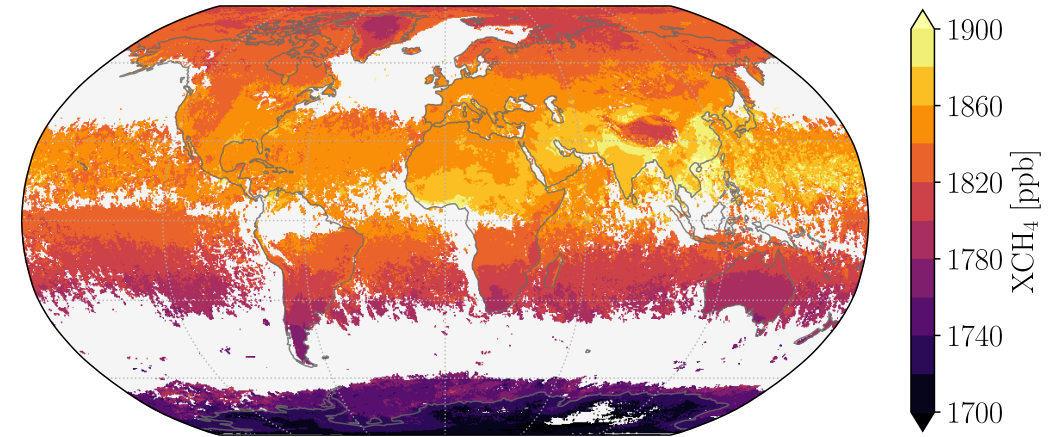
Remote observations: TROPOMI

High resolution data
(up to $7.0 \times 5.5 \text{ km}^2$)

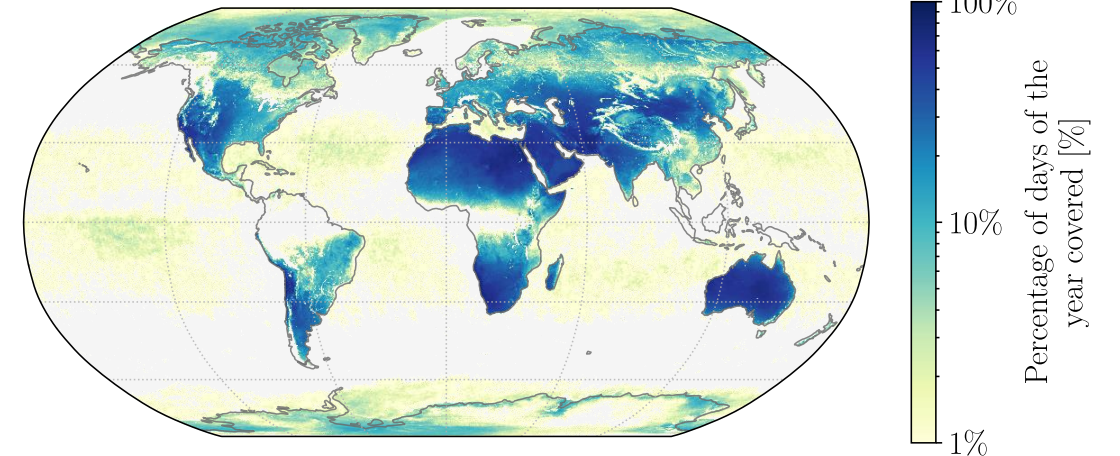
Global daily coverage since 2018
(kind of)

WFMD product covers high latitudes ^[1]

TROPOMI mean XCH₄ for 2018



TROPOMI year XCH₄ coverage for 2018



[1] Schneising et al. (2023). Advances in retrieving XCH₄ and XCO from Sentinel-5 Precursor: improvements in the scientific TROPOMI/WFMD algorithm. In *Atmos. Meas. Tech.*

TROPOMI

Atmospheric total column

General constrain over
atmosphere

142,000,000 pixels per year

NOAA

Point measurement

Constrain near-surface
concentrations

1,200 measurements per year

WHY

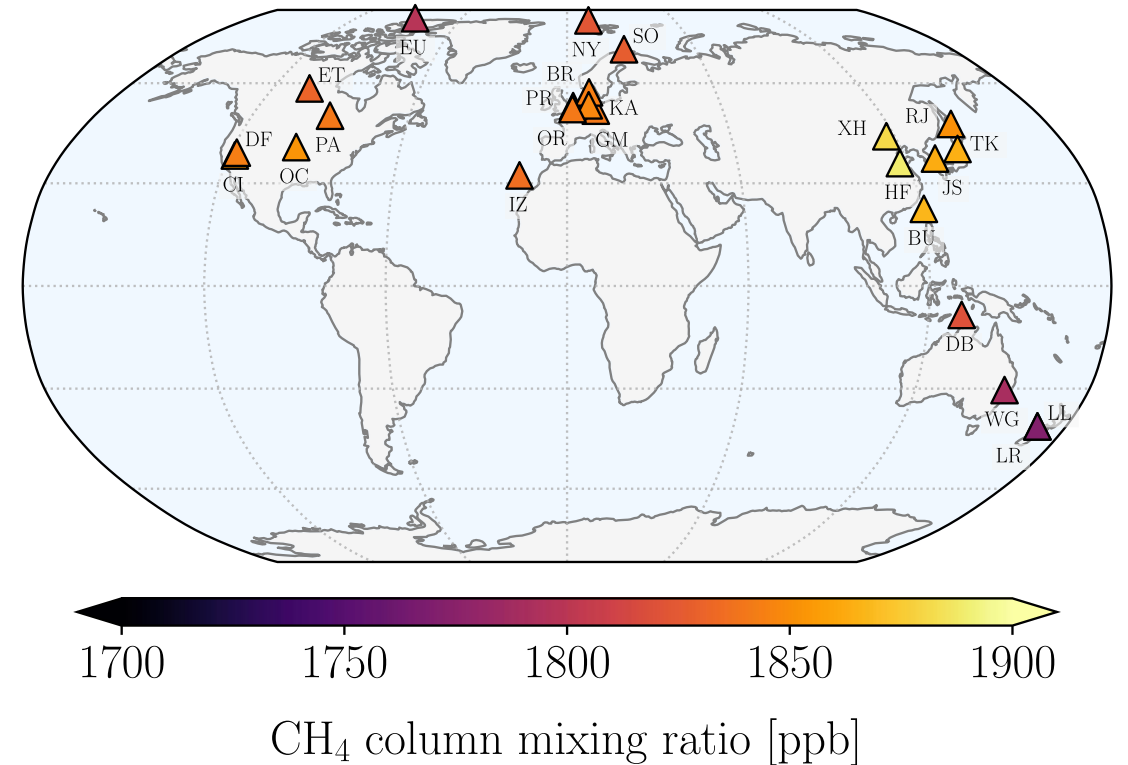
Ground measurements: TCCON

Ground-based total column observations

Accurate and precise,
widely used for validation

Sites not globally distributed

Site mean total column for 2018



1. Motivation
2. Observations and measurements

3. Background

Cost function

$$\min_x J(x) = J_{bg}(x) + \sum_k J_{obs}(x)$$

- Aim to find the background state x to minimize our cost function

Cost function

$$J_{obs}(x) = \sum_i \frac{(F(x_i) - y_i)^2}{\sigma_i^2}$$

- Aim to find the background state x to minimize our cost function
- Sampling model F at the time and point of observations y
- Variance σ^2 comprises both model sampling error and observation error

Cost function

$$J_{obs}(x) = \frac{1}{I^2} \sum_i \frac{(F(x_i) - y_i)^2}{\sigma_i^2}$$

- Aim to find the background state x to minimize our cost function
- Sampling model F at the time and point of observations y
- Variance σ^2 comprises both model sampling error and observation error
- Inclusion of inflation factor I decreases weight of cost function

Inflation factor for TROPOMI

- Constant factor applied as variance inflation in previous works
- Factors used:
 - $I = \sqrt{50}$ or $I = \sqrt{150}$
- TROPOMI need higher inflation factor to compensate amount of pixels ($I = \sqrt{10000}$)
- Massive reduction ignores more isolated pixels

PROBLEM

Weighting factors of satellite data in TM5-4dvar
33rd international TM5 meeting, December 2022

Johann Rasmus Nüß¹
N. Daskalakis¹ and M. Vrekoussis^{1,2,3}

¹IUP-UB; ²MARUM; ³CARE-C

Sixteen years of MOPITT satellite data strongly constrain Amazon CO fire emissions

Stijn Naus^{1,2}, Lucas G. Domingos^{3,4},
John B. Miller⁷, Emanuel
Helen M. Worden¹², Jo

Monitoring emissions from the 2015 Indonesian fires using CO satellite data

Narcisa Nechita-Banda¹, Maarten Krol^{1,2,3}, Guido R. van der Werf⁴,
Johannes W. Kaiser⁵, Sudhanshu Pandey³, Vincent Huijnen⁶,
Cathy Clerbaux^{7,8}, Pierre Coheur⁸, Meritxell
s Röckmann¹

How much CO was

M. Krol^{1,2,3}, W. Peters¹, P. Hoogh
P. Bergamaschi⁶, M. El Hajj⁷, J.

CURRENT

Cost function

$$J_{obs}(x) = \sum_i \frac{(F(x_i) - y_i)^2}{I_i^2 \cdot \sigma_i^2}$$

- Aim to find the background state x to minimize our cost function
- Sampling model F at the time and point of observations y
- Variance σ^2 comprises both model sampling error and observation error
- Inclusion of inflation factor I decrease weight of cost function
- Use of individual value for each observation based on spatial density of points

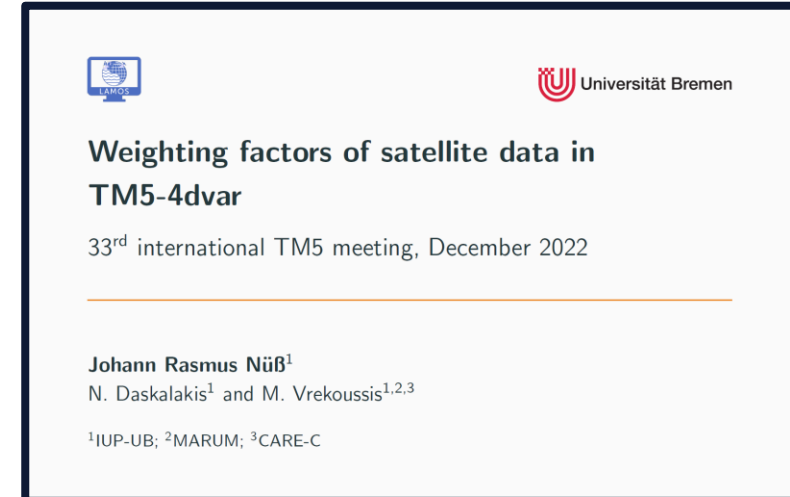
Variable inflation factor

- Density of points estimation based on the distance
- **Kernel Density Estimation** or Parzen–Rosenblatt window method [2]

$$I = \sum \exp\left(-\frac{d^2}{2h^2}\right)$$

APPROACH

[2] Rosenblatt, M. (1956). Remarks on Some Nonparametric Estimates of a Density Function. In *The Annals of Mathematical Statistics* (Vol. 27, Issue 3, pp. 832–837). Institute of Mathematical Statistics.

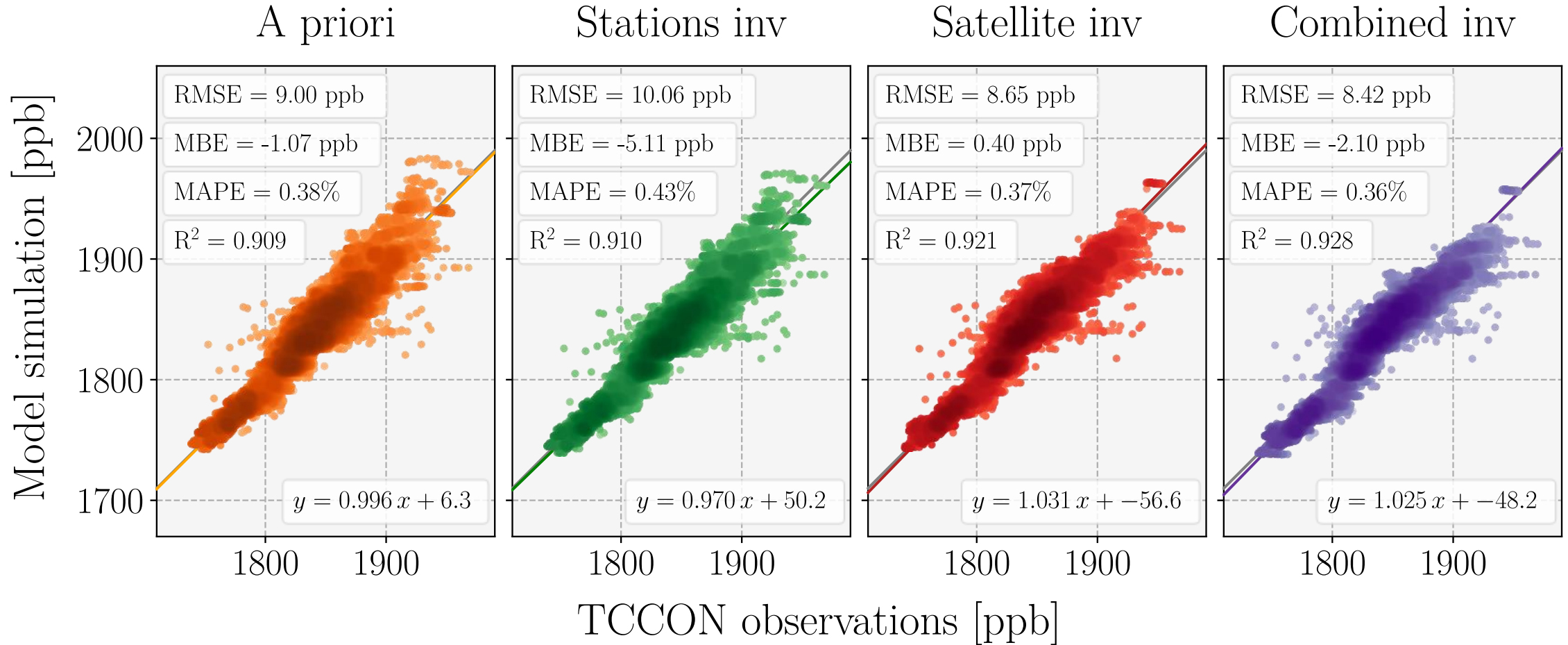


The slide features the logos of IUP (International Union of Pure and Applied Chemistry) and Universität Bremen at the top. The title is 'Weighting factors of satellite data in TM5-4dvar', and the subtitle is '33rd international TM5 meeting, December 2022'. The authors listed are Johann Rasmus Nüß¹, N. Daskalakis¹, and M. Vrekoussis^{1,2,3}. A horizontal line separates the title from the author information. At the bottom, the affiliations are listed as ¹IUP-UB; ²MARUM; ³CARE-C.

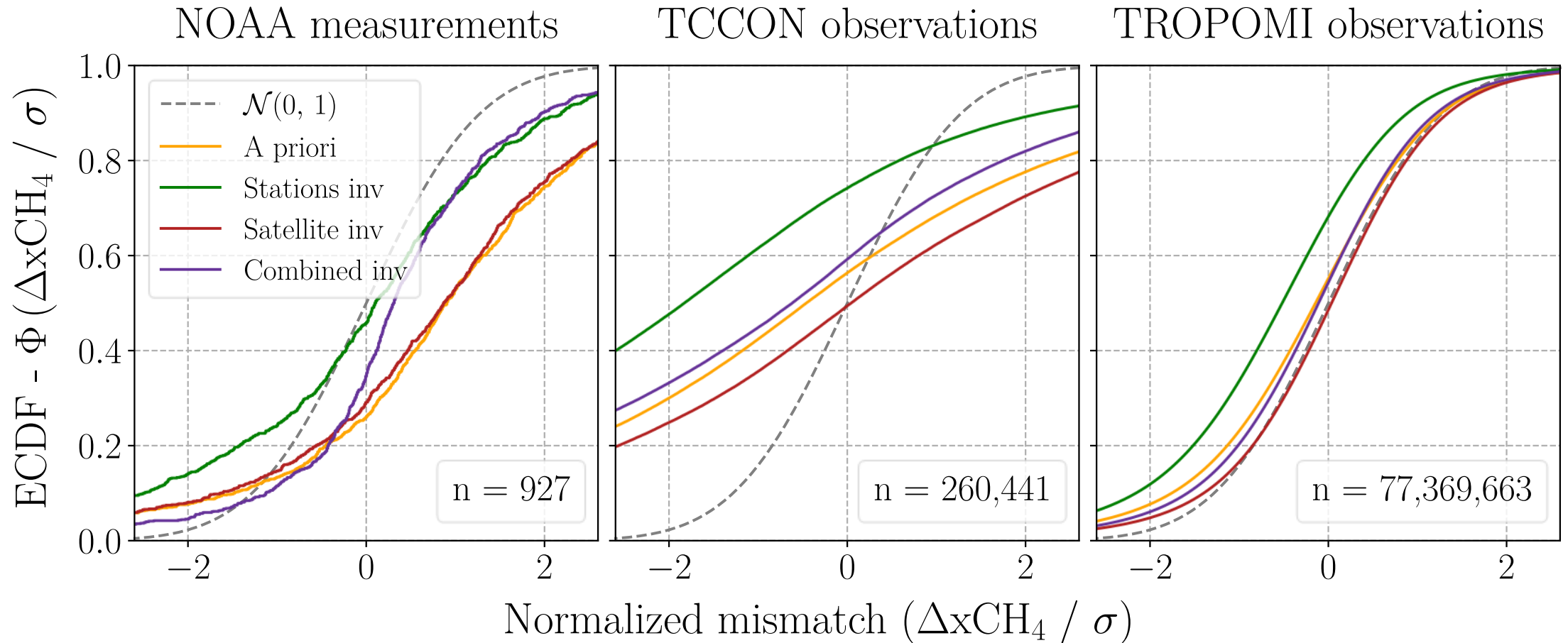
1. Objective
2. Observations and measurements
3. Background

4. Simulations with adaptative factor

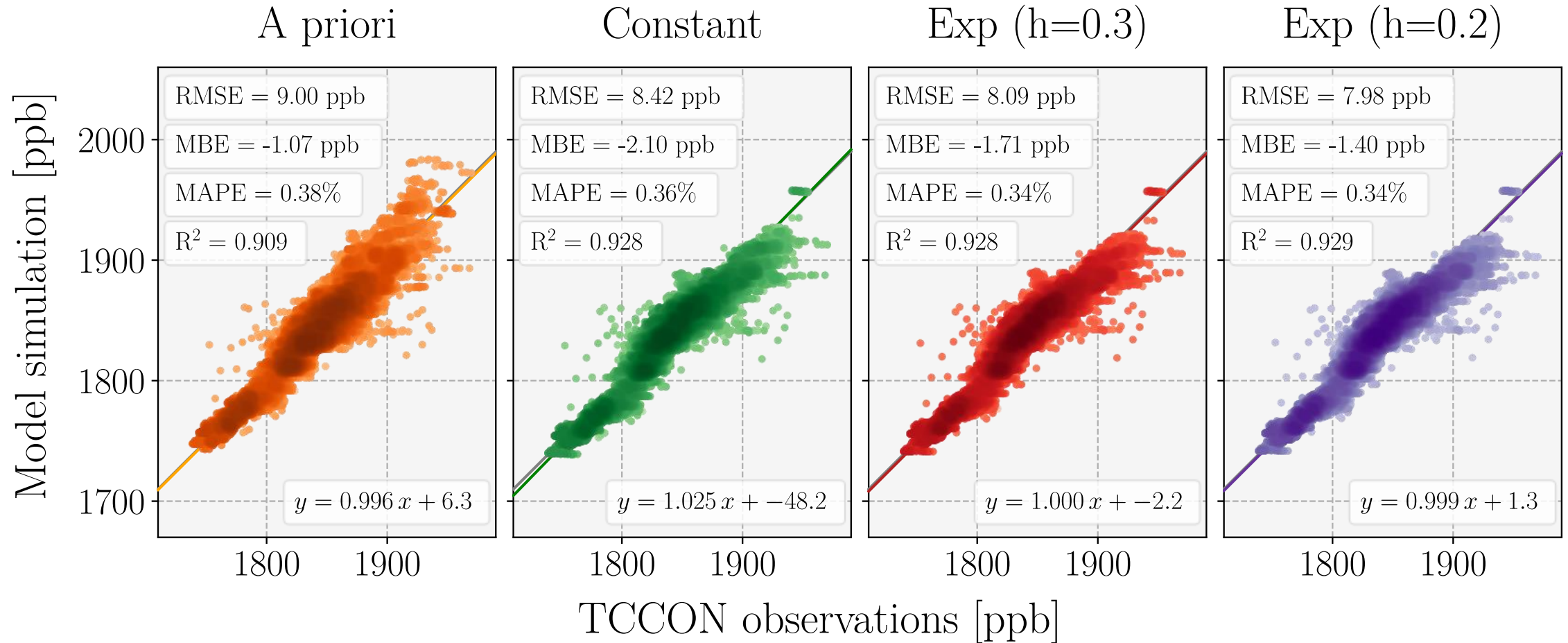
First simulation with a constant factor



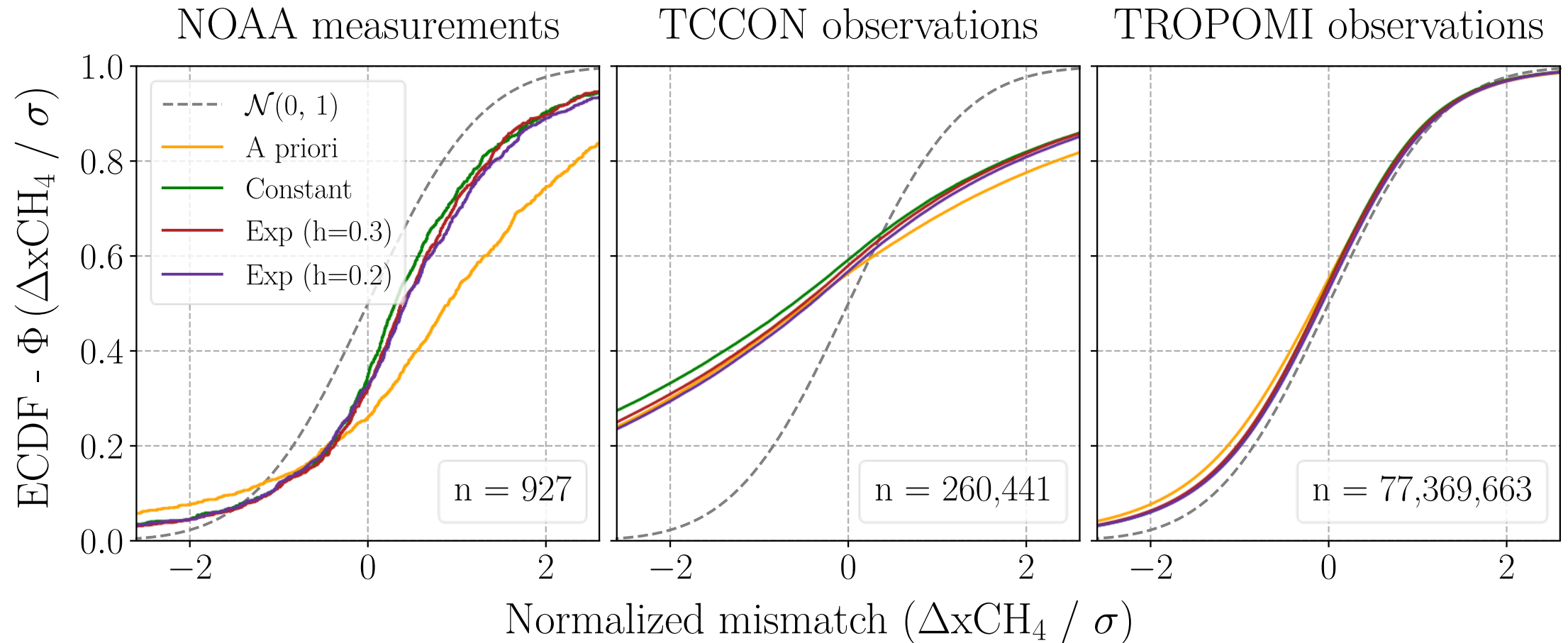
First simulation with a constant factor



Simulations with adaptative factors

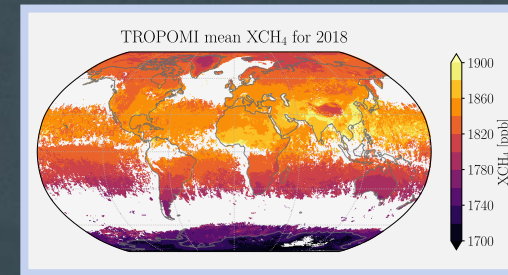


Simulations with adaptative factors

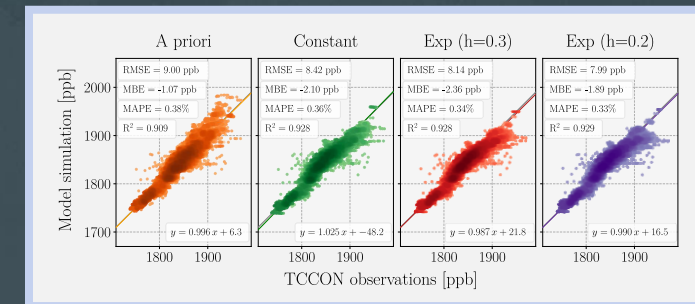


Summary

- TROPOMI provides added information but too many pixels
- Implementation of adaptive inflation factor on TMVar
- Some improvements on inversions comparing with TCCON



$$I = \sum \exp\left(-\frac{d^2}{2h^2}\right)$$



On CH₄ inversions using TROPOMI, and how to better combine different measurements (maybe...)

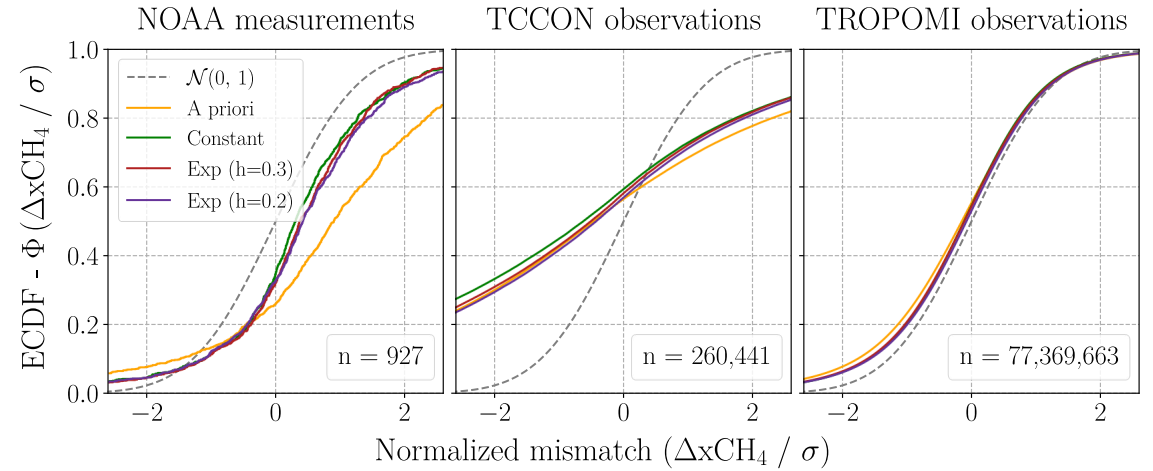
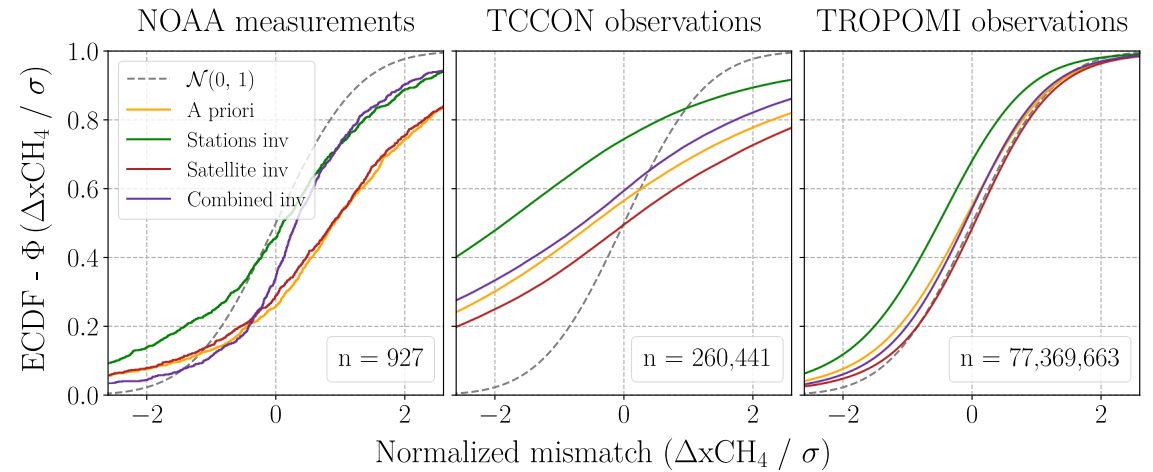
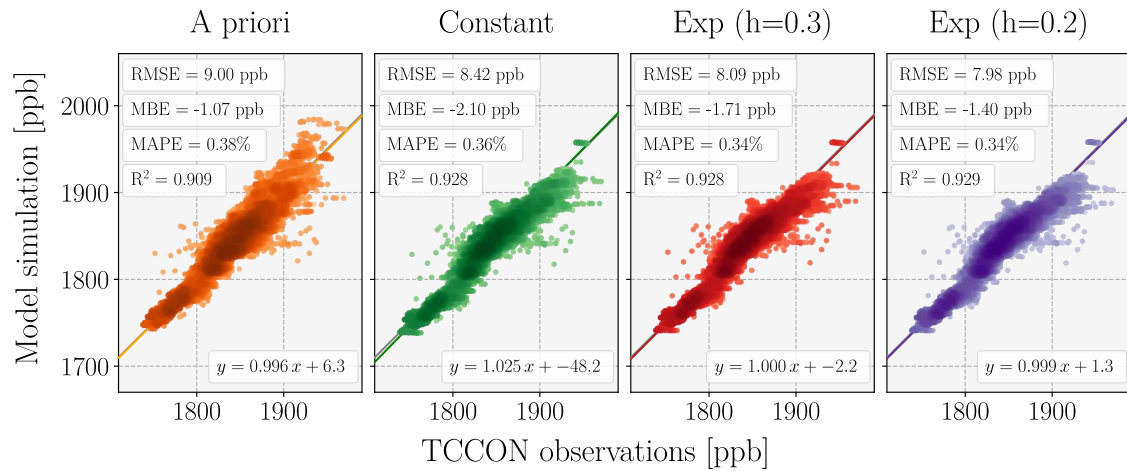
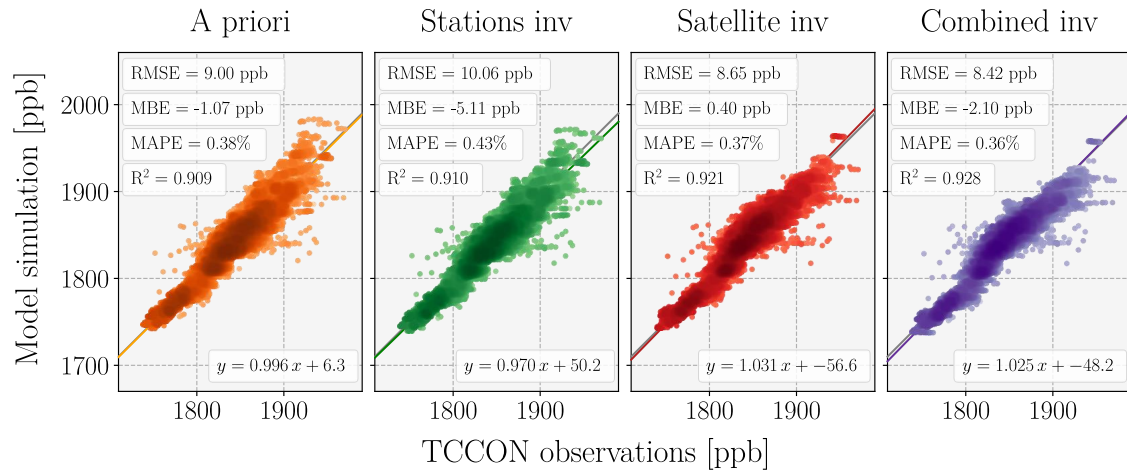
Santiago Parraguez Cerda

Laboratory for Modelling and Observation of the Earth System (LAMOS)

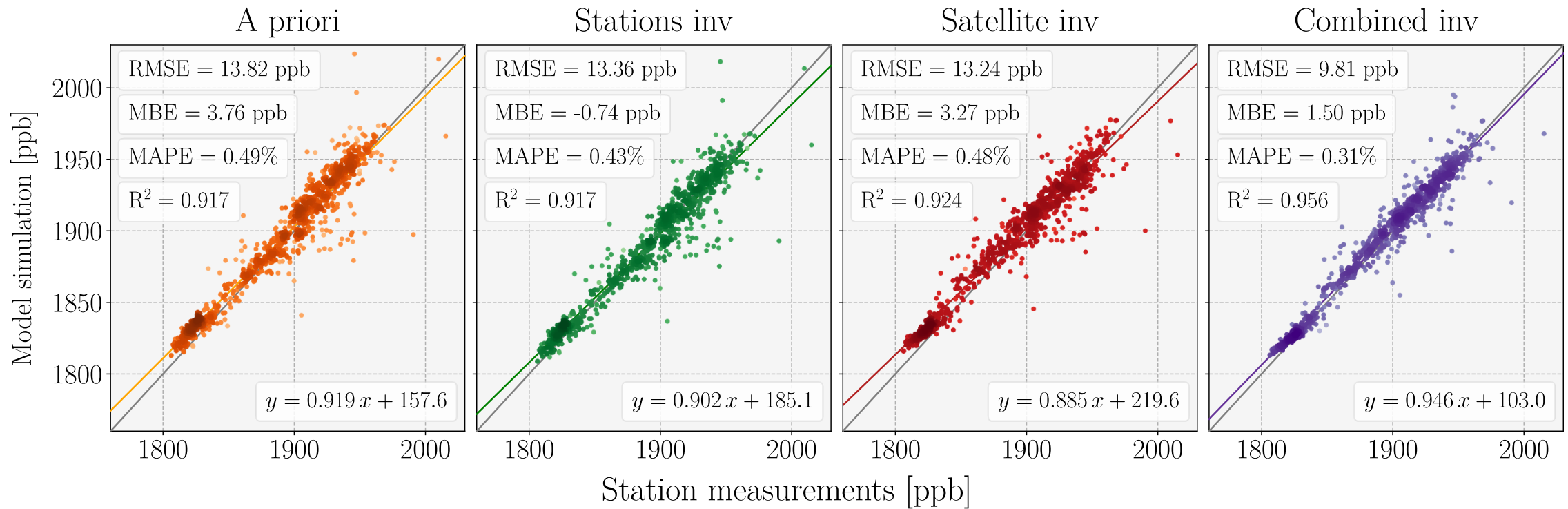
Rasmus Nüß, Nikos Daskalakis, Arjo Segers, Oliver Schneising,
Michael Buchwitz, Mihalis Vrekoussis, Maria Kanakidou

35th International TM5 Meeting
21-22 October 2024
Wageningen, The Netherlands

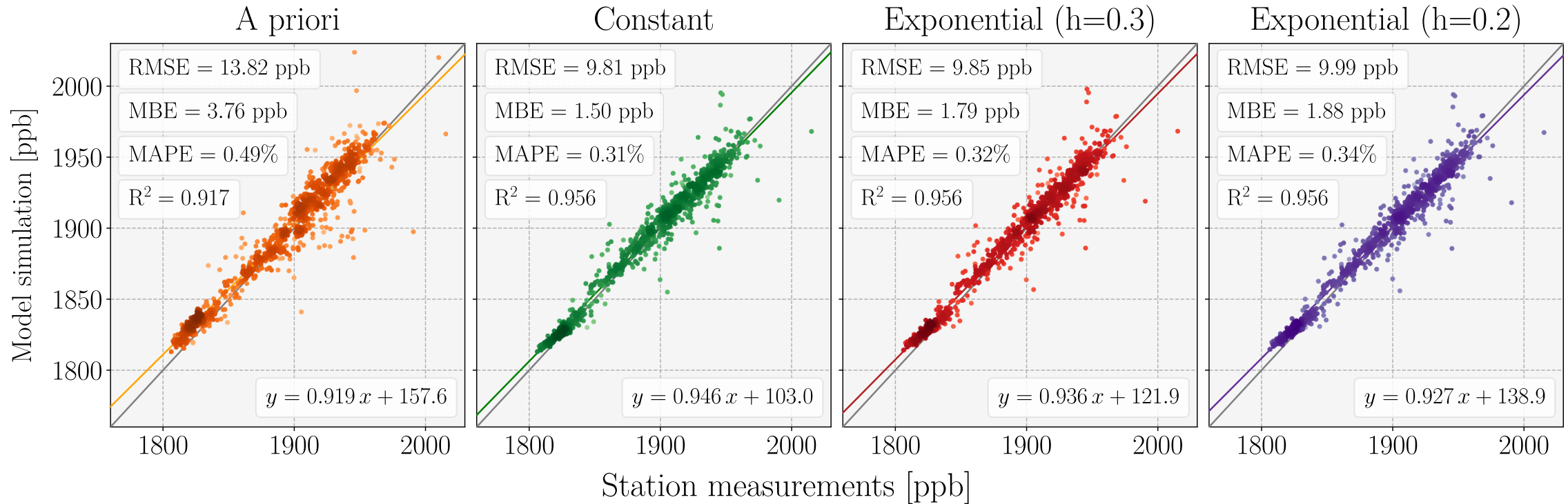
Comparison of results



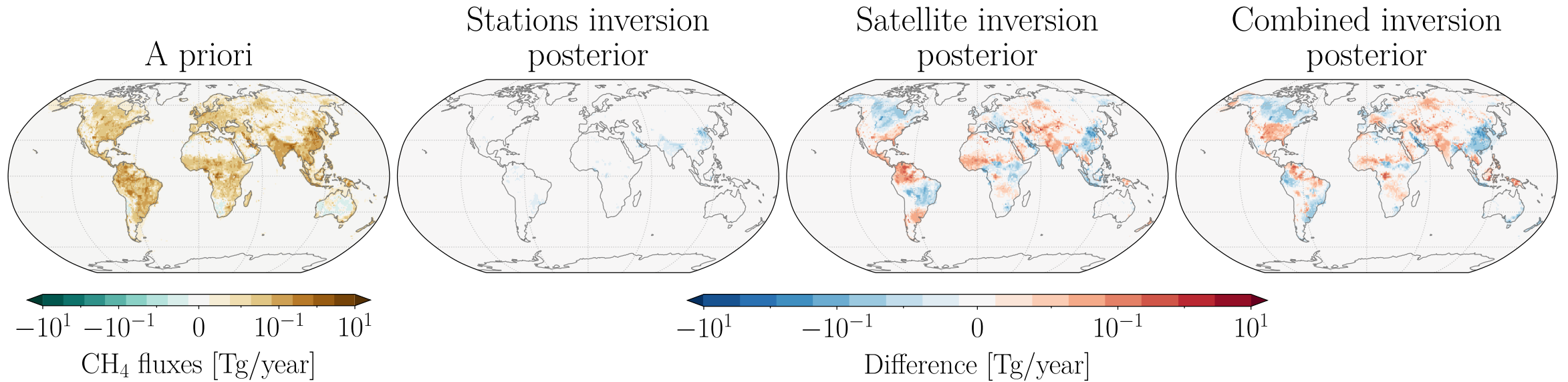
First simulation with a constant factor



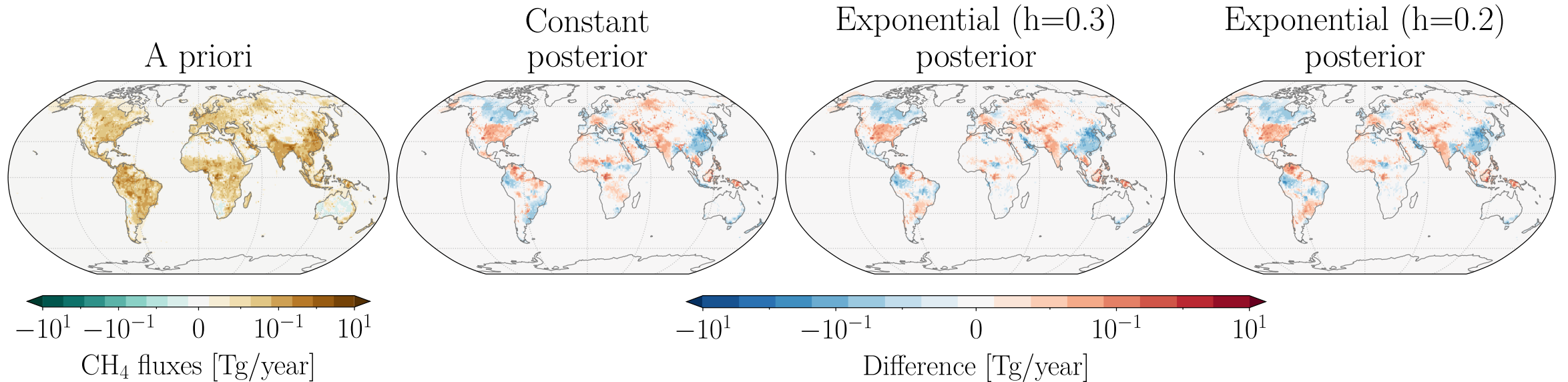
Simulations with adaptative factor



Emissions for base simulation



Emissions for simulation with adaptive factor



Total emissions per simulation

	A priori	Only stations	Only TROPOMI	Constant inflation	Exponential (h=0.3)	Exponential (h=0.2)
Total annual emissions [Tg/year]	585.61	572.11	584.51	575.50	575.39	577.97