Environnement et Changement climatique Canada
Environment and Climate Change Canada

Mathematical Approaches of Atmospheric Constituents Data Assimilation and Inverse Modeling
Session 7 – Parametric Kalman filtering (TCPL 201)

# PvKF Assimilation of GOSAT Methane in the Hemispheric CMAQ: Design and Results using Optimal Error Statistics with an Application for Emissions Inversion


Presenter: Sina Voshtani[1]

Co-authors: Richard Ménard[2], Thomas W. Walker[3], Amir Hakami[3]

[1] Department of Physics, University of Toronto
[2] Air Quality Research Division, Environment and Climate Change Canada
[3] Department of Environmental Engineering, Carleton University


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# Outline:

## Background

- Data Assimilation and Inverse Modelling
- Importance of Atmospheric Methane

## Motivation

- Gaps and Limitations
- Questions

## Tools

- Model and Observations
- Covariance Modeling and Parameter Estimation

## Project

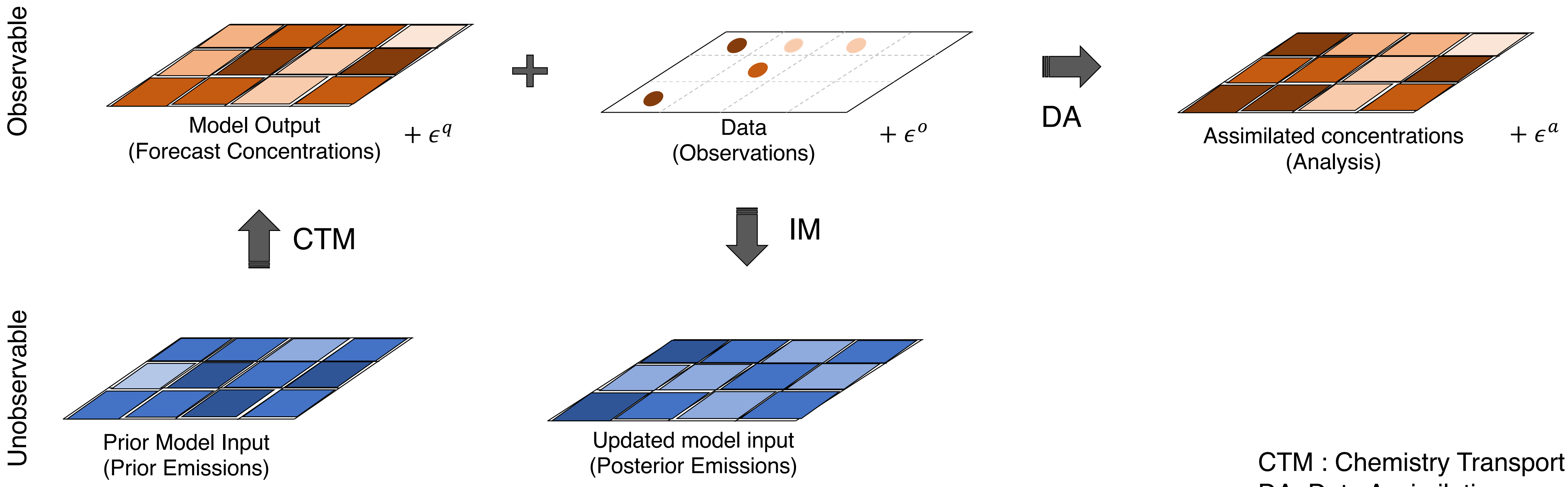
- Part I: **Design of an Assimilation System for Methane**
- Part II: **Assimilation Results with Optimal Error Statistics**
- Part III: **Assimilation Use in Methane Emissions Inversion**

## Future Work

# Data Assimilation and Inverse Modelling

are statistical frameworks to:

- Obtain consistent, precise, and evolving 3-dimensional picture of the atmosphere
- Fill in data gaps and inferring information about unobserved variables

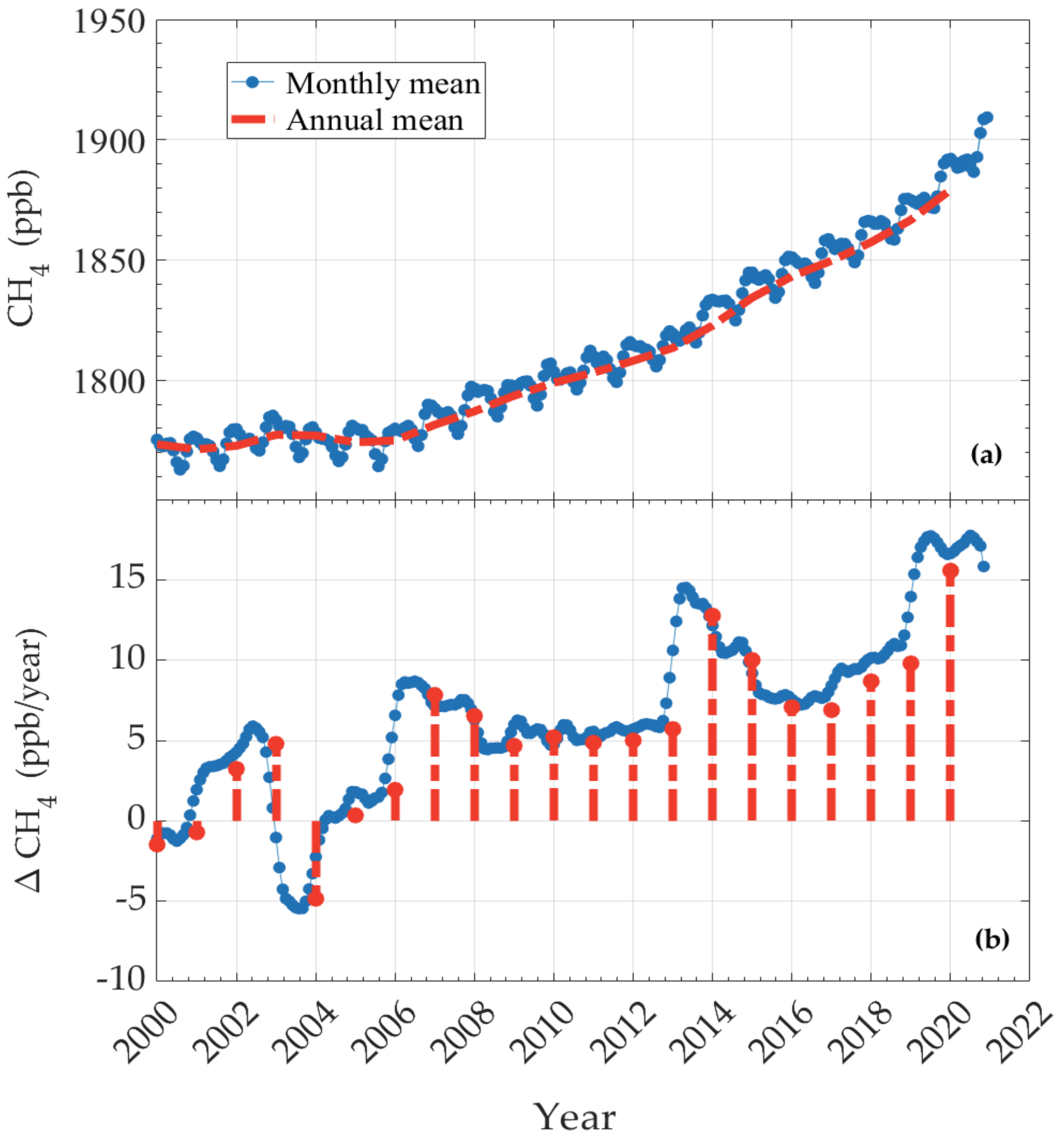



CTM : Chemistry Transport Model
DA: Data Assimilation
IM: Inverse Modelling (or Inversion)

# Why Atmospheric Methane?

Because of the large **climate** and **air quality** impact

- Largest anthropogenic radiative forcing after $CO_2$
- Short lifetime and ~30 times greater GWP than $CO_2$
- Outsized influence on near-term climate change
- Large air quality impact, (e.g., $O_3$ production)
- Global average concentration acceleration after 2007




GWP: Global Warming Potential

Data obtained from Dlugokencky (2022)

# Gaps and Limitations in the Past Methane Studies

## 1. Challenges in Emissions Inversion

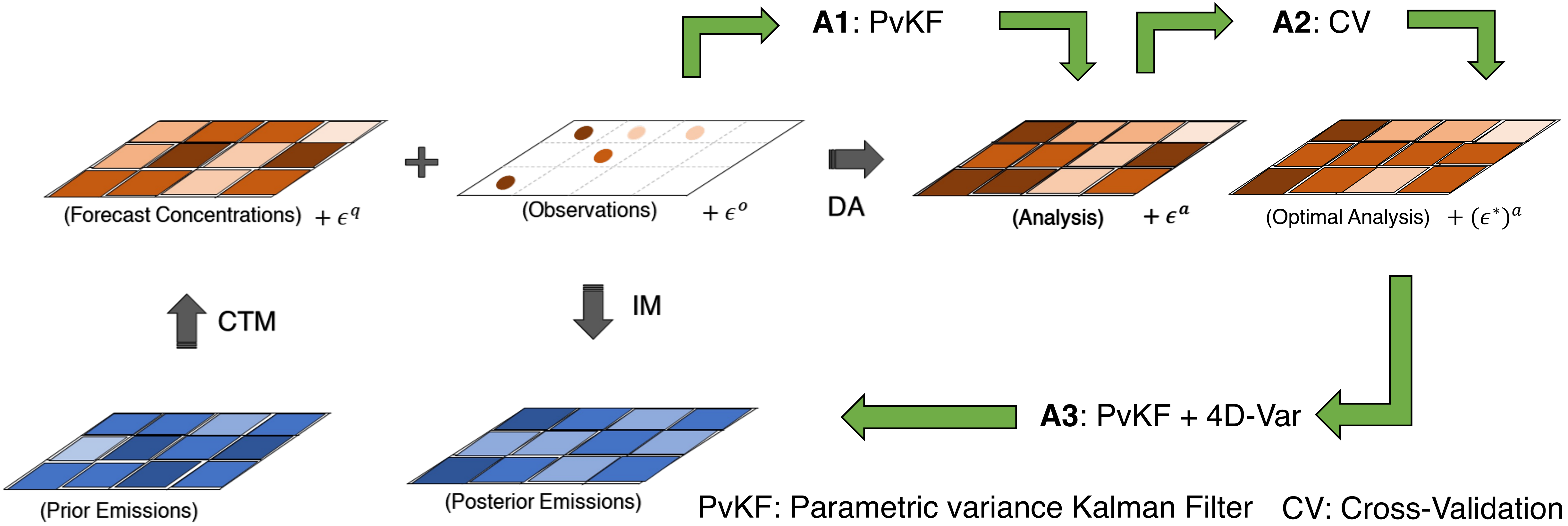
- Scale, temporal, and spatial resolution (Turner et al., 2015; Zavala-Araiza et al., 2017)
- Initial and boundary conditions (Bousserez et al. 2016; Bergamaschi et al. 2018)
- Contradiction in the result of different inversions (Ganesan et al., 2019; Miller et al., 2019)
- High computations to estimate the state errors (Yu et al., 2021; Voshtani et al., 2022a)

## 2. Limitations in Estimation Problem

- Perfect model assumptions (Janardanan et al., 2020; Zhang et al., 2021)
- Error statistics are already optimal (Voshtani et al., 2022b)
- Separate evaluations on the error statistics (Voshtani et al., 2022b)
- Concentration uncertainties and error correlations in the observation space (Voshtani et al., 2023; in review)

# Research Questions?

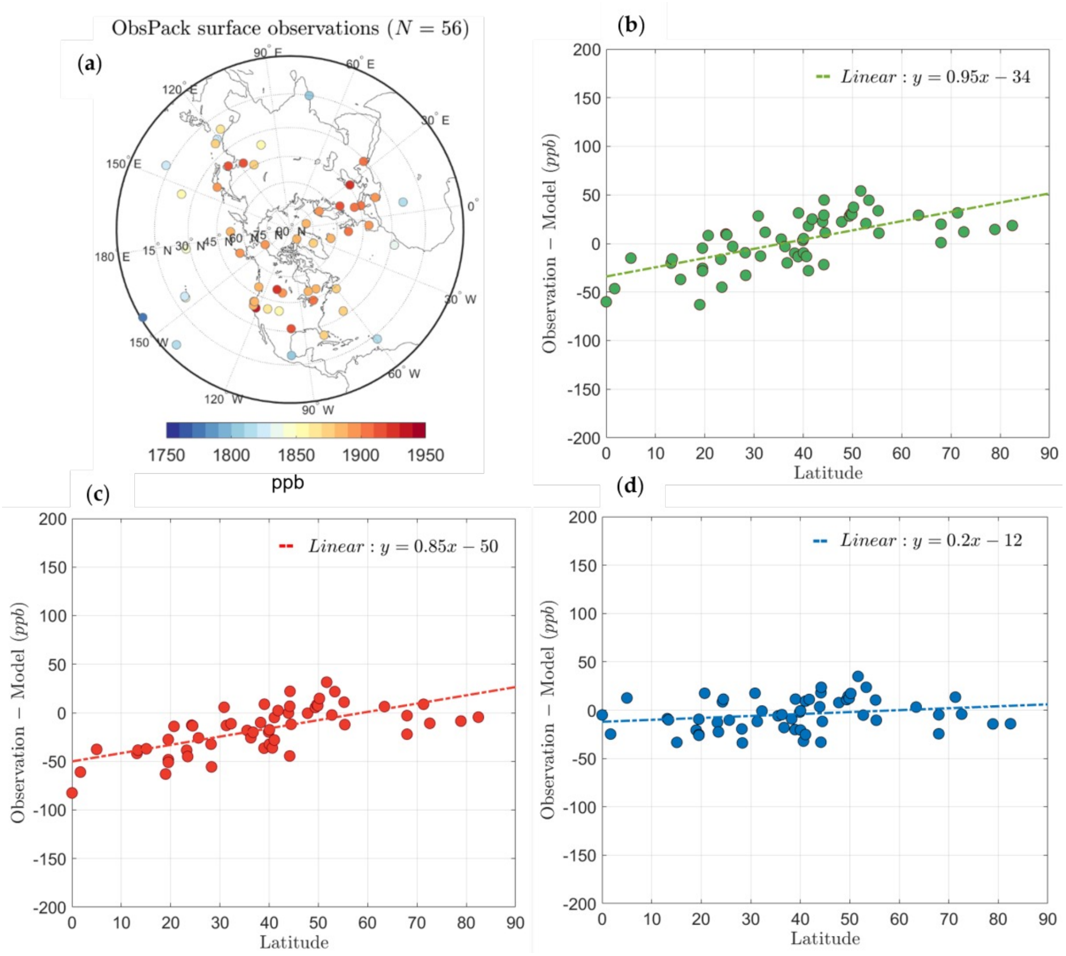
**Q1**: How to obtain a low-cost yet powerful DA system, capable of estimating uncertainties?
**Q2**: What is the impact of optimal error statistics on the analysis?
**Q3**: Can we improve on 4D-Var inversion using optimal analysis and their uncertainties?




PvKF: Parametric variance Kalman Filter CV: Cross-Validation

# Model and Data (+ Adaptation)

Bias correction (I)




**Model**: Hemispheric CMAQ v5 and CMAQ-ADJ

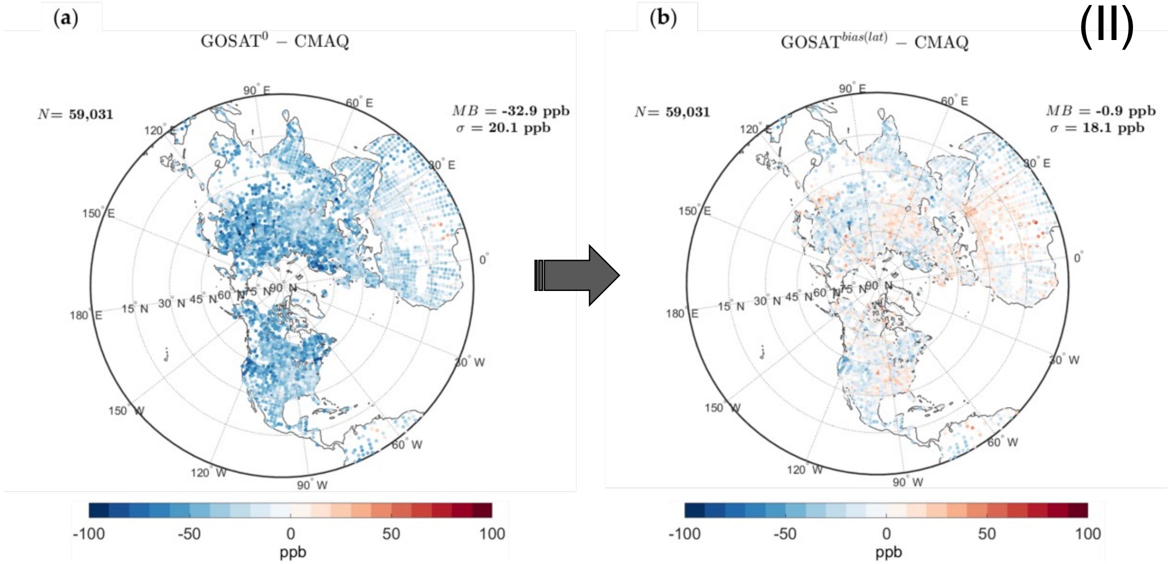
- Processing Emissions:
  Anthropogenic (EDGAR v6) + Natural (WetCHARTs v3.0)
- Modifying chemical mechanism of gas-phase chemistry in CCTM:

$$CH_4 + OH \rightarrow CH_3 + H_2O$$

**Data**: GOSAT observations

- Bias correction relative to ObsPack surface observations
- Quality control (i.e., removing outliers)

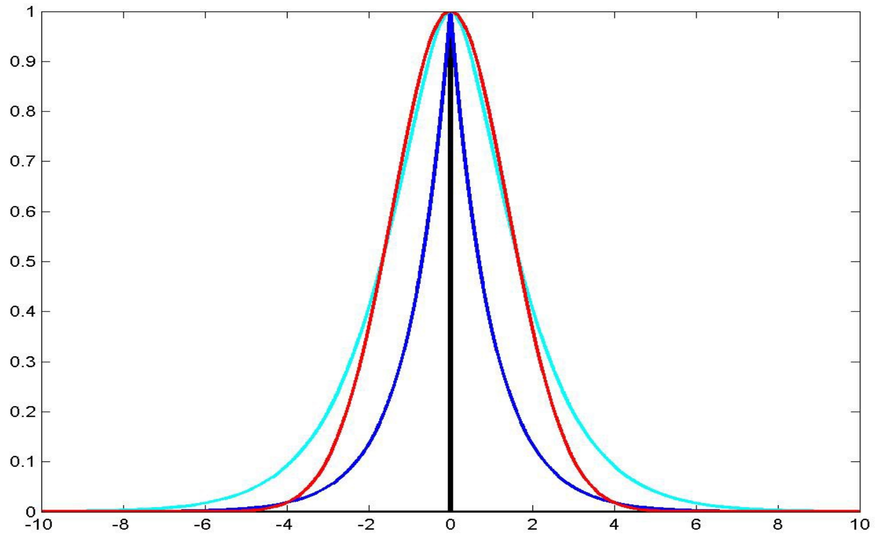
(II)



# Covariance Modelling

Examples of suitable correlation functions:

- FOAR: $C(\|\mathbf{r}-\mathbf{r}'\|) = \exp\left(-\frac{\|\mathbf{r}-\mathbf{r}'\|}{L}\right)$
- SOAR: $C(\|\mathbf{r}-\mathbf{r}'\|) = \left(1+\frac{\|\mathbf{r}-\mathbf{r}'\|}{L}\right)\exp\left(-\frac{\|\mathbf{r}-\mathbf{r}'\|}{L}\right)$
- Gaussian: $C(\|\mathbf{r}-\mathbf{r}'\|) = \exp\left(-\frac{\|\mathbf{r}-\mathbf{r}'\|^2}{2L^2}\right)$




$$\mathbf{P}^f_{n\times n} = \mathbf{\Sigma}^f_t \mathbf{C}\,\mathbf{\Sigma}^f_t$$

Forecast error

$$P(\mathbf{r},\mathbf{r}',t) = \sigma(\mathbf{r},t)C(\mathbf{r},\mathbf{r}',t)\sigma(\mathbf{r}',t)$$

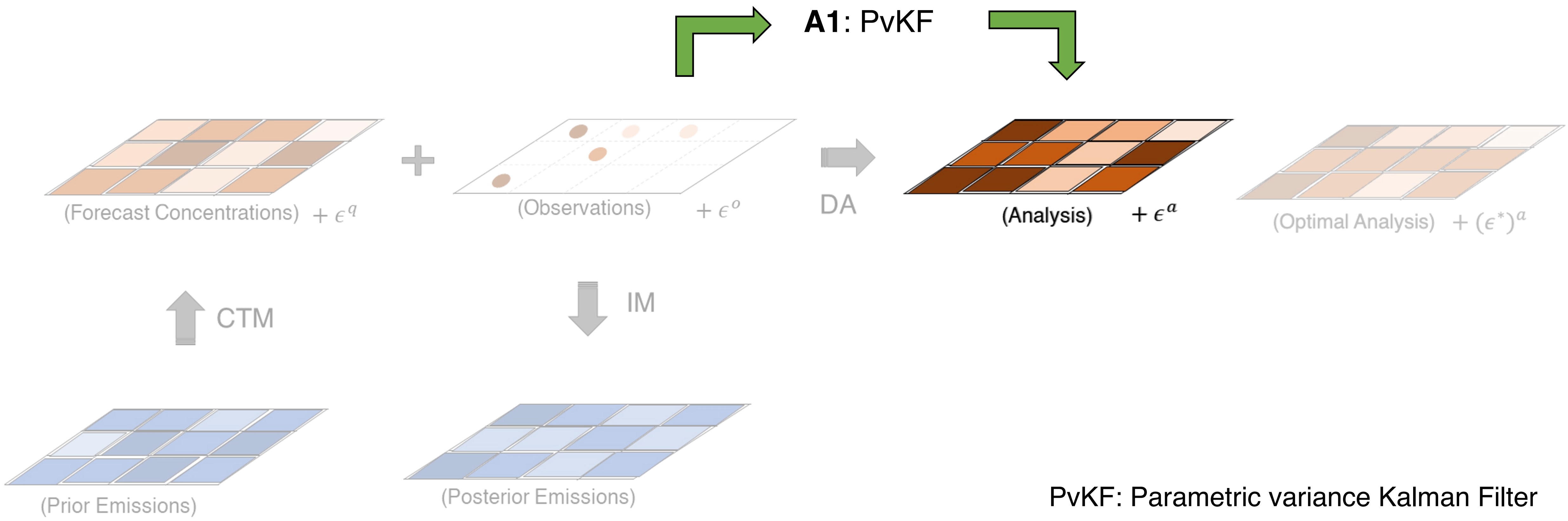
$$C(\mathbf{r},\mathbf{r}') = C(\|\mathbf{r}-\mathbf{r}'\|)$$

$$\mathbf{R}_{m\times m} = \left(f^o\varepsilon^m\right)^2\mathbf{I}$$

$$\mathbf{Q}_{n\times n} = \left(f^q\varepsilon^q\right)^2\mathbf{I}$$

We will estimate $\boldsymbol{\alpha} = \{f^o, f^q, L, \ldots\}$

# **Q1**: How to obtain a low-cost DA system, capable of estimating uncertainties?




PvKF: Parametric variance Kalman Filter

# **Part I**: Development of PvKF Assimilation

Forecast step

1. Transport of the model state

$$\frac{\partial c}{\partial t}+\mathbf{V}\cdot\nabla c-\frac{1}{\rho}\nabla\cdot\left(\rho\mathbf{K}\nabla c\right)+\mathrm{R}=\mathrm{E}$$

2. Advection of error variance

$$\frac{\partial\sigma^2}{\partial t}+\mathbf{V}\cdot\nabla\sigma^2=q$$

Analysis step

1. Covariance function convolution

$$\zeta = 1,\dots,m$$

$$H_{\mathbf{x}}[P^f(\mathbf{x},\mathbf{x}',t)] \Leftrightarrow \mathbf{H}\,\mathbf{P}^f$$

$$\zeta = 1,\dots,m$$

$$H_{\mathbf{x}'}[P^f(\mathbf{x},\mathbf{x}',t)] \Leftrightarrow \mathbf{P}^f\mathbf{H}^T$$

$$H_{\mathbf{x}}\left[H_{\mathbf{x}'}\left(P^f(\mathbf{x},\mathbf{x}',t)\right)\right] \Leftrightarrow \mathbf{H}\mathbf{P}^f\mathbf{H}^T$$

2. Matrix inversion

$$\mathbf{\Gamma}=\mathbf{H}\mathbf{P}^f\mathbf{H}^T+\mathbf{R}$$

$\mathbf{\Gamma}b=d$ $\longrightarrow$ *Cholesky decomposition*

3. Analysis increment/
Analysis error variance reduction

$$\zeta = 1,\dots,m$$

$$\mathbf{X}^a=\mathbf{X}^f+\mathbf{K}(\mathbf{Y}^o-\mathbf{H}\mathbf{X}^f)$$

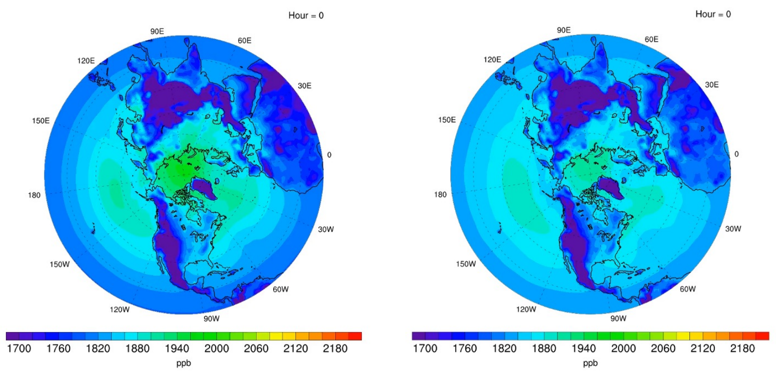
$$\mathbf{P}^a=\mathbf{P}^f-(\mathbf{H}\mathbf{P}^f)^T(\mathbf{H}\mathbf{P}^f\mathbf{H}^T+\mathbf{R})^{-1}(\mathbf{H}\mathbf{P}^f)$$

- Large state-space problem (e.g., ~1.5e6 elements)
- Produces forecast and analyses and explicitly evolve its error variance
- Computationally advantageous compared to 4D-Var and EnKF
- Accounts for model imperfection
- High potential for real-time or operational assimilation

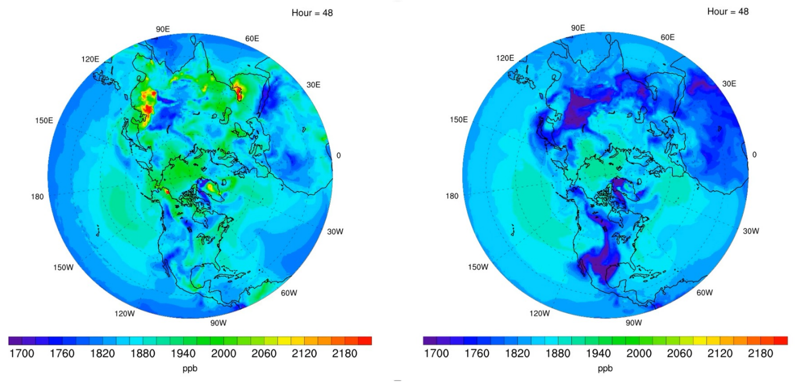
# **Part I**: Evolution of the State

Methane Analysis (with DA) vs. Methane Model (without DA)

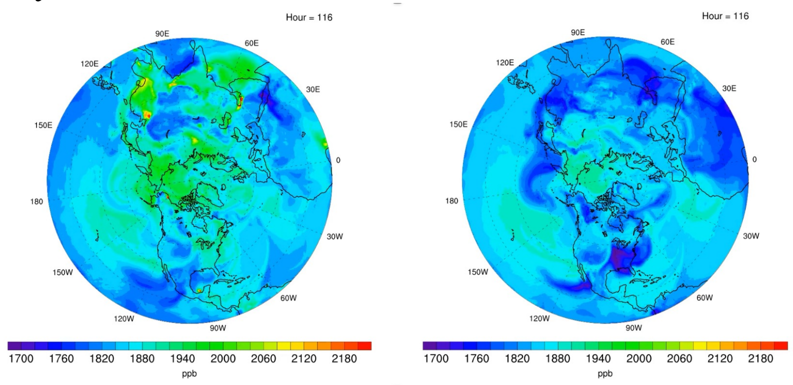
Day 0



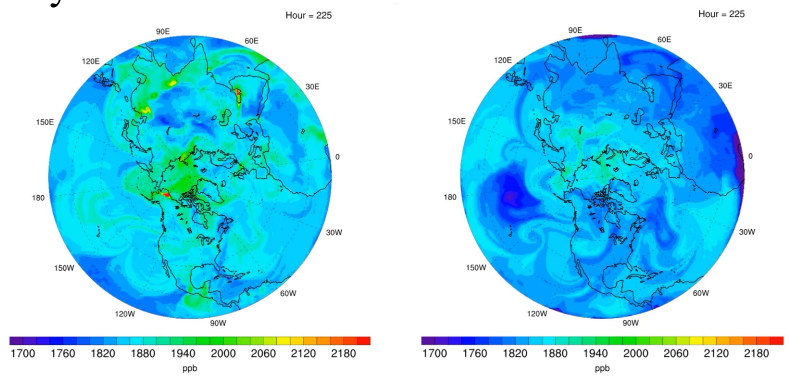

Day 4



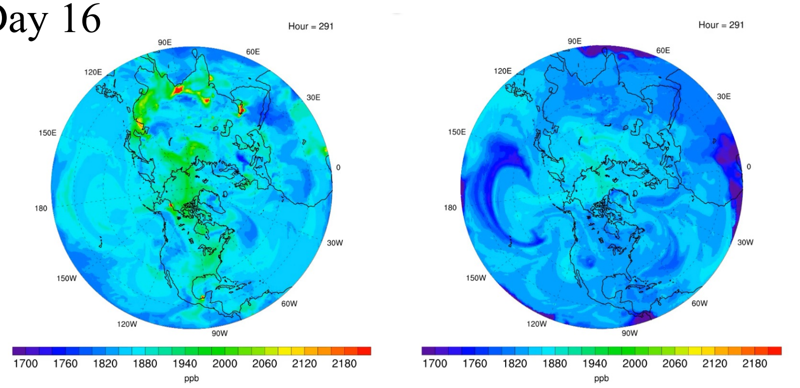

Day 8



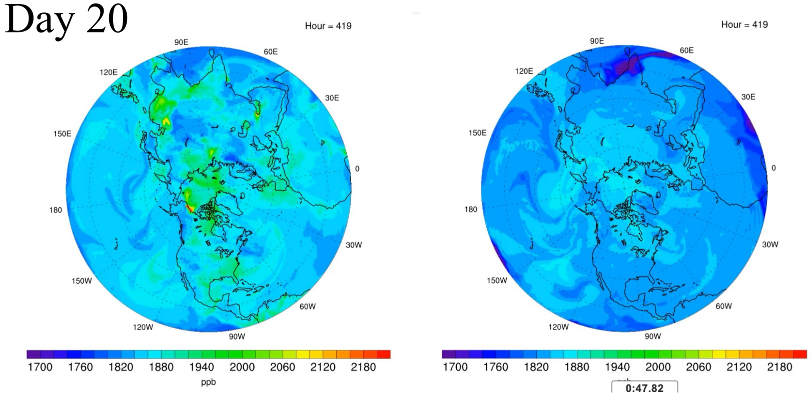

Day 12




Day 16

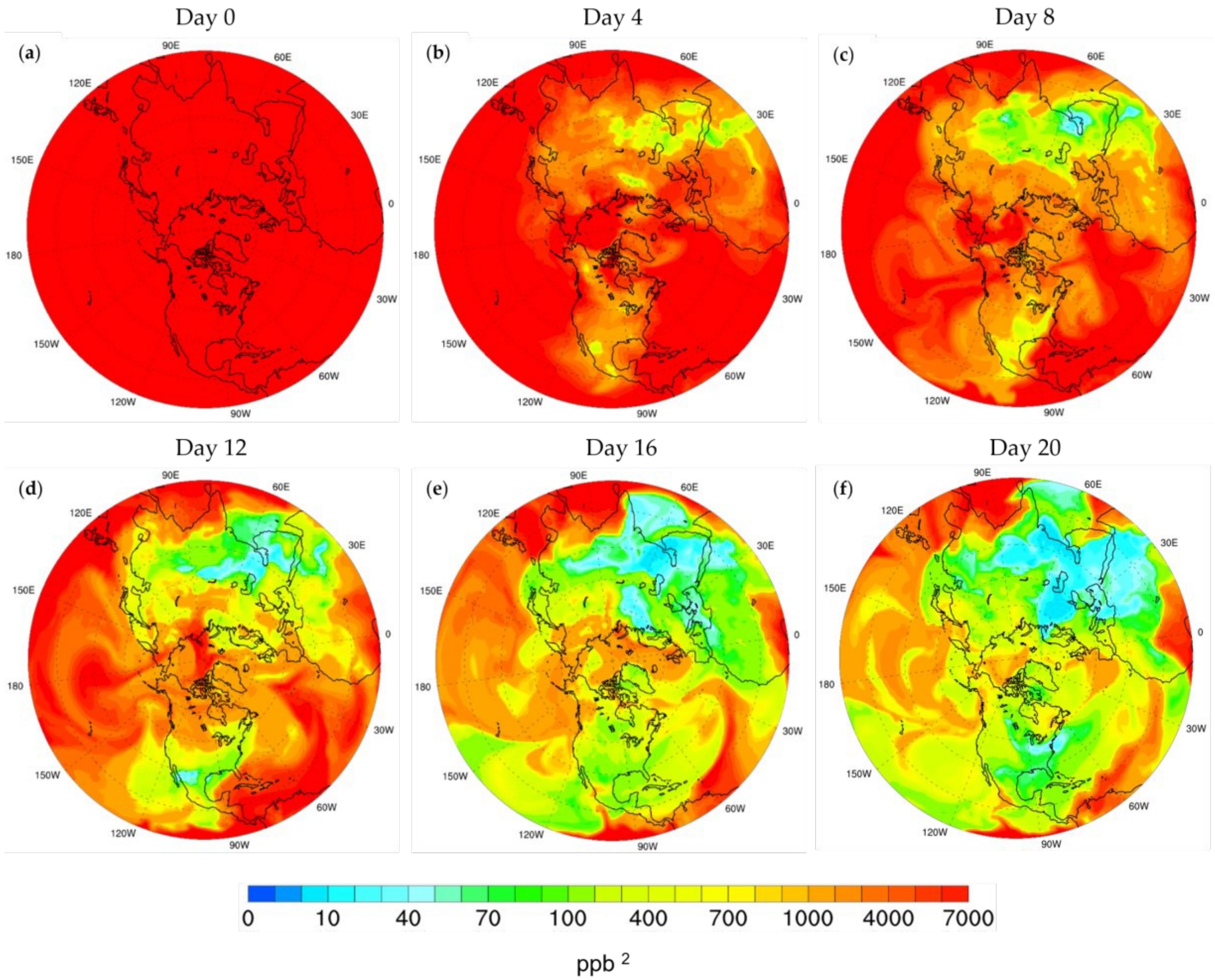



Day 20



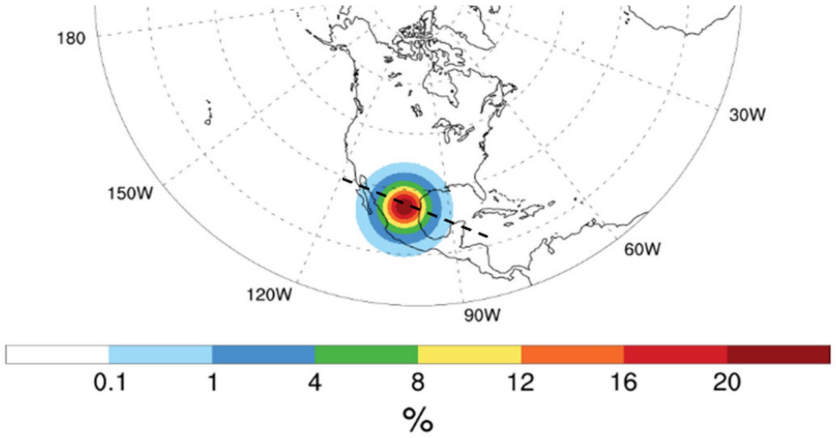
# **Part I**: Evolution of the Error Variance

Methane Analysis Error Variance:

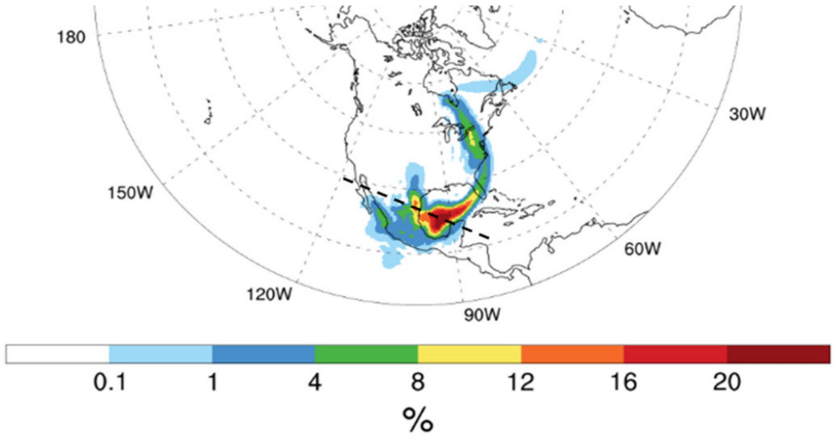


# **Part I**: Verification with Single Observation

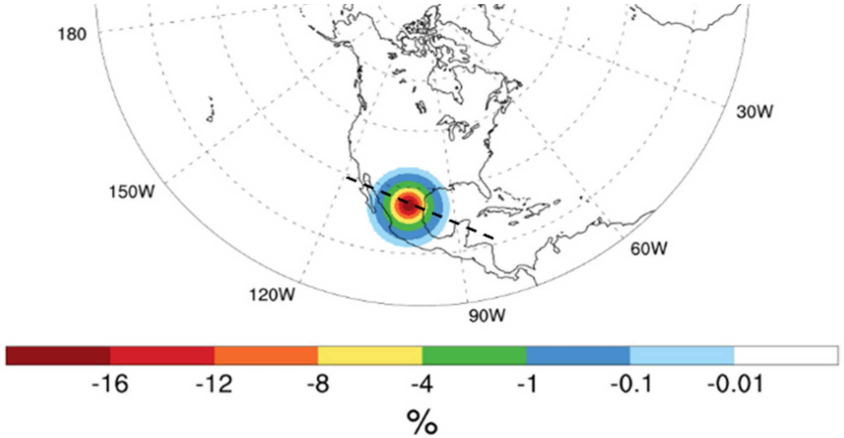
**Analysis** increment (Day 0)



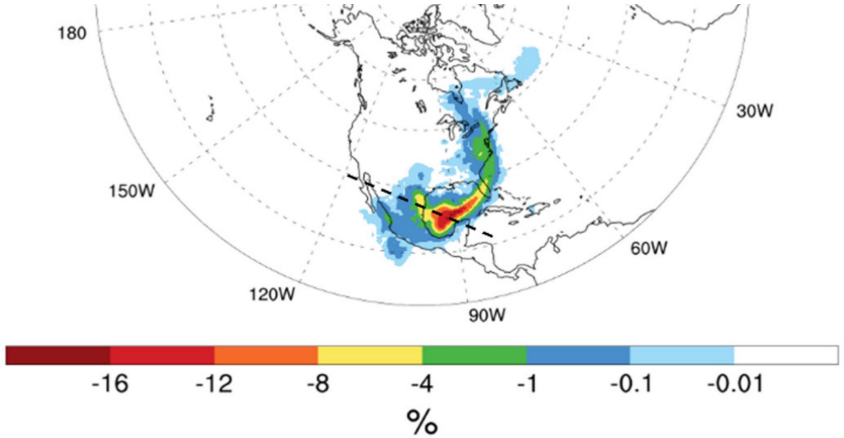

**Analysis** increment (Day 3)




**Error variance** reduction (Day 0)



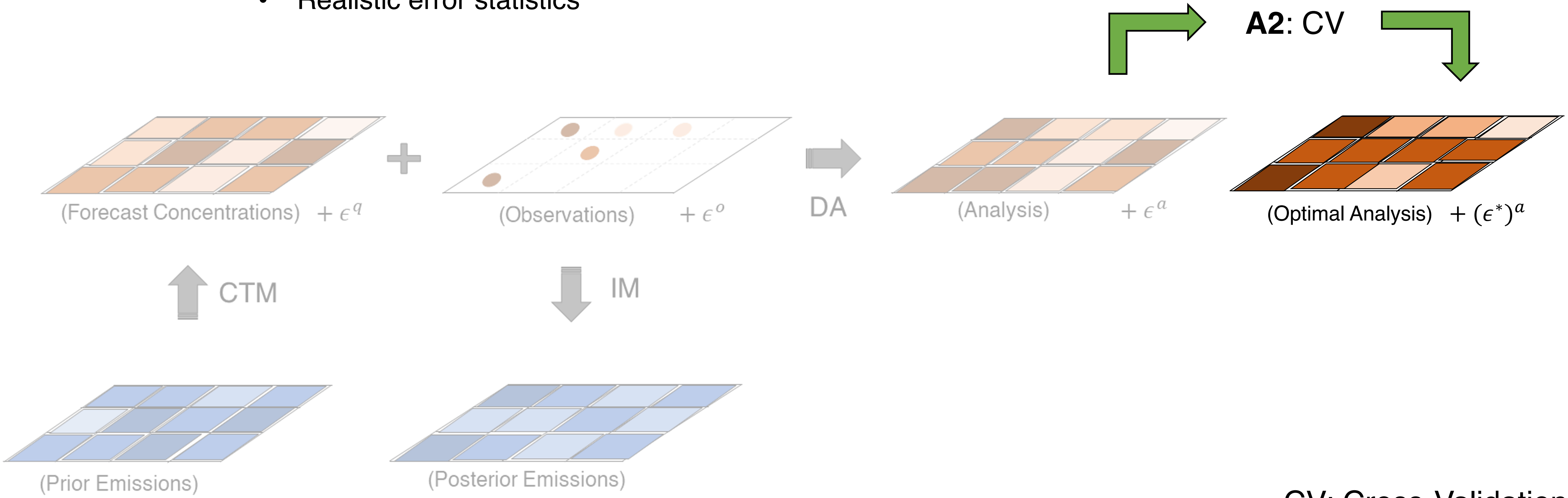

**Error variance** reduction (Day 3)



# **Q2**: What is the impact of optimal error statistics on the Analysis?

We want to obtain

- Optimal (true) analysis
- Realistic error statistics




CV: Cross-Validation

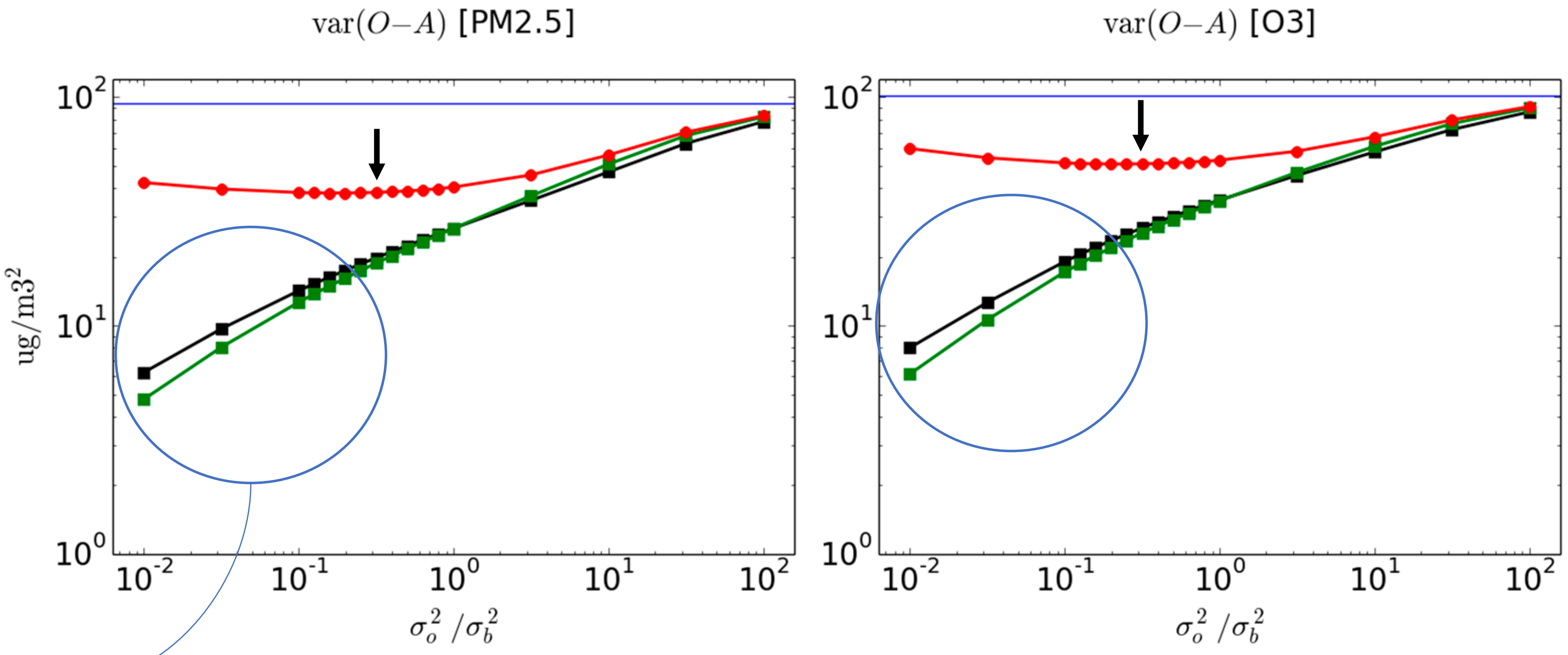
# **Part II**: Why Cross-Validation?

Because it does not assume that the analysis is already optimal

$$tr(\mathbf{A}(\boldsymbol{\alpha})) = J = \left\langle (O-A)^2 \right\rangle \quad \longrightarrow \quad \arg\min_{\boldsymbol{\alpha}} J(\boldsymbol{\alpha}) \Rightarrow \text{optimal } \mathbf{A}(\boldsymbol{\alpha})$$

$$\boldsymbol{\alpha} = \{f^o, f^q, L, \ldots\}$$

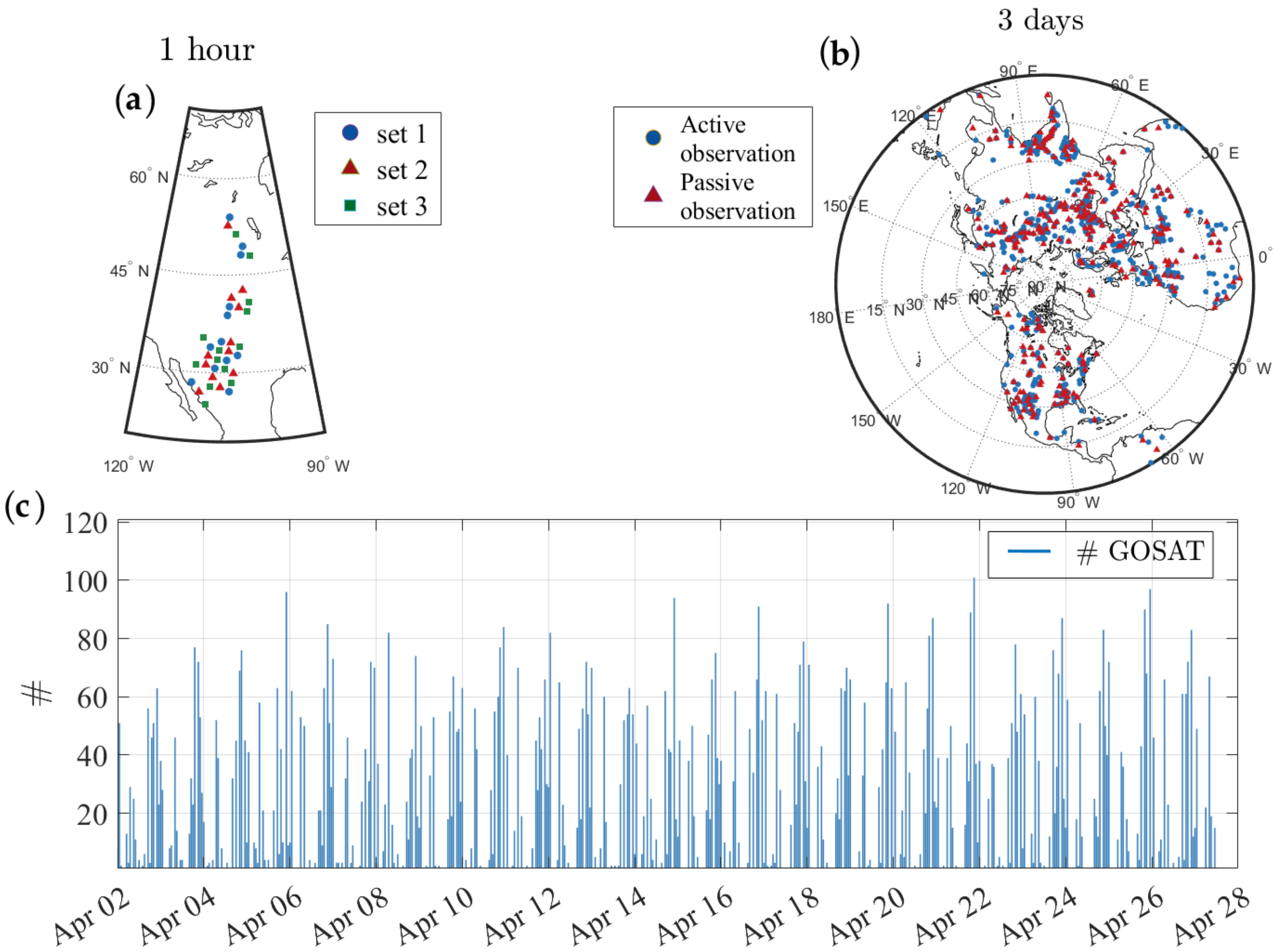
| With CV | Without CV |
| --- | --- |
| | $J = \left\langle (O-A)^2 \right\rangle$ |
| $J_c = \left\langle (O-A)_c^2 \right\rangle$ | $J = \left\langle (O-A)^2 \right\rangle$ |
| Uncorrelated | Correlated |




Overestimation

(Ménard and Deshaies-Jacques, 2018a)

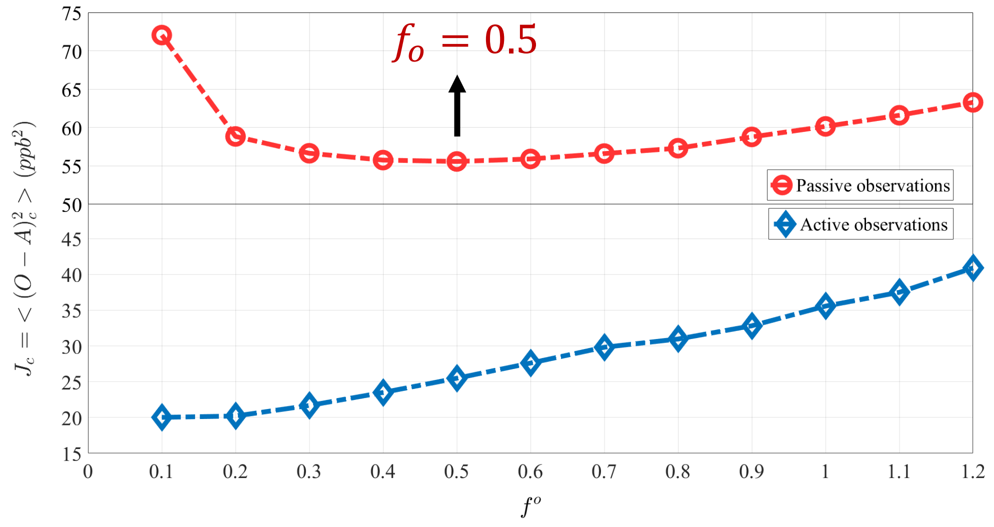
# **Part II**: Cross-Validation with GOSAT

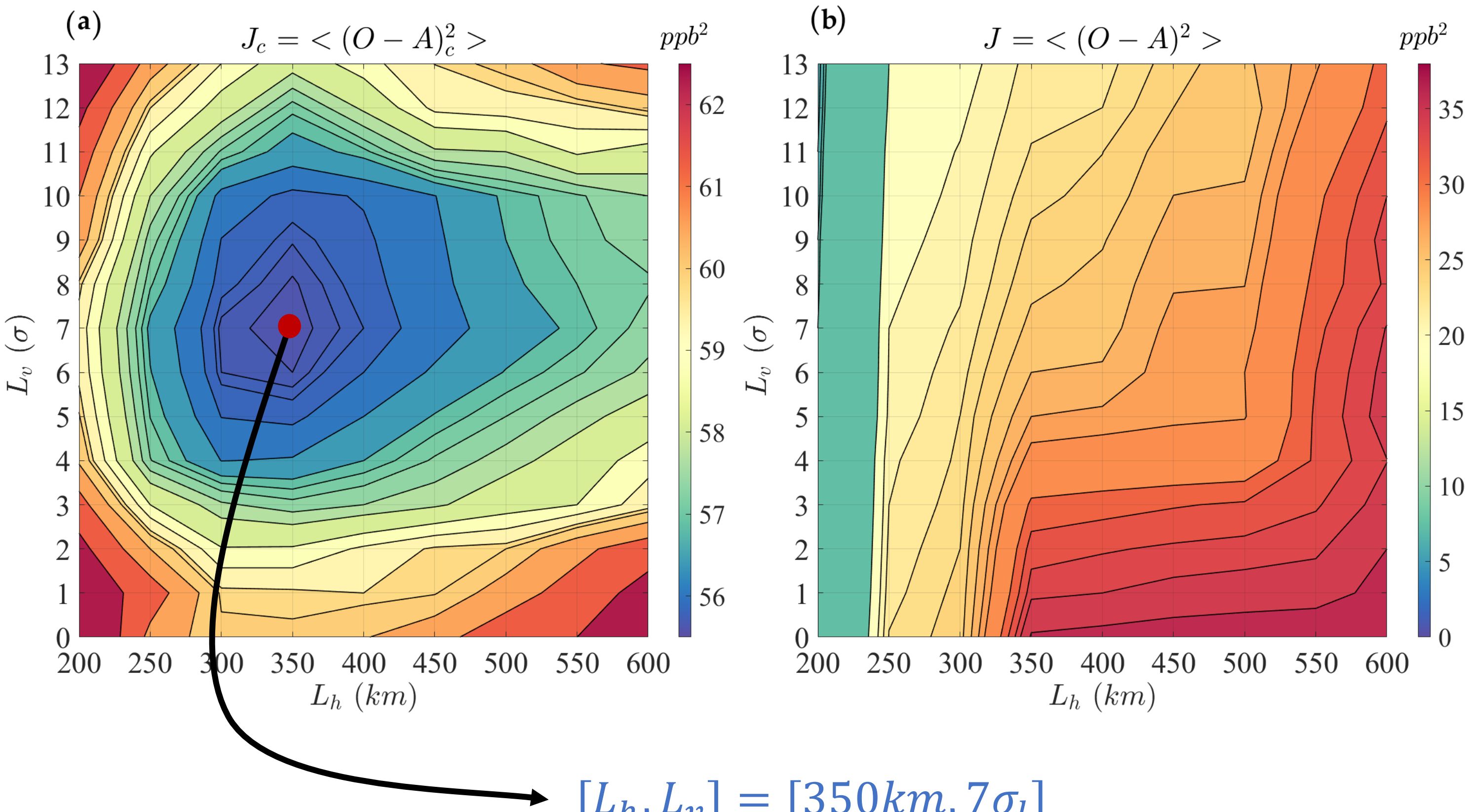


# **Part II**: Estimate Error Covariances Parameters

Optimizing CV cost function to obtain error parameters, corresponding to optimal solution.

| itr/Step \ Parameters | $L_h$ | $L_v$ | $f^o$ | $J_c = \langle (O-A)_c^2 \rangle$ |
|---|---|---|---|---|
| initial | 500 km | $1\sigma$ | 1 | 62.4 ppb$^2$ |
| itr 0/step 1 | 500 km | $1\sigma$ | 0.45 | 60.5 ppb$^2$ |
| itr 0/step 2 | 350 km | $7\sigma$ | 0.45 | 55.9 ppb$^2$ |
| itr 1/step 1 | 350 km | $7\sigma$ | 0.5 | 55.6 ppb$^2$ |
| itr 1/step 2 | 350 km | $7\sigma$ | 0.5 | 55.6 ppb$^2$ |




$[L_h, L_v] = [350km, 7\sigma_l]$

# **Part II**: Impact of Optimal Estimation

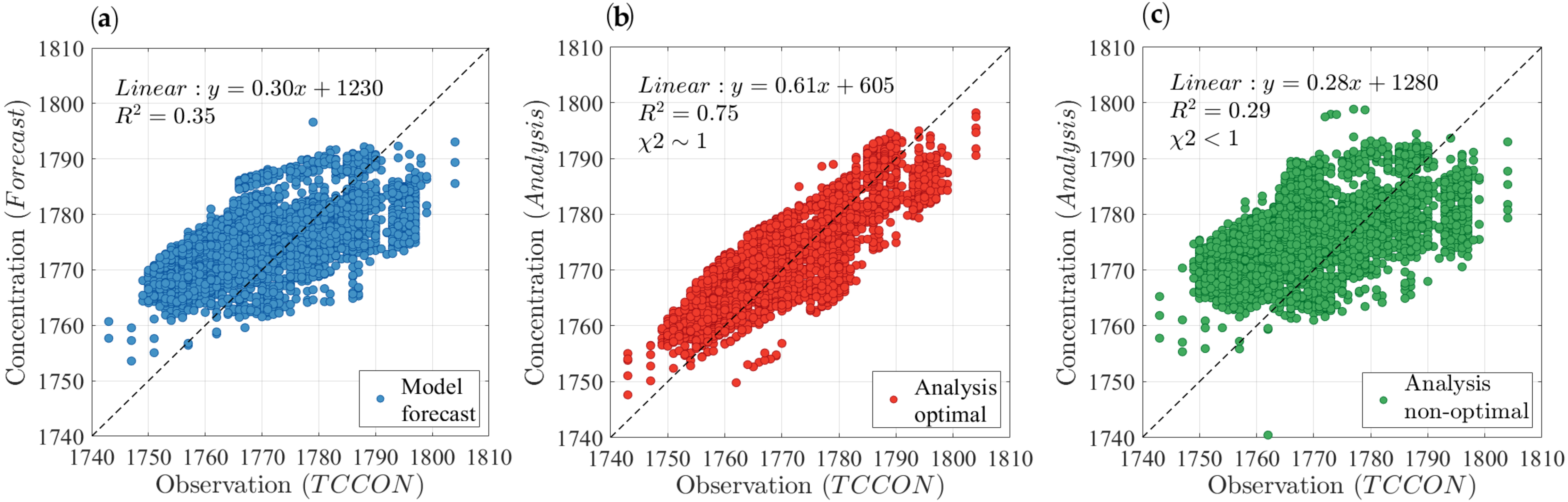
Optimal estimation parameters:

$$f^o = 0.5, f^i = 0.45, f^q = 0.018, L_h = 350\ \mathrm{km}, L_v = 7\sigma$$

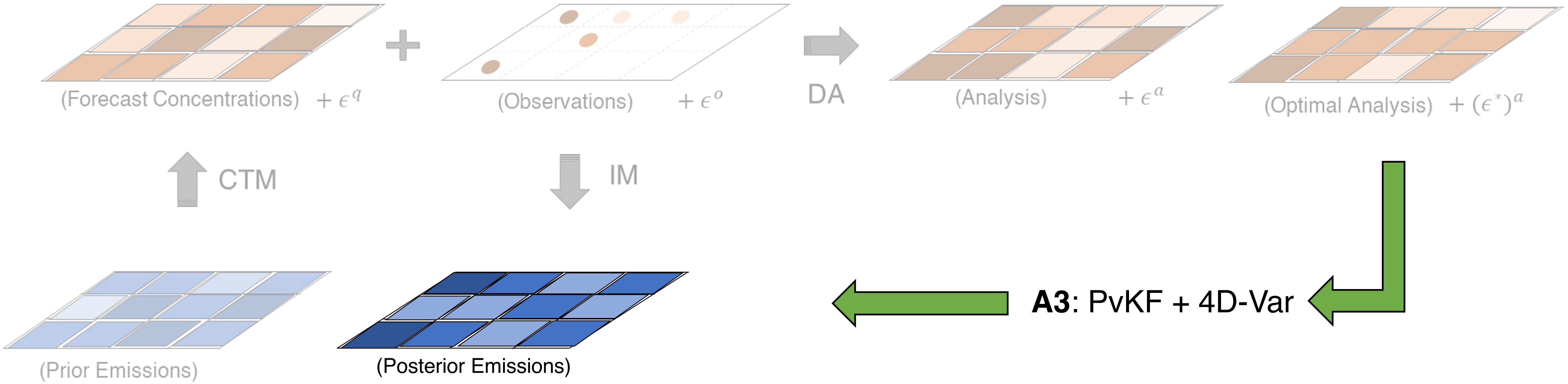
Non-optimal estimation but commonly used parameters:

$$f^o = 1.2, f^i = 0.45, f^q = 0, L_h = 600\ \mathrm{km}, L_v = 1\sigma$$

Optimality of error parameters has a crucial impact on the assimilation result.

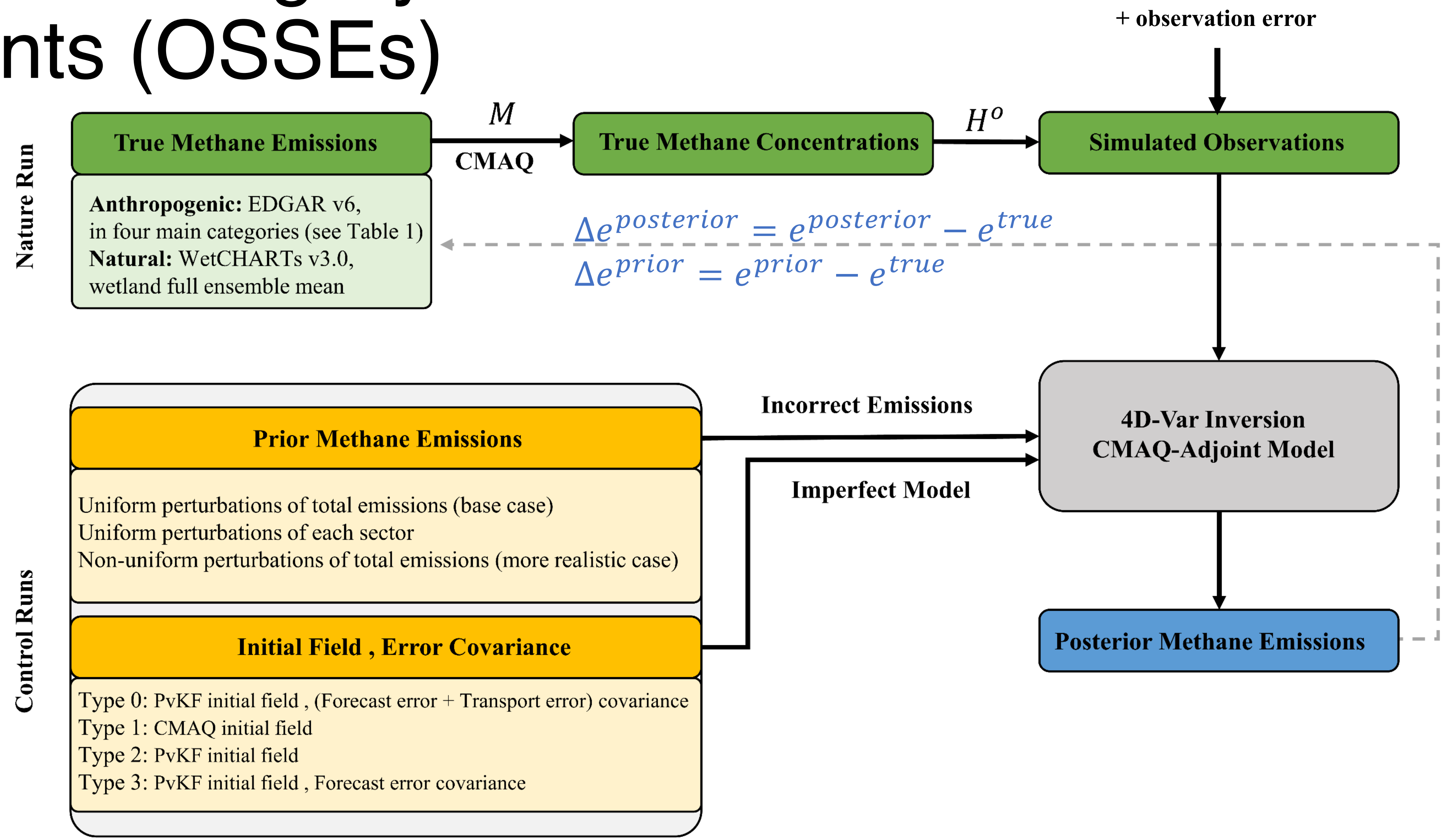


# **Q3**: Can we improve on 4D-Var inversion using optimal analysis and their uncertainties?



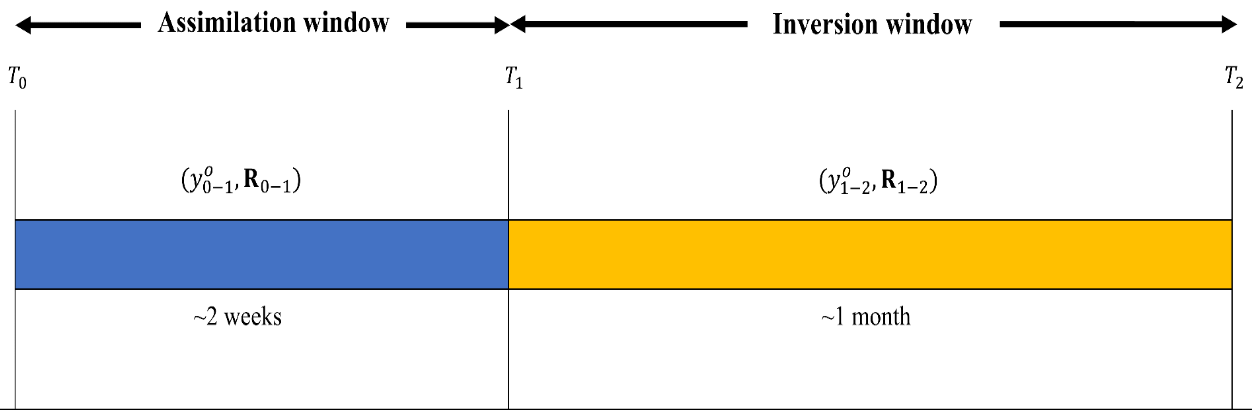
# **Part III**: Observing System Simulation Experiments (OSSEs)

To evaluate the proposed inversion:



# **Part III**: Use of PvKF Assimilation for Emissions Inversion (4D-Var)

$y$: Observations
$x$: Emission scaling factor
$c$: Model/assimilation concentration
$\mathbf{R}$: Observation error covariance
$\mathbf{P}$: Forecast error covariance
$\mathbf{Q}$: Model transport error covariance
$\mathbf{A}$: Analysis error covariance




| | Experiments | | | | Assumptions |
|---|---|---|---|---|---|
| **Classical form (Previous studies)** | 1 | $M$ | $c_1^f$ | $\mathbf{P}^f_{1-2} = \emptyset$ | Perfect forecast field<br>Perfect model |
| | 2 | PvKF | $c_1^a$ | $\mathbf{P}^f_{1-2} = \emptyset$ | Perfect analysis field<br>Perfect model |
| **Other variation** | 3 | PvKF | $(c_1^a, \mathbf{A}_1)$ | $\mathbf{P}^f_{1-2}(\mathbf{A}_1)$ | Imperfect analysis field<br>Perfect model |
| **This study** | 4* | PvKF | $(c_1^a, \mathbf{A}_1)$ | $\mathbf{P}^f_{1-2}(\mathbf{A}_1, \mathbf{Q})$ | Imperfect analysis field<br>Imperfect model |

# **Part III**: Different From of 4D-Var Cost Functions

| Type # | Cost function | | $c_1^a$ | $\mathbf{P}(\mathbf{A}_1)$ | $\mathbf{P}(\mathbf{Q})$ |
|---|---|---|---|---|---|
| Type 0: | $J_0(x)=\frac{1}{2}\gamma(x-x_b)^T\mathbf{B}^{-1}(x-x_b)+\sum_{t=0}^{n}\frac{1}{2}\left(y_t^o-H_t(c_1^a,x)\right)^T\left(H^o\mathbf{P}_t^f(\mathbf{A}_1,\mathbf{Q})H^{o\,T}+\mathbf{R}_t\right)^{-1}\left(y_t^o-H_t(c_1^a,x)\right)$ | This study | ✓ | ✓ | ✓ |
| Type 1: | $J_1(x)=\frac{1}{2}\gamma(x-x_b)^T\mathbf{B}^{-1}(x-x_b)+\sum_{t=0}^{n}\frac{1}{2}\left(y_t^o-H_t(c_1^f,x)\right)^T(\mathbf{R}_t)^{-1}\left(y_t^o-H_t(c_1^f,x)\right)$ | Classical form | ✗ | ✗ | ✗ |
| Type 2: | $J_2(x)=\frac{1}{2}\gamma(x-x_b)^T\mathbf{B}^{-1}(x-x_b)+\sum_{t=0}^{n}\frac{1}{2}\left(y_t^o-H_t(c_1^a,x)\right)^T(\mathbf{R}_t)^{-1}\left(y_t^o-H_t(c_1^a,x)\right)$ | | ✓ | ✗ | ✗ |
| Type 3: | $J_3(x)=\frac{1}{2}\gamma(x-x_b)^T\mathbf{B}^{-1}(x-x_b)+\sum_{t=0}^{n}\frac{1}{2}\left(y_t^o-H_t(c_1^a,x)\right)^T\left(H^o\mathbf{P}_t^f(\mathbf{A}_1)H^{o\,T}+\mathbf{R}_t\right)^{-1}\left(y_t^o-H_t(c_1^a,x)\right)$ | Other variation | ✓ | ✓ | ✗ |

$c_1^a$ : optimal analysis field
$\mathbf{P}(\mathbf{A}_1)$: propagated analysis error covariance
$\mathbf{P}(\mathbf{Q})$ : propagated modelling (transport) error covariance

# **Part III**: Uniform Perturbations

This study

Classical form

Other variation

$c_1^a$ ✓ P(A$_1$) ✓ P(Q) ✓

$c_1^a$ ✗ P(A$_1$) ✗ P(Q) ✗

$c_1^a$ ✓ P(A$_1$) ✗ P(Q) ✗

$c_1^a$ ✓ P(A$_1$) ✓ P(Q) ✗

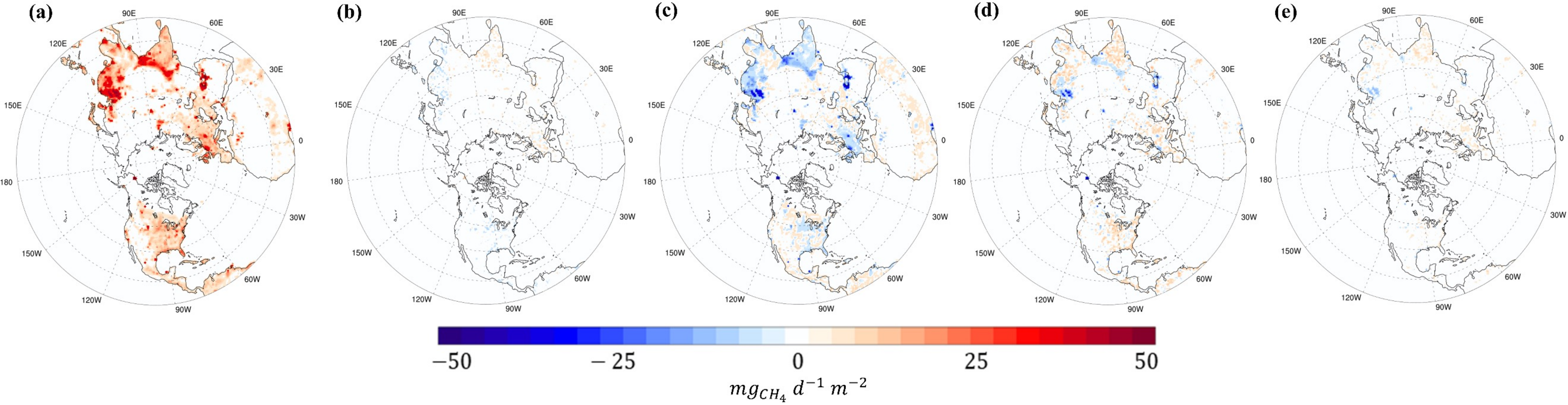
$\Delta e^{prior}$

Type 0: $\Delta e_{J_0}^{posterior}$

Type 1: $\Delta e_{J_1}^{posterior}$

Type 2: $\Delta e_{J_2}^{posterior}$

Type 3: $\Delta e_{J_3}^{posterior}$



# **Part III**: Uniform Perturbations

This study

$c_1^a$ ✓ $\mathbf{P}(\mathbf{A}_1)$ ✓ $\mathbf{P}(\mathbf{Q})$ ✓

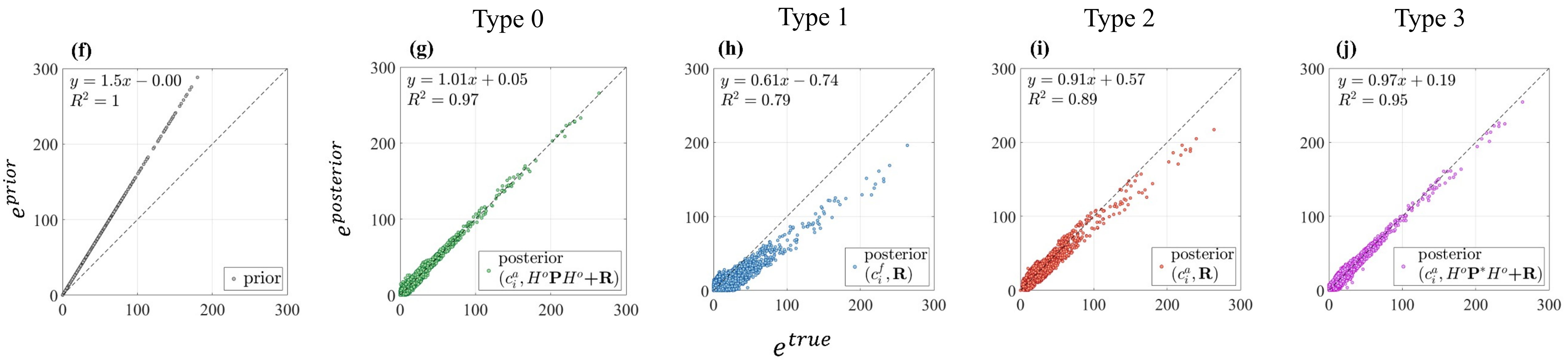
Classical form

$c_1^a$ ✗ $\mathbf{P}(\mathbf{A}_1)$ ✗ $\mathbf{P}(\mathbf{Q})$ ✗

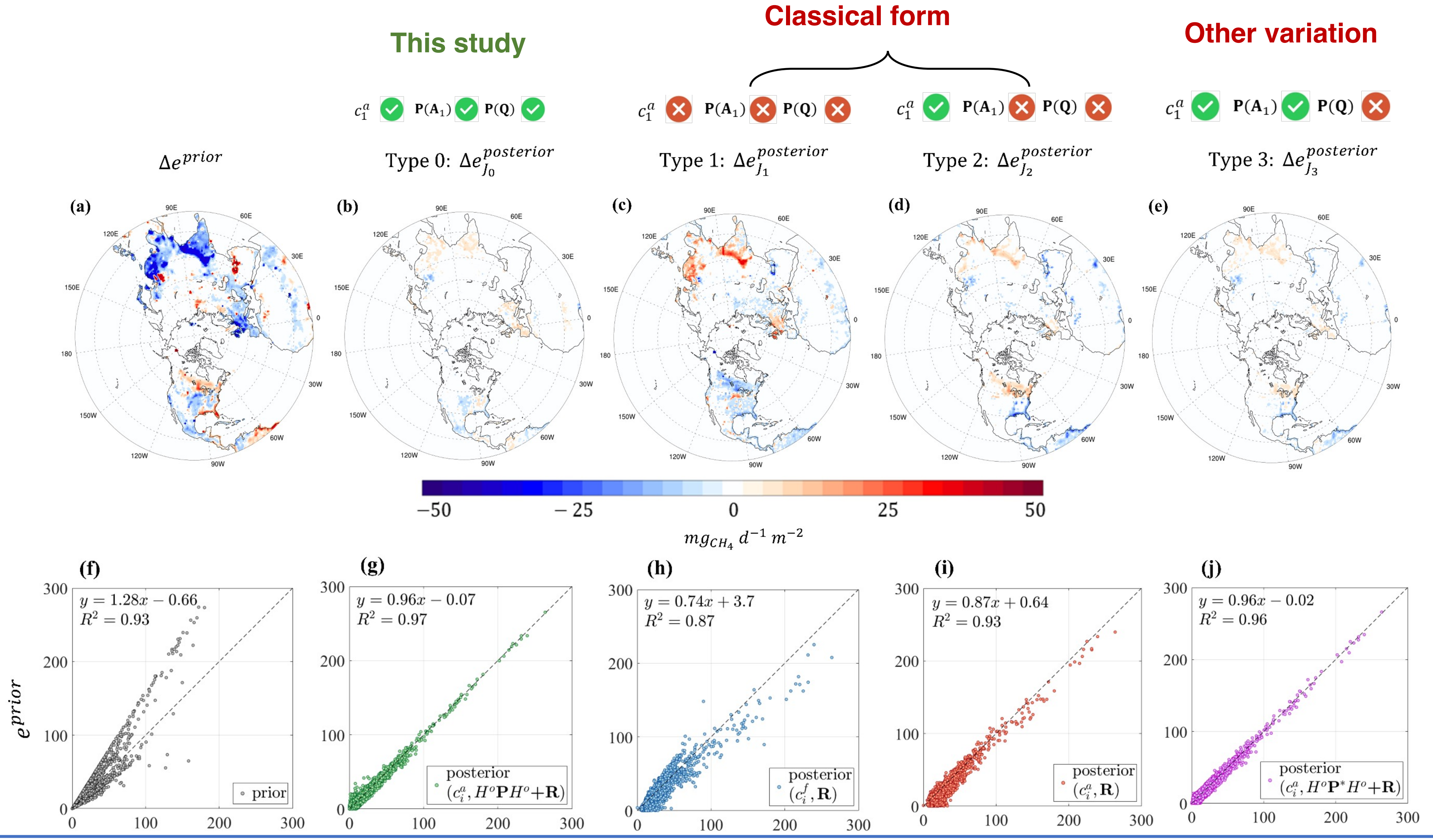
$c_1^a$ ✓ $\mathbf{P}(\mathbf{A}_1)$ ✗ $\mathbf{P}(\mathbf{Q})$ ✗

Other variation

$c_1^a$ ✓ $\mathbf{P}(\mathbf{A}_1)$ ✓ $\mathbf{P}(\mathbf{Q})$ ✗



# **Part III**: Non-uniform Perturbations



# Conclusions & Future Work

(**I**) PvKF assimilation is a stand-alone DA framework that improves our understanding of atmospheric methane estimation

- No need to assume a perfect model
- Provides an (continuous) **estimation of methane analysis and its uncertainties cost-effectively**

(**II**) Realistic error statistics and optimal analysis play a key role in PvKF assimilation

- Optimal analysis is obtained by **optimizing error statistics using cross-validation**
- Non-optimal error covariances can lead to an analysis even worse than the model forecast

(**III**) PvKF assimilation can be used in conjunction with an inversion system

- **Improve the typical 4D-Var inversion results** by providing more sophisticated form of error correlations and initial optimal analysis field

**Suggestions for future work**

- Extending PvKF assimilation framework to a jointly source-state estimation (i.e., emissions error will be estimated as part of the solution)
- Further development of PvKF assimilation for other species such as short-lived pollutants (likely requires evolving error correlations)
- Conducting PvKF with dense satellite observations (e.g., TROPOMI) for high-resolution inversion in regional domain (e.g., CONUS)
- Application of PvKF analysis to remove (measurement) biases over remote area such as oceans

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# Thank you!

sina.voshtani@utoronto.ca