Data Assimilation and Machine Learning for Air Quality Forecasts - Emission Inversion

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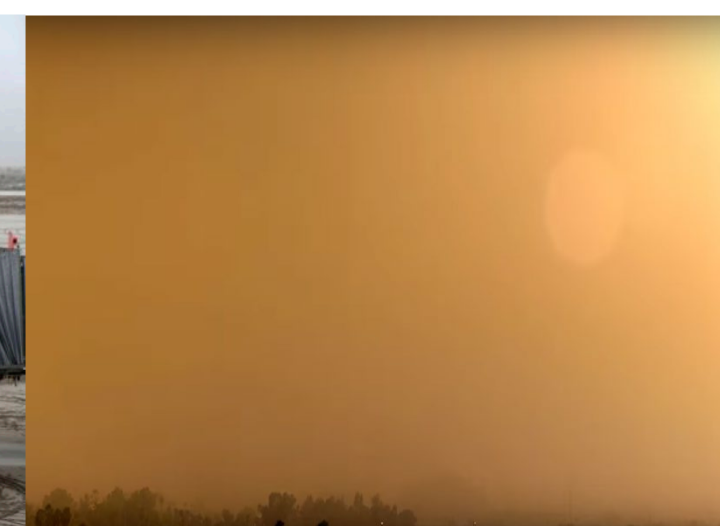

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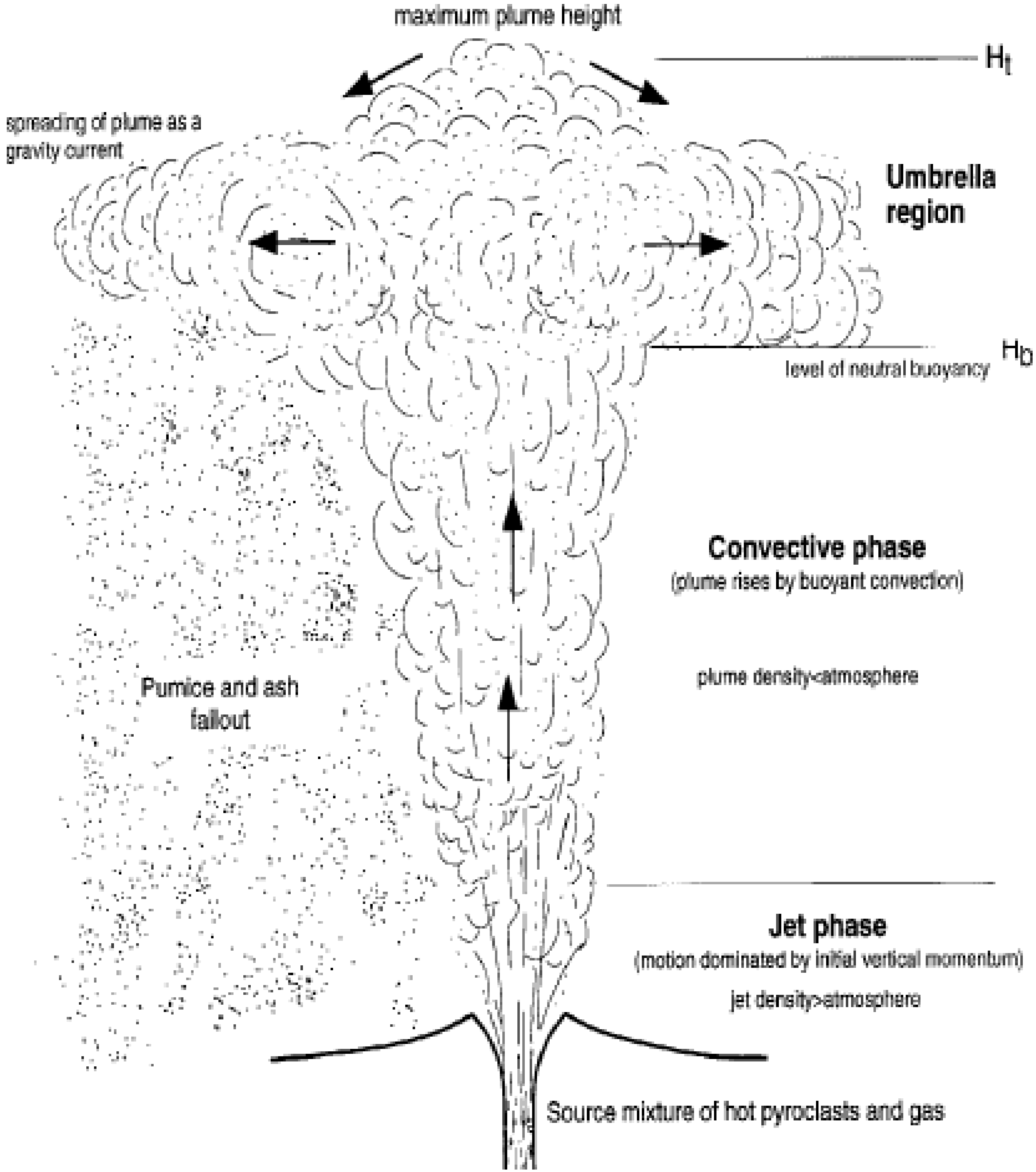
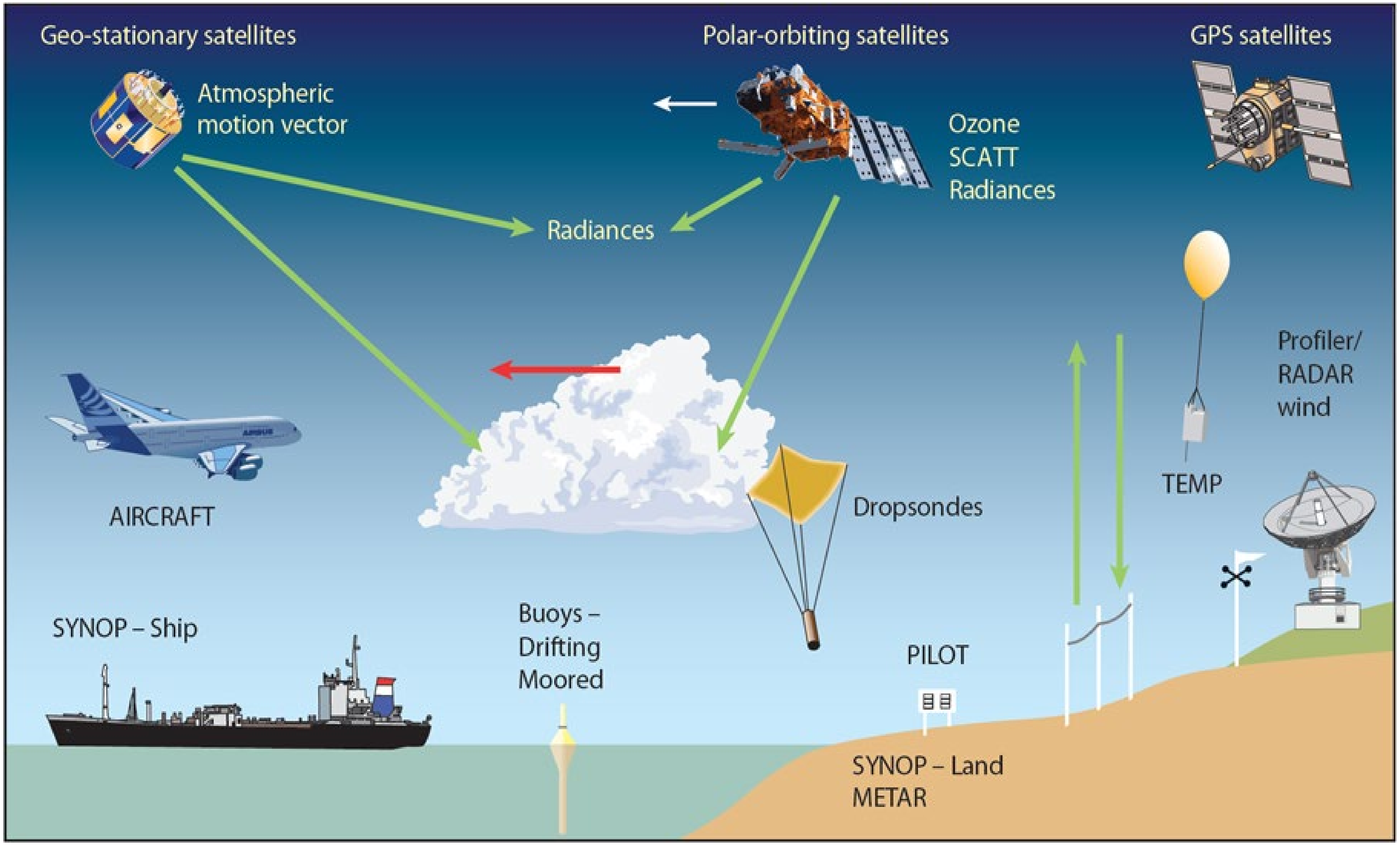
Hazard of volcanic ash:
An accurate forecast is important!


maximum plume height
H_t
spreading of plume as a gravity current
Umbrella region
H_b
level of neutral buoyancy
Convective phase
(plume rises by buoyant convection)
plume density<atmosphere
Pumice and ash fallout
Jet phase
(motion dominated by initial vertical momentum)
jet density>atmosphere
Source mixture of hot pyroclasts and gas

Observations of volcanic ash activity



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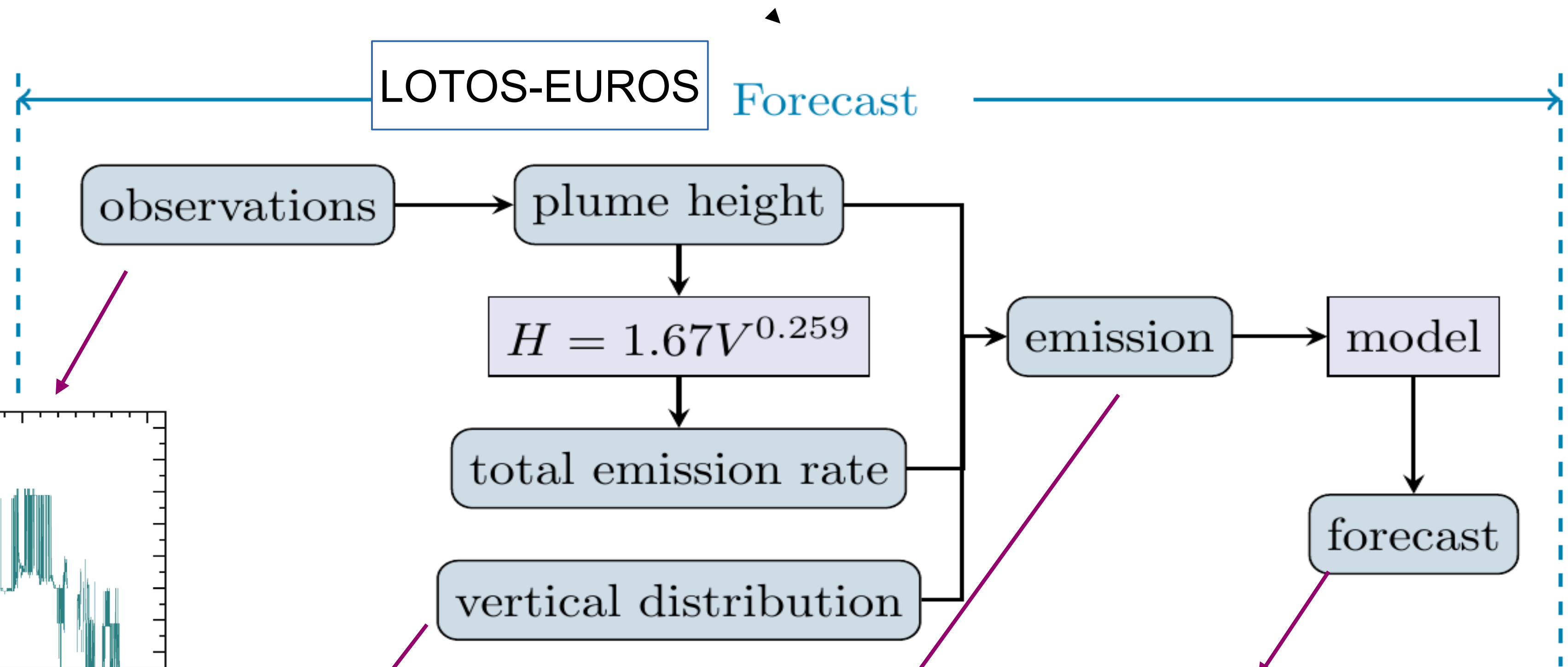
Emission observation: plume height



Ground-based observations of plume height: Lidar, radar

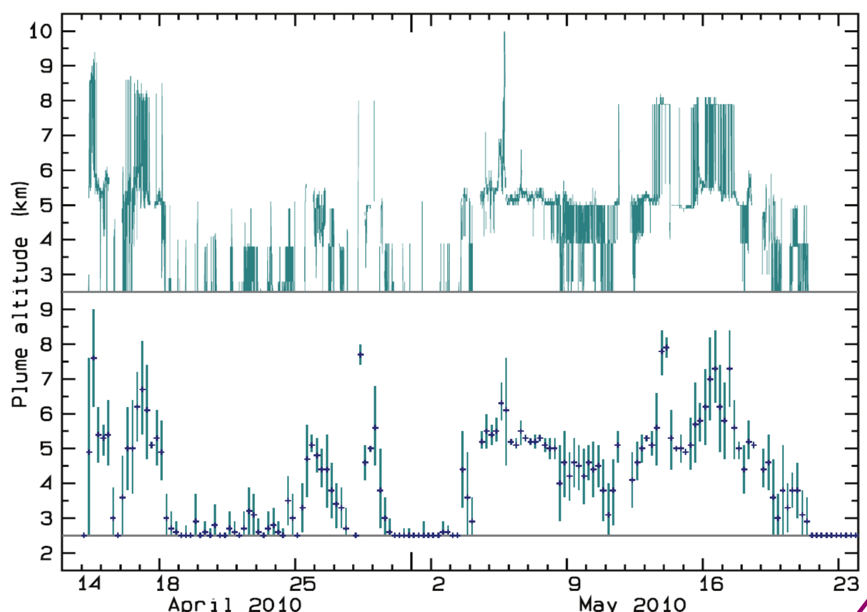


Illustration of the vertical profile of emission

Ash columns of forecast ash plume

Predefined vertical distribution:
Umbrella-shaped,
Exponentially-distributed,
Poisson-distributed

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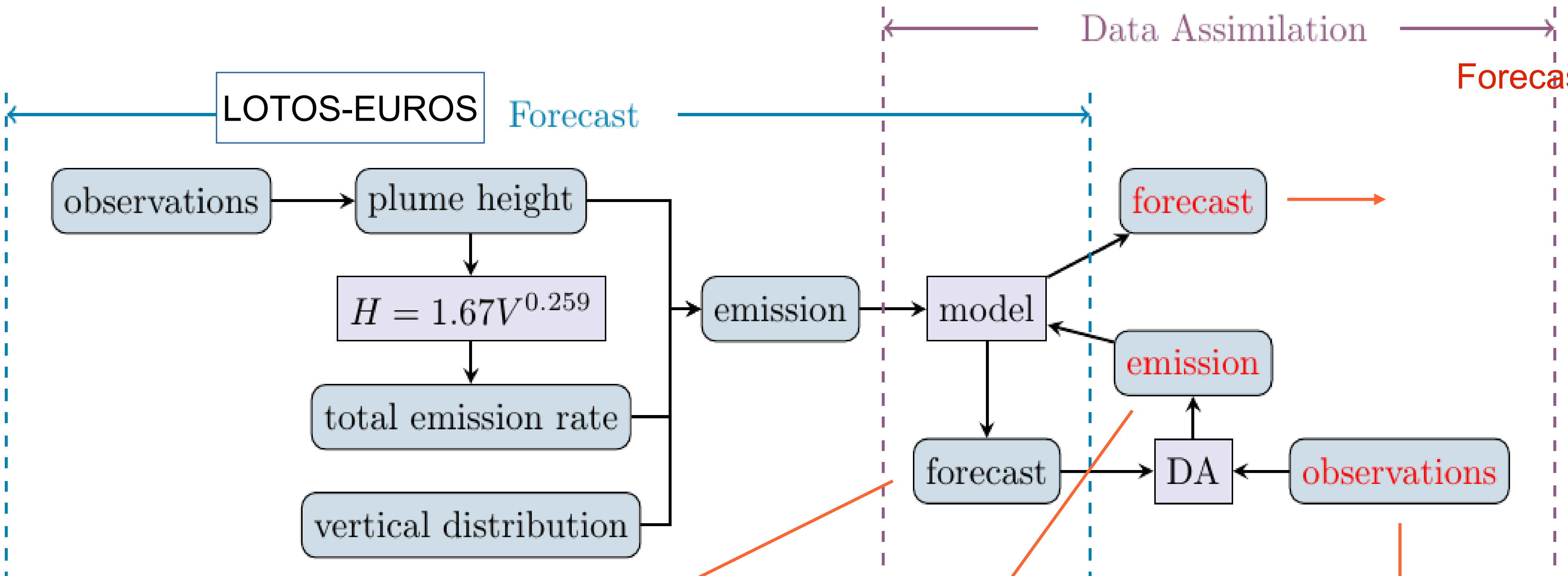
Forecast of volcanic ash cloud

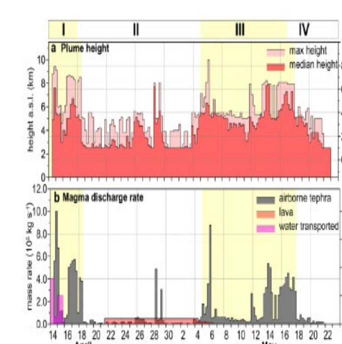


Forecast after DA

Forecast before DA

Illustration of emission after DA

Ash mass loading retrieved from satellite data;
Plume height from ground-based observations



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Data Assimilation

Data assimilation combines information of observations and models and their errors to get a best estimate of atmospheric state (or other parameters)

N(0,B_k)

$$X_k^f = M_k(X_{k-1}^a, u) + w_{k-1}$$

$$y_k = H_k(X_k) + v_k$$

N(0,R_k)

The prior and likelihood are

$$f(X) \propto \exp(-\frac{1}{2}(X - X^f)^T B_k^{-1}(X - X^f)),$$ and

$$f(y \mid X) \propto \exp(-\frac{1}{2}(X - y)^T R_k^{-1}(X - y))$$

Posterior: $f(X \mid y) \propto f(X) f(y \mid X) \propto \exp(-\frac{1}{2} J(X))$

Minimize the cost function J:

$$J(X^a) = (X^a - X^f)^T B_k^{-1}(X^a - X^f) + (X^a - y)^T R_k^{-1}(X^a - y)$$

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Chemical Transport Model – LOTUS-EUROS

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} + V\frac{\partial C}{\partial y} + W\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}\left(K_h\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_h\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right)$$
$$+E+R+Q-D-H$$

Emissions

Transport
(advection, diffusion, radiation**)**

Model

sedimentation
(wet/dry deposition)

Chemical reactions

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Using 4D-Var to estimate the emissions

Model representation:

$$\begin{aligned}\mathbf{x}_k &= M_k(\mathbf{x}_{k-1}, \mathbf{u}_k + \mathbf{w}_k),\\ \mathbf{y}_k &= H_k(\mathbf{x}_k) + \mathbf{v}_k.\end{aligned}$$

Model uncertainty lies in the emission 'u'

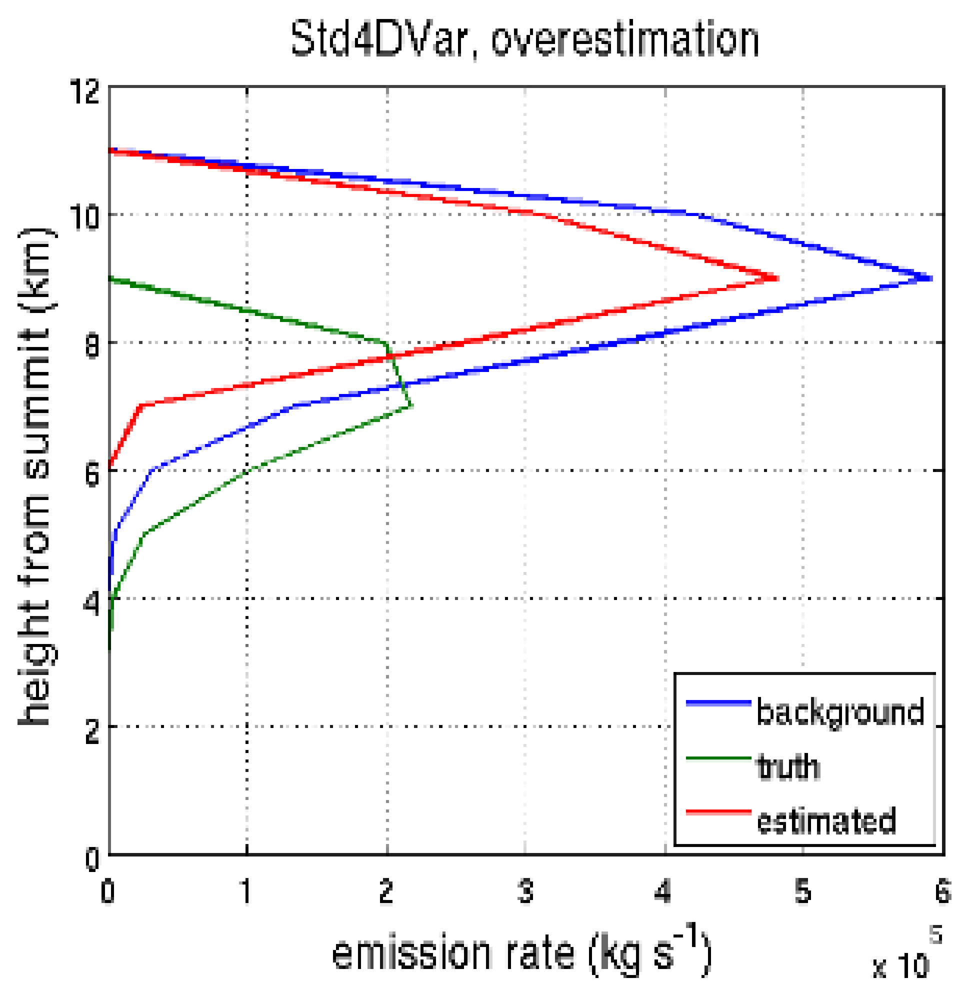
Measurement uncertainty (error) v_k

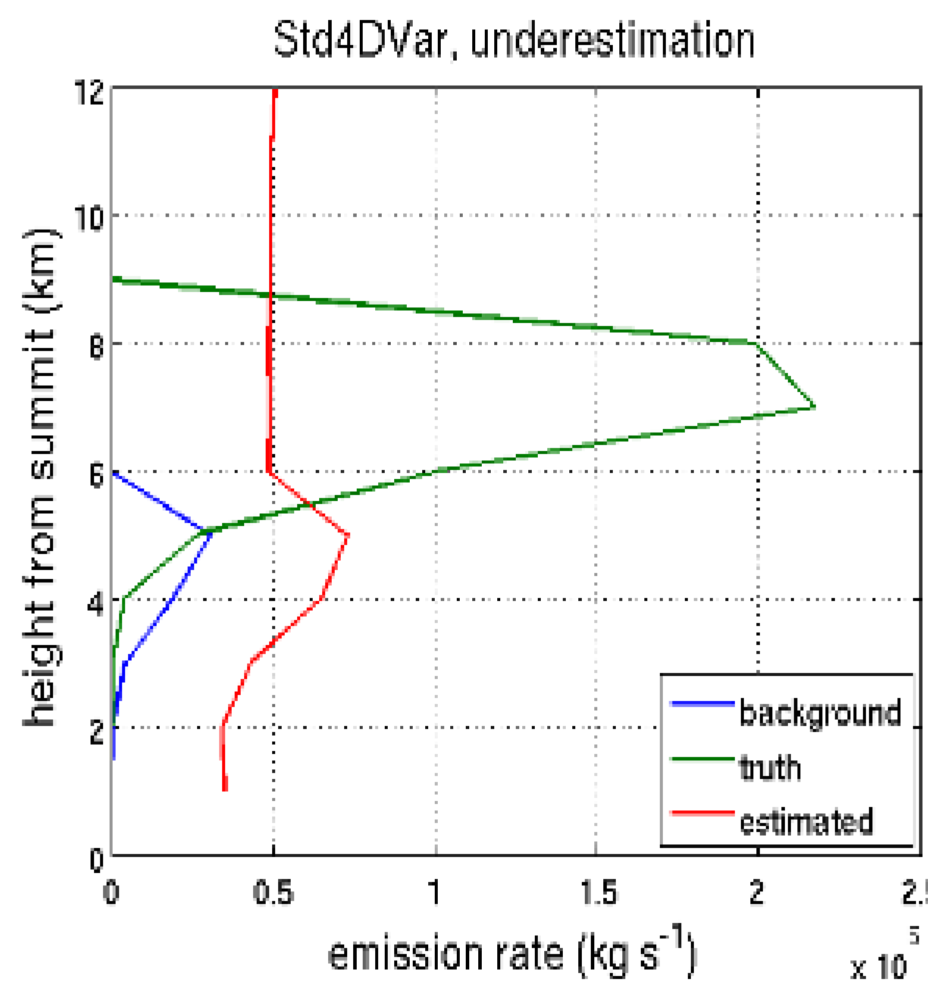
Typical cost function of standard 4DVar:

$$J(\mathbf{u}_k) = \frac{1}{2}\sum_{k=0}^{N}\left(\mathbf{u}_k - \mathbf{u}_k^b\right)^T \mathbf{B}_k^{-1}\left(\mathbf{u}_k - \mathbf{u}_k^b\right) + \frac{1}{2}\sum_{k=0}^{N}(\tilde{\mathbf{y}}_k - \mathbf{y}_k)^T \mathbf{R}_k^{-1}(\tilde{\mathbf{y}}_k - \mathbf{y}_k)$$

$$= J^b + J^o,$$

Ill-conditioned problem
due to ‘spurious relationship’



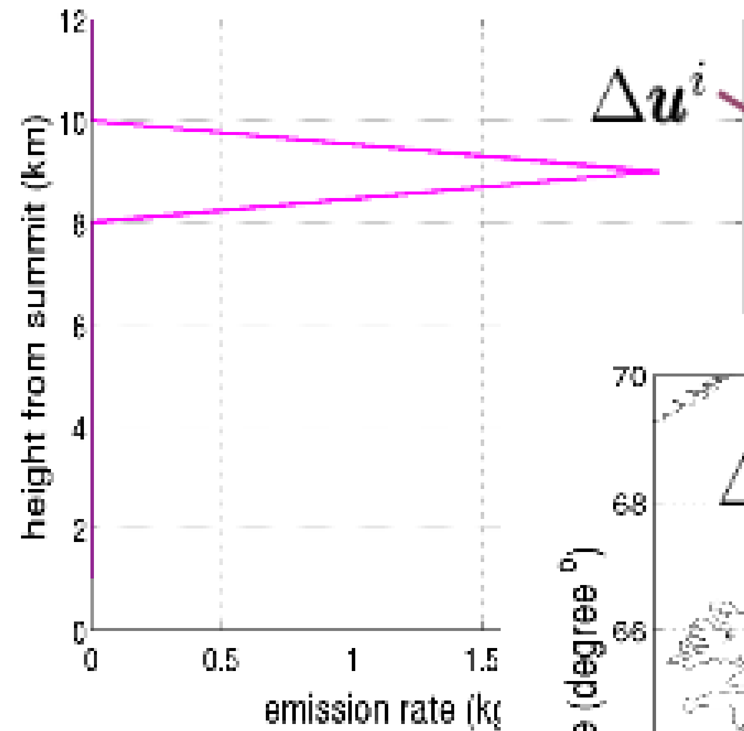


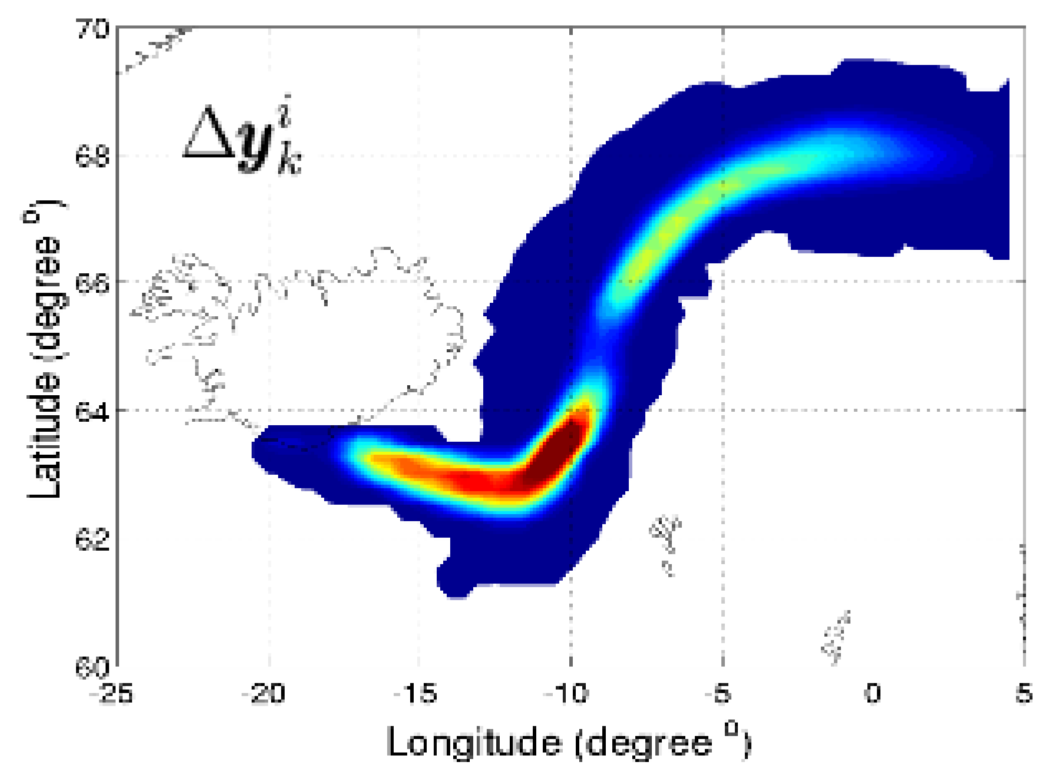
Trajectory-based 4D-Var

Assumption/observation:
Horizontal transport is stronger than vertical transport and diffusion.

The emission is assumed to be a linear combination of the perturbation sets:

$$\boldsymbol{u} = \boldsymbol{u}^b + \sum_{i=1}^{p} \beta^i \Delta \boldsymbol{u}^i,$$





Trajectories
:

$$\boldsymbol{y}_k^0 = \mathcal{H}_k(\mathcal{M}_k(\boldsymbol{x}_{k-1}, \boldsymbol{u}^b)).$$

$$\Delta \boldsymbol{y}_k^i = \mathcal{H}_k(\mathcal{M}_k(\boldsymbol{x}_{k-1}, \boldsymbol{u}^b + \Delta \boldsymbol{u}^i)) - \boldsymbol{y}_k^0.$$

The reformulated cost function of Trj4DVar:

$$\begin{aligned} J(\boldsymbol{\beta}) &= \frac{1}{2} \sum_{k=1}^{Nt} \left(\sum_{i=1}^{p} \beta^i \Delta \boldsymbol{y}_k^i + \boldsymbol{y}_k^0 - \boldsymbol{y}_k \right)^T [\mathbf{R}_k]^{-1} \left(\sum_{i=1}^{p} \beta^i \Delta \boldsymbol{y}_k^i + \boldsymbol{y}_k^0 - \boldsymbol{y}_k \right) \\ &+ \frac{1}{2} \left(\boldsymbol{u} - \boldsymbol{u}^b \right)^T [\mathbf{B}_k]^{-1} \left(\boldsymbol{u} - \boldsymbol{u}^b \right) \\ &= J^o + J^b, \end{aligned}$$

Given:

$$\mathbf{x}_k = M_k(\mathbf{x}_{k-1}, \mathbf{u}_k + \mathbf{w}_k), \tag{1}$$

$$\mathbf{y}_k = H_k(\mathbf{x}_k) + \mathbf{v}_k . \tag{2}$$

with $\mathbf{u} = \mathbf{u}^b + \sum_{i=1}^{p} \beta^i \Delta \mathbf{u}^i$ Eq.(2) can be rewritten as

$$\begin{aligned}
\mathbf{y}_k &\approx H_k[M_k(\mathbf{x}_{k-1}, \mathbf{u}^b)] + \sum_{i=1}^{p} \beta^i \mathbf{H}_k \mathbf{M}_k(\mathbf{x}_{k-1}, \mathbf{u}^b) \Delta \mathbf{u}^i + \mathbf{v}_k \\
&\approx \mathbf{y}_k^0 + \sum_{i=1}^{p} \beta^i \{ H_k[M_k(\mathbf{x}_{k-1}, \mathbf{u}^b + \Delta \mathbf{u}^i)] - \mathbf{y}_k^0 \} + \mathbf{v}_k \\
&= \mathbf{y}_k^0 + \sum_{i=1}^{p} \beta^i \Delta \mathbf{y}_k^i + \mathbf{v}_k , \qquad (5)
\end{aligned}$$

leading to the trajectory-based 4D-Var formulation:

$$\begin{aligned}
J(\beta) &= \frac{1}{2} \sum_{k=1}^{Nt} \left(\sum_{i=1}^{p} \beta^i \Delta \mathbf{y}_k^i + \mathbf{y}_k^0 - \mathbf{y}_k \right)^{\mathrm{T}} [\mathbf{R}_k]^{-1} \left(\sum_{i=1}^{p} \beta^i \Delta \mathbf{y}_k^i + \mathbf{y}_k^0 - \mathbf{y}_k \right) \\
&\quad + \frac{1}{2} \sum_{k=1}^{Nt} (\mathbf{u} - \mathbf{u}^b)^{\mathrm{T}} [\mathbf{B}_k]^{-1} (\mathbf{u} - \mathbf{u}^b) + \mu \|\nabla \mathbf{u}\|^2 \\
&= J^o + J^b + J^r ,
\end{aligned}$$

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Satellite
Data
assimilation

Estimates of emissions in twin experiments

E15 2010 eruption events as a case study: LOTOS-EUROS model, meteorological situation, synthetic observations

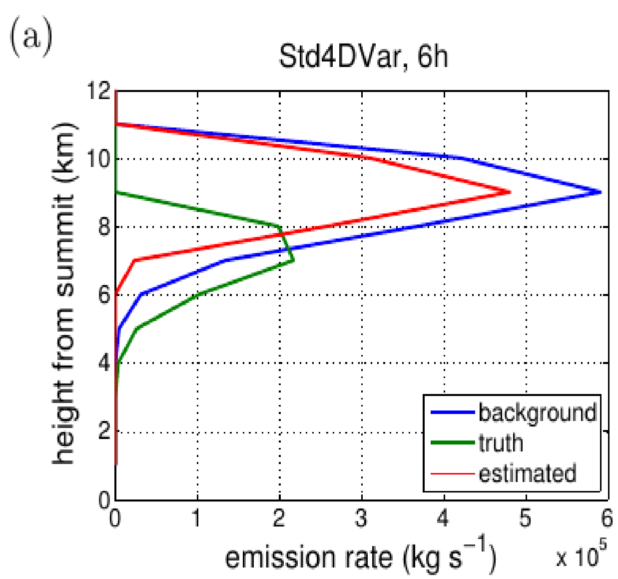
Testing the methodology:

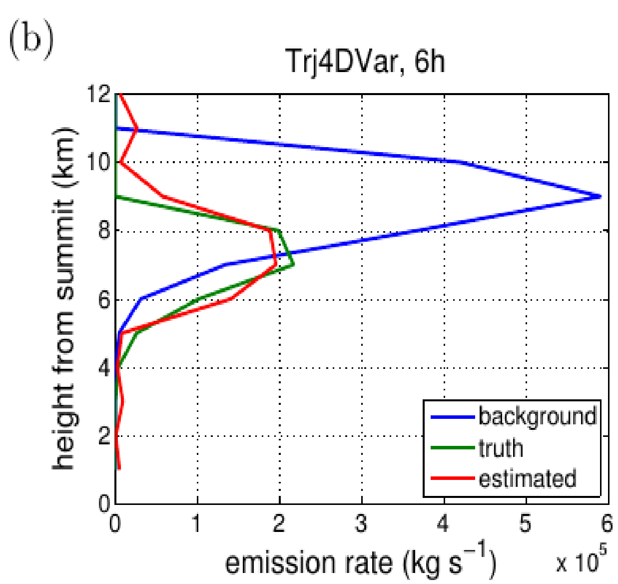
- Standard 4D-Var vs.
- Trajectory-based 4D-Var

- Deterministic model

- Observations: synthetic ash column data

- 6-hour assimilation window





Testing some of the choices:

- Trajectory-based 4D-Var

- Stochastic model

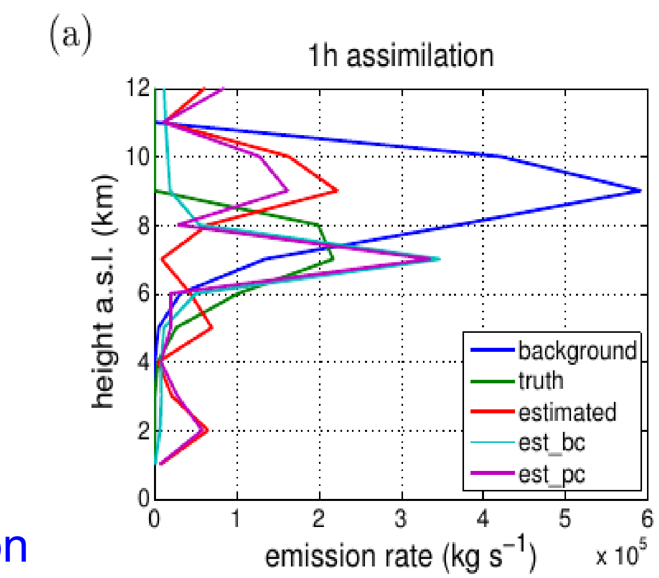
- Observations: synthetic ash columns with 50% uncertainty & plume height and mass eruption rate

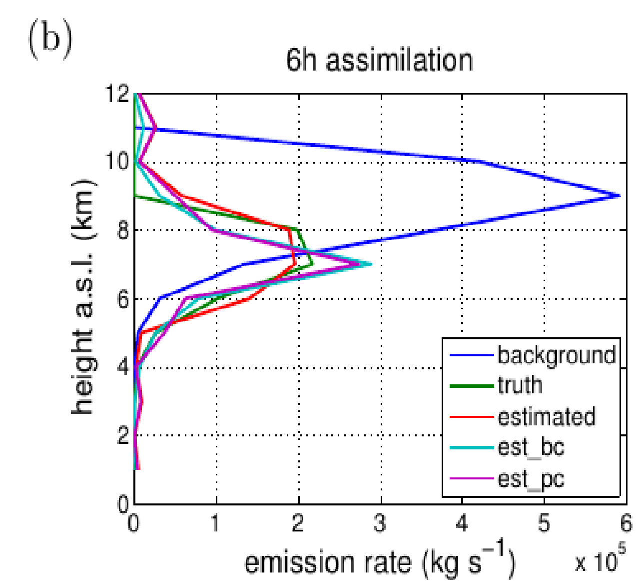
Settings and choices:

- Length of assimilation windows

- Uncertainties of Observations

- Schemes to integrate
- multi-observations





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Lu, S., Lin, H.X., Heemink, A.W., Fu, G., and Segers, A.J. (2016). Estimation of Volcanic Ash Emissions Using Trajectory-Based 4D-Var Data Assimilation. ***Monthly Weather Review*** *144, 575-589.*

Dust storm emission inversion using multiple data sources

Dust storm models
(chemical transport model)

- **Emissions;**
- **Transport;**

  advection, diffusion, radiation
- **Sedimentations.**

  wet, dry deposition

$$\frac{\partial C}{\partial t}+U\frac{\partial C}{\partial x}+V\frac{\partial C}{\partial y}+W\frac{\partial C}{\partial z}$$

$$=\frac{\partial}{\partial x}\left(K_h\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_h\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right)$$

$$+E+R+Q-D-H$$

Example: Lotos-Euros/Dust over East Asia

2.1. Data assimilation with Lotos-Euros: algorithm

Data assimilation: to find a solution that fits both the observation and priori.

Traditional 4 dimensional variational (4DVar) data assimilation:

$$J(\delta \boldsymbol{f}) = \frac{1}{2}\,\delta \boldsymbol{f}\;\mathbf{B}^{-1}\;\delta \boldsymbol{f} + \frac{1}{2}\sum_{i=1}^{k}(\mathbf{H}_i\mathbf{M}_i\delta \boldsymbol{f} + \boldsymbol{d}_i)^T\,\mathbf{O}_i^{-1}\,(\mathbf{H}_i\mathbf{M}_i\delta \boldsymbol{f} + \boldsymbol{d}_i)$$

$$\boldsymbol{d}_i = \mathcal{H}_i(\;\mathcal{M}_i(\boldsymbol{f})\;) - \boldsymbol{y}_i$$

$\mathbf{M}_i$ **full tangent linear model**
Order of **O(10^5)**

Reduced-tangent-linearization 4DVar

$$\mathbf{B} = \mathbf{U}\mathbf{U}^T \approx \tilde{\mathbf{U}}\tilde{\mathbf{U}}^T$$

$$\delta \boldsymbol{f} \approx \tilde{\mathbf{U}}\delta \boldsymbol{w}$$

$$J(\delta \boldsymbol{w}) = \frac{1}{2}\delta \boldsymbol{w}^T\delta \boldsymbol{w} + \frac{1}{2}\sum_{i=1}^{k}(\mathbf{H}_i\tilde{\mathbf{M}}_i\tilde{\mathbf{U}}\delta \boldsymbol{w} + d_i)^T\,\mathbf{O}_\mathbf{i}^{-1}\,(\mathbf{H}_i\tilde{\mathbf{M}}_i\tilde{\mathbf{U}}\delta \boldsymbol{w} + d_i)$$

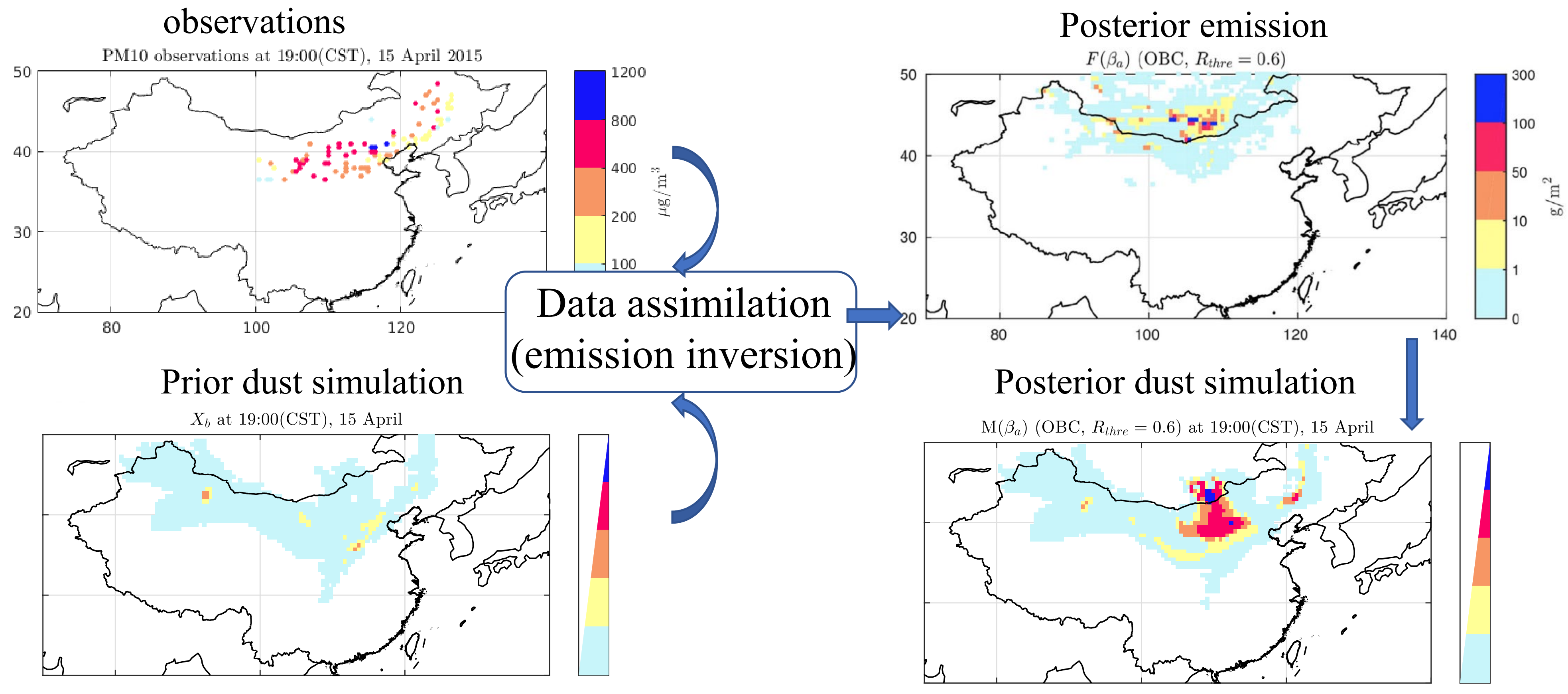
$\tilde{\mathbf{M}}_i$ **reduced tangent linear model**
Order of **O(10^2)**

Sensitivity-based parameter filters: To reduce the size of $\delta \boldsymbol{f}$, improve the computation efficiency

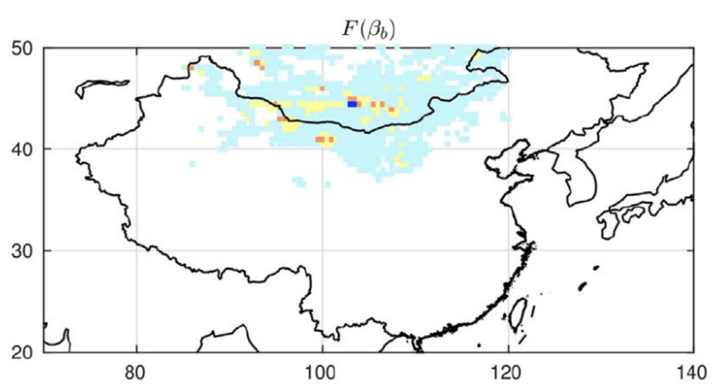
Dust storm emission inversion using multiple data sources

2.1 Data assimilation with Lotos-Euros: assimilating PM10

China MEP monitoring network:
- PM_{10}, $PM_{2.5}$, SO_2, NO_X, O_3
- wide coverage
- high accuracy
- hourly measured
- Over 1,500 sites



Prior emission

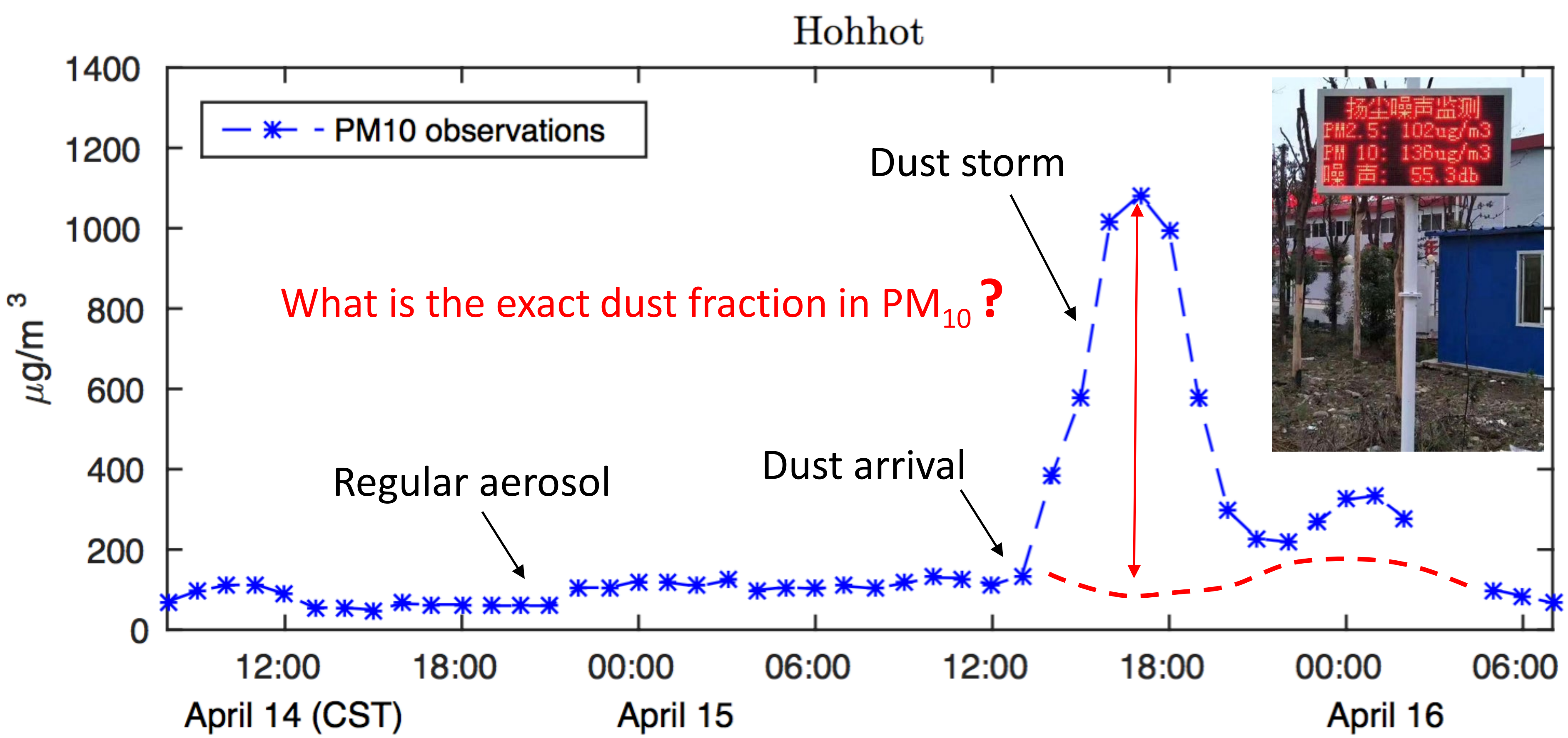


***J.Jin** et al., 2018, Spatially varying parameter estimation …, Atmospheric Environments*

Dust storm emission inversion using multiple data sources

2.2 Machine learning based observation bias correction: bias/baseline

Existence of bias in PM10 concentration for its use in data assimilation



- **PM10 observation is a sum of non-dust and dust aerosols, thus includes a bias when representing the dust concentration.**
- **Issue:** the data assimilation algorithm cannot calculate whether the error is caused by the model deficiency or observation bias.
- **Challenge:** bias with strong spatial and temporal variability
- **Why not full aerosol model???**

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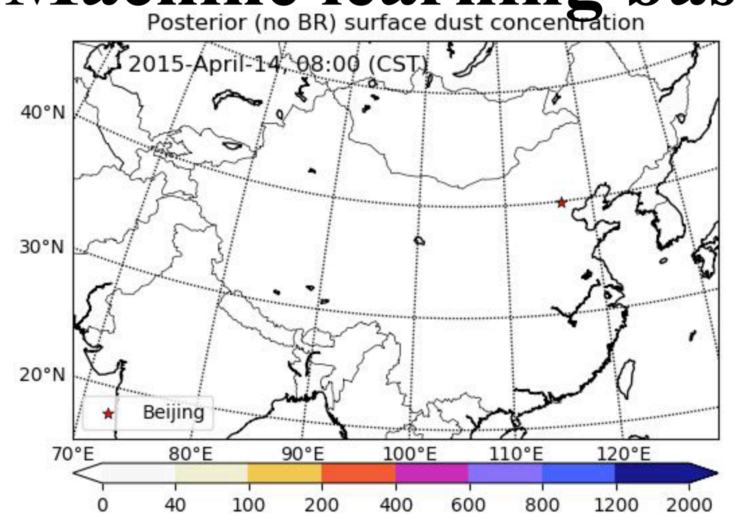
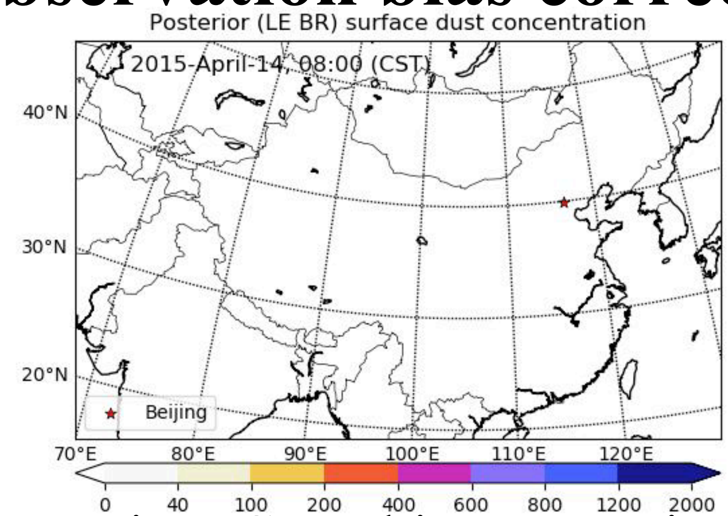
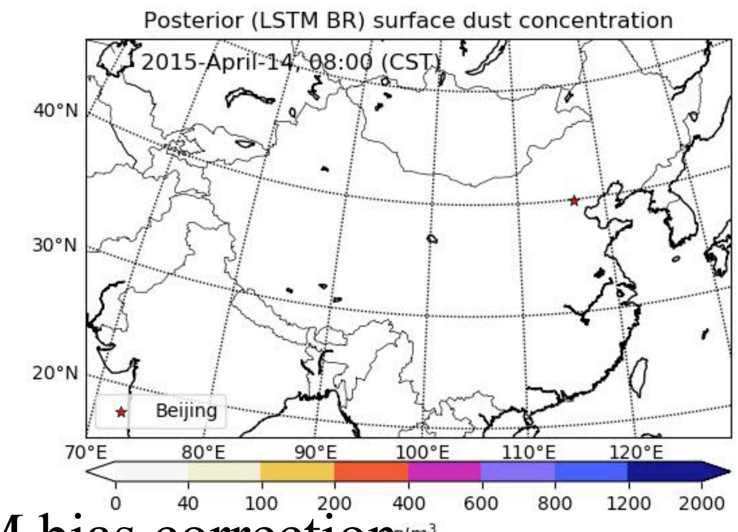
2.2 Machine learning based observation bias correction: assimilation evaluation



Posteriors no bias correction



Posteriors CTM bias correction



Posteriors LSTM bias correction

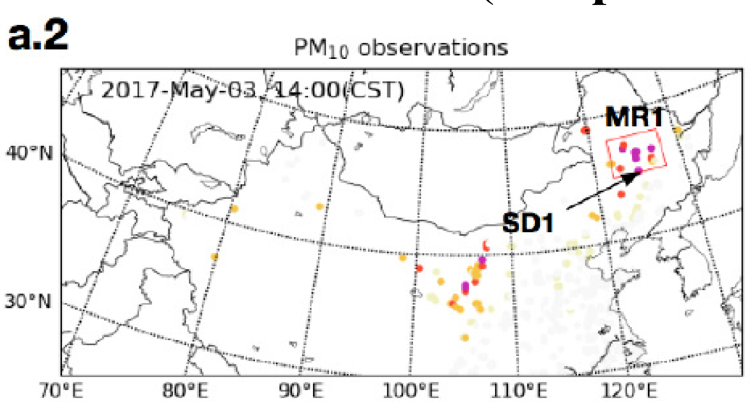
- Assimilation of machine learning bias corrected data gives the most accurate posterior;
- **Direct assimilation of PM_{10} causes overestimation of dust simulations.**

J.Jin *et al, Machine learning for observation bias correction with application to dust storm data assimilation. (ACP Discussion)*

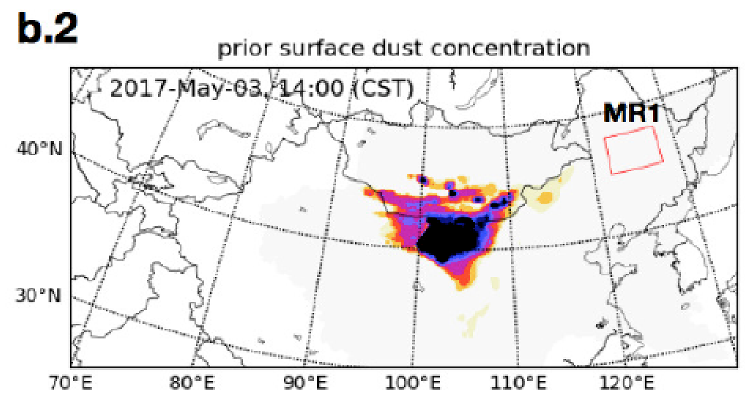
H.X.Lin, ***J.Jin*** *et al. air quality forecast through integrated data assimilation and machine learning. ICCART, Prague, 2019.*

2.3 Emission detection using adjoint: no dust simulated in northeast China

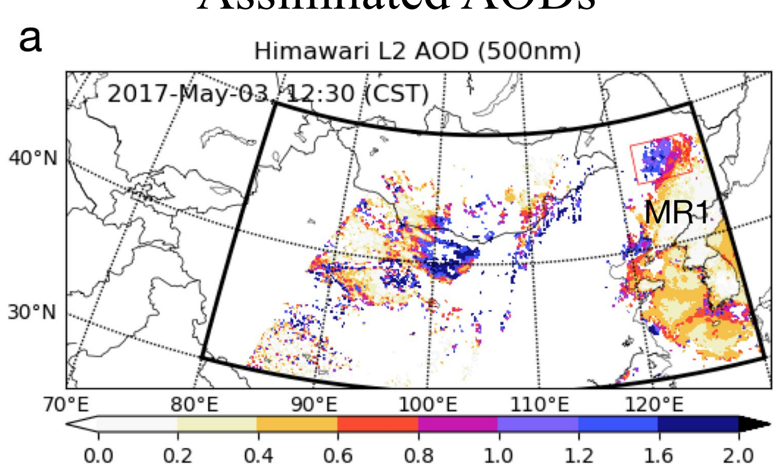
PM10 observations (**independent**)



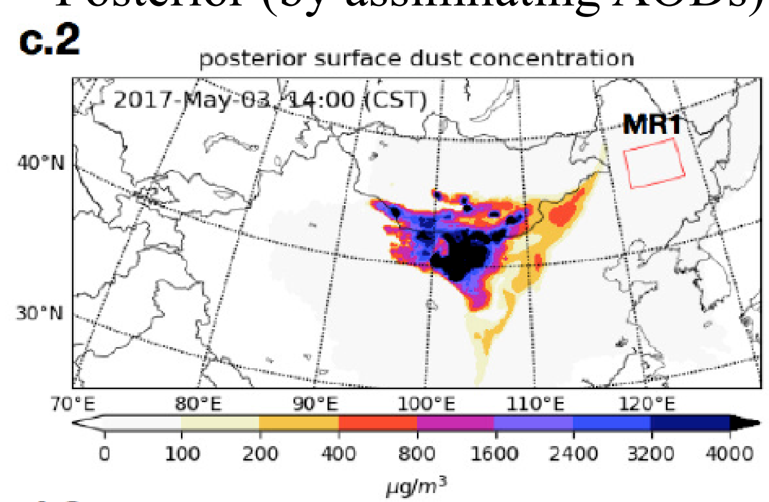
Prior



Assimilated AODs



Posterior (by assimilating AODs)



- No dusts are simulated in prior or posterior model;
- Other **two** dust outbreaks are also not reproduced.
- **Solution: to detect the (missing) sensitive emissions for the dust outbreak**

2.3 Emission detection using adjoint: theory

- CTM Model: $x^{i+1} = \mathcal{M}^i(x^i,\ f^i)$
- Sensitivity calculation
- Linearized model operator: $\frac{\partial x^{i+1}}{\partial f^i} = \frac{\partial \mathcal{M}^i}{\partial f^i} = \mathrm{M}^i_f$ and $\frac{\partial x^{i+1}}{\partial x^i} = \frac{\partial \mathcal{M}^i}{\partial x^i} = \mathrm{M}^i_x$

finite difference: **accurate but intensive**

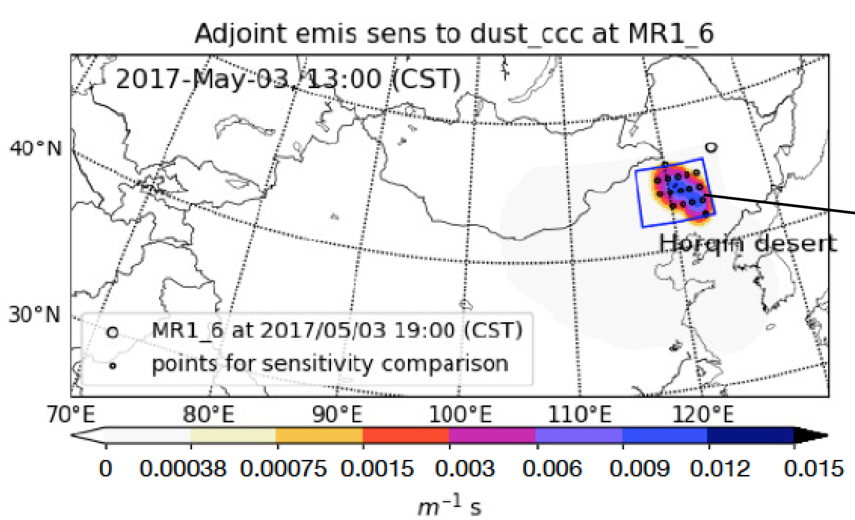
$\boxed{(x^i,\ f^i)}$ forward model $\boxed{x^{i+1}}$

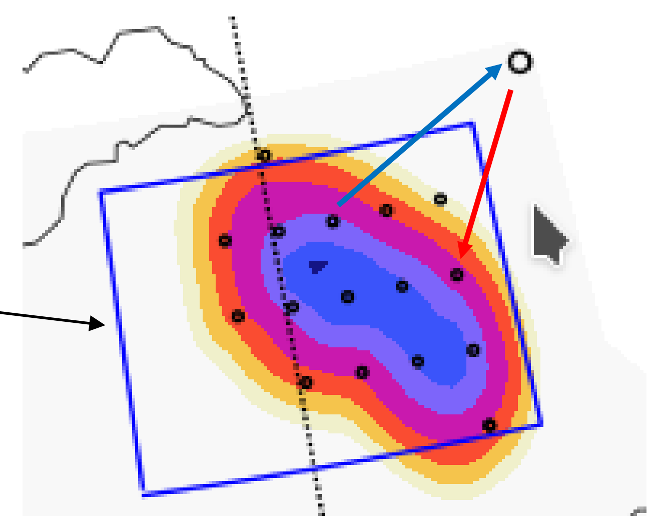
backward model

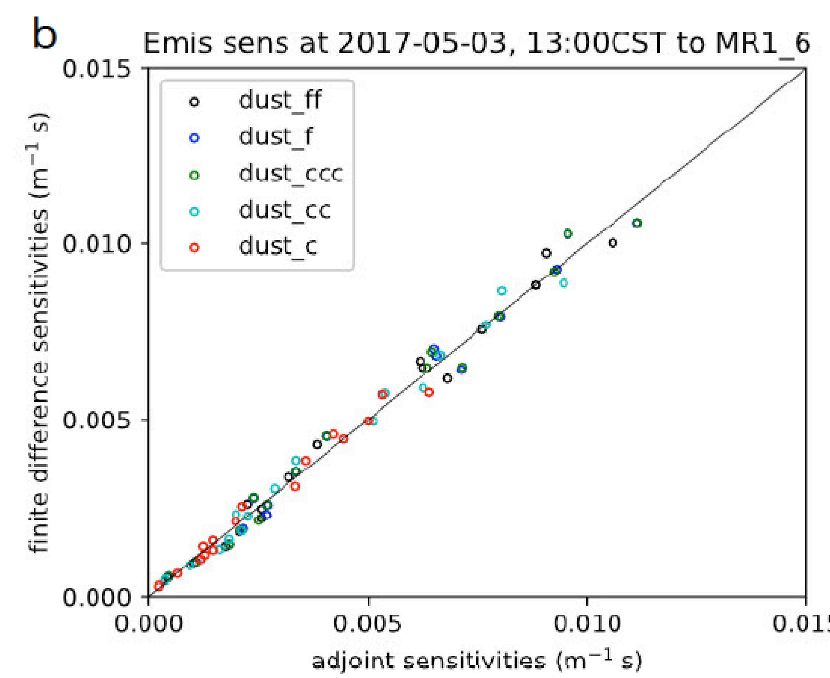
adjoint method: **efficient but ……**

Gradient of model response J to parameters: $\nabla_{f^j}\mathcal{J}(x^i) = (\mathrm{M}^j_f)^T \cdot (\mathrm{M}^{j+1}_x)^T \cdots (\mathrm{M}^{i-1}_x)^T \cdot \{\frac{\partial \mathcal{J}(x^i)}{\partial x^i}\}^T$

(adjoint vs. finite difference):







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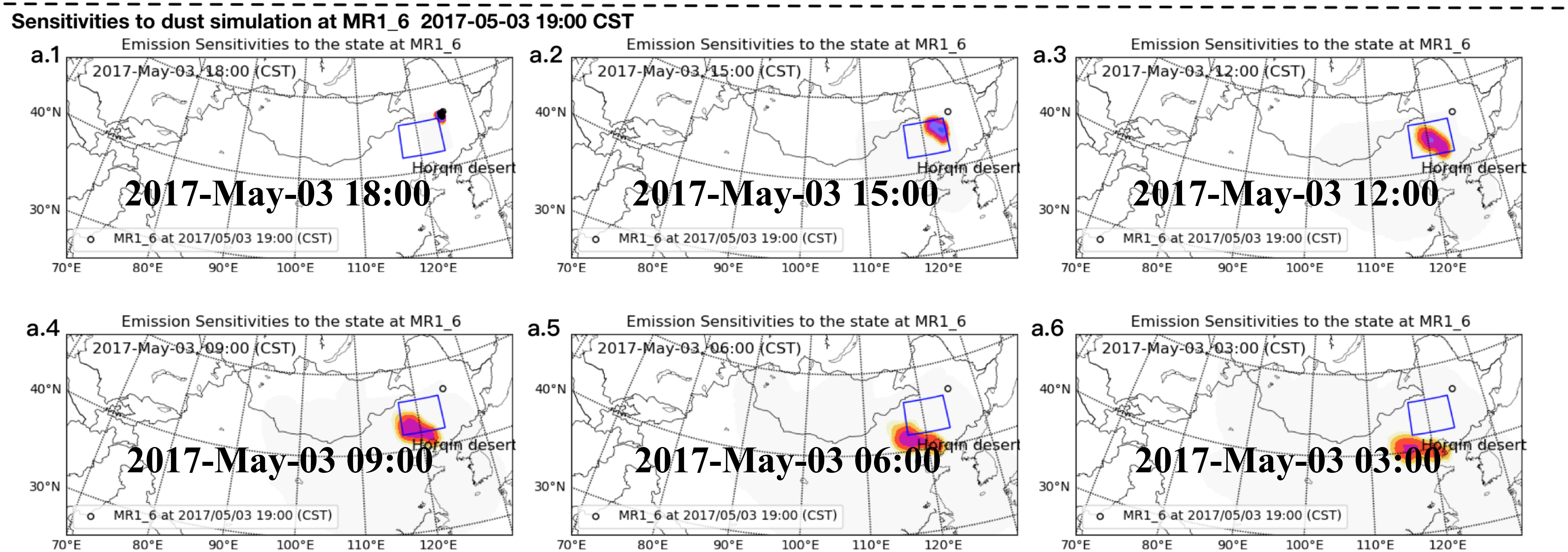
2.3 Emission detection using adjoint: emission backtracking

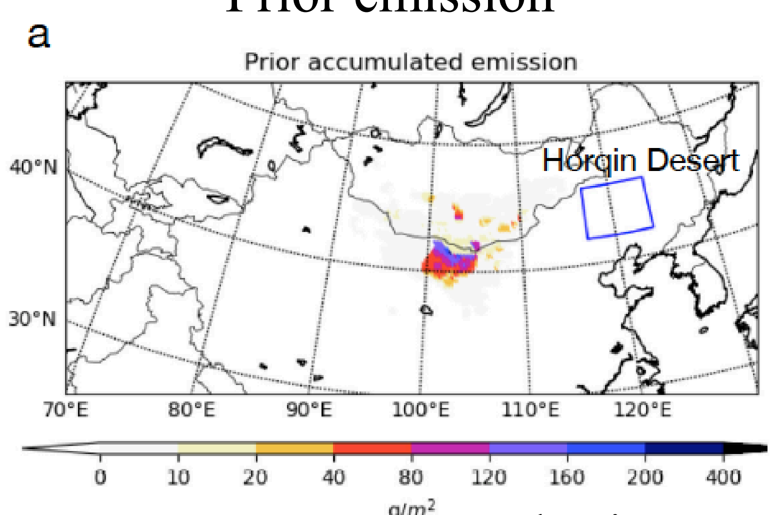
Time series of emission sensitivities to a state X at **2017-May-03 19:00**



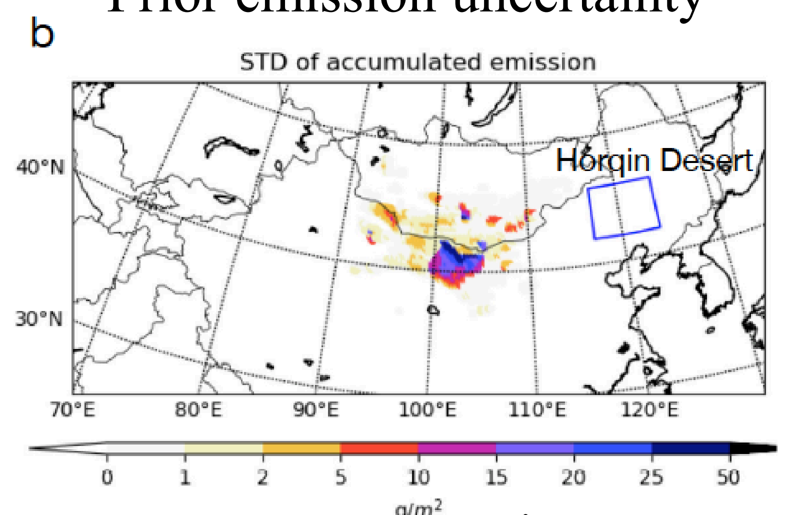
Dust storm emission inversion using multiple data sources

2.3 Emission detection using adjoint: guided emission reconstruction

Prior emission

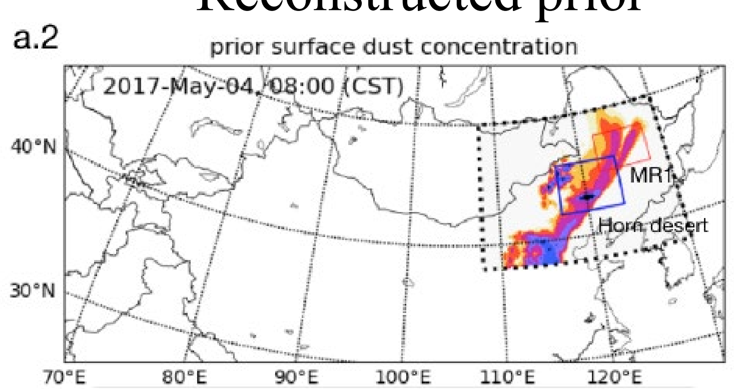


Prior emission uncertainty

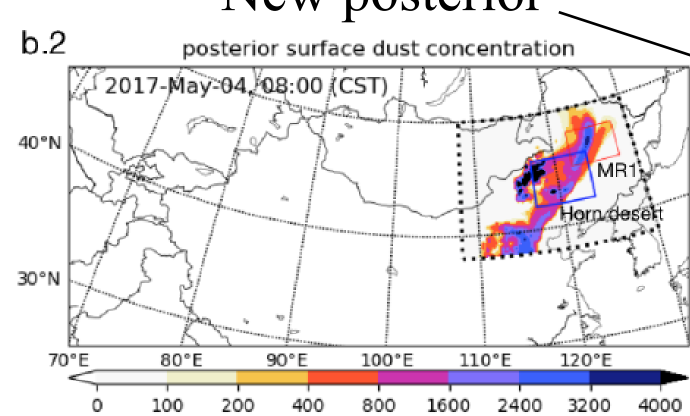


Landcover over **Horqin**

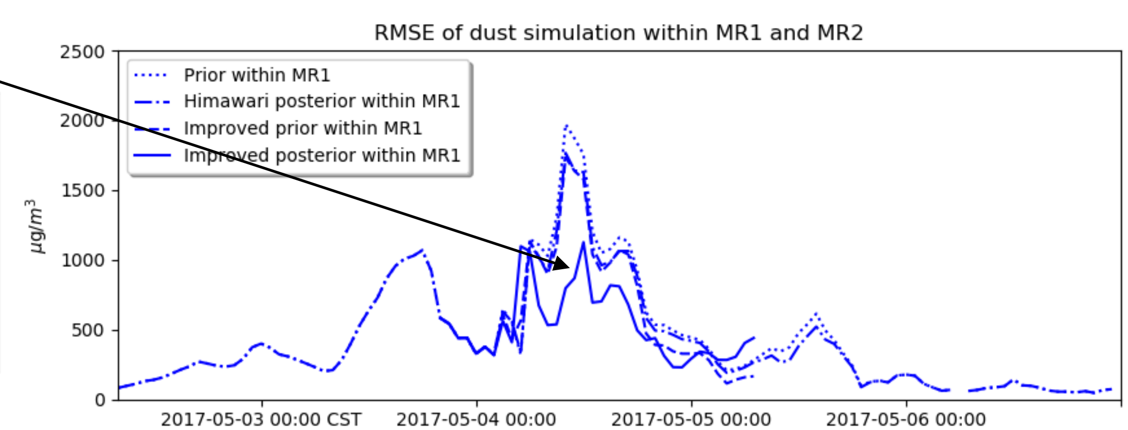
Reconstructed prior



New posterior

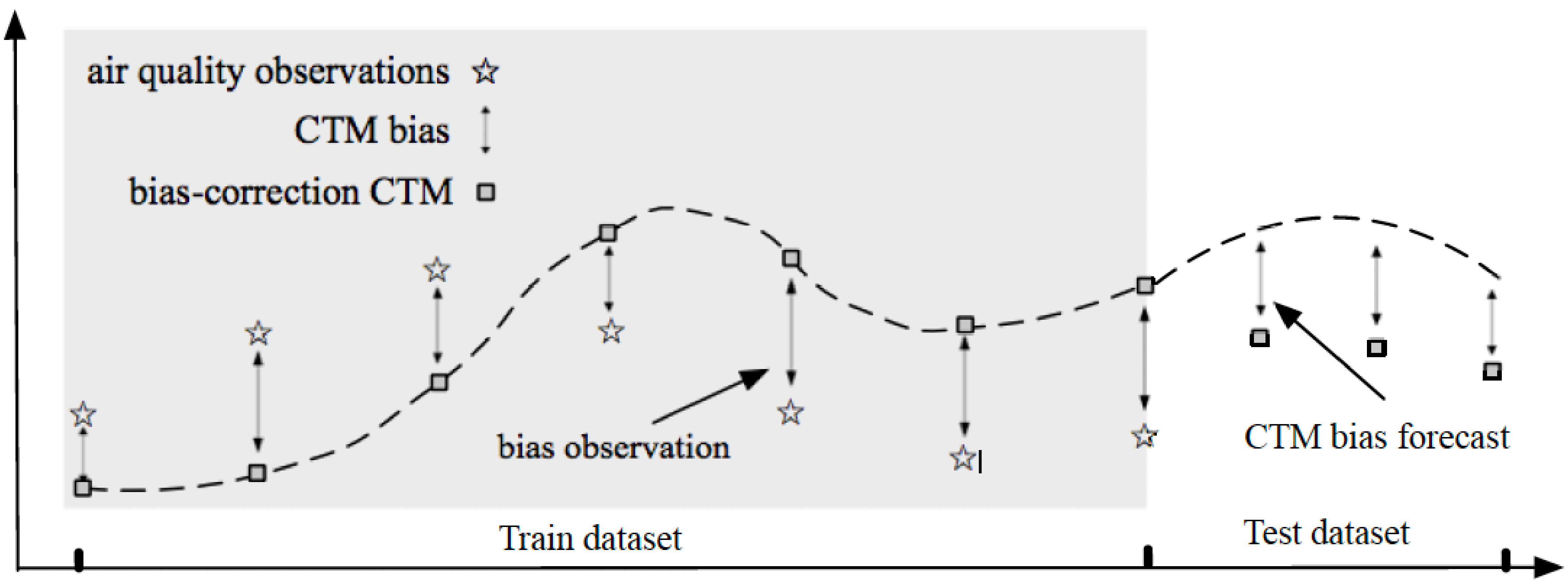


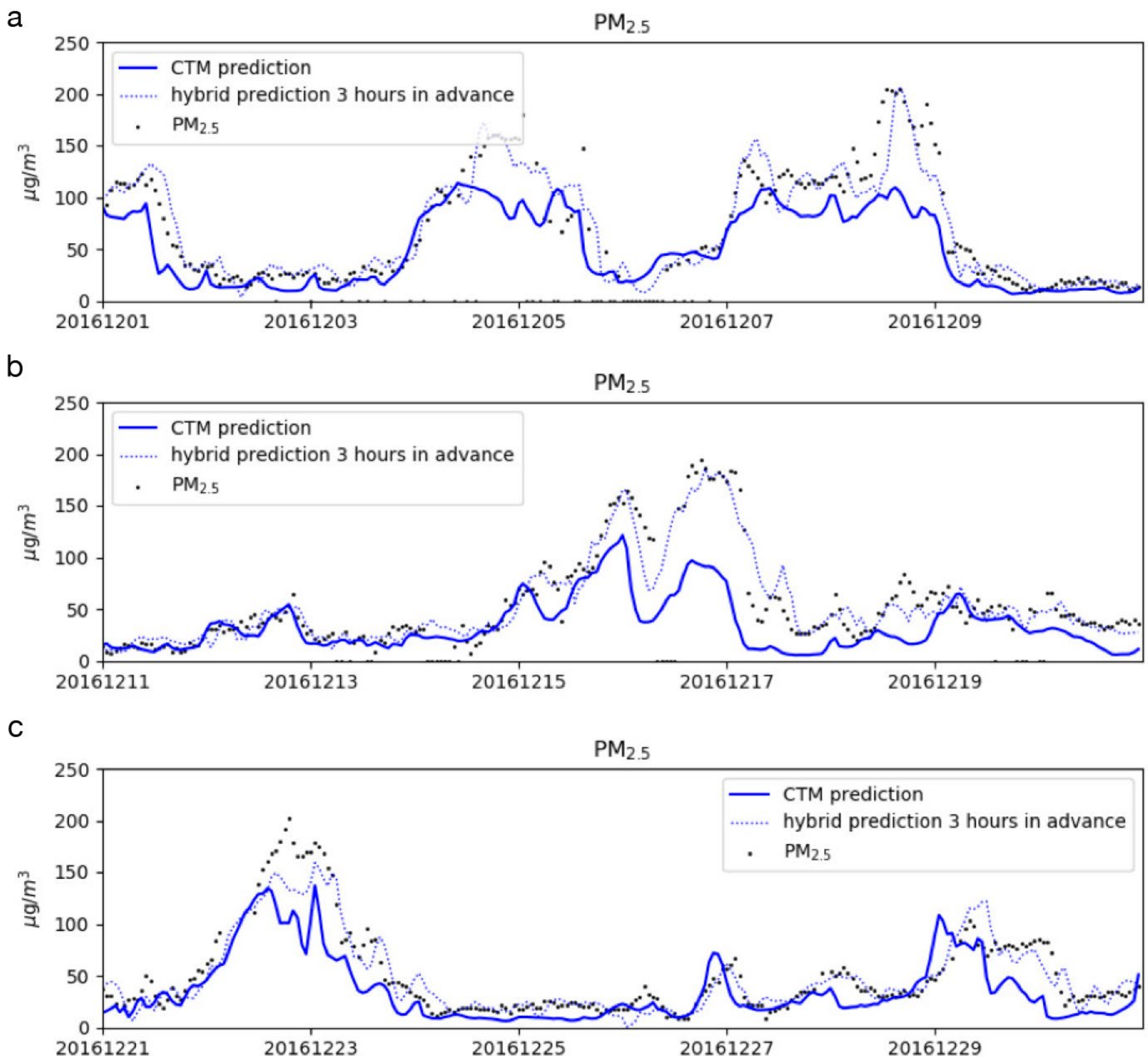
RMSE



J.Jin *et.al.*, Source backtracking for dust storm emission inversion using an adjoint method.
Atmospheric Chemistry and Physics, 2021

2.4 Machine Learning: error bias correction





Improved forecast after ML bias correction

Figure 4: Time series of the $PM_{2.5}$ observation, CTM prediction and hybrid forecasts with 3 hours in advance. (a): Dec 01-10; (b): Dec 11-20; (c): Dec 21-30.

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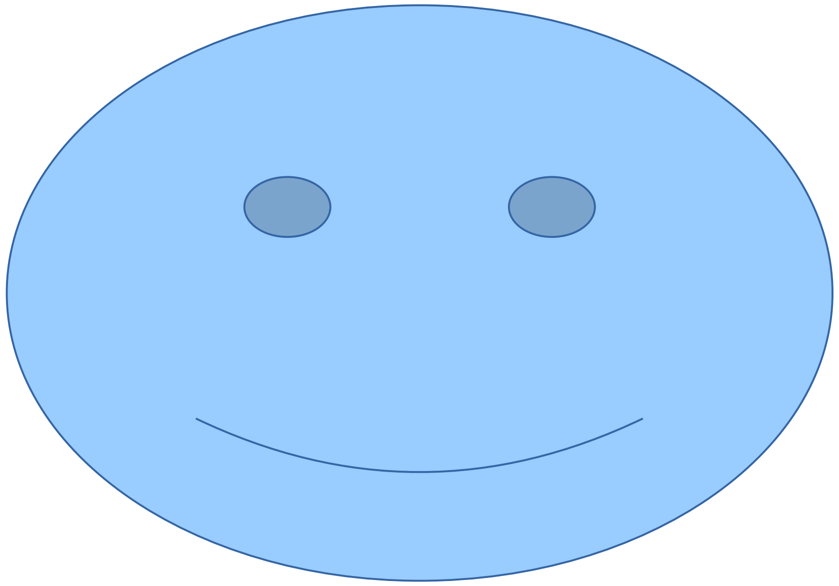
Data assimilation and machine learning for air quality forecasts

- Trajectory-based 4DVar is effective in estimating volcano eruption plume shapes using satellite data
- The integration of machine learning and data assimilation results in more accurate air quality forecast during dust storms.
- Inclusion of physical model knowledge further enhances the learning process in (atmospheric) modeling.
- Integration ML and DA opens many new possibilities, such as filling unmodelled prrocess in CTM with ML, using an ML surrogate to replace computation intensive (sub)models, …

Challenges

- Explainable ML model
- Can DA sometimes converge to ‘truth’ (certainty)? Accurate Uncertainty quantification is the key.
- Computational cost
- …



Thank you!

References

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