Added-value of chemical data assimilation in the stratosphere:

A discussion about DA fundamentals
with some results from the International Study Group
(Ménard[1] and Errera[2], co-PI)

by Richard Ménard[1],

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SPARC Data Assimilation Workshop
Paris, October 15, 2015

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Thus to bring added-value of CDA requires the development of of state-of-the-art data assimilation for atmospheric composition

Outline

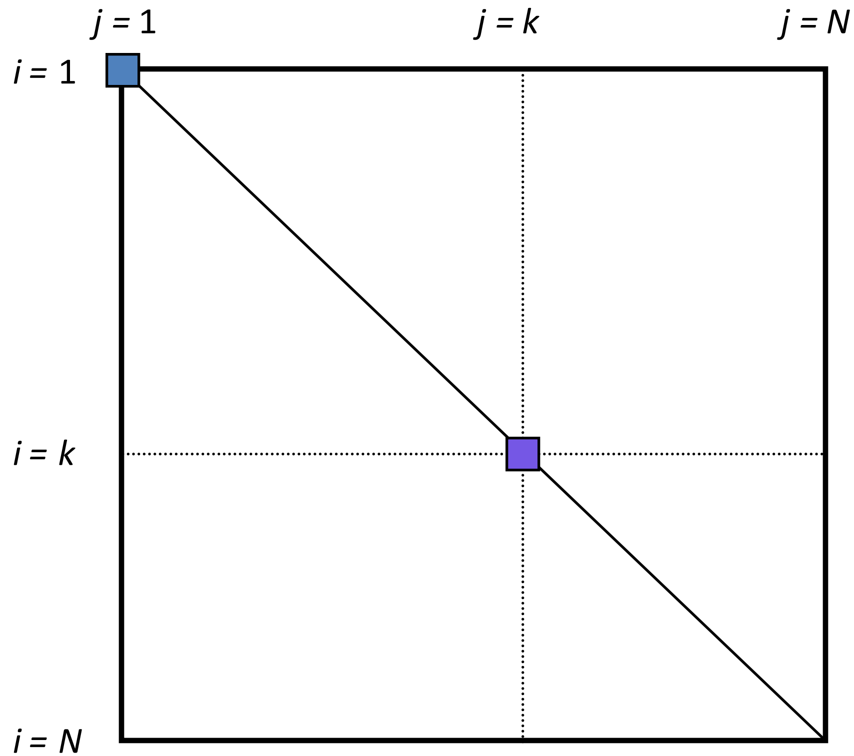
- ❑ Fundamentals of CDA
- ❑ Estimation of error statistics
- ❑ Quantification of chemical ozone loss
- ❑ Forecasting chemical composition
- ❑ Facilitate satellite/data intercomparison (Quentin talk)
- ❑ Interaction with NWP (more to be said in this workshop)
  - ozone radiation interaction
  - tracer-wind estimation

Fundamentals of CDA

Underlying physical law in chemical composition is ***mass conservation, or relative mass (mixing ratio)***
takes the form of the advection equation $\frac{\partial \mu}{\partial t} + \mathbf{V} \cdot \nabla \mu = 0$

Seminal observation made by Roger Daley in 1995 (result not published)

Error covariance evolution under advection



Initial error covariance

$$\mathbf{P} = \lfloor \mathbf{p}_1 , \mathbf{p}_2 , \ldots , \mathbf{p}_N \rfloor$$

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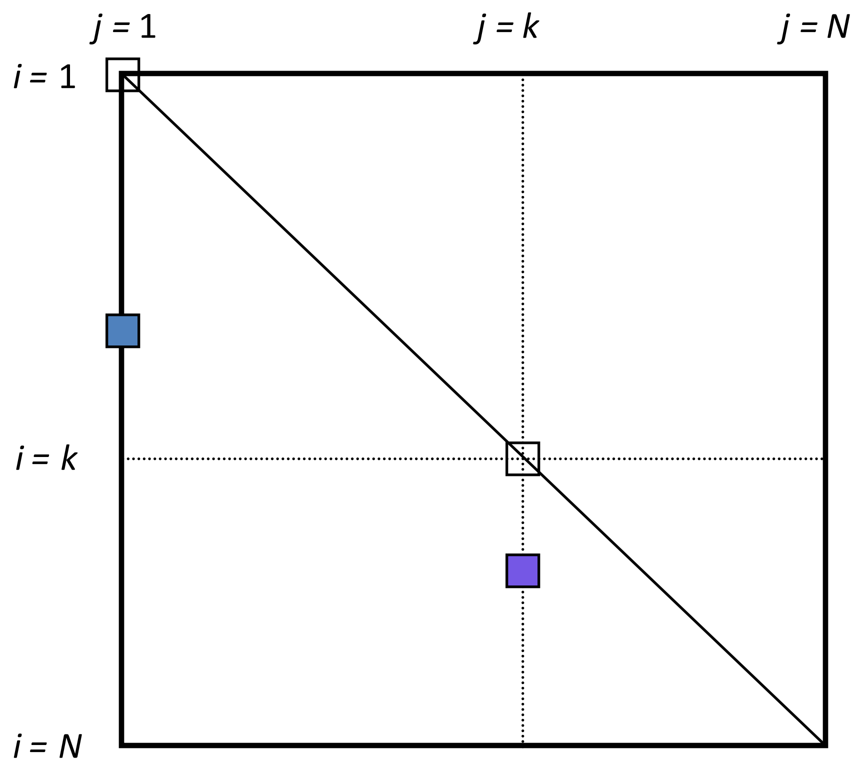
M is a linear advection model

$$\mathbf{M}\,\mathbf{P} = \left\lfloor \mathbf{Mp}_1\,,\, \mathbf{Mp}_2\,,\ \ldots\,, \mathbf{Mp}_N \right\rfloor$$



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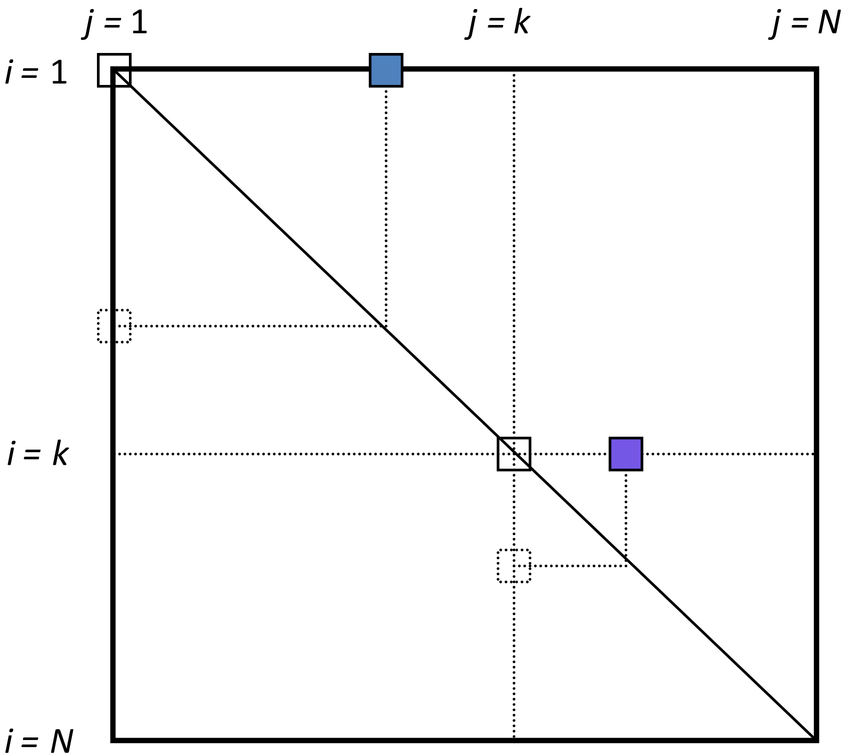
🎬Matrix transpose $(\mathbf{M}\,\mathbf{P})^T$



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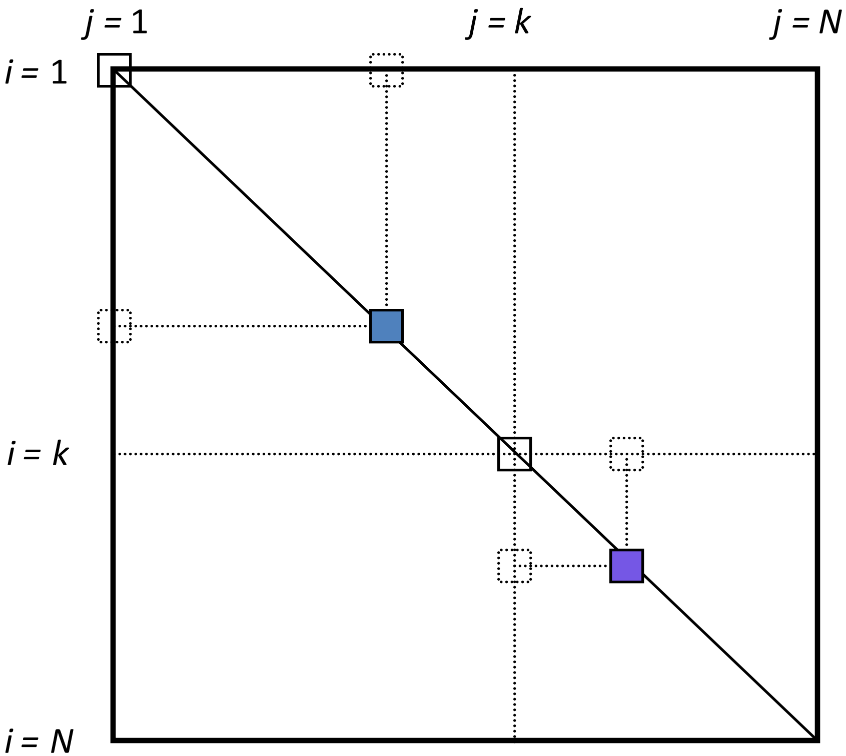

advection of error variance !

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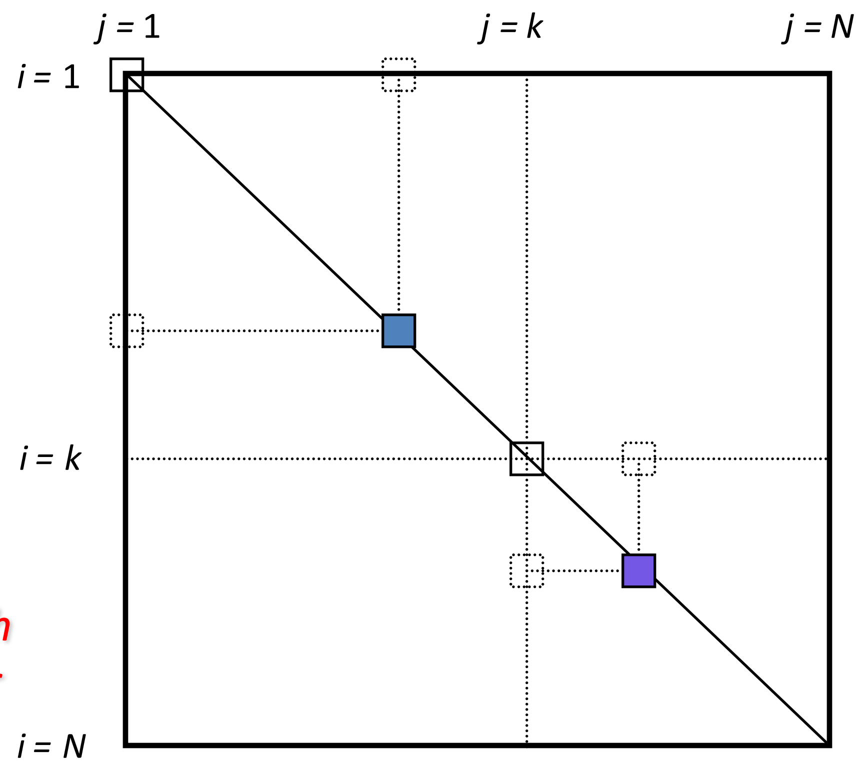


M is a linear advection model

$$\mathbf{P}^f = \mathbf{M}(\mathbf{MP})^T$$

There is no advection of error variance with meteorological data assimilation, the error variance and error correlations are linked and inseparable

advection of error variance !

Transport of errors and its spatial covariance (Cohn 1996)

Mass conservation $\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{V}) = 0$ n is the number density (molecules m^{-3}).

Mixing ratio is a conserved quantity $\frac{D\mu}{Dt} = \frac{\partial \mu}{\partial t} + \mathbf{V} \cdot \nabla \mu = 0$

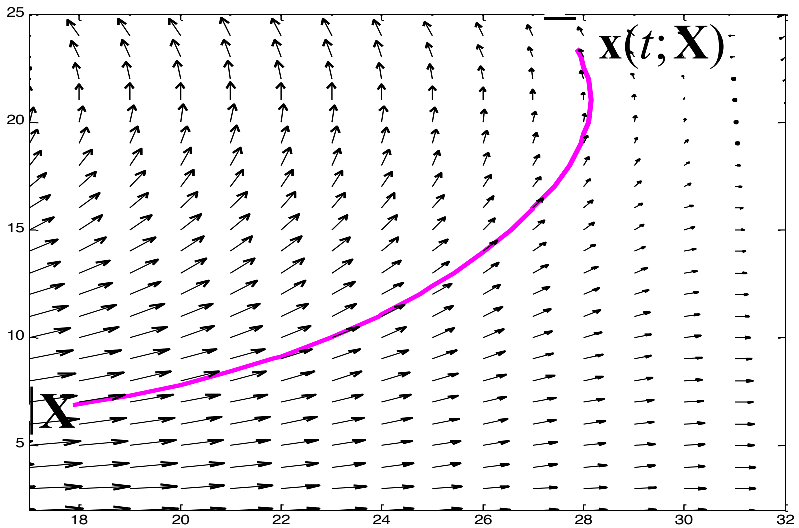
Lagrangian description

trajectories

$$\mathbf{x}(t;X) = \int_0^t \mathbf{V}(x(\tau),\tau)\,d\tau$$

conservation

$$\mu(\mathbf{x}(t;\mathbf{X}),t) = \mu(\mathbf{X},0)$$



True mixing ratio is governed by
(q = physical processes, errors in winds) $\frac{\partial \mu^t}{\partial t} + \mathbf{V} \cdot \nabla \mu^t + q = 0$

The mixing ratio error $\varepsilon = \mu - \mu^t$ obey

$$\boxed{\frac{D\varepsilon}{Dt} = \frac{\partial \varepsilon}{\partial t} + \mathbf{V} \cdot \nabla \varepsilon = q}$$

The solution proposed by Cohn (1996)

- Propagate the spatial error covariance **function**

then

- Discretize the covariance function on a model grid to obtain an error covariance **matrix**

Flip-flop between discretized and spatially continuous formulations is also present with adjoint models and 4D-Var

- finite difference of adjoint (FDA)

- adjoint of finite difference models (AFD)

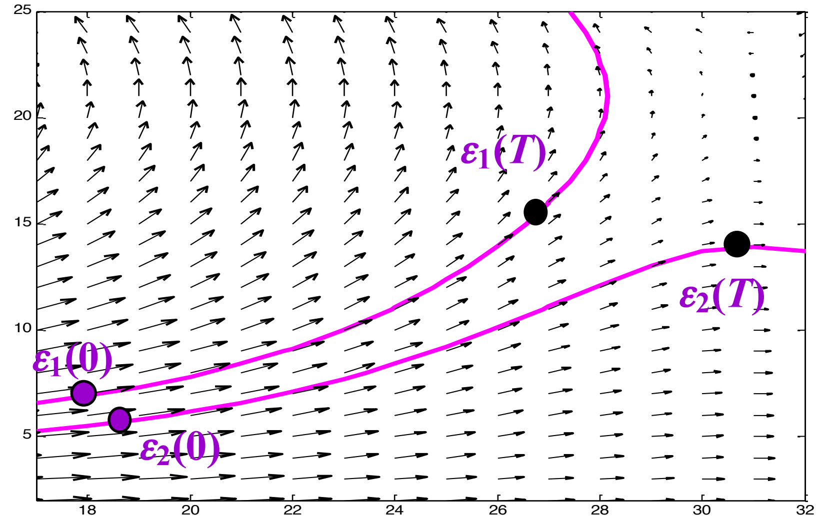
(*Sirkes and Tziperman 1997, Hourdin and Talagrand 2006, Henze et al. 2007, Haines et al 2014*)

Covariance **function** $P(\mathbf{x_1},\mathbf{x}_2,t) = \left\langle \varepsilon_1(\mathbf{x_1},t)\ \varepsilon_2(\mathbf{x}_2,t)\right\rangle$ with $\mathbf{x_1} = (x_1, y_1)$ and $\mathbf{x_2} = (x_2, y_2)$
defined over a 4-dimensional space (x_1, y_1, x_2, y_2) and time t

assume no model error

$$\frac{\partial \varepsilon_1}{\partial t} + \mathbf{V_1} \cdot \nabla_1 \varepsilon_1 = 0$$

$$\frac{\partial \varepsilon_2}{\partial t} + \mathbf{V}_2 \cdot \nabla_2 \varepsilon_2 = 0$$



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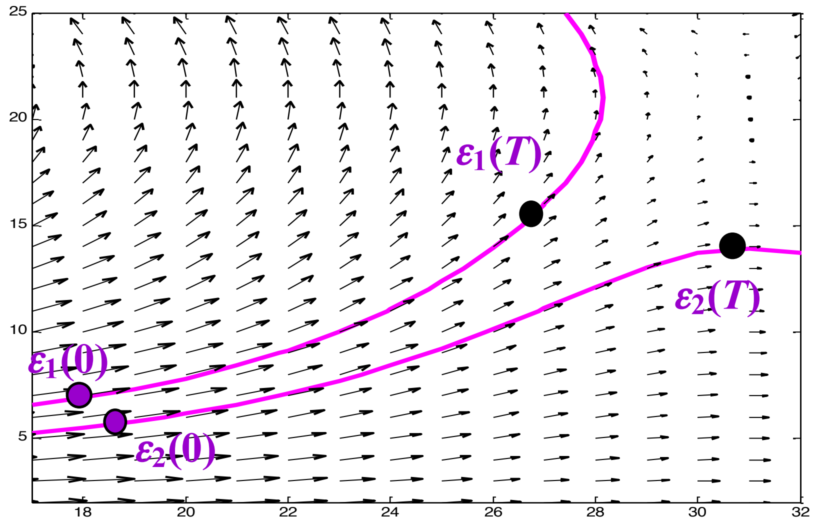
$$\varepsilon_2 \frac{\partial \varepsilon_1}{\partial t} + \varepsilon_2 \mathbf{V_1} \cdot \nabla_1 \varepsilon_1 = 0$$

$$\varepsilon_1 \frac{\partial \varepsilon_2}{\partial t} + \varepsilon_1 \mathbf{V}_2 \cdot \nabla_2 \varepsilon_2 = 0$$



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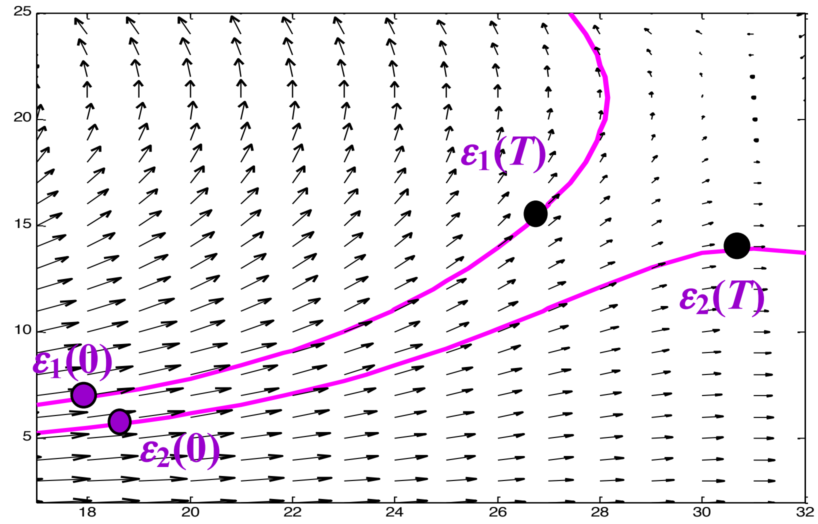

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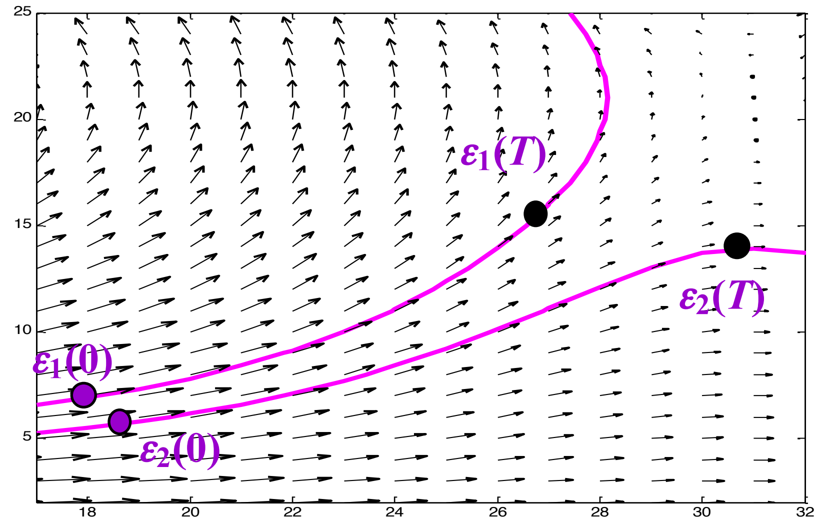

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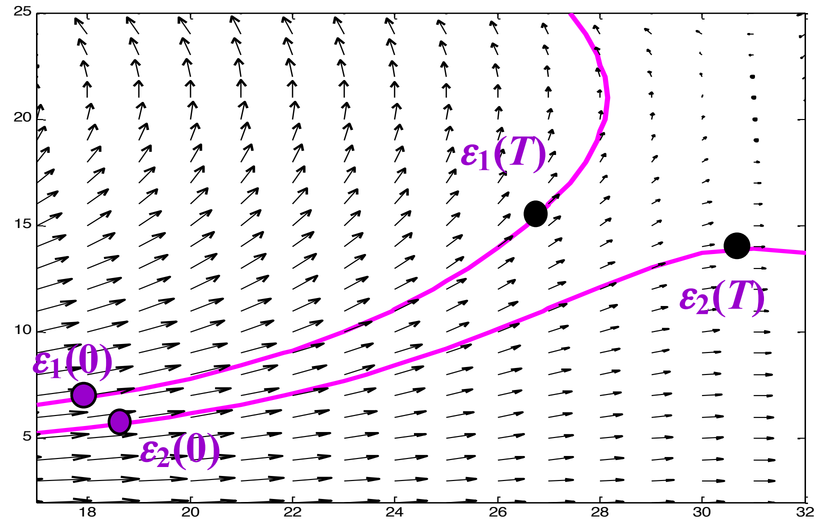
$$\left\langle \varepsilon_2 \frac{\partial \varepsilon_1}{\partial t} + \varepsilon_1 \frac{\partial \varepsilon_2}{\partial t} \right\rangle + \mathbf{V_1} \cdot \nabla_1 \langle \varepsilon_1 \varepsilon_2 \rangle + \mathbf{V_2} \cdot \nabla_2 \langle \varepsilon_1 \varepsilon_2 \rangle = 0$$



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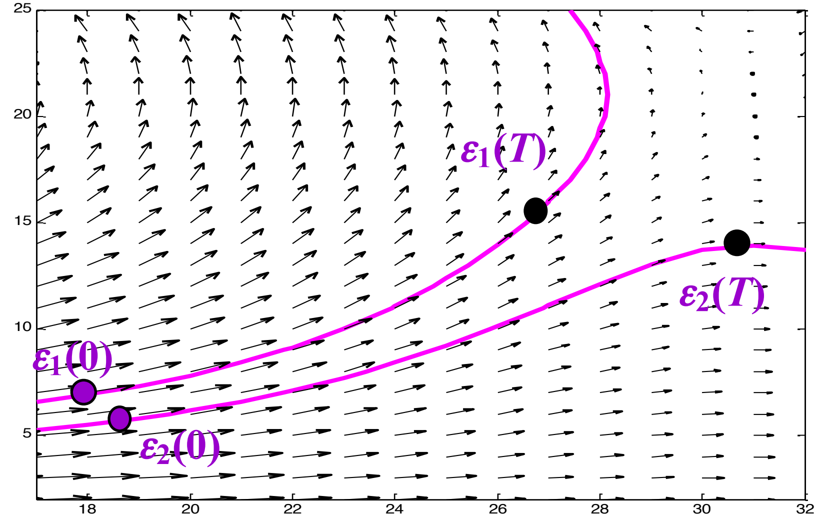
$$\frac{\partial \langle \varepsilon_1 \varepsilon_2 \rangle}{\partial t} + \mathbf{V_1} \cdot \nabla_1 \langle \varepsilon_1 \varepsilon_2 \rangle + \mathbf{V_2} \cdot \nabla_2 \langle \varepsilon_1 \varepsilon_2 \rangle = 0$$



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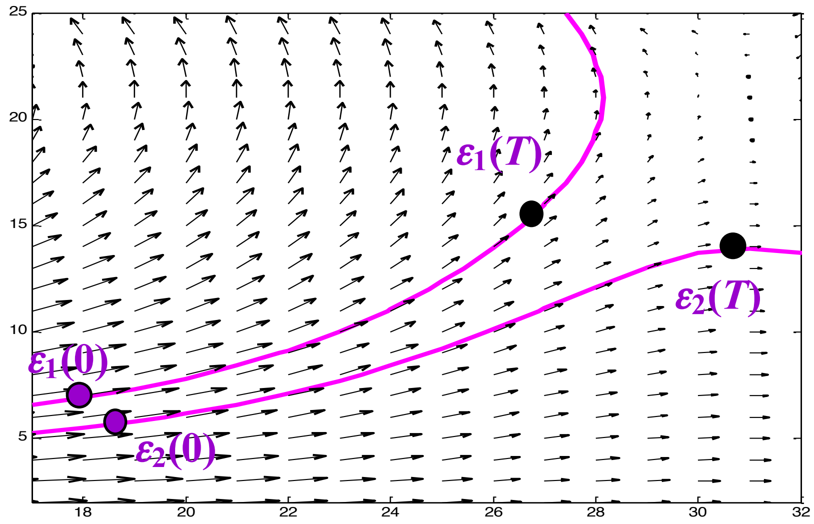
$$\frac{\partial P}{\partial t} + \mathbf{V_1} \cdot \nabla_1 P + \mathbf{V_2} \cdot \nabla_2 P = 0$$



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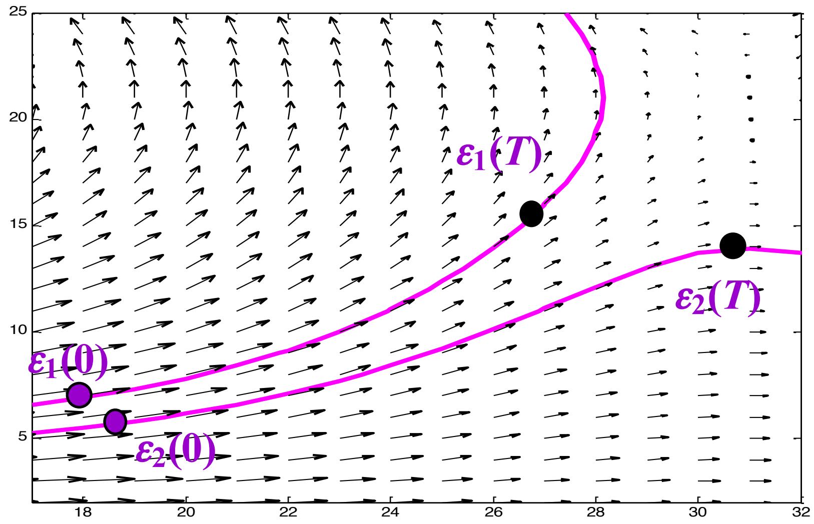
$$P(\boldsymbol{X_1}(0), \boldsymbol{X_2}(0)) = P(\boldsymbol{X_1}(T), \boldsymbol{X_2}(T))$$

the error covariance is conserved between a pair of Lagrangian points



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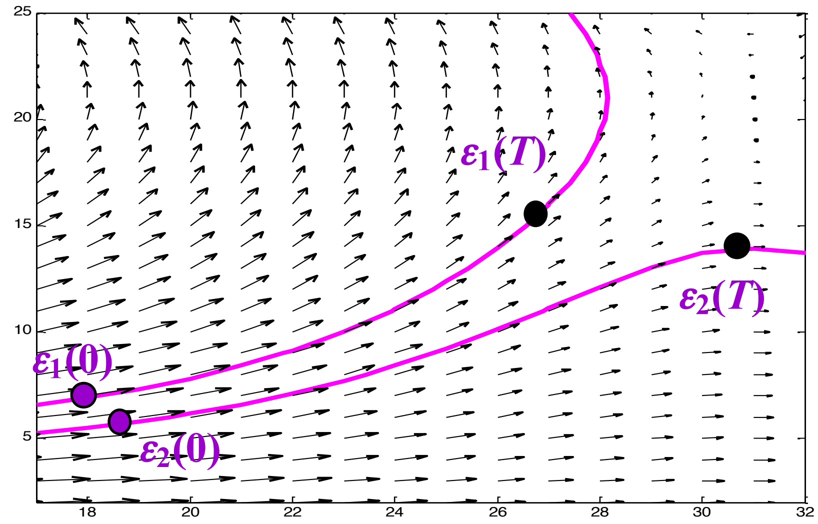

in particular the error variance is conserved along the trajectory or obey the advection equation

With random model error q with spatial covariance $\langle q(\mathbf{x}_1)\, q(\mathbf{x_2}) \rangle = Q(\mathbf{x_1}, \mathbf{x_2})$

$$\frac{\partial P}{\partial t} + \mathbf{V}_1 \cdot \nabla_1 P + \mathbf{V}_2 \cdot \nabla_2 P = Q$$

The error variance obeys

$$\boxed{\frac{D\sigma^2}{Dt} = \frac{\partial \sigma^2}{\partial t} + \mathbf{V} \cdot \nabla \sigma^2 = \sigma_q^2(\mathbf{x}, t) \equiv Q(\mathbf{x}, \mathbf{x}, t)}$$

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Relative error formulation

Define the relative error $\sigma^* = \dfrac{\sigma}{\mu}$, and using the mass conservation $\dfrac{D\mu}{Dt} = 0$ we get

$$\frac{D(\sigma^*)^2}{Dt} = (\sigma_q^*)^2$$

and if we neglect model error variance

$$\frac{D\sigma^*}{Dt} = 0$$

the relative error is conserved !

Sequential filter

(Menard et al. 2000, Khatattov et al. 2000, Dee 2003, Eskes et al. 2003, Marchand et al. 2004, Rösevall et al. 2007, van der A et al. 2010)

This error variance evolving scheme with a fixed error correlation is known as the sequential filter (or suboptimal Kalman filter)

Has been applied to 3D CTM of long-lived species in

- Stratosphere (UARS, GOME, flight planning)
- Troposphere (MOPITT)

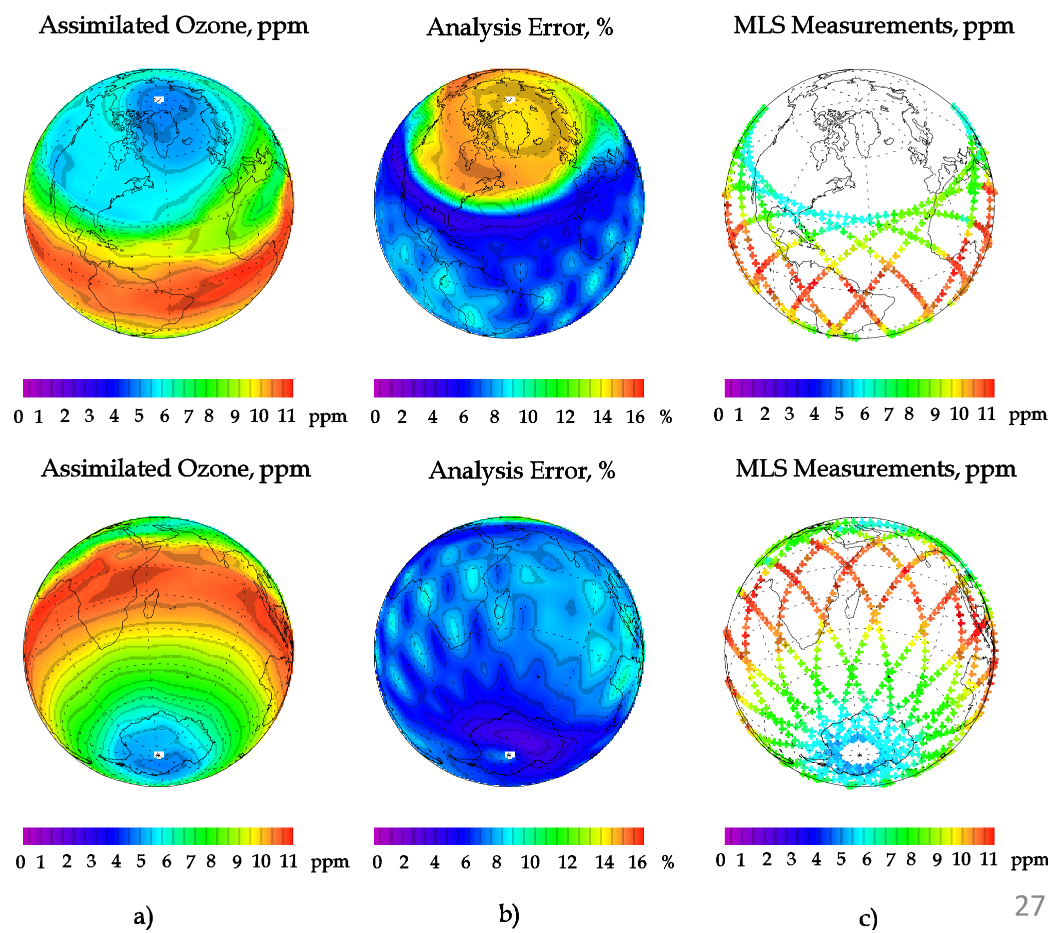
also to multispecies, and to

- humidity in the troposphere

Using a Choleski decomposition (small matrices ~ 2000 or less) and

$$\mathbf{v}^a(\mathbf{x}_i) = \mathbf{v}^f(\mathbf{x}_i) - \mathbf{p}_i^T\left(\mathbf{HP}^f\mathbf{H}^T + \mathbf{R}\right)^{-1}\mathbf{p}_i$$

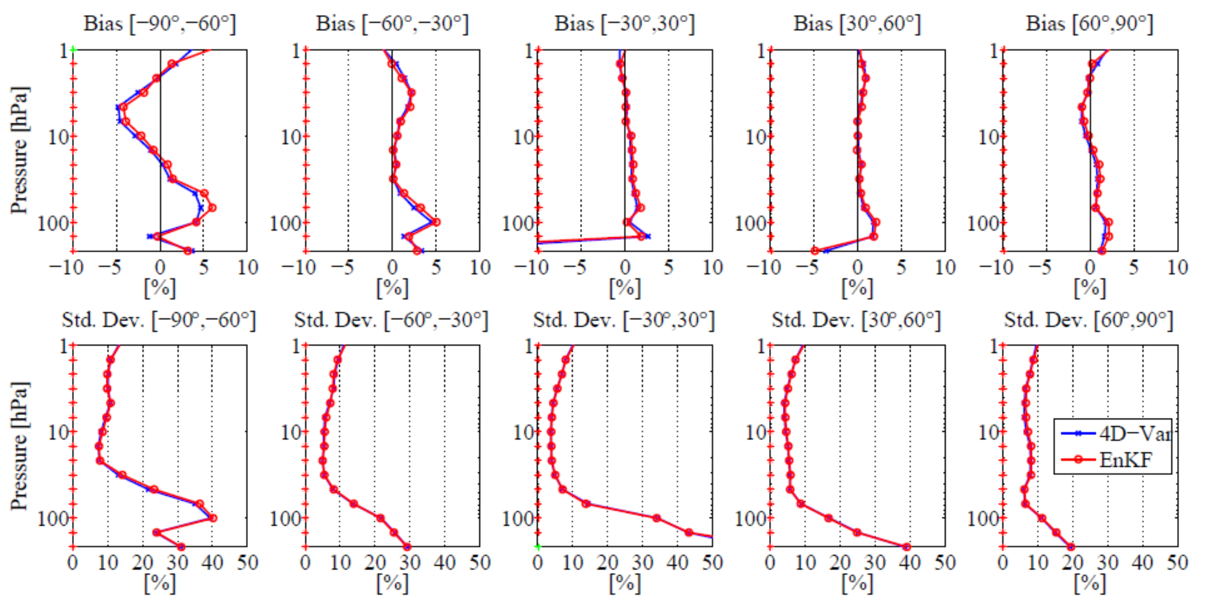
where $\mathbf{p}_i$ is the column of $\mathbf{P}^f$ associated with $\mathbf{x}_i$ we get the analysis error variance



Data assimilation methods for atmospheric composition

EnKF vs 4D-Var

Comparison EnKF-4DVar tracer (O3 assimilation)
Skachko et al 2014 GMD



The OmF are computed for September-October 2008

and for chemical transport

Sequential filter

Error statistics

(Ménard, QJRMS 2015)

Necessary and *sufficient* conditions to have the **true** error covariances in observation space

(a) $\mathbf{H}\widetilde{\mathbf{K}} = \mathbf{HK}$ the gain is equal to the Kalman gain

⟹ The analysis error variance is minimum

(b) $\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T + \widetilde{\mathbf{R}} = \left\langle (O-B)(O-B)^T \right\rangle$ the innovation covariance consistency

⟹ $\chi^2 = p$ or $J_{\min} = p/2$

Desroziers scheme

$$\widetilde{\mathbf{R}}_{i+1} = \left\langle (O-A_i)(O-B)^T \right\rangle \quad \text{....(1)}$$

$$\mathbf{H}\widetilde{\mathbf{B}}_{i+1}\mathbf{H}^T = \left\langle (A_i-B)(O-B)^T \right\rangle \quad \text{....(2)}$$

where A_i is the analysis interpolated in the observation space and derived from i-th estimates, $\widetilde{\mathbf{R}}_i$ and $\mathbf{H}\widetilde{\mathbf{B}}_i\mathbf{H}^T$

- Can estimate the full error covariance $\widetilde{\mathbf{R}}_{i+1}$ or $\mathbf{H}\widetilde{\mathbf{B}}_{i+1}\mathbf{H}^T$ but not both, because $\widetilde{\mathbf{R}}_{i+1}$ and $\mathbf{H}\widetilde{\mathbf{B}}_{i+1}\mathbf{H}^T$ are not independent.

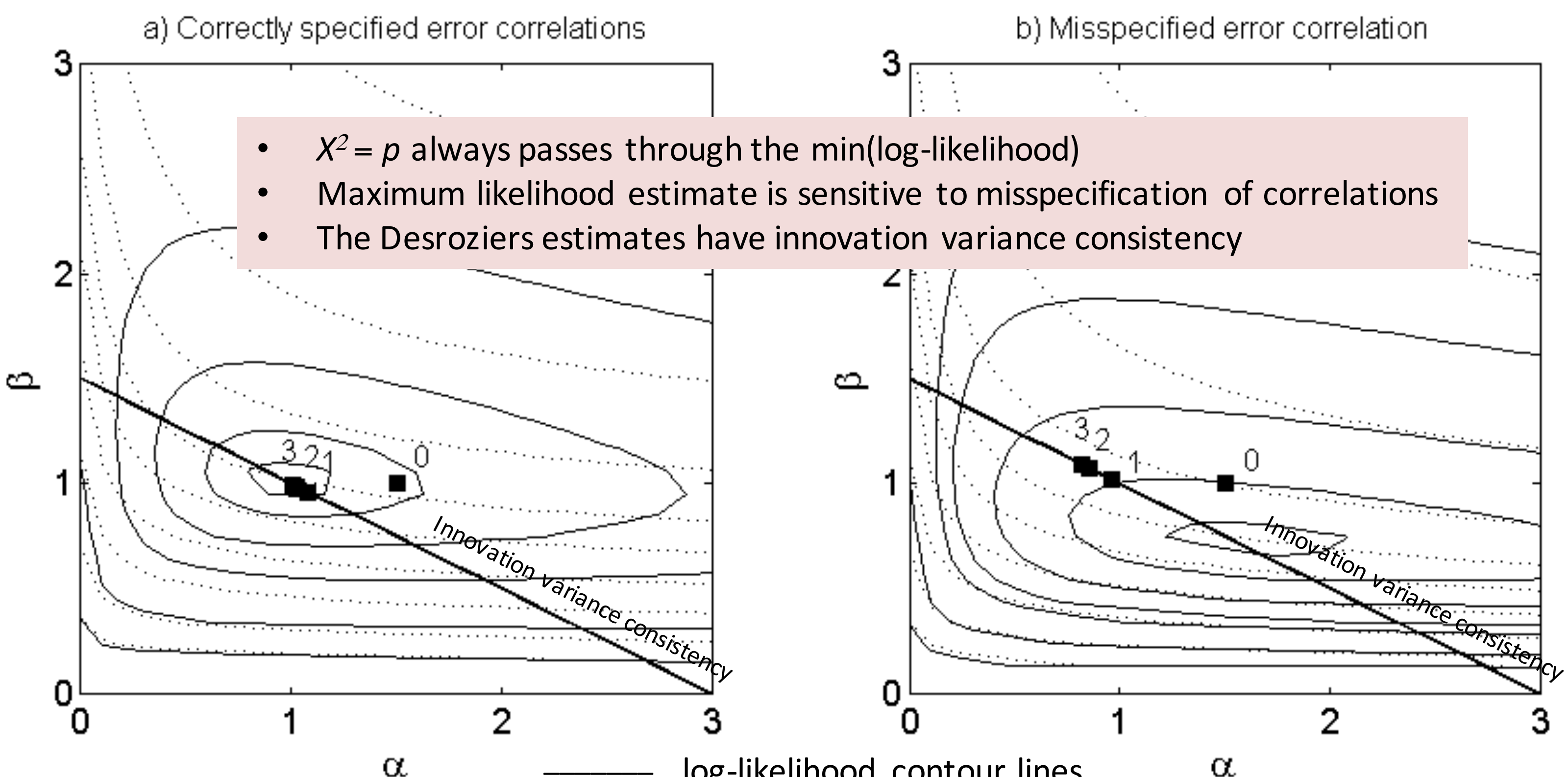
- The accuracy of $\widetilde{\mathbf{R}}_\infty$ depends on how $\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T$ is different from the true $\mathbf{HBH}^T$ In an EnKF we could assume that $\mathbf{H}\widetilde{\mathbf{B}}\mathbf{H}^T$ is close to the truth and thus $\widetilde{\mathbf{R}}_\infty \approx \mathbf{R}$

- Estimation of variance scaling factor for $\widetilde{\mathbf{R}}$ and $\widetilde{\mathbf{B}}$ depends on accurate correlations. Reliable using analysis increments, but more sensitive using variational method

Estimation of scaling factors α (obs) and β (background) using the *Analysis Increment Method* (Desroziers et a. 2005)

$$\alpha_{i+1} = tr\left\langle (O - A(\alpha_i, \beta_i))(O - B)^T \right\rangle \qquad \beta_{i+1} = tr\left\langle (A(\alpha_i, \beta_i) - B)(O - B)^T \right\rangle$$

Example with $\mathbf{H} = \mathbf{I}$ True estimates ↔ α = β = 1



- $X^2 = p$ always passes through the min(log-likelihood)
- Maximum likelihood estimate is sensitive to misspecification of correlations
- The Desroziers estimates have innovation variance consistency

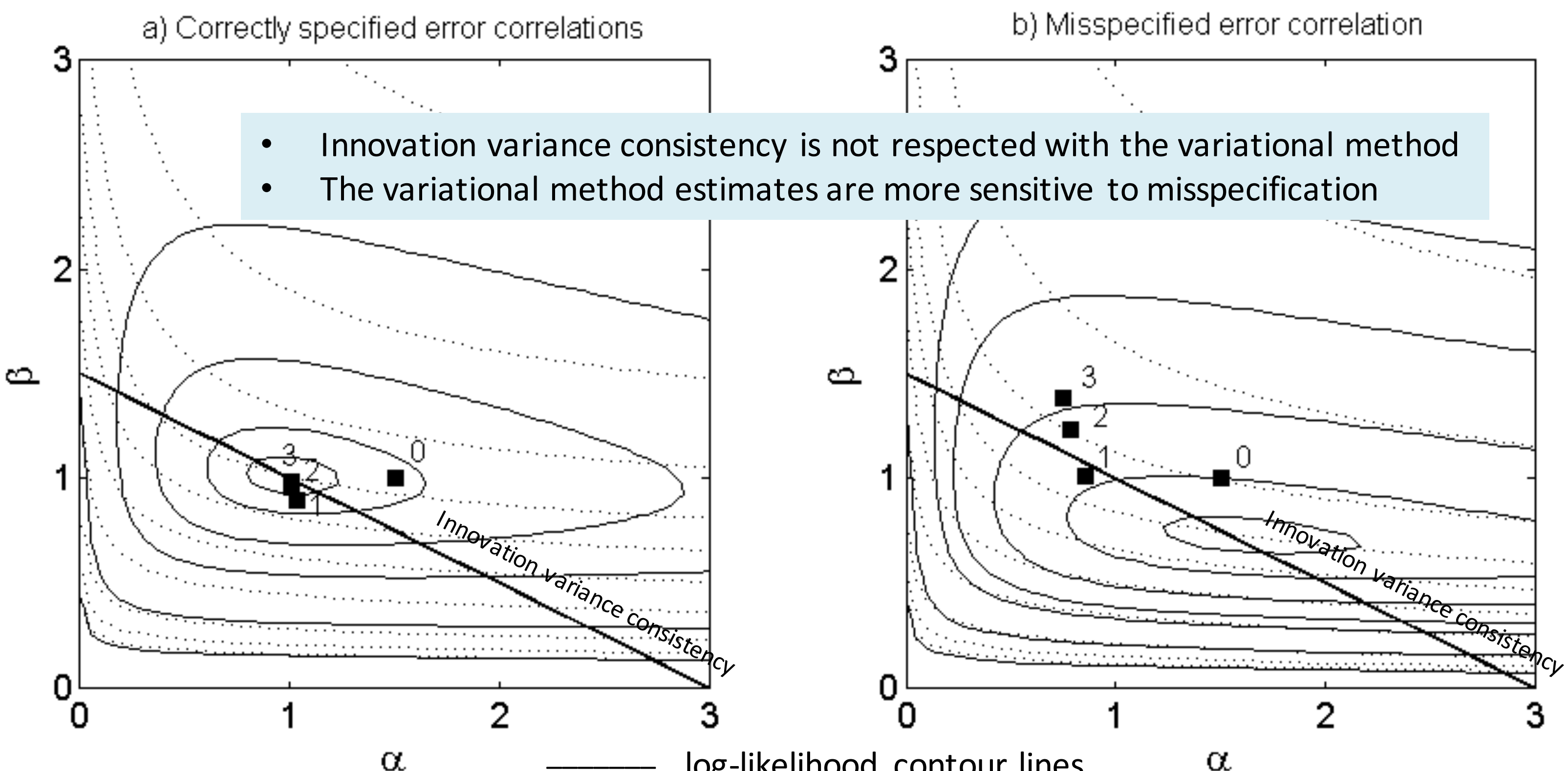
———— log-likelihood contour lines

………. χ^2 contours lines

Estimation of scaling factors α (obs) and β (background) using the *Variational Method* (Desroziers and Ivanov 2001)

$$s_{i+1}^{o} = \frac{J^{o}(\mathbf{x}^{a})}{\frac{1}{2}tr[\mathbf{I} - \mathbf{HK}(s_i^o, s_i^b)]} \qquad s_{i+1}^{b} = \frac{J^{b}(\mathbf{x}^{a})}{\frac{1}{2}tr[\mathbf{HK}(s_i^o, s_i^b)]}$$

Example with $\mathbf{H} = \mathbf{I}$ True estimates ↔ α = β = 1



- Innovation variance consistency is not respected with the variational method
- The variational method estimates are more sensitive to misspecification

——— log-likelihood contour lines

.... χ^2 contours lines

Estimation of observation error and model error variances in an EnKF

(1) Observation error using the *Analysis Increment Method*

(2) Model error using the X^2 diagnostic

(Skachko et al. 2015 in preparation)

Observation error adjustable parameter

$$\mathbf{R}_k(i,j) = \begin{cases} (r\,\sigma_y(i)|_k)^2, & \text{if } i = j \\ 0, & \text{if } i \neq j, \end{cases} \qquad (1)$$

where

- r, *adjustable* observation error parameter
- $\sigma_y(i)$, i-th observation error at time k provided by retrieval team

Model error adjustable parameter

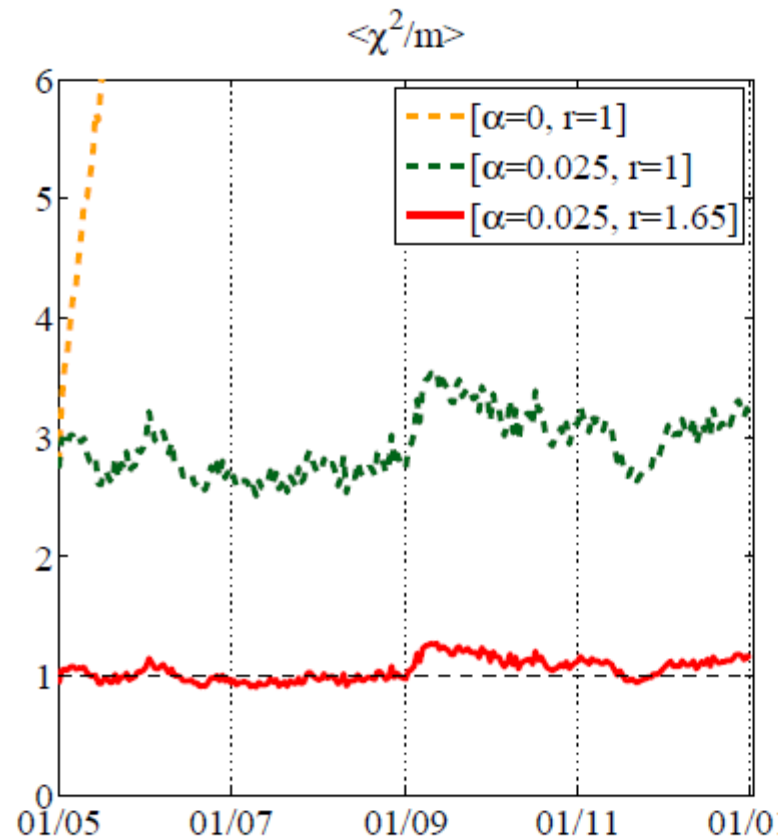
- Approximated using ensemble
- Model error term is considered
  $\mathbf{x}_i^f(t_k) = M(\mathbf{x}_i^a(t_{k-1})) + \alpha\boldsymbol{\eta}(t_k), \quad i \in [1, N]$
  - α, *adjustable* background error parameter
  - added in the model space at each time step

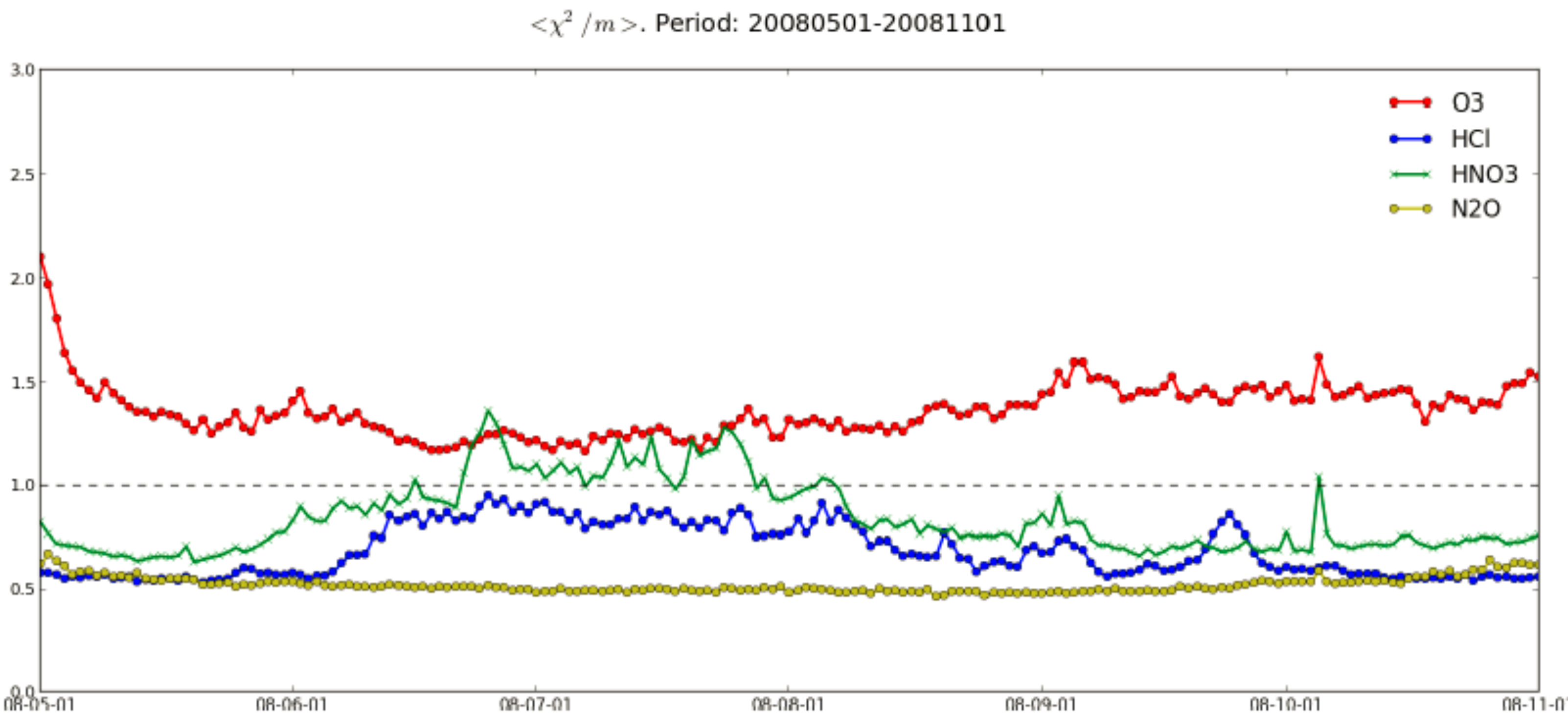
χ^2-test (Ménard and Chang (2000))

$\chi^2 = \mathbf{d}^T(\mathbf{HBH}^T + \mathbf{R})^{-1}\mathbf{d}$:

- Stable
- Around 1 when normalized with m, number of obs
- Defined by values of α and r

Empirical value of α is found model error variance parameter





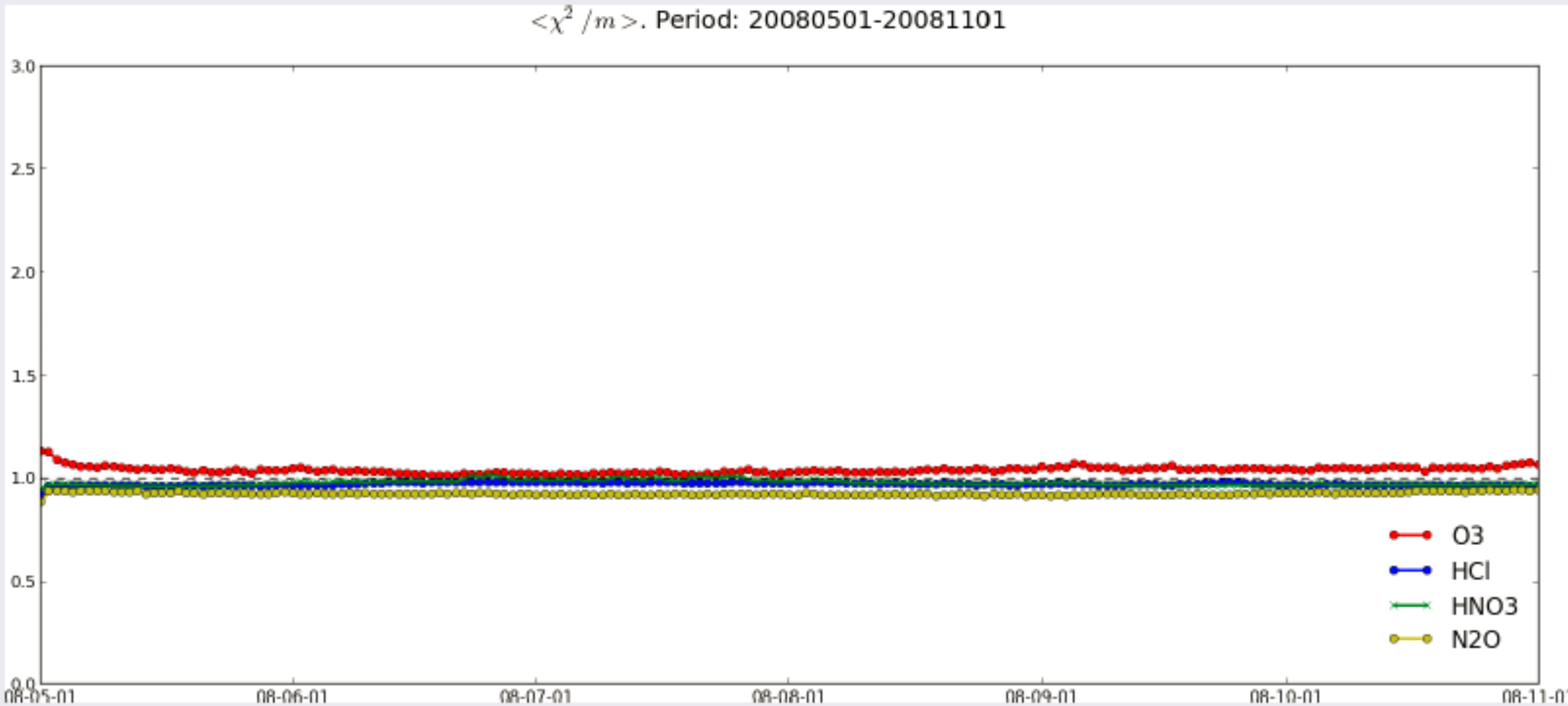
- Empirical α = 0.025 (model error variance parameter)
- r is not calibrated

- One value of model error variance fits all species assimilation
- Milewski and Bourqui (2011,2013) found that model error in a CTM is due primarily to the errors in the driving winds

- Estimation of r:

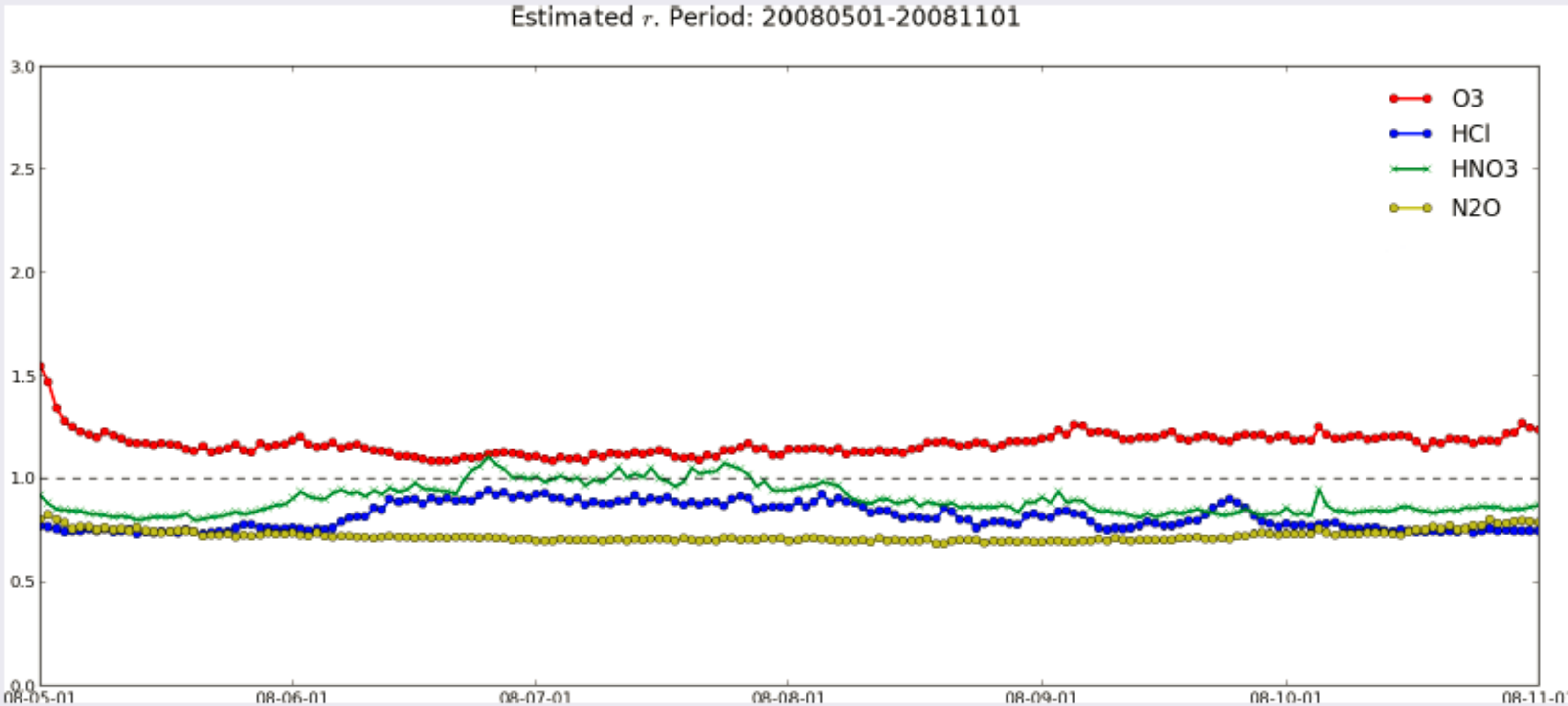
$$r^2 = \left\langle (O-A)(O-B)^T / \sigma_y^2(i) \right\rangle$$

$\langle \chi^2 / m \rangle$ using estimated obs.error



- Empirical α
- Estimated r

Estimation of parameter *r*

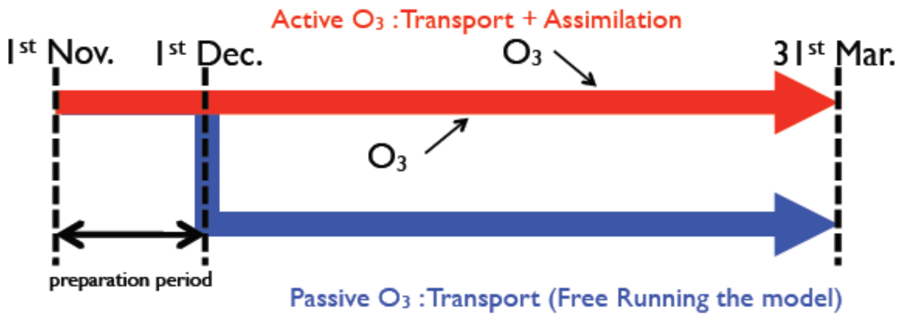


we could take it one step further and estimate the full observation error covariance,
Or practically estimate the error variance at each levels and
and estimate observation error horizonal and vertical correlations

Ozone loss estimation - A problem of model bias estimation

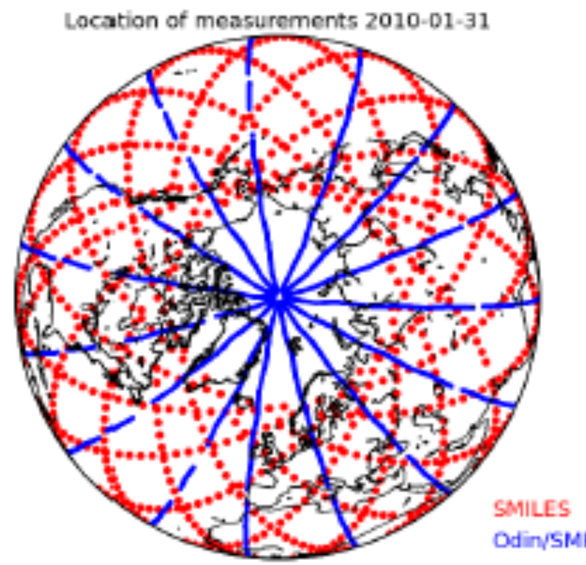
(Rosevall et al. 2007, Sagi et al., ACP 2014)

To separate ozone variation into "transport" and "chemical" processes



$$O_{3loss} = O_{3active} - O_{3passive}$$

ODIN SMR limb measurements



Using an accurate transport model

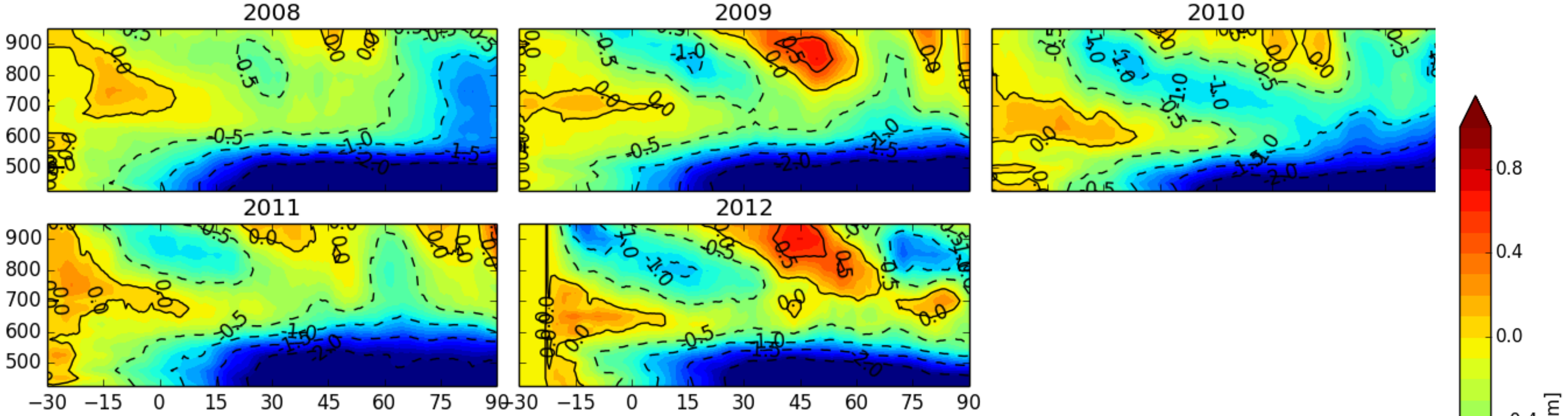
- Prather 2D isentropic
- Vertical upwind scheme driven by diabatic heating

Estimation method

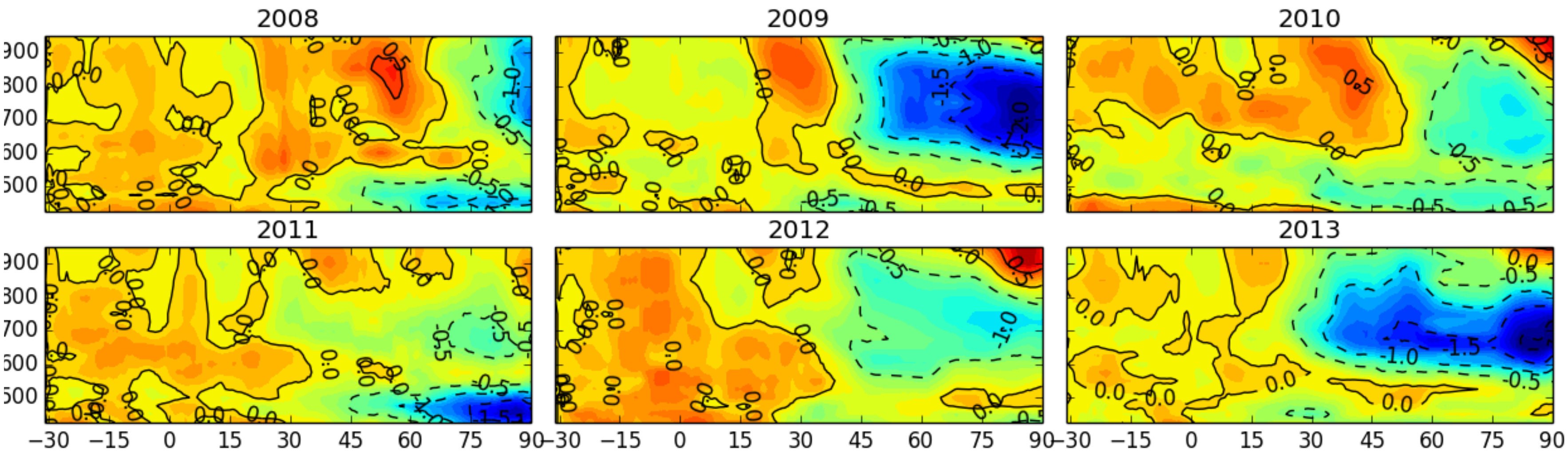
- Estimates of the **chemical** ozone loss
- Not tied to any threshold value

Chemical ozone loss - vortex mean average (70- 90 equivalent latitude s)

Antarctic ozone loss - from December 1st



Arctic ozone loss - from August 1st



Interpretation and equivalence of the method (Ménard and Sagi, work in progress)

- The difference between $\mathbf{x}_n^a$ (analysis) and $\mathbf{x}_n^T$ (pure transport) is the accumulated transport of analysis increments $\Delta\mathbf{x}_n^a = \mathbf{x}_n^a - \mathbf{x}_n^f$

$$\mathbf{x}_n^a - \mathbf{x}_n^T = \sum_{p=0}^{n-1} M_{n,n-p}\ \Delta\mathbf{x}_{n-p}^a$$

where $M_{n,n-p}$ is the model transport from time n-p to n .
(assumptions: (1) M is linear and (2) $\mathbf{x}_0^a = \mathbf{x}_0^T$)

mean analysis increments vs accumulated transport of analysis increments

diagnosis of model error bias — estimation of model error bias

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mean analysis increments vs accumulated transport of analysis increments

diagnosis of model error bias — estimation of model error bias

- **Equivalent formulation** The accumulated analysis increment can be calculated using a bias evolution equation

$$\begin{aligned}
\mathbf{x}_n^a &= \mathbf{x}_n^f + \mathbf{K}_n(\mathbf{y}_n - \mathbf{H}_n\mathbf{x}_n^f) \\
\mathbf{x}_{n+1}^f &= M_{n+1,n}\,\mathbf{x}_n^a \\
\mathbf{x}_{n+1}^T &= M_{n+1,n}\,\mathbf{x}_n^T \\
\mathbf{b}_{n+1} &= M_{n+1,n}\,\mathbf{b}_n + \Delta\mathbf{x}_n^a
\end{aligned}$$

with initial conditions

$$\mathbf{x}_0^a = \mathbf{x}_0^T$$

$$\mathbf{b}_0 = 0$$

Forecasting chemical composition

Impact measured using anomaly correlation
(correlation of forecast against analyses)

```
11/08        12/08        13/08 .....                                05/10

|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|------------------| ANALYSES
|----------------|  (24hr)
|------------------------------|  (48hr)                                    FORECAST
| ---------------------------------------------| (72hr)
```

ANOMALY CORRELATION ***r***

$$r = \frac{\sum_{i=1}^{n} (x_f - x_c - M_{f,c})_i (x_a - x_c - M_{a,c})_i \cos\varphi_i}{\sqrt{\sum_{i=1}^{n} (x_f - x_c - M_{f,c})_i^2 \cos\varphi_i} \sqrt{\sum_{i=1}^{n} (x_a - x_c - M_{a,c})_i^2 \cos\varphi_i}}$$

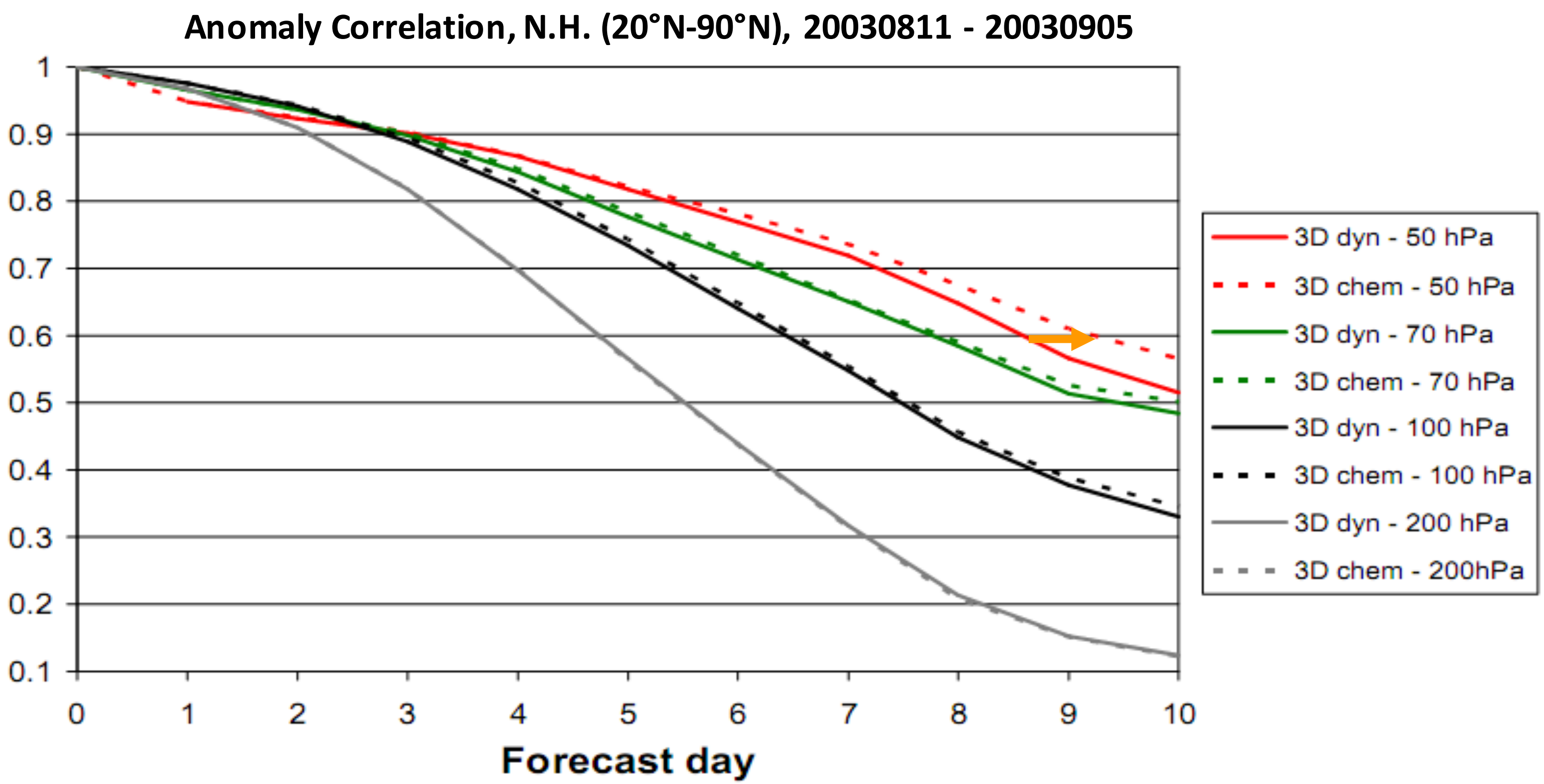
AREA MEAN

$$M_{f,v} = \frac{\sum_{i=1}^{n} (x_f - x_v)_i \cos\varphi_i}{\sum_{i=1}^{n} \cos\varphi_i}$$

Ozone-radiation impact on NWP

de Grandpré *et al.*, Mon. Wea. Rev., 2009 :

- MIPAS assimilation of ozone ➾ big improvement of *T* forecast skill in lower strato:



The LINOZ scheme (McLinden et al., 2000)

$$\frac{dq}{dt} = (P-L)|^o + \frac{\partial(P-L)}{\partial q}\bigg|_o (q-q^o) + \frac{\partial(P-L)}{\partial T}\bigg|_o (T-T^o) + \frac{\partial(P-L)}{\partial c_{o_3}}\bigg|_o (c_{o_3} - c_{o_3}^o).$$

q **is the ozone volume mixing ratio, *T* is the temperature, C_{O3} is the column ozone above the level "l", *P* and *L* are the production and loss terms and q_o, T_o *and* C^o_{o3} are climatological parameters. The partial derivatives coefficients have been pre-computed using a photochemical box model and are read as lookup tables in the GEM NWP model.**

—— RMSE

----- BIAS

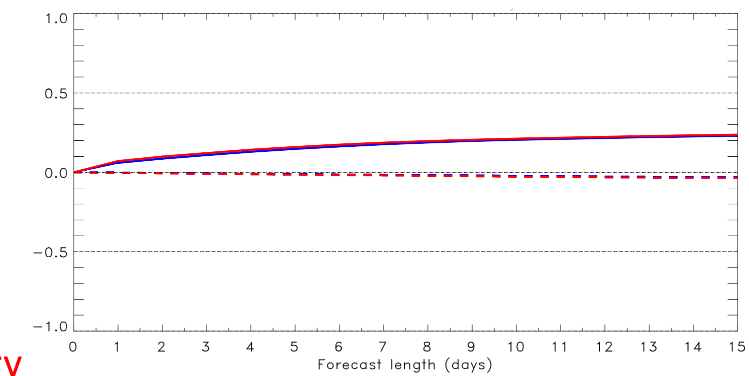
--- BIRA --- LINOZ ---- FK

Forecast verification against analyses

BIRA: Comprehensive chemistry

LINOZ: Linearized chemistry

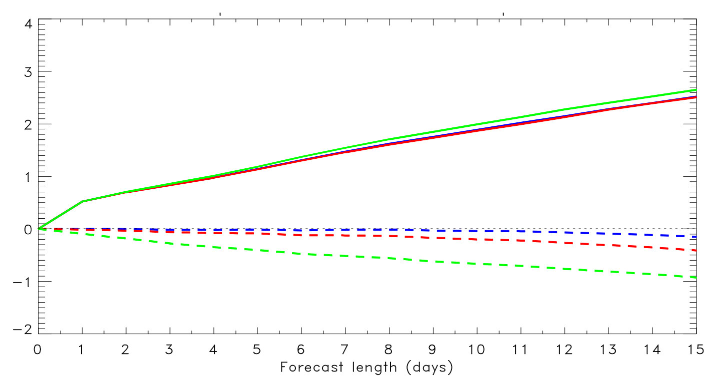
FK : Ozone zonal monthly climatology



Ozone (ppmv)

50 hPa

(NH)



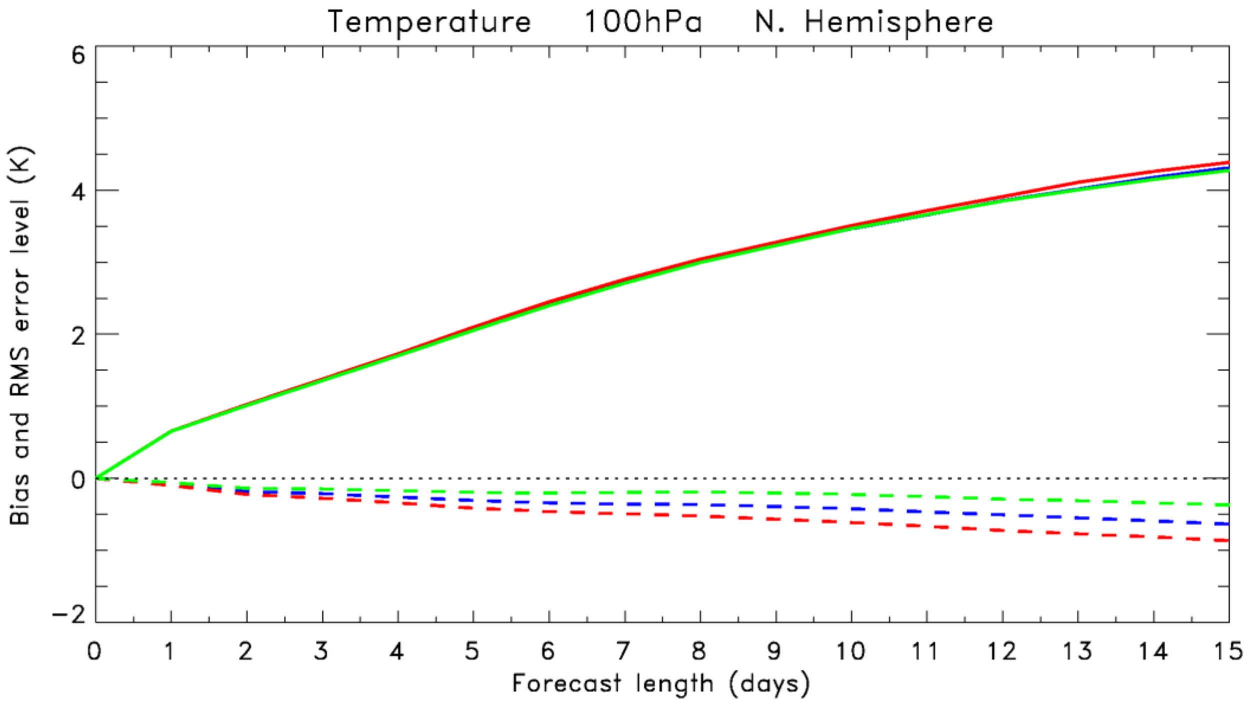
Temperature (K)

50 hPa

(NH)

Forecast verification against analyses
BIRA: Comprehensive chemistry
LINOZ: Linearized chemistry
FK : Ozone zonal monthly climatology

We have improvement 50 hPa and higher up. But lower down at 100 hPa - the reverse is observed

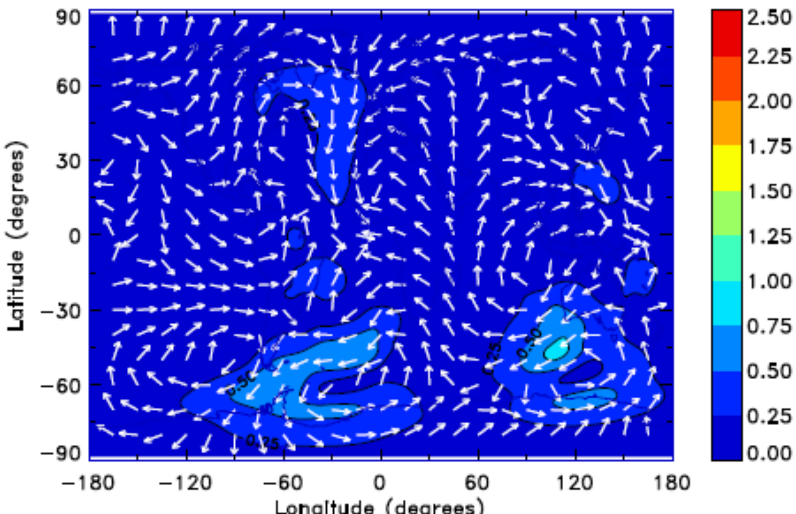


No clear why? MIPAS observations at 100 hPa ?
or other radiative processes / cancellation of errors ?

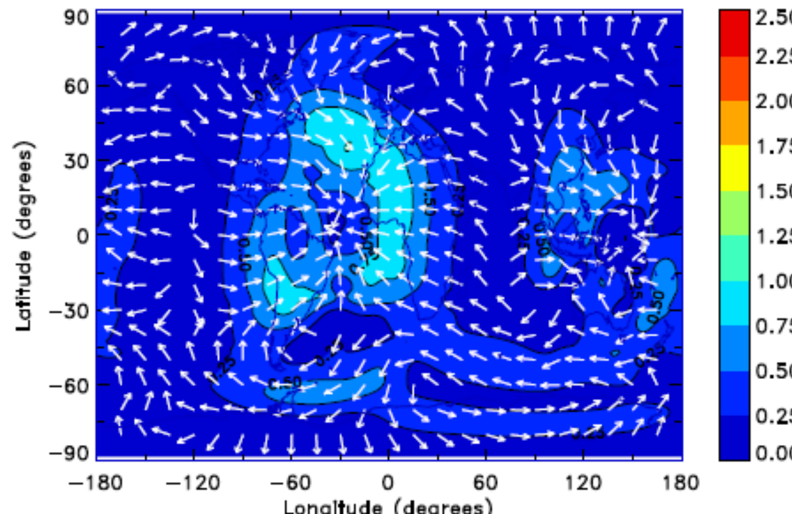
Tracer-wind using 4D Var in an NWP model

Limb observations from MIPAS / Using 1x1° Canadian NWP GEM model

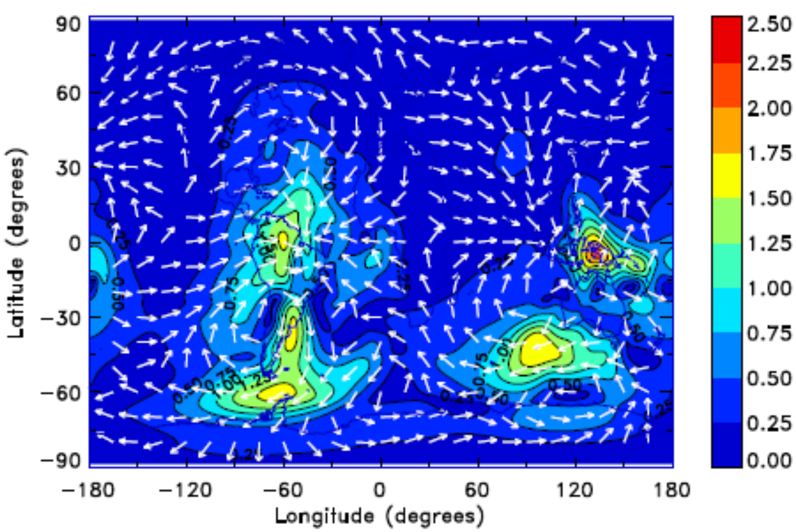
CH_4



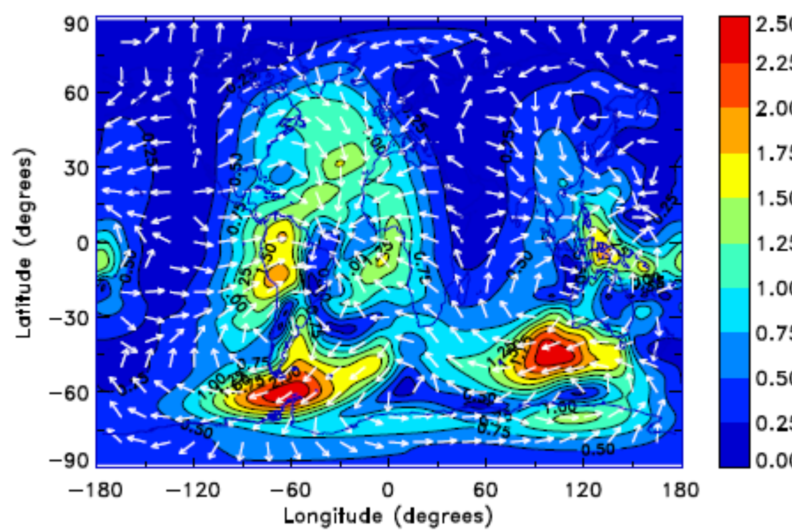
O_3



N_2O



Together



Wind increments from TOVS and chemical species are of comparable magnitude

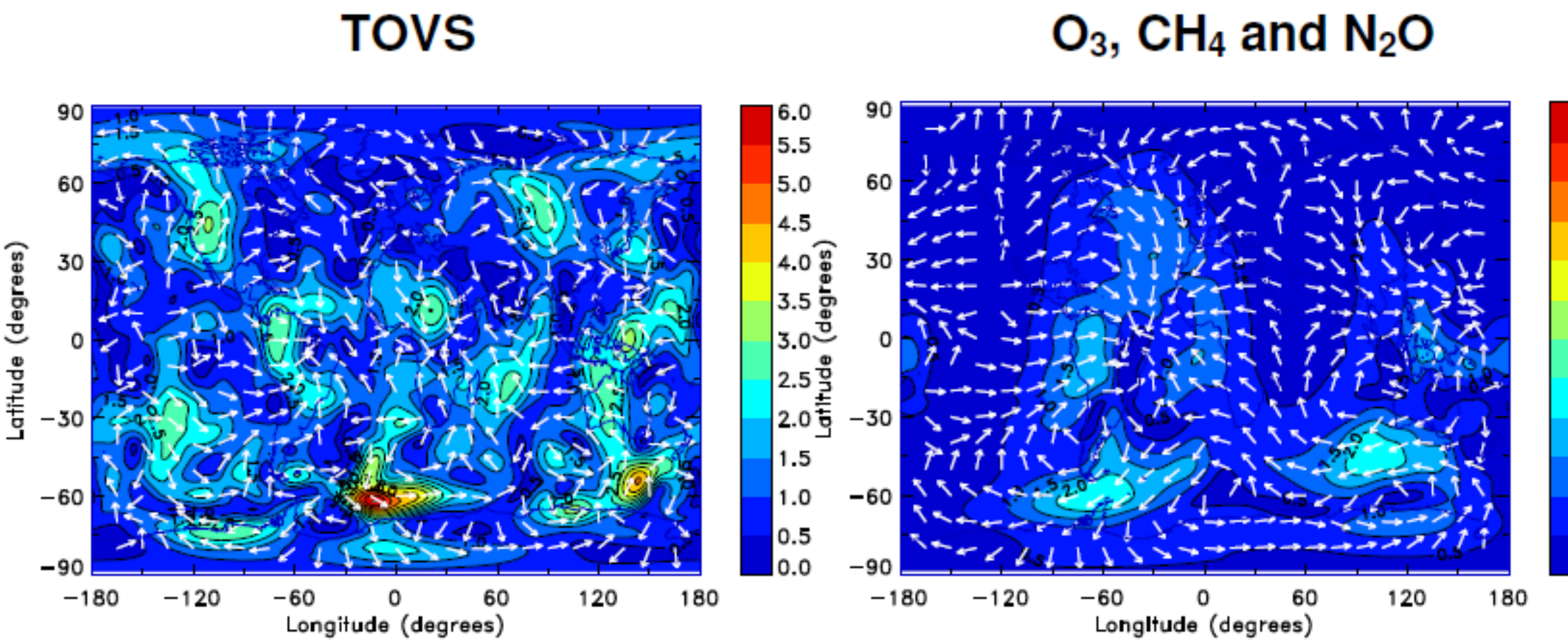
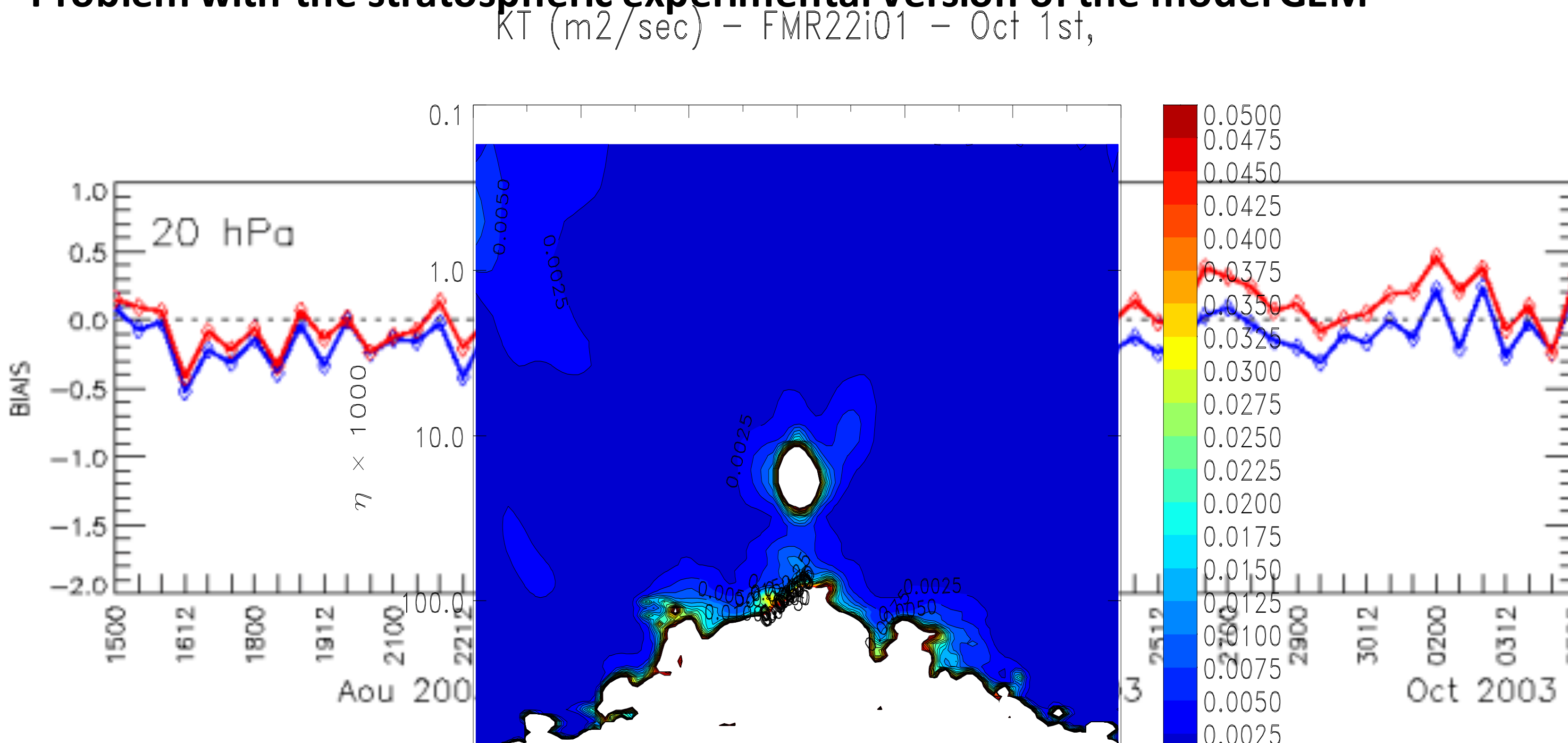


Figure 14.14 Wind increments at 10 hPa obtained from TOVS and chemical species when simultaneously assimilated in 4D-Var.

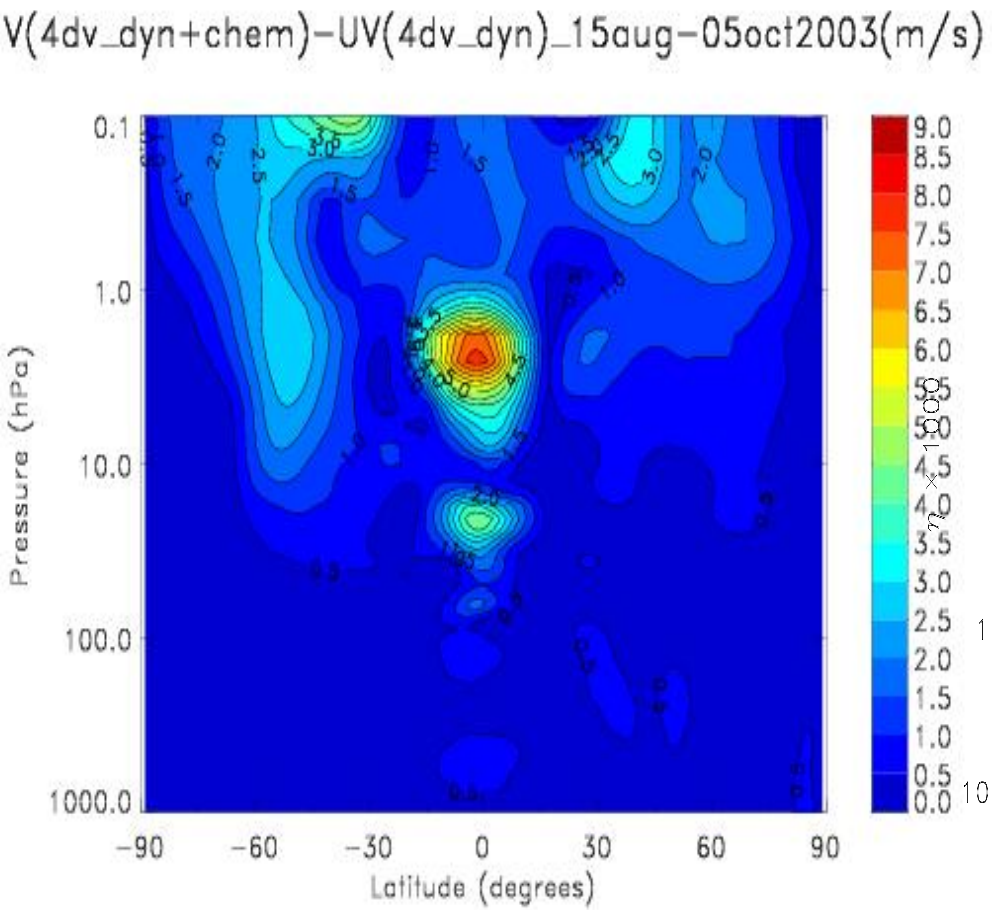
Problem with the stratospheric experimental version of the model GEM

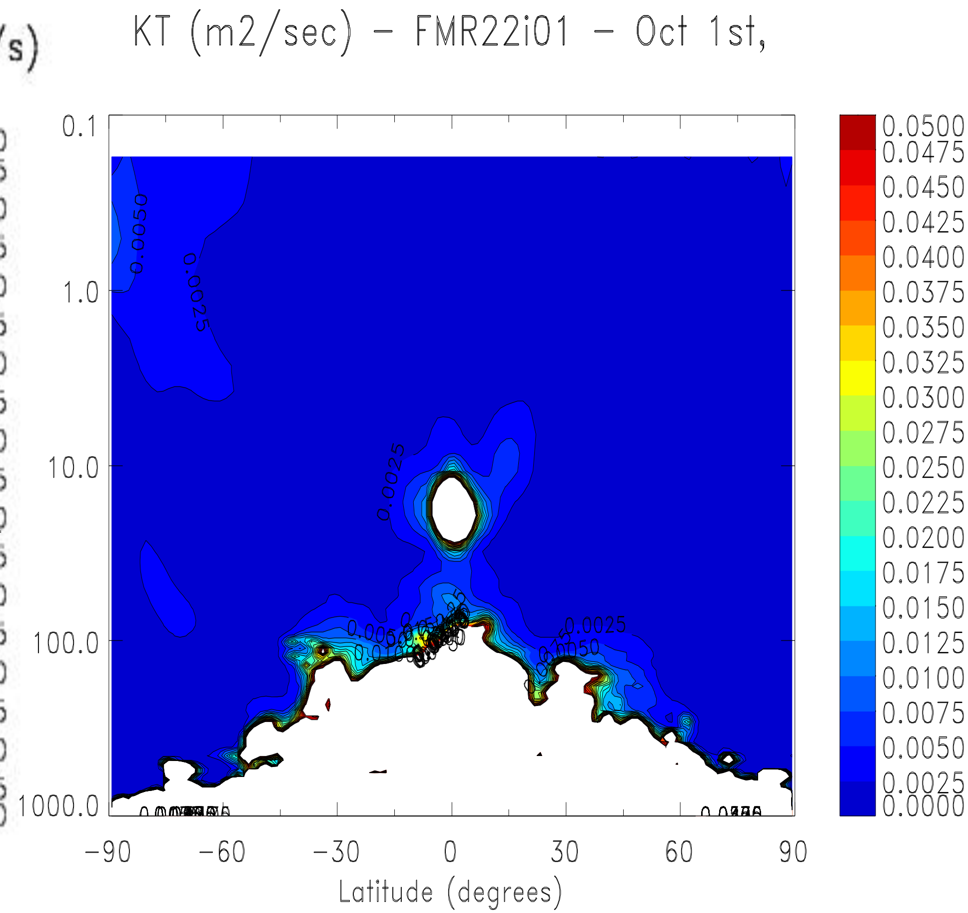


O-P temperature time series between RAOBS and the 3D-Var (blue) and 4D-var (red) assimilation cycles at 20 hPa in the North Hemisphere.

Temperature bias that increases with time

Important to have a good meteorological model





Difference between the wind vector intensity of the analyses obtained from two assimilation cycles done with and without the assimilation of ozone, methane and nitrous oxide. The results are averaged over the period from August 15 to October 5, 2003. The zonal mean of this average is shown here.

Perspectives on stratospheric applications

- Improving the CDA methodology is needed in order to obtain added-value to assimilation products
  - A more effective use of obs can be achieved by improving error covariances
  - Adding retrieval consistency in the obs operator (Kernels or ML estimation)
  - Quality control and bias correction
- In the past CDA have also been oversold – e.g. infering unobserved species
- Methodologies based on CDA are being developed to estimate missing processes (e.g. chemical ozone loss).
- Coupling with NWP remain difficult on short time scales
  - o Ozone –radiation interaction is not seen to be positive in LS/UT region
  - o Tracer-wind. Analysis increment on winds are consistent and significant, but may develop biases
- Radiative impact of GH species on seasonal and climatic time scales maybe important

The end

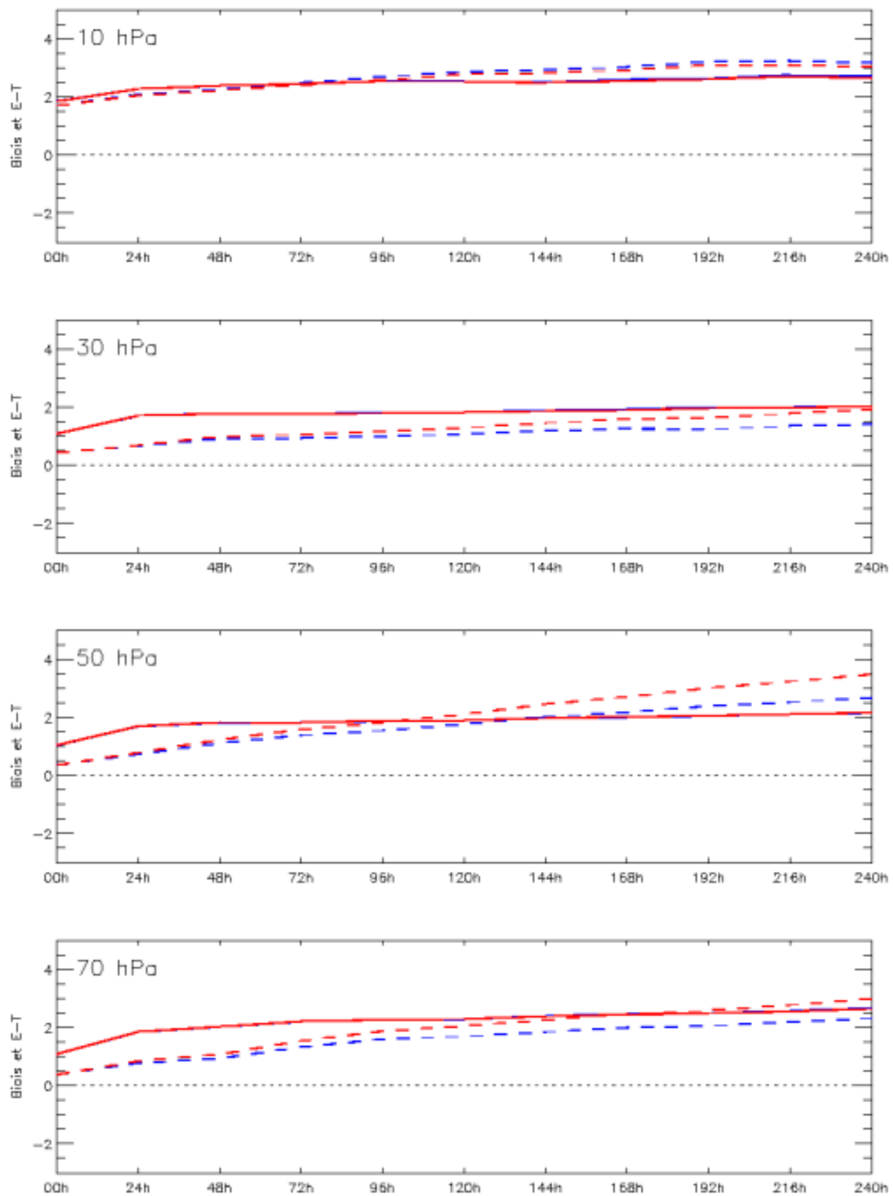


Figure 10.4.4: Time series of radiosonde observations minus forecast (O-F) mean temperature differences (dashed) and standard deviations (solid) for the period Jan 1st to Feb 28th 2009 at 10, 30, 50 and 70 hPa in the tropics [20S-20N]. Results from non-interactive (blue) and interactive (red) ensemble ozone forecasts as in Figure 10.4.1.