3D-FGAT assimilation of MIPAS-IMK (and GOMOS) chemical data

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Outline

- Description of MIPAS-IMK dataset & set-up for assimilation of NO_2, HNO_3, $ClONO_2$, O_3
- Optimization and impact of error statistics
- Comparison between MIPAS-ESA analyses and MIPAS-IMK analyses
- Assimilation of Overhead Column Densities
- One slide on GOMOS assimilation
- Conclusions

Setup of chemistry assimilation experiments

- Forward model (GEM-BACH) has full and interactive chemistry but assimilation system does not have adjoint of chemistry → 4D-VAR chem not available. (120x240 grid, 80 levels up to 0.1hPa)
- Using 3D-FGAT scheme with window of 6h:
  O-F computed at obs time but analysis increments (A-F) do not account for temporal correlation over 6h.
- Dyn variables overwritten every 6h by analyses from a previous 4D-VAR experiment
  (similar to CTM-based assimilation)
- Short experiments: 2003/08/11 – 2003/09/05

Datasets actually assimilated

- MIPAS-ESA retrievals: offline dataset (v4.61).
  T; N_2O, CH_4 (tracers) ; H_2O, O_3,, HNO_3 (chem & adv) ; NO_2 (chem) .

- **MIPAS-IMK retrievals: same + $ClONO_2$**
  (intermediate-lived chlorine reservoir; very important for polar ozone depletion)**.**
  Tailor-made dataset with full coverage for 2003/08/11 to 2003/09/05.

  Each profile was delivered with averaging kernels and
  a priori profiles (T, H_2O, NO_2).

  Did not assimilate H_2O (lack of time), N_2O and CH_4
  (more biased than MIPAS-ESA w.r.t. HALOE)

- GOMOS retrievals: offline ESA dataset (v6.0f).
  Used only O_3 and NO_2 during *night time* (dark limb)

Approx. in dealing with retrieval products

Retrievals and constraints applied in retrievals give rise to non-diagonal solution covariance matrices **R** (for random error).

In addition, constraints also result in non-identity averaging kernel matrices **A**.

In data assimilation (of the retrieval products) via minimization of the cost function:

$$J(x) = \frac{1}{2}\left(x - x^f\right)^T \mathbf{B}^{-1}\left(x - x^f\right) + \frac{1}{2}\left(y - \mathbf{H}(x)\right)^T \mathbf{R}^{-1}\left(y - \mathbf{H}(x)\right)$$

- Assim. system assumes obs error covariance matrix **R** is diagonal.
- Never the case but we should keep vertical correlations between errors as small as possible.
- Correct way to compare obs ***y*** and model profiles ***x*** at different resolutions is to apply the averaging kernels **A** to the model variable **x**.
- **A** becomes part of the obs operator **H.**
- Application of **A** (varying for each profile) not implemented in this project.

MIPAS-IMK retrieval products: Dealing with artificially high vertical resolution

MIPAS-IMK data is delivered with an artificially high vertical resolution relying on a regularization constraint to ensure smoothness.

This is another type of a priori information and impacts both **R** and **A**.

For assimilation, it was decided to at least reduce the retrieved profiles to the same resolution as the measurement.

Two approaches applied:

- vmr profile thinning - using only altitudes closest to tangent heights.
- produce overhead column densities with lower boundaries at tangent heights (for even better consistency with a diagonal **R**)

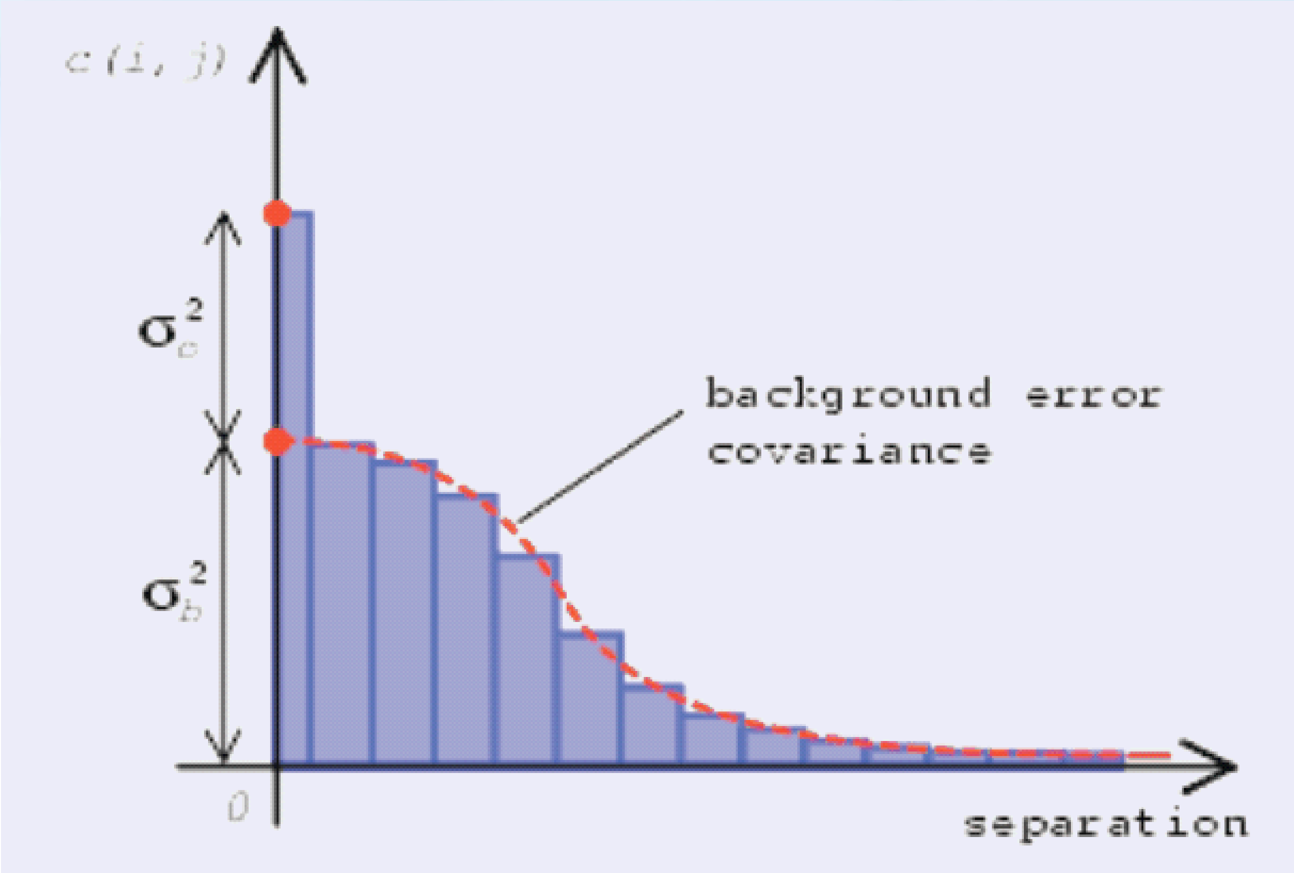
Optimization of error variances by Hollingsworth-Lönnberg (H-L) method and its impact

Error statistics

- First assimilation pass
  uses "educated guesses" for error std. dev.:
  - Background error std. dev. σ_b
    from previous MIPAS-ESA experiments
  - Observation error std. dev. $\sigma_o = \sqrt{(0.1 * vmr)^2 + \sigma_i^2}$
    (σ_i=precision error std. dev. from retrieval team)
- Second assimilation pass
  uses the result of first pass to estimate error variances which allow optimal assimilation…

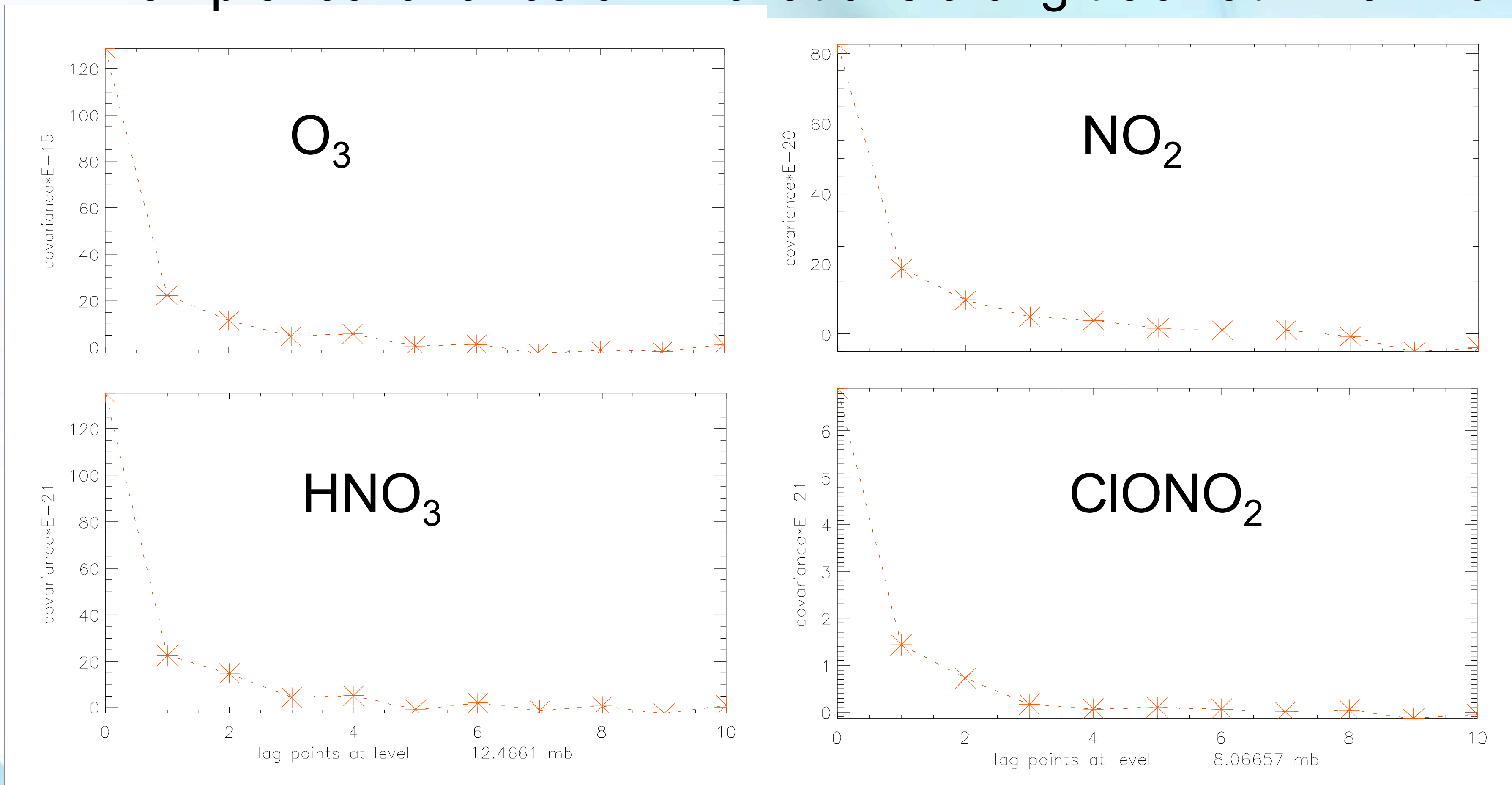
Estimation of σ_o^2 and σ_b^2 from 1st pass assim

Plot the covariances between innovations (O-F) as a function of distance along the satellite track. Assuming that σ_b are spatially correlated and σ_o horizontally uncorrelated (Hollingsworth and Lonnberg, 1986) :



Estimation of σ_o^2 and σ_b^2 from 1st pass assim

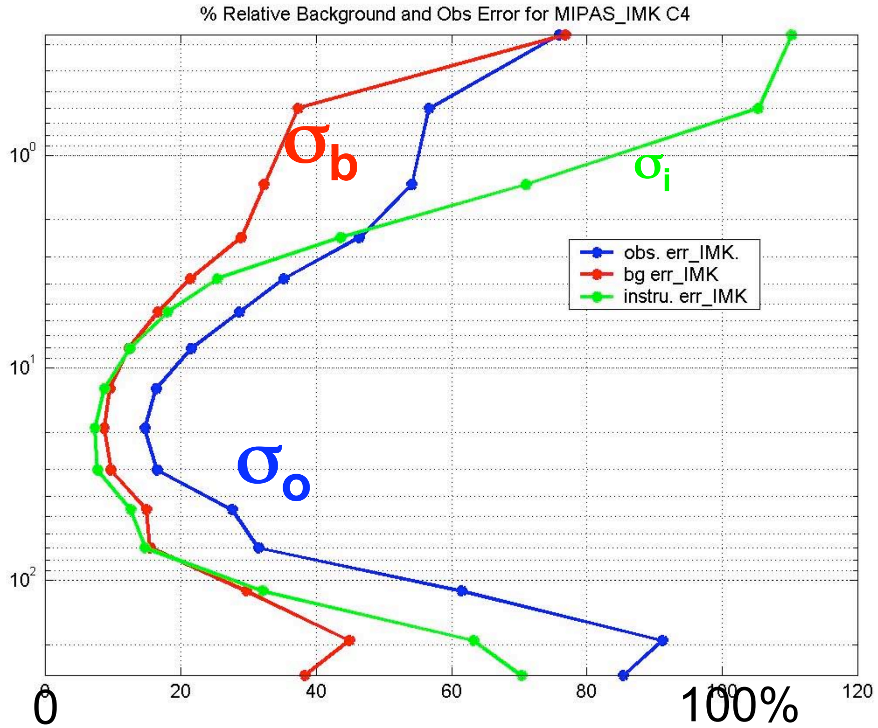
Exemple: covariance of innovations along track at ~ 10 hPa



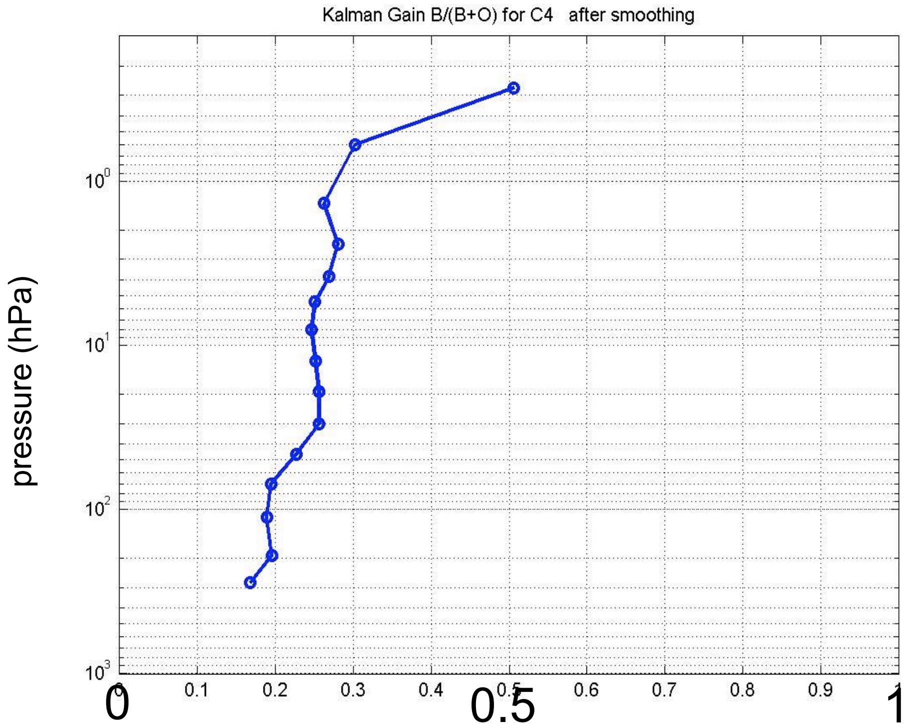
Estimation of σ_o^2 and σ_b^2 from 1st pass assim

Result: "relative error std. dev." (σ/|o| in %), fct of *p* but not fct of lat:

$ClONO_2$ *vmr*



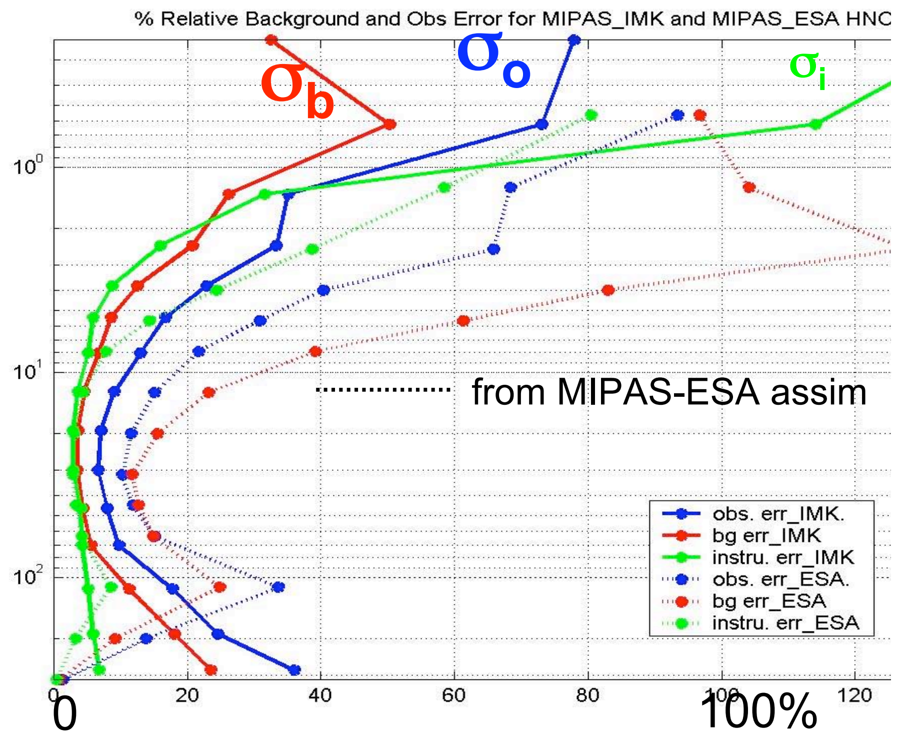
Kalman gain, $\sigma_b^2/(\sigma_b^2 + \sigma_o^2)$



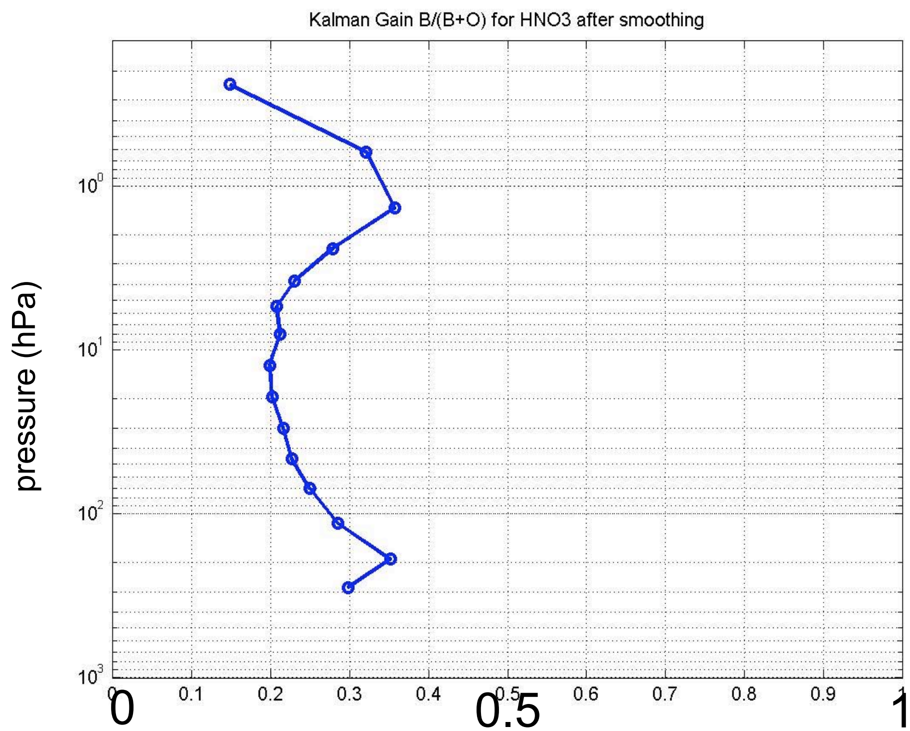
Estimation of σ_o^2 and σ_b^2 from 1st pass assim

Result: "relative error std. dev." ($\sigma/|o|$ in %), fct of *p* but not fct of lat:

HNO_3 *vmr*



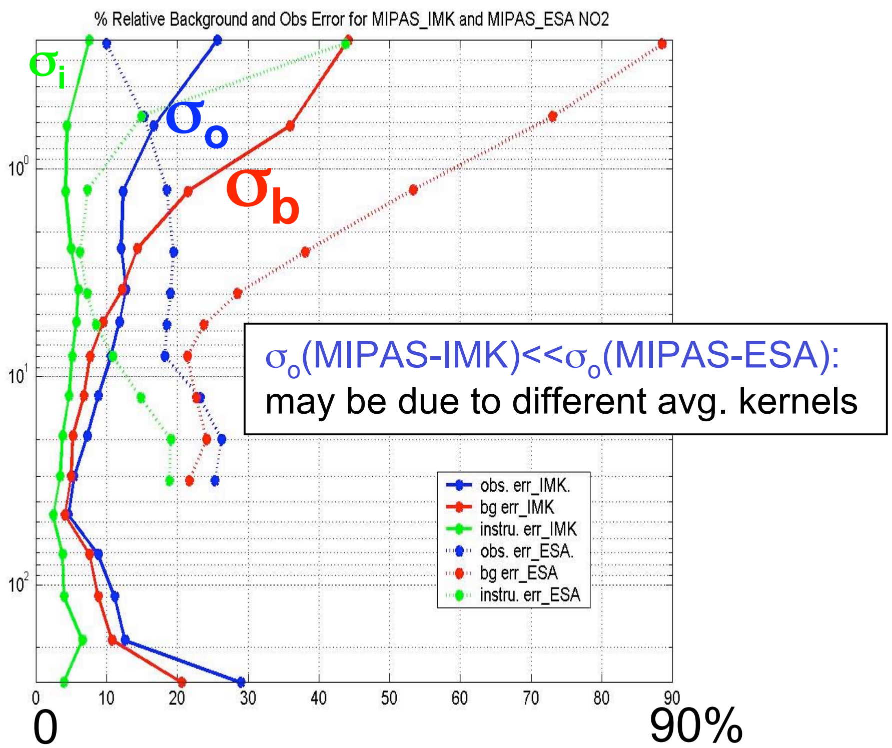
Kalman gain, $\sigma_b^2/(\sigma_b^2 + \sigma_o^2)$



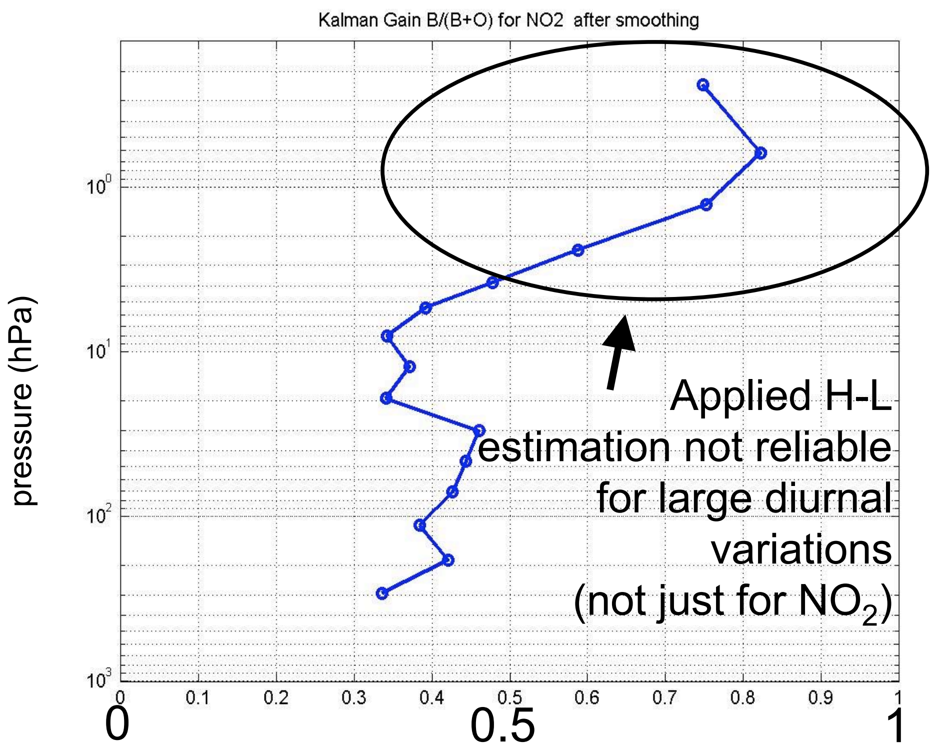
Estimation of σ_o^2 and σ_b^2 from 1st pass assim

Result: "relative error std. dev." ($\sigma/|o|$ in %), fct of *p* but not fct of lat:

NO_2 *vmr*



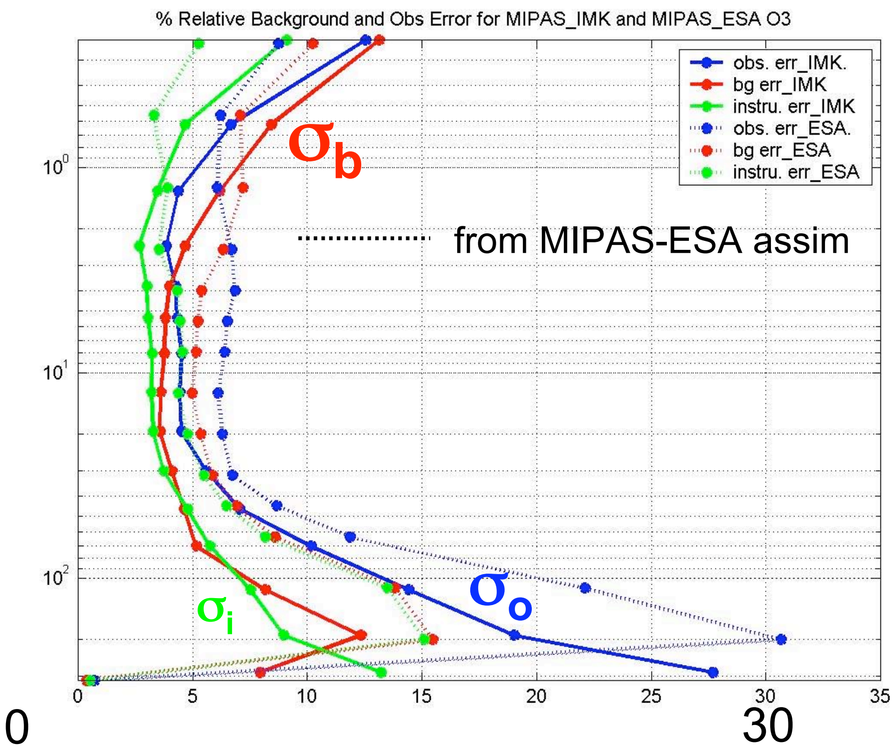
Kalman gain, $\sigma_b^2/(\sigma_b^2 + \sigma_o^2)$



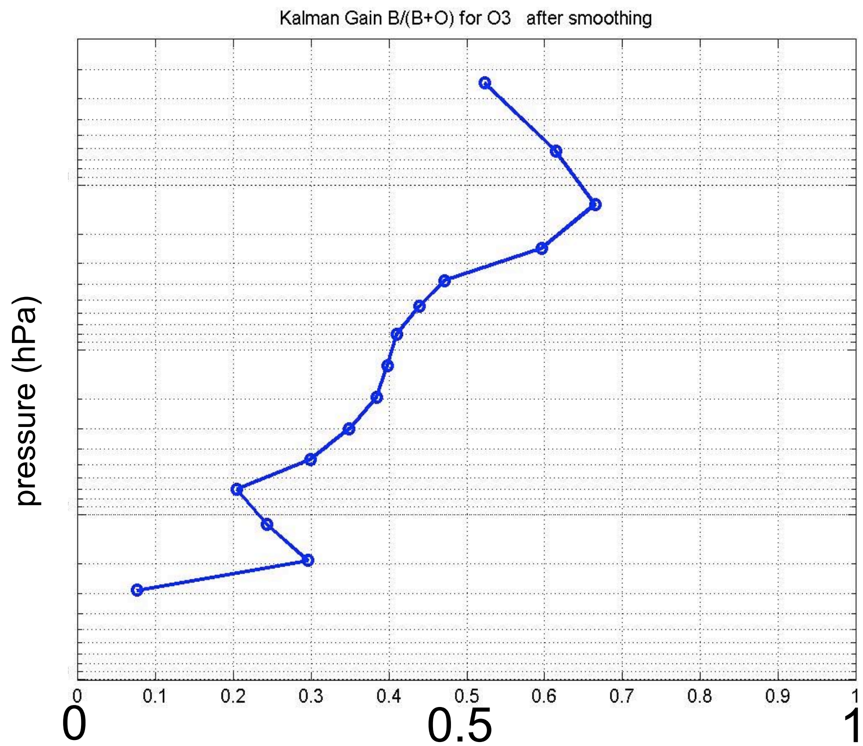
Estimation of σ_o^2 and σ_b^2 from 1st pass assim

Result: "relative error std. dev." (σ/|o| in %), fct of *p* but not fct of lat:

O_3 *vmr*



Kalman gain, $\sigma_b^2/(\sigma_b^2 + \sigma_o^2)$



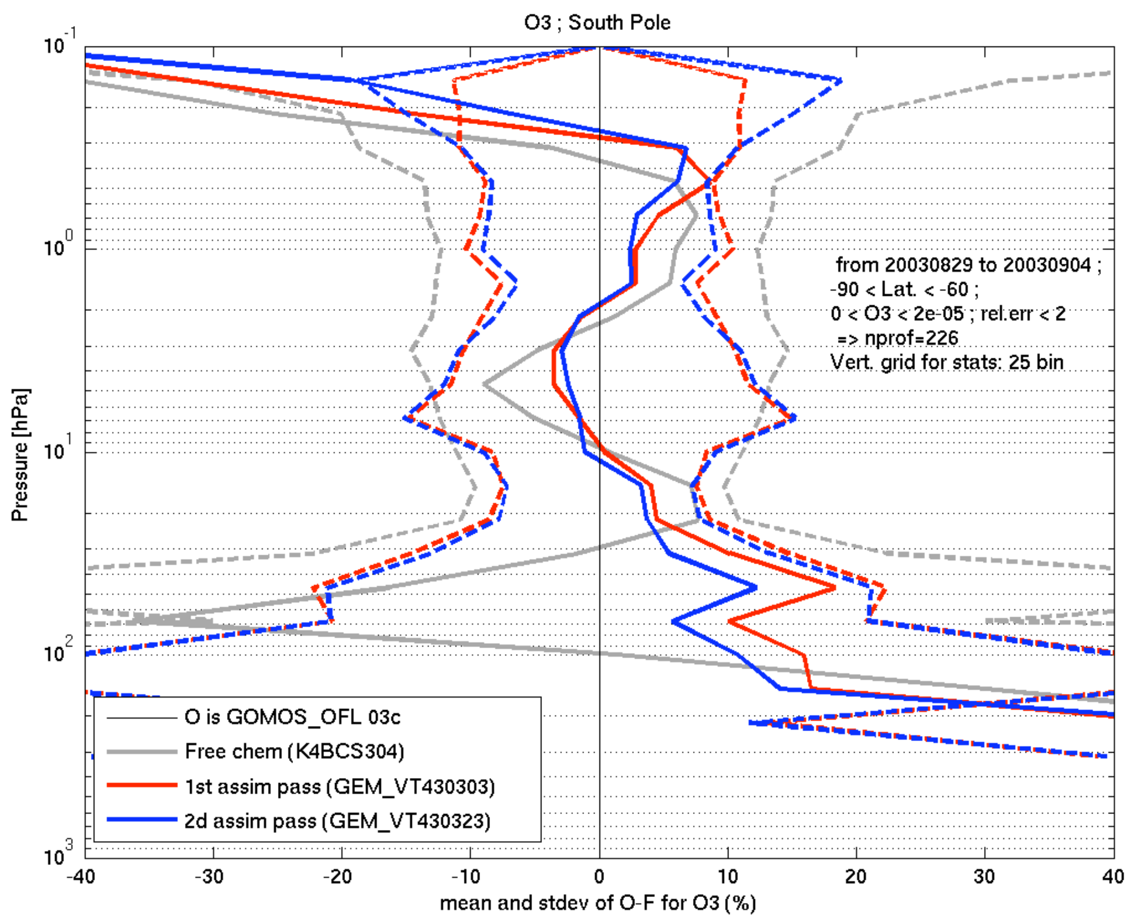
Impact of optimized error variances

Best case:

Ozone, South Pole

Compared with GOMOS (independent instr), the **2d assim pass** has a smaller bias than the **1st assim pass**

(12% instead of 17% at 45hPa)



Comparison of MIPAS-IMK assimilation (O_3, NO_2, HNO_3, $ClONO_2$) With MIPAS-ESA assimilation (O_3, NO_2)

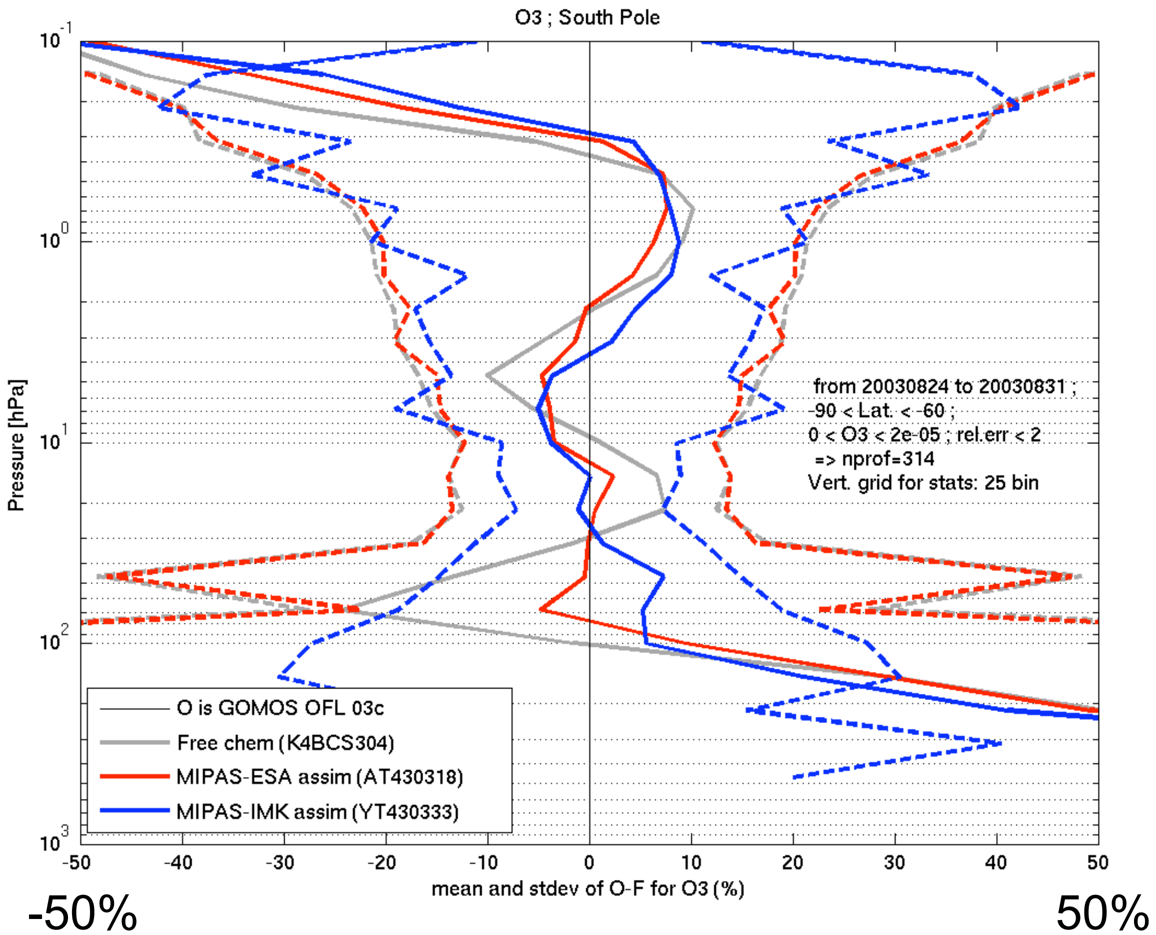
Setup is identical:

- dyn variables from same 4D-VAR experiment
- same model, same 3D-FGAT assimilation scheme
- error variances obtained from 1st pass + H-L method in both cases

→ All differences should be due to:

- different retrievals (for same MIPAS obs) and different data selection criteria
- presence/absence of $ClONO_2$ and HNO_3

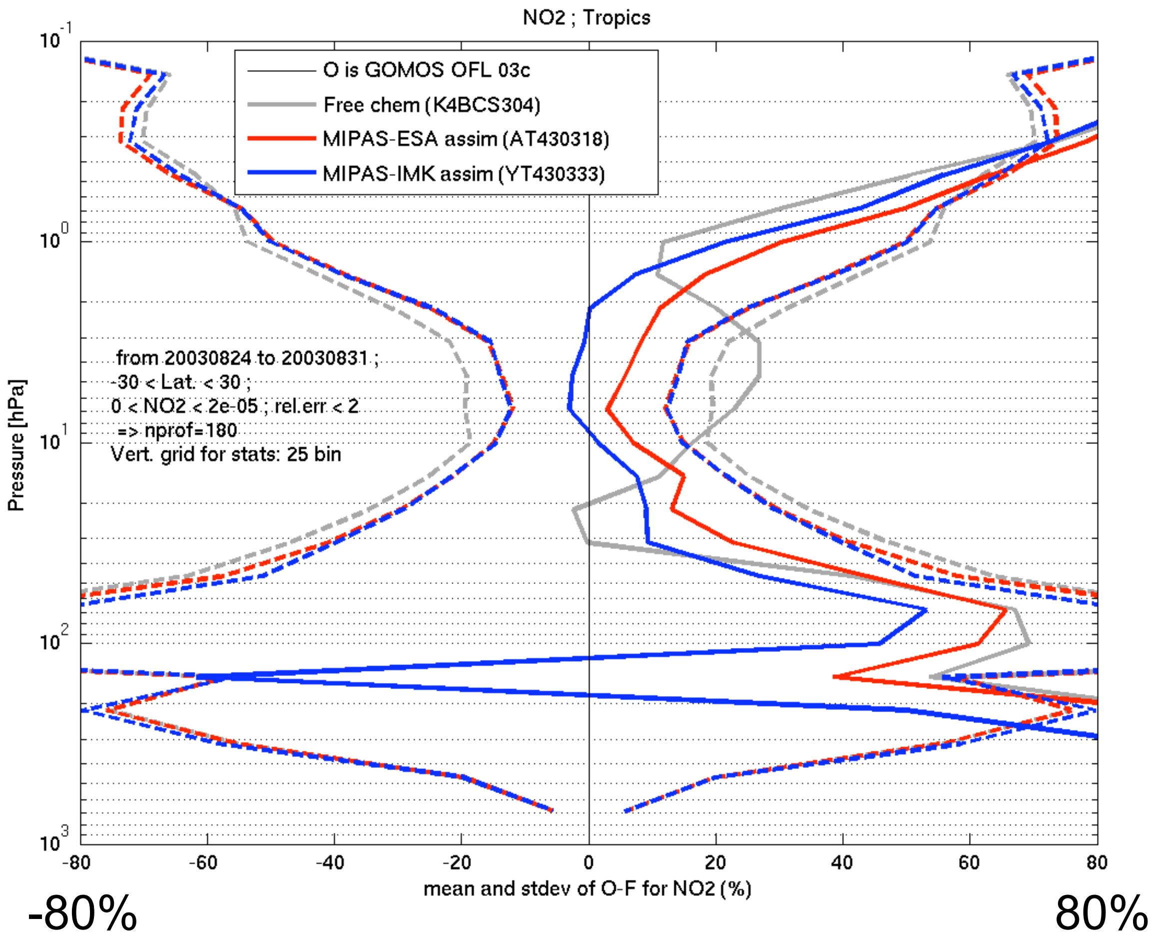
MIPAS-ESA *vs* MIPAS-IMK: ozone (South Pole)



Ozone at South Pole, comparing with GOMOS (indep obs): bias similar but stdev(O-F) smaller using **MIPAS-IMK** than **MIPAS-ESA**, especially in lower strato

In tropics, analyses of both retrievals compare equally well with GOMOS (not shown)

MIPAS-ESA *vs* MIPAS-IMK: NO_2 (tropics)



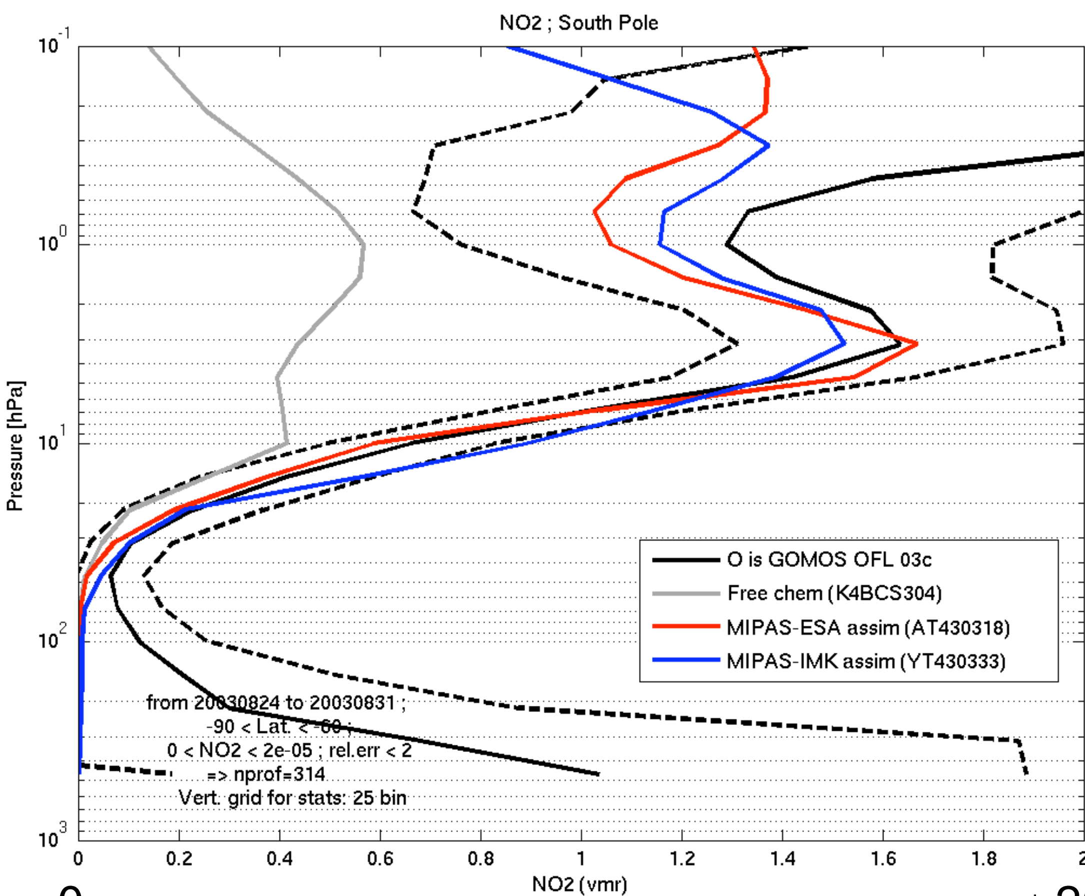
Tropical NO2 (at night), comparing with GOMOS (indep obs): forecasts using **MIPAS-IMK** have much smaller bias than forecasts using **MIPAS-ESA**

Results still quite poor except in middle stratosphere:

- model deficiencies (aerosols)
- 3D-FGAT scheme and H-L implementation not appropriate for large diurnal variations

MIPAS-IMK chemical data assimilation

MIPAS-ESA *vs* MIPAS-IMK: NO_2 (South Pole)

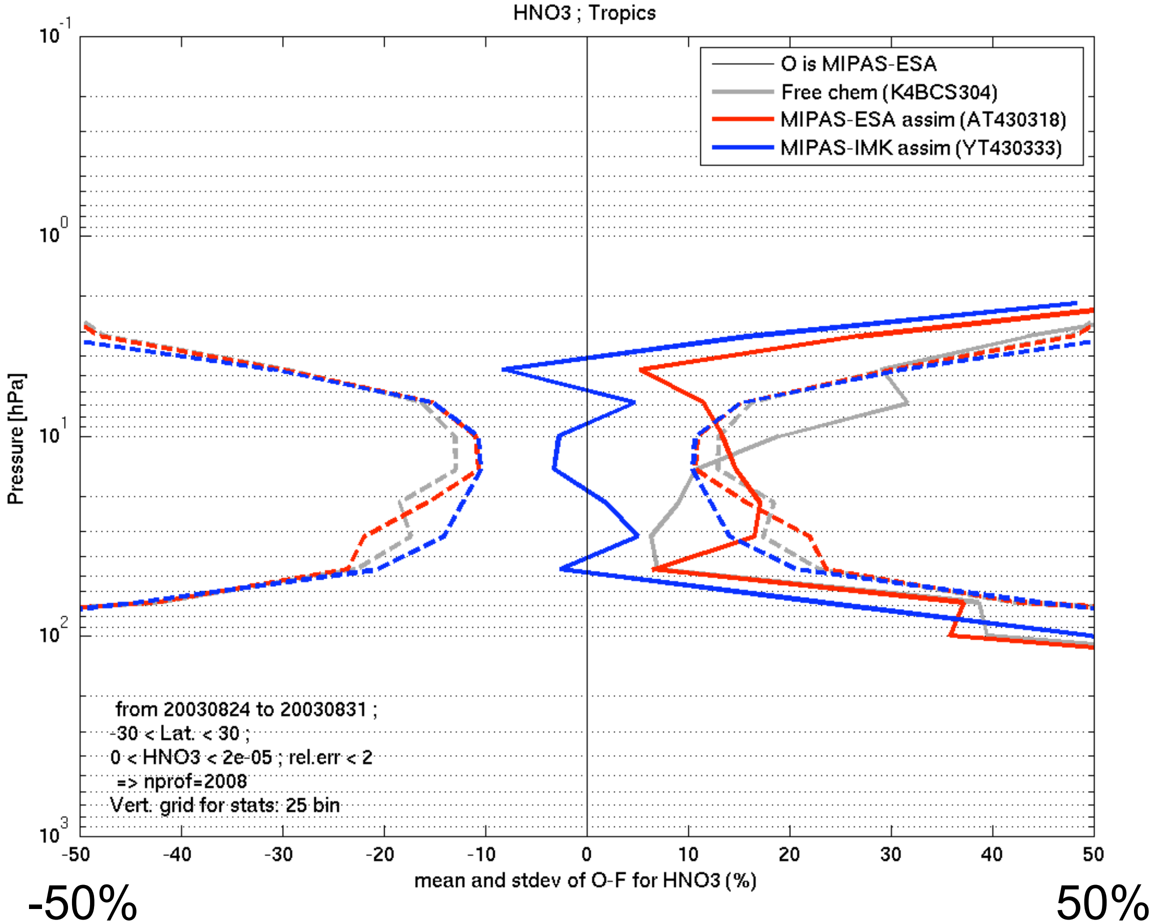


0   20 ppbv

NO_2 in polar vortex is most difficult : **model** has nothing to simulate NOx production in MLT (aurorae etc)
→ simulated NO_2 <u>much</u> too small

- Assim still improves results a lot, but here **MIPAS-ESA** delivers better results overall than **MIPAS-IMK**

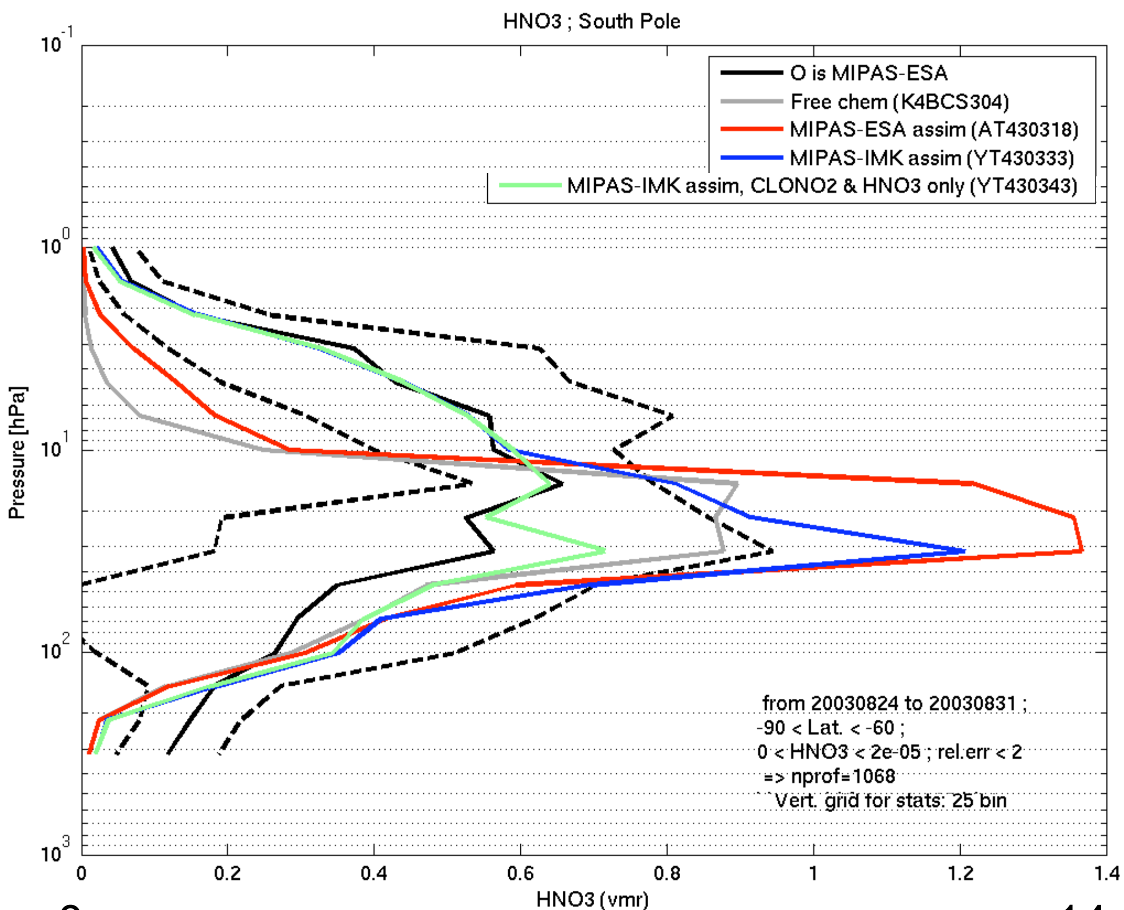
MIPAS-IMK: HNO_3 (tropics)



Tropical HNO3 :
MIPAS-IMK assim works much better than **MIPAS-ESA** assim (of O_3 and NO_2 only; excludng HNO_3).

Note: Comparison with *MIPAS-ESA obs*

MIPAS-IMK: HNO_3 (South Pole)



MIPAS-IMK assim as compared to MIPAS-ESA assim (excluding HNO_3) and MPAS-ESA with no assim.

Still, MIPAS-IMK is very bad in lower strato. We know that NO_2 is a big problem at South Pole. We have **another MIPAS-IMK assimilation which did not use NO_2**

MIPAS-ESA *vs* MIPAS-IMK: conclusions

- For common assim. species, **MIPAS-IMK retrievals provide as good or better analyses than MIPAS-ESA retrievals**.
- Only exception is ***NO_2 in (Southern) Polar vortex***, where MIPAS-ESA assimilation worked a little better than MIPAS-IMK assimilation.
  Both experiments correct most of the (very large) model underestimation.
- But in both experiments, this NO_2 correction has a very negative impact on HNO_3
- What about $ClONO_2$?

Assimilation of overhead column densities instead of volume mixing ratios: the case of $ClONO_2$

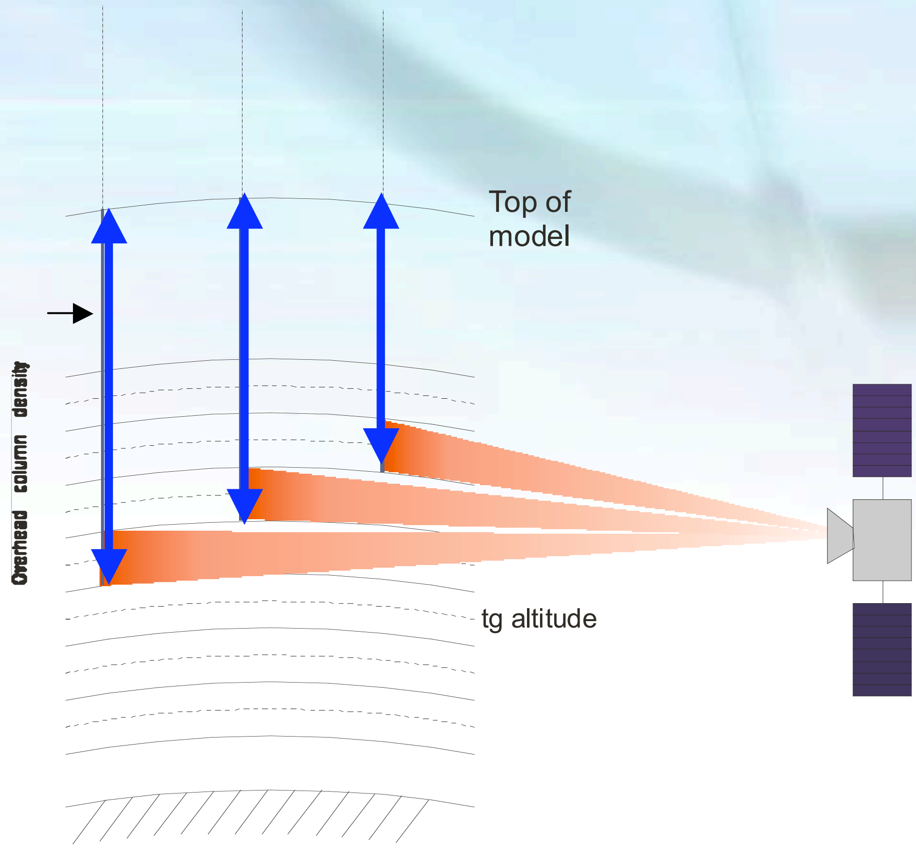
Conversion to overhead column densities

All results previously shown assim. the *vmr* closest to tg altitude.

Tried alternative method: convert MIPAS-IMK *vmr* to overhead column densities (*ocd*) at each tg altitude and assim this.

ocd errors should be less correlated than the full-resolution and reduced resolution *vmr* profiles. This should be more consistent with the measured integrals and with a diagonal **R**.

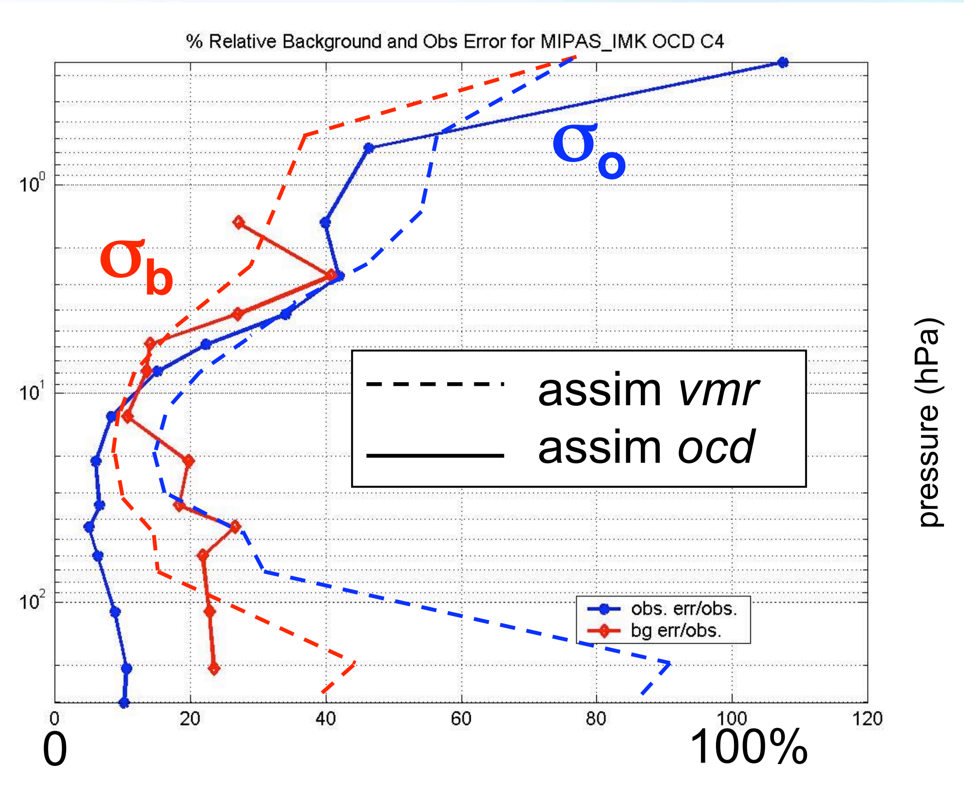
However, broad weighting functions are introduced via change in **H** as compared to the reduced resolution *vmr.*



Estimation of σ_o^2 and σ_b^2 from 1st pass assim

Result: "relative error std. dev." ($\sigma/|o|$ in %), fct of *p* but not fct of lat:

$ClONO_2$



For lower-strato $ClONO_2$, the H-L estimation from 1st pass assim of *ocd* delivers much larger background error std. dev. and much smaller obs error std. dev. than from 1st pass assim of *vmr*.

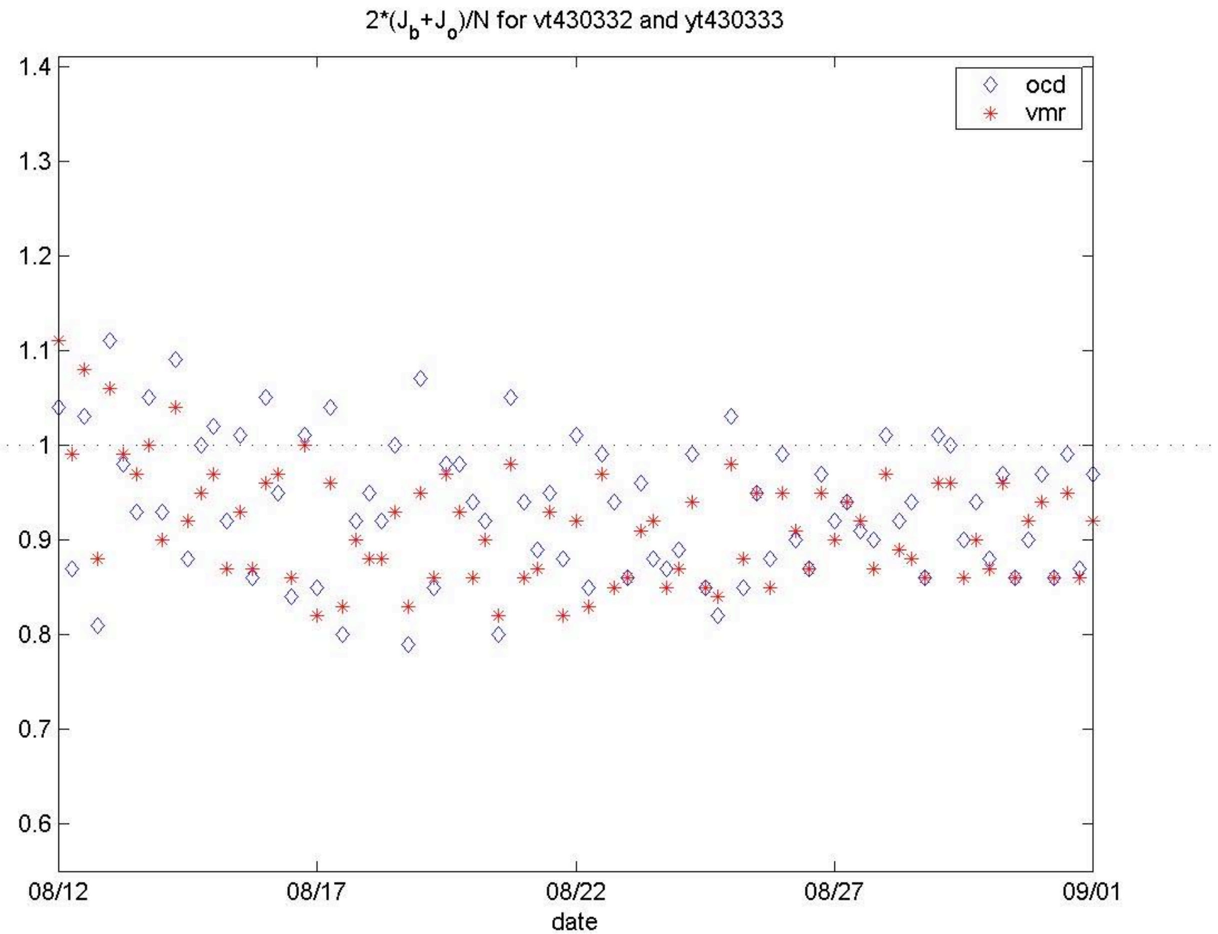
→ Smaller O-P relative random error std. dev. for vertical integrals/summations.

Note: For 1st pass of assimilation, assigned arbitrary relative error std. dev. of 10% for the *ocd*

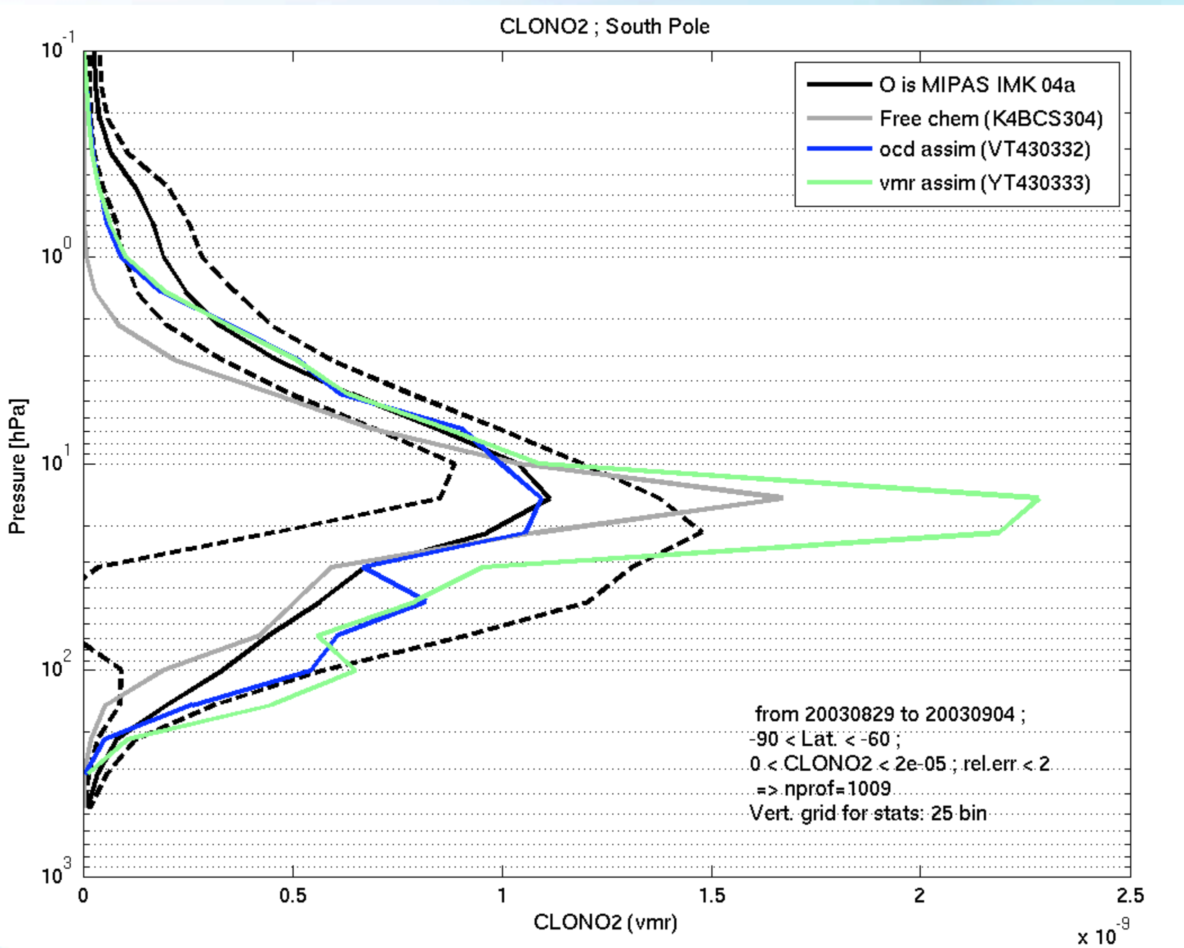
Normalized χ^2 diagnostic (2^{nd} assim. pass)

From assim. of the 4-species.

Values from the 1^{st} pass were > ~2



Is it better to assimilate overhead columns ?



For $ClONO_2$ at South Pole, the answer is yes: ***ocd* assim** works better than ***vmr* assim**. But…

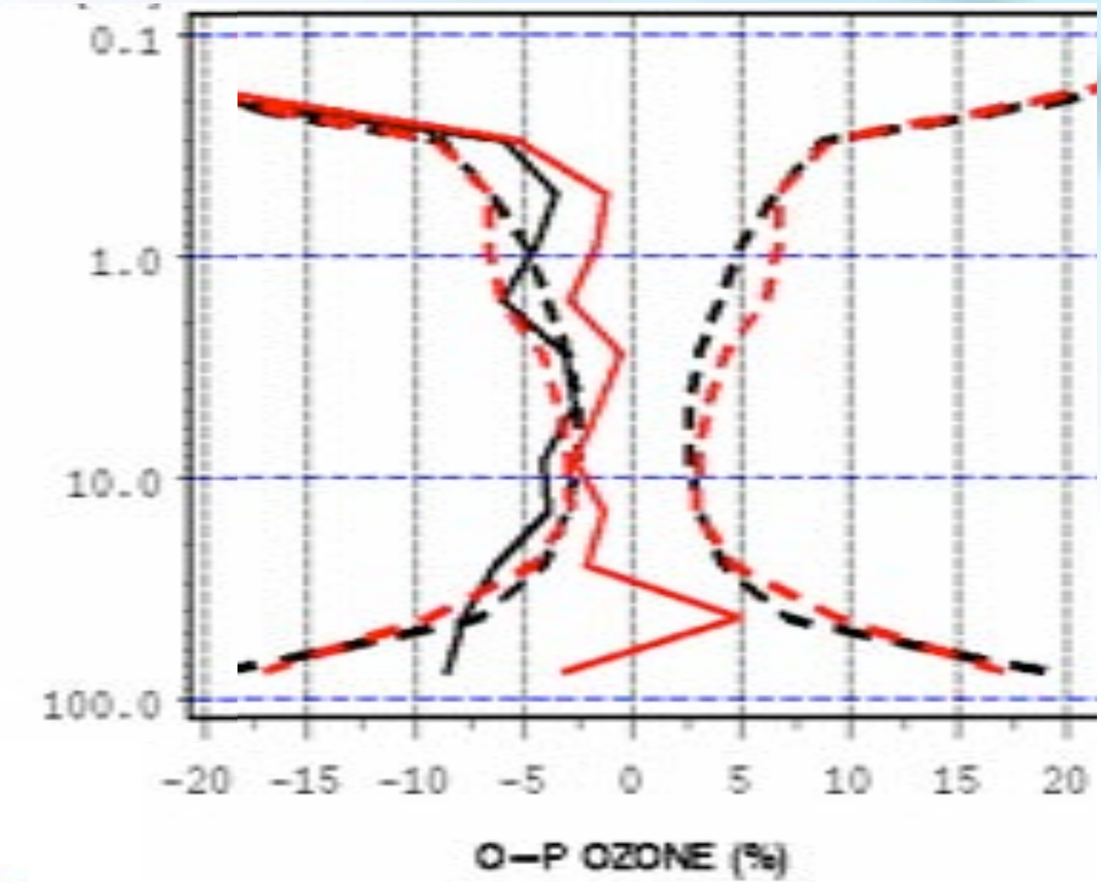
- Results partly due to interaction with NO_2: outcome not as clear when NO_2 is not assimilated
- For HNO_3 & NO_2 the answer is no (*vmr* assim works better than *ocd* assim)

One slide on the assimilation of GOMOS O_3

(using night-time obs
from occultations of a subset of stars)

Impact of GOMOS assimilation: O_3

In the Tropics, using **HALOE** as reference:



assim MIPAS-ESA *vmr*
assim GOMOS *vmr*

→ Assim of GOMOS reduces bias more than assim of MIPAS-ESA (but std dev larger)

Conclusions

- Assimilation of MIPAS-IMK
  - Optimized error statistics using 1st pass assim and Hollingsworth-Lönnberg method: improves quality of short-term forecasts (especially ozone in polar vortex…)
  - MIPAS-IMK assim compares better with independent obs (GOMOS) than MIPAS-ESA assim, except for…
  - NO_2 in polar vortex, very difficult for model (MLT production) and for assimilation scheme (NO_2 too short-lived)
  - NO_2 assimilation corrects well NO_2 simulation, but has very negative impact on HNO3 and (probably) $ClONO_2$
  - Tried assimilating overhead column densities (*ocd*) rather than *vmr* closest to tg altitudes. Had positive impact only for $ClONO_2$. Possible reason to be verified (impact from simultaneous NO_2 assim combined with applied obs error std dev?).
  - We must first improve our understanding of NO_2 assimilation and its interaction with other species
- Assimilation of GOMOS
  - Ozone analyses are less biased than MIPAS-ESA analyses but have less precision

Merci

Thank you

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