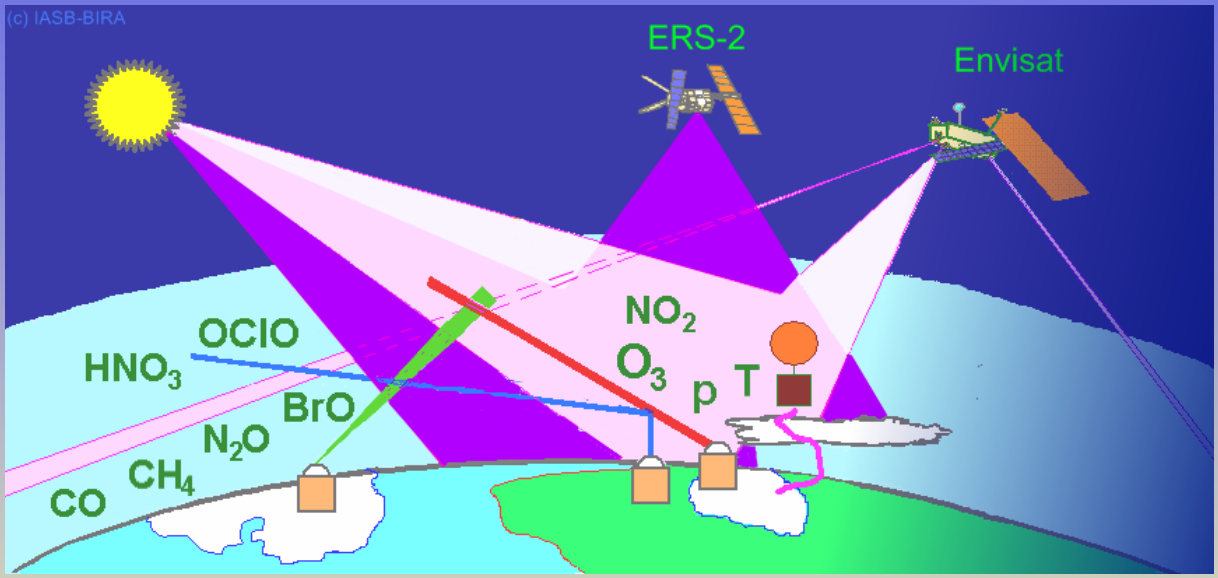
8th SPARC Data Assimilation Workshop, 20-22 June 2011, Brussels, Belgium

Improved observation operators for the chemical data assimilation of atmospheric trace gases



J.-C. Lambert [1], S. Vandenbussche [1], R.J.D. Spurr [2], and T. von Clarmann [3]

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Improved observation operators for the chemical data assimilation of atmospheric trace gases

1. The ideal observation operator?
2. Pragmatic observation operators
3. Illustrations
   1. Assessment of smoothing errors
   2. Interpretation of comparisons
   3. Optimised co-location criteria
4. Conclusion

Funded by EC FP4 ESMOS and SCUVS, BELSPO/ProDEx SECPEA and EC FP6 GEOmon. Continuation with BELSPO/ProDEx A3C and EC FP7 NORS.

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The ideal observation operator?

For an ideal data assimilation...

Observation operators used in chemical data assimilation

low the tropopause.

2.2 The 4D-Var system

Data assimilation is done using 4D-Var (Talagrand and Courtier, 1987). This method optimizes the model initial conditions to reproduce a set of observations over a time window. This is done by minimizing the following objective function, $J(\mathbf{x})$ (also denoted cost function) (Talagrand and Courtier, 1987) using the standard notation of Ide et al. (1997):

$$J(\mathbf{x}) = \frac{1}{2}[\mathbf{x}(t_0) - \mathbf{x}^b(t_0)]^T \mathbf{B}_0^{-1}[\mathbf{x}(t_0) - \mathbf{x}^b(t_0)] + \frac{1}{2}\sum_{i=0}^{N}(\mathbf{y}^o(t_i) - H(\mathbf{x}(t_i)))^T \mathbf{R}_i^{-1}(\mathbf{y}^o(t_i) - H(\mathbf{x}(t_i))) \quad (1)$$

given the model evolution equation

$$\mathbf{x}(t_i) = M_{i-1}[\mathbf{x}(t_i - 1)] \quad (2)$$

where $\mathbf{x}(t_i)$ represents the model state vector at time t_i, $\mathbf{x}^b(t_0)$ is the first guess and $\mathbf{B}_0$ is the background error covariance matrix of $\mathbf{x}^b(t_0)$. Vectors $\mathbf{y}^o(t_i)$ and matrix $\mathbf{R}_i$ are, respectively, the observation state vector and the error covariance matrix associated with the observations at time t_i. The observation operator H maps the model state into the observation space and M is the model operator that calculates the time evolution of the model state. Minimization of Eq. (1) requires the knowledge of the gradient of J. This is done

Errera et al., *Atmos. Chem. Phys.*, 8, 2008

are assimilated by the BASCOE system to constrain its CTM outputs, while HALOE and POAM-III data are monitored by the system and used for a posteriori evaluation of the BASCOE analyses. Assimilated data are volume mixing ratio at the location of the tangent point and the observation operator interpolates linearly the model values at the eight grid points to the surrounding tangent point of any available observation at ±15 min of the model time step. In the monitoring procedure, the BASCOE observation operator is used only to map the analyses at HALOE and POAM-III locations. Finally, BASCOE analyses interpolated at observation locations (as

Underlying assumption: $H(x(t_i))$ reproduces perfectly smoothing and sampling characteristics of the observation.

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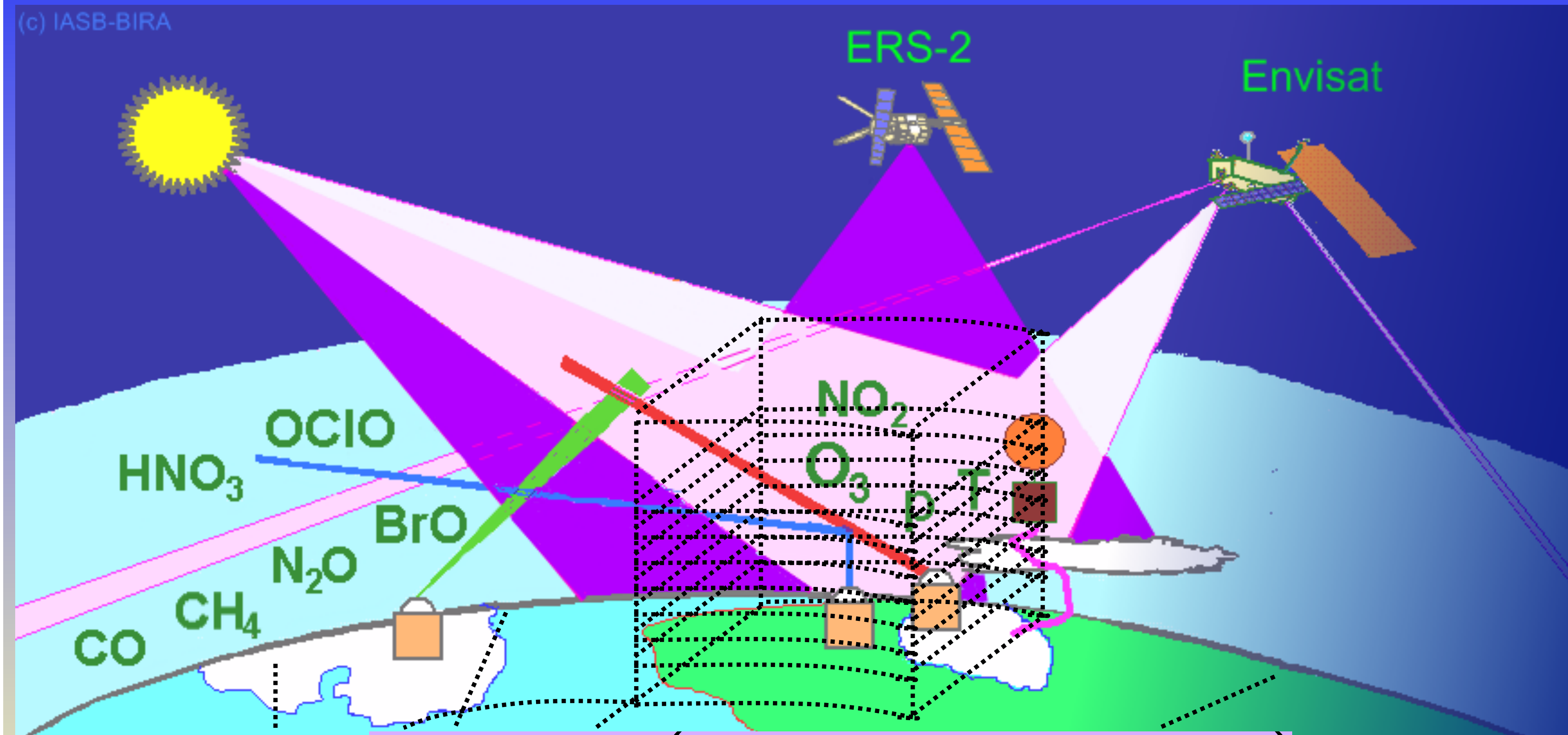
Observation operator for an ideal ingestion?

Air masses probed by GOME, Envisat and NDACC ground-based instruments



$$\varepsilon_{smoothing} = f\left((A_1 - A_2).S_{atmos.}.(A_1 - A_2)^T\right)$$

in the vertical **AND** horizontal dimensions

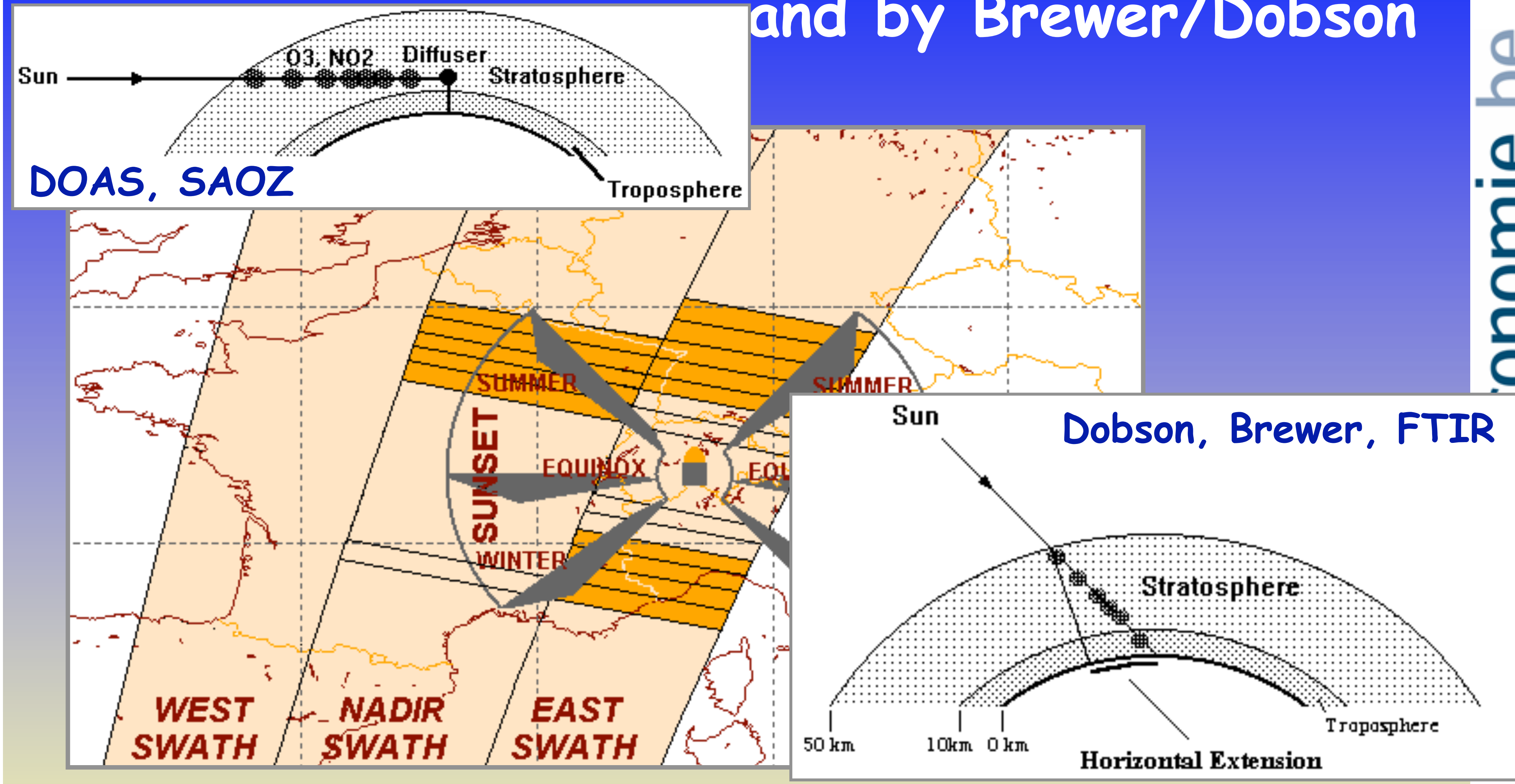
⇒ Pragmatic observation operators

- The main objective is to reduce apparent discrepancies generated by smoothing and sampling differences.
  - Match at best the characteristics of the retrieved information (e.g., no instrument measures "within a circle of 500km radius")
  - Smoothing errors depend on species, atmospheric state, and use
  - Provide essential characteristics like the barycentre and spread of the retrieved information, and possibly its shape.
- Operators are expected to provide more than just an adaptation of the resolution. They should also indicate the sensitivity versus altitude, and show where there is no (significant) information from the measurement, e.g., below clouds or after severe instrumental degradation.
- Operators must be affordable in terms of design (i.e., RT tools exist or can be adapted at reasonable cost) and use (e.g., no heavy RT calculation for every single ingestion).

Pragmatic observation operators

… for an optimised selection and
ingestion of observations

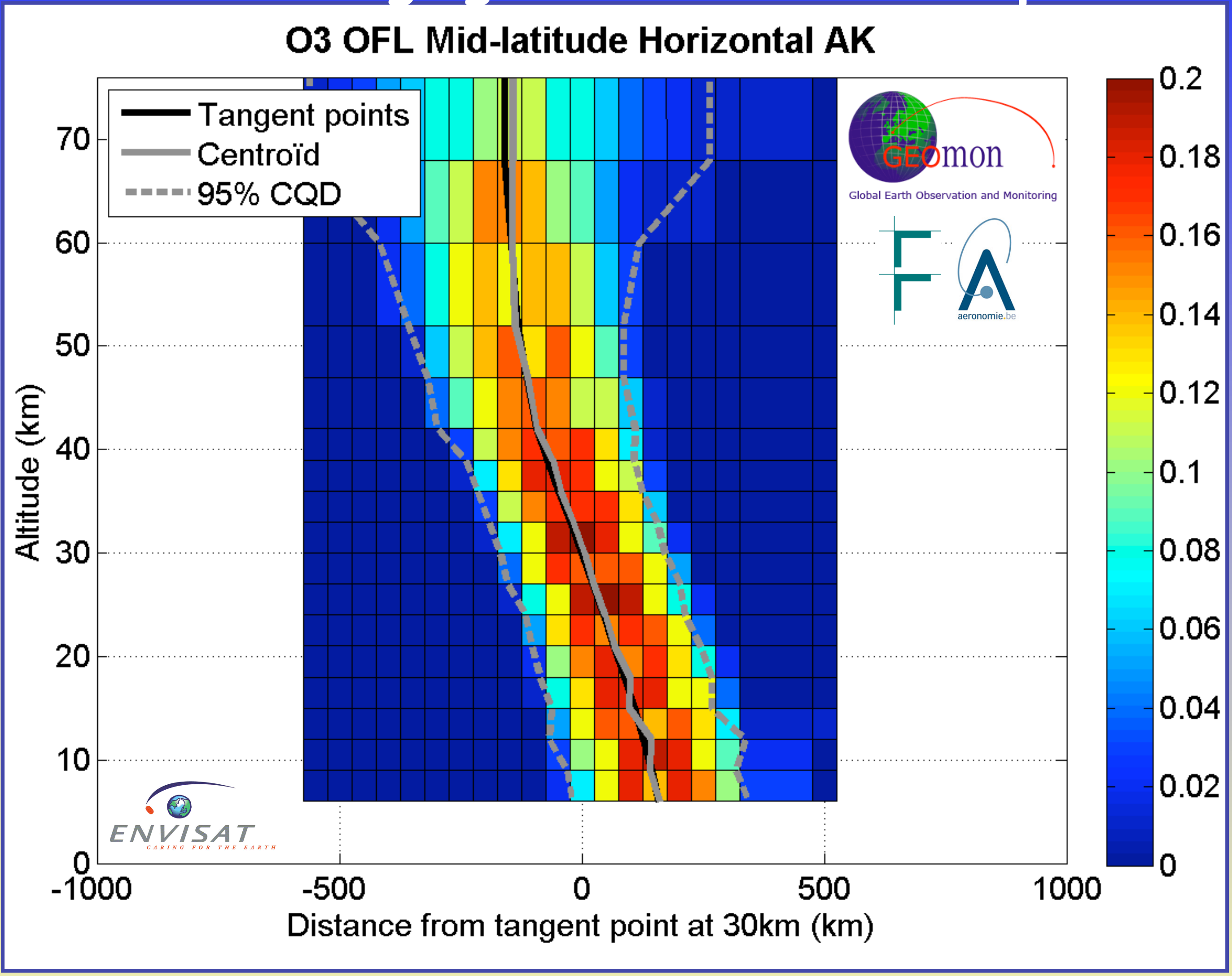
Horizontal smoothing by ground-based DOAS and by Brewer/Dobson



Evidence of effects in GOME validation studies (Lambert *et al.*, QO_3OS, 1996)

Horizontal smoothing by MIPAS: O_3

2-D horizontal Averaging Kernels for a 1D profile retrieval



von Clarmann et al, AMT, 2, 47-54, 2009

MIPAS processor settings ESA IPF 4.61/nominal mode

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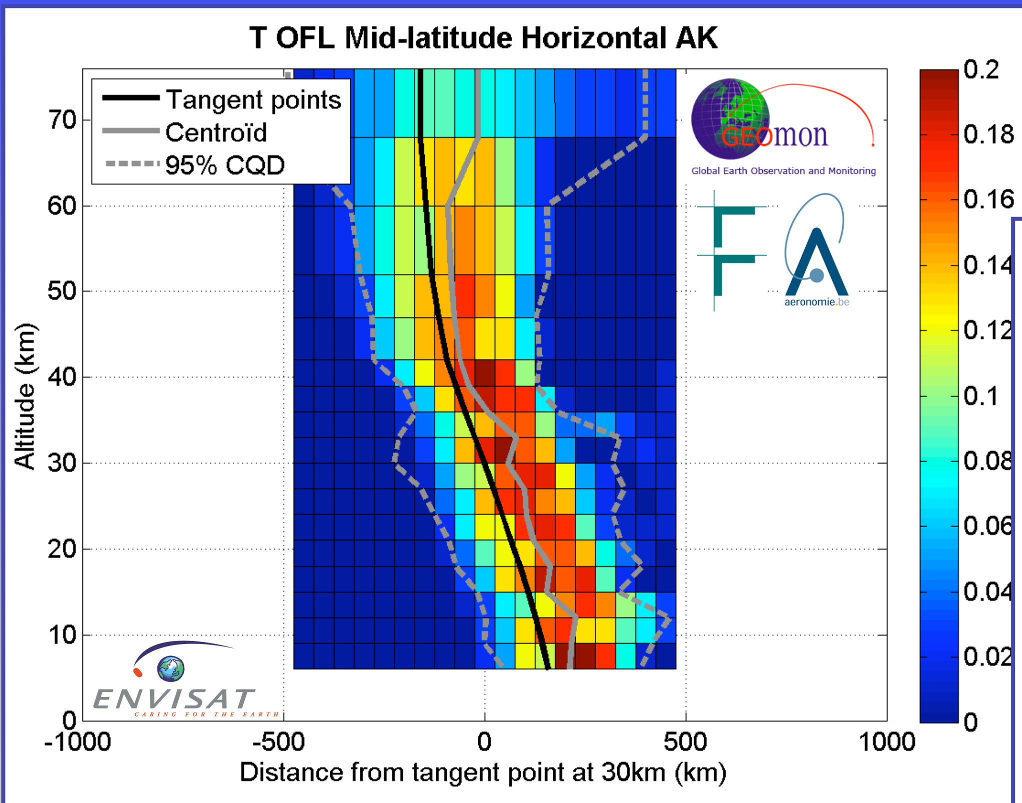
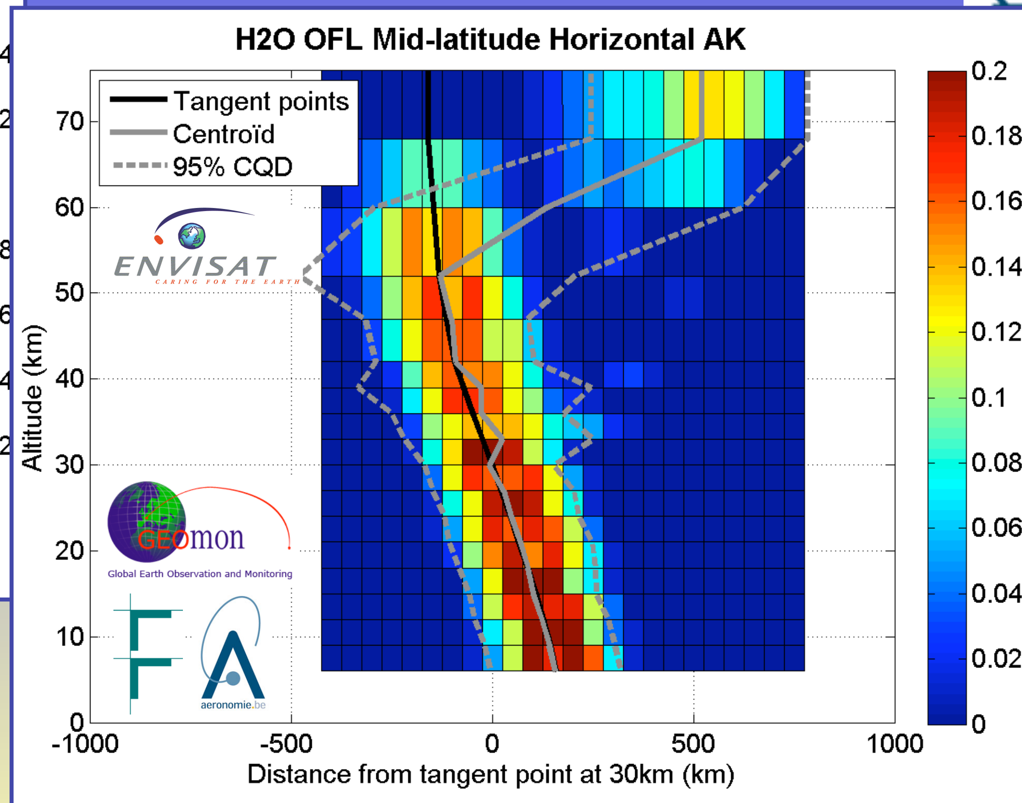
Horizontal smoothing by MIPAS: T and H_2O

2-D horizontal Averaging Kernels for a 1D profile retrieval

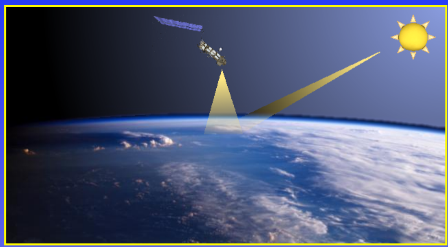


MIPAS processor settings ESA IPF 4.61/nominal mode

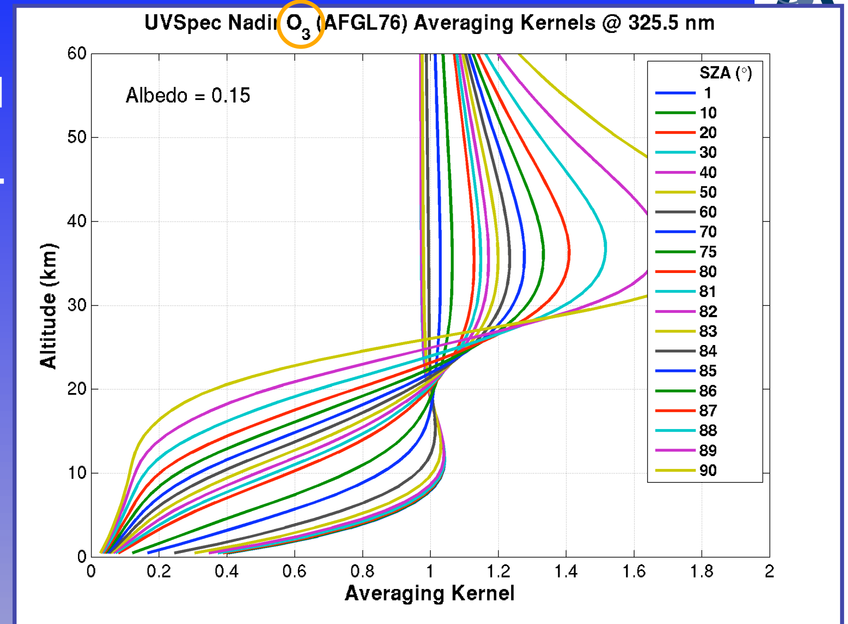


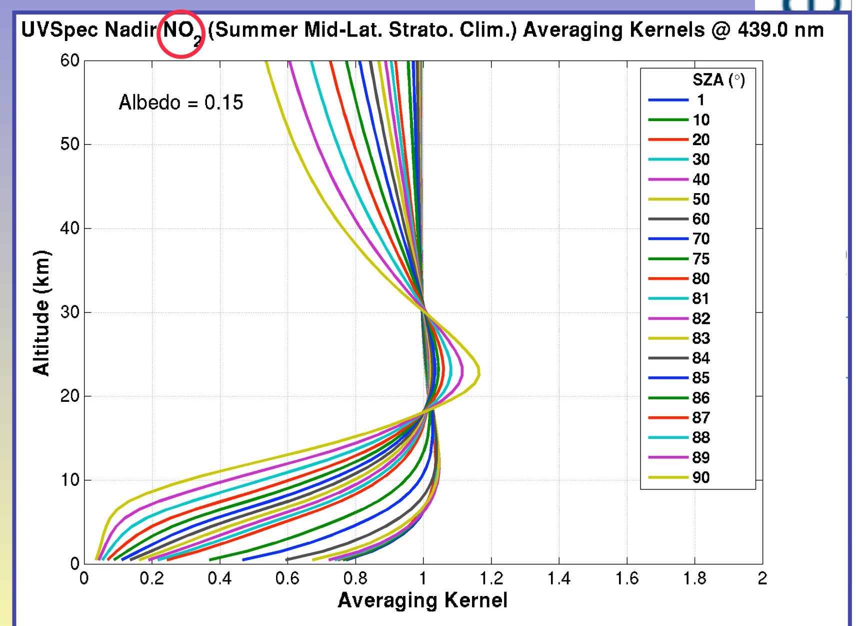
von Clarmann et al, AMT, 2, 47-54, 2009

1D vertical averaging kernels for GOME

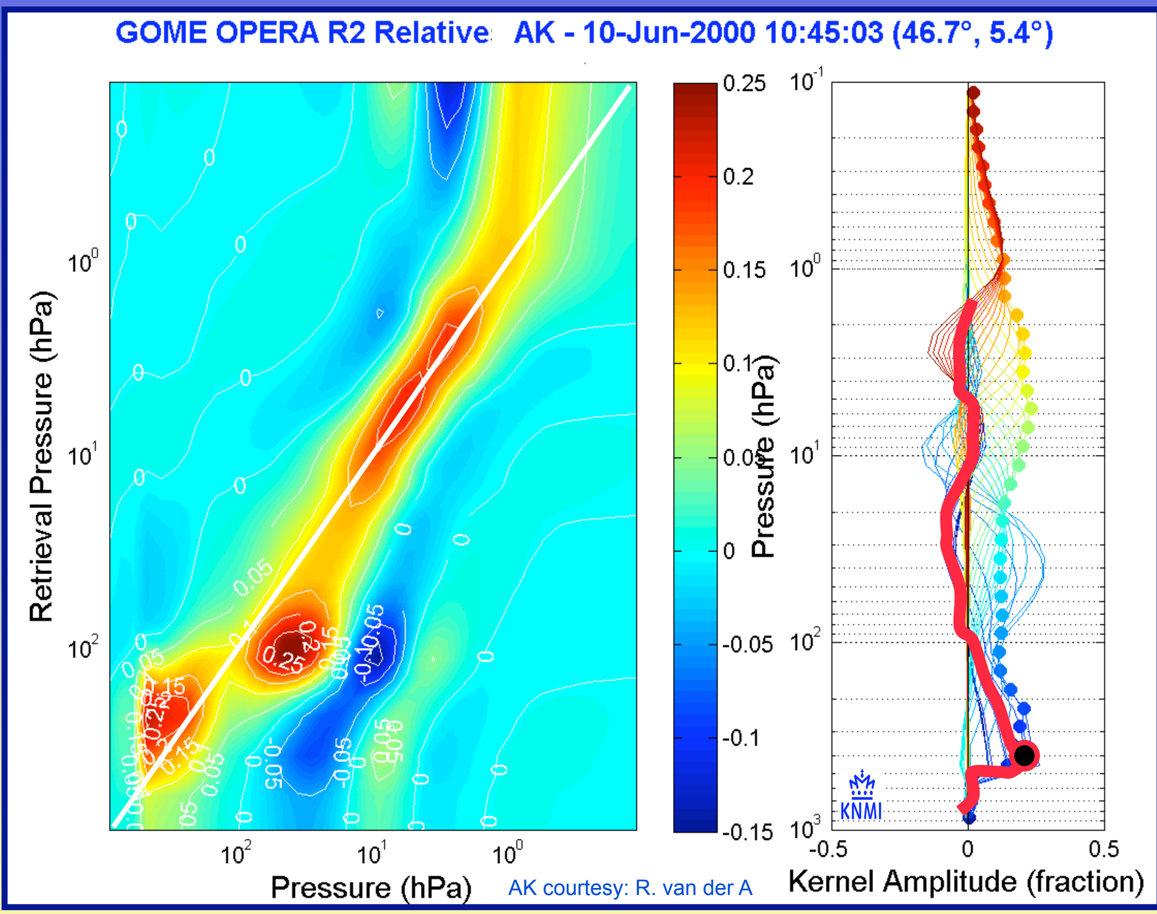


O_3 and NO_2 COLUMN RETRIEVAL



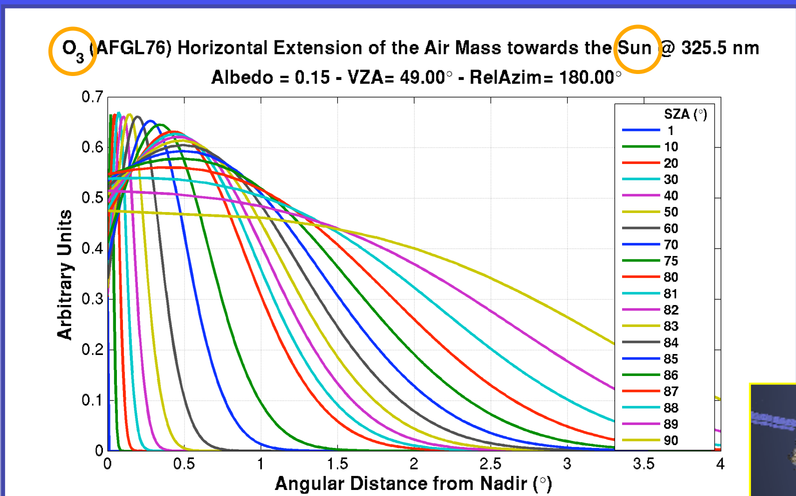


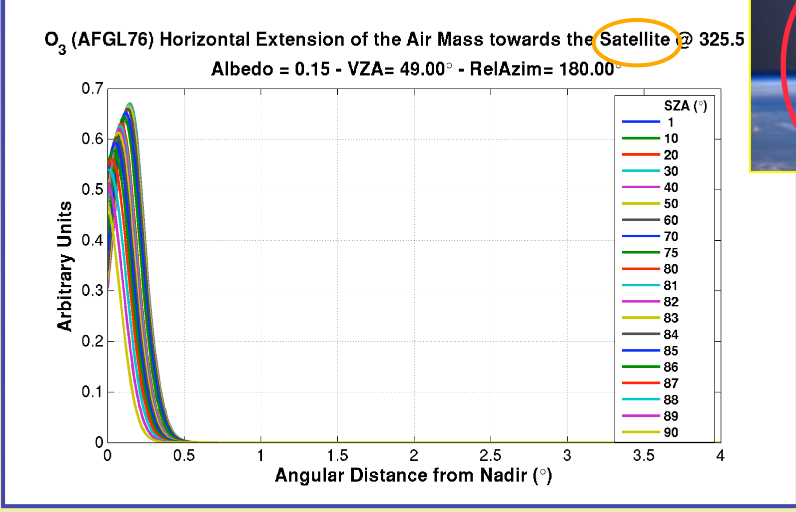
OZONE PROFILE RETRIEVAL

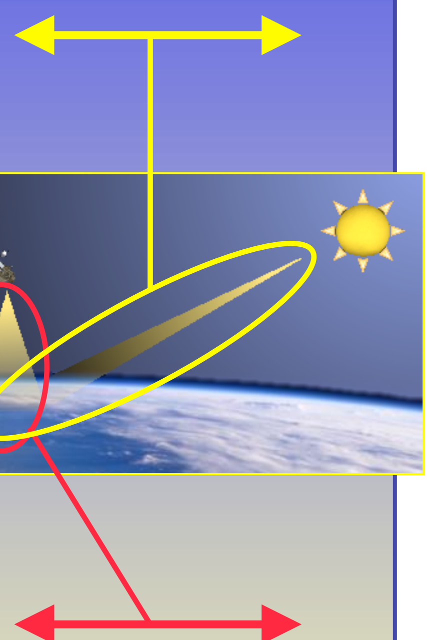


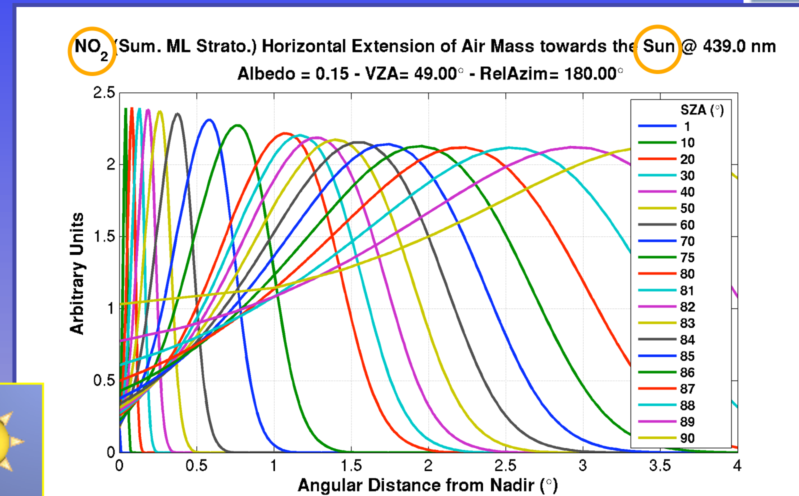
Horizontal smoothing by GOME-2

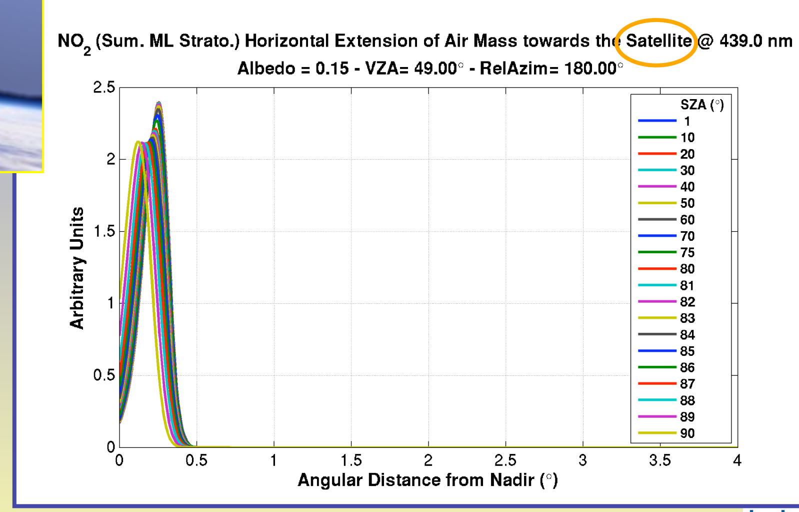
Horizontal dilution between Sun, scatterer and satellite











Vandenbussche et al., GEOmon, 2011

Example: GOME-2 observation operators for O_3 and (stratospheric) NO_2 columns

Dilution between Sun and scatterer

$$dil90_{Sun}(O_3) = 4.10^{-3} * SZA + 2.10^{-14} * \exp(0.35 * SZA) + 16.10^{-3} * \exp(6.10^{-4} * SZA^2)$$

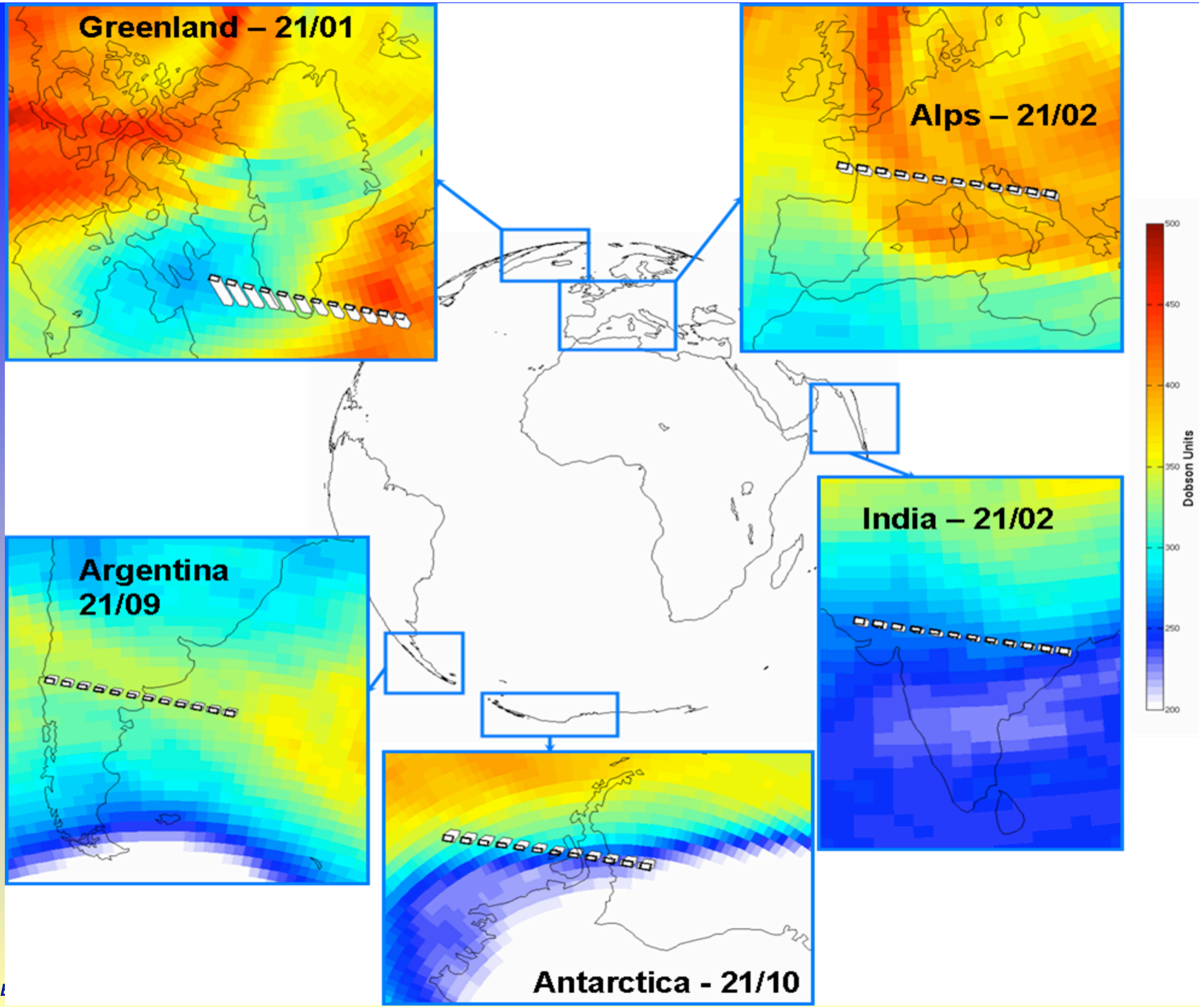
$$dil90_{Sun}(NO_2) = 43.10^{-4} * SZA + 312.10^{-10} * \exp(0.2 * SZA) + 33.10^{-3} * \exp(5.10^{-4} * SZA^2)$$

Dilution between scatterer and satellite

$$dil90_{satellite}(O_3) = 0.0051 * VZA$$

$$dil90_{satellite}(NO_2) = 0.0056 * VZA$$

Smoothing by GOME-2: O_3 column

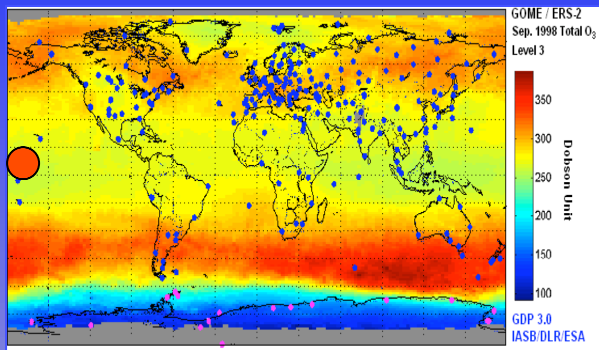


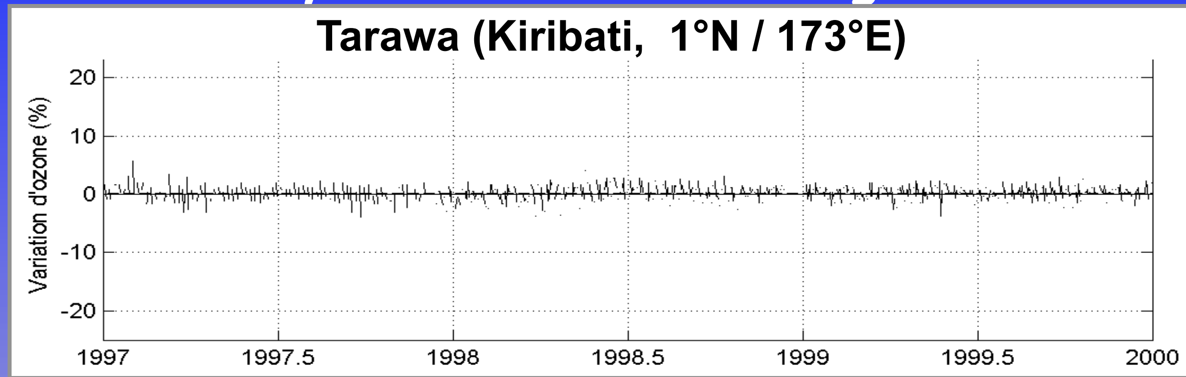
Illustrations (1)

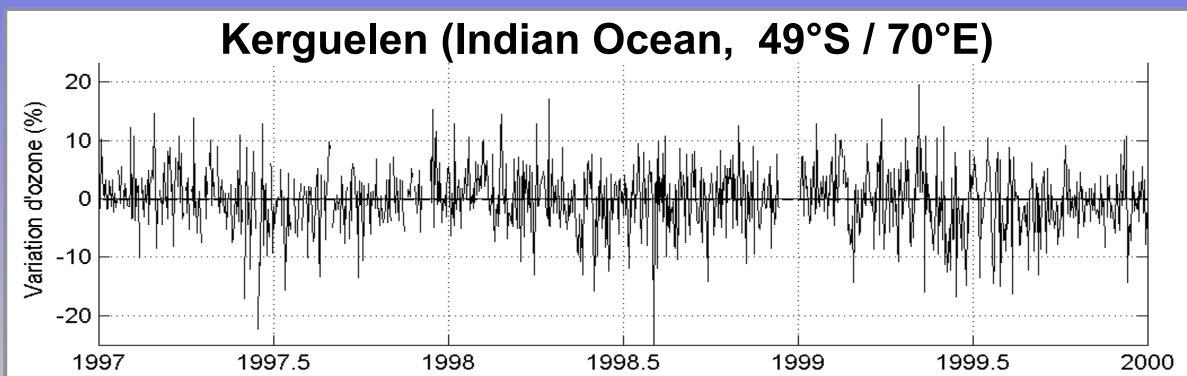
Smoothing error assessments

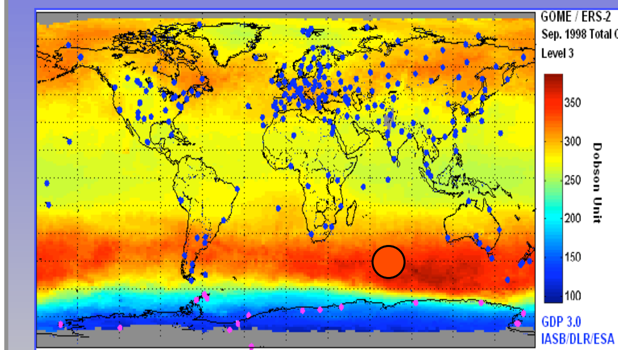
Smoothing error for O_3 column measurements –

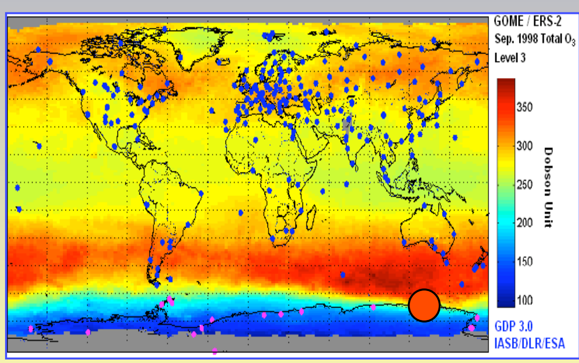
Ground-based zenith-sky observation at twilight

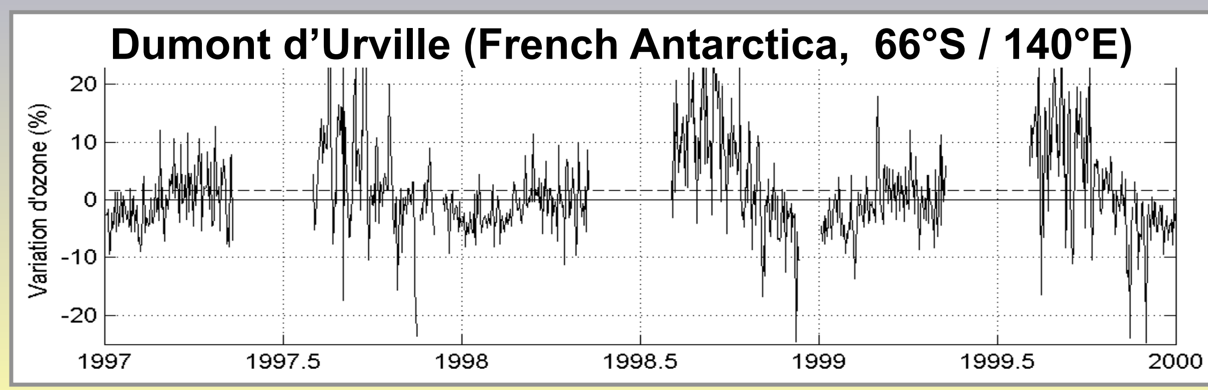






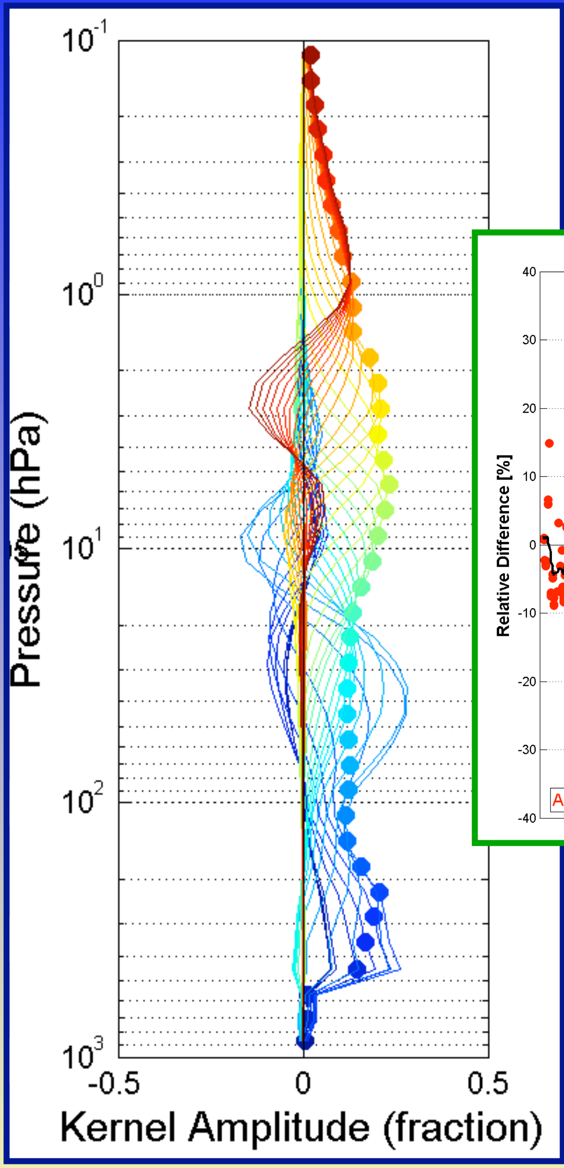


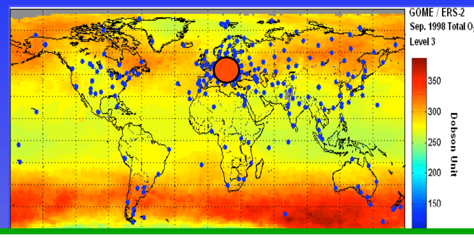


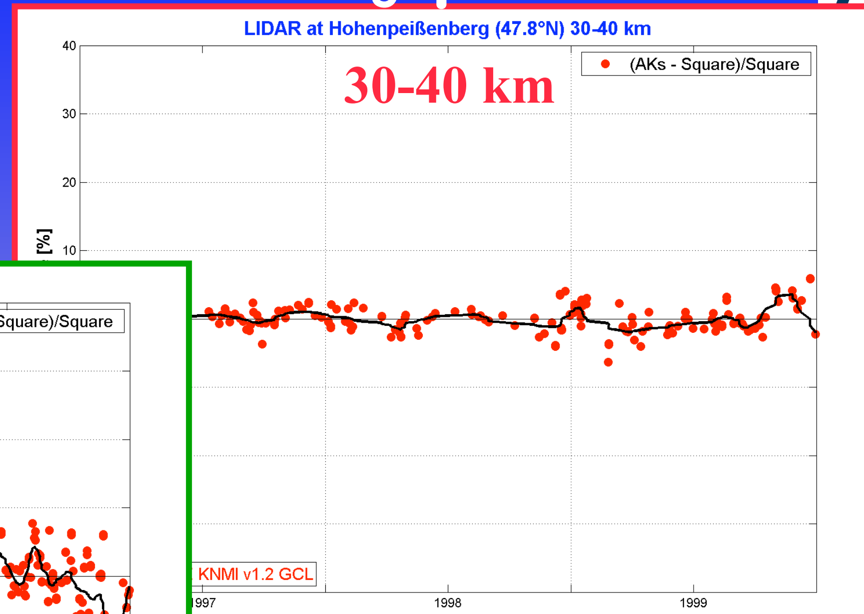


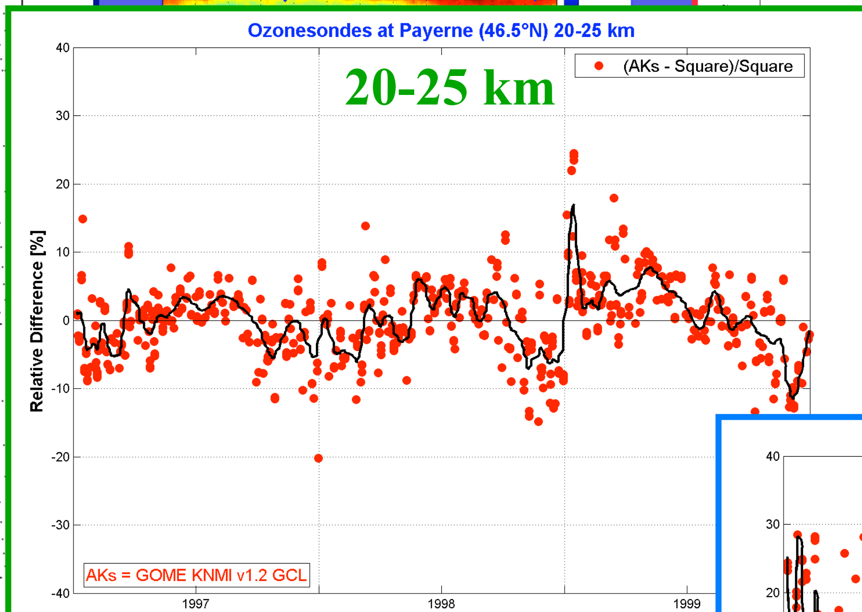
Lambert, ULB, 2006

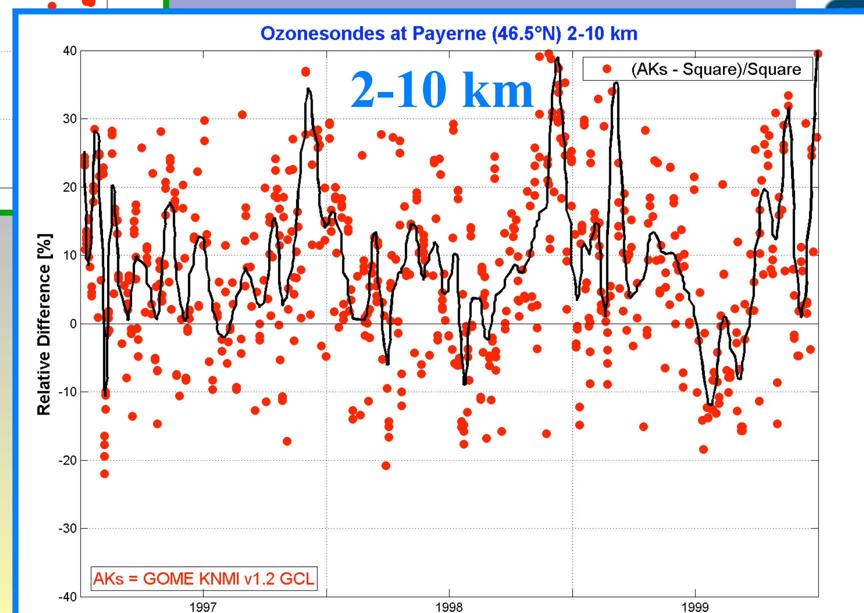
Vertical smoothing error for GOME O_3 profiles







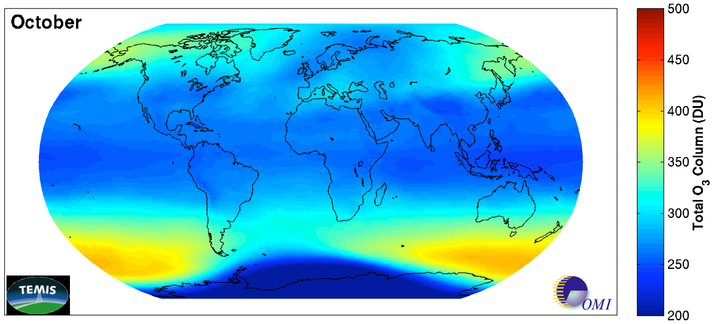


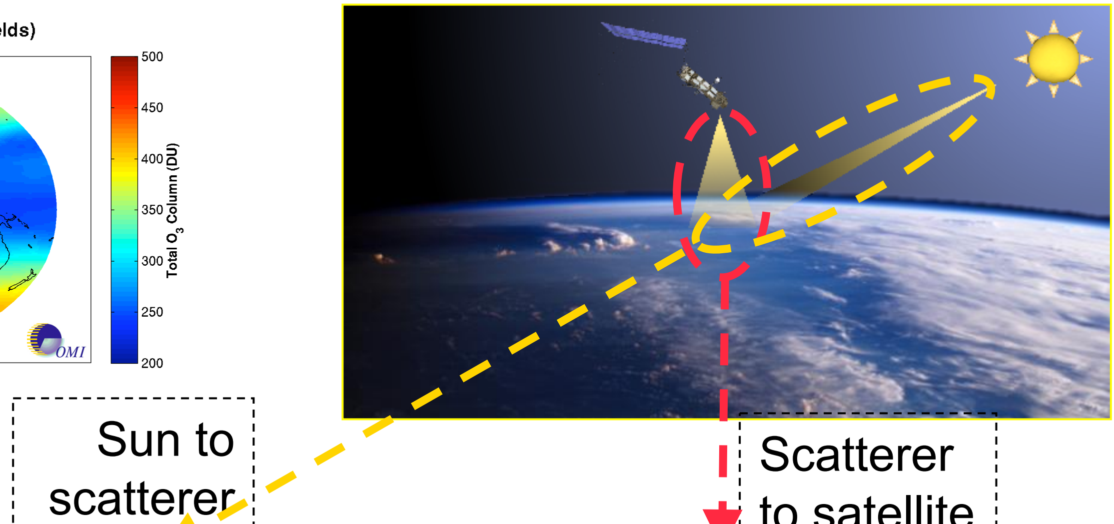


Lambert et al., 2004; De Clercq et al., 2006

Horizontal smoothing errors by GOME-2

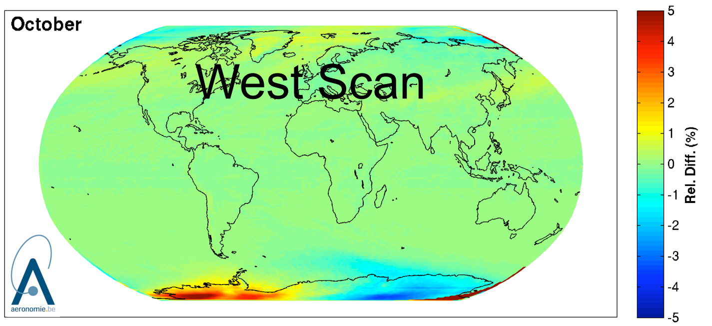
Average Total O_3 Column (TEMIS OMI assimilated fields)



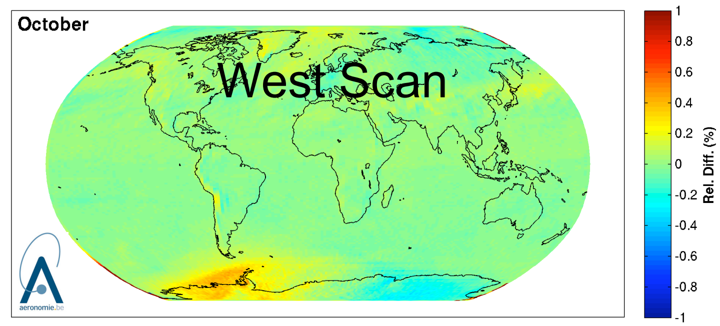


Vandenbussche et al., 2011

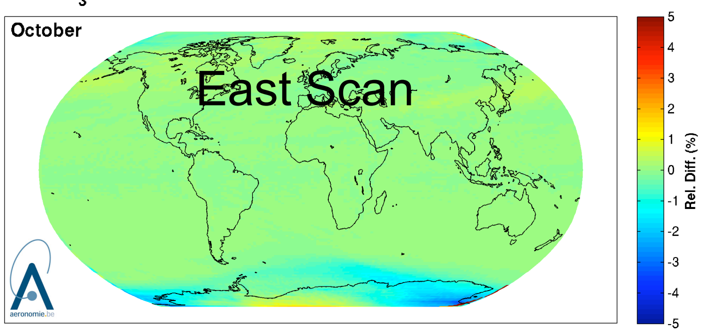
Rel. Diff. btw Total O_3 Column in a GOME-2 Technical Pixel and Pixel Diluted towards the Sun



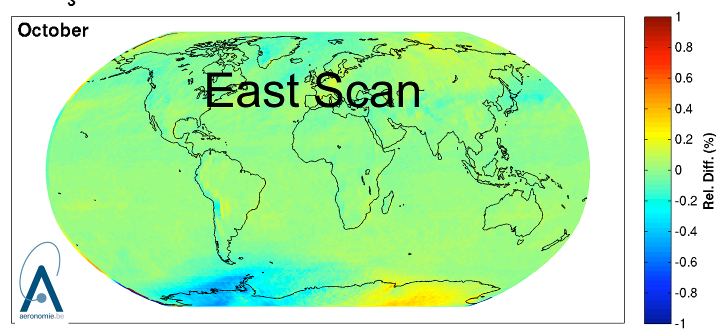
Rel. Diff. btw Total O_3 Column in a GOME-2 Technical Pixel and Pixel Diluted towards the Satellite



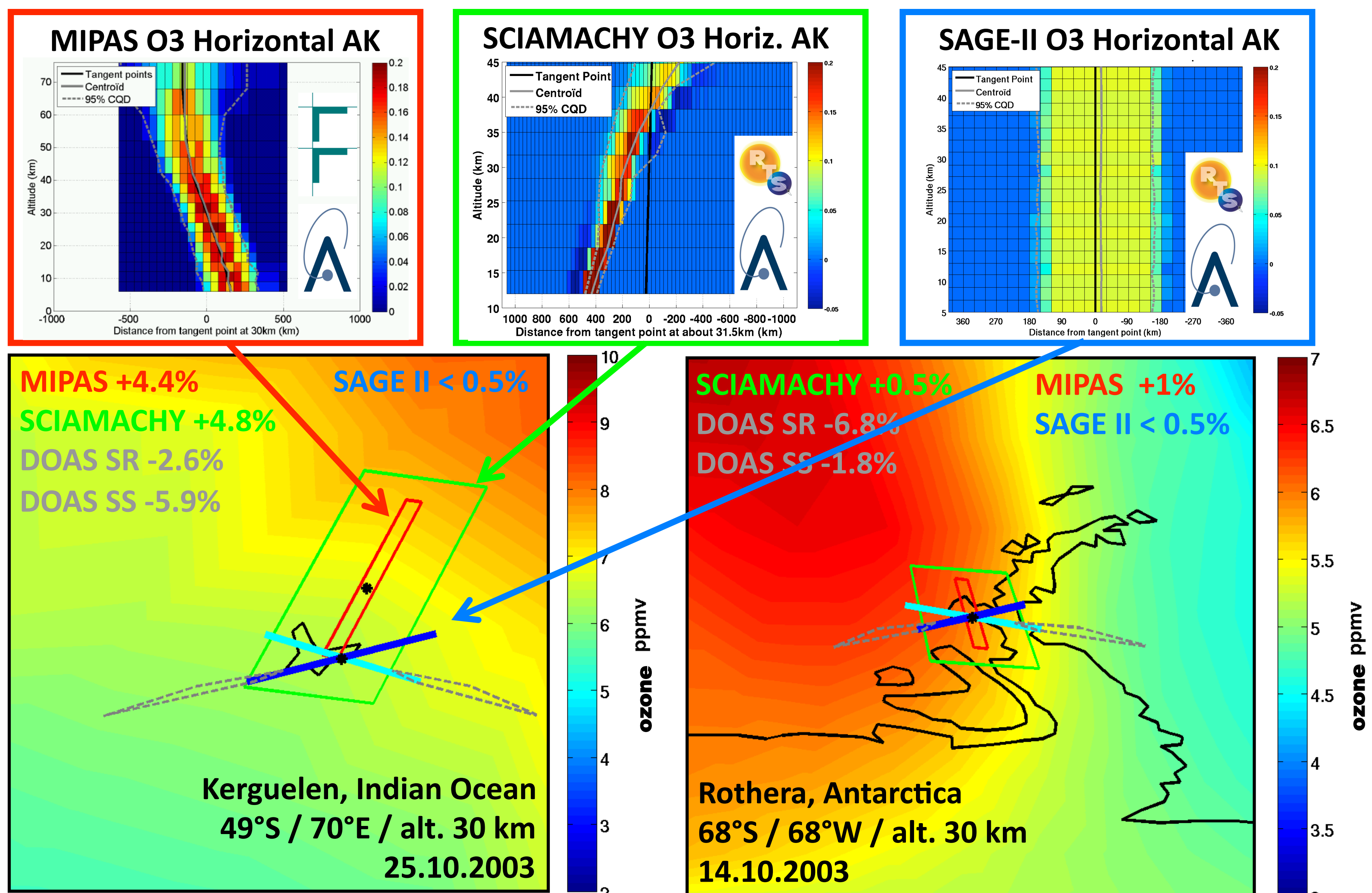
Rel. Diff. btw Total O_3 Column in a GOME-2 Technical Pixel and Pixel Diluted towards the Sun



Rel. Diff. btw Total O_3 Column in a GOME-2 Technical Pixel and Pixel Diluted towards the Satellite



O_3P horizontal smoothing error estimates
for MIPAS, SCIAMACHY, SAGE-II, GB-DOAS



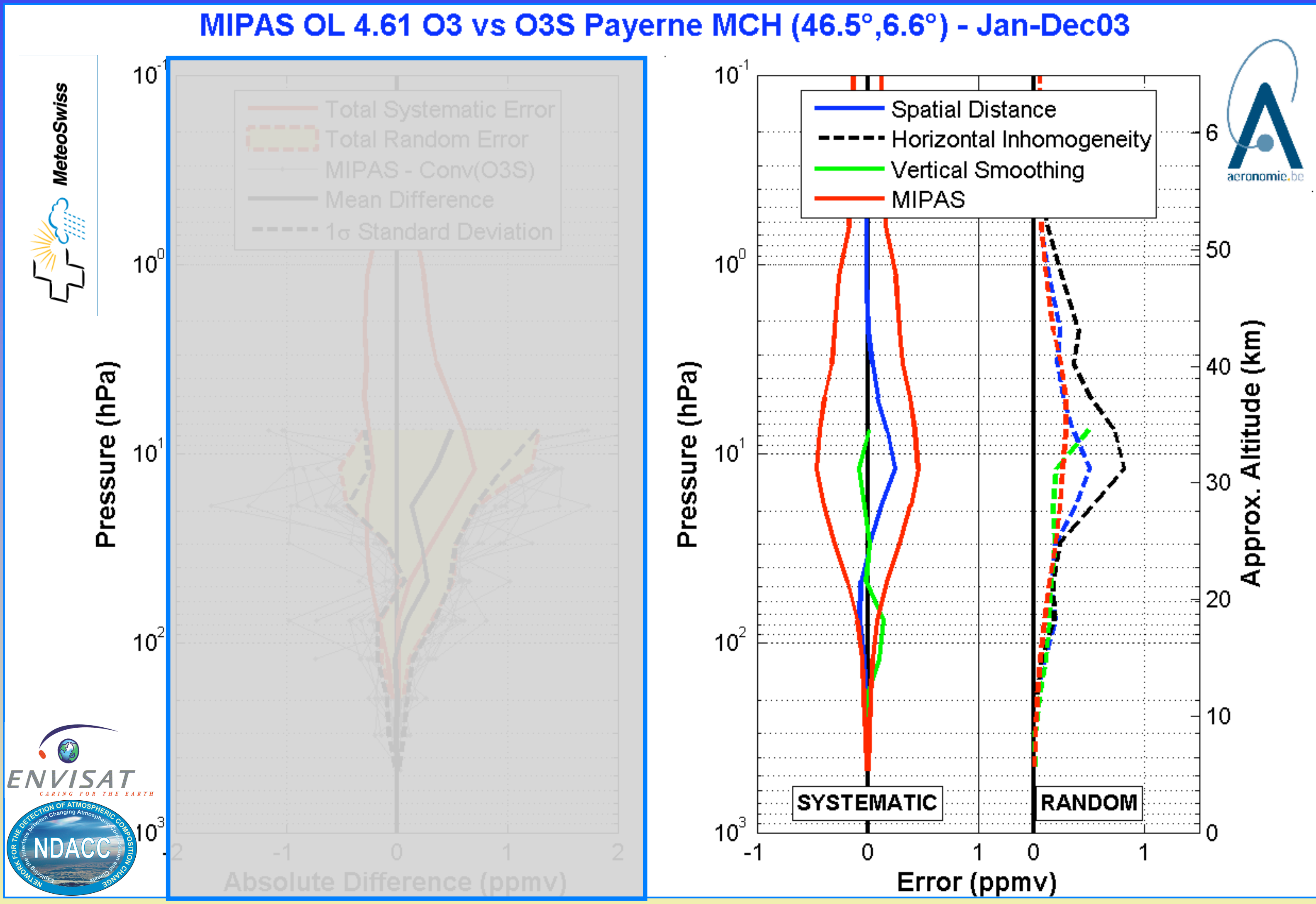
S. Vandenbussche et al., GEOmon, 2011

Illustrations (2)

Interpretation of comparisons

Error budget of a data comparison

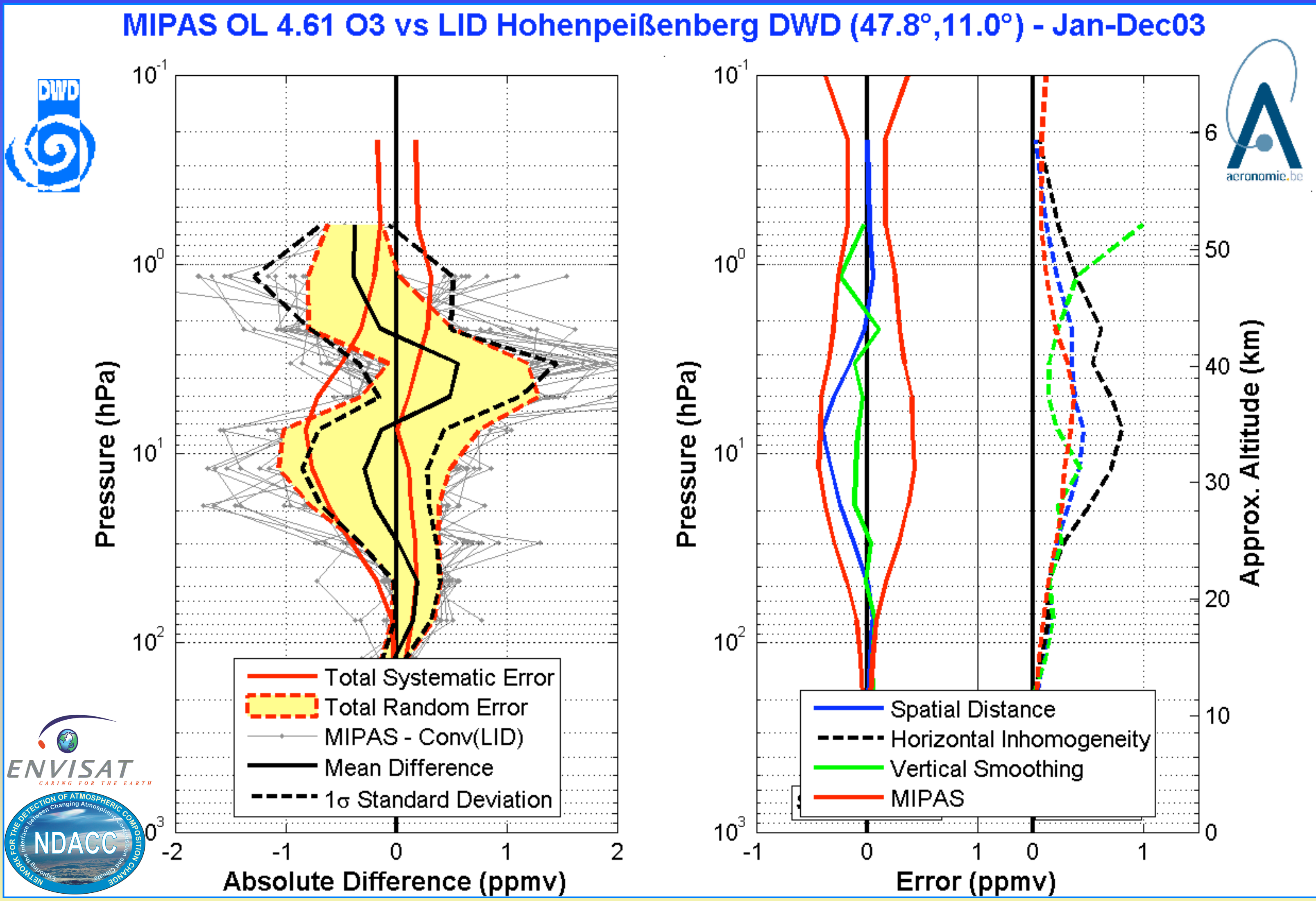
Error budget of MIPAS validation vs. ozonesondes



Method described in Section 4.1 of Cortesi *et al.*, ACP 2007

Error budget of a data comparison

Error budget of MIPAS validation vs. lidar



Method described in Section 4.1 of Cortesi *et al.*, ACP 2007

Illustrations (3)

Optimised co-location criteria for better comparisons, tracer-tracer correlations etc.

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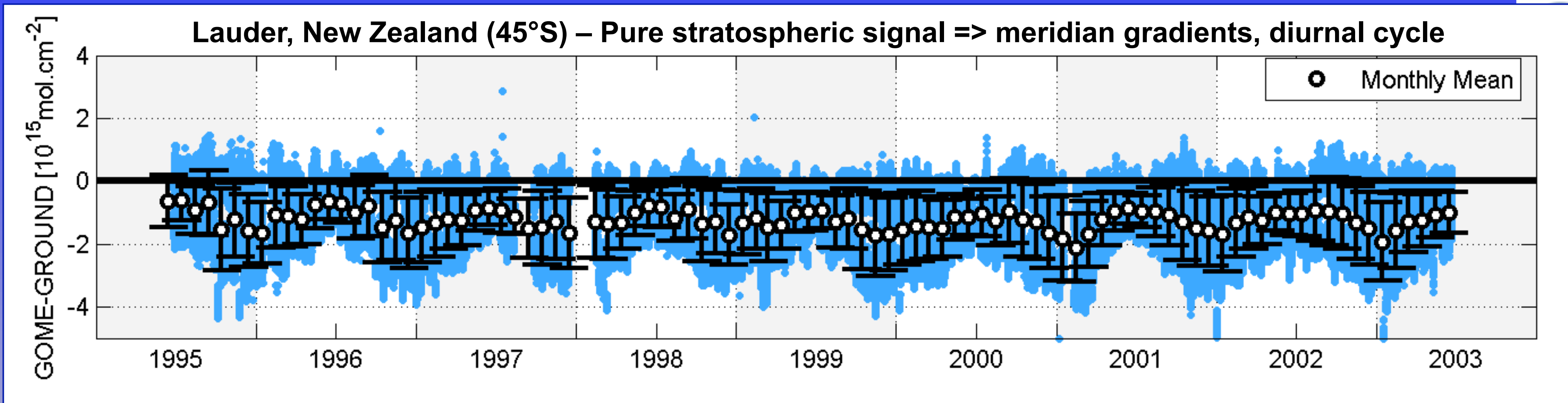
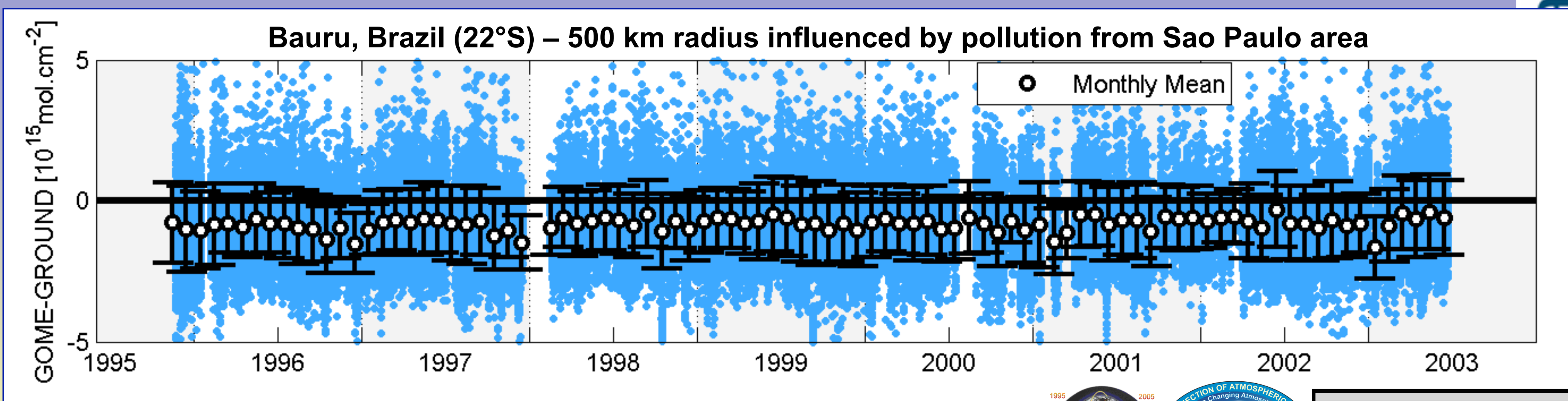
Co-location for satellite NO_2 validation

Selection within 500km radius: pollution, meridian gradients, diurnal cycle…

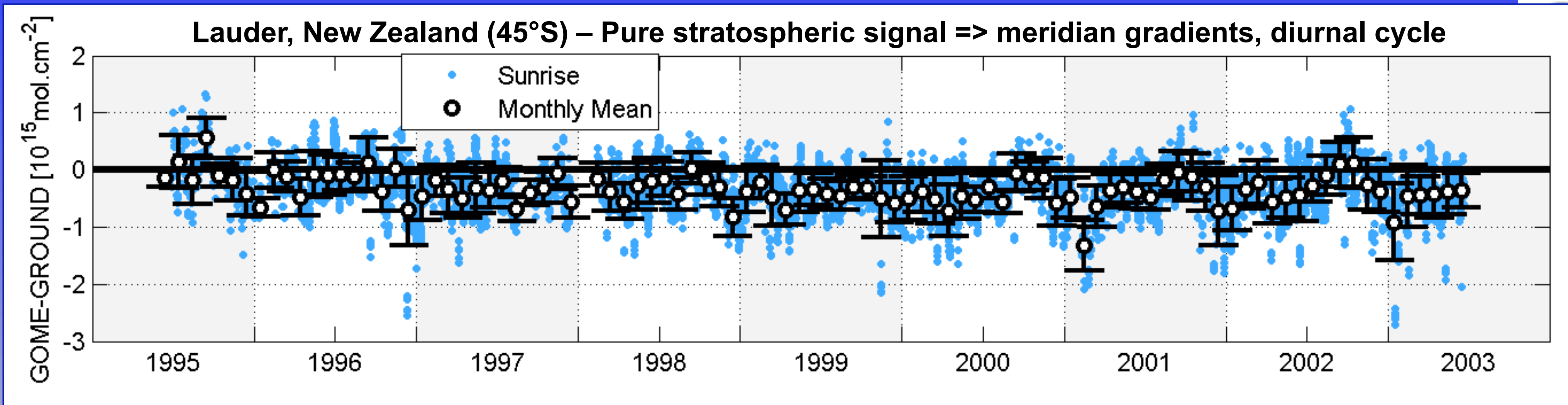


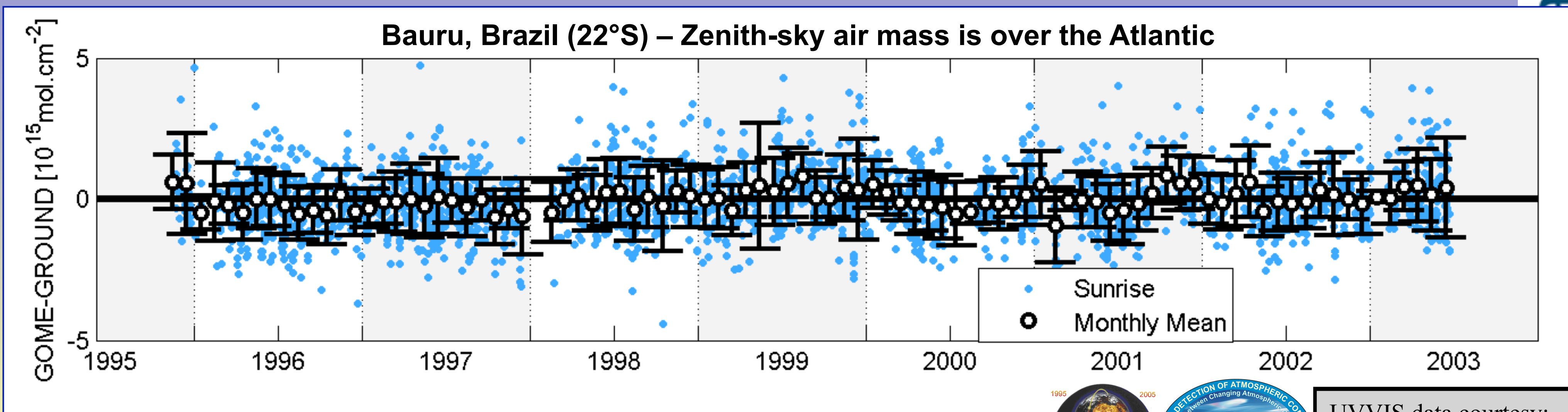


UVVIS data courtesy:
CNRS / UNESP (Bauru)
and NIWA (Lauder)

Co-location for satellite NO_2 validation

Selection based on observation operators





UVVIS data courtesy:
CNRS / UNESP (Bauru)
and NIWA (Lauder)

Tracer-tracer correlations and hydrogen budget

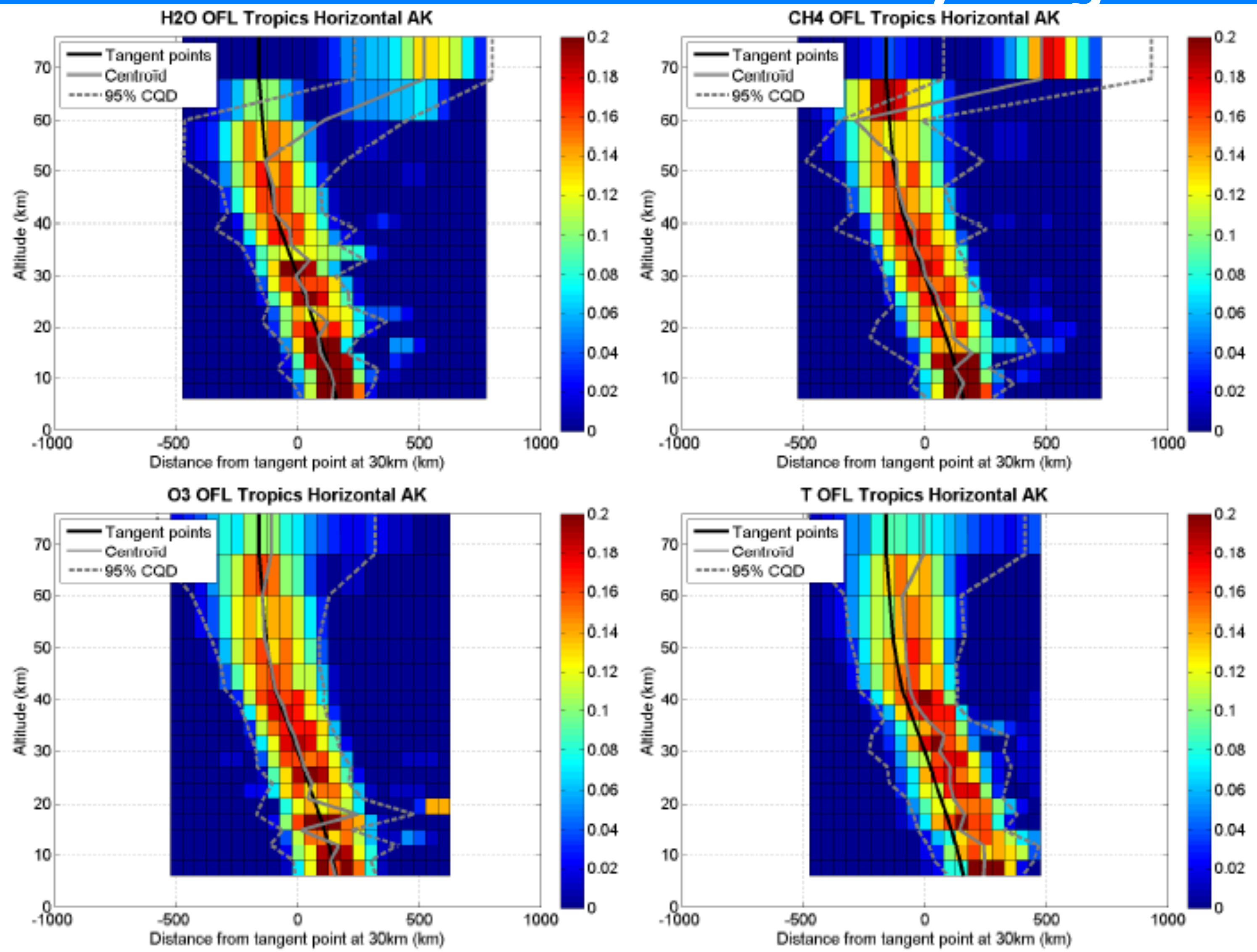


Figure 9.6: Horizontal averaging kernels for the MIPAS off-line retrieval of water vapour, methane, ozone and temperature vertical profiles, calculated for a tropical standard atmosphere. The colour scale

Lambert et al., ISSI, 2011 (with figures adapted from von Clarmann et al., AMT 2009)

Conclusion

- Bias and noise introduced by neglecting smoothing and sampling errors can spoil the value of a data comparison.
- The problem is a combined effect of measurement properties (measurement + retrieval) and of atmospheric properties.
- The problem is multi-dimensional.
- Observation operators have been/are being published for major remote sensing techniques and a few key molecules. Feedback from the DA community is welcome !
- Consideration of smoothing/sampling issues has demonstrated value for:
  - Optimising co-location criteria
  - Assessing smoothing errors of an individual observation system
  - Assessing discrepancies due to differences in smoothing and sampling
- More accurate error assessments need modelled/assimilated fields at ~1° horizontal resolution.
- Information content aspects of merged data sets might be an issue.

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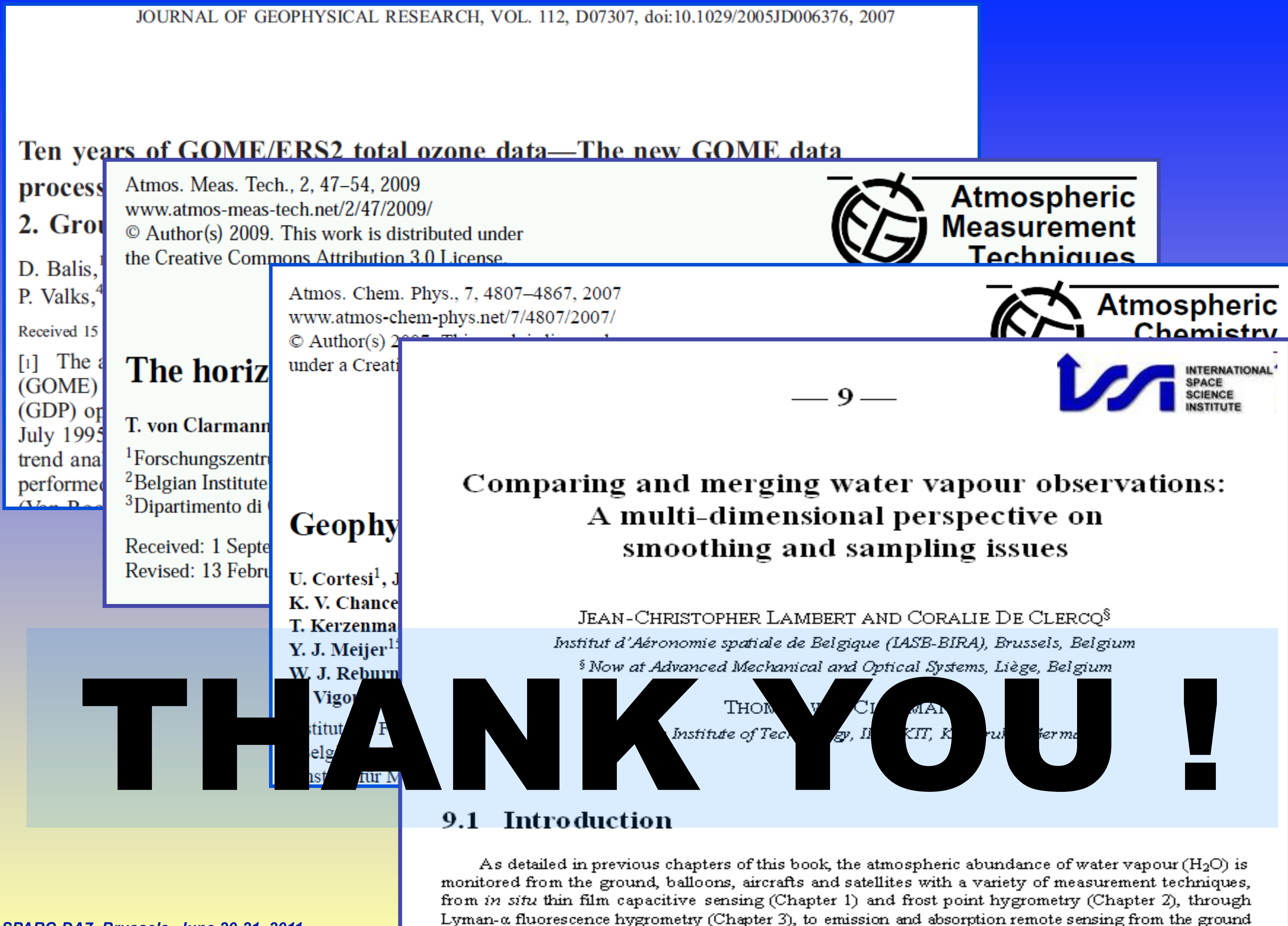
JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 112, D07307, doi:10.1029/2005JD006376, 2007

Ten years of GOME/ERS2 total ozone data—The new GOME data process
2. Grou

D. Balis,[1]
P. Valks,[4]

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Atmos. Meas. Tech., 2, 47–54, 2009
www.atmos-meas-tech.net/2/47/2009/
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Atmospheric Measurement Techniques

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Atmospheric Chemistry

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Vigo

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INTERNATIONAL SPACE SCIENCE INSTITUTE

Comparing and merging water vapour observations: A multi-dimensional perspective on smoothing and sampling issues

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THOM
Institute of Tec

9.1 Introduction

As detailed in previous chapters of this book, the atmospheric abundance of water vapour (H_2O) is monitored from the ground, balloons, aircrafts and satellites with a variety of measurement techniques, from *in situ* thin film capacitive sensing (Chapter 1) and frost point hygrometry (Chapter 2), through Lyman-α fluorescence hygrometry (Chapter 3), to emission and absorption remote sensing from the ground

THANK YOU !

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