# Validation and Use of Satellite Atmospheric Composition Products

June 15, 2009

ACC Workshop, ESA,  Frascati Italy

L. Flynn, NOAA/NESDIS

with material borrowed

from numerous presentations

GSICS: Global Space-based Inter-Calibration System
ICVS: Inter-satellite Calibration and Validation System

- My first topic addresses efforts to create consistent measurements/products from the satellite instruments used to make atmospheric composition products. The next slides present some GSICS and ICVS results available from:

**http://www.star.nesdis.noaa.gov**

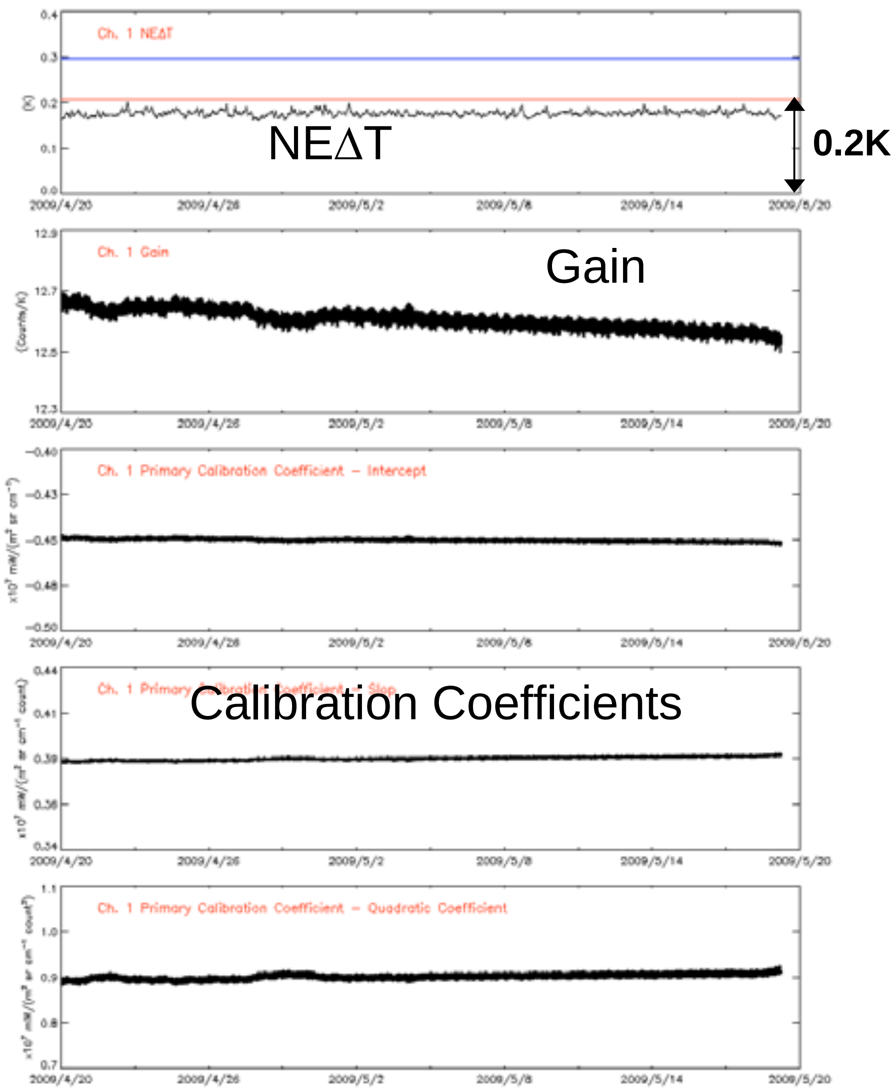
**/smcd/spb/calibration/icvs/GSICS/ and**

**/smcd/spb/icvs/**

- We have started discussions with the Level 1 and Level 2 product providers and validation researchers to use Simultaneous Nadir Overpass and In-Phase Orbits approaches to inter-compare BUV measurements and products. The initial target pair is EOS Aura OMI and MetOp-A GOME-2.

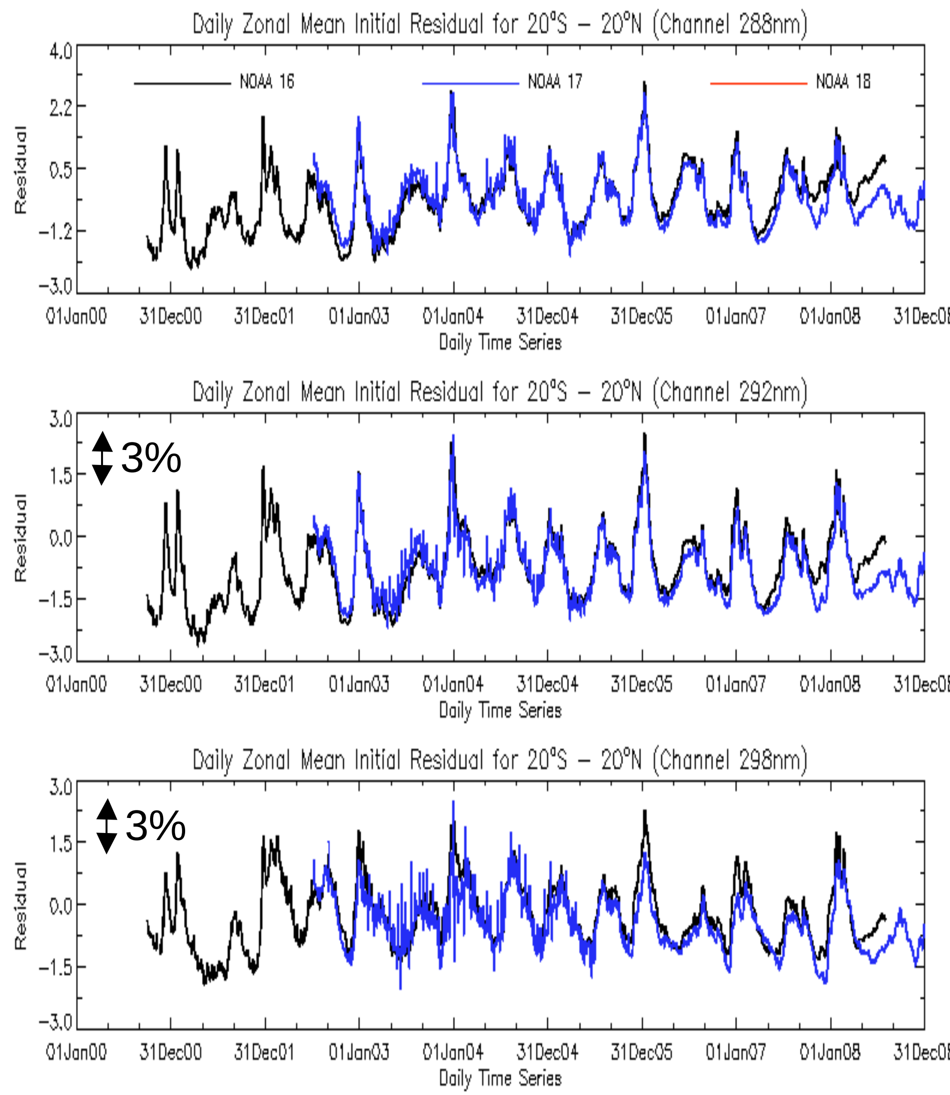
http://www.star.nesdis.noaa.gov/smcd/spb/icvs/index.php

Satellite Instrument Monitoring
NOAA-19 AMSU-A Channel 1




Time Since Launch

Satellite Product Monitoring
NOAA SBUV/2 Initial Residuals
Channels 4, 5, and 6

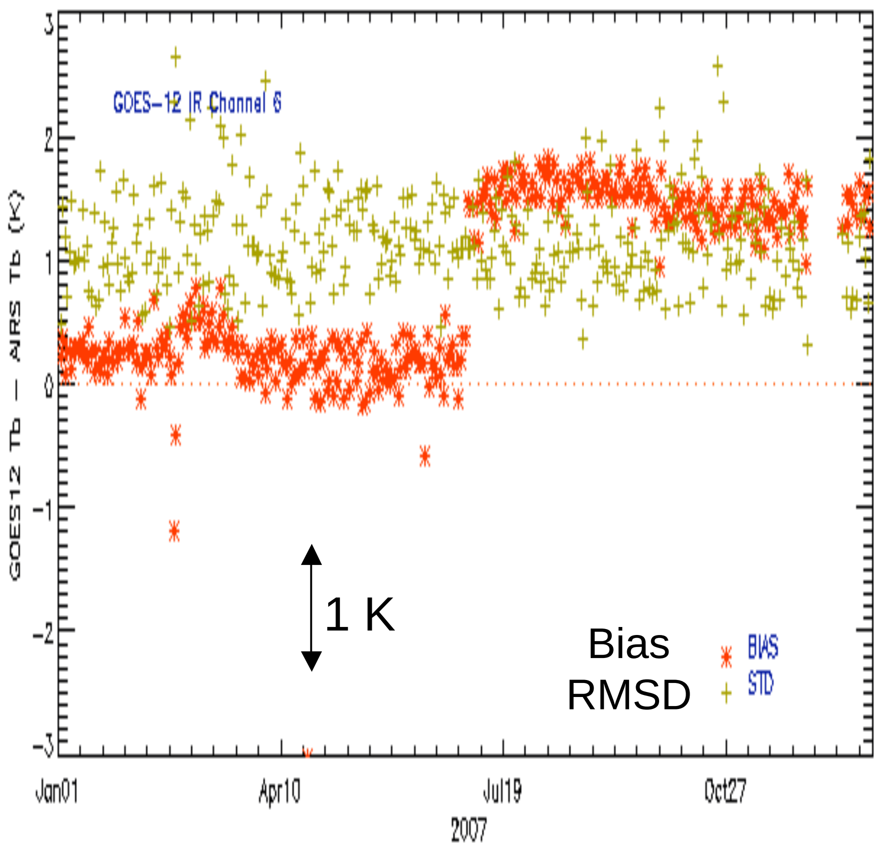



Last Seven Years

http://www.star.nesdis.noaa.gov
/smcd/spb/calibration/icvs/GSICS/products.php

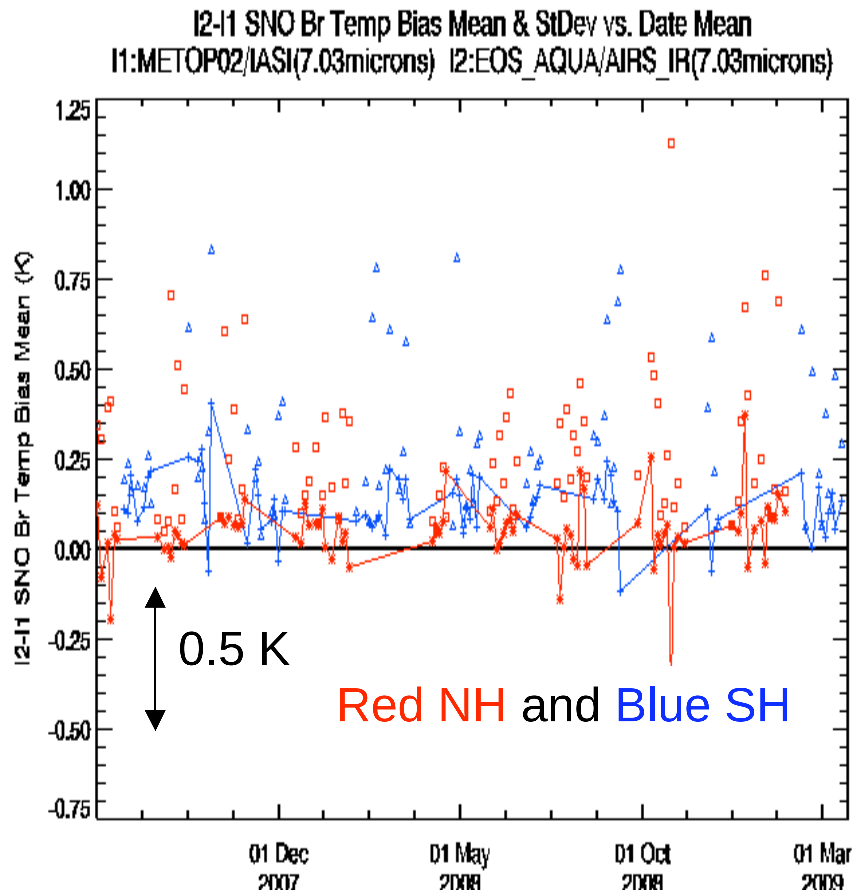
# Simultaneous Nadir Overpass (SNO) match up Comparisons

**GEO-LEO GOES-12 to Aqua AIRS Tb Comparison: Channel 6 (13.3 µm); 2007**




2007

**LEO-LEO IASI to Aqua AIRS Tb Comparison: 7.03 µm Bias and RMSD**

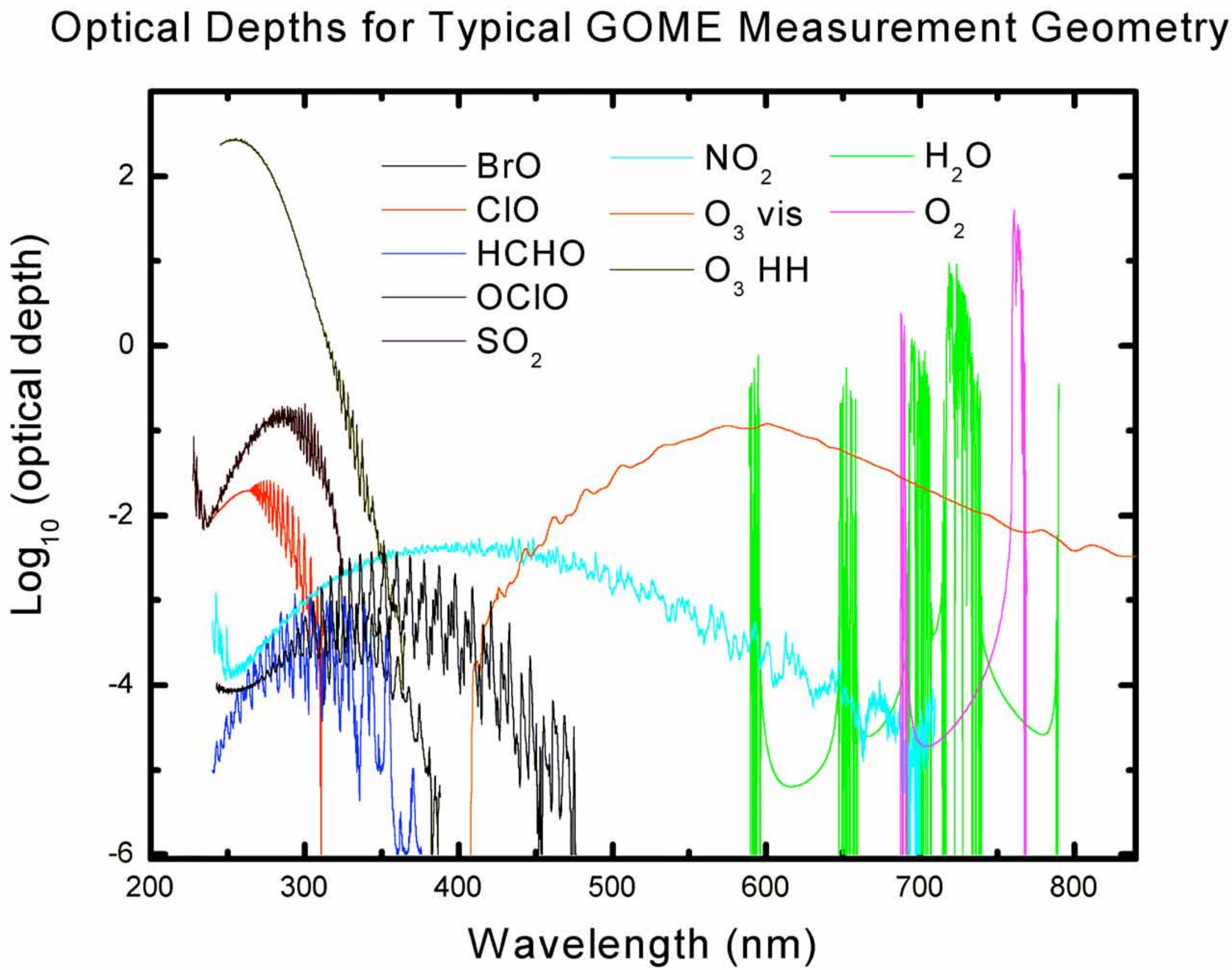



2007 to 2009

# Information in Satellite Trace Gas Retrievals

- DOAS Retrievals:
  - What information is in a DOAS trace gas column retrieval?
  - What should be provided with the column amount to make it more useful?
  - Trace gas “absorption darkness”
- Ozone Profile Retrievals – The problem of the *A Priori*:
  - What information is in an ozone profile retrieval?
  - How should this information be assimilated?

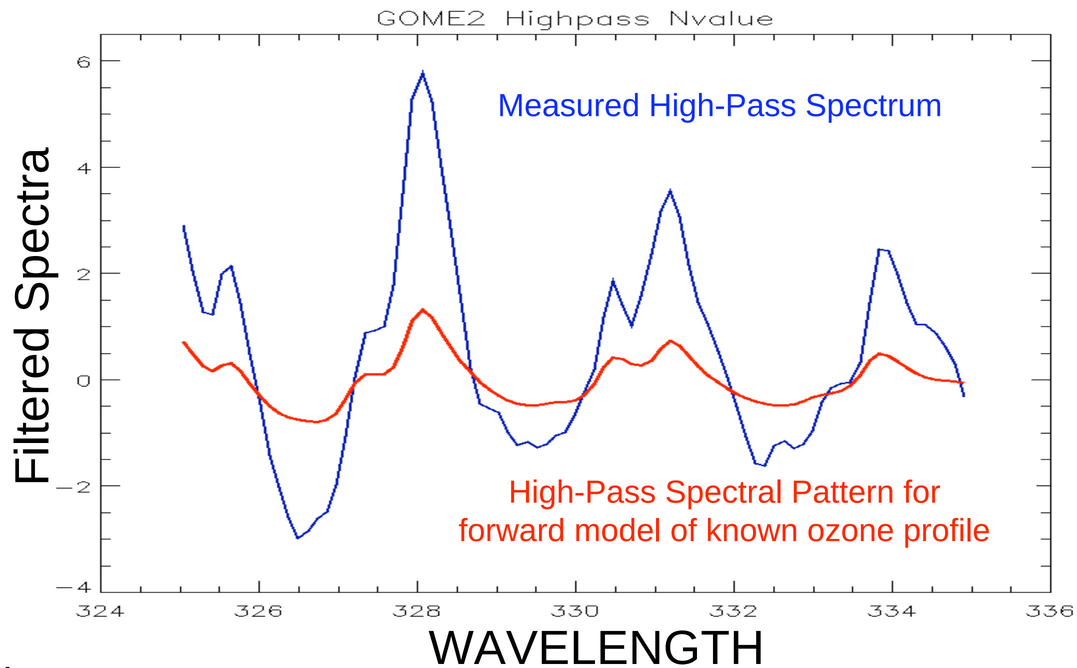
# Which Absorbers are Optically Thin?




From a presentation by *Kelly Chance, et al. -- Harvard-Smithsonian Center for Astrophysics*

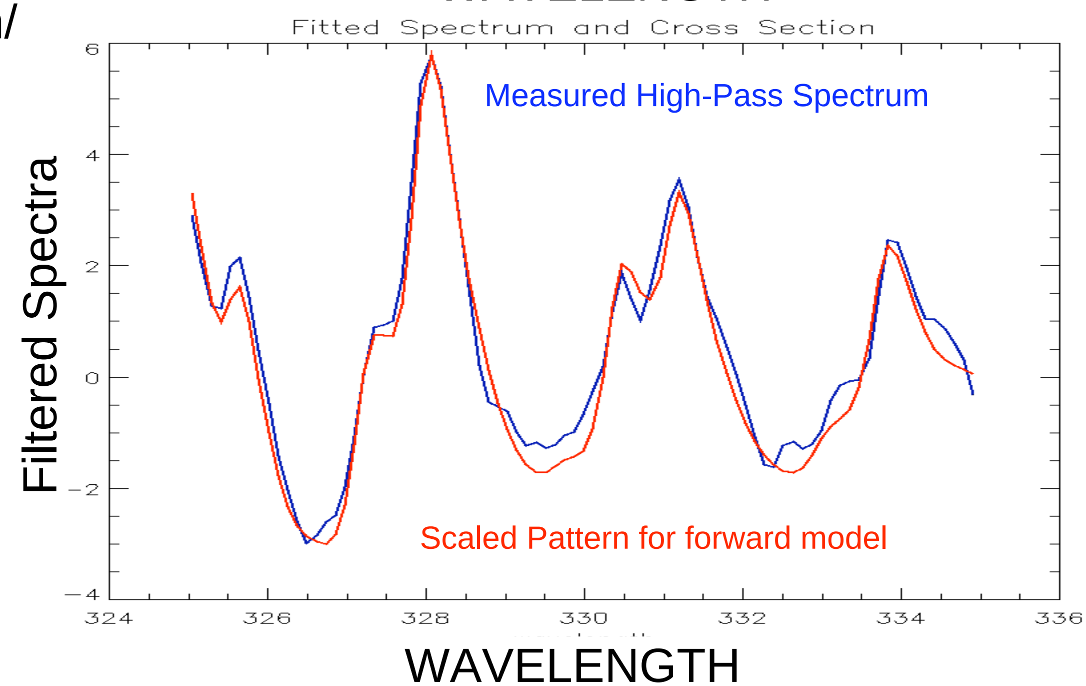
# Example of Spectral Fitting

**Before fitting**
**Pattern for known Ozone amount**

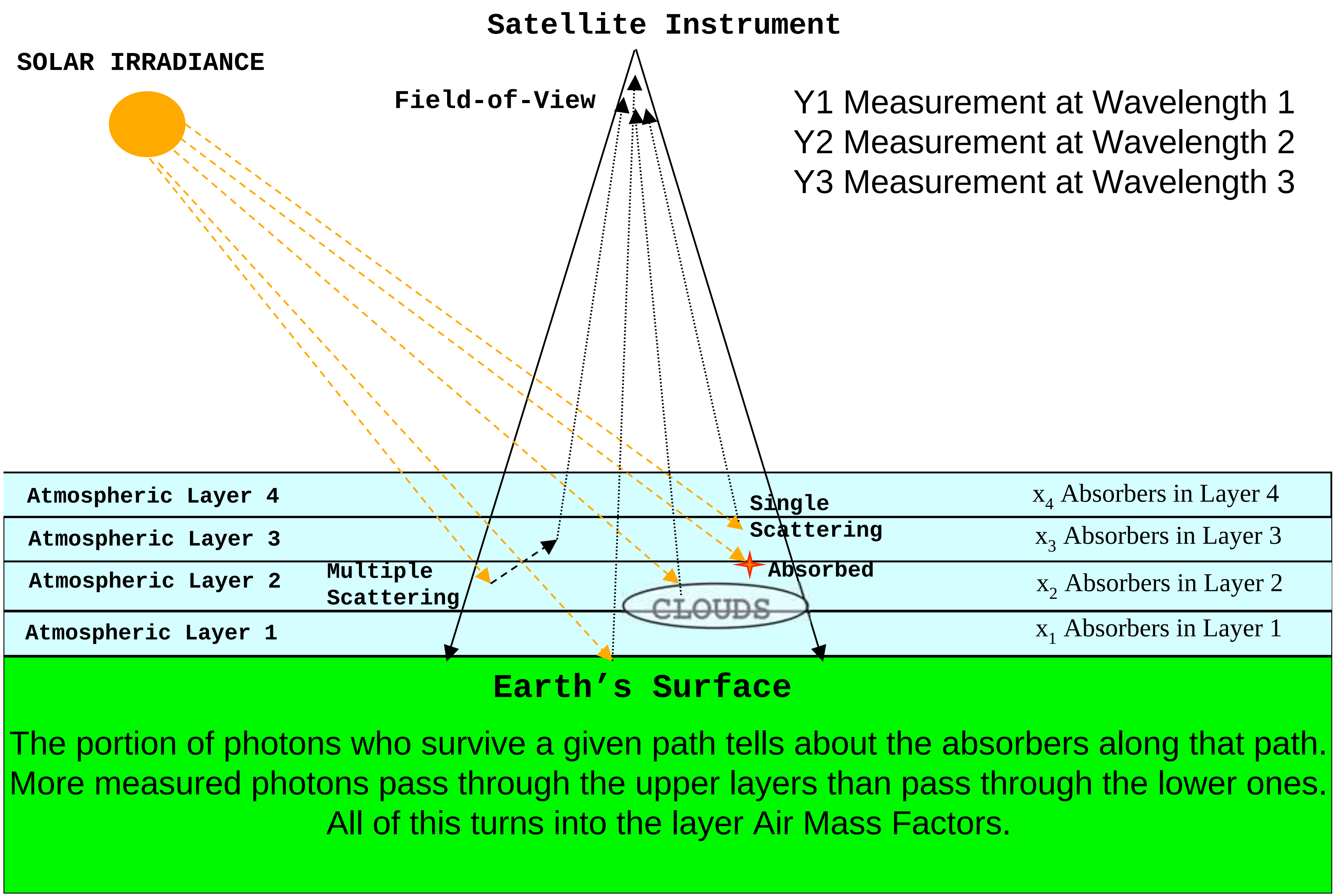



Assumes optically thin absorber and scaled profile shape.
Additional work for table interpolation/ look-up or profile shape changes.

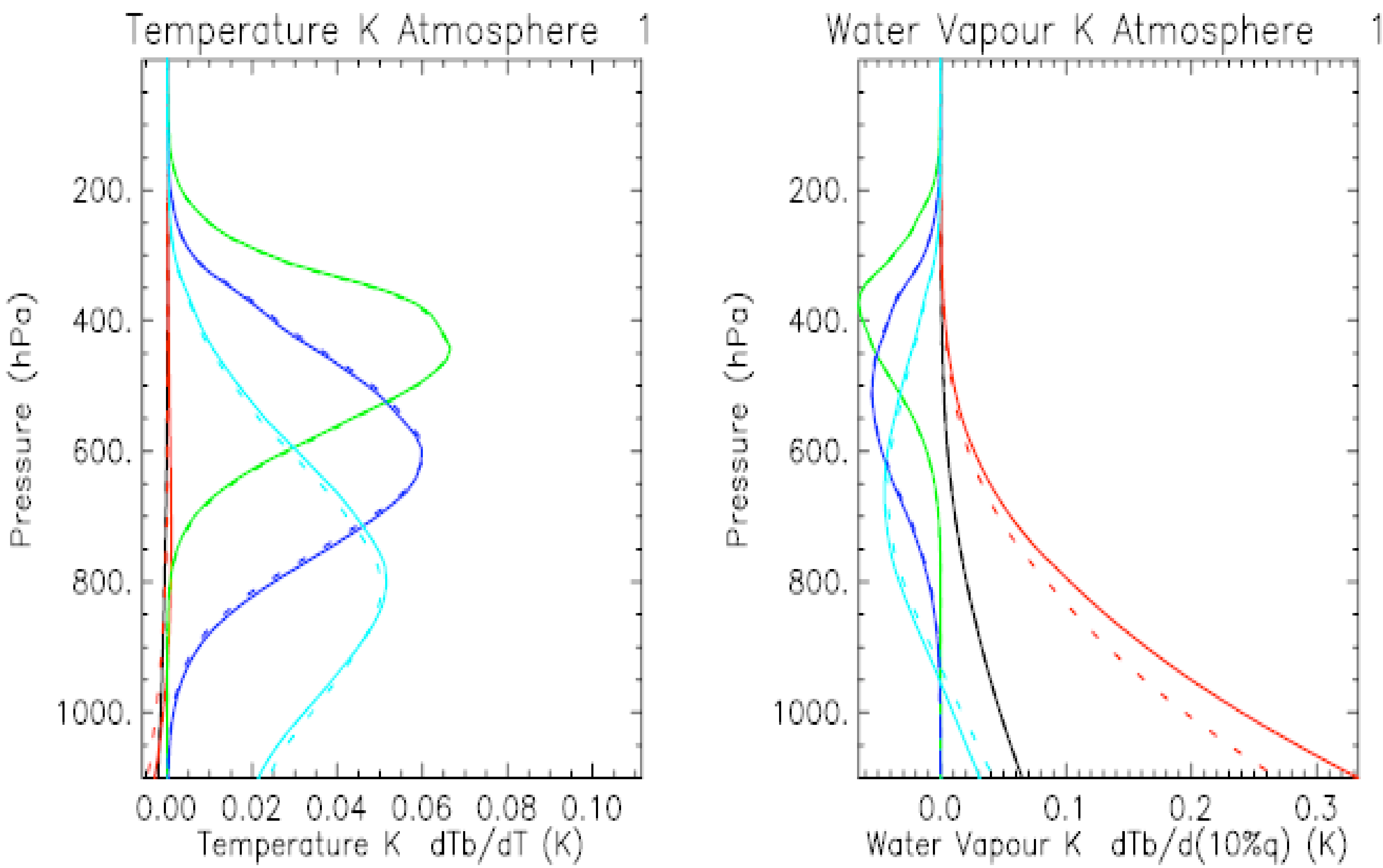
**After fitting**
**Scaling to find the fit gives an estimate of the ozone amount in the observed spectrum**



# Backscatter Photon Path Schematic



- DOAS retrievals convert patterns in the measurements into column estimates of trace gases. These can be considered as pseudo measurements that are functions of the assumed profiles. The retrieved quantities' dependence on the height distribution of the absorber can provide partial derivatives (Jacobians).
- The measurement errors due to instrument calibration are usually small.* The main error sources are inaccurate information on cloud and surface reflectivity, and cloud and aerosol heights and ODs. Additional errors come from limited discretization of the atmosphere and cross-section uncertainties.
- *Different approaches to remove patterns in solar or Earth spectra may produce biases. Tropospheric estimates have often removed the stratospheric component in some self-consistent way.




Temperature and water vapor Jacobians for the US Standard Atmosphere for AMSU-B. Black–channel 1, Red–channel 2, Green–channel 3, Blue–channel 4, Cyan–channel 5 Dashed lines are for MHS. Figure from *Comparison of Simulated Radiances, Jacobians and Information Content for the Microwave Humidity Sounder and the Advanced Microwave Sounding Unit–B*. *Thomas J. Kleespies, Philip Watts*

H. J. Eskes and K. F. Boersma, 2003, *Averaging kernels for DOAS total-column satellite retrievals,* **Atmos. Chem. Phys., 3**, 1285–1291.

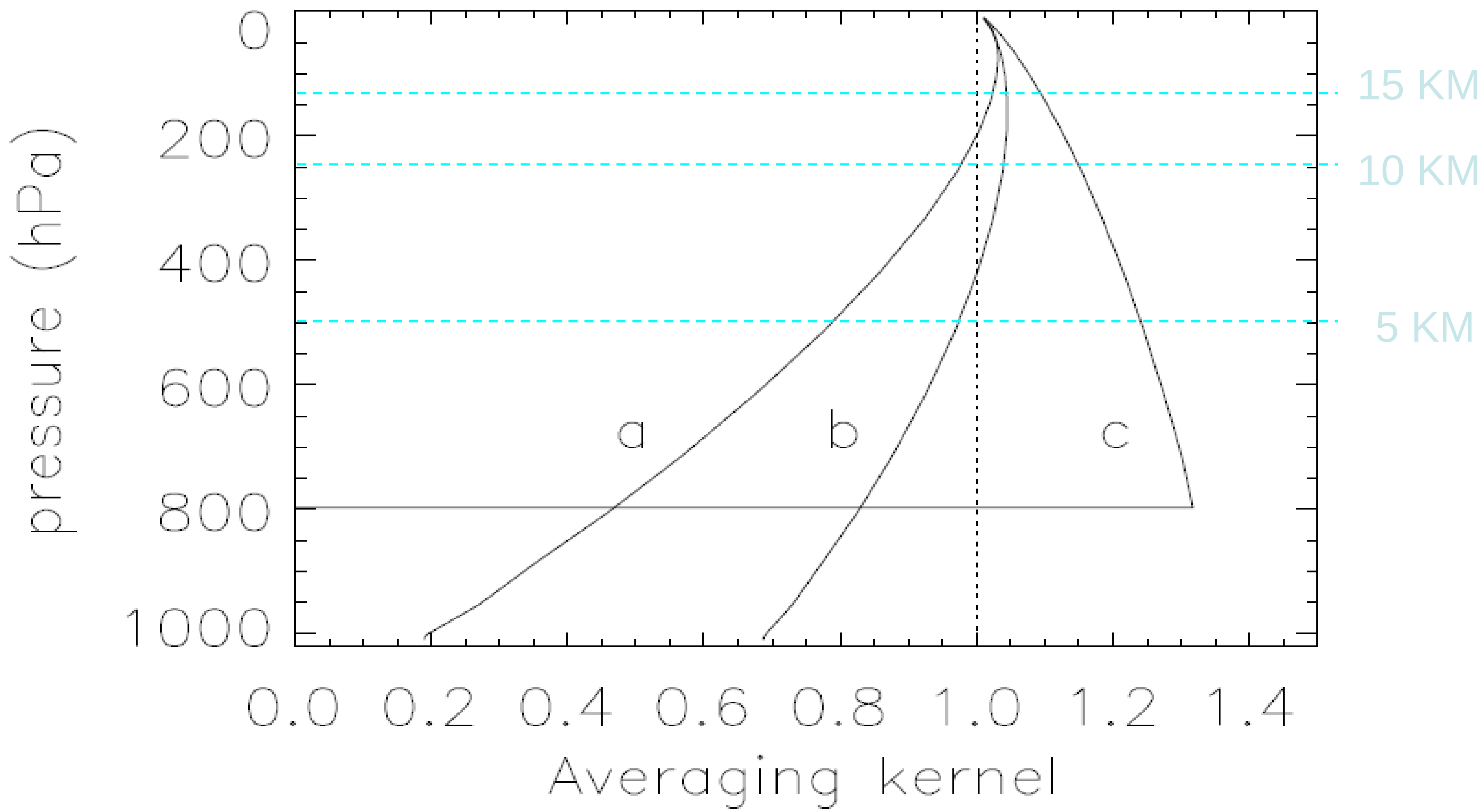
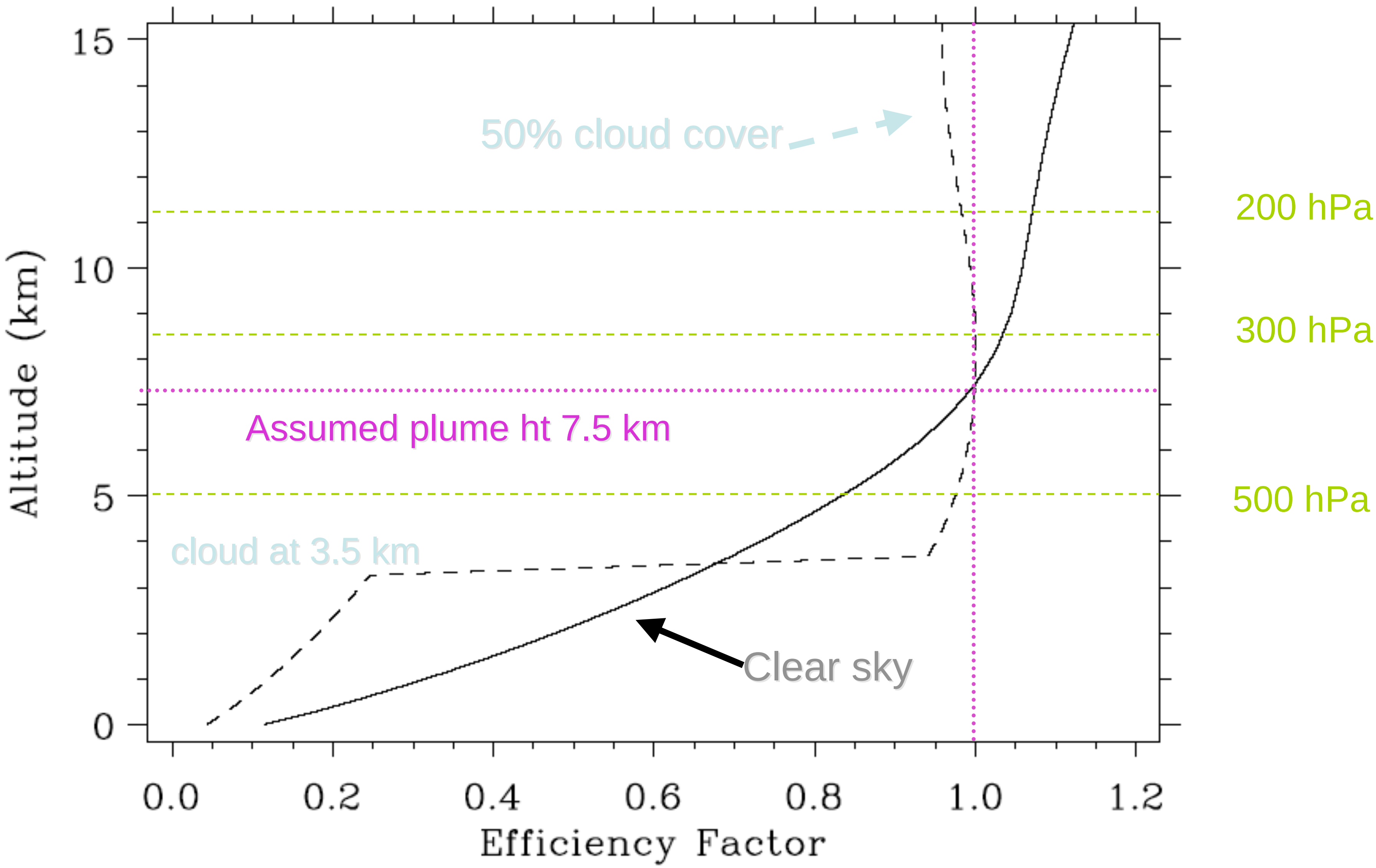


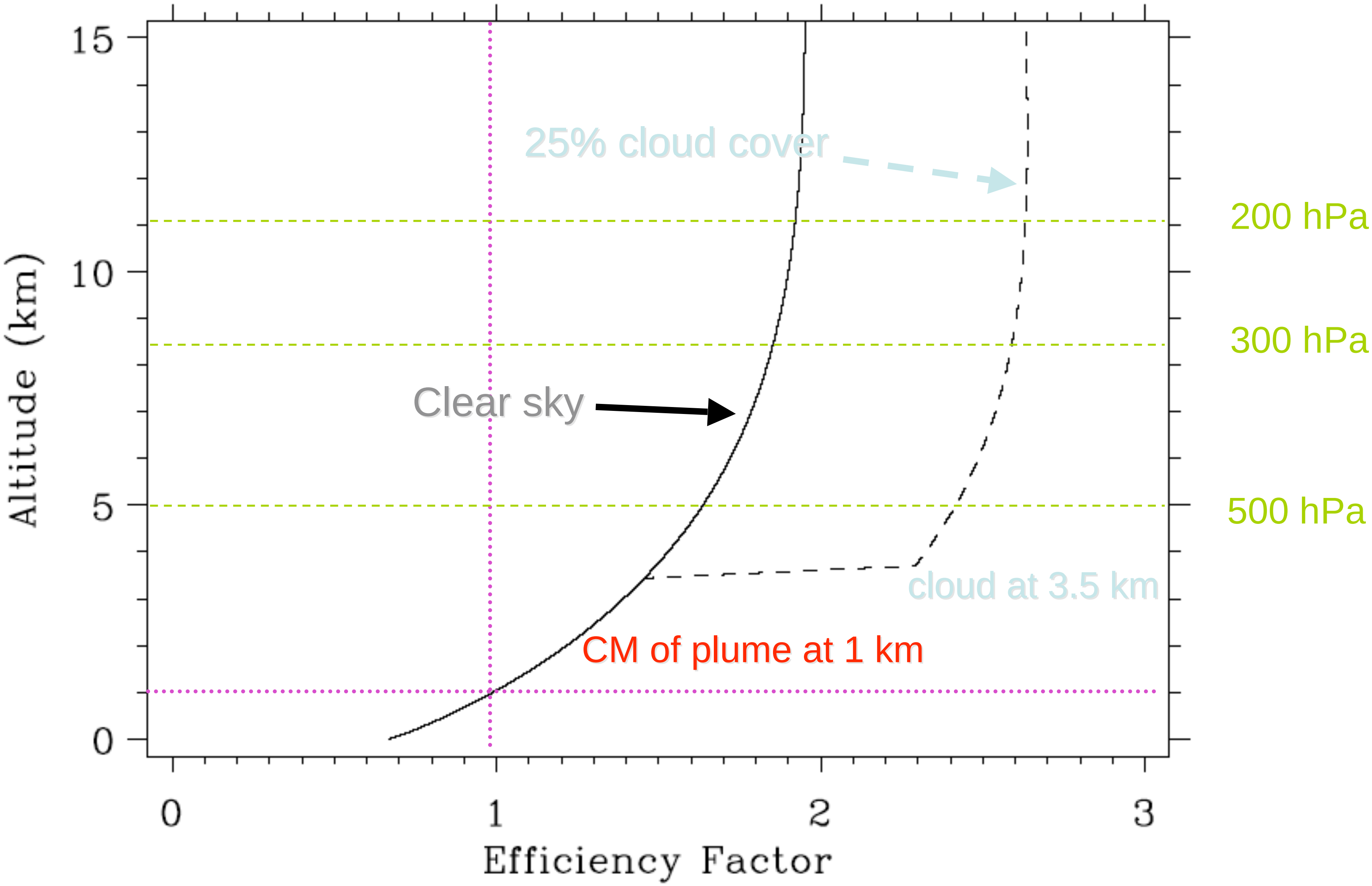

**Fig. 1.** Example of DOAS averaging kernels at 437 nm: **(a)** clear pixel with a surface albedo of 0.02; **(b)** clear pixel with a surface albedo of 0.15; **(c)** pixel with an optically thick cloud and cloud top at 800 hPa.

# Sensitivity to $SO_2$ Plume Height




From a Presentation by P.K. Bhartia, NASA GSFC, on OMI

# Sensitivity to $NO_2$ Plume Height




From a Presentation by P.K. Bhartia, NASA GSFC, on OMI

For trace gas column retrievals, we will want to know the retrieved column total, Cr; the assumed profile for the retrieval/observation, **X**r; the forecast/background profile, **X**f, and the layer retrieval efficiencies, **W**. The DOAS retrieval cannot distinguish between profiles with the same weighted column sums, WC, given by

$$WC(\mathbf{X}) = \sum_i (\mathbf{W}_i * \mathbf{X}_i)$$

One form of the assimilation cost function could use the difference between the weighted model column and the weighted retrieval column as the measurement constraint.

$$\Delta WC(\mathbf{X}) = WC(\mathbf{X}) - WCr(\mathbf{X}r) = \sum_i [\mathbf{W}_i * (\mathbf{X}_i - \mathbf{X}r_i)]$$

The measurement covariance would have a general component related to the accuracy of the spectral product and fit, and layer-dependent terms related to the accuracy of the forward model. Notice that the Jacobians are simply

$$\mathbf{K}_i = \mathbf{W}_i = \partial WC(\mathbf{X}) / \partial \mathbf{X}_i$$

# Maximum Likelihood Retrieval – Optimal Estimation

- **Model Discretization**
  - **The atmosphere is represented as set of pressure layers defined by a set of discrete pressures {**$p_i$**}.**
  - **The ozone profile is represented by the ozone amounts in each layer {**$x_i$**}.**
- **A set of *A Priori* Profiles {**$x_A$**} and Covariance matrices, {**$S_A$**}, are obtained from balloonsonde and occultation climatological data. These are mean profiles with small scale structure lost in the average.**
- **A set of measurements, {**$y_{Mj}$**} is made and the error covariance,** $S_M$**, is provided.**
- **Radiate Transfer Forward Models** $y_j$**=F(**$x$**,**$\lambda_j$**) are used to calculate the radiance/irradiance ratio (and partial derivatives with respect to ozone layer amounts) for each measurement channel,** $\lambda_j$**, for the appropriate *A Priori* Profile.**
- **The Measurement Jacobians (Partial Derivatives) ,** K [kij = ∂ Fλj/ ∂ xi **partial derivatives of the forward model for wavelength** $\lambda_j$ **with respect to layer ozone** $x_i$**] are used to give a Linearization of the forward model changes with respect to ozone profile changes.**

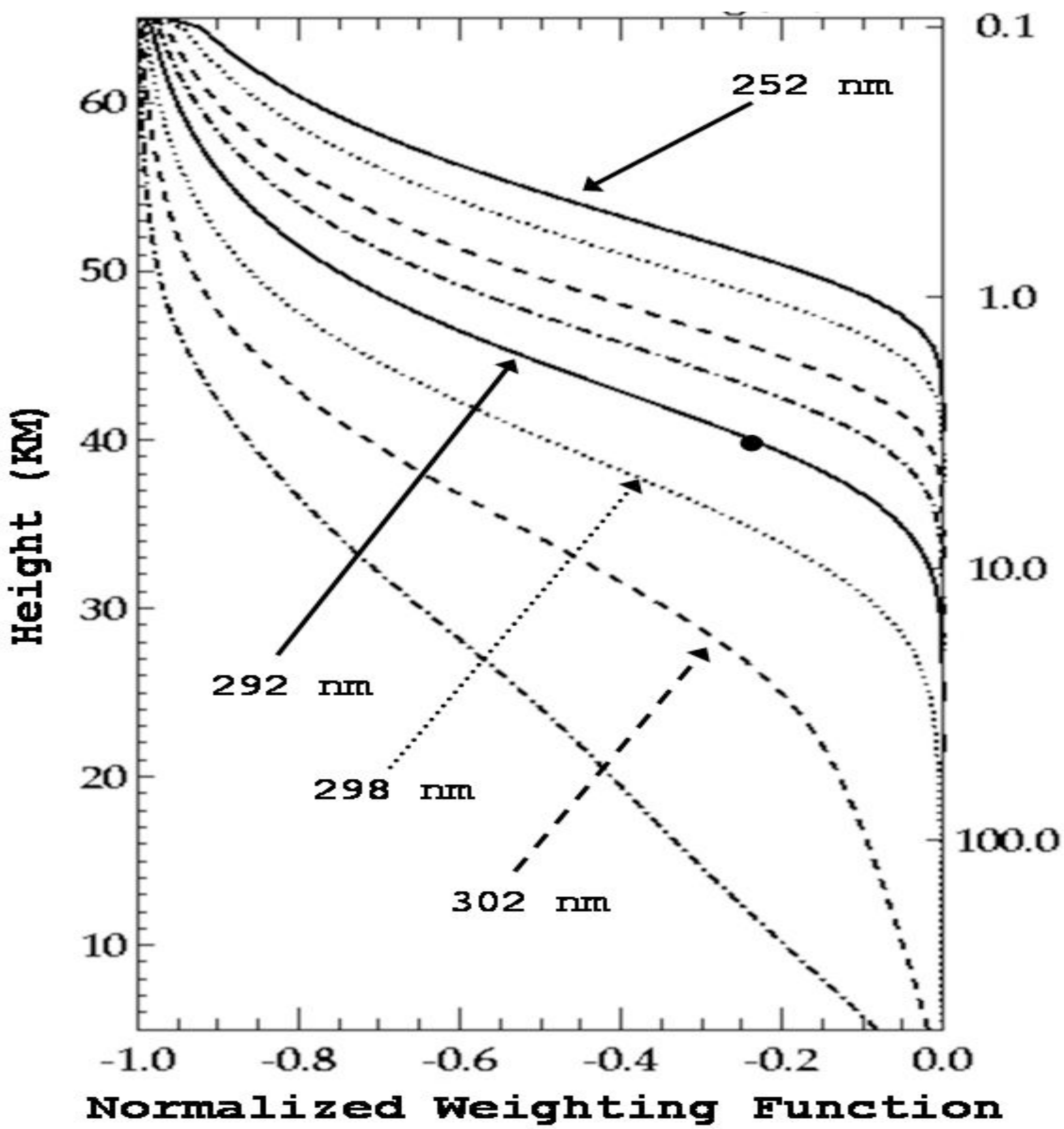
$$\mathbf{y} = \mathbf{F}(\mathbf{x}) \approx \mathbf{F}(\mathbf{x}_A) + \mathbf{K}_A(\mathbf{x} - \mathbf{x}_A),$$ **$y_j$ is the estimate at $\lambda_j$**

References:

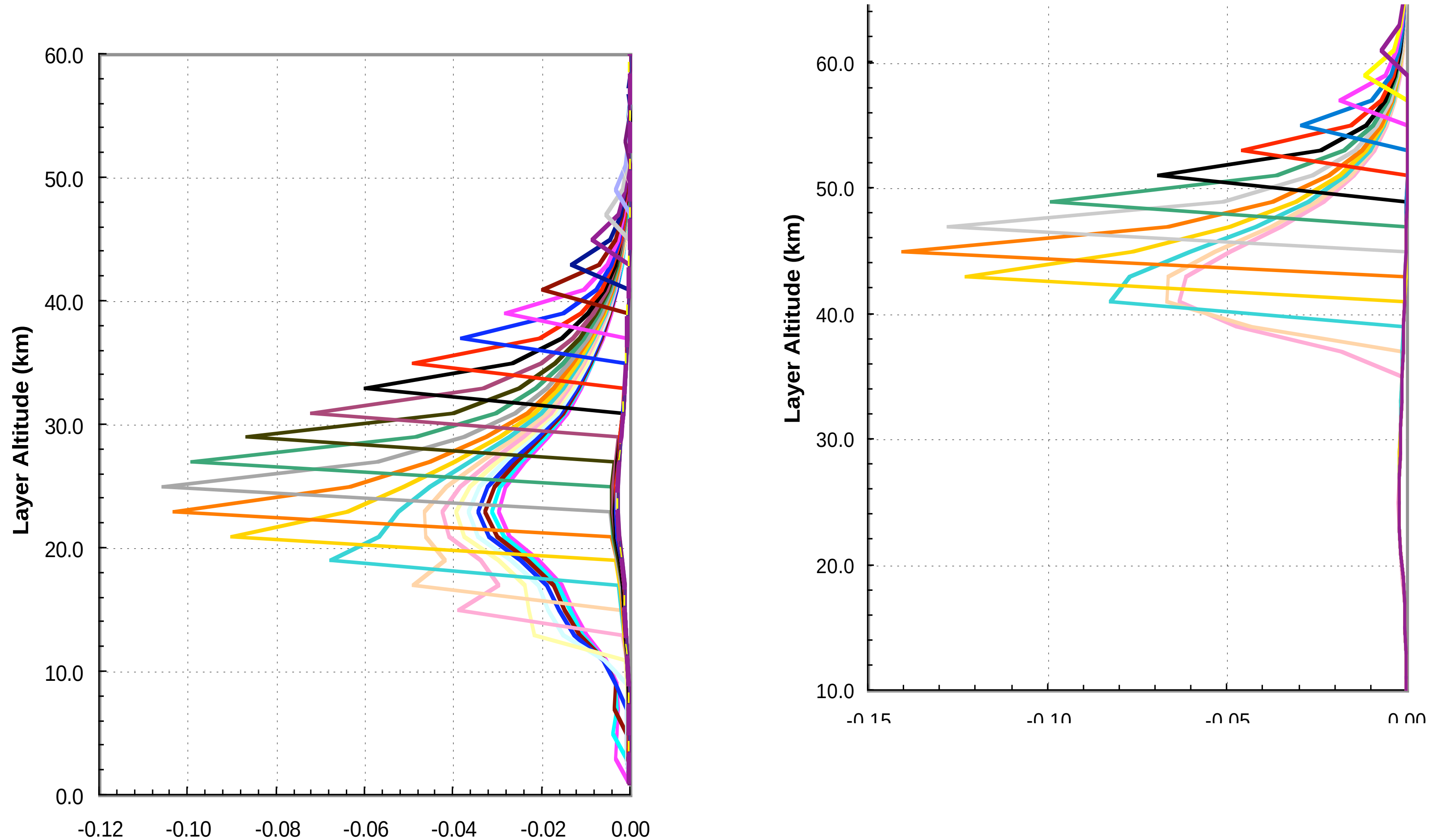

Rodgers, C. D., Retrieval of Atmospheric Temperature and Composition From Remote Measurements of Thermal Radiation, *Rev. Geophys. and Space Phys*., 14, p609-624, 1976.

Rodgers, C. D., The Characterization and Error Analysis of Profiles Retrieved from Remote Sounding Measurements, *J. Geophys. Res*., 95, p5587-5595, 1990.

# Normalized Weighting Functions

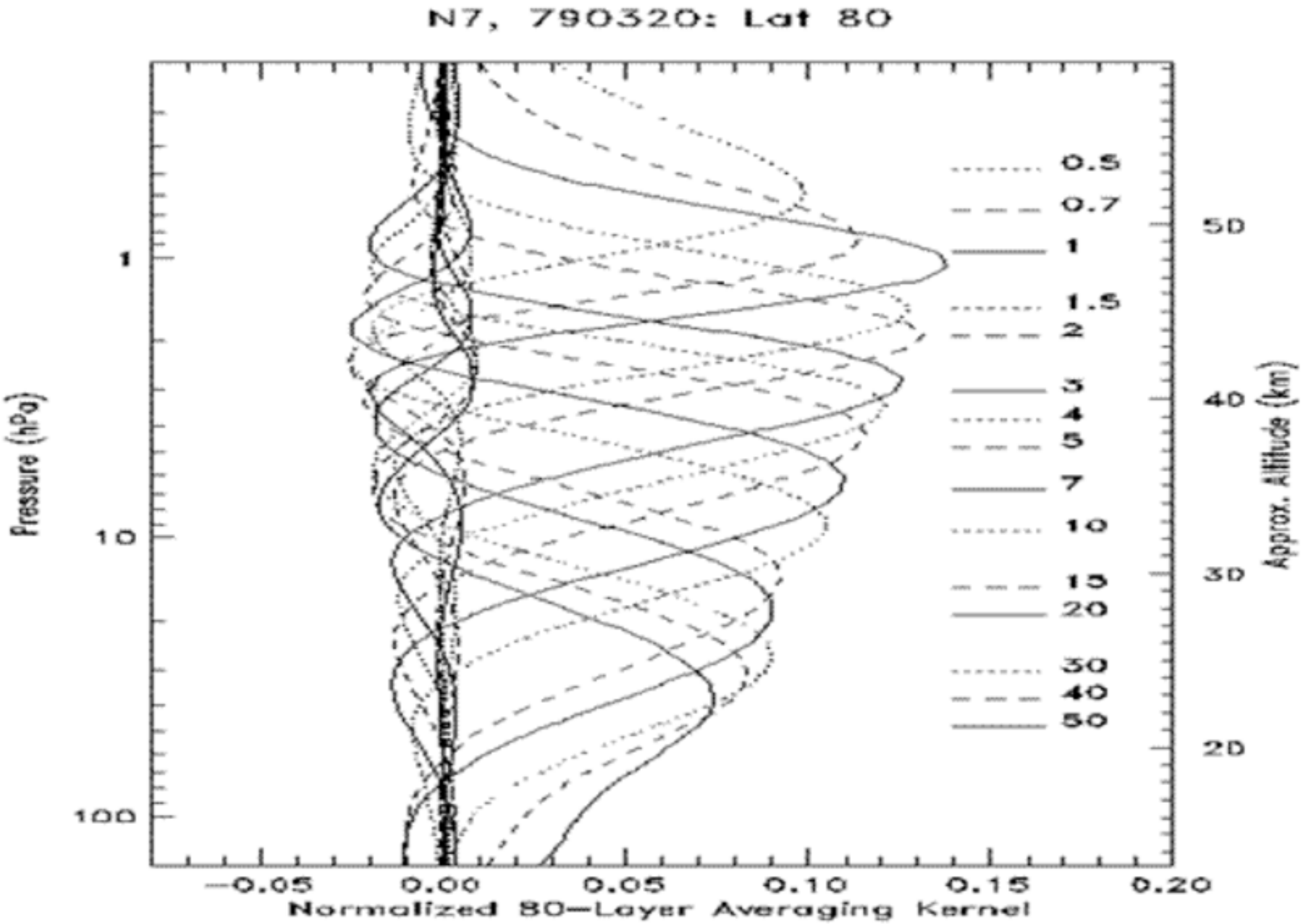



Measurement Jacobians (Partial Derivatives) with respect to ozone layer amounts for the eight shortest SBUS Wavelengths – 252, 273, 283, 288, 292, 298, 302, and 306 nm. Photon Penetration for 325 DU of ozone 30º Solar Zenith Angle. Each curve is normalized by its peak sensitivity. The ozone absorption cross section decreases with increasing wavelength so the photons for longer wavelengths penetrate deeper into the atmosphere.




Sensitivity of channel limb radiances to layer ozone changes for 1-km layers for a 40º SZA and mid-latitude 325-DU profile. Each curve gives the ratio of changes in the limb radiance for a given tangent height to changes in the ozone amounts as a function of altitude. The changes in the natural log of both quantities are used to give a % radiance change per % ozone change interpretation to the results. The curves give radiances for observation tangent heights spaced out every 2 km.

The plot on the left is for the 600-nm channel. The grey curve with the highest peak is for the 25-km tangent height case. The plot on the right is for the 305-nm channel. The orange curve with the highest peak is for the 45-km tangent height case.




**Averaging kernels as fractional layer changes for a high latitude profile and viewing condition for SBUV instruments**

The Averaging Kernel or impulse response, $\mathbf{A}$, is the product of the Jacobian of partial derivatives of the measurements with respect to the ozone profile layers, $\mathbf{K}$, and the measurement retrieval contribution function, $\mathbf{D}y$:

$$\mathbf{A} = \mathbf{D}y \# \mathbf{K}$$

For a linear problem, the retrieved profile, $\mathbf{X}r$, is the sum of the *A Priori* Profile, $\mathbf{X}a$, plus the product of the Averaging Kernel, $\mathbf{A}$, and the difference between the Truth Profile, $\mathbf{X}t$, and $\mathbf{X}a$:

$$\mathbf{X}r = \mathbf{A} \# [\mathbf{X}t - \mathbf{X}a] + \mathbf{X}a$$

The measurement change, $\Delta\mathbf{M}$, is the Jacobian times a profile change, $\Delta\mathbf{X}$:

$$\Delta\mathbf{M} = \mathbf{K} \# \Delta\mathbf{X}$$

The retrieval change, $\Delta\mathbf{X}r$, is the contribution function times the measurement change, $\Delta\mathbf{M}$:

$$\Delta\mathbf{X}r = \mathbf{D}y \# \Delta\mathbf{M}$$

The difference between the satellite measurements and those corresponding to a forecast profile, **X**f, can be approximated by:

$$\Delta \mathbf{M}\text{f} = \mathbf{M}\text{res} - \mathbf{K} \# (\mathbf{X}\text{f} – \mathbf{X}\text{r})$$

where **M**res is the retrieval measurement residual. The profile that would have been retrieved using the **X**f as an *A Priori*, **X'r,** is then approximated by

$$\mathbf{X'r} = \mathbf{X}\text{f} + \mathbf{D}\text{y} \# \Delta \mathbf{M}\text{f}$$

or

$$\mathbf{X'r} = \mathbf{X}\text{f} + [\mathbf{X}\text{r} – \mathbf{X}\text{a}] – \mathbf{A} \# [\mathbf{X}\text{f} – \mathbf{X}\text{a}]$$

This approach preserves any difference between the *A Priori* and the forecast profile that lie in the measurement null space.

# Discussion

- How are DOAS Retrieval columns used in practice?
- How are total ozone and ozone profiles used?
- What can be done to get more information in the lower atmosphere?
  - Tropospheric residuals
  - Smaller FOVs
  - Better cloud and surface information
  - Optically thick considerations
  - Temperature sensitivity
  - Cloud clearing

# Short list of parameters to provide with DOAS retrievals

- Column amount
- Assumed profile
- Cloud pressure, fraction, and reflectivity
- Surface reflectivity
- Layer retrieval sensitivity
- DOAS goodness of fit
- Cross section source
- ?

# Background

# Assimliation Equations

$$\mathbf{J}(\mathbf{x}) = \left(\mathbf{x} - \mathbf{x}^b\right)^T \mathbf{B}^{-1}\left(\mathbf{x} - \mathbf{x}^b\right) + \left(\mathbf{y}^o - \mathbf{y}(\mathbf{x})\right)^T (\mathbf{O} + \mathbf{F})^{-1} \left(\mathbf{y}^o - \mathbf{y}(\mathbf{x})\right) \qquad (1)$$

where $\mathbf{x}^b$ is a background estimate of the model state vector usually given by a short term forecast, $\mathbf{x}$ is the desired solution, $\mathbf{y}^o$ is the vector of observations, $\mathbf{y}(\mathbf{x})$ is an operator which transforms the model state vector into the same form as the observations, and **B, O** and **F** are the background, observational and forward modelling error covariance matrices respectively. For this purpose, $\mathbf{y}(\mathbf{x})$ is the radiative transfer operator. Neglecting the possibility of multiple minima, the most probable solution is where the gradient of $\mathbf{J}(\mathbf{x})$ is zero:

$$\nabla \mathbf{J}(\mathbf{x}) = \mathbf{B}^{-1}\left(\mathbf{x} - \mathbf{x}^b\right) - \mathbf{K}(\mathbf{x})^T \ (\mathbf{O} + \mathbf{F})^{-1} \left(\mathbf{y}^o - \mathbf{y}(\mathbf{x})\right) = 0 \qquad (2)$$

where $\mathbf{K(x)}$ is the matrix of partial derivatives of $\mathbf{y(x)}$ with respect to the elements of $\mathbf{x}$, or the jacobian. The information content can be estimated from the covariance matrix which is the Hessian of (1) (Rodgers, 1976)

$$\mathbf{S} \ = \ \left\{\left(\mathbf{B}^{-1} \ - \mathbf{K}(\mathbf{x})^T \ (\mathbf{O} + \mathbf{F})^{-1} \mathbf{K}(\mathbf{x})\right)^{-1}\right\}^{1/2} \qquad (3)$$

- The second topic is on how to use the information in the retrieved estimates. The assimilation and modelers are just starting to get to these problems. They can handle biases and don't mind variances, but covariances, a priori, and retrieval efficiencies are just on the drawing table. There are additional pitfalls, such as the use of a "Clean Sky" spectrum to get the reference stratospheric NO2 loading. This can produce large differences in the stratospheric fields between retrieval algorithms which should be self-canceling for the tropospheric estimates but not the column or slant column.
- Assumed profile, averaging kernels, a prioris, covariances, measurement response, efficiency factors, Jacobians, assimilation of measurements, DOAS Slant columns
- The second topic is more of a discussion on the use of averaging kernels, retrieval efficiencies, a prioris, and other retrieval information in validation studies and product applications. This would consider some ideas taken from ozone profiles experiences and from my conversations with modelers as well as some ideas presented by H. Eskes and F. Boersma in their paper. I think it would be useful for the Level 2 product developers, validation study providers, and user community to exchange information on what can be provided, what it can help to do, and what information can be best brought into the models.

# Discussion Topic on Satellite Atmospheric Chemistry Trace Gas Product Content

- Assumed/A Priori/Retrieved profile (Covariance)
- Profile sensitivity (Layer sensitivity or Averaging Kernel)
- Measurement precision error estimate
- Measurement residuals
- Retrieval accuracy estimates
- Cloud fraction and Cloud “Top” pressure
- Algorithm version
- Stratosphere internal consistency

# Tutorial on DOAS retrieval Information

- Slant column
- Assumed profile – Air Mass Factor (Mirror)
- Total column
- Retrieval Sensitivity to changes (How many of the photons see a given layer?)
- www.atmos-chem-phys.org/acp/3/1285/ Atmospheric Chemistry and Physics, “Averaging kernels for DOAS total-column satellite retrievals,” H. J. Eskes and K. F. Boersma, Atmos. Chem. Phys., 3, 1285–1291, 2003. “Error Analysis for Tropospheric NO2 Retrieval from Space,” K.F. Boersma, H.J. Eskes and E.J. Brinksma, *J. Geophys. Res.* **109** D04311, doi:10.1029/2003JD003962, 2004.

We want to minimize sum of the following inverse variance weighted deviations

$$\mathbf{J(x)} = \left( (\mathbf{x}-\mathbf{x}_A)^{\mathrm{T}} \mathbf{S}_A^{-1} (\mathbf{x}-\mathbf{x}_A) + (\mathbf{y}-\mathbf{y}_M)^{\mathrm{T}} \left(\mathbf{S}_M\right)^{-1} (\mathbf{y}-\mathbf{y}_M) \right)$$

This leads to the and iterative solution of the form

$$\mathbf{x}_{\mathbf{n+1}} = \mathbf{x}_A + \mathbf{S}_A \mathbf{K}_{\mathbf{n}}^{\mathrm{T}} (\mathbf{K}_{\mathbf{n}} \mathbf{S}_A \mathbf{K}_{\mathbf{n}}^{\mathrm{T}} + \mathbf{S}_M)^{-1} [(\mathbf{y}_M - \mathbf{y}_{\mathbf{n}}) - \mathbf{K}_{\mathbf{n}} (\mathbf{x}_A - \mathbf{x}_{\mathbf{n}})]$$

where the linearization estimate is recomputed at each step

$$K_{i\,j} = \partial F_j(\mathbf{x}) / \partial x_i$$

to find the partial derivatives of the forward model for wavelength $\lambda_j$ with respect to layer ozone $x_i$.

The Measurement errors due to instruments are small. The main error sources are cloud and surface reflectivity, and cloud and aerosol heights and ODs. Additional errors come from limited discretization of the atmosphere.

$$MC = \sum_i (\mathbf{w}_i * \mathbf{r}_i)$$

$$FC = \sum_i (\mathbf{w}_i * \mathbf{f}_i)$$

We want to minimze the absolute difference of MC and FC.

$$\mathbf{x_{n+1}} = \mathbf{x}_A + \mathbf{S}_A \mathbf{K_n}^{\mathrm{T}} (\mathbf{K_n} \mathbf{S}_A \mathbf{K_n}^{\mathrm{T}} + \mathbf{S}_M)^{-1} [(\mathbf{y}_M - \mathbf{y_n}) - \mathbf{K_n} (\mathbf{x}_A - \mathbf{x_n})]$$

$$K_{i\,j} = \partial F_j(\mathbf{x}) / \partial x_i$$

$$\mathbf{x_{n+1}} = \mathbf{x}_A + \mathbf{S}_A \mathbf{K_n}^{\mathrm{T}} (\mathbf{K_n} \mathbf{S}_A \mathbf{K_n}^{\mathrm{T}} + \mathbf{S}_M)^{-1} [(\mathbf{y}_M - \mathbf{y_n}) - \mathbf{K_n}(\mathbf{x}_A - \mathbf{x_n})]$$

$$\mathbf{J(x)} = \left( (\mathbf{x} - \mathbf{x}_A)^{\mathrm{T}} \mathbf{S}_A^{-1} (\mathbf{x} - \mathbf{x}_A) + (\mathbf{y} - \mathbf{y}_M)^{\mathrm{T}} (\mathbf{S}_M)^{-1} (\mathbf{y} - \mathbf{y}_M) \right)$$

$$\mathbf{y} = \mathbf{F(x)} \approx \mathbf{F}(\mathbf{x}_A) + \mathbf{K}_A (\mathbf{x} - \mathbf{x}_A), \quad y_j \text{ } \mathit{is\ the\ estimate\ at}\ \lambda_j$$

$K_{ij} = \partial F_j(\mathbf{x}) / \partial x_i$ Partial derivative of the forward model for wavelength lambda j with respect to layer ozone xi.

$$x_{n+1} = x_0 + S_x K_n^T (K_n S_x K_n^T + S_\varepsilon)^{-1} [(y - y_n) - K_n (x_0 - x_n)] \tag{10}$$

In this equation, $x_0$ is the a priori profile. The solution starts with a first-guess profile $x_1$, from which the kernels $K_1$ and measurements $y_1$ are evaluated, and proceeds through $n$ iterations until the retrieved profiles stop changing to within a specified tolerance. Although $x_1$ is not required to be the same as $x_0$, they are made the same in the buv algorithm. Strictly speaking, since measured radiances are used in constructing $x_0$, one does not have a true a priori profile to which the

# Forward Models, Jacobians, and Bandpass

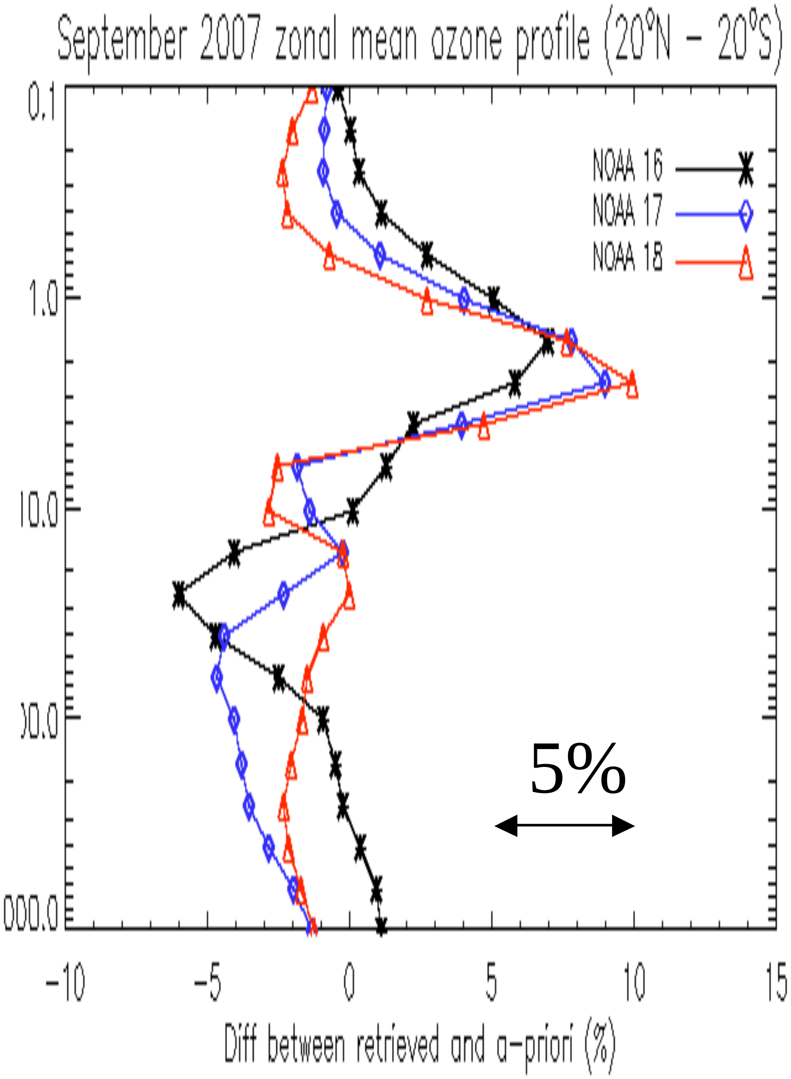
- Various Radiative Transfer Forward Models are used
  - TOMRAD - successive iteration of the auxiliary equation, Dave [1964]
  - LIDORT -discrete ordinate radiative transfer code, Spurr [2006]
  - Spherical RT Code, Herman (1994)
  - Single Scattering - quadrature of RT integrals
- All involve discetization or layering to represent the atmosphere. Clouds are often modeled as Lambertian reflective surfaces. Specialized codes are used for aerosols.
- Partial derivatives are obtained by discrete differences, adjoint computation methods (tangent linear), and analytically
- Wavelength bandpass results are approximated by using discrete representation of the bandpass at a limited number of channels and the corresponding solar weighting or by using effective (average) parameters in the radiative transfer models.
- Ring effect (inelastic scattering) is usually handled separately.

* References are in the Note Pages.

# Operational SBUV/2 Zonal Means 20S-20N

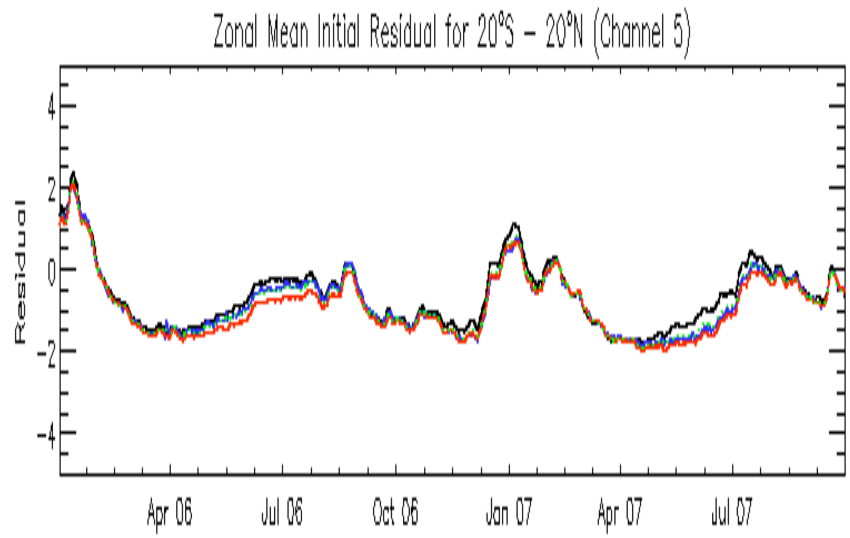
http://www.star.nesdis.noaa.gov/smcd/spb/calibration/icvs/

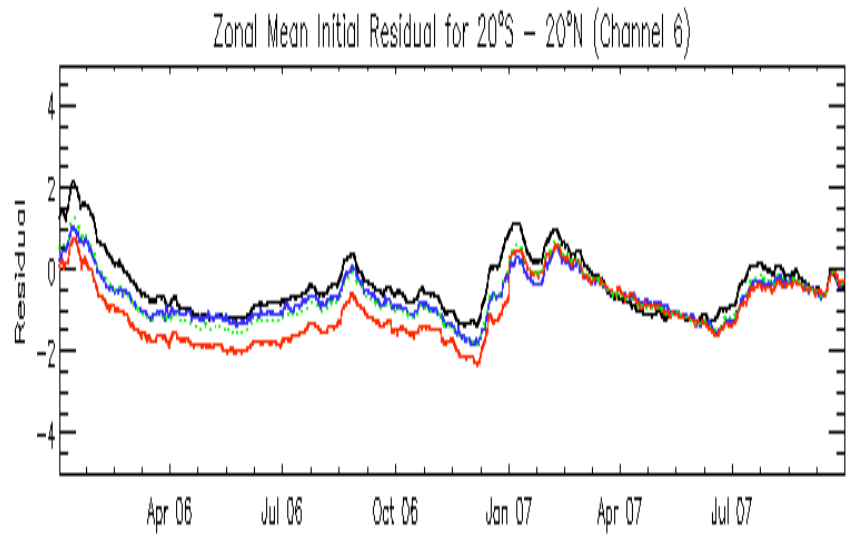
Pressure hPa

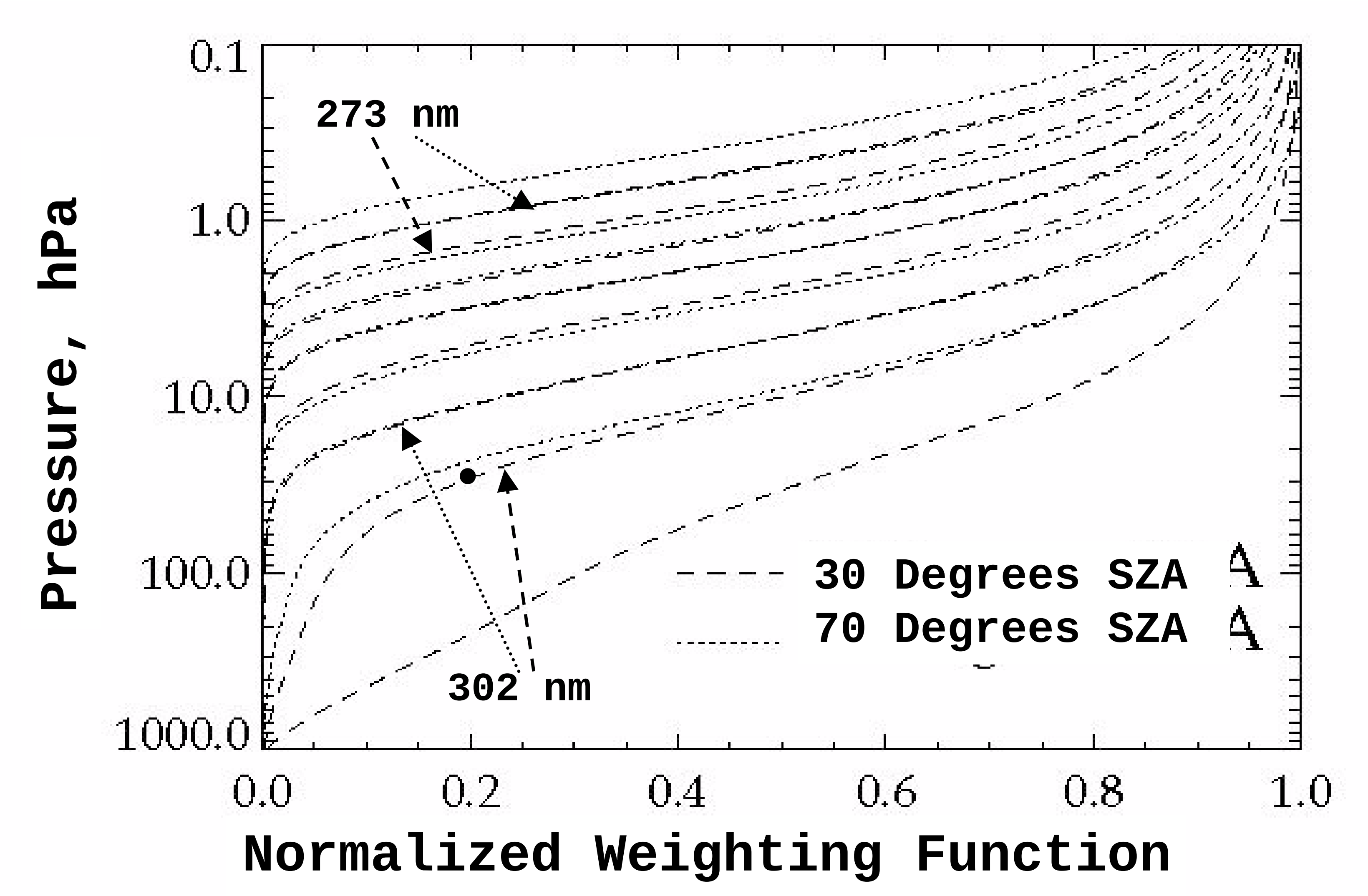



Retrieved Profile minus A Priori.

Initial Residual






Measurement Jacobians (Partial Derivatives) for the eight shortest SBUS wavelengths – 252, 273, 283, 288, 292, 298, 302, and 306 nm. Each curve is normalized by its peak sensitivity. The ozone absorption cross section decreases with increasing wavelength so the photons for longer wavelengths penetrate deeper into the atmosphere. Results are shown for a standard 325 DU atmosphere at two Solar Zenith Angles.

- FCDRs and NPP...
- Eskes, Boersma

Information in DOAS retrievals of column amounts.

Satellite instruments are making

This monograph examines practical questions for users of DOAS retrievals.

Eskes

The retrieval depends strongly on aspects like clouds, the assumed profile shape, surface albedo, the presence of a stratospheric background and aerosols.

Use Eskes notation.

Information for retrieval record:

1. Slant Path Column OD Units, Air Mass Factor, and Column Estimate
2. Profile layer amounts and Air Mass Factor sensitivities

Single channel optical absorption due to $NO_2$.

Change in OA for change in layer

Column and layers consistent with OA

Was a proportional retrieval used? More work to compute layer sensitivities.

Questions:

1. Is a new profile consistent with the measurement?
2. How would the column and layer amounts change if a new profile shape was used?
3. How would the column and layer amounts change if layer i was known?
4. If layer i changes by x% from the estimate profile how would the retrieval change?
5. If we have another estimate of the column and profile and a covariance matrix for it, how do we combine the DOAS measurement? What is the covariance matrix for the DOAS result? How do parameter and measurement uncertainties combine?

# Input Required by the DOAS Algorithms

- Forward Model results for trace gas profile sensitivity (Physical spectral patterns) and slant path calculations
- Differential Optical Absorption Spectroscopy (DOAS) Spectral Windows
- Radiance (corrected for calibration, polarization, non-linearity and dark current)
- Irradiance (corrected for calibration, polarization, non-linearity, goniometry and dark current)
- Wavelength Scales and Bandpasses for Earth and Solar
- Geolocation information
- Satellite viewing angles and solar zenith and azimuth angles
- Ancillary data sets (climatology, forecast or retrieved)

# Reflectivity and Cloud Top Pressure

- Algorithms require information on Clouds for reflectivity, cloud fraction, and ghost column estimation.
- The Cloud Top Pressures from IR measurements give a lower value than the effective pressure sensed by UV photons.
- In addition to climatologies, three methods are in use to estimate UV cloud top pressures directly from the measurements
  - Rotational Raman scattering (Ring effect) fills in Fraunhoffer lines. The filliing-in depends on the pressure at the scattering location.
  - The O2-O2 absorption (collision complex) at 477.7 nm varies with the pressure
  - Oxygen A-band absorption at 761-nm varies with the neutral atmospheric patn/

# DOAS Trace Gas Products

| **Retrieved species** | **Fitting window** | **Reference spectra** |
|---|---|---|
| $O_3$ | 325 - 335 nm | $O_3$, Ring |
| $O_3$, $NO_2$ | 425 - 450 nm | $O_3$, $NO_2$, Ring |
| HCHO | 336.5 - 357.5 nm | HCHO, $O_3$, $NO_2$, BrO, $O_4$, Ring |
| BrO | 345.6 - 359.0 nm | BrO, $NO_2$, $O_3$, (OClO), Ring |
| $SO_2$ | 313.5 - 327.0 nm | $SO_2$, $O_3$, Ring |
| OClO | 357.0 - 381.5 nm | OClO, $NO_2$, $O_4$ |