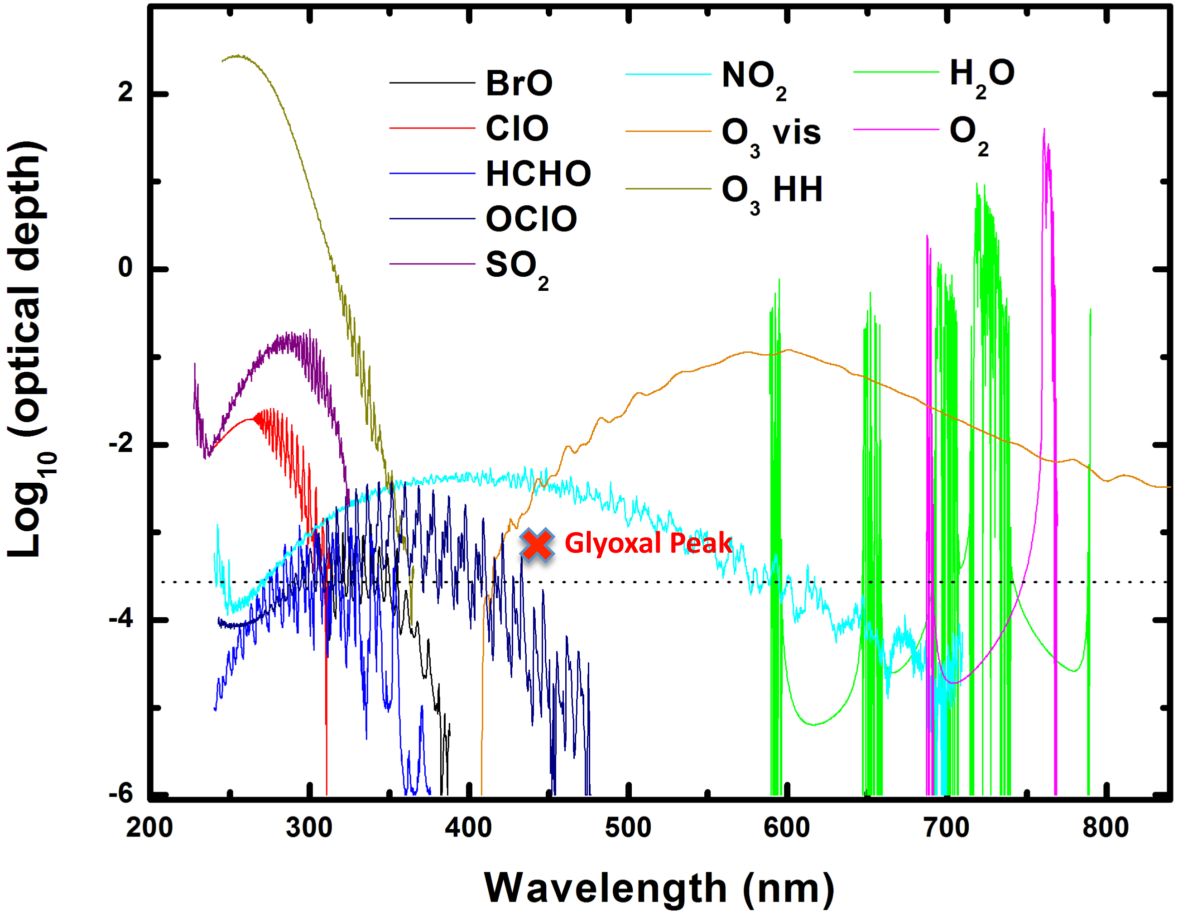
Satellite UV-Vis Measurements

What Can We See From Space?

Optical Depths for Typical GOME Measurement Geometry



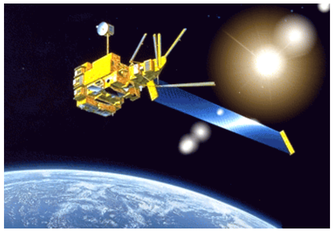
Minimum fit (so far)

ATMOSPHERIC MEASUREMENTS FROM UV-VISIBLE

1978

TOMS/

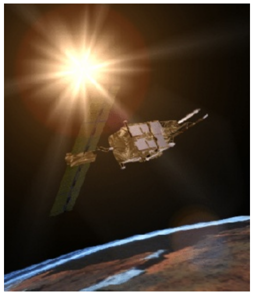
Nimbus 7 (78-94)
Meteor-3 (78-94)
ADEOS (96)
EP (96-06)



Total O_3 (derived tropospheric column), AI, SO_2
Global coverage ~daily
UV-vis

1995

GOME/ERS-2



O_3, NO_2, HCHO, BrO, OClO, H_2O, SO_2
Global coverage 3 days
UV-vis

2002

SCIAMACHY/ ENVISAT

O_3, NO_2, HCHO, BrO, OClO, H_2O, SO_2, CO, CH_4
Global coverage 3 days
UV-vis-near IR

2005

OMI/AURA

O_3, NO_2, HCHO, BrO, OClO, H_2O, SO_2
Daily Global coverage
UV-vis

2007

GOME-2/ METOP-A

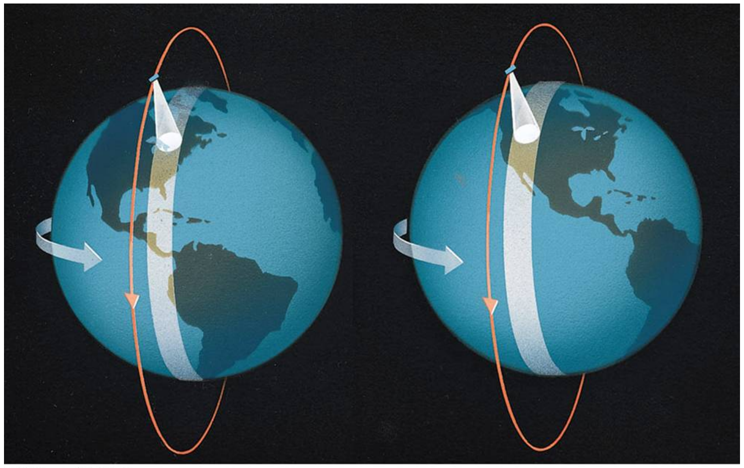
(Stolen from C. Heald)

Properties of UV-Vis Retrievals

- Scattering is important at these wavelengths
- Emission is not
- Spectral lines are not resolved by satellite instruments.
- Optical depths of absorbing species are typically weak (O(1%) or less) (The exception is ozone in the UV)

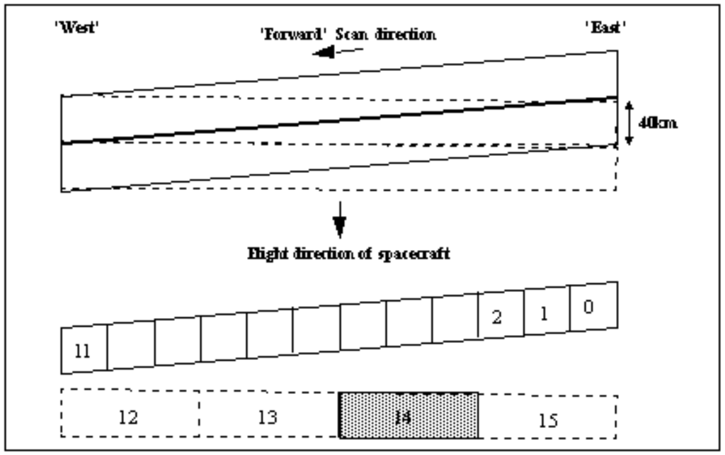
Nadir LEO Measurements

Both OMI and Gome 2 are in low earth orbit (~800km) circling from pole to pole, crossing the equator at the same local time each orbit.



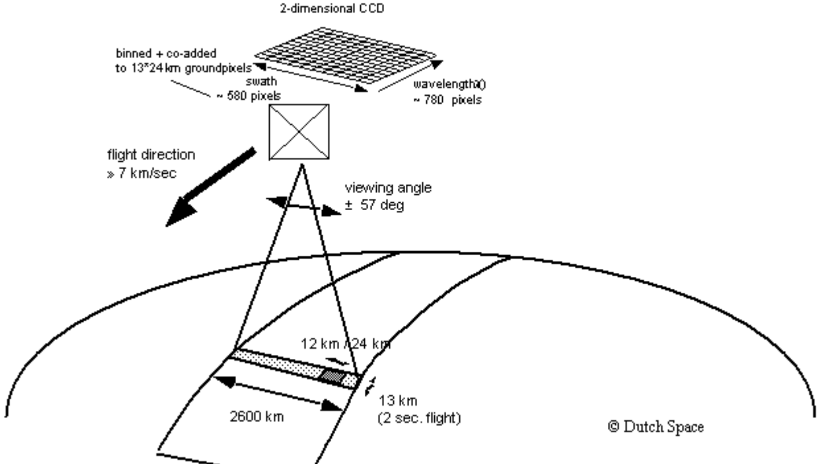
© 2007 Thomson Higher Education

Whisk Broom Scanner (Gome-2)



Mirror scans across satellites path, reflecting light to a single detector

Push Broom Scanner (OMI)

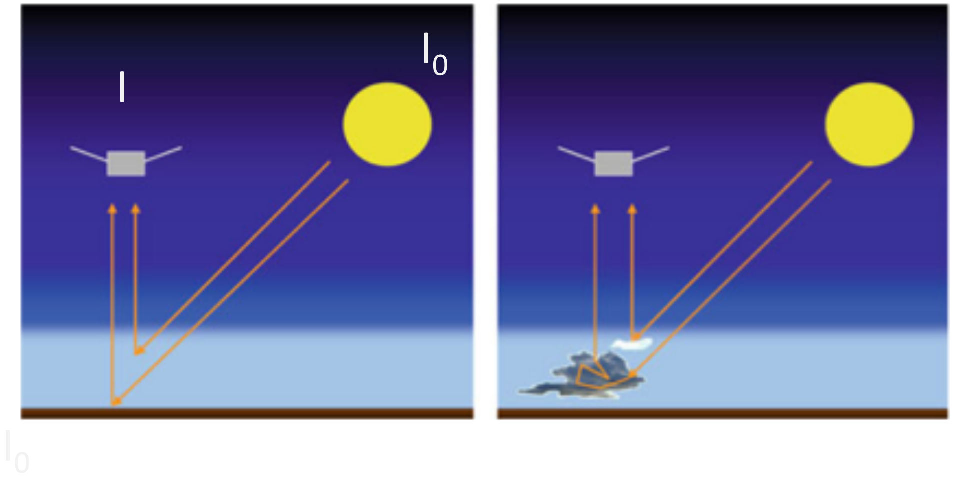


A line of detectors is arranged perpendicular to satellites path

UV-Vis Trace Gas Retrievals are a Two Step Process

A two step process:

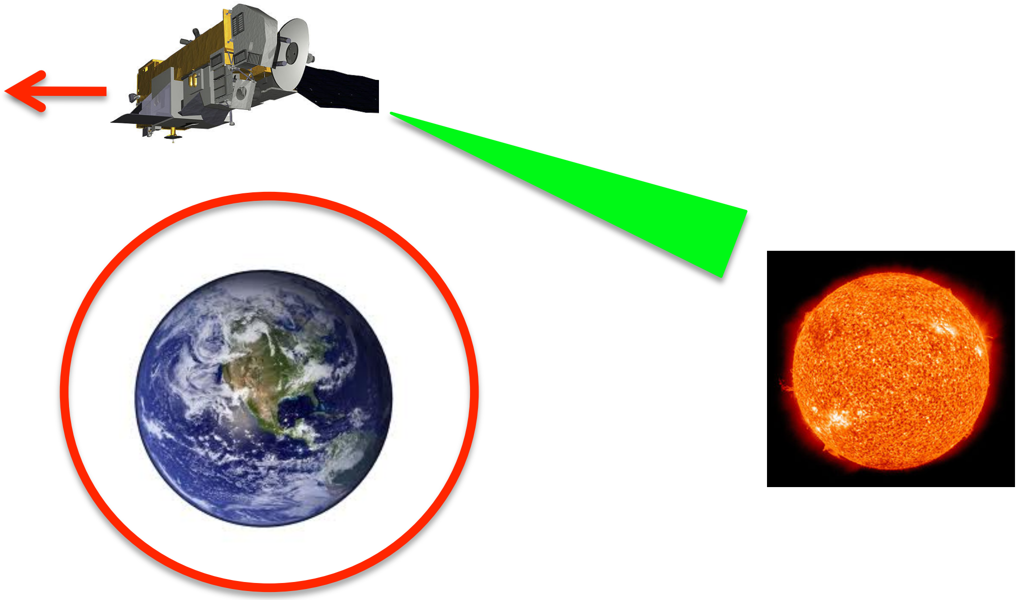
1) Measure slant column density (SCD) from backscattered radiation observed by satellite



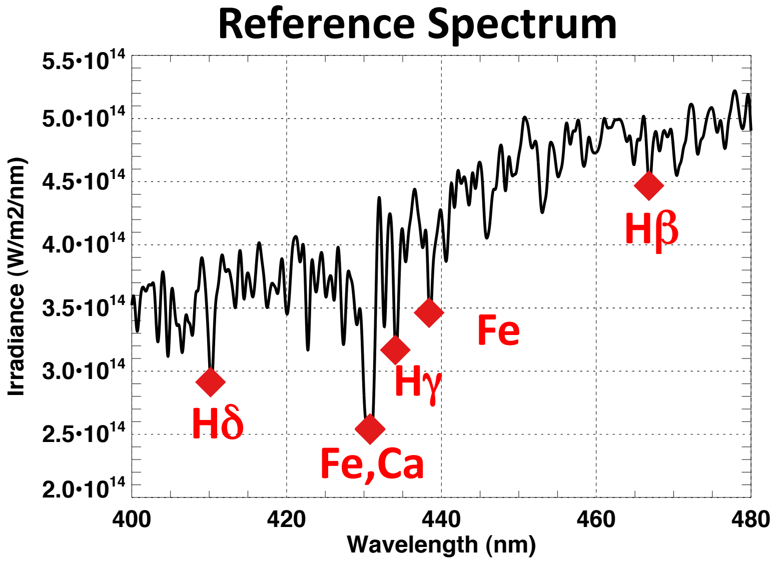
2) Calculate air mass factor (AMF) with a radiative transfer model to convert SCD to a vertical column density (VCD)

$$AMF = \frac{SCD}{VCD}$$

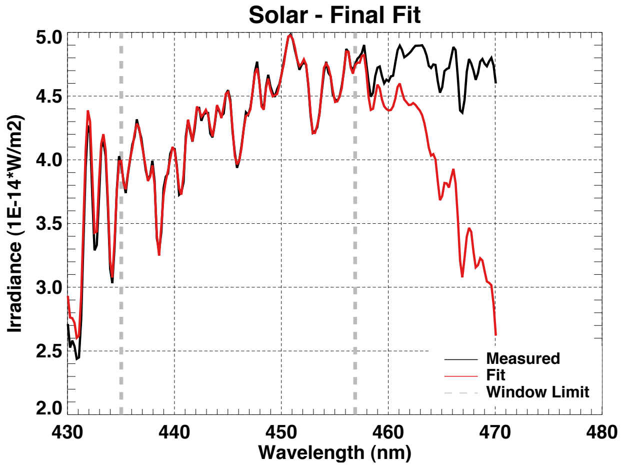
Characterising the Source Spectrum



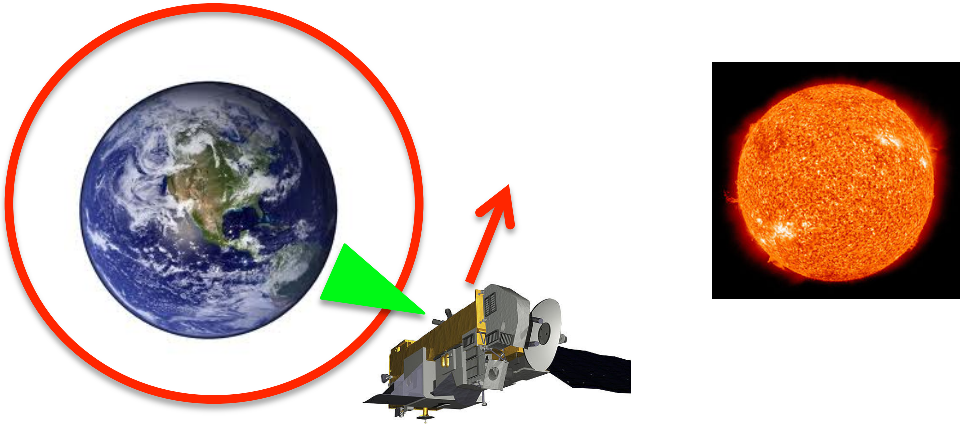
- Fit reference solar spectrum to the measured to determine solar wavelength grid and Instrument Line Shape.

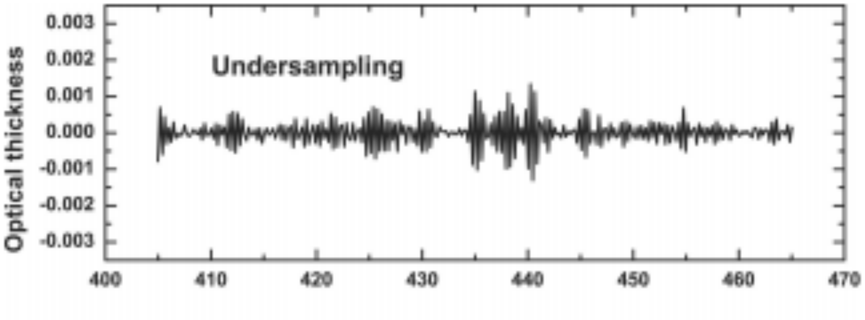


Fit to observed



Accounting for the Doppler shift





- The measured irradiance spectrum is doppler-shifted relative to the earth radiances. This must be corrected if it to be used as a 'source' spectrum
- Observed solar spectrum is splined to the earthshine radiance grid
- The detector undersamples the solar spectrum (below nyquist frequency) – We include an additional "undersampled spectrum" in the spectrum fitting process calculated using a high resolution reference solar spectrum

SCD Determination (Direct Fitting)

State of atmosphere (x) are determined by minimising the difference between an observed spectrum (y) and model spectrum (F)

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x}\in\mathbb{R}^n}{\arg\min} \sum_{i=1}^{m} (y_i - F_i(\boldsymbol{x}, \boldsymbol{b}))^2$$

Spectrum Model (F)

$$F(\lambda) = [\underset{\substack{\uparrow \\ \text{Source Spectrum}}}{I_0}(\lambda)\exp(-\underset{\substack{\uparrow \\ \text{Trace Gas Absorption}}}{\tau}(\lambda)) + \underset{\substack{\uparrow \\ \text{Common Mode}}}{R}(\lambda)]\,\underset{\substack{\uparrow \\ \text{Scaling Polynomial}}}{P_{sc}}(\lambda) + \underset{\substack{\uparrow \\ \text{Baseline Polynomial}}}{P_{bl}}(\lambda)$$

Source Spectrum

Spectrum Model (F)

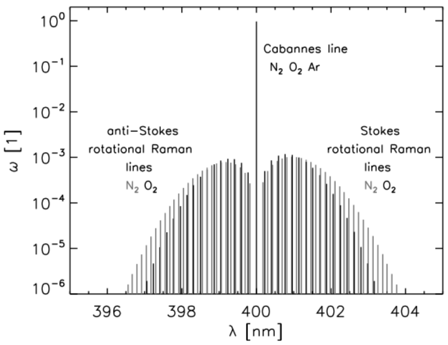
$$F(\lambda) = [I_0(\lambda)] \exp(-\tau(\lambda)) + R(\lambda)] P_{sc}(\lambda) + P_{bl}(\lambda)$$

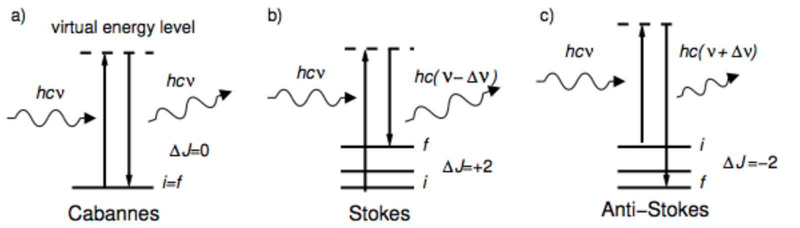
$$I_0(\lambda) = b_{sol}(\lambda) + x_u b_u(\lambda) + x_r b_r(\lambda)$$

Solar Spectrum Measured By Satellite

Undersampling Correction

Ring Spectrum – Rotational Raman scattering of O_2 and N_2 “fills in” I_0



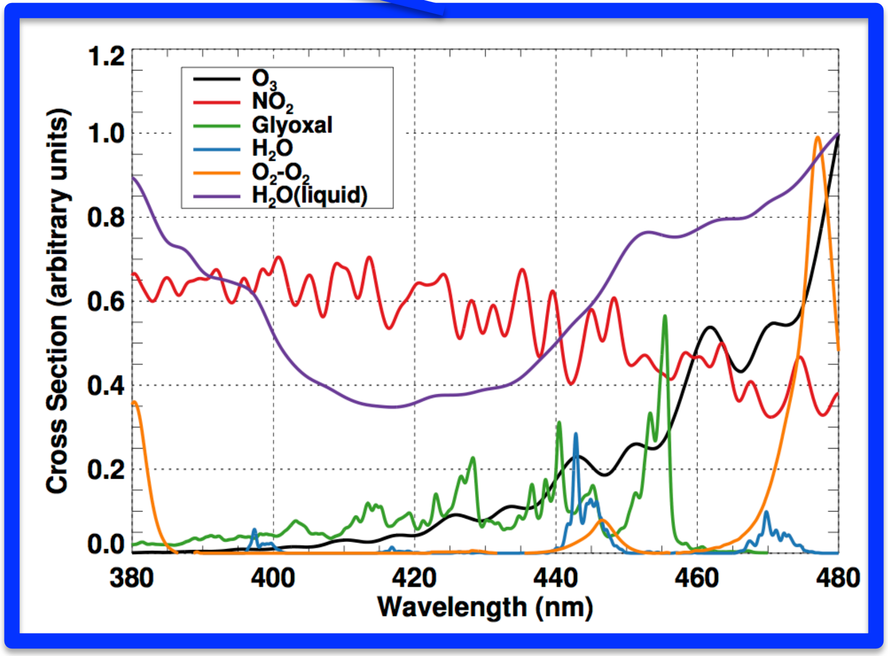


Trace Gas Absorption

Spectrum Model (F)

$$F(\lambda) = [I_0(\lambda)\exp(-\tau(\lambda)) + R(\lambda)]\,P_{sc}(\lambda) + P_{bl}(\lambda)$$

$$\tau(\lambda) = \sum_j x_j b_j(\lambda)$$



Common Mode Spectrum

Spectrum Model (F)

$$F(\lambda) = [I_0(\lambda)\exp(-\tau(\lambda)) + R(\lambda)]\, P_{sc}(\lambda) + P_{bl}(\lambda)$$

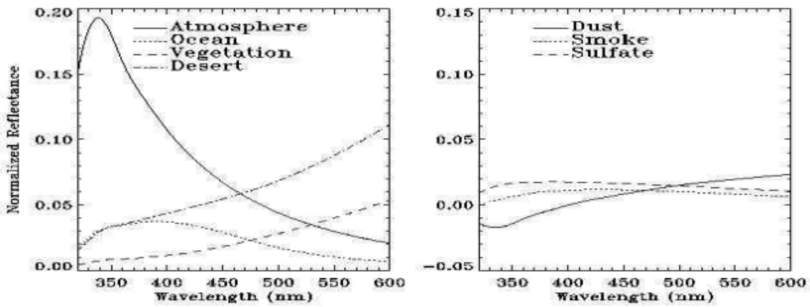
Mean Residual Spectrum

Broad-band Corrections

Spectrum Model (F)

$$F(\lambda) = [I_0(\lambda)\exp(-\tau(\lambda)) + R(\lambda)]\, P_{sc}(\lambda) + P_{bl}(\lambda)$$

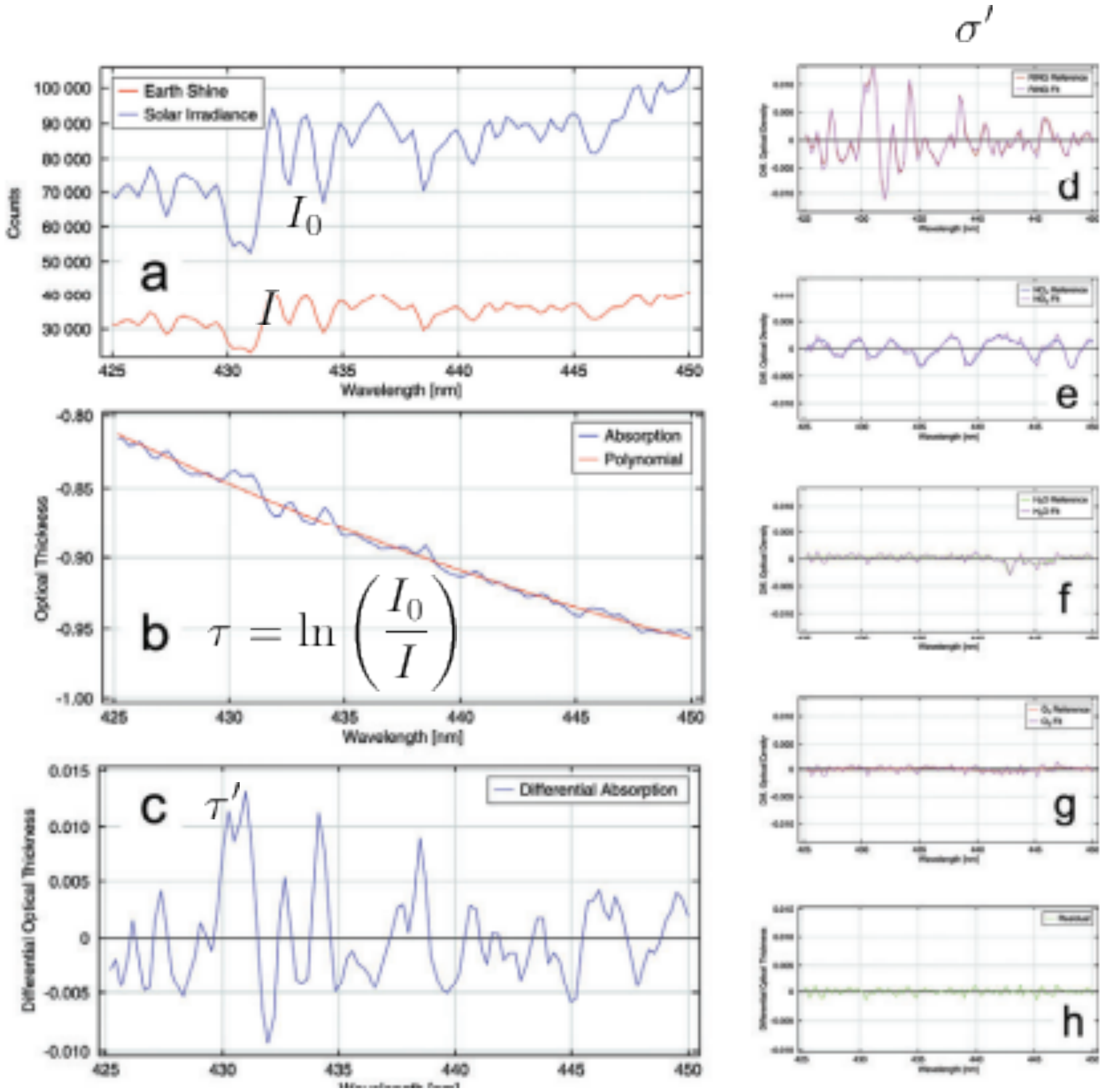
Closure Polynomials – Account for Rayleigh Scattering, Mie Scattering (clouds + aerosols), Wavelength dependence of surface albedo, Instrument errors, Errors in cross sections...



SCD Determination (DOAS)

1) Calculate optical thickness (plot b)
2) Subtract polynomial to get differential optical thickness (plot c)
3) Fit differential optical cross section (also filtered w/ polynomial)

$$\tau' = \sum_i \sigma_i' SCD_i + \sum_p c_p \lambda^p$$



Richter (2006)

Air Mass Factors

Goal: Convert SCDs determined through direct spectral fitting to a more geophysically relevant Quantity – the VCD

The Air Mass factor is the ratio of the slant to vertical column

$$A = \frac{N_s}{N_v}$$

Because the atmosphere is optically thin we can decouple radiative transfer from species concentrations

$$A = \int_0^\infty W(z)S(z)dz$$

Scattering Weights (Radiative Transfer Model)

Species Vertical Profile (Chemical Transport Model)

AMF Slides Stolen from Colette Heald

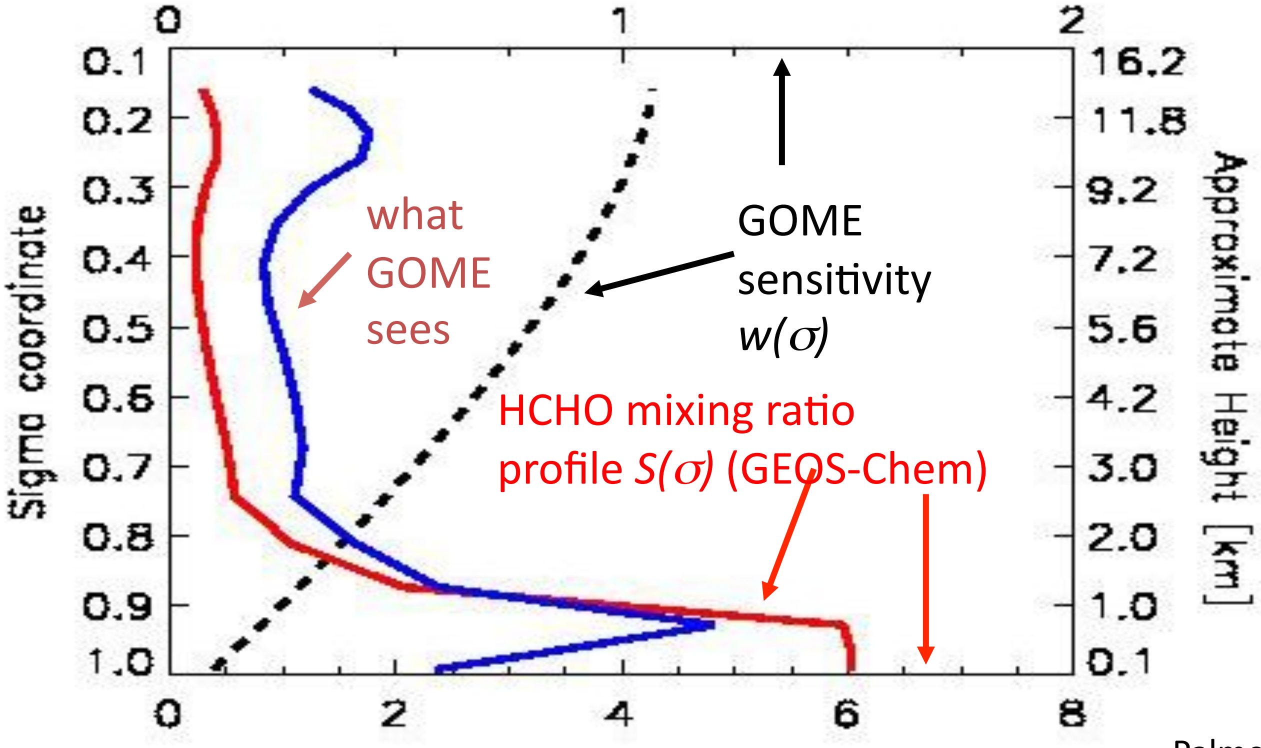
http://www.atmos.colostate.edu/~heald/teaching.html

AMF FORMULATION FOR A SCATTERING ATMOSPHERE

$$AMF = AMF_G \int_0 S(z)\, w(z)\, dz$$

Account for vertical instrument sensitivity (scattering increases towards the surface, inhibits the view of the lower atmosphere) + how this is convolved with the distribution of species X

Example from GOME formaldehyde (HCHO) measurements



what GOME sees

GOME sensitivity $w(\sigma)$

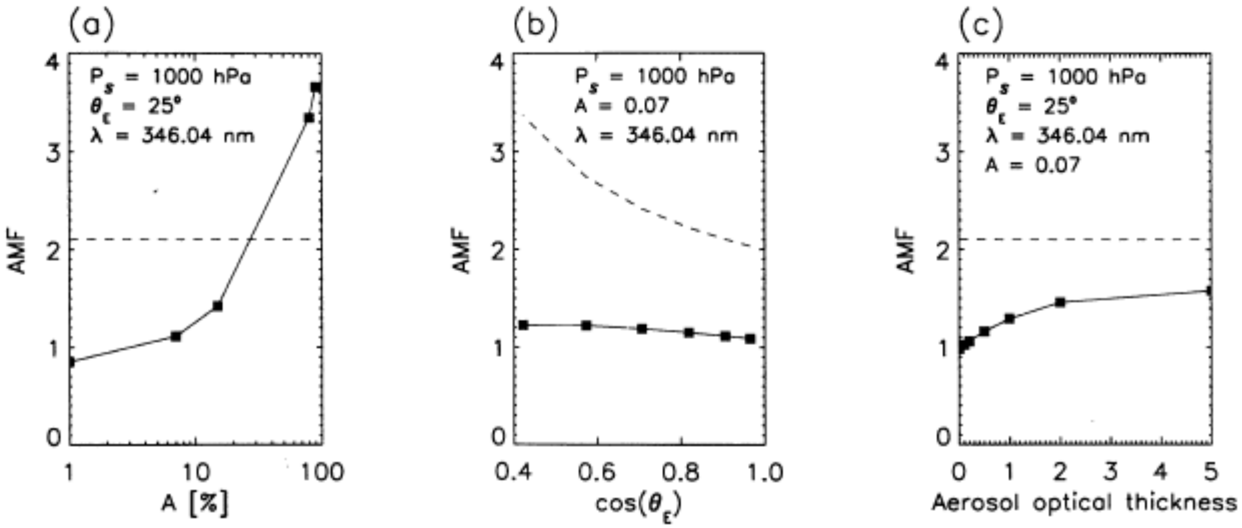
HCHO mixing ratio profile $S(\sigma)$ (GEOS-Chem)

$AMF_G = 2.08$
actual $AMF = 0.71$

Palmer et al., 2001

WHAT ARE AMFs SENSITIVE TO?

Scattering weights are most sensitive to the surface albedo and aerosol loading



Palmer et al., 2001

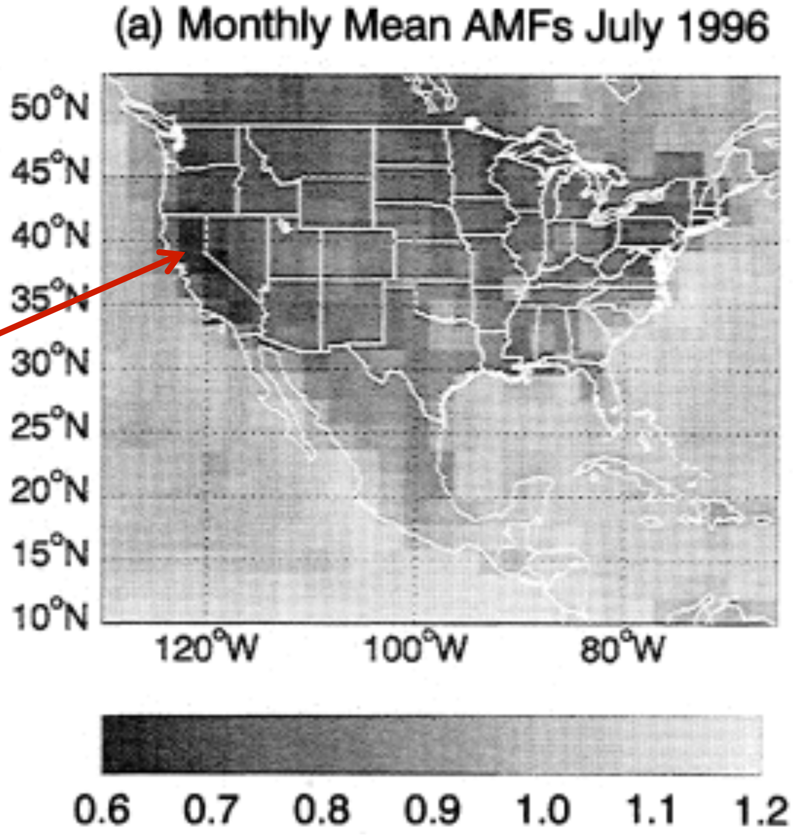
- Increasing A allows more solar radiation into the lower atmosphere = increasing observational sensitivity
- Relatively insensitive to angle between sun & satellite (θ_E): with larger angle physical path increase (AMF_G larger) but scattering along the path reduces the sensitivity
- Aerosols increase the sensitivity to HCHO in this example: increasing AOD from 0.1 to 1.0 (typical range) increases AMF by 30%

Scattering decreases the sensitivity to species
AMF is typically ½ AMF_G

HOW VARIABLE ARE AMFs?

If most of the species X is in the BL, where the instrument is not as sensitive, the AMF will be lower to compensate → ocean AMFs are higher than over land

Continuing with our HCHO example…



Also see particularly low AMFs in California due to shallow BL

Given this variability, it is inappropriate to use single S(z) for tropospheric species

* We should all be grateful that journals no longer charge for on-line colour

Palmer et al., 2001

RETRIEVAL CONSIDERATIONS

1. CLOUDS: Cloud droplets scatter radiation and complicate the interpretation…

Generally try to filter for < 40% cloudy conditions to ensure higher quality retrievals

2. AEROSOLS: Important sensitivity to aerosols means it's important to include these in the scattering weight calculations.

3. ARTIFACTS: GOME solar diffuser plate bias: daily varying global bias – tricky correction!

4. STRATOSPHERIC CONTRIBUTION: For species with significant part of the column in the stratosphere, must develop a technique to remove this contribution.

4. SHAPE FACTOR: continual improvement of shape factors from model. Also shape factors may vary at spatial scales higher than represented by models…

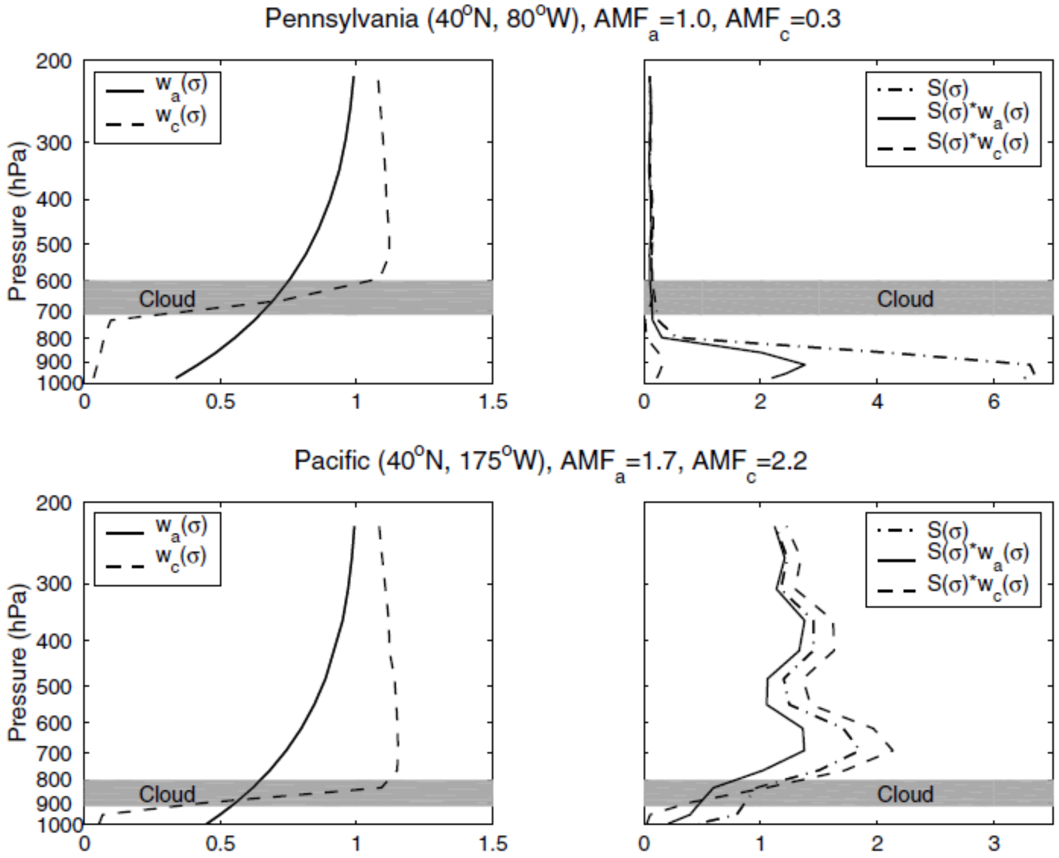
THE ROLE OF CLOUDS

Clouds enhance sensitivity to species above clouds and reduce (obscure) sensitivity for below cloud

Early retrievals tried to limit cloud contamination by keeping $F_{cloud}<40\%$

Later techniques: more sophisticated approach to separately estimate AMF for cloudy & clear scenes and combine based on cloud fraction

$$A = \frac{A_{clr} R_{clr} (1 - f) + A_{cld} R_c f}{R_{clr} (1 - f) + R_{cld} f}$$



clr=clear-sky
cld=cloudy
R=reflectivity
f=cloud fraction

Advantages:
(1)correct cloud effects on backscatter
(2) retrieve in partly cloud scenes

Martin et al., 2002

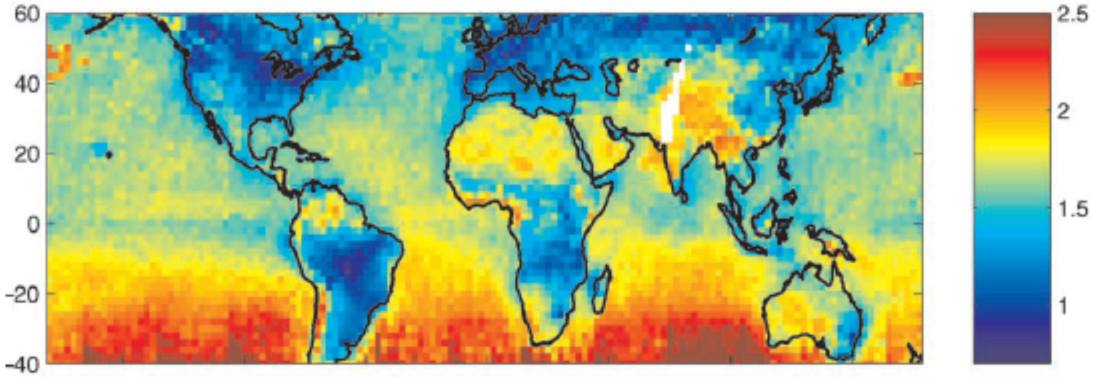
VARIABILITY OF AMFs and CLOUDS

$AMF_c > AMF_a$ when little NO_2 is below the cloud (oceans)

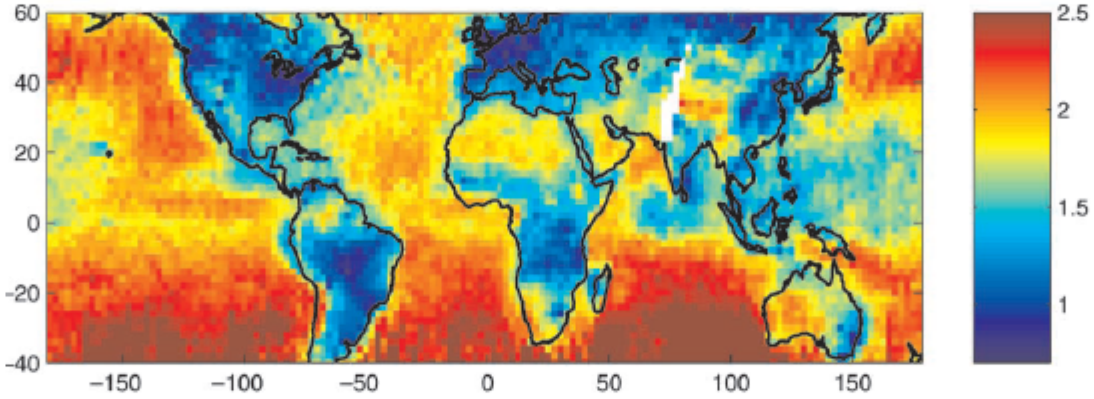
$AMF_c < AMF_a$ when cloud obscures BL NO_2 (land)

July AMFs for NO_2

Clear-sky AMFs



Actual AMFs (accounting for clouds)



Note high spatial variability in the cloud correction

Martin et al., 2002

Satellite Retrieval Error Budgets

UV-Vis Retrieval Error Budget

The Vertical column density (N_v) for a typical UV-Vis retrieval is given by

$$N_v = \frac{N_s - N_{s0}}{A} + N_{v_0}^{CTM}$$

Assuming that errors in the slant column, AMF and background VCD are uncorrelated the error in the vertical column is

$$\sigma_{N_v}^2 = \left(\frac{\partial N_v}{\partial N_s} \underset{\uparrow}{\sigma_{N_s}} \right)^2 + \left(\frac{\partial N_v}{\partial A} \underset{\uparrow}{\sigma_A} \right)^2 + \left(\frac{\partial N_v}{\partial N_{v_0}} \underset{\uparrow}{\sigma_{N_{v0}^{CTM}}} \right)^2$$

Error from the spectrum fit

Error in AMF Calculation

Error in Model Background

Slant Column Retrieval Error (σ_{Ns})

In our slant column retrieval we fit a set of variables **x** to a spectrum of radiance values **y**. These are related by a forward function **f**

$$y = f(x,b) + \varepsilon$$

We employ a retrieval method **R** (e.g. least squares fit to spectrum) to estimate **x**

$$\hat{x} = R(y,\hat{b},x_a)$$

In practice we use a Forward model **F** that approximates the forward function with error **Δf**

$$F(x,b) = f(x,b) - \Delta f(x,b)$$

After linearising the forward model and retrieval method we arrive at

$$\hat{x} = (I - A)x_a + Ax + G_y\left(K_b(b - \hat{b}) + \Delta f + \varepsilon\right)$$

Where $G_y = \frac{\partial R}{\partial y}$ $K_b = \frac{\partial F}{\partial b}$ $A = G_y \frac{\partial F}{\partial x}$

Slant Column Retrieval Error (σ_{Ns})

If the errors in the spectrum are not weighted, A=I

$$\hat{x} = x + G_y\left(K_b(b - \hat{b}) + \Delta f + \varepsilon\right)$$

Parameter Errors **Forward Model Errors** **Random Noise**

We can now propagate these errors to understand their impact on x

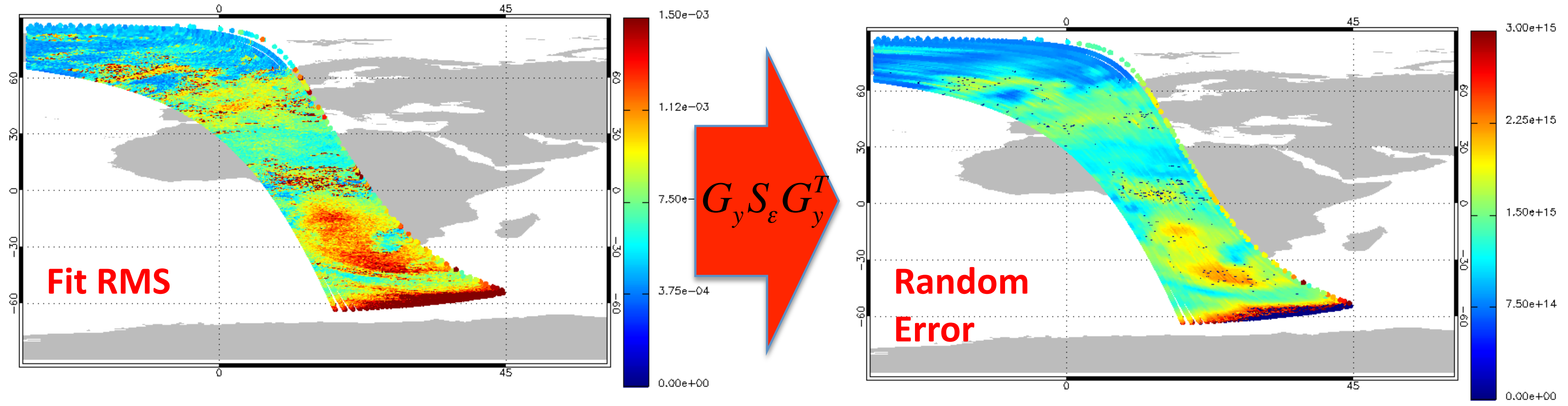
Random Noise	$G_y S_\varepsilon G_y^T$
Parameter Errors	$G_y K_b S_b K_b^T G_y^T$
Forward Model Errors	$G_y S_{\Delta f} G_y^T$

Random Noise Error

$$G_y S_\varepsilon G_y^T$$

We can estimate the error covariance matrix for random noise from the fit residuals.

$$S_\varepsilon = \left(\frac{n}{m - n + 1} RMS^2 \right) \bullet I_{m \times m}$$

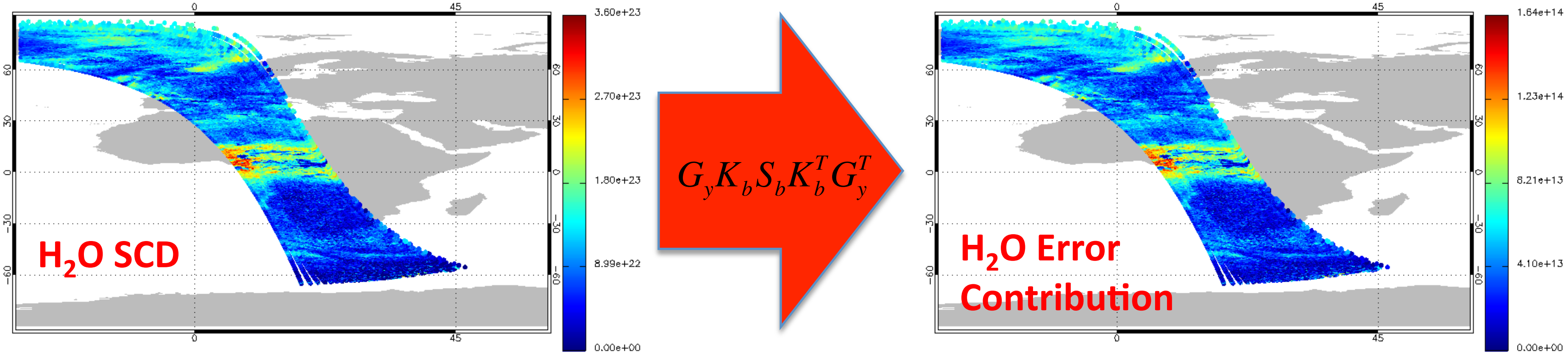


This error can be beaten down by space/time averaging

$$\overline{\sigma} = \frac{\sigma}{\sqrt{\# \, measurements}}$$

Fitting Parameter Error

S_b is computed from the relative errors specified from the literature. It is assumed that there is no covariance between cross section values at different wavelengths (though there may be due to common experimental conditions). Since there should not be covariance between different reference cross sections, S_b takes a block diagonal form, allowing total parameter error to be decomposed into the contributions from different interfering species.



$$G_y K_b S_b K_b^T G_y^T$$

These errors are systematic as the same cross sections are used for each spectrum fit

Forward Model Errors $G_y S_{\Delta f} G_y^T$

Errors due to not simulating the correct physics. These errors are tricky to estimate

For the UV-Vis retrievals the forward model is given by

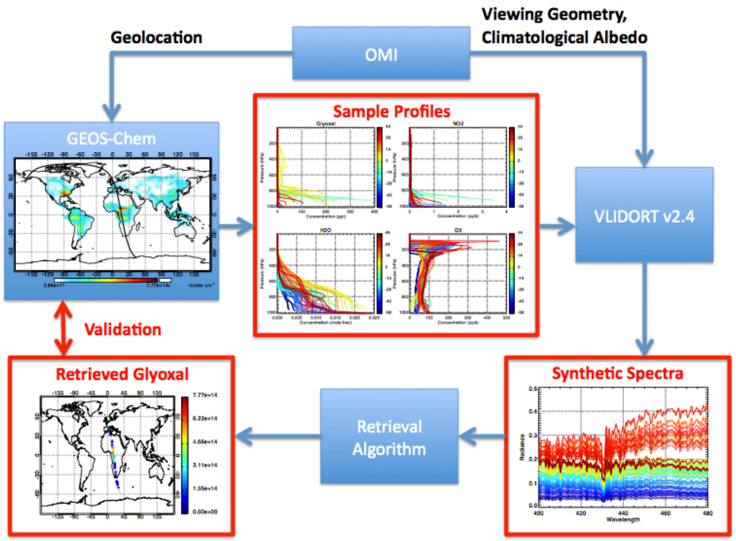
$$F(\lambda) = [I_0(\lambda)\exp(-\tau(\lambda)) + R(\lambda)]\,P_{sc}(\lambda) + P_{bl}(\lambda)$$

Source Spectrum **Gas Absorption**

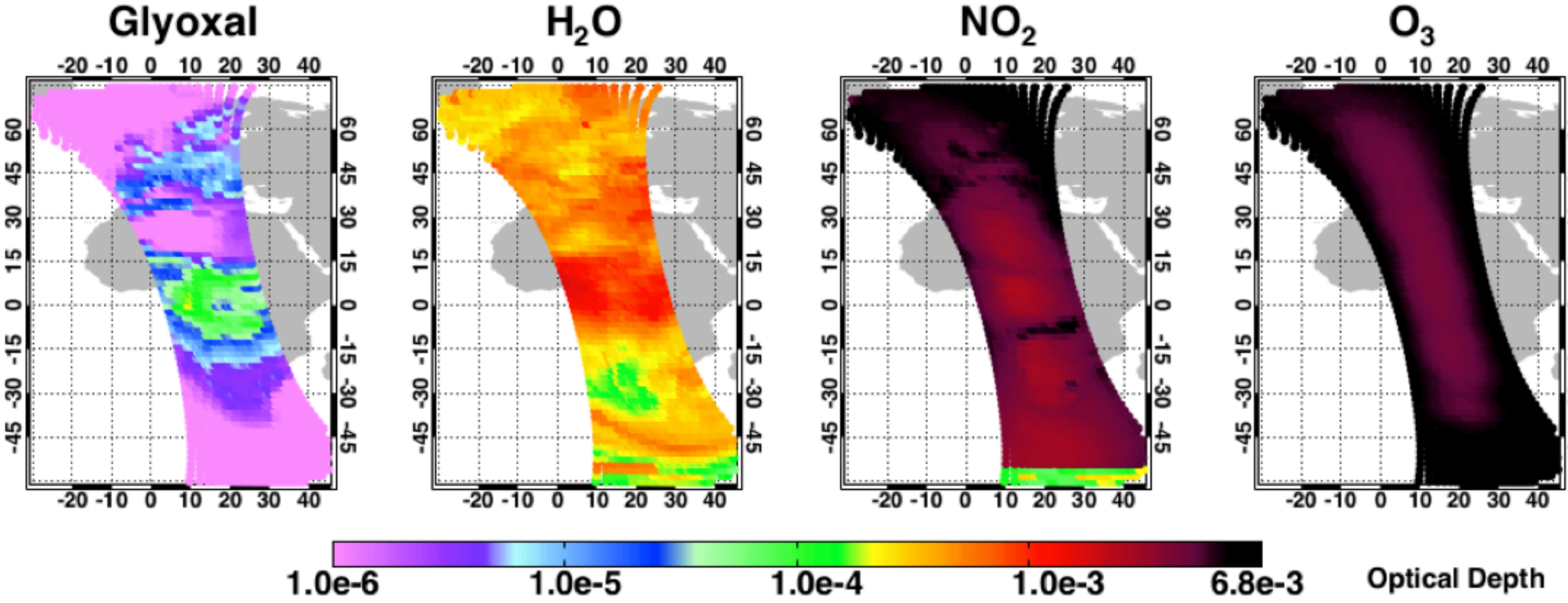
Empirical Polynomial Corrections

Q_m accounts for instrument baseline offsets
P_n accounts for many physical phenomena
- Rayleigh & Mie Scattering
- Wavelength dependent surface reflectance
- Instrument effects (e.g. detector efficiencies)

Other potential error sources
- Higher order Raman Scatter
- Ignored absorbers
- Wavelength dependence of slant column densities

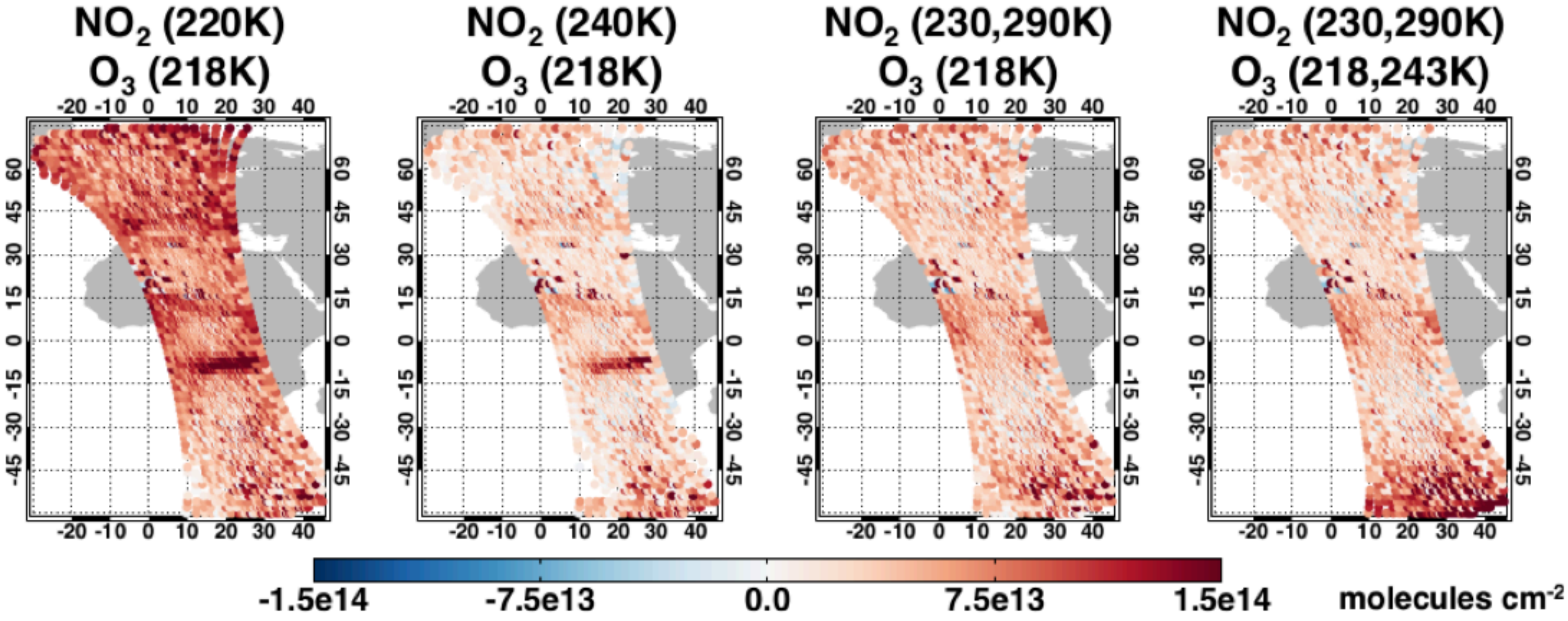


Glyoxal optical depths are really low relative to interfering species



Small errors in fitting other species can lead to big errors in retrieved glyoxal!

Cross Section Temperature Dependence



NO_2 (220K) O_3 (218K)

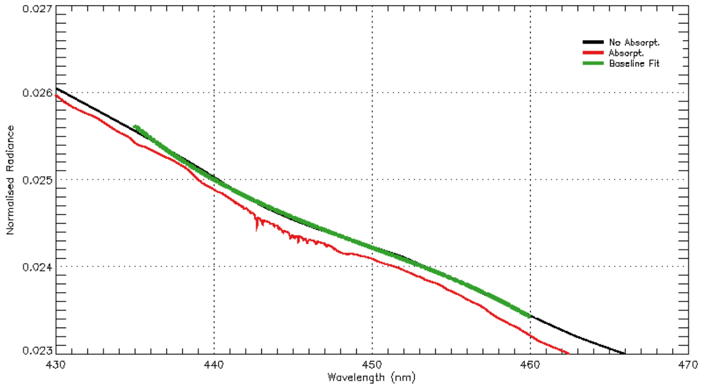
NO_2 (240K) O_3 (218K)

NO_2 (230,290K) O_3 (218K)

NO_2 (230,290K) O_3 (218,243K)

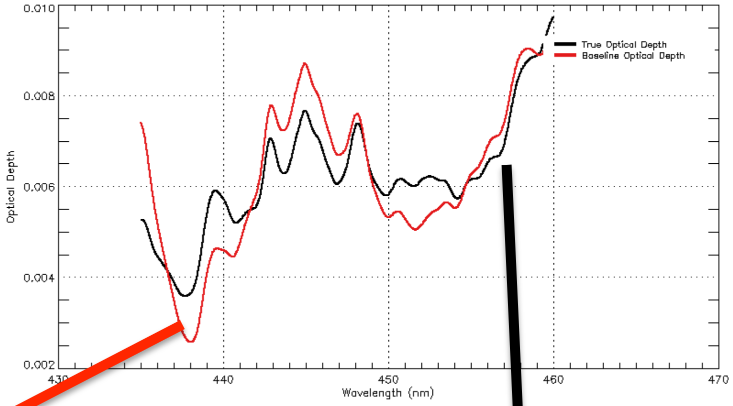
Importance of Broad Band Corrections

Baseline Fit (Pure Rayleigh Atmosphere)

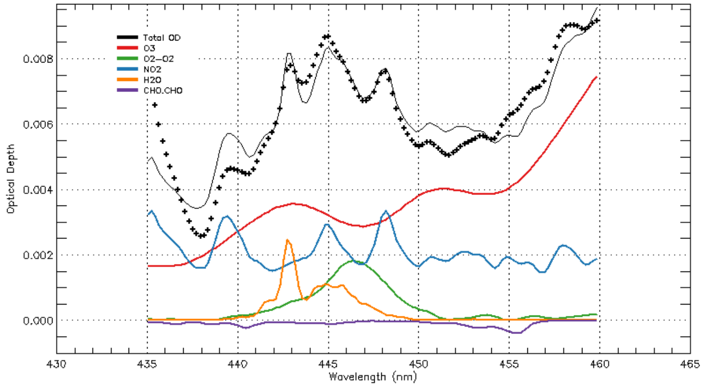


$$\tau = \ln\left(\frac{I_0}{I}\right)$$

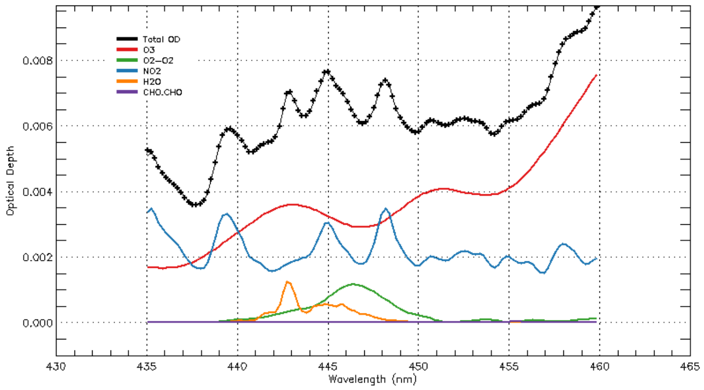
Total Optical Depth



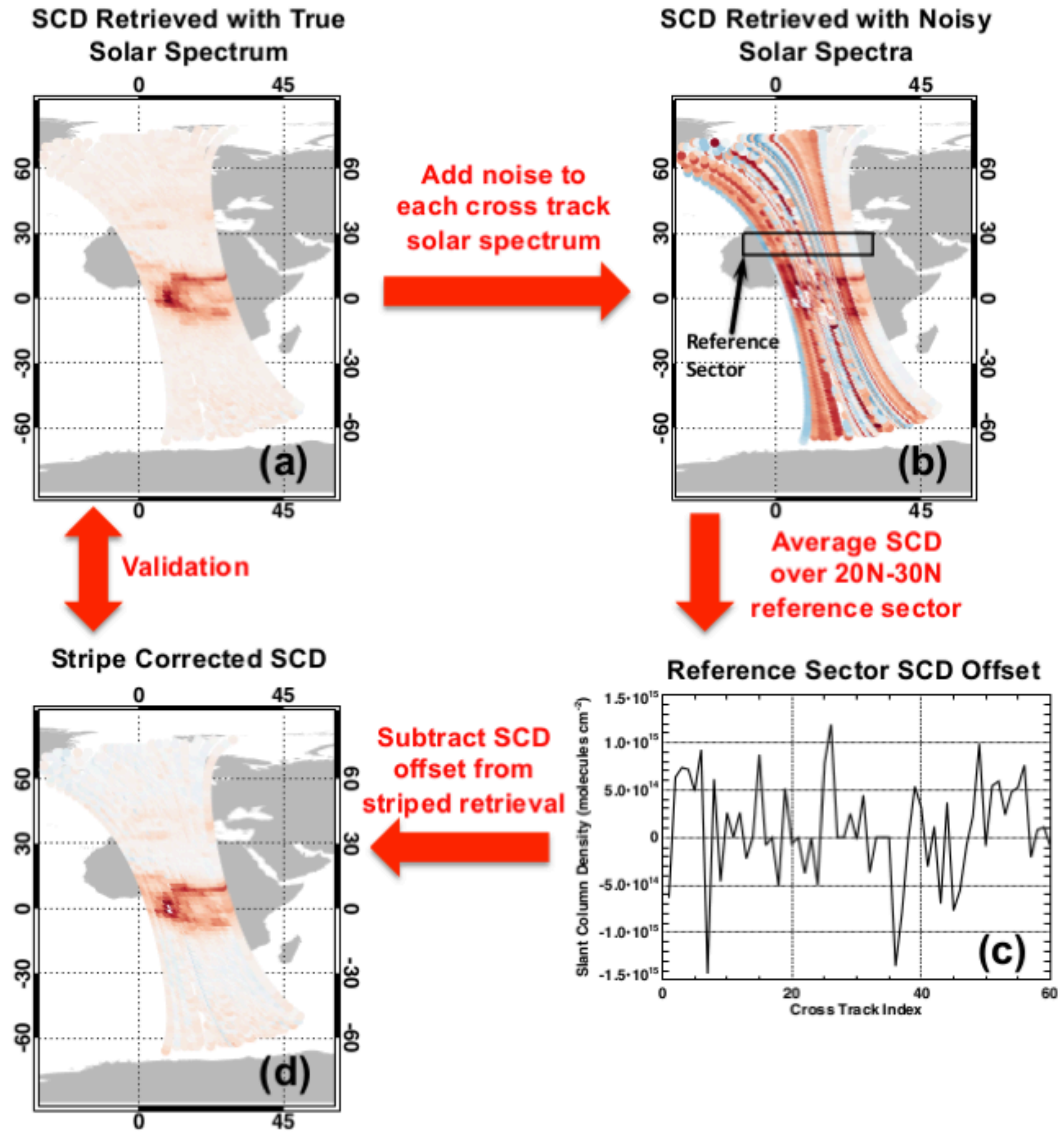
OD Fit with Polynomial Baseline



OD Fit with True Baseline

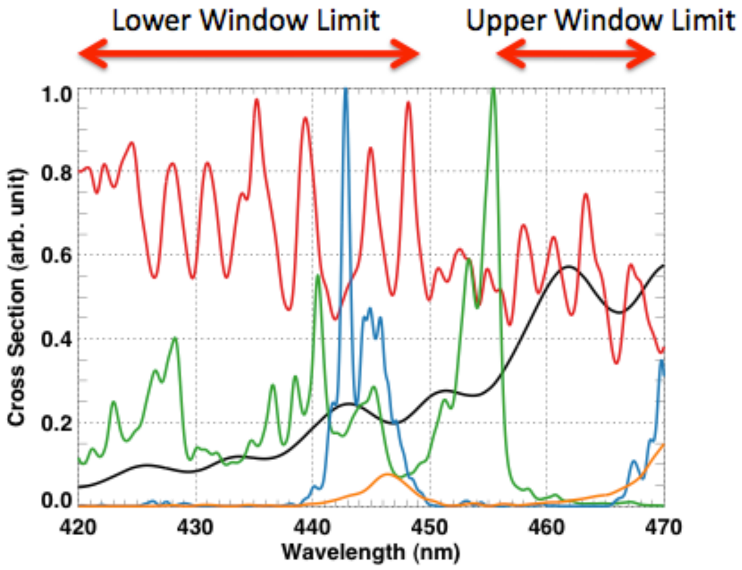


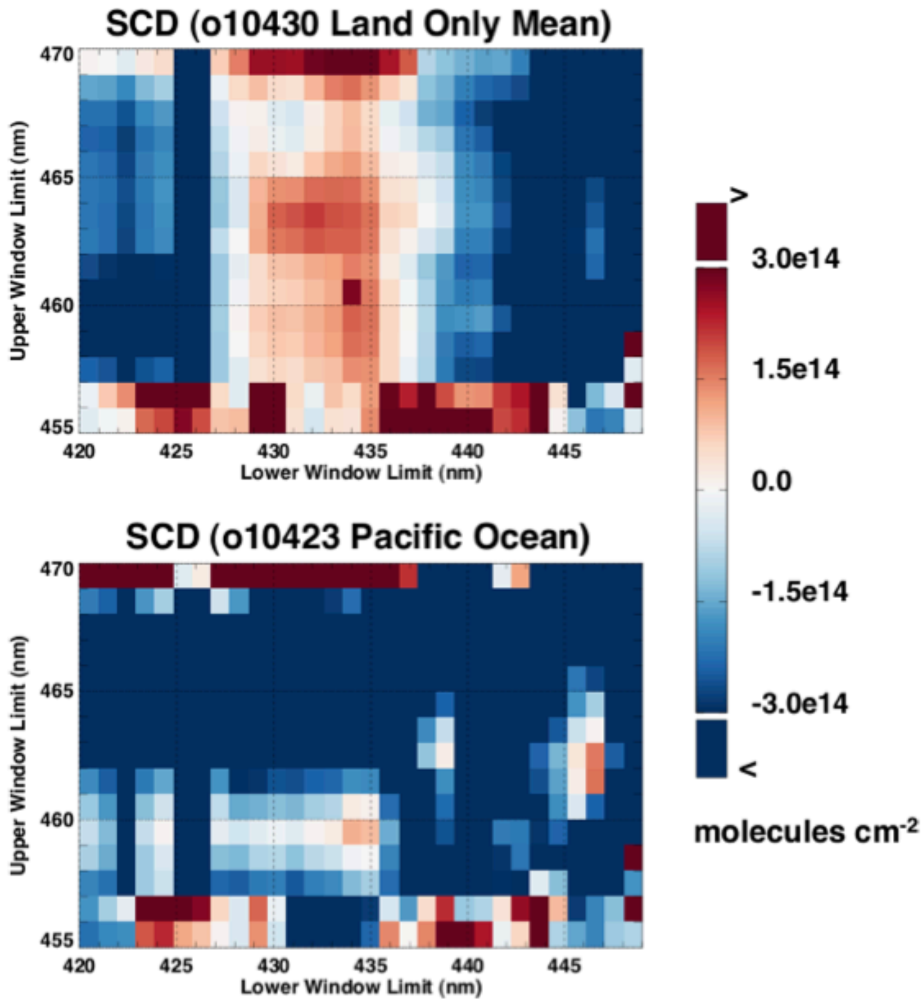
Background Offsets are induced by Noise in the Solar Spectrum



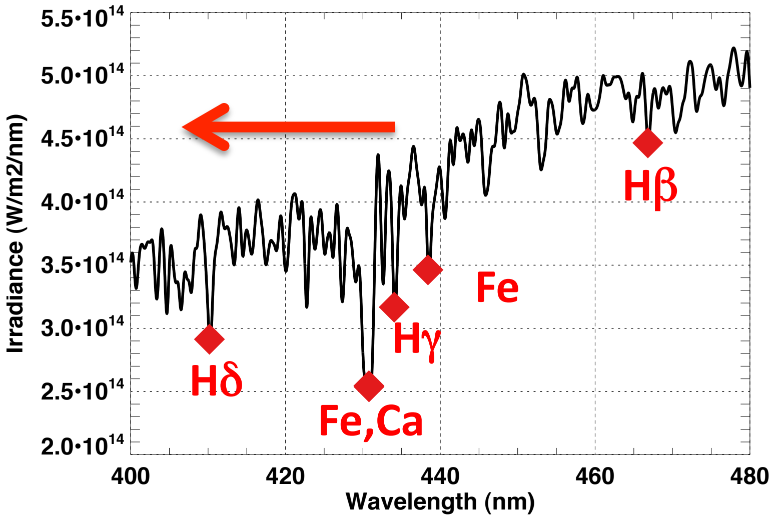
Since OMI measures 60 spectra across track, there are 60 offsets (stripes)

Retrieval Dependence on Fit Window

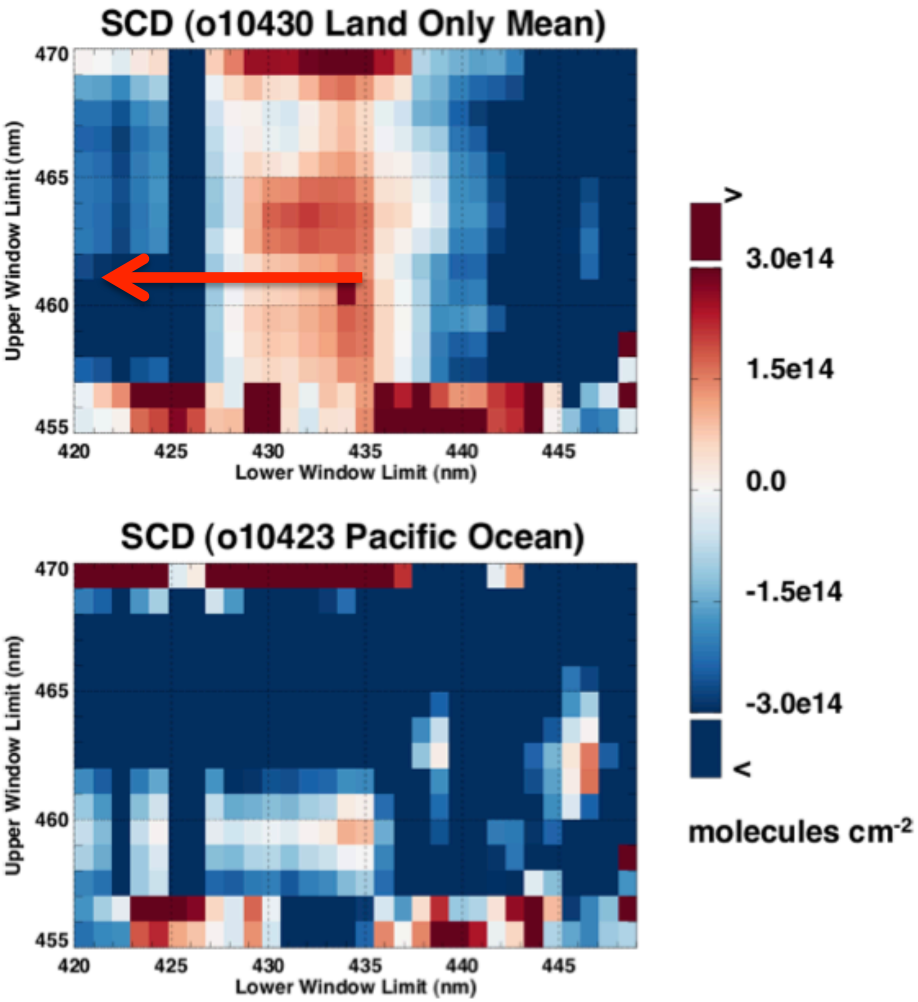




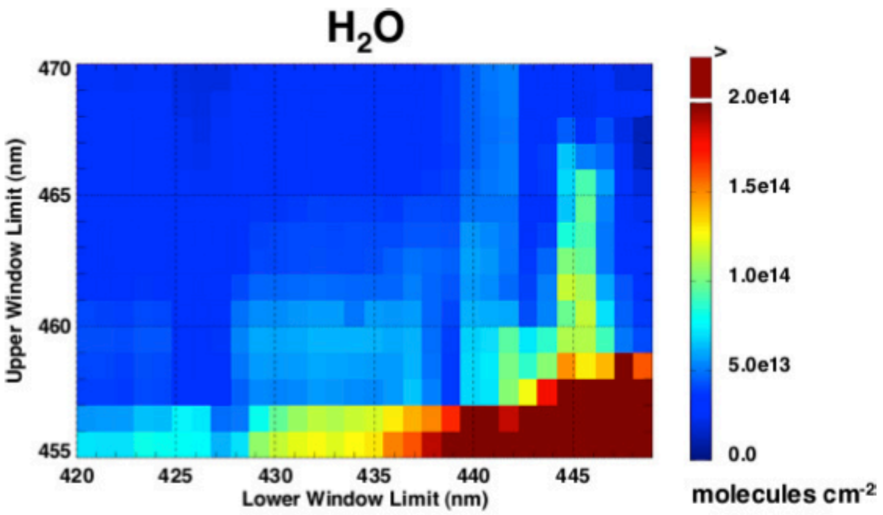
Retrieval Dependence on Fit Window

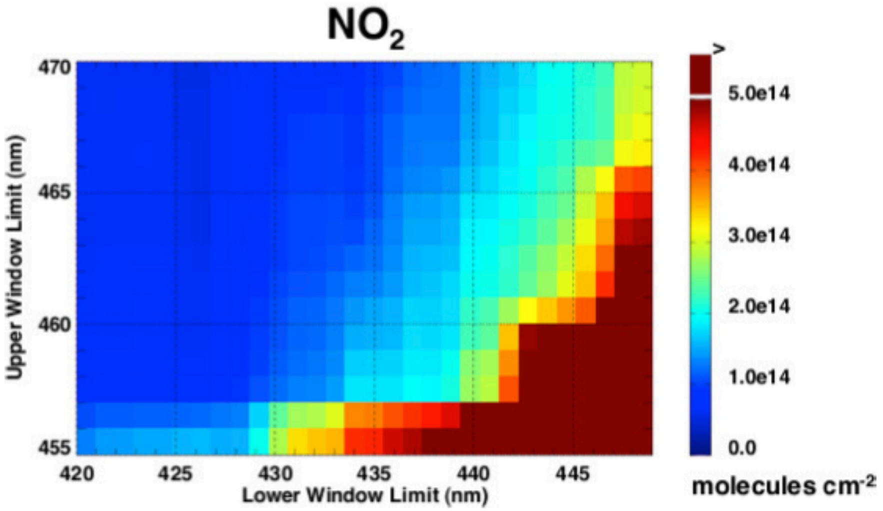


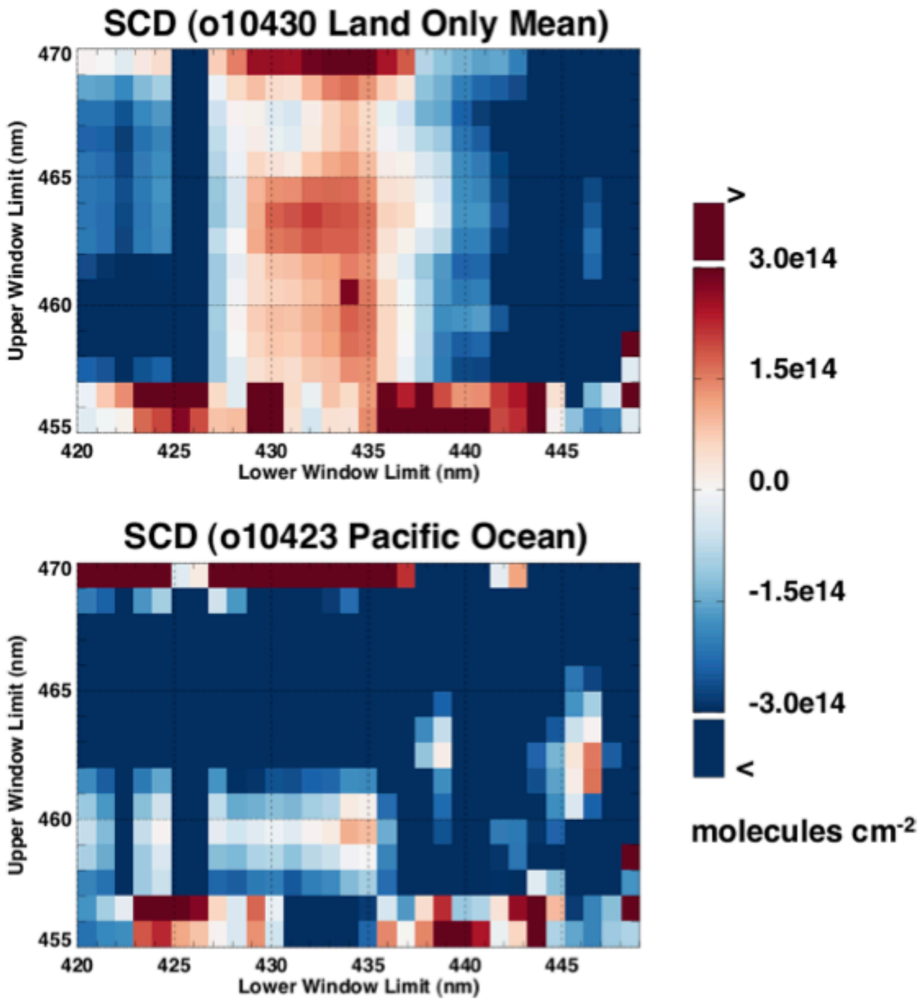
Strong Solar lines below 435nm
Interference from inelastic scattering?



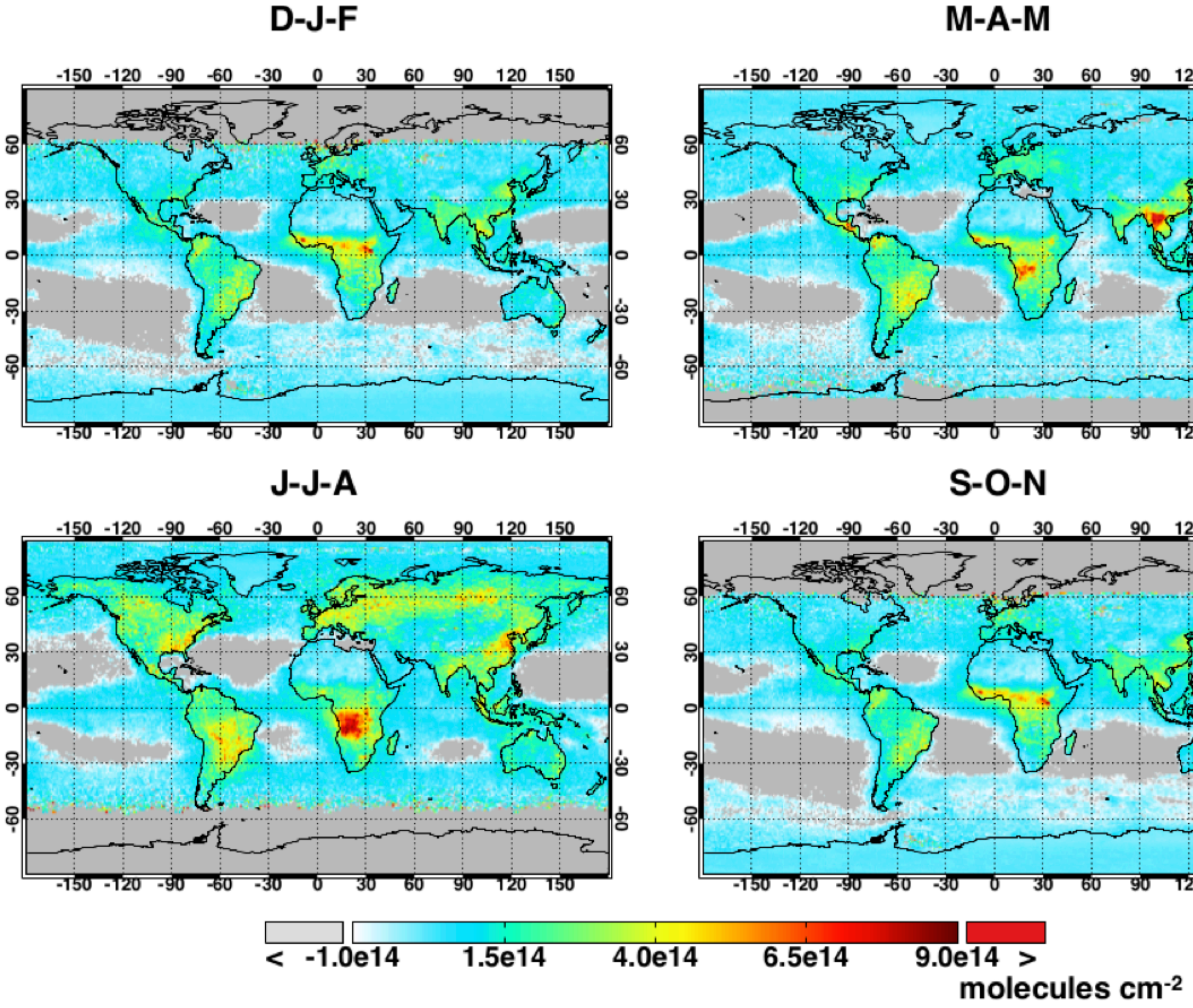
Retrieval Dependence on Fit Window







Retrieval errors above 435nm may be due to cross section error


D-J-F
M-A-M
J-J-A
S-O-N
-150
-120
-90
-60
-30
0
30
60
90
120
150
60
30
0
-30
-60
< -1.0e14
1.5e14
4.0e14
6.5e14
9.0e14 >
molecules cm-2