NIWA
Taihoro Nukurangi

MAX-DOAS NO_2 profiles

Tim Hay [1,2], Paul Johnston [1], Karin Kreher [1],
Alan Thomas [1], Robyn Schofield [3],
Adrian McDonald [2]

(1) NIWA, Lauder, New Zealand
(2) University of Canterbury, Christchurch, NZ
(3) Alfred Wegener Institute, Potsdam, Germany

CINDI

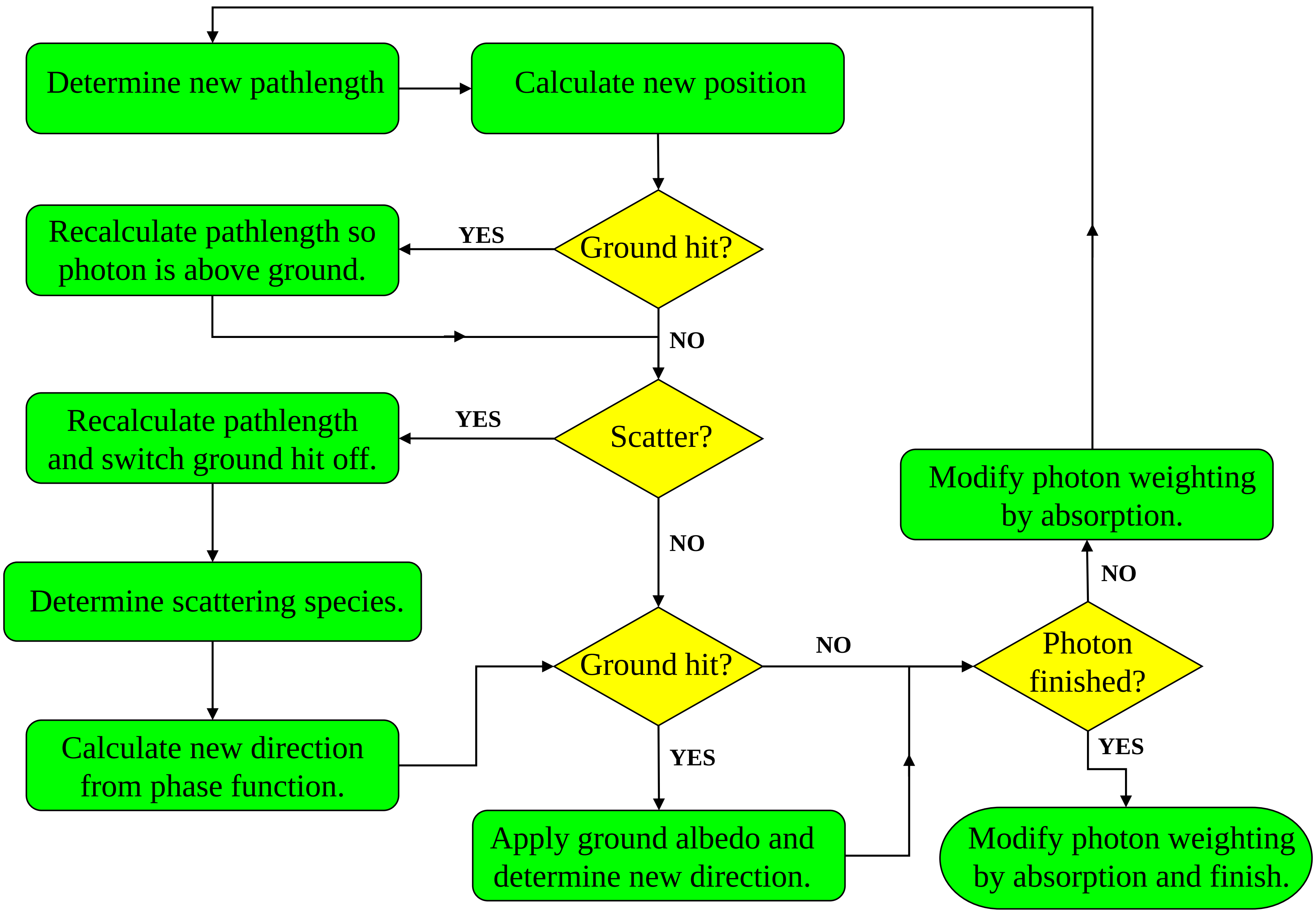
Outline

- Forward model - radiative transfer
- Retrieval algorithm
- Results – profiles
- Summary

Forward Model - Radiative Transfer

- NIMO spherical Monte Carlo RTM
- Calculates radiances and box AMFs
- Input parameters:
  - P,T profiles
  - Trace gases: σ, ρ profiles
  - Aerosol: *k* profile, ω, and g for $P_{HG}(\theta)$
  - Wavelengths
  - Surface albedo, instrument altitude, topography (DEM)
  - Field of view
  - SZAs, azimuths and elevation angles

Core ray tracing algorithm



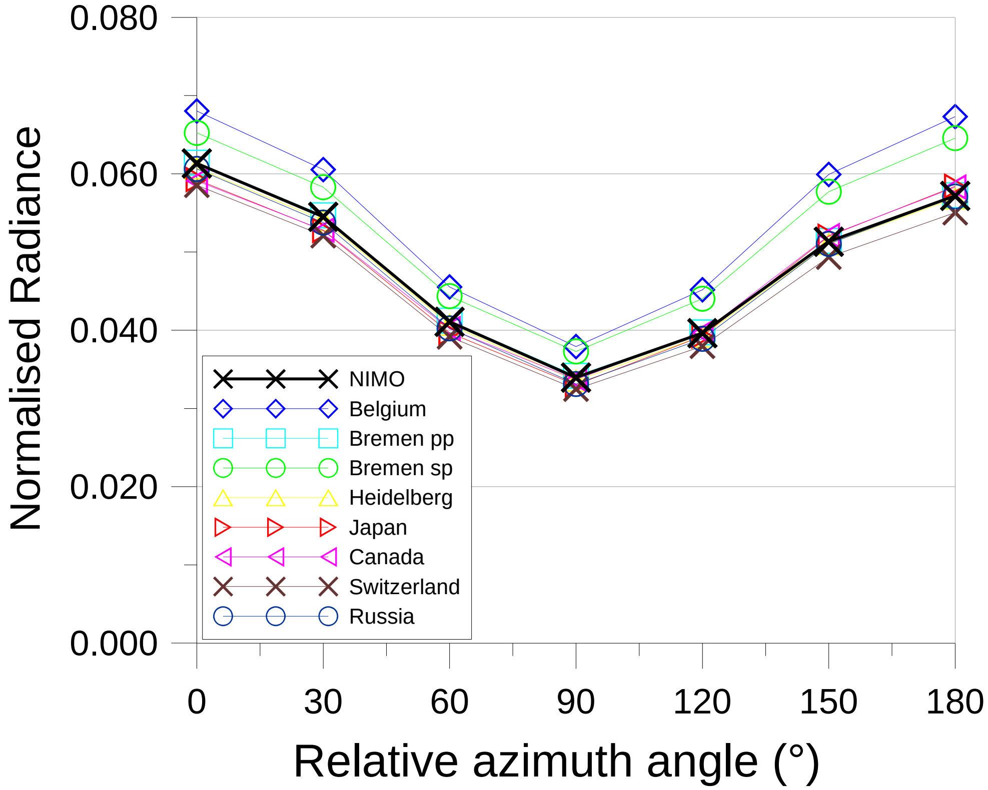
Path calculation

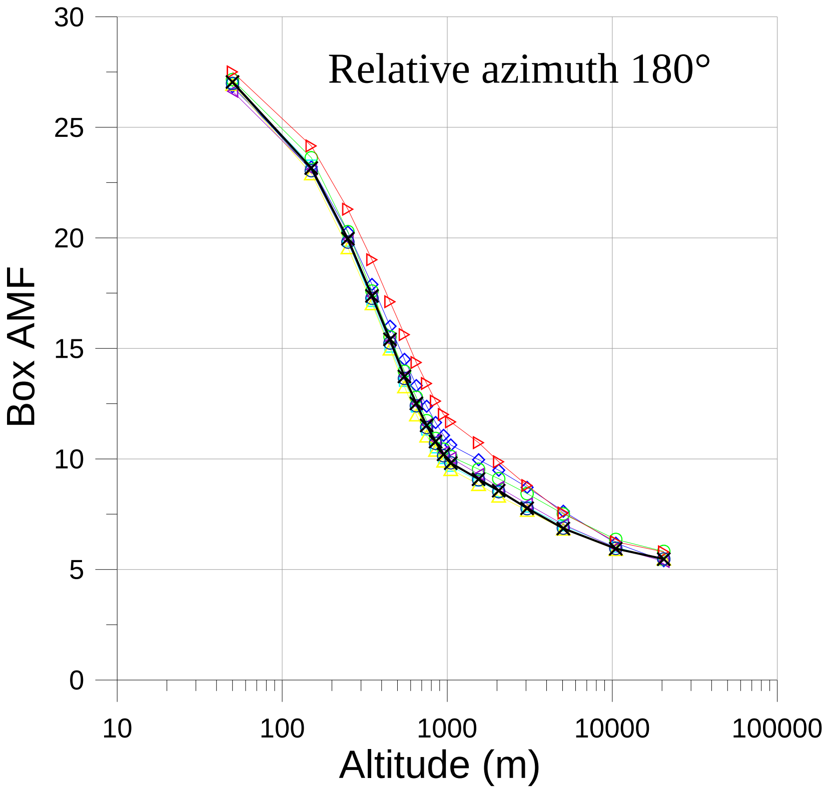
- An altitude grid is selected or read in from a file.
- The photon path is retraced to determine the pathlength through each layer.
- The pathlengths are weighted by the normalized intensity of the photon.
- The LZA in each layer is determined from geometry and a small correction is made for refraction.
- The mean, intensity-weighted paths are then:

$$Path_z = \frac{\sum_{i=1}^{m} \xi_i \cdot l_i}{\sum_{i=1}^{m} \xi_i}$$

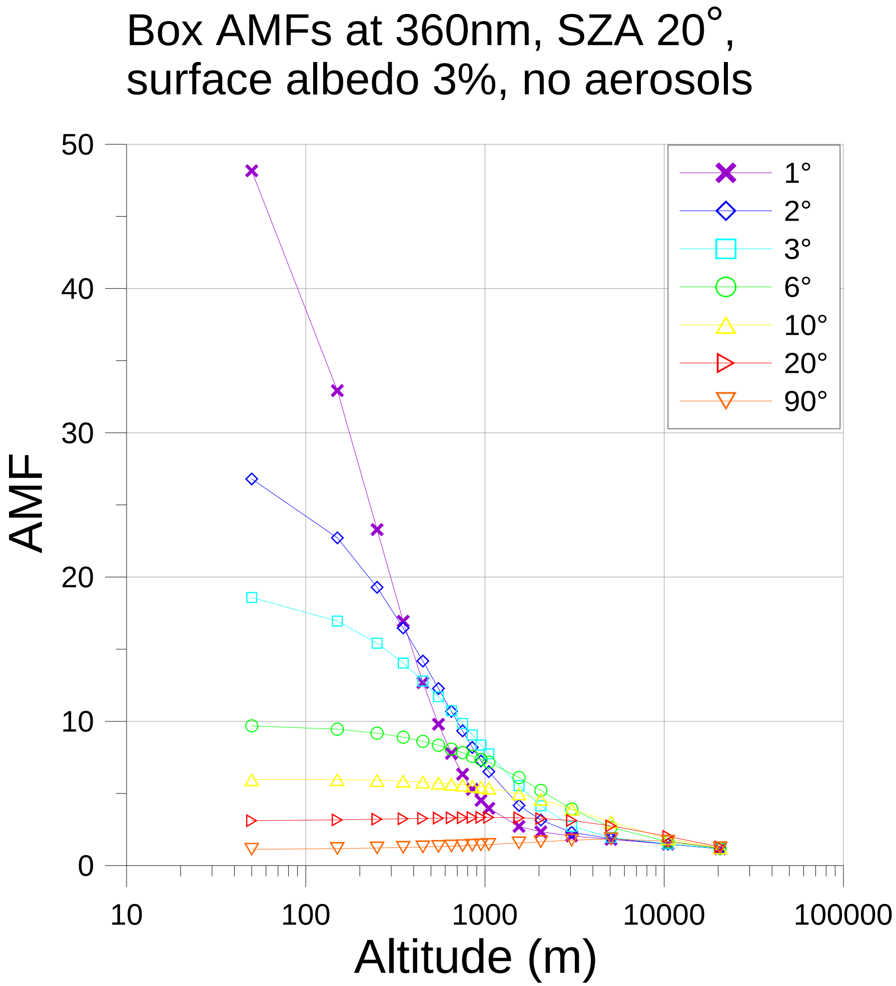
RTM comparison – Wagner et al. 2007

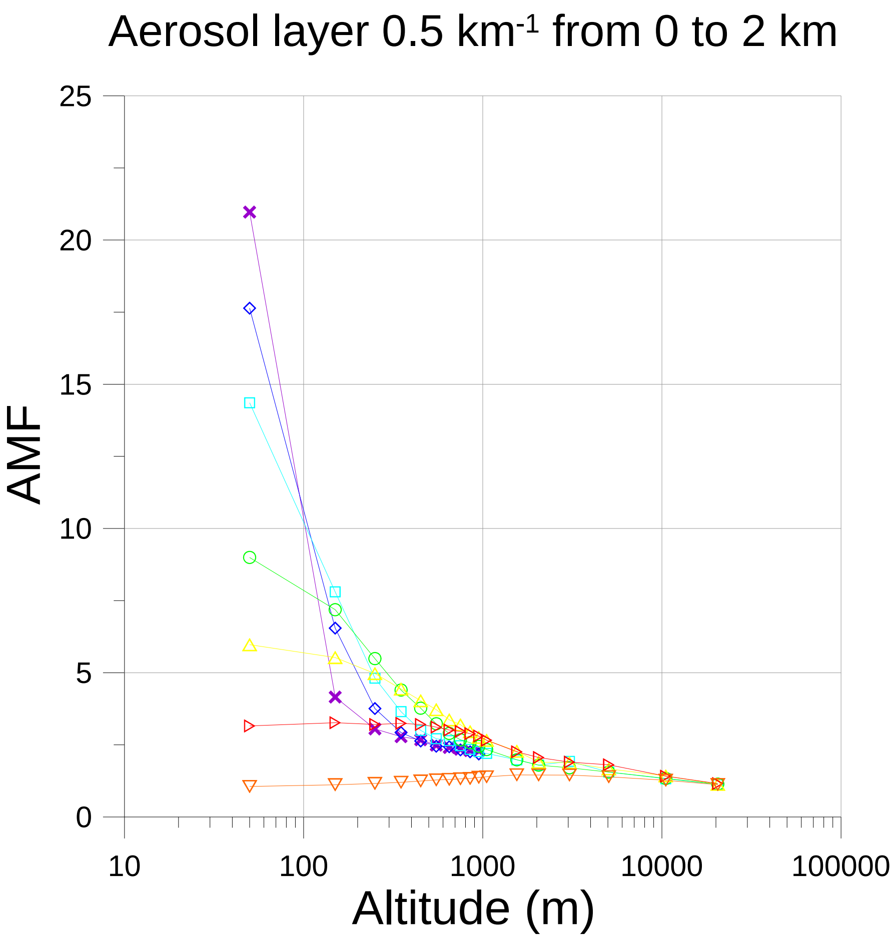
- 577 nm, SZA 80°, elevation 2°, surface albedo 3%
- Aerosol layer 0.1 km-1 from 0 to 1 km



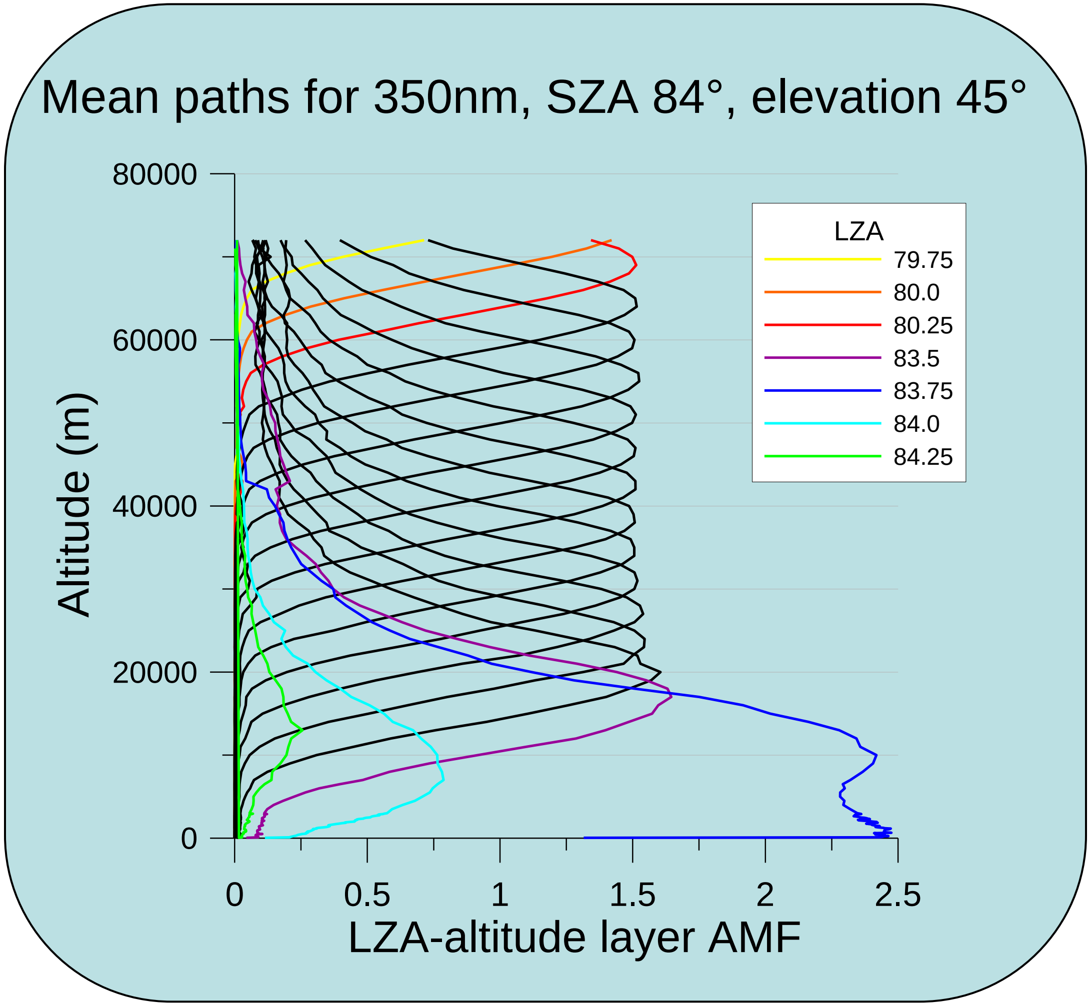


Sensitivity to elevation angle and aerosols





Forward Model – Weighting Functions



- Mean intensity weighted pathlengths in each layer.
- 40m layers, 0.25° LZA step
- One NIMO table for each geometry.
- One altitude profile for each LZA interval.
- Σ paths over all LZAs = box-AMF x Δz.

SCD calculation

- For each measurement SZA and azimuth calculate F(x) :

$$I = \prod_{\vartheta=1}^{m} \prod_{z=1}^{n} \exp\left[-\ (k_0 + \sigma \cdot \rho(\vartheta, z)) \cdot L(\vartheta, z)\right]$$

$$I^* = \prod_{\vartheta=1}^{m} \prod_{z=1}^{n} \exp\left[-\, k_0 \cdot L(\vartheta, z)\right]$$

  - $k_0(z) = \Sigma\, [k_{Ray}(z) + k_{HG}(z) + k_{O3}(z) + k_{\mathrm{other}}(z)]$
  - σ – cross-section of the absorber
  - ρ – absorber density at LZA index θ, altitude layer z
  - L – mean intensity weighted pathlength for θ, z

- From Lambert-Beers Law :

$$\mathrm{SCD} = \frac{1}{\sigma}\left(-\ln\left(\frac{I}{I^*}\right)\right)$$

Weighting functions

- $\mathbf{K} = \delta\mathbf{y} / \delta\mathbf{x}$ = sensitivity of measurements to state vector
- $y = DSCD = SCD_{Off\text{-}Axis} - SCD_{reference}$

1) Start with $\mathbf{x}_a$ = array of ρ profiles at retrieved SZAs
2) Perturb each layer of each profile in turn with a set mixing ratio amount, δx
3) Recalculate DSCDs for all measurement geometries
4) One element of **K** is then: $(y_p - y) / \delta x$
5) Repeat sequence to calculate all rows of K.

The inversion

- Optimal estimation – 'n-form' of non-linear Gauss-Newtonian iteration (Rogers 2000):

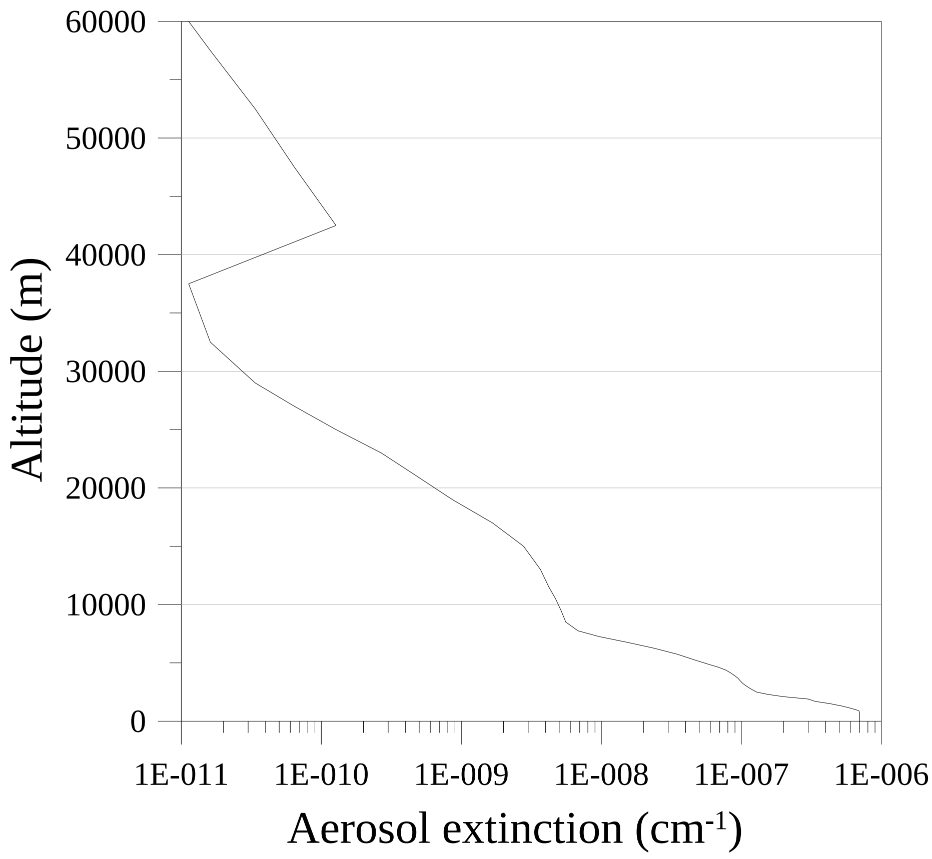
$$\mathrm{x}_{i+1} = \mathrm{x}_a + (\mathbf{S}_a^{-1} + \mathbf{K}_i^T \mathbf{S}_\epsilon^{-1} \mathbf{K}_i)^{-1} \mathbf{K}_i^T \mathbf{S}_\epsilon^{-1} [\mathbf{y} - \mathbf{F}(\mathrm{x}_i) + \mathbf{K}_i (\mathrm{x}_i - \mathrm{x}_a)]$$

- $\mathbf{S}_\varepsilon$ = measurement error covariance matrix
- $\mathbf{S}_a$ = *a priori* error covariance matrix

- Repeat forward model with new x_i ⟹ new **K** and $\mathbf{F}(x_i)$
- Convergence when $\mathbf{K}d\mathbf{x} < 0.2 \sqrt{\mathbf{S}_\varepsilon}$ ⟹ FM: final **K**, $\mathbf{F}(x_i)$

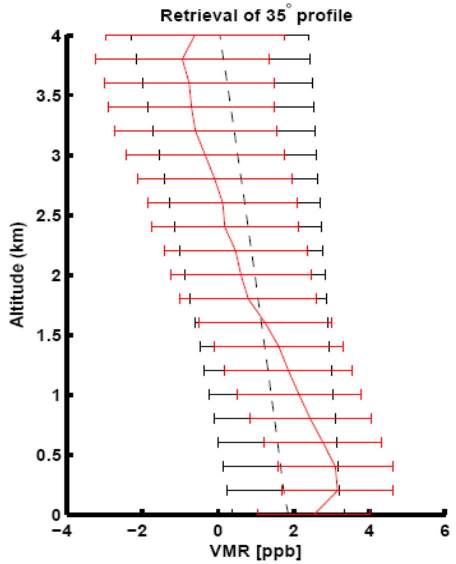
Settings

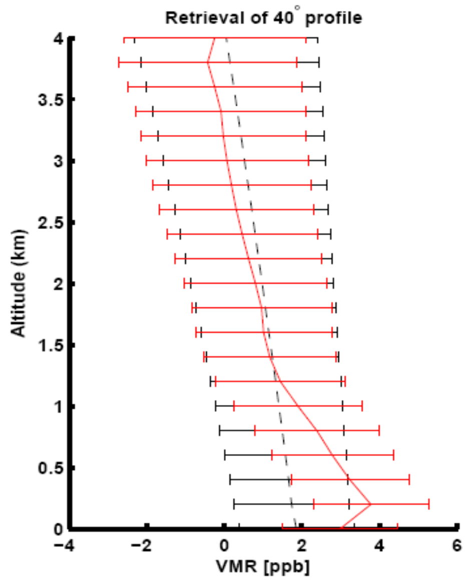
Prescribed Aerosol profile

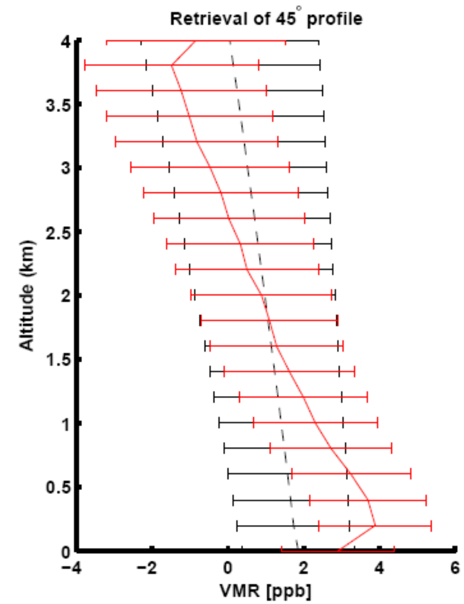


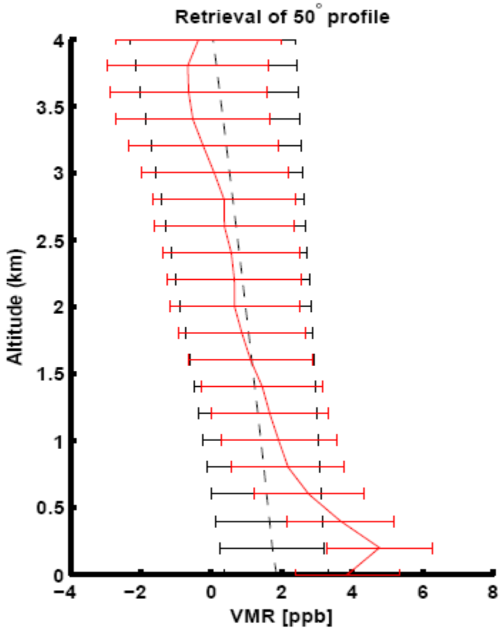
- Fixed *a priori* profile of 2ppb at surface to 0.1ppb at 4km
- Covariance error of 0.8

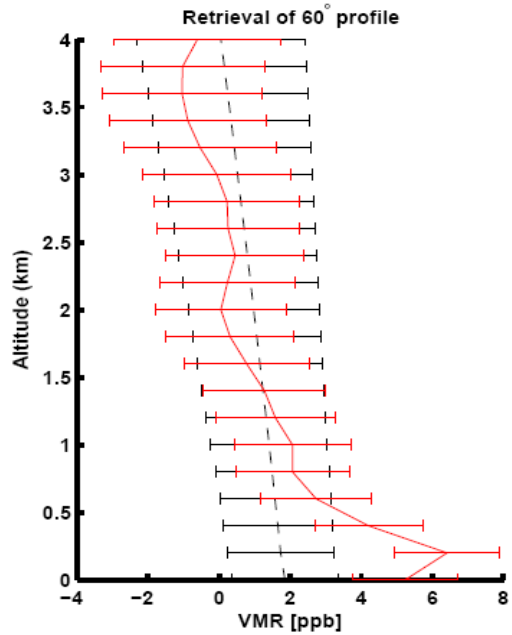
Retrieved profiles for 24th June AM

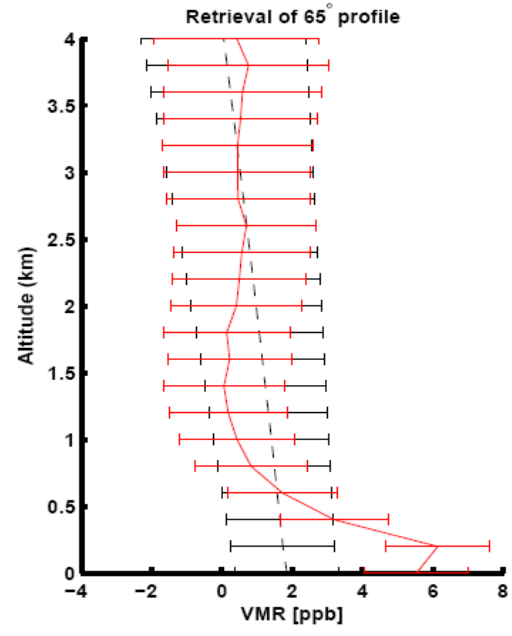




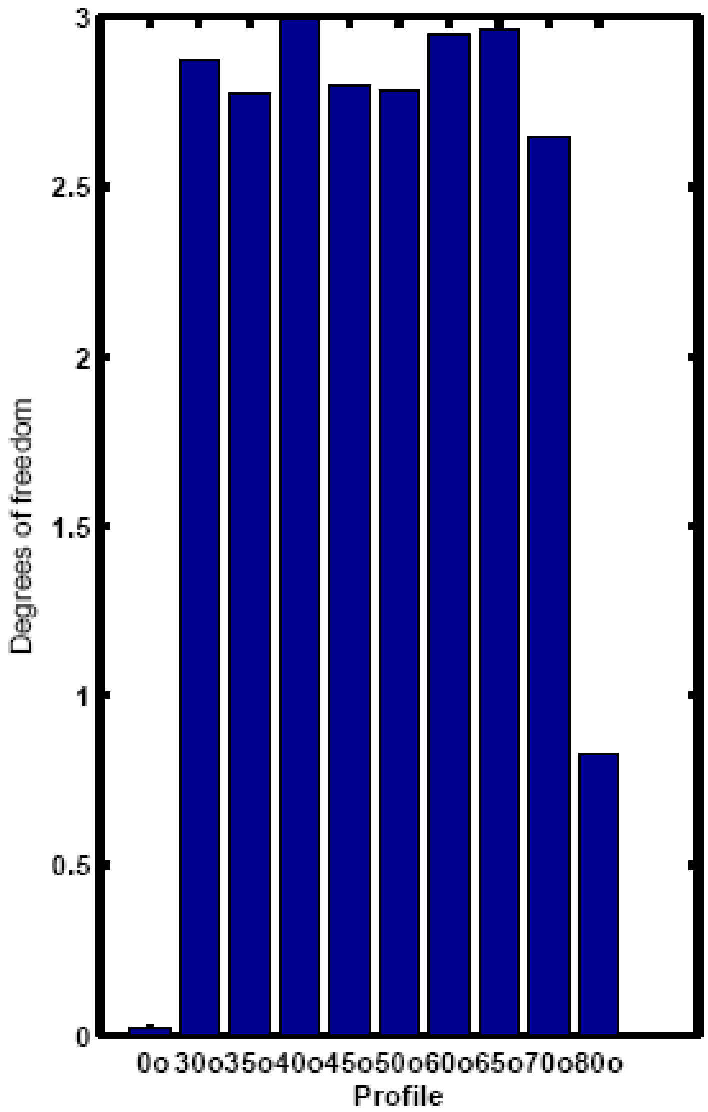




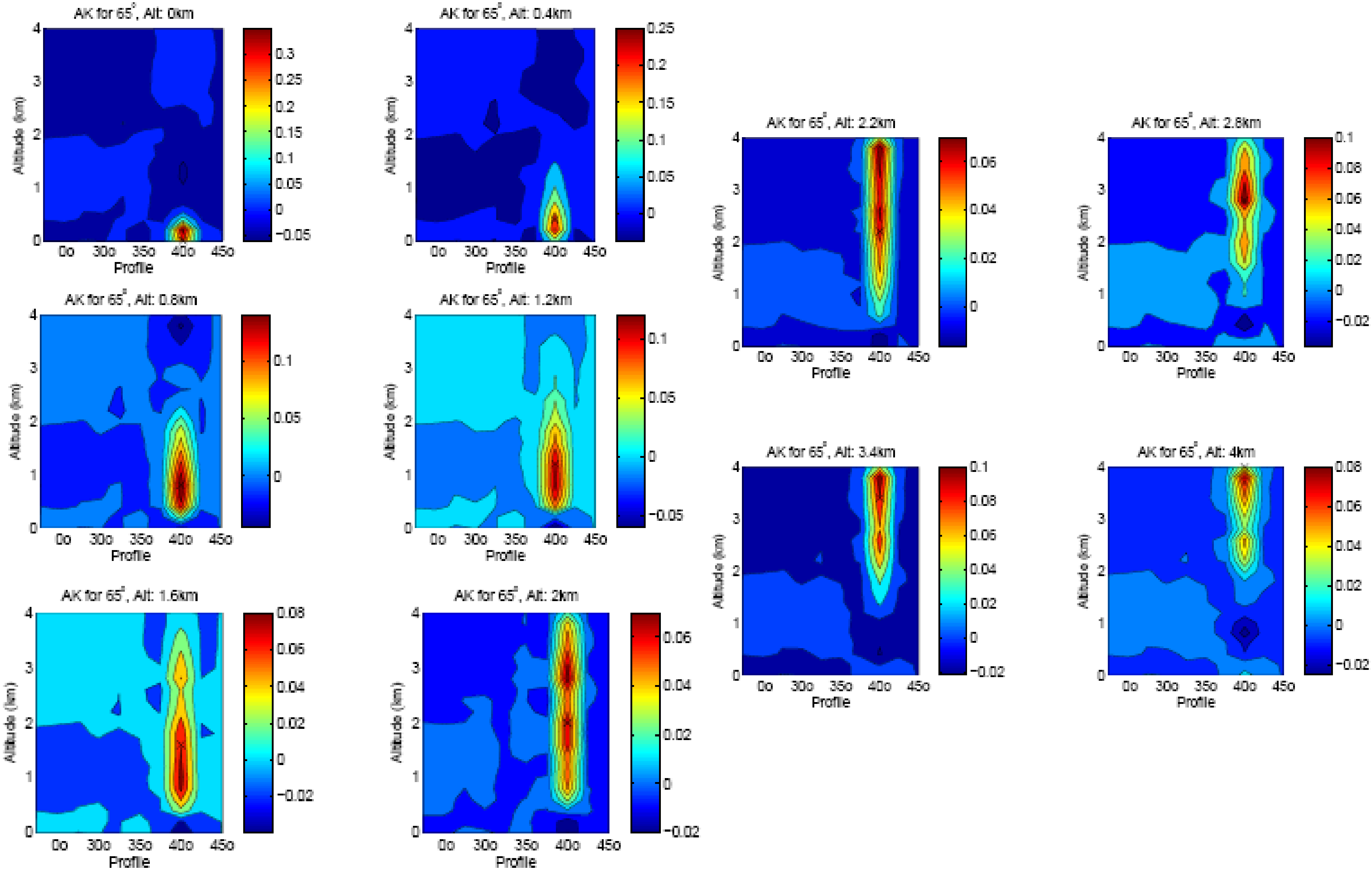




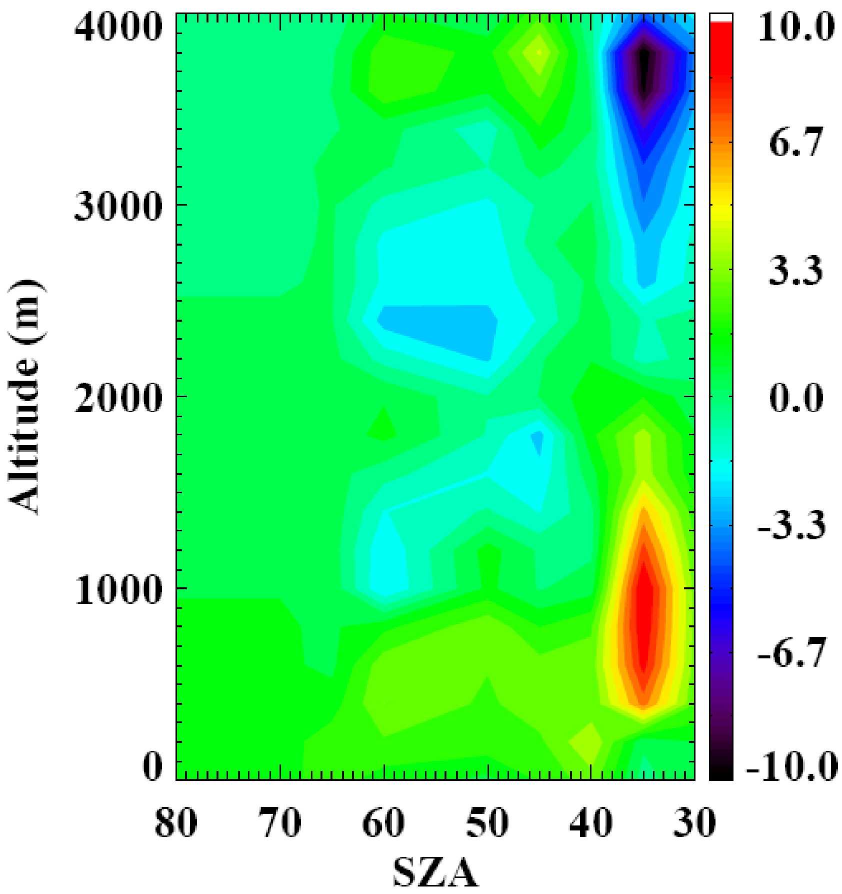
DFS, 24th June, AM



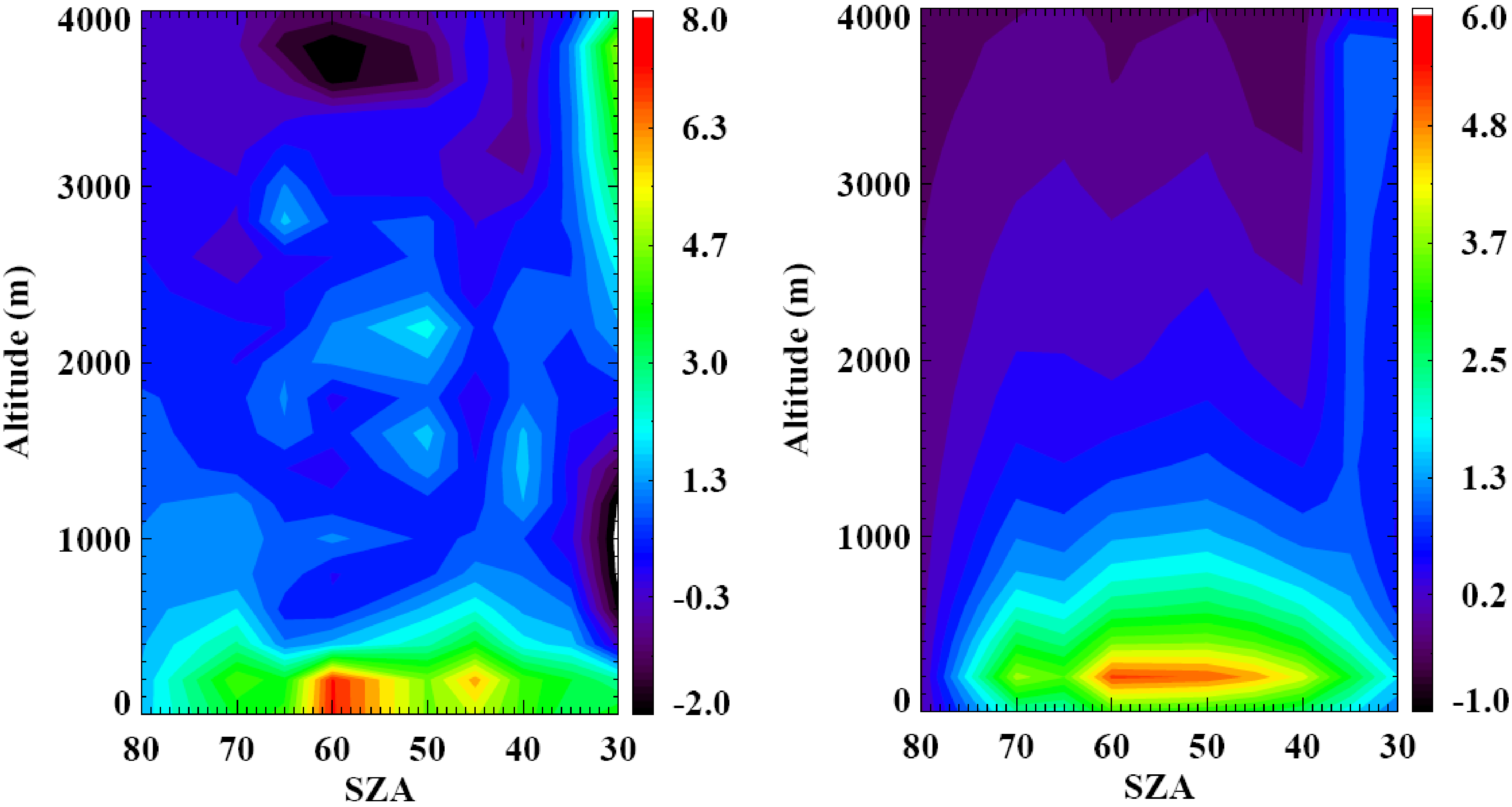
Averaging Kernels for 24th June, AM



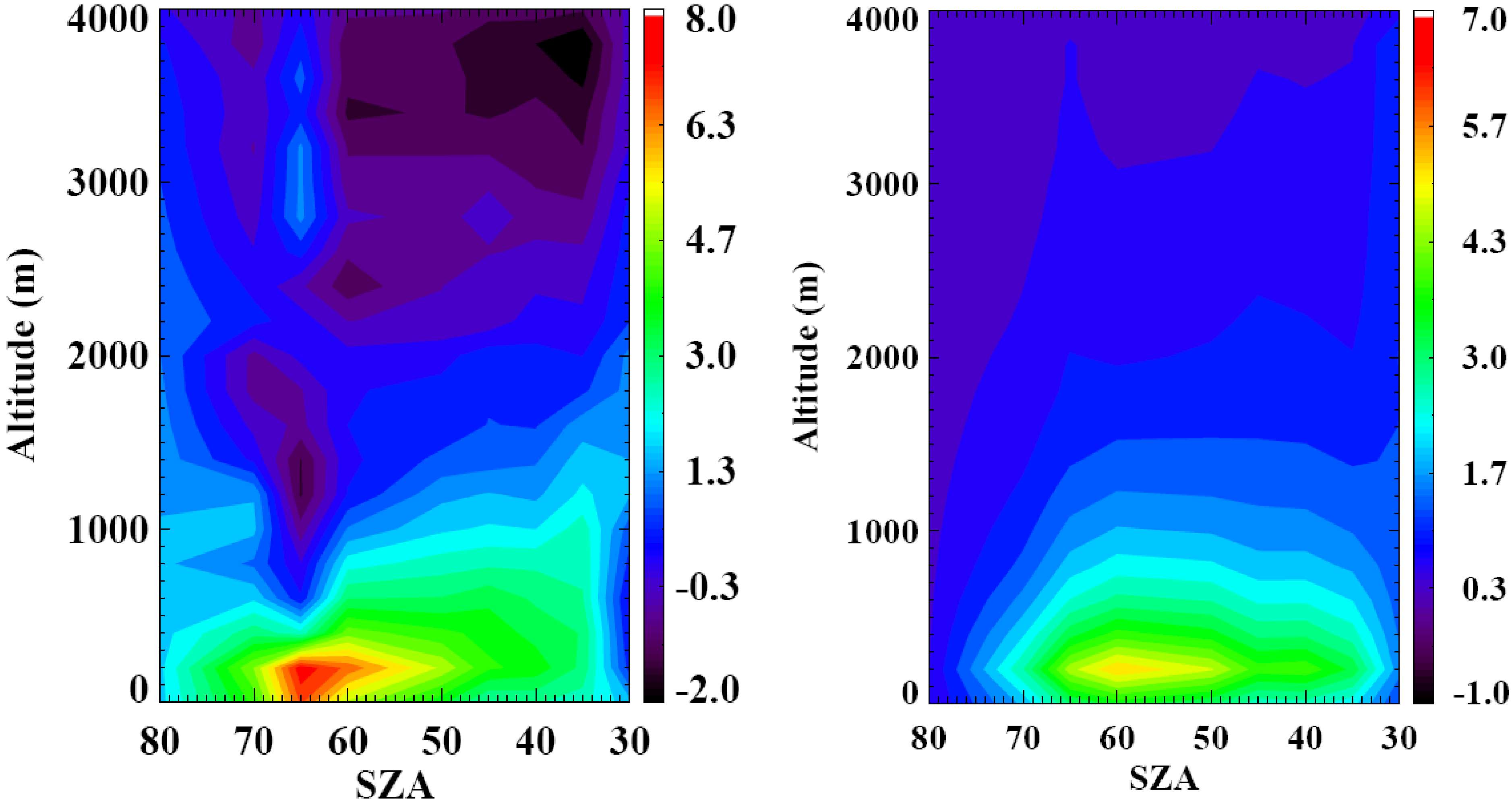
NO_2 (ppb) 18th June, AM



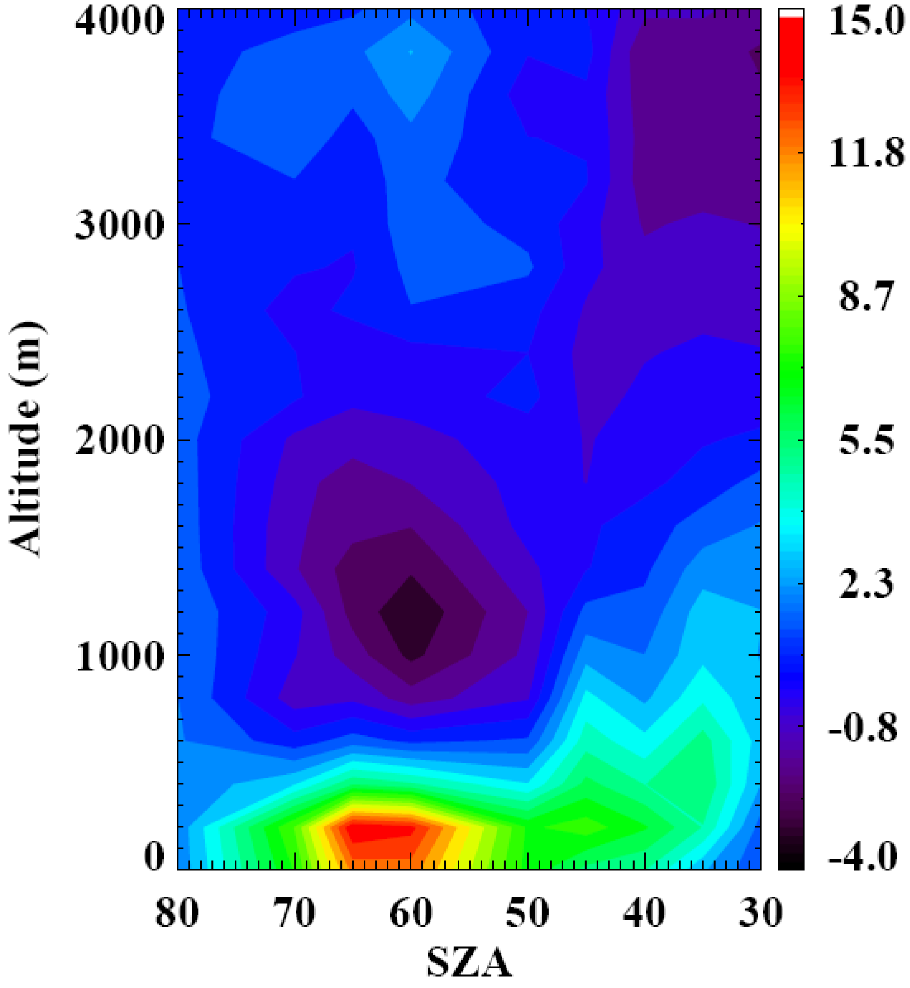
NO_2 (ppb) 23rd June, AM



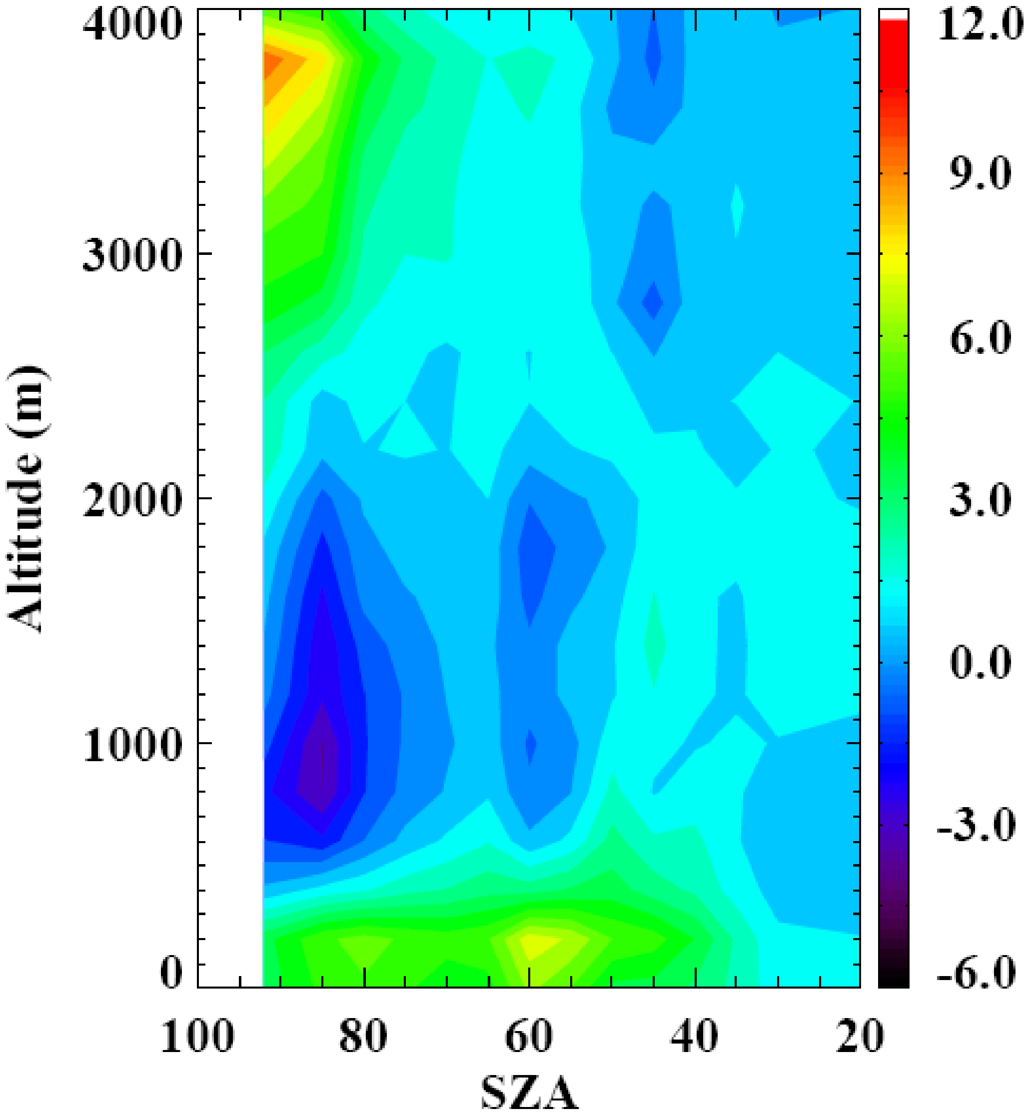
NO_2 (ppb) 24th June, AM



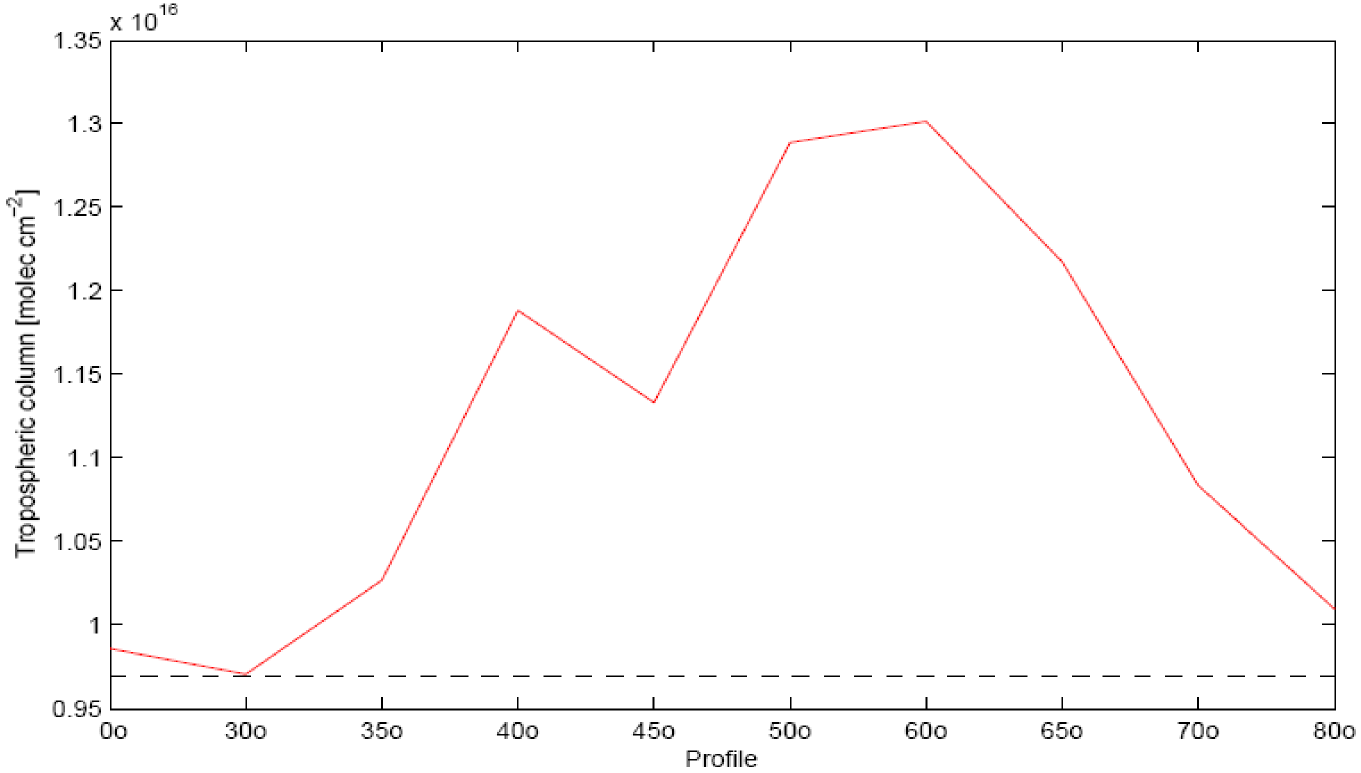
NO_2 (ppb) 25th June, AM



NO_2 (ppb) 2 July, AM



Vertical columns



Summary and Outlook

- MAX-DOAS measurements contain most profile information in lowest 1 km
- Very sensitive to aerosols – need accurate FM
- Retrieved profiles are strongly influenced by x_a and S_a

- Simplify algorithm:

  - retrieve one scan at a time without LZA dependence

  - use Kalman smoothing
- Compare with log version
- Implement aerosol retrieval