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"Retrieval of Temperature and Constituents from the High Resolution Dynamics Limb Sounder (MLS)"

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Please note: These are preliminary notes intended for internal distribution only.

Retrieval of Temperature and Constituents from the High Resolution Dynamics Limb Sounder

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HIRDLS Instrument Overview

- HIRDLS = High Resolution Dynamics Limb Sounder
- Infrared limb-scanning radiometer
- Stirling cycle cryo-cooled detectors and cold-filters operating at $\sim$65 K
- US-UK collaboration
  - Co-PIs: John Gille (Univ. Colorado), John Barnett (Univ. Oxford)
- EOS-Aura satellite (HIRDLS, MLS, TES, OMI)
  - Launch July 2003
- $\sim$705 km altitude Sun-synchronous Orbit
  - 98° inclination
  - 1:45pm ascending node
- Measure infrared limb-radiance samples in 21 spectral channels.
- Retrieve vertical profiles of atmospheric temperature, pressure, geopotential height gradients, constituent mixing ratios and aerosol extinction.

HIRDLS Science Objectives

- Chemical Composition
  - H_2O, O_3, NO_2, HNO_3, CFC11, CFC12, N_2O, CH_4, $ClONO_2$, N_2O_5
- Stratospheric Aerosols, PSCs, Cirrus
- Dynamics and Transport
- Momentum, Energy and Potential Vorticity Balances
- Validation of Numerical Models
- Climatologies and Trends
- Upper Troposphere

HIRDLS Measurements

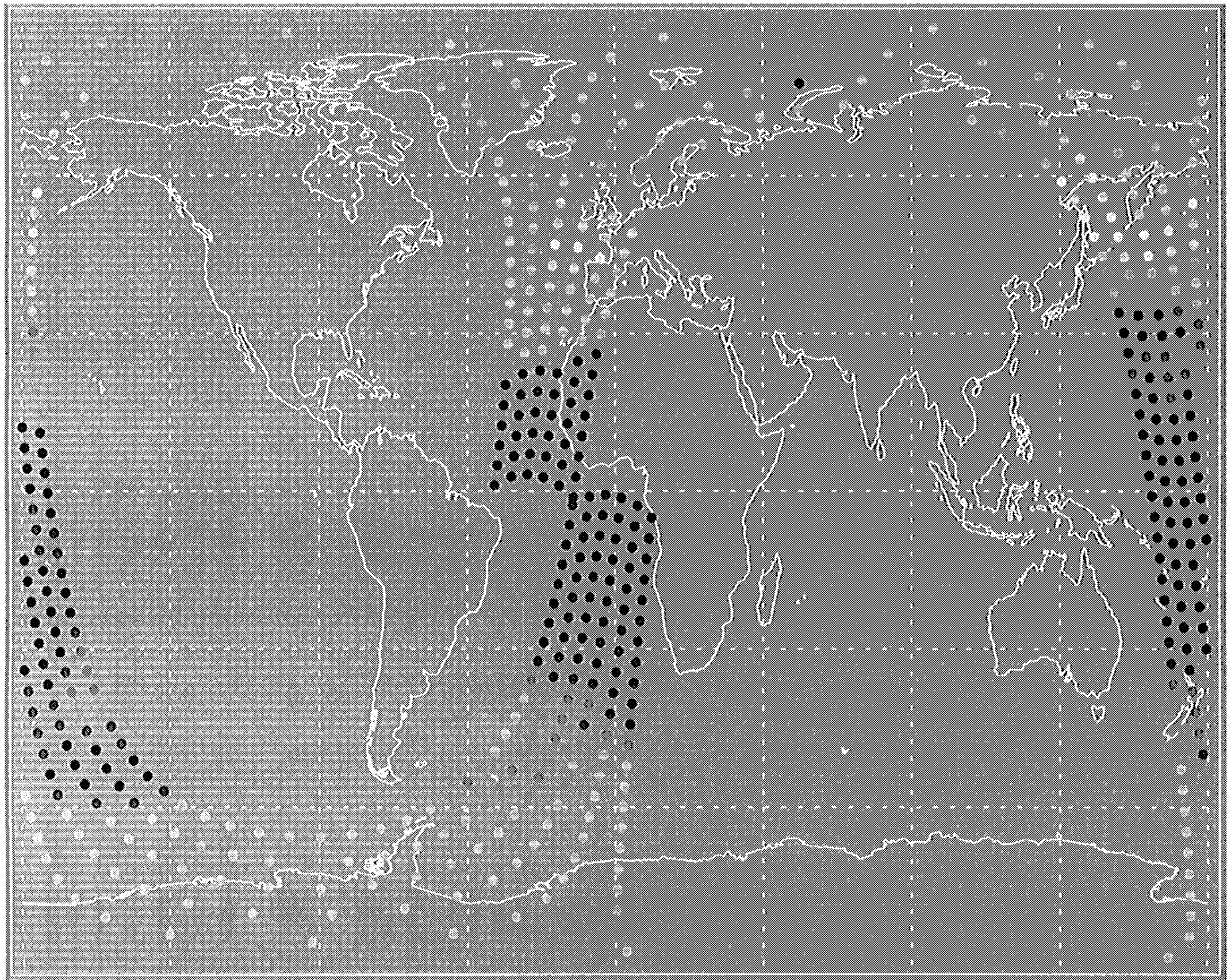
- infrared limb emission 555 – 1650 cm^{-1}
  - 21 spectral channels (band-pass filters)
- elevation scan every $\sim$10 s
  - vertical coverage 8–80 km
  - vertical field of view $\sim$1.25km
  - relative pointing knowledge $\sim$1.0 arcsec or 14m at the limb
- viewing aft-direction with azimuth step range $+21^\circ$ to -43°
- operating lifetime $\sim$5 yrs

HIRDLS Scan Modes

- Standard scan sequences provide flexible data acquisition modes tailored to address a wide range of scientific problems. Range of atmospheric phenomena to be investigated impose different and sometimes conflicting operational constraints.
  - Global Mode: default acquisition mode for normal scientific operation. Complete global coverage (pole to pole) in 12^h with 5° by 5° profile spacing. Provides the long-term requirement for homogeneous monitoring of the atmosphere.

HIRDLS Global Scan Mode - 1 swath

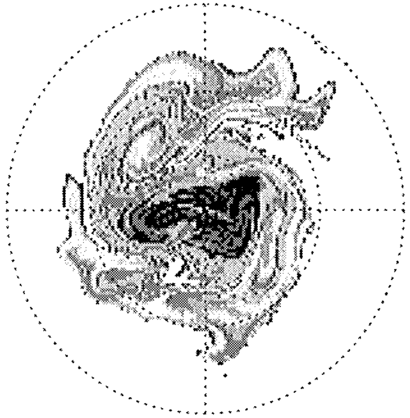
HIRDLS 1-Orbit 5x5 Global Mode Swath Coverage



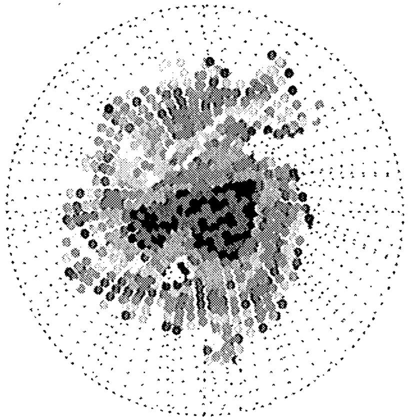
HIRDLS Global Mode Coverage

c.f. Northern Hemisphere post-Pinatubo aerosol extinction

Contour Advection



HIRDLS



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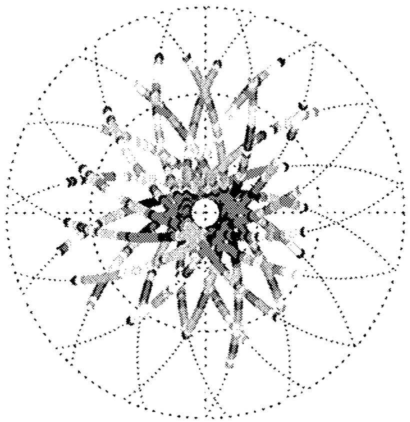


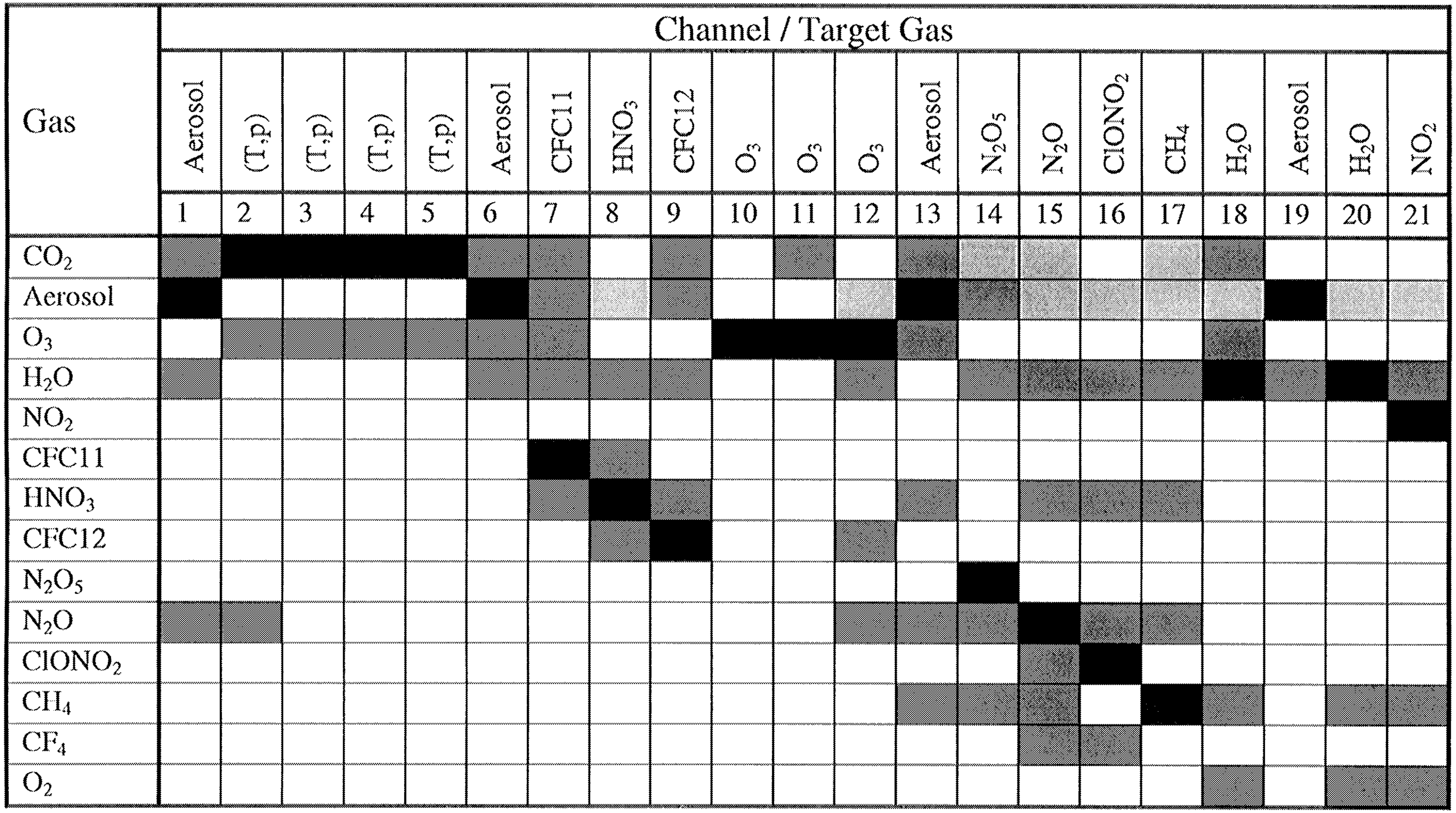
HIRDLS Retrievals

- Operational considerations
  - $>$ 7000 profiles $\times$ 12 products per day
- Inversion scheme
  - Level-1 calibrated radiances $\rightarrow$ Level-2 products
  - Optimal Estimation maximum a posteriori (MAP) Rodgers (2000)

HIRDLS Sounding Channels

Identification of the target gases (black), and the strong (dark grey) and minor (light grey) contaminants in the HIRDLS sounding channels.

HIRDLS Sounding Channels



Retrieval Scheme

- The **retrieval scheme** defines the sequence in which the retrievals are to be carried out. The Table shows a possible configuration for the retrieval of all catalogued Level-2 products

  (i) retrieval sequence steps

  (ii) radiance channels

  (iii) contaminant species

  (iv) grouping of multiple retrieval products.

- Two complete passes through the retrieval sequence are required to correct for **line of sight gradients**

Retrieval Scheme

	Target	Contaminants						Channels			
1	T/p	CO_2	O_3	N_2O	H_2O		Aerosol	2	3	4	5
2	Aerosol	H_2O	N_2O	CO_2	O_3	HNO_3	CH_4	1	6	13	19
3	H_2O	CH_4	O_2				Aerosol	18	20		
4	O_3	CO_2	H_2O	N_2O	CFC12		Aerosol	10	11	12	
5	NO_2	H_2O	CH_4	O_2			Aerosol	21			
6	HNO_3	H_2O	CO_2	O_3			Aerosol	8			
	CFC11							7			
	CFC12							9			
7	N_2O_5	H_2O	CO_2	HNO_3	CF_4		Aerosol	14			
	N_2O							15			
	$ClONO_2$							16			
	CH_4							17			

Retrieval Schemes

- **Target gas(es)** is (are) the species to be retrieved from a radiance channel or combination of channels
- **Contaminants** are the species specified as contributing to the emission within a radiance channel but which are not being retrieved at the current retrieval step. These may be fixed gases, or taken from the climatology data, or obtained from data retrieved independently from other radiance channels at an earlier processing stage

Climatological Data

Climatological data are required for each contaminant species in the HIRDLS channels and are conveniently stored as gridded data. The spatial and temporal gridding resolution depends on the variability of the particular species, i.e. 1-D profiles are adequate for well-mixed gases such as CO_2, but 2-D zonal mean spatial distributions will be required for most species. Some species will only require a single fixed distribution in time, while others will be represented as seasonal or monthly distributions.

Diurnally varying species will require special treatment to factor in the change as a function of solar zenith angle or local time as appropriate.

HIRDLS Climatological Data

Field	Temporal	Spatial
CO_2	Fixed	1-D Profile
O_3	Monthly	2-D Zonal Mean
H_2O	Monthly	2-D Zonal Mean
NO_2	Monthly, Diurnal	2-D Zonal Mean
CFC11	Monthly	2-D Zonal Mean
HNO_3	Monthly	2-D Zonal Mean
CFC12	Monthly	2-D Zonal Mean
N_2O_5	Monthly, Diurnal	2-D Zonal Mean
N_2O	Monthly	2-D Zonal Mean
$ClONO_2$	Monthly, Diurnal	2-D Zonal Mean
CH_4	Monthly	2-D Zonal Mean
CF_4	Monthly	2-D Zonal Mean
O_2	Fixed	1-D Profile
Aerosol	Background to Volcanic	2-D Zonal Mean
Temperature	Monthly	2-D Zonal Mean
Height	Monthly	2-D Zonal Mean

A Priori Data

The *a priori* data consist of a profile and covariance matrix for each of the HIRDLS target species. They are required to constrain the retrieval solution.

The *a priori* profile represents prior knowledge of the state of the atmosphere at the time and location of measurement and the *a priori* covariances represent the associated uncertainty.

The *a priori* data for HIRDLS will be derived from climatological data.

HIRDLS Level-2 retrieval flow

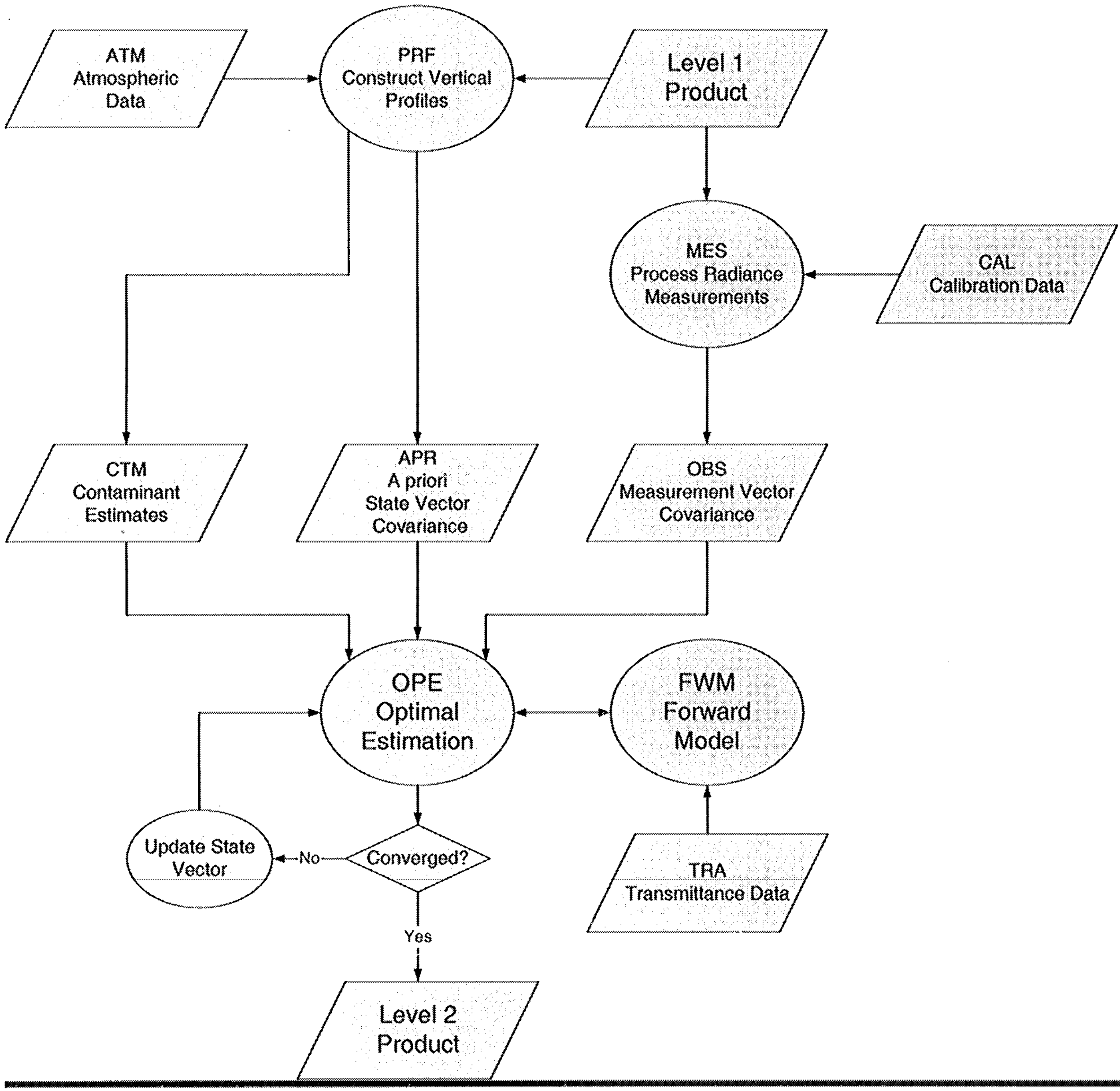
The retrieval sequence consists of 7 steps, a two-stage process being used to achieve the line of sight gradient correction.

Each product that is retrieved is then used to generate line of sight gradients which are used in the second pass of the retrieval sequence.

Here we only consider the radiance samples obtained during a single up or down scan. The flexibility of the HIRDLS instrumentation allows more complex observation modes and retrieval schemes to be devised in which the horizontal variability along the line of sight may be probed in greater detail.

An overview of the Level-2 retrieval flow is shown in the Figure. The instrument data input is via the Level-1 data product which consists of geolocated and time-stamped limb radiance samples. Ancilliary data, such as the climatology data, transmittance data etc. are also required inputs to the Level-2 processor.

HIRDLS Level-2 retrieval flow



Radiative Transfer for Infrared Limb-Sounding

The channel radiance, $R(s_o, h)$, received when viewing a particular tangent altitude, h, at an observation point, s_o, along the ray path is given by,

$$R(s_o, h) = \int_{-\infty}^{s_o} \int_{\Delta\nu} B(\nu, T(s)) \frac{d\tau(\nu, q(s), s)}{ds} f(\nu) d\nu ds \qquad (1)$$

where s is the position along the ray path which has its tangent point at h, ν the wavenumber, B the Planck function, which depends the temperature T, and τ the transmittance from s to s_o, which depends on the gas mixing ratio q. The channel filter response function is $f(\nu)$ and extends over a spectral passband of width $\Delta\nu$.

Forward Models

Simulation of calibrated Level-1 radiances

- Absorption coefficient look-up table
  - absorption coefficient (gas/channel combination) stored as a 3D table look-up (wavenumber, pressure, temperature)
  - large table size ($\sim$Gb)
  - monochromatic calculation - line-by-line accuracy - slow to execute
  - generation of parameterized models
- Fast Forward Model based on Curtis-Godson approximation
  - transmittance (gas/channel combination) parameterized as a 3D table look-up (pressure, temperature, absorber mass)
  - modest table size ($\sim$Mb)
  - fast analytic weighting function calculation
  - assumes multiplicative property for multiple gases in a channel
  - since $\sim$2–3 % accuracy is insufficient for T/p sounding channels a modified scheme is under development

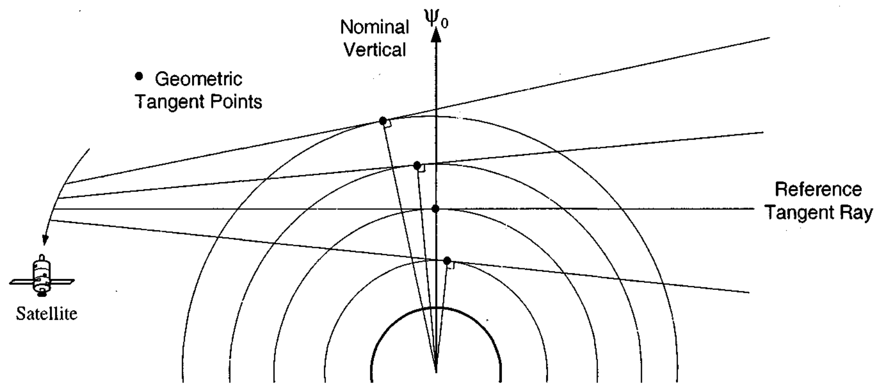
Line-of-sight Gradients

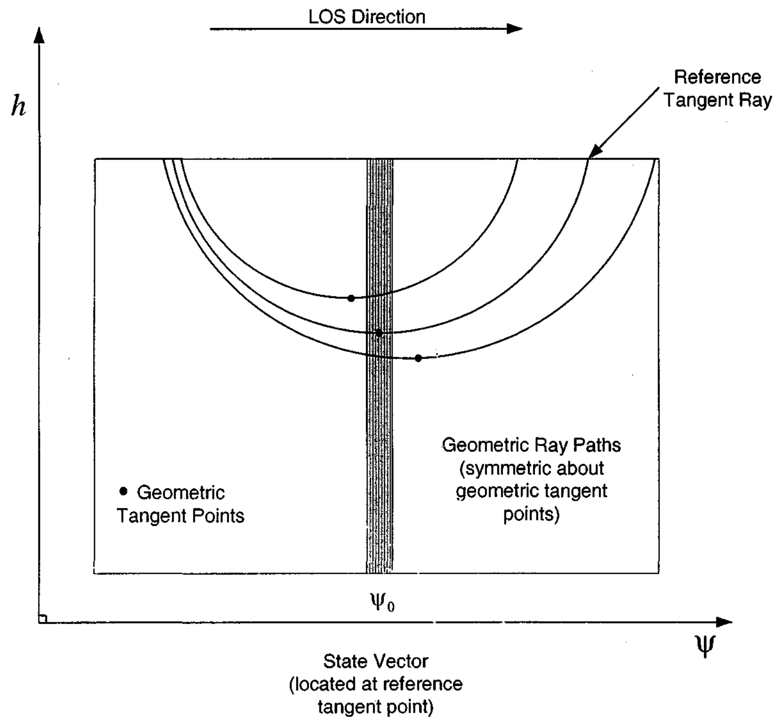
- The atmospheric limb-radiance is dependent on horizontal thermal and constituent mixing ratio gradients which invalidates assumptions of spherical symmetry of the limb-path.
  - sensitivity to thermal gradients increases with decreasing wavelength (Planck function dependence) for same opacity.
  - optically thin channels are less sensitive to gradients
  - typical errors of 2–3 K in temperature for a gradient of 1 K per 100 km
- Two-Pass approach
  - first pass
    * assume horizontal homogeneity (flat 2D-LOS field)
    * retrieve products
  - second pass
    * calculate 2D-LOS fields from the retrieved data
    * retrieve products

Geometry for the limb-sounding problem

The atmospheric layer boundaries must be chosen to ensure that sufficient layers are used for an accurate radiative transfer calculation. The Figure shows a 2D vertical (height, Earth centred angle) cross-section, (h, ψ), along the line of sight. As the the limb-sounder scans up or down the atmosphere a locus of geometrical tangent point altitudes are defined which do not lie on a vertical through the Earth's centre. A reference tangent height is selected which is used to define the nominal vertical profile location, ψ_0, along the line of sight and its (latitude, longitude) position on the Earth. The state vector is located at this reference position as is the origin of the 2D coordinate system atmospheric profiles used in the retrieval.

Geometry for the limb-sounding problem

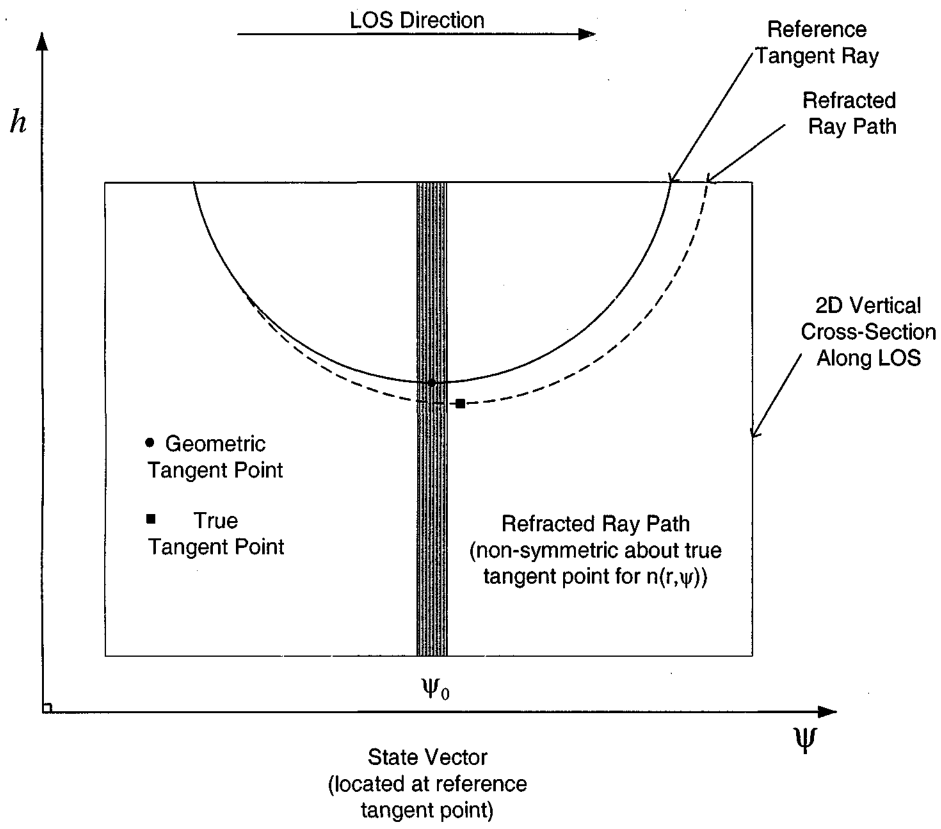




Atmospheric Refraction

The Figure shows schematically that atmospheric refraction deviates the light ray from the geometric path resulting in a true tangent point which is lower in altitude and further from the satellite than the geometric (or apparent) tangent point location. This is the true path through the atmosphere and it must be modelled adequately to achieve an accurate radiative transfer calculation.

Atmospheric Refraction



Temperature, Pressure, H_2O in vertical plane along LOS are used to calculate the Refractive Index of Air and derivatives.

$$T(h,\psi),\ P(h,\psi),\ H_2O(h,\psi) \longrightarrow n(h,\psi), \left.\frac{\partial n}{dh}\right|_{\psi}, \left.\frac{\partial n}{d\psi}\right|_{h}$$

Ray Tracing Algorithm calculates the Refracted Ray Path $h(s), \theta(s), \psi(s)$

Interpolation of 2D fields along LOS generates the required LOS path quantities

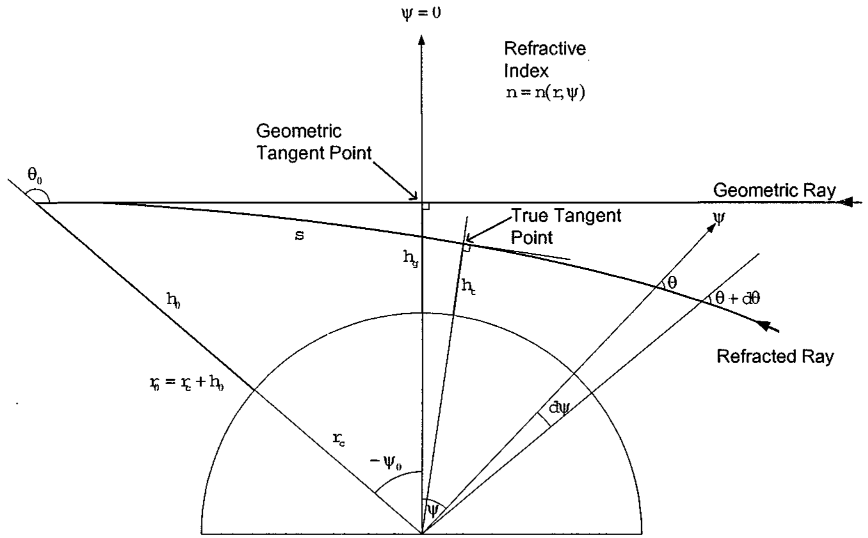
$$T_{LOS}(s) = T[h(s), \psi(s)]$$
$$P_{LOS}(s) = P[h(s), \psi(s)]$$
$$VMR_{LOS}(s) = VMR[h(s), \psi(s)]$$

Ray Path Coordinates

The atmosphere is modelled on a 2-D (h, ψ) grid and the ray path through the atmosphere is described by coordinates (h, ψ, θ) for a given instrument geometric tangent height view.

The intersections of the view vector with the top of the atmosphere (TOA) defined by an arc of radius, $r_{toa} = h_{toa} + R_c$, give the $(r_{toa}, \psi_{toa}, \theta_{toa})$ coordinates required to initialize the ray tracing algorithm.

Ray Path Coordinates



rc = Radius of Curvature of Geoid at (lat,lon) location of the reference tangent point in the direction of LOS

Refractive Index of Air

$n = n(r)$ - horizontal homogeneity

$n = n(r, \psi)$ - LOS variation in T, p, H_2O

Initial Conditions for Ray Tracing : Solve for $r(s)$ distance from RoC

$\theta(s)$ zenith angle

$\psi(s)$ RoC centred angle

$$s = 0$$

$$r(0) = r_0$$

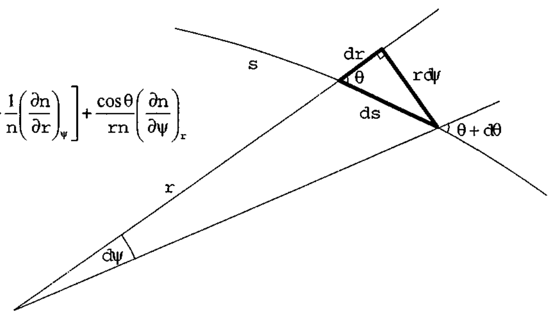
$$\theta(0) = \theta_0$$

$$\psi(0) = -\psi_0$$

$$\frac{d\theta}{ds} = -\sin\theta \left[\frac{1}{r} + \frac{1}{n}\left(\frac{\partial n}{\partial r}\right)_{\psi} \right] + \frac{\cos\theta}{rn}\left(\frac{\partial n}{\partial \psi}\right)_{r}$$

$$\frac{dr}{ds} = \cos\theta$$

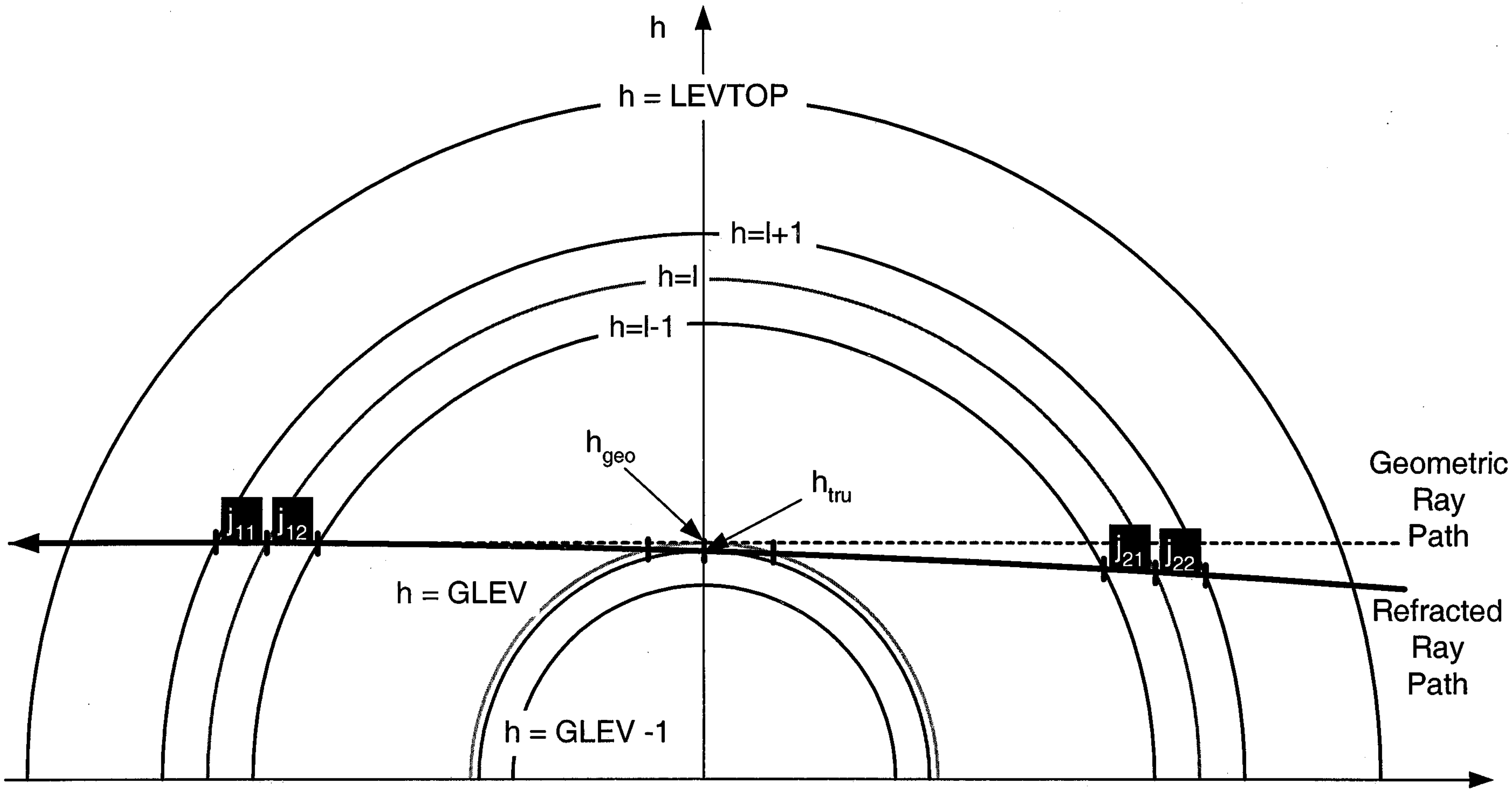
$$\frac{d\psi}{ds} = \frac{\sin\theta}{r}$$

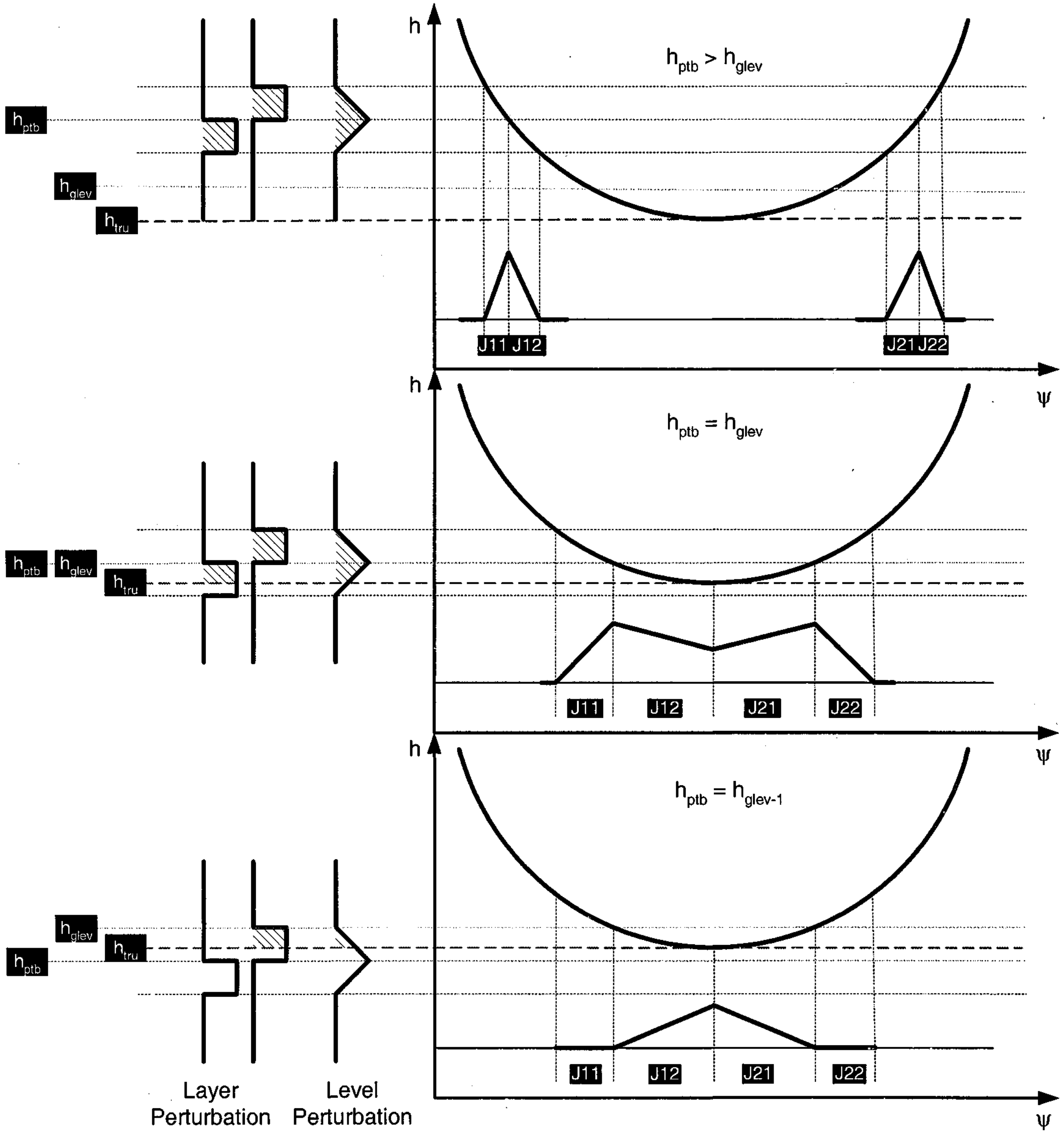


Forward Model Derivatives

The relationship between perturbations at an atmospheric level and for an atmospheric layer. The geometric height of a perturbed level is denoted by h_{ptb}, and the perturbation takes the form of a triangular function, the apex centered at h_{ptb} and the two base vertices at the geometric levels above and below h_{ptb}.

Line-of-sight schematic for weighting function calculations. An atmospheric perturbation at height, $h = l$, affects the line of sight segments on either side of the true tangent point at $j_{11}, j_{12}, j_{21}, j_{22}$.




h
$h_{ptb} > h_{glev}$
h_{ptb}
h_{glev}
h_{tru}
J11 J12
J21 J22
h
ψ
$h_{ptb} = h_{glev}$
h_{ptb}
h_{glev}
h_{tru}
J11
J12
J21
J22
h
ψ
$h_{ptb} = h_{glev-1}$
h_{glev}
h_{tru}
h_{ptb}
J11
J12
J21
J22
Layer Perturbation
Level Perturbation
ψ

Weighting Functions

The weighting function matrix, K_{hl}, for a state vector quantity, q, defined on levels, where R_h is the radiance calculated for the refracted atmospheric path associated with the geometric tangent height, h, and l is the vertical perturbation level is given by,

$$K_{hl} = \frac{\partial R_h}{\partial q_l}$$

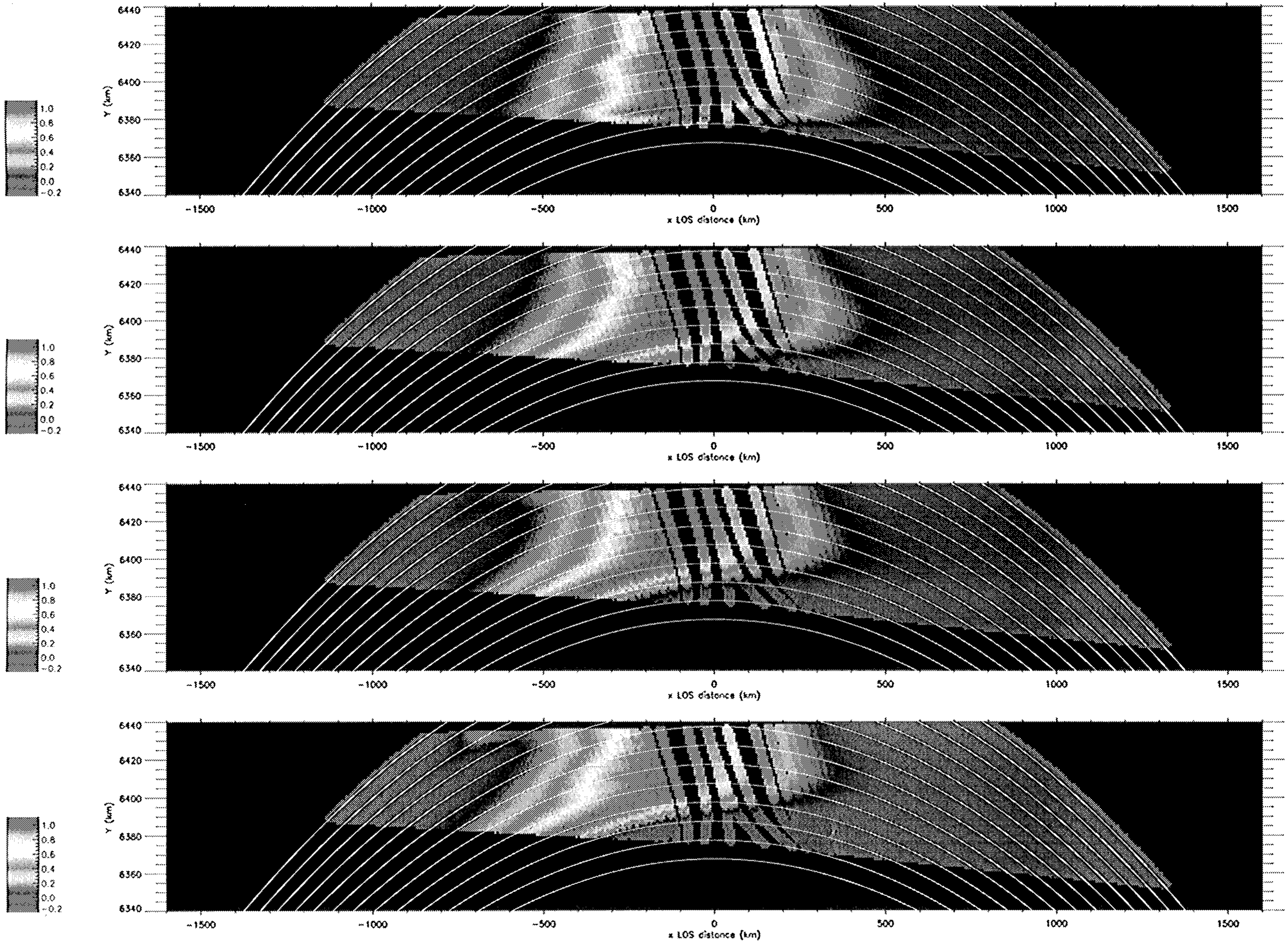
These are related to the layer defined quantities, $\bar{q}$, by a summation over the LOS indices, $i = j_{11}, j_{12}, j_{21}, j_{22}$

$$K_{hl} = \sum_i \frac{\partial R_h}{\partial \bar{q}_i} \frac{\partial \bar{q}_i}{\partial q_l} = \sum_i \bar{K}_{hi} \frac{\partial \bar{q}_i}{\partial q_l} \tag{2}$$

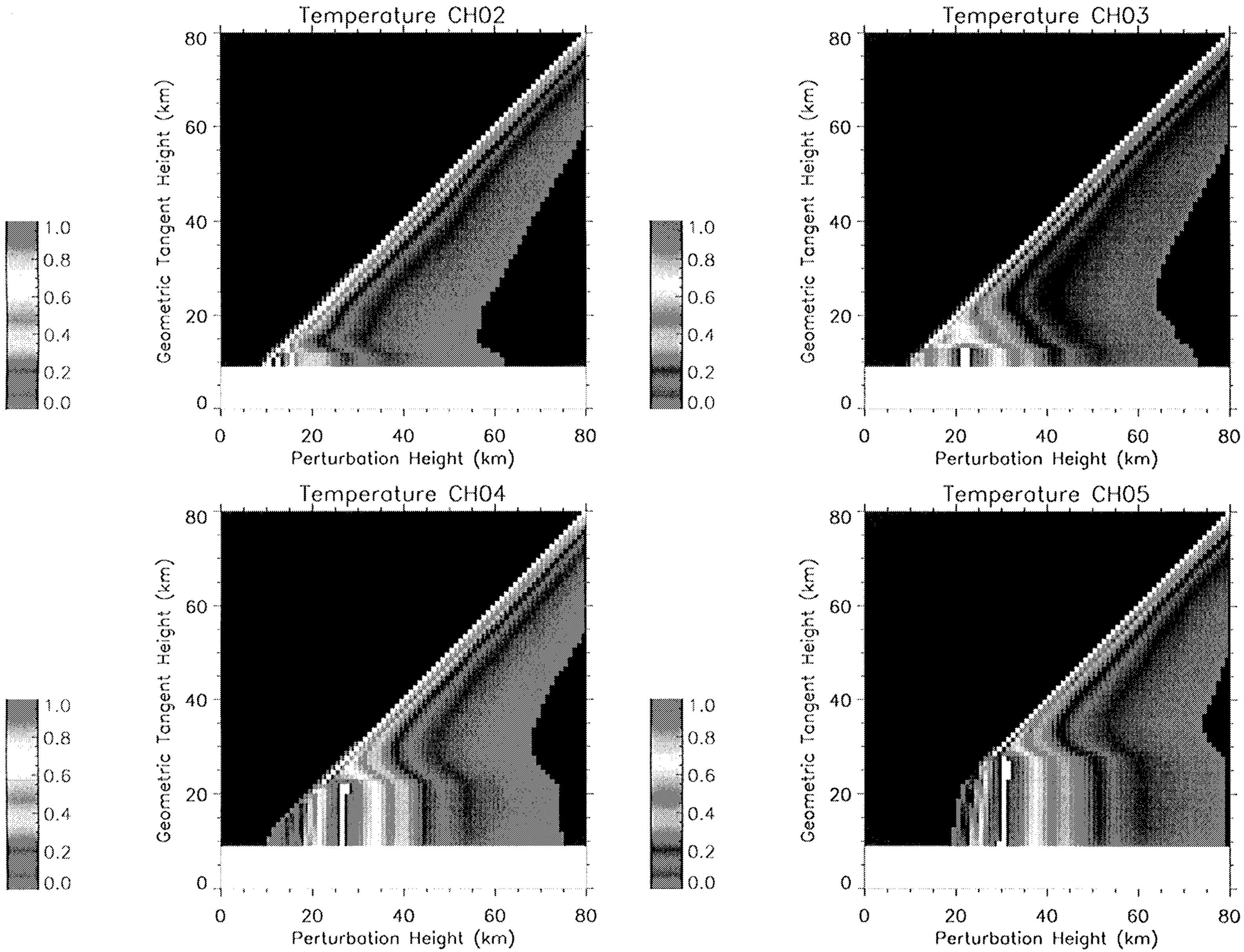
Weighting Functions

- Tropical AFGL atmosphere homogeneous with LOS angle
- LOS-layer weighting functions along a ray path $\frac{\partial R_h}{\partial \bar{q}_i}$
  - pixel position corresponds to mid-points of 1 km vertical layers
  - maximum response is normalized to unity along each LOS path
  - 50 % max. response shown by green/yellow contour
  - 10 km interval shells from Earth's surface to 120 km shown in white
- Vertical-level weighting functions $\mathbf{K}$-matrix $\frac{\partial R_h}{\partial q_l}$

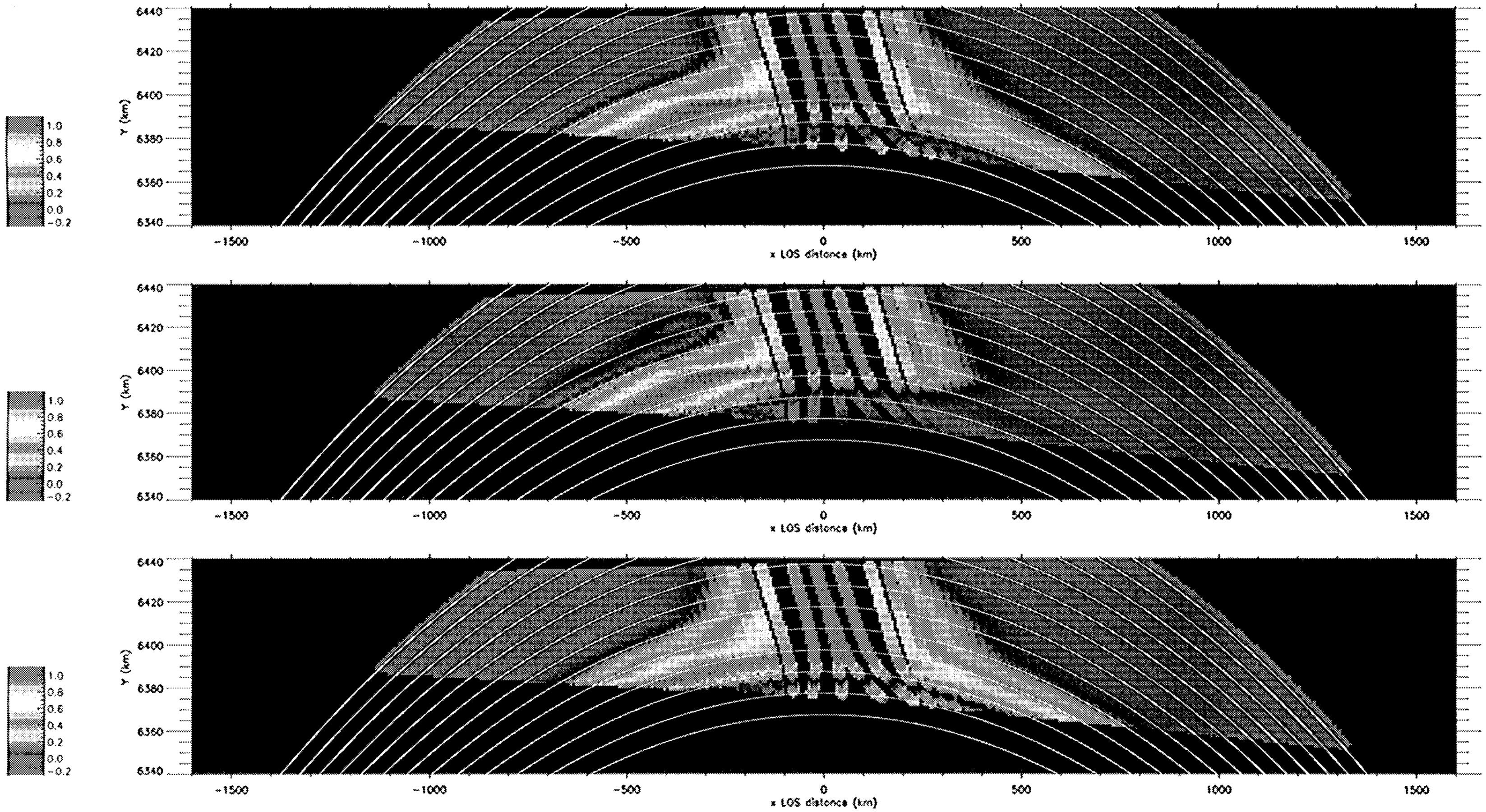
LOS Temperature Weighting Functions



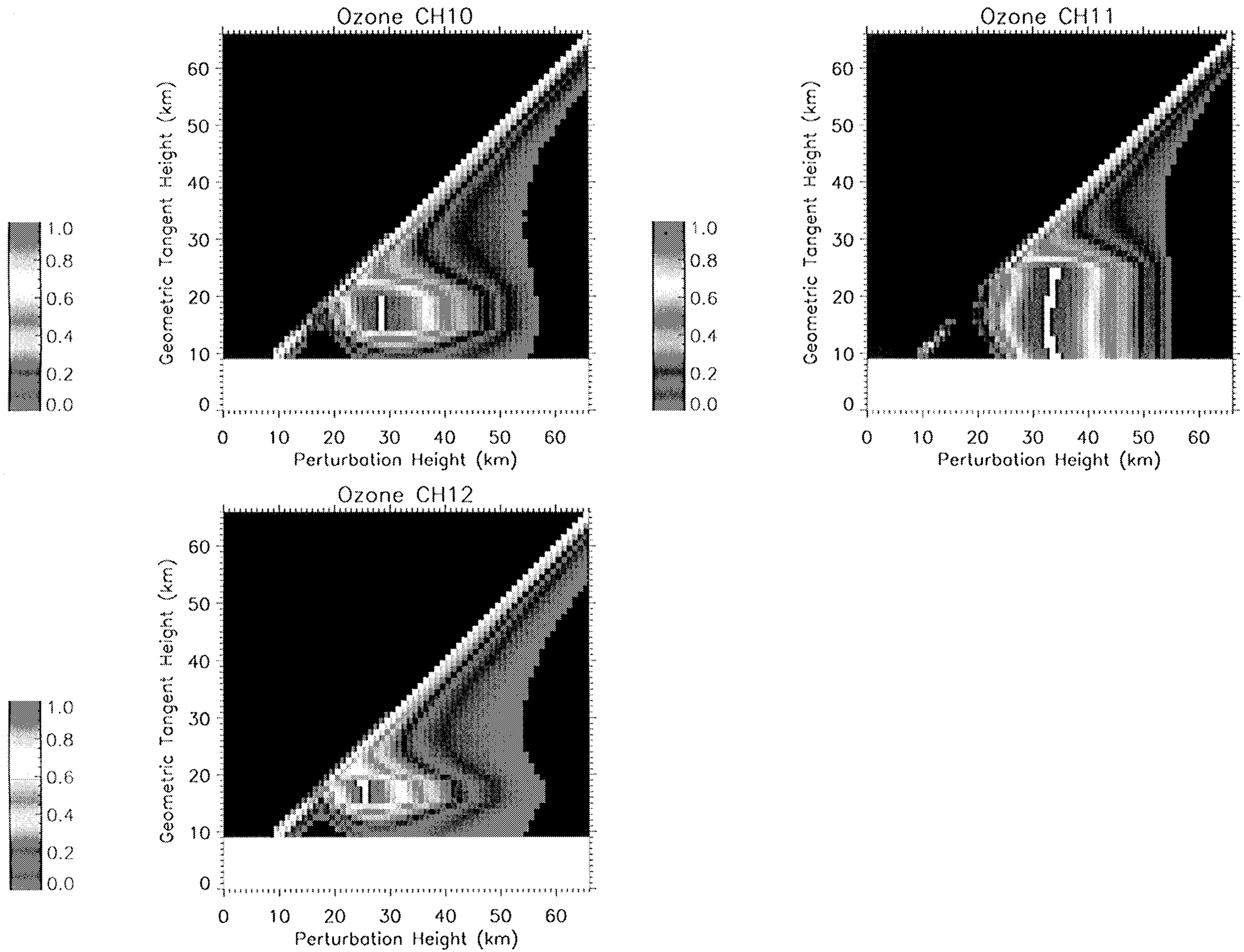
Level Temperature Weighting Functions



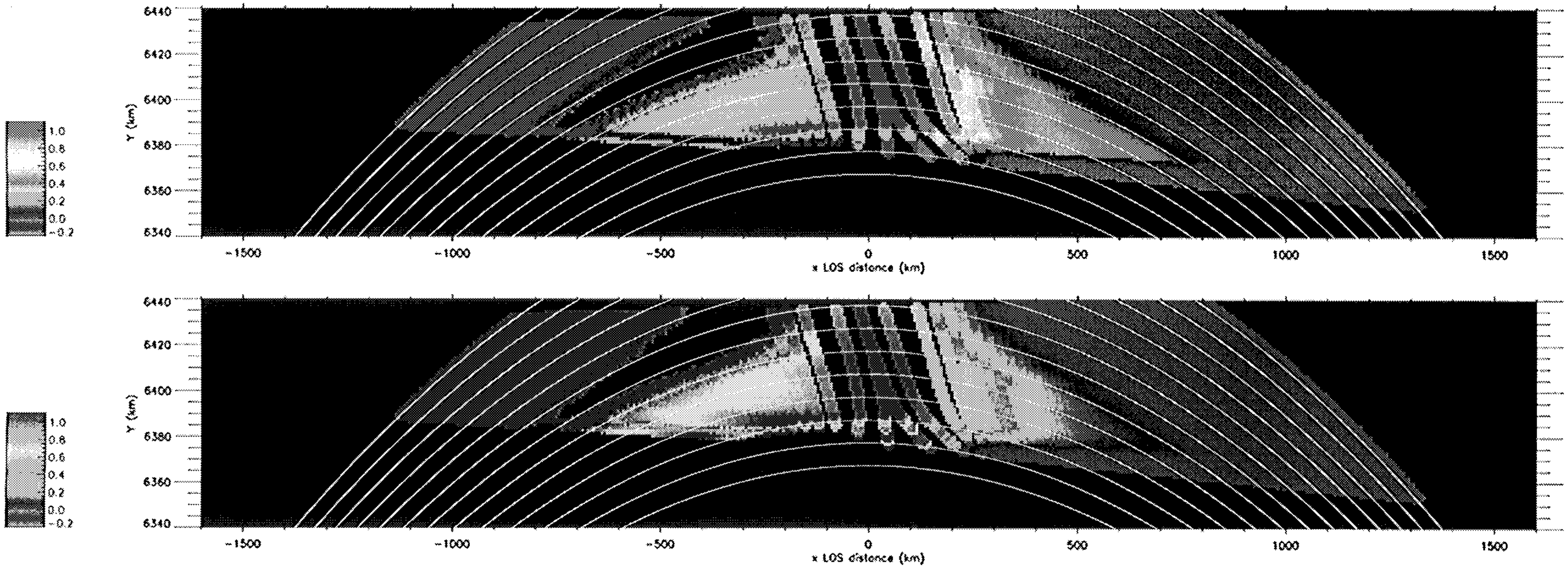
LOS Ozone Weighting Functions



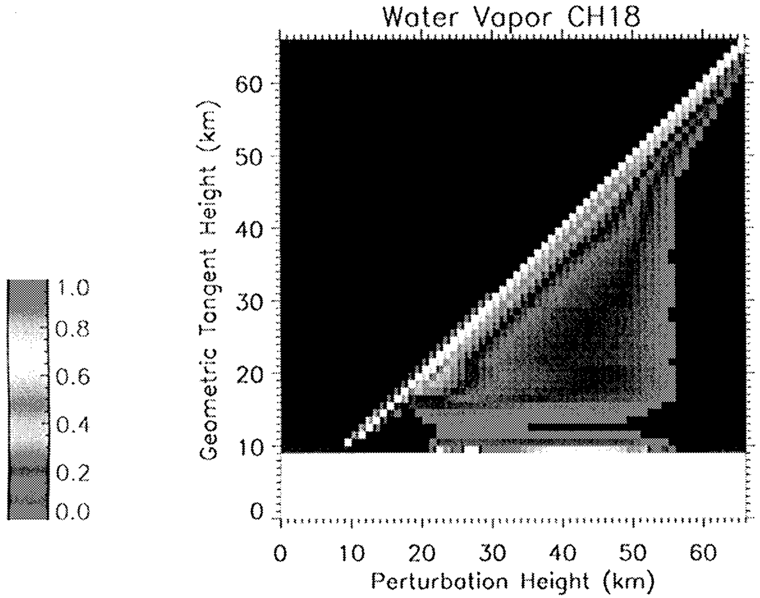
Level Ozone Weighting Functions

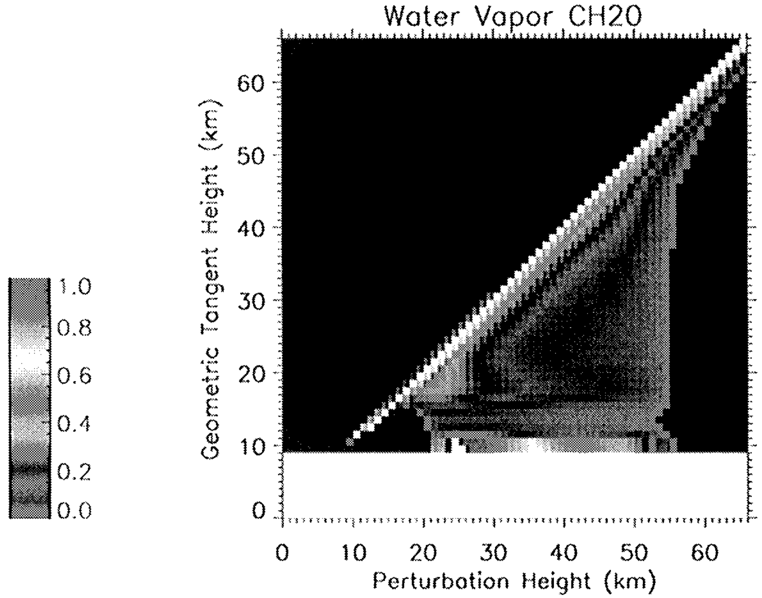


LOS Water Vapour Weighting Functions



Level Water Vapour Weighting Functions





Retrieval of Temperature and Pressure

- The retrieval of temperature and pressure will be performed jointly on a relative height grid from 4 channels (2,3,4,5).
- Absolute pointing knowledge of the line-of-sight is not required. However, the relative altitudes of the retrieval grid must be known to high precision. A reference pressure, $p_0(z_0)$, is chosen corresponding to an altitude surface in the stratosphere.
- The temperature profile is retrieved by making use of the ideal gas equation to relate temperature, T, density, ρ, and pressure, p,

$$p = \frac{\rho}{M_r} RT \tag{3}$$

where R is the gas constant and M_r is the relative molecular mass of air.

Retrieval of Temperature and Pressure

- The hydrostatic equation is integrated to obtain the pressure profile,

$$\ln p(z) = \ln p_0(z_0) + \int_{z_0}^{z} \frac{M_r g(\phi, z)}{RT(z)} dz \tag{4}$$

where $g(\phi, z)$ is the gravatational acceleration at latitude, ϕ, altitude, z

- The state vector for this retrieval contains the reference pressure, $\ln p_0(z_0)$, and the temperature profile, $T(z)$.

Multiple Product Retrievals

The retrieval of multiple products simultaneously from multiple sounding channels is achieved using the generality of the retrieval algorithm which allows the state and measurement vectors to be composed of the concatenation of the individual product profiles and channel radiances, respectively. The measurement error covariance, *a priori* vector and covariance matrix, and weighting function matrix must also be composed accordingly. The simultaneous retrieval is most effective for the products which have significant contamination in several sounding channels.

In principle T/p and all constituents could be retrieved simultaneously from the 21 channels in a "full-up" retrieval. In practice, some caution is advisable in performing the initial retrievals after launch of the instrument to reduce the complexity of diagnosing potential problems with real data from the radiance channels.

Retrieval Overview

The aim of any physical retrieval algorithm is to obtain profiles of the atmospheric constituents (contained in the "state vector") for which the radiative transfer model ("forward model") predicts synthesized radiances which are consistent with the measured radiances ("measurement vector") and the *a priori* information.

Measurement vector and error covariance

The measurement vector, y, has m elements consisting of the vertical profiles of calibrated Level-1 radiances for the channels selected for the retrieval,

$$\mathrm{y} = \{y_c(z_{l_c})\} \tag{5}$$

where the indices, l_c, specify the altitudes, z_{l_c}, to be used for a channel, c. The instrument noise, ϵ_y, is assumed to be uncorrelated between channels (i.e. no cross-talk) and to have zero mean.

The measurement error covariance, $\mathrm{S_y}$, is an $(m \times m)$ matrix, where the diagonal elements are equal to the variances of the instrument noise, σ_y^2, and the off-diagonal elements are zero,

$$\mathrm{S_y} = \mathcal{E}\left\{\epsilon_y \epsilon_y^{\mathsf{T}}\right\}; \quad S_y(i,j) = \begin{cases} \sigma_y^2(i) & \text{if } i = j, \\ 0 & \text{if } i \neq j \end{cases} \tag{6}$$

State vector

The state vector, $\mathbf{x}$, has n elements consisting of the quantities to be retrieved e.g. temperature profile, reference pressure and/or constituent mixing ratio profiles at the required altitude ranges,

$$\mathbf{x} = \{x_q(z_{l_q})\} \tag{7}$$

where the indices, l_q, specify the altitudes, z_{l_q}, to be used for a retrieved quantity, x_q.

A priori vector

The *a priori* data give an independent estimate of the state of the atmosphere and its uncertainty. The influence of the *a priori* on the retrieval is to provide stabilization against the possible gross amplification of noise associated with direct inversion of the measurements. All the quantities in the state vector require *a priori* data.

The *a priori* vector, $\mathbf{x_a}$, has n elements with the same structure as the state vector,

$$\mathbf{x_a} = \{x_{q_a}(z_{l_q})\} \tag{8}$$

where the same indices as in Eqn 7, l_q, specify the altitudes, z, to be used for an *a priori* quantity, x_{q_a}.

A priori covariance

The *a priori* covariance, $\mathrm{S_{x_a}}$, is an $(n \times n)$ matrix, where the diagonal elements are the variances and the off-diagonal elements represent the inter-level correlations characterized by a correlation length, l,

$$S_{x_a}^{ij} = \sqrt{S_{x_a}^{ii} S_{x_a}^{jj}} \; \exp(-|z_i - z_j|/l) \qquad (9)$$

Forward Model

We define the act of measurement to be,

$$\mathbf{y} = f(\mathbf{x}, \mathbf{b}) + \epsilon_y \tag{10}$$

where f is identified as the "forward function" and represents the physics of the measurement including the characterization of the instrument and the radiative transfer process. The true atmospheric state is described by the vector $\mathbf{x}$ and $\mathbf{b}$ is a vector of "forward function parameters" which are quantities that affect the radiative transfer but which are not being retrieved. The error term is given by the vector ϵ_y with covariance matrix $\mathbf{S_y}$ and includes measurement noise. The forward model, $\mathbf{f}$, is used to calculate synthesized radiances, $\hat{\mathbf{y}}$, and can be represented by,

$$\hat{\mathbf{y}} = \mathbf{f}(\hat{\mathbf{x}}, \hat{\mathbf{b}}) \tag{11}$$

where $\hat{\mathbf{x}}$ and $\hat{\mathbf{b}}$ are estimation vectors for the state and model parameters, respectively. This represents an approximation to the true forward transfer process and results in a forward model error.

Inverse Model

The inverse model, I, relates the retrieved state to the true state and can be represented formally by,

$$\hat{\mathbf{x}} = I(\mathbf{y}, \hat{\mathbf{b}}, \mathbf{x_a}, \mathbf{c}) \tag{12}$$

where $\mathbf{x_a}$ is a vector of *a priori* data corresponding to the state vector and $\mathbf{c}$ are other data not explicitly included in the forward model e.g. the starting guess vector for $\mathbf{x}$.

Weighting Functions

The state vector is defined on a geometric altitude grid and the radiances are labelled according to the same grid. Then the definition of a weighting function is :

$$K_{hl} = \frac{df_h}{dx_l} \tag{13}$$

where df_h is the predicted change in radiance at the satellite, originating along the ray path labelled by the geometric altitude index, h, due to a change in the quantity, dx_l, at the geometric altitude index, l.

Cost Function

The process we use to obtain a solution for $\mathbf{x}$ is an optimal estimation algorithm. The scalar cost function, constructed assuming Gaussian errors for both the *a priori* estimate and measurements, is given by,

$$\Phi(\mathbf{x}) = (\mathbf{x} - \mathbf{x_a})^{\mathsf{T}} \mathbf{S}_{\mathbf{x_a}}^{-1} (\mathbf{x} - \mathbf{x_a}) + (\mathbf{y} - \mathbf{f}(\mathbf{x}))^{\mathsf{T}} \mathbf{S}_{\mathbf{y}}^{-1} (\mathbf{y} - \mathbf{f}(\mathbf{x})) \qquad (14)$$

The first term of Eqn 14 is a penalty function which constrains the solution to the *a priori* state with a weighting dependent on the *a priori* covariances. The second term is the familiar χ^2-statistic which evaluates the “distance” between the measured and the synthesized radiances with a weighting dependent on the measurement error covariances.

MAP Solution

The **maximum a posteriori** solution is obtained by minimizing the cost function with respect to $\mathbf{x}$,

$$\nabla_{\mathbf{x}}\Phi(\mathbf{x}) = g(\mathbf{x}) = 0 = \mathbf{S}_{\mathbf{x_a}}^{-1}(\mathbf{x} - \mathbf{x_a}) - \mathbf{K}^{\mathsf{T}}\mathbf{S}_{\mathbf{y}}^{-1}(\mathbf{y} - \mathbf{f}(\mathbf{x})) \tag{15}$$

where

$$\mathbf{K} = \frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \tag{16}$$

is the weighting function matrix $(m \times n)$ which represents the sensitivity of the forward model to the retrieved quantities. Rearranging Eqn 15 yields the following nonlinear equation for $\hat{\mathbf{x}}$,

$$\hat{\mathbf{x}} = \mathbf{x_a} + \mathbf{S}_{\mathbf{x_a}}\mathbf{K}^{\mathsf{T}}\mathbf{S}_{\mathbf{y}}^{-1}(\mathbf{y} - \mathbf{f}(\hat{\mathbf{x}})) \tag{17}$$

Gauss-Newtonian Iteration

We seek an efficient numerical method of obtaining the solution to Eqn 17 and a Newtonian iteration scheme may be employed if the system is only moderately non-linear and the initial guess value of the state vector is in the vicinity of the solution,

$$\mathbf{x}_{i+1} = \mathbf{x}_i - [\mathbf{H}(\mathbf{x}_i)]^{-1} \nabla_{\mathbf{x}} \Phi(\mathbf{x}_i) \qquad (18)$$

where the second derivative of the cost function is known as the Hessian matrix,

$$\mathbf{H}(\mathbf{x}) = \nabla^2_{\mathbf{x}} \Phi(\mathbf{x}) = \nabla_{\mathbf{x}} g(\mathbf{x}) \approx \mathbf{S}_{\mathbf{x_a}}^{-1} + \mathbf{K}^{\top} \mathbf{S}_{\mathbf{y}}^{-1} \mathbf{K} \qquad (19)$$

and the iteration scheme is called the inverse Hessian method. If $\Phi(\mathbf{x})$ is exactly a quadratic form then Eqn 18 gives the solution in one step.

Iteration Equation

On substituting Eqns 15 and 19 into Eqn 18 we obtain the iteration equation for $\hat{\mathbf{x}}$, where (hopefully) $\mathbf{x}_i \to \hat{\mathbf{x}}$ as the iteration proceeds,

$$\mathbf{x}_{i+1} = \mathbf{x}_i + (\mathbf{S}_{\mathbf{x_a}}^{-1} + \mathbf{K}_i^{\top}\mathbf{S}_{\mathbf{y}}^{-1}\mathbf{K}_i)^{-1}(\mathbf{K}_i^{\top}\mathbf{S}_{\mathbf{y}}^{-1}[\mathbf{y} - \mathbf{f}(\mathbf{x}_i)] - \mathbf{S}_{\mathbf{x_a}}^{-1}(\mathbf{x}_i - \mathbf{x_a})) \tag{20}$$

The solution covariance including the *a priori* and measurement noise terms is given by,

$$\mathbf{S_x} = (\mathbf{S}_{\mathbf{x_a}}^{-1} + \mathbf{K}^{\top}\mathbf{S}_{\mathbf{y}}^{-1}\mathbf{K})^{-1} \tag{21}$$

Steepest Descent

However, we must consider situations where an initial estimate of the state vector is so far from the solution that a quadratic hypersurface is not a good approximation to the shape of the cost function. The simple method of steepest descent is then more appropriate,

$$\mathbf{x}_{i+1} = \mathbf{x}_i - \gamma^{-1} \nabla_{\mathbf{x}} \Phi(\mathbf{x}_i) \quad (22)$$

where γ determines the step size in the search for the minimum.

Marquardt-Levenberg Method

The Marquardt-Levenberg method combines the inverse Hessian and steepest descent approaches,

$$\mathbf{x}_{i+1} = \mathbf{x}_i - [\mathbf{H}(\mathbf{x}_i) + \gamma \mathbf{I}_n]^{-1} \nabla_{\mathbf{x}} \Phi(\mathbf{x}_i) \tag{23}$$

The value of γ controls the search strategy, for $\gamma \to 0$ the inverse Hessian method dominates and for $\gamma \to \infty$ the steepest descent dominates with a small step size. The prescription for changing the value of γ is dependent on the convergence behaviour. If $\Phi(\mathbf{x}_{n+1}) > \Phi(\mathbf{x}_n)$ then reject $\mathbf{x}_{n+1}$ and increase γ, whereas if $\Phi(\mathbf{x}_{n+1}) < \Phi(\mathbf{x}_n)$ then accept $\mathbf{x}_{n+1}$ and decrease γ. In general, the search procedure starts out as a slow steepest descent method and, as the iteration proceeds and the solution is approached more closely, the search turns to the faster inverse Hessian method.

Scaled Iteration Equation

Because the state vector elements may have widely varying magnitudes and different dimensions a convenient scaling can be achieved by replacing $\gamma \mathbf{I}$ with $\gamma \mathbf{S}_{\mathbf{x_a}}^{-1}$ in which case the iteration equation becomes,

$$\mathbf{x}_{i+1} = \mathbf{x}_i + [(1+\gamma)\mathbf{S}_{\mathbf{x_a}}^{-1} + \mathbf{K}_i^\top \mathbf{S}_{\mathbf{y}}^{-1} \mathbf{K}_i]^{-1} \{\mathbf{K}_i^\top \mathbf{S}_{\mathbf{y}}^{-1} [\mathbf{y} - \mathbf{f}(\mathbf{x}_i)] - \mathbf{S}_{\mathbf{x_a}}^{-1} (\mathbf{x}_i - \mathbf{x_a})\} \tag{24}$$

This equation can be derived formally by applying a scaling transformation to Eqn 23 using $\tilde{\mathbf{x}} = \mathbf{S}_{\mathbf{x_a}}^{-\frac{1}{2}} \mathbf{x}$, $\tilde{\mathbf{y}} = \mathbf{S}_{\mathbf{y}}^{-\frac{1}{2}} \mathbf{y}$, $\tilde{\mathbf{K}} = \mathbf{S}_{\mathbf{y}}^{-\frac{1}{2}} \mathbf{K} \mathbf{S}_{\mathbf{x_a}}^{\frac{1}{2}}$, $\tilde{\mathbf{S}}_{\mathbf{x_a}}^{-1} = \mathbf{I}_n$, $\tilde{\mathbf{S}}_{\mathbf{y}}^{-1} = \mathbf{I}_m$, simplifying and transforming back to the unscaled quantities.

Convergence Criterion

The iteration process must be stopped at a suitable point which prevents

(i) over-running the iteration, resulting in time-wasting computational effort

(ii) under-running the iteration and therefore not converging on an answer lying within a negligible difference from the optimal solution.

A practical convergence test is to stop the iteration when the difference between the last two iterates scaled by the estimated error is smaller than a pre-defined tolerance fraction, ϵ, i.e.

$$d_i^2 = (\mathbf{x}_{i+1} - \mathbf{x}_i)^\top \hat{\mathbf{S}}^{-1} (\mathbf{x}_{i+1} - \mathbf{x}_i) < \epsilon\, n \qquad (25)$$

An upper limit must obviously be set on the maximum number of iterations allowed to curtail "runaway" retrievals which never converge.

Retrieval Quality Control

If the retrieval converges then a number of tests are carried out including :

(i) Consistency of the retrieval with the measurements and *a priori* data.
The standard χ^2-test is applied to Eqn 14 to determine whether there is a statistically significant deviation which indicates an abnormally poor fit. This should follow a χ^2 distribution with m degrees of freedom since there are $n+m$ measurements (the *a priori* data are considered as virtual measurements) to which n parameters have been fitted. The retrieval is accepted as successful if the value of the χ^2-statistic satisfies, for example, the 99.9 % confidence level.

(ii) Consistency of the retrieval with the *a priori* data.
The retrieved state vector is compared to the *a priori* state vector. A poor fit in this case may be indicative of an anomalous atmospheric event in progress i.e. the atmospheric variability has exceed that specified by the *a priori* covariance.

It is useful to record and examine the χ^2-distribution for a complete set of retrievals accumulated over a processing period.

Retrieval Characterization

The retrieved state can be expressed as a **weighted mean** of the true and *a priori* states and the noise contribution,

$$\hat{\mathrm{x}} = \mathrm{Ax} + (\mathrm{I} - \mathrm{A})\mathrm{x_a} + \mathrm{D_y}[\mathrm{K_b}(\mathrm{b} - \hat{\mathrm{b}}) + \Delta\mathrm{f}(\mathrm{x}, \mathrm{b}) + \epsilon_y] \qquad (26)$$

where

$$\mathrm{A} = \mathrm{D_y K} = \frac{\partial \hat{\mathrm{x}}}{\partial \mathrm{x}} \qquad (27)$$

is the **averaging kernel matrix** which represents the sensitivity of the retrieved state to perturbations of the true state.

Retrieval Characterization

$$\mathbf{D_y} = \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{y}} = \left(\mathbf{S}_{\mathbf{x_a}}^{-1} + \mathbf{K}^\top \mathbf{S}_{\mathbf{y}}^{-1} \mathbf{K}\right)^{-1} \mathbf{K}^\top \mathbf{S}_{\mathbf{y}}^{-1} \tag{28}$$

is the **contribution function** matrix (sensitivity of the retrieval to the measurement vector).

Introducing the **forward model error** term $\Delta\mathbf{f}(\mathbf{x}, \mathbf{b})$ into the retrieval

$$\Delta\mathbf{f}(\mathbf{x}, \mathbf{b}) = f(\mathbf{x}, \mathbf{b}) - \mathbf{f}(\mathbf{x}, \mathbf{b}) \tag{29}$$

allows for the fact that the measurements may be known to a much higher accuracy than the expected accuracy of the forward model.

Retrieval Characterization

$$\mathbf{K} = \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \tag{30}$$

is the **weighting function** matrix (sensitivity of the forward model radiances to the state vector), and

$$\mathbf{K_b} = \frac{\partial \mathbf{f}}{\partial \mathbf{b}} \tag{31}$$

is the **model parameter** matrix (sensitivity of the forward model radiances to the forward model parameters.

$$\mathbf{D_a} = \frac{\partial \hat{\mathbf{x}}}{\partial \mathbf{x_a}} = \left(\mathbf{S}_{\mathbf{x_a}}^{-1} + \mathbf{K}^\top \mathbf{S}_{\mathbf{y}}^{-1} \mathbf{K}\right)^{-1} \mathbf{S}_{\mathbf{x_a}}^{-1} = \mathbf{I} - \mathbf{A} \tag{32}$$

is the **a priori contribution function** matrix (sensitivity of the retrieval to the *a priori* vector).

Retrieval Error Analysis

Rearranging the terms in Eqn 26 yields,

$$\begin{aligned}
\hat{\mathbf{x}} - \mathbf{x} = (\mathbf{A} - \mathbf{I})(\mathbf{x} - \mathbf{x_a}) & \quad \text{...smoothing error ...} \epsilon_s \\
+ \mathbf{D_y K_b}(\mathbf{b} - \hat{\mathbf{b}}) & \quad \text{...model parameter error ...} \epsilon_b \\
+ \mathbf{D_y} \Delta \mathbf{f}(\mathbf{x}, \mathbf{b}) & \quad \text{...forward model error ...} \epsilon_f \\
+ \mathbf{D_y} \epsilon_y & \quad \text{...retrieval noise ...} \epsilon_n
\end{aligned} \tag{33}$$

The **smoothing error** (*a priori* error) is given by

$$\epsilon_s = (\mathbf{A} - \mathbf{I})(\mathbf{x} - \mathbf{x_a}) \tag{34}$$

and the retrieval error covariance contribution is,

$$\mathbf{S}_{\epsilon_s} = \mathcal{E}\left\{\epsilon_s \epsilon_s^\top\right\} = (\mathbf{A} - \mathbf{I})\mathbf{S_{x_a}}(\mathbf{A} - \mathbf{I})^\top = \mathbf{D_a}\mathbf{S_{x_a}}\mathbf{D_a}^\top \tag{35}$$

Retrieval Error Analysis

The **model parameter error** is,

$$\epsilon_b = \mathbf{D_y K_b}(\mathbf{b} - \hat{\mathbf{b}}) \tag{36}$$

and the retrieval error covariance contribution is,

$$\mathbf{S}_{\epsilon_b} = \mathcal{E}\left\{\epsilon_b \epsilon_b^\top\right\} = \mathbf{D_y K_b S_b K_b^\top D_y^\top} \tag{37}$$

where $\mathbf{S_b} = \mathcal{E}\left\{(\mathbf{b} - \hat{\mathbf{b}})(\mathbf{b} - \hat{\mathbf{b}})^\top\right\}$ is the error covariance of the model parameters, $\mathbf{b}$.

The **forward model error** is,

$$\epsilon_f = \mathbf{D_y} \Delta \mathbf{f} \tag{38}$$

and the retrieval error covariance contribution is,

$$\mathbf{S}_{\epsilon_f} = \mathcal{E}\left\{\epsilon_f \epsilon_f^\top\right\} = \mathbf{D_y S_f D_y^\top} \tag{39}$$

Retrieval Error Analysis

where $\mathrm{S_f} = \mathcal{E}\left\{\Delta f \Delta f^{\mathsf{T}}\right\}$ is the error covariance of f. An estimate of the error in the operational forward model will be obtained by comparison with line-by-line models.

The **retrieval noise** is given by

$$\boldsymbol{\epsilon_n} = \mathbf{D_y}\boldsymbol{\epsilon_y} \tag{40}$$

and the retrieval error covariance contribution is,

$$\mathbf{S_{\epsilon_n}} = \mathcal{E}\left\{\boldsymbol{\epsilon_n}\boldsymbol{\epsilon_n}^{\mathsf{T}}\right\} = \mathbf{D_y S_y D_y^{\mathsf{T}}} \tag{41}$$

The **full solution covariance** is given by the sum of the error covariance matrices,

$$\begin{aligned} \mathbf{S_x} &= \mathbf{S_{\epsilon_n}} + \mathbf{S_{\epsilon_s}} + \mathbf{S_{\epsilon_b}} + \mathbf{S_{\epsilon_f}} \\ &= \mathbf{D_y S_y D_y^{\mathsf{T}}} + \mathbf{D_a S_{x_a} D_a^{\mathsf{T}}} + \mathbf{D_y K_b S_b K_b^{\mathsf{T}} D_b^{\mathsf{T}}} + \mathbf{D_y S_f D_y^{\mathsf{T}}} \\ &= \left(\mathbf{S_{x_a}^{-1}} + \mathbf{K^{\mathsf{T}} S_y^{-1} K}\right)^{-1} + \mathbf{D_y K_b S_b K_b^{\mathsf{T}} D_b^{\mathsf{T}}} + \mathbf{D_y S_f D_y^{\mathsf{T}}} \end{aligned} \tag{42}$$

Error Terms and Sources

Retrieval Error Term	Error Source	
Smoothing error	Intrinsic resolution	
Forward model parameter error	Ancilliary data error	Contaminant species
	Instrument error	Calibration
		Field-of-view
		Pointing jitter
		Detector misalignment
		Spectral filter
	Spectroscopy error	Line shape, line mixing, continuum
Forward model error	Temperature/pressure error	
	Approximations	
Measurement error	Instrument noise	

Pre-launch algorithm testing

The pre-launch **retrieval testing** consists of making simulated data retrievals corresponding to expected atmospheric conditions which are derived either from model data or previous measurements. The error analyses will incorporate estimates of the error sources shown in the Table obtained from instrument calibration and test data.

Random errors include instrument, detector and electronic noise, which we consider together to form the radiometric measurement noise. Line of sight pointing jitter also makes an important radiometric random noise contribution.

Systematic errors occur due to the instrument model (field of view response, detector misalignment, spectral filter response, calibration gain and off-set), ancillary data (climatological contaminant species abundances), spectroscopy (line shape, line mixing and continuum emission) and the forward model (transmittance approximations, retrieved temperature/pressure values).

Pre-launch Simulated Atmospheres

- Homogeneous atmosphere
- Gradients in Temperature and Constituent Fields
  - polar vortex
  - tropical stratospheric reservoir
  - diurnal species variations
- Atmospheric perturbations
  - influence of *a priori* atmosphere
  - ozone hole
  - stratospheric sudden warming
  - volcanic eruption
- Clouds and Aerosols
  - cirrus
  - polar stratospheric clouds
  - background - volcanic aerosols

Post-launch error analysis

- Post-launch error analysis is concerned with internal data validation and uses the information from in-flight instrument performance studies e.g.
  - estimates of uncorrected scan dependent stray radiances from satellite pitch-up events
  - time-series of space and black-body views
  - profile-to-profile / orbit-to-orbit repeatability measurements

Level-2 Product Errors

- Reporting **correlated errors** in the Level-2 product poses something of a problem
  - **diagonal terms** of a covariance matrix are the familiar error variances which are normally reported in the retrieved product as standard deviations (1 σ).
  - additional **data quality indicators** should be available in the Level-2 product to allow the assessment of the influence of the a priori on the retrieved quantity e.g. a negative sign in the error value to flag the altitudes where most of the information comes from the a priori.

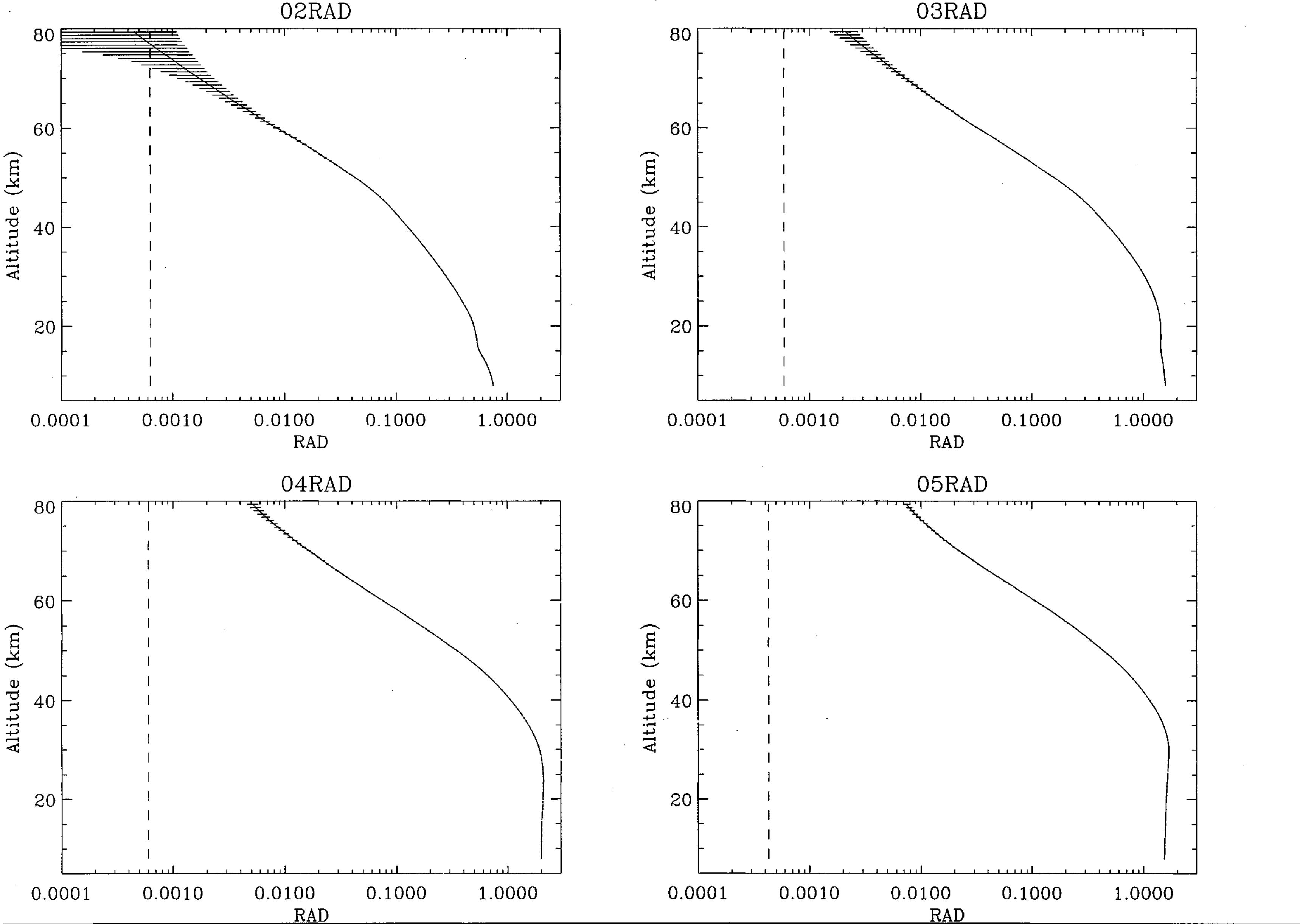
AFGL Profile Retrievals

- A retrieval characterization and error analysis has been performed for the AFGL tropical atmosphere profiles.
- Random error sources apart from the measurement error are represented by a single "forward model error" term consisting of 0.3 % of the channel radiance. Detailed information on individual error components will become available during the HIRDLS calibration and testing phases and these will be used in the final assessments.
- The following figures show the results of calculations of radiance profiles, weighting functions, averaging kernels and random error contributions. The random error contributions, consisting of the measurement error, forward model error and *a priori* error, are the square roots of the diagonals of the respective covariance matrices.

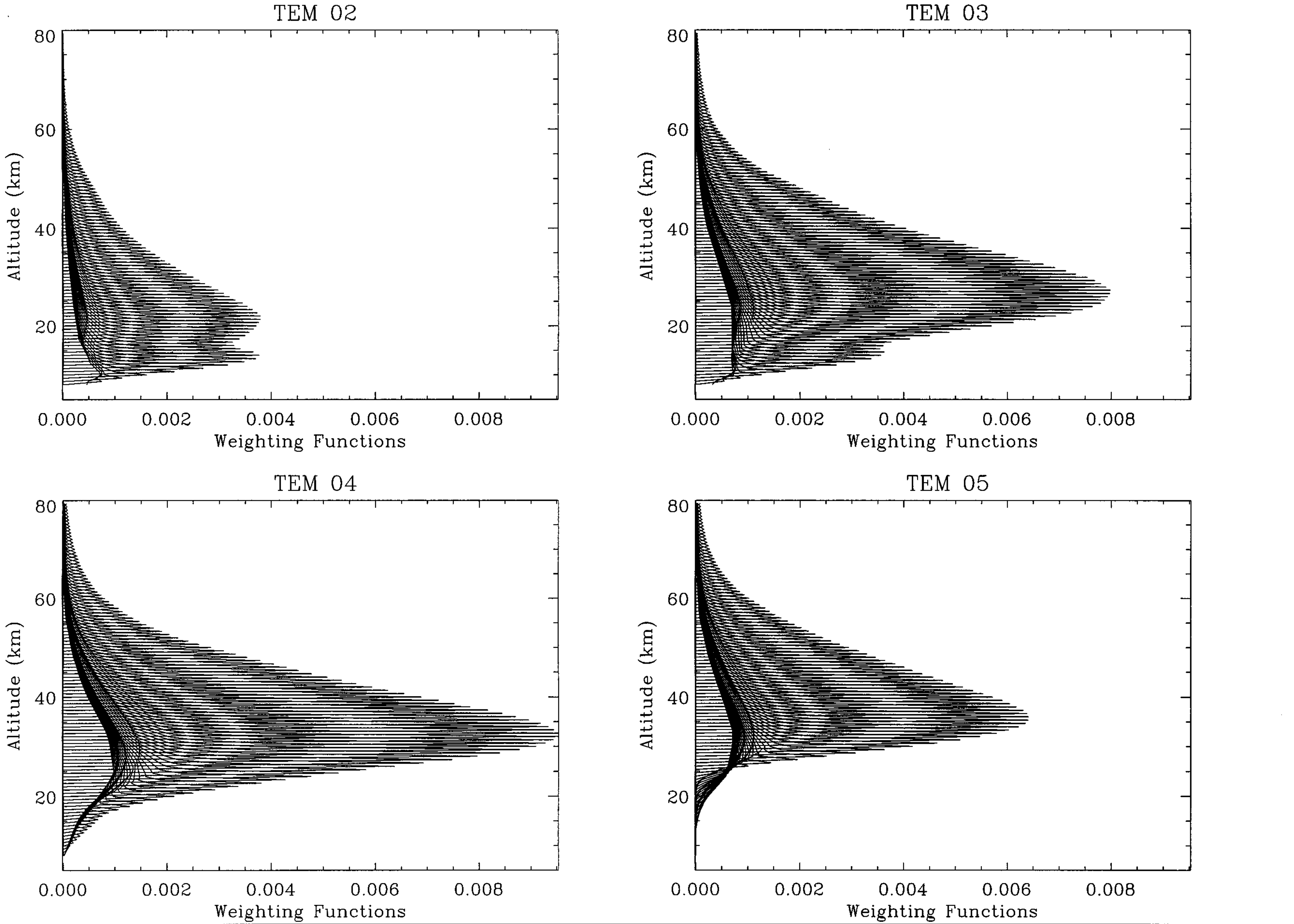
AFGL Temperature/Pressure Retrieval

- The retrieval of temperature and pressure at a reference altitude is performed jointly using 4-sounding channels (2,3,4,5).
- The diagonal elements of the *a priori* covariance matrix, $S_{x_a}^{ii}$ were set at $(20\ K)^2$ and the off-diagonal elements were calculated using a $l = 10$ km correlation length.

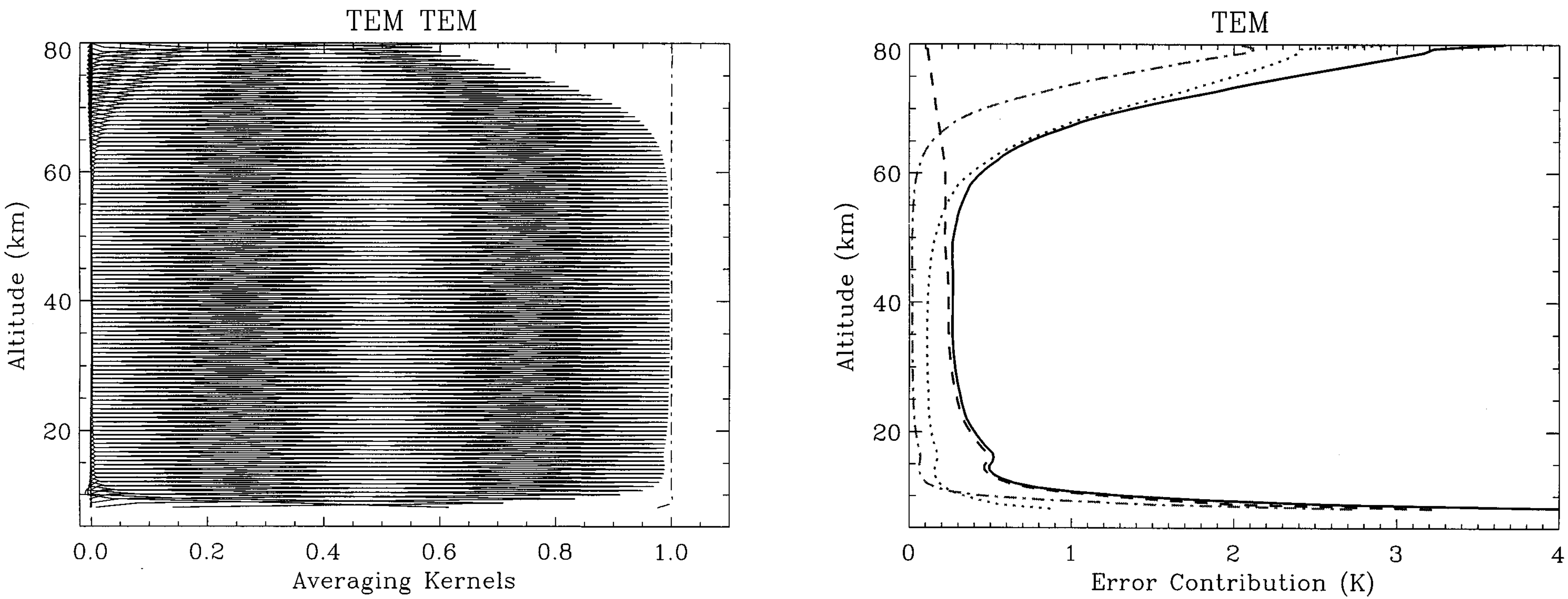
Radiance profiles ($Wm^{-2}sr^{-1}$) for the HIRDLS temperature sounding channels (2,3,4,5) calculated for the AFGL tropical atmosphere



Weighting functions, $\partial R/\partial T$, for the HIRDLS temperature sounding channels (2,3,4,5) calculated for the AFGL tropical atmosphere



Averaging kernels and random error contributions for the temperature retrieval.

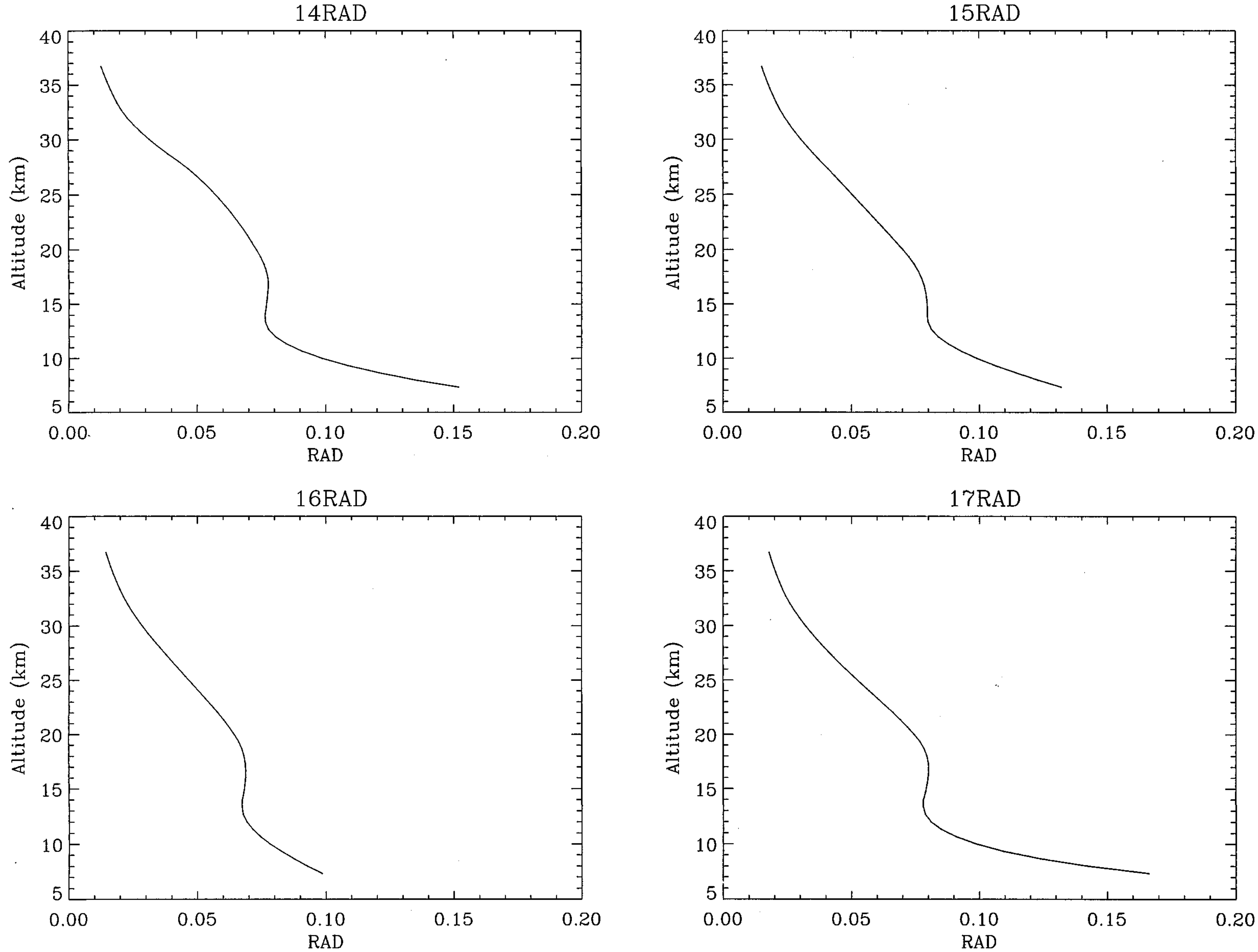


(a) Averaging kernels and (b) random error contributions for the HIRDLS temperature sounding channels calculated for the AFGL tropical atmosphere. The dot-dash line in (a) represents the sum of the averaging kernel rows. In (b) the solid line represents the total error and the dotted, dashed and dot-dashed lines represent the measurement noise, forward model and *a priori* error contributions, respectively.

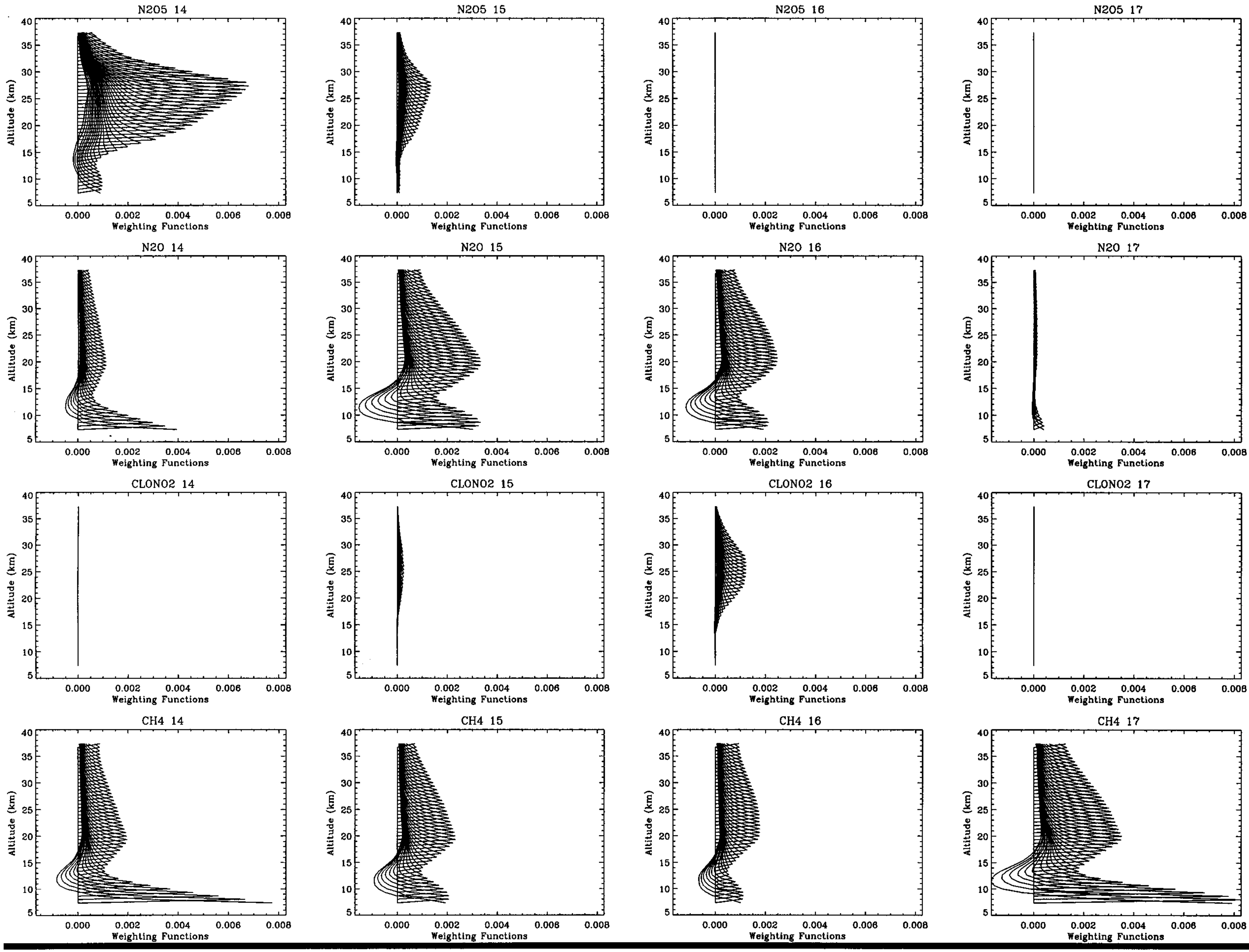
AFGL N_2O, N_2O_5, $ClONO_2$, and CH_4 retrieval

The retrieval of N_2O, N_2O_5, $ClONO_2$, and CH_4 will be performed jointly from 4 channels (14,15,16,17). The diagonal elements of the *a priori* covariance matrix, $S_{x_a}^{ii}$ were set at $(75\ \%VMR)^2$ and the off-diagonal elements were calculated using a $l = 10$ km correlation length

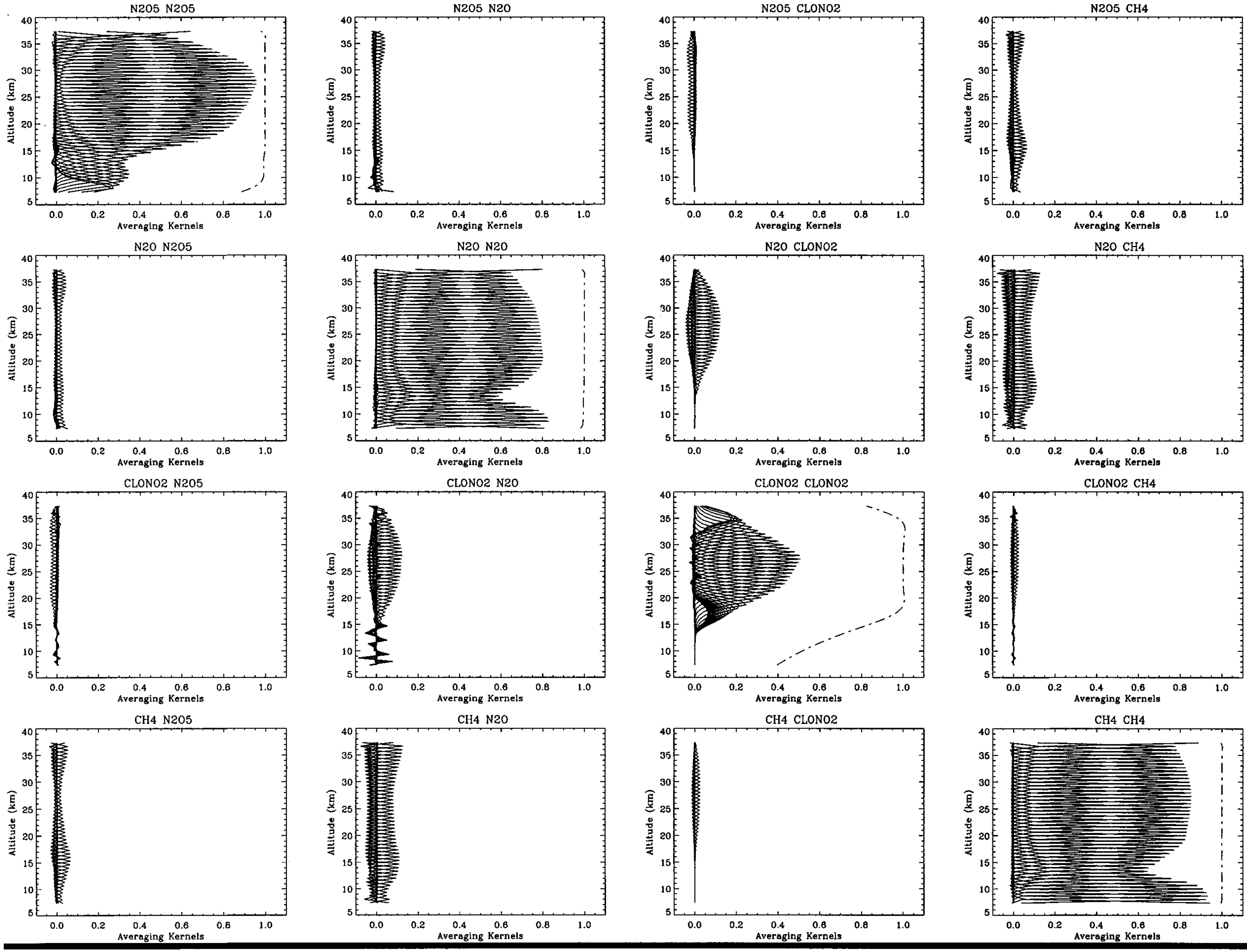
Radiance profiles ($Wm^{-2}sr^{-1}$) for the HIRDLS sounding channels (14,15,16,17) calculated for the AFGL tropical atmosphere.



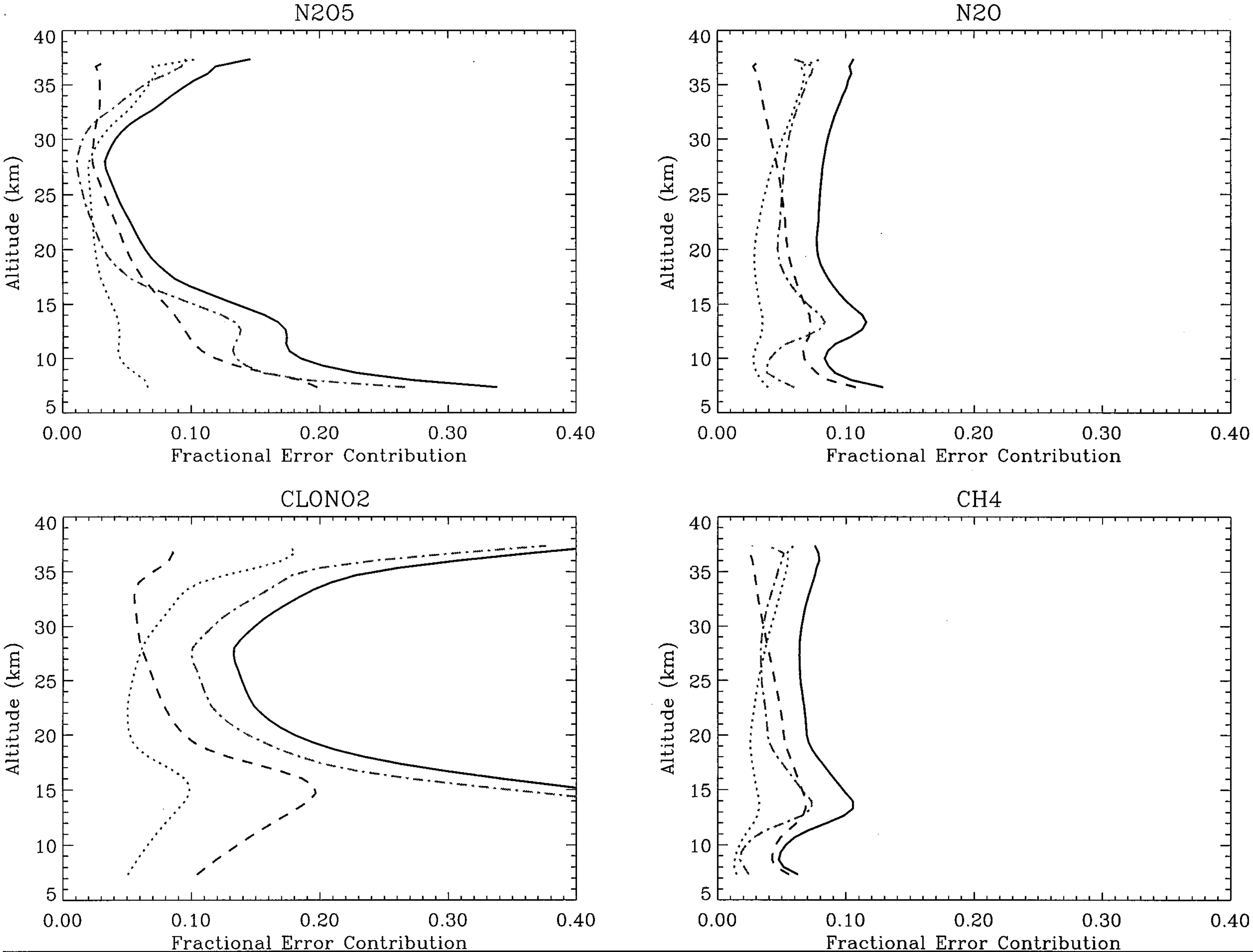
Weighting functions, $\partial R/\partial \ln(VMR)$, for the HIRDLS sounding channels (14,15,16,17) calculated for the AFGL tropical atmosphere



Averaging kernels for the joint retrieval of N_2O, N_2O_5, $ClONO_2$, and CH_4



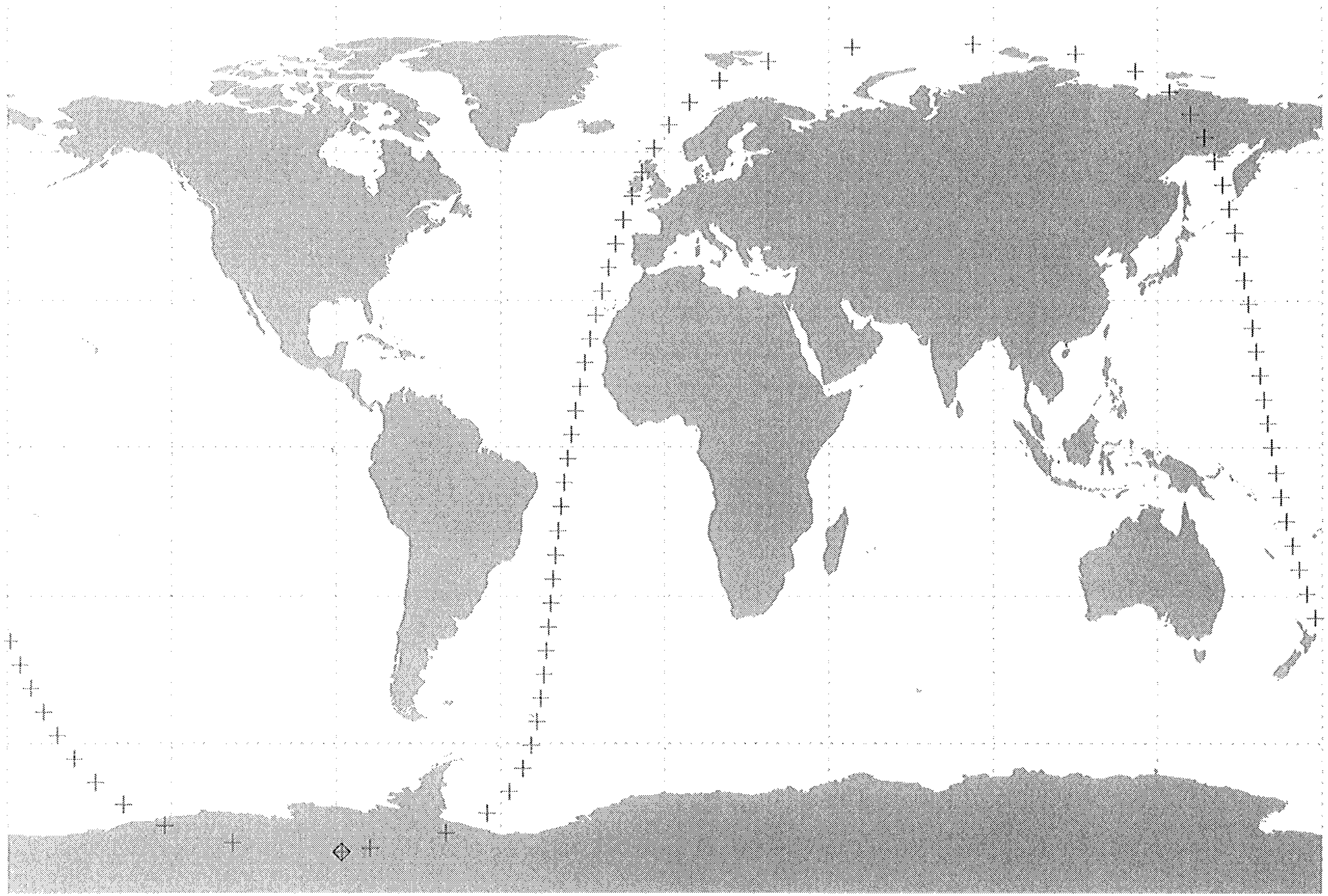
Fractional random error contributions for the joint retrieval of N_2O, N_2O_5, $ClONO_2$, and CH_4



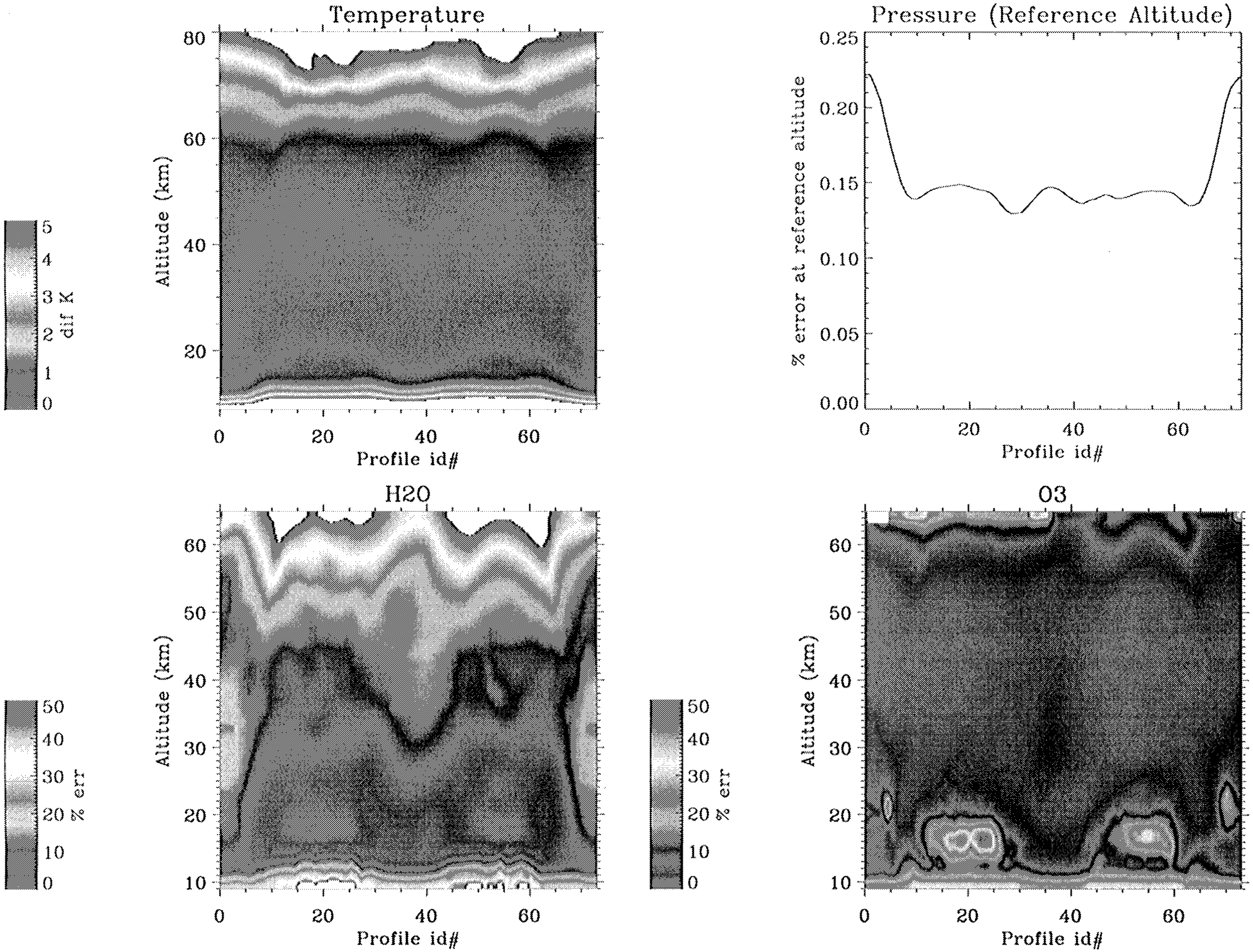
EOS-Aura Intercomparison Exercise

- A retrieval characterization and error analysis has been performed for the Aura Algorithm Working Group Intercomparison Excercise.
- NCAR Mozart Model - Model for OZone And Related chemical Tracers
  - 3-D global chemical transport model (CTM)
  - 20 min time-step
- CIRA T/p + NCAR SOCRATES 2D Model used for *a priori* and initial guess data.
- Ficticious circular orbit - 73 profiles along track
- Clear sky conditions - no clouds or aerosols
- Contaminants are given their "true" model data values in the retrieval
- Random error sources apart from the measurement error are represented by a single "forward model error" term consisting of 0.3 % of the channel radiance
- No propagation of T/p errors into the constituent retrievals
- The following figures show the total retrieval errors.

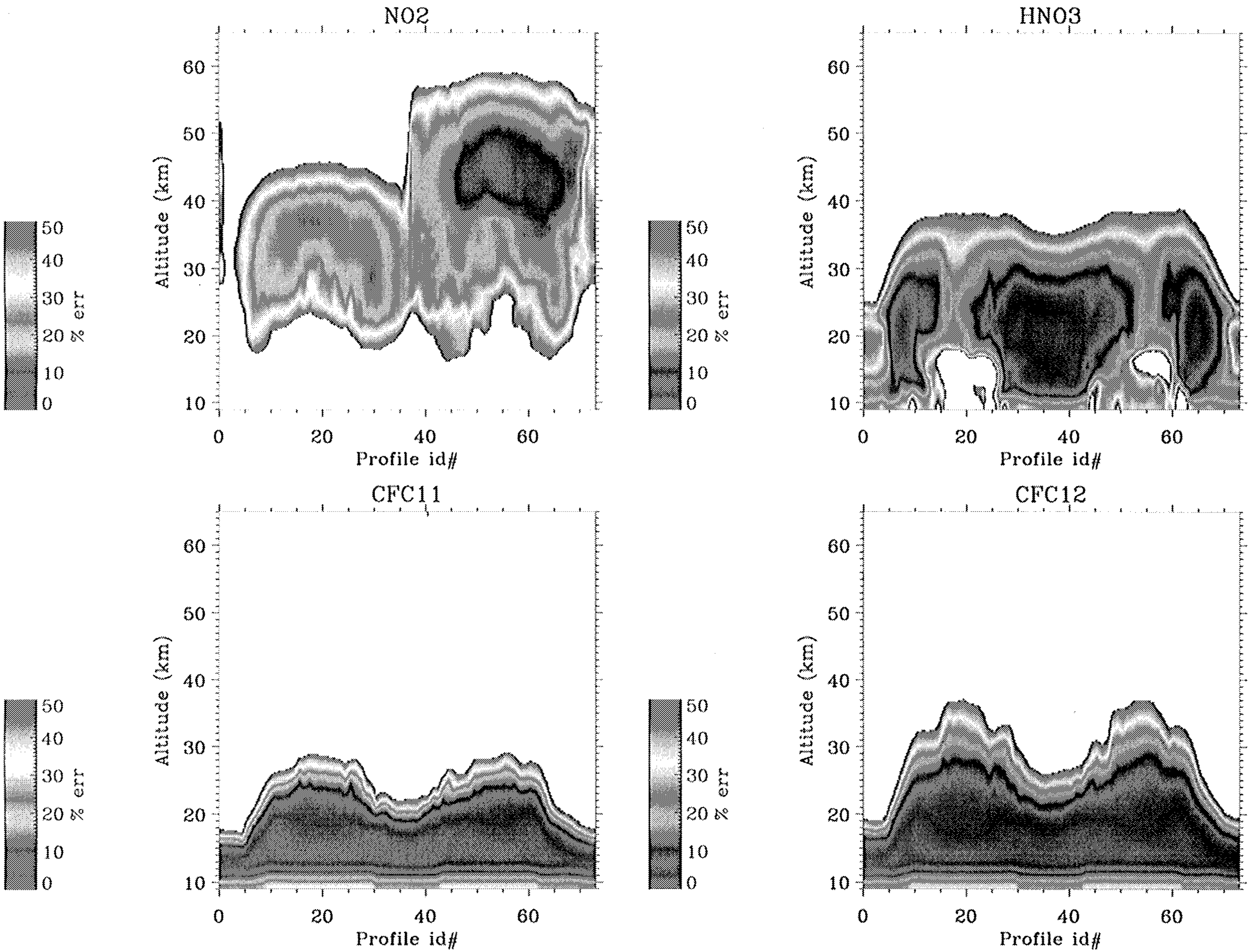
EOS-Aura Intercomparison Orbit



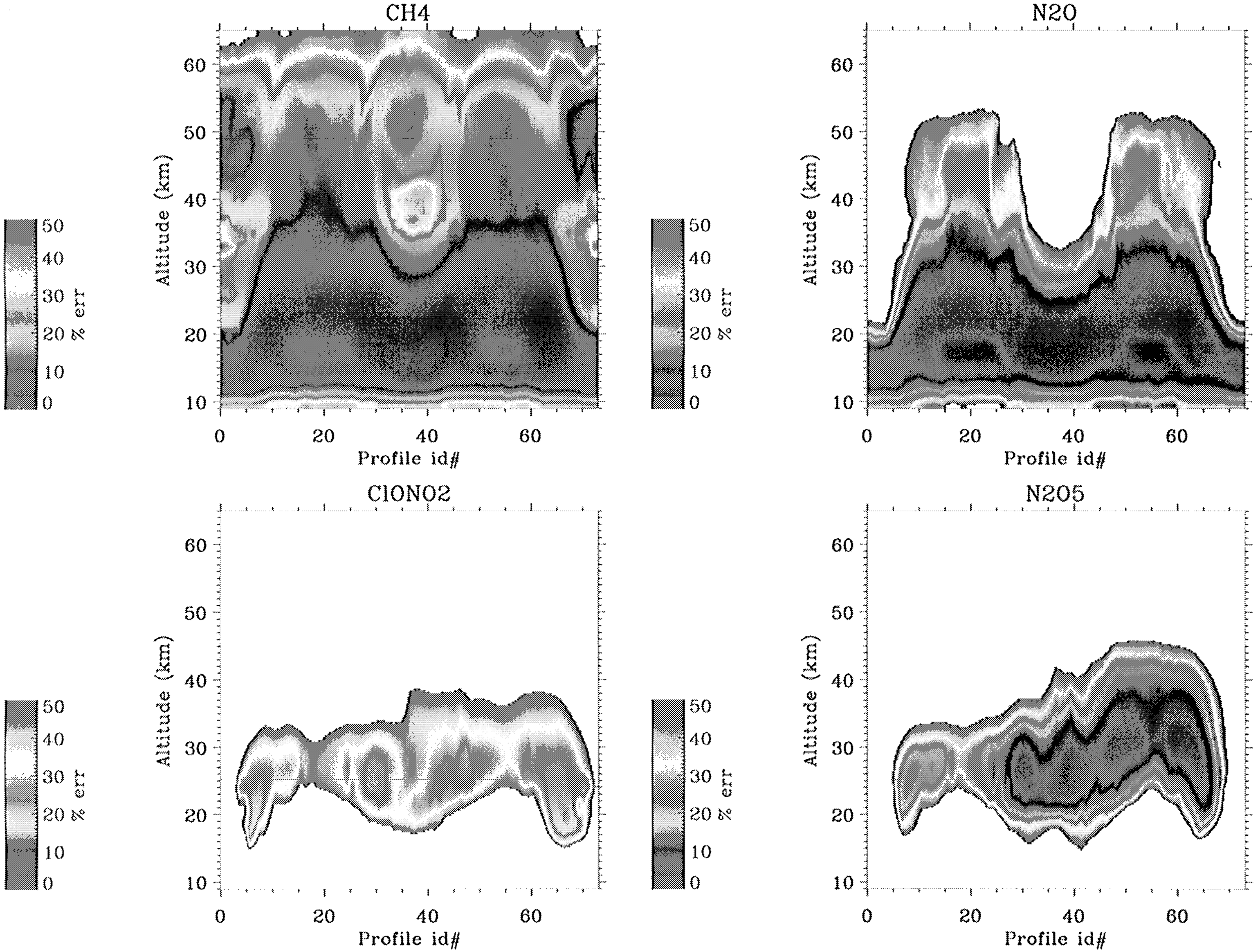
Retrieval Error



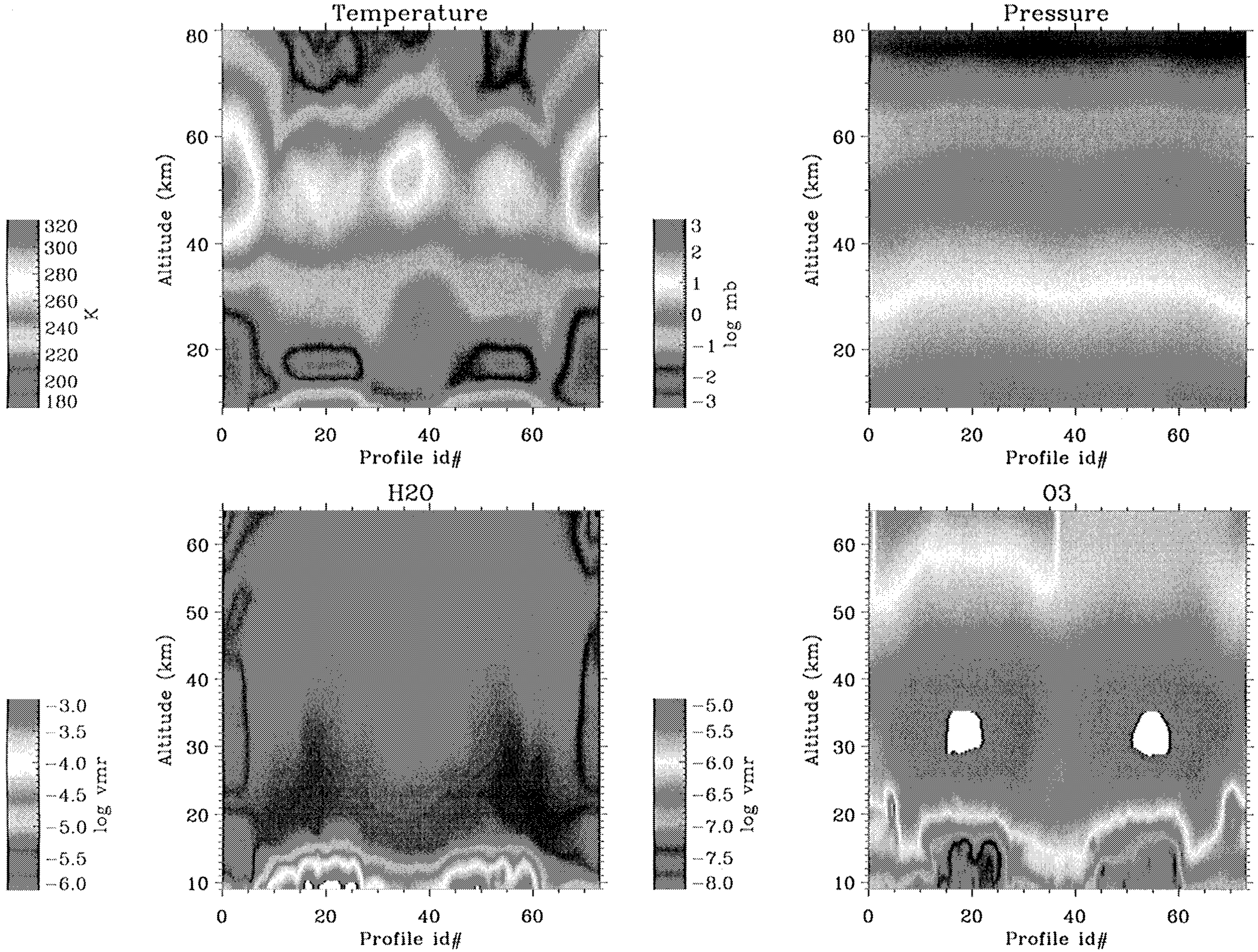
Retrieval Error



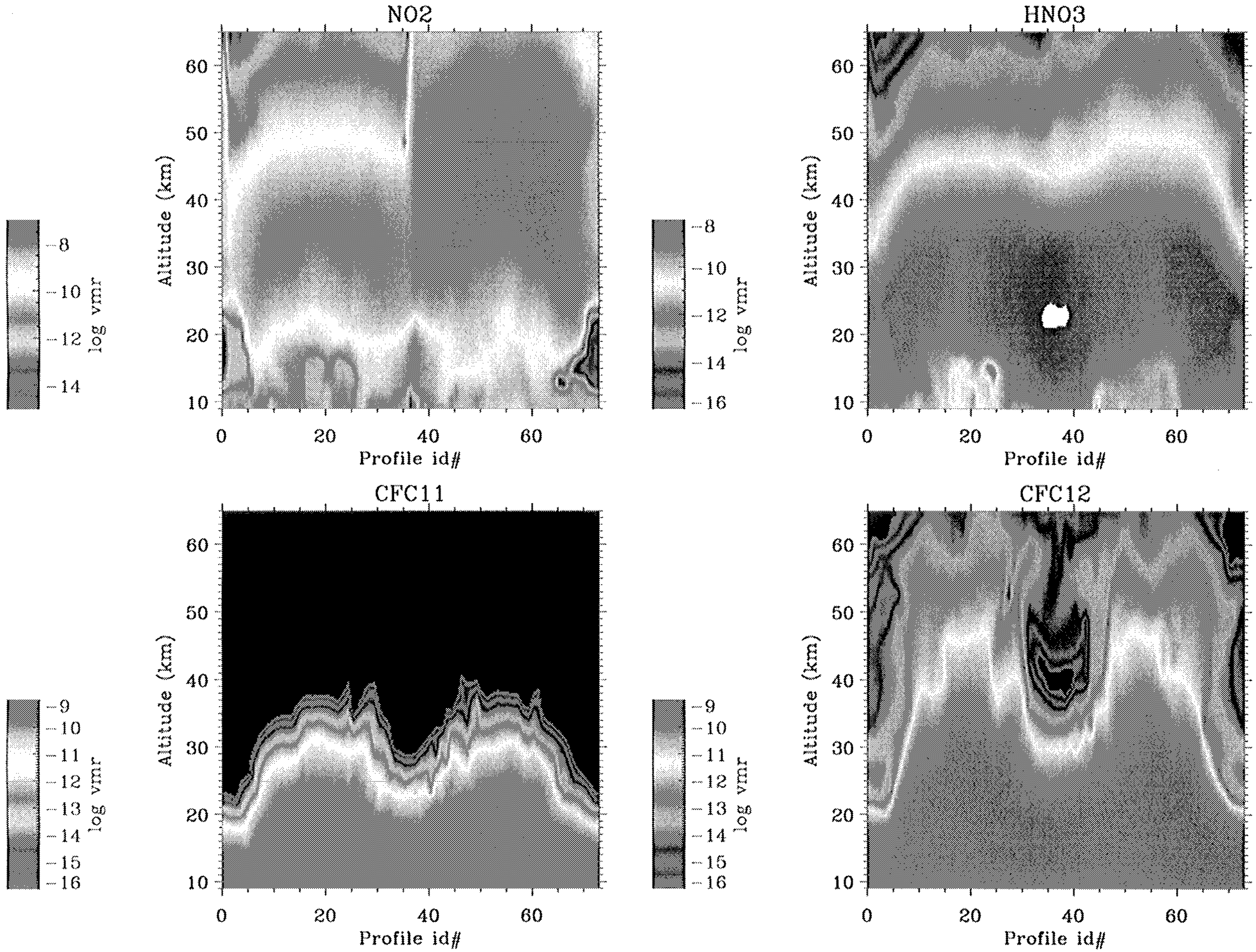
Retrieval Error



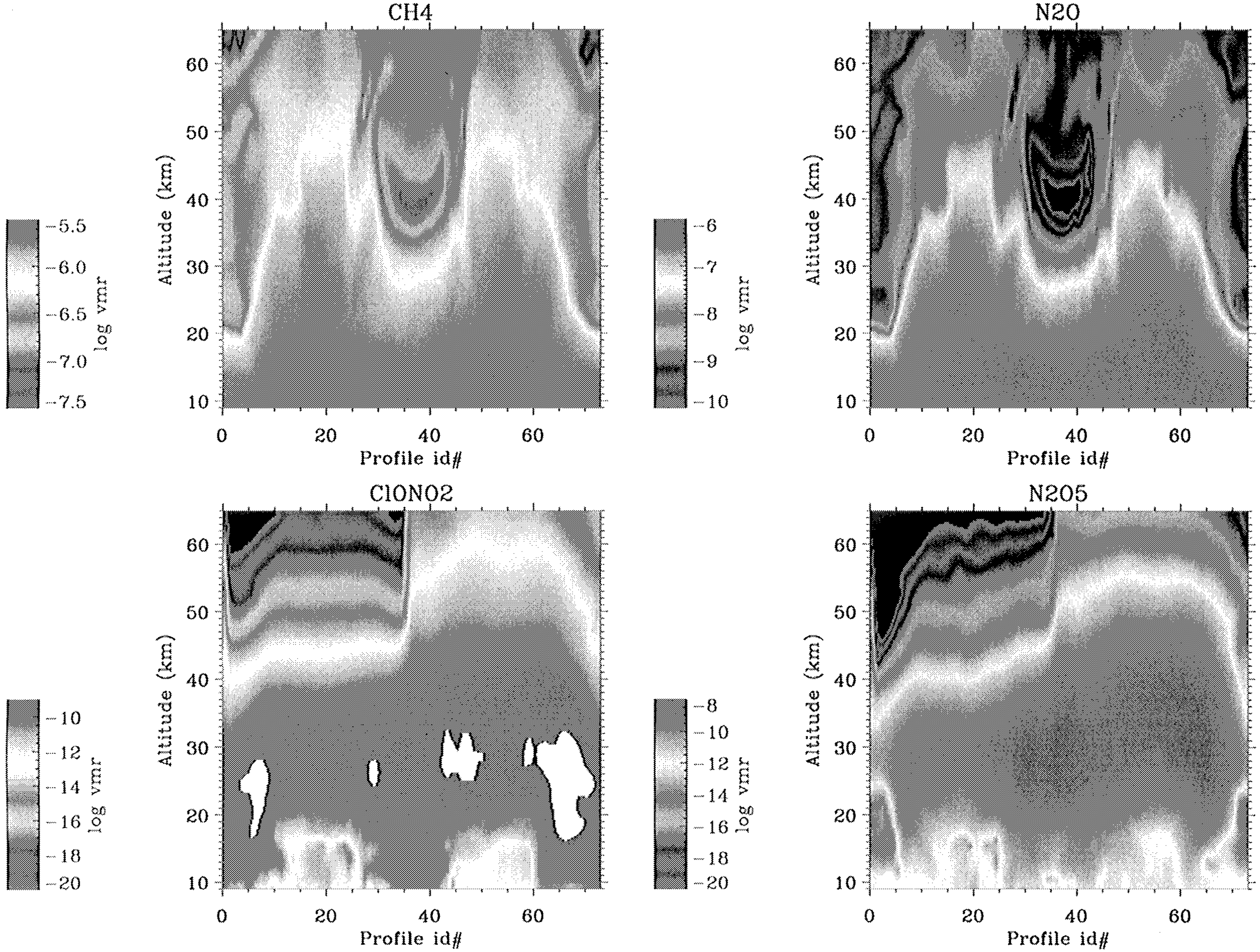
Model Data


Temperature
Pressure
H2O
O3
Altitude (km)
Profile id#
K
320
300
280
260
240
220
200
180
log mb
3
2
1
0
−1
−2
−3
log vmr
−3.0
−3.5
−4.0
−4.5
−5.0
−5.5
−6.0
−5.0
−5.5
−6.0
−6.5
−7.0
−7.5
−8.0

Model Data



Model Data


CH4
N2O
ClONO2
N2O5
Altitude (km)
Profile id#
log vmr
-5.5
-6.0
-6.5
-7.0
-7.5
-6
-7
-8
-9
-10
-10
-12
-14
-16
-18
-20
-8
-10
-12
-14
-16
-18
-20
10
20
30
40
50
60
0
20
40
60

```fortran
SUBROUTINE H2ROE_RetVal( DrvDat, Pnt, LevHgt, Los2D, Toa, RayPath, SpectFilt, CGTraDat, CGPathTra, OptEst, Prf, FIRSTR, ErrLoc )
  !*******************************************************************
  !$Header: H2ROE_RetVal.f90, 9, 8/6/2001 5:51:14 PM, Alyn Lambert$
  ! example subroutine error handling and dignostic prints removed
  !*******************************************************************
  USE H2RSS_Mod, ONLY : H2RSS_DrvDatType, H2RSS_PntType, H2RSS_LevHgtType, H2RSS_ToaType, H2RSS_PrfType, &
       H2RSS_OptEstType
  USE H2RRT_Mod, ONLY : H2RRT_RayPathType, H2RRT_Los2DType
  USE H2RLD_Mod, ONLY : H2RLD_SpectFiltType, H2RLD_CGTraDatType
  USE H2RMA_Mod, ONLY : H2RMA_MakApr, H2RMA_MakDSF
  USE H2RCG_Mod, ONLY : H2RCG_CGPathTraType
  IMPLICIT NONE

  !! Arguments
  TYPE(H2RSS_DrvDatType),    INTENT(INOUT) :: DrvDat    ! retrieval block driver data (n.b. OUT because LSTWTG is set)
  TYPE(H2RSS_PntType),       INTENT(IN)    :: Pnt       ! retrieval pointers
  TYPE(H2RSS_LevHgtType),    INTENT(INOUT) :: LevHgt    ! geolocation data
  TYPE(H2RSS_ToaType),       INTENT(IN)    :: Toa       ! top of atmosphere structure
  TYPE(H2RRT_Los2DType),     INTENT(INOUT) :: Los2D     ! 2D atmosphere
  TYPE(H2RRT_RayPathType),   INTENT(INOUT) :: RayPath   ! ray path structure
  TYPE(H2RLD_SpectFiltType), INTENT(IN)    :: SpectFilt ! spectral filter data loaded by retrieval driver
  TYPE(H2RLD_CGTraDatType),  INTENT(IN)    :: CGTraDat  ! transmittance tables loaded by retrieval driver
  TYPE(H2RCG_CGPathTraType), INTENT(INOUT) :: CGPathTra ! saved path transmittances
  TYPE(H2RSS_OptEstType),    INTENT(INOUT) :: OptEst    ! vectors and matrices used in optimal estimation (allocated arrays)
  TYPE(H2RSS_PrfType),       INTENT(INOUT) :: Prf       ! profile data
  LOGICAL,                   INTENT(INOUT) :: FIRSTR    ! if .TRUE. save FM into INIRAD (1st calc. radiance)
  TYPE(H2_ErrLoc_Type),      INTENT(OUT)   :: ErrLoc    ! error handling

  !! Locals
  TYPE(H2RSS_OptEstType)                   :: OE        ! vectors and matrices used in optimal estimation ( subsets of OptEst )
  CHARACTER(LEN=15)                        :: ErrId     ! error id
  CHARACTER(LEN=80)                        :: ErrMsg    ! error message
  INTEGER(I4B)                             :: NITER     ! iteration counter
  REAL(R8B)                                :: gamma     ! Marquardt-Levenberg step size parameter
  LOGICAL                                  :: CONVERGED ! convergence monitor flag
  CHARACTER(LEN=10)                        :: RetMethod ! retrieval method

  REAL(R8B), ALLOCATABLE, DIMENSION(:,:) :: SXAI    ! matrix inverse of SXA
  REAL(R8B), ALLOCATABLE, DIMENSION(:,:) :: KT      ! matrix transpose of KMN
  REAL(R8B), ALLOCATABLE, DIMENSION(:,:) :: SYI     ! matrix inverse of SY
  REAL(R8B), ALLOCATABLE, DIMENSION(:,:) :: KT_SYI  ! matrix product KT # SYI
  REAL(R8B), ALLOCATABLE, DIMENSION(:,:) :: MAT     ! matrix eqn MAT = (KT#SYI#(YM-FM) + SXAI#(XA-XN))
  REAL(R8B), ALLOCATABLE, DIMENSION(:,:) :: DM      ! matrix eqn DM = INVERT((1.0D0 + gamma)*SXAI + KT#SYI#KMN)
  REAL(R8B), ALLOCATABLE, DIMENSION(:,:) :: DMI     ! matrix inverse of DM
  REAL(R8B), ALLOCATABLE, DIMENSION(:,:) :: YM_FM   ! vector difference of measurment and forward model vectors (YM - FM)
  REAL(R8B), ALLOCATABLE, DIMENSION(:,:) :: XA_XN   ! vector difference of apriori and state vectors (XA - XN)
  REAL(R8B), ALLOCATABLE, DIMENSION(:)   :: XNP     ! updated state vector XNP = XN + DMI#MAT

  REAL(R8B), ALLOCATABLE, DIMENSION(:)   :: SAVEX   ! saved state vector
  REAL(R8B), ALLOCATABLE, DIMENSION(:)   :: SAVEF   ! saved forward model vector
  REAL(R8B), ALLOCATABLE, DIMENSION(:,:) :: SAVEK   ! saved weighting function matrix

  REAL(R8B), ALLOCATABLE, DIMENSION(:)   :: SAVET   ! saved Prf%T
  REAL(R8B), ALLOCATABLE, DIMENSION(:)   :: SAVEP   ! saved Prf%P
  REAL(R8B), ALLOCATABLE, DIMENSION(:,:) :: SAVEV   ! saved Prf%V

  REAL(R8B)                              :: PHIN    ! Phi(XN)  value of cost function at XN
  REAL(R8B)                              :: PHINP1  ! Phi(XNP) value of cost function at new location XNP
  REAL(R8B)                              :: di2     ! convergance diagnostic

  LOGICAL                                :: LBLWUP       ! set .TRUE. if retrieval blows up
  LOGICAL                                :: UpdatePath   ! set .TRUE. if new RayPath is to be computed
  LOGICAL                                :: FAIL, SINGLR
  !! Exe
```

```
UpdatePath = .FALSE.
FIRSTR     = .TRUE.

!! make XA, SXA first guess XN, determine NX
CALL H2RMA_MakApr( DrvDat%PRDGAS, DrvDat%NPRDCT, LevHgt%LevRef, Pnt%PDCTLV, Pnt%NPDTLV, DrvDat%APRLEN, &
     LevHgt%Z, Prf%P, Prf%T, Prf%PApr, Prf%PAprErr, Prf%TApr, Prf%TAprErr, Prf%V, Prf%VErr, &
     OptEst%XN, OptEst%XA, OptEst%SXA, OptEst%NX )

!! point to array subsets
OE%NX  = OptEst%NX
OE%MY  = OptEst%MY
OE%XN  => OptEst%XN(1:OE%NX)
OE%SX  => OptEst%SX(1:OE%NX,1:OE%NX)
OE%XA  => OptEst%XA(1:OE%NX)
OE%SXA => OptEst%SXA(1:OE%NX,1:OE%NX)
OE%YM  => OptEst%YM(1:OE%MY)
OE%FM  => OptEst%FM(1:OE%MY)
OE%SY  => OptEst%SY(1:OE%MY,1:OE%MY)
OE%SM  => OptEst%SM(1:OE%MY,1:OE%MY)
OE%SF  => OptEst%SF(1:OE%MY,1:OE%MY)
OE%ST  => OptEst%ST(1:OE%MY,1:OE%MY)
OE%SR  => OptEst%SR(1:OE%MY,1:OE%MY)
OE%KMN => OptEst%KMN(1:OE%MY,1:OE%NX)

ALLOCATE( SXAI(OE%NX,OE%NX) )
ALLOCATE( KT(OE%NX,OE%MY) )
ALLOCATE( SYI(OE%MY,OE%MY) )
ALLOCATE( KT_SYI(OE%NX,OE%MY) )
ALLOCATE( MAT(OE%NX,1) )
ALLOCATE( DM(OE%NX,OE%NX) )
ALLOCATE( DMI(OE%NX,OE%NX) )
ALLOCATE( YM_FM(OE%MY,1) )
ALLOCATE( XA_XN(OE%NX,1) )
ALLOCATE( XNP(OE%NX) )

ALLOCATE( SAVEX(OE%NX) )
ALLOCATE( SAVEF(OE%MY) )
ALLOCATE( SAVEK(OE%MY,OE%NX) )

ALLOCATE( SAVET(SIZE(Prf%T)) )
ALLOCATE( SAVEP(SIZE(Prf%P)) )
ALLOCATE( SAVEV(SIZE(Prf%V(:,1)), SIZE(Prf%V(1,:))) )

!! invert the apriori covariance matrix SXA
CALL H2ROE_MTXINV( OE%NX, OE%NX, OE%NX, OE%SXA, SXAI, SINGLR, FAIL, ERRMSG )

CONVERGED = .FALSE.
NITER = 0

RetMethod = 'ML' ! only one retrieval method

SELECT CASE(RetMethod)

CASE('ML') !! Marquardt-Levenberg

   !! call forward model
   CALL H2ROE_CGFMRad( DrvDat, Pnt, LevHgt, Los2D, RayPath, SpectFilt, CGTraDat, CGPathTra, &
        OE, Prf, FIRSTR, ErrLoc )

   !! adjust FM/SY with forward model bias/errors
   CALL H2RMA_MakDSF( OE%FM, OE%MY, OE%SM, OE%SF, OE%ST, OE%SR, OE%SY, SYI )

   gamma = 100.0D0  ! ensure starts with steepest descent
```

```

      !! calculate cost function
      PHIN = H2ROE_ClcPhi( OE%XN, OE%XA, SXAI, OE%YM, OE%FM, SYI )

      UpdatePath = ANY( DrvDat%PRDGAS(:) == 'CO2' ) ! set update path if T/p retrieval

      ITERATE : DO

         niter = niter + 1

         KT     = TRANSPOSE(OE%KMN)
         KT_SYI = MATMUL(KT, SYI)

         YM_FM(:,1) = (OE%YM(:) - OE%FM(:))
         XA_XN(:,1) = (OE%XA(:) - OE%XN(:))

         !! MAT = (KT#SYI#(YM-FM) + SXAI#(XA-XN))
         MAT = MATMUL(KT_SYI, YM_FM) + MATMUL(SXAI, XA_XN)

         !! DM = (1.D0 + gamma)*SXAI + (KT#SYI#K)
         DM = (1.0D0 + gamma)*SXAI + MATMUL( KT_SYI, OE%KMN )

         !! invert the DM matrix
         CALL H2ROE_MTXINV ( OE%NX, OE%NX, OE%NX, DM, DMI, SINGLR, FAIL, ERRMSG )

         !! generate the state vector update XNP = XN + INVERT((1.0D0 + gamma)*SXAI + KT#SYI#K) # MAT
         XNP = OE%XN + RESHAPE( MATMUL(DMI, MAT), (/ OE%NX /) )

         !! convergence diagnostic (scalar) di2 = (XNP-XN)^T # MAT
         di2 = DOT_PRODUCT( XNP-OE%XN, MAT(:,1) )

         !! save current info in case we don't move to a better location
         SAVET = Prf%T     ; SAVEP = Prf%P     ; SAVEV = Prf%V
         SAVEX = OE%XN     ; SAVEF = OE%FM     ; SAVEK = OE%KMN
         OE%XN = XNP

         !! decompose XN and update atm. profiles
         CALL H2ROE_DecomX( DrvDat%PRDGAS, OE%XN, LevHgt%Top, LevHgt%LevRef, DrvDat%NPRDCT, &
              Pnt%NPDTLV, Pnt%PDCTLV, LevHgt%GeoHRef, LevHgt%SinLat, Prf%TApr, &
              Prf%T, Prf%P, Prf%E, LevHgt%Z, Prf%V, LBLWUP, ErrLoc )

         !! update the LO2 2D atmosphere
         CALL H2ROE_UpdateLOS2D( DrvDat, Pnt, Prf, LevHgt, Toa, RayPath, UpdatePath, Los2D, ErrLoc )

         !! call forward model
         CALL H2ROE_CGFMRad( DrvDat, Pnt, LevHgt, Los2D, RayPath, SpectFilt, CGTraDat, CGPathTra, &
              OE, Prf, FIRSTR, ErrLoc )

         !! adjust FM/SY with forward model bias/errors
         CALL H2RMA_MakDSF( OE%FM, OE%MY, OE%SM, OE%SF, OE%ST, OE%SR, OE%SY, SYI )

         !! calculate cost function
         PHINP1 = H2ROE_ClcPhi( OE%XN, OE%XA, SXAI, OE%YM, OE%FM, SYI )

         IF (PHINP1 > PHIN) THEN !! revert to previous XN and increase gamma

            OE%XN = SAVEX ; OE%FM = SAVEF ; OE%KMN = SAVEK

            !! don't update PHIN
            gamma = MIN( 1.D33, gamma * 10.D0 )

            !! revert to previous atm.
            Prf%T = SAVET ; Prf%P = SAVEP ; Prf%V = SAVEV

```

```
           !! revert to previous LO2 2D atmosphere
           CALL H2ROE_UpdateLOS2D( DrvDat, Pnt, Prf, LevHgt, Toa, RayPath, UpdatePath, Los2D, ErrLoc )

        ELSE  !! accept new XN and decrease gamma

           !! update PHIN
           PHIN = PHINP1
           gamma = MAX( 1D-33, gamma * 0.1D0 )

           !! accept new atm (already called DECOMX)

        END IF

        CONVERGED = (di2 < DrvDat%epsilon*OE%NX)
        IF (niter >= DrvDat%MaxItr .OR. CONVERGED) EXIT ITERATE

     ENDDO ITERATE

  CASE DEFAULT
  END SELECT

  !! calculate solution covariance SX = INVERT(SXAI + KT#SYI#KMN)
  CALL H2ROE_MTXINV ( OE%NX, OE%NX, OE%NX, SXAI + MATMUL( MATMUL(KT,SYI), OE%KMN ), OE%SX, &
       SINGLR, FAIL, ERRMSG )

  !! decompose solution covariance SX onto atm. error profiles
  CALL H2ROE_DecomXerr( DrvDat%PRDGAS, OE%XN, OE%SX, OE%SXA, LevHgt%LevRef, DrvDat%NPRDCT, Pnt%PDCTLV, &
       Pnt%NPDTLV, Prf%PErr, Prf%TErr, Prf%VErr, LBLWUP, ErrLoc )

  !! Add Apriori test

  !! Add Radiance test

  !! Add diagnostics

  DEALLOCATE( SXAI, KT, SYI, KT_SYI, MAT, DM, DMI, YM_FM, XA_XN, XNP, SAVEX, SAVEF, SAVEK, SAVET, SAVEP, SAVEV )
  RETURN

END SUBROUTINE H2ROE_RetVal
```