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"The Empirical Optimal Estimation Method Applied to the Inversion of Atmospheric FTIR Remote Sensing Data"

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

The empirical optimal estimation method applied to the inversion of atmospheric FTIR remote sensing data.

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OUTLINE

- Principle of FTIR remote sensing
- Inversion
  - Total columns
  - Improved total columns
  - vertical profiles
- Characterisation of the retrieval
- Application:

  1996-2001 time series of O_3 at the Jungfraujoch

FTIR REMOTE SENSING

- Principle of Michelson interferometry:

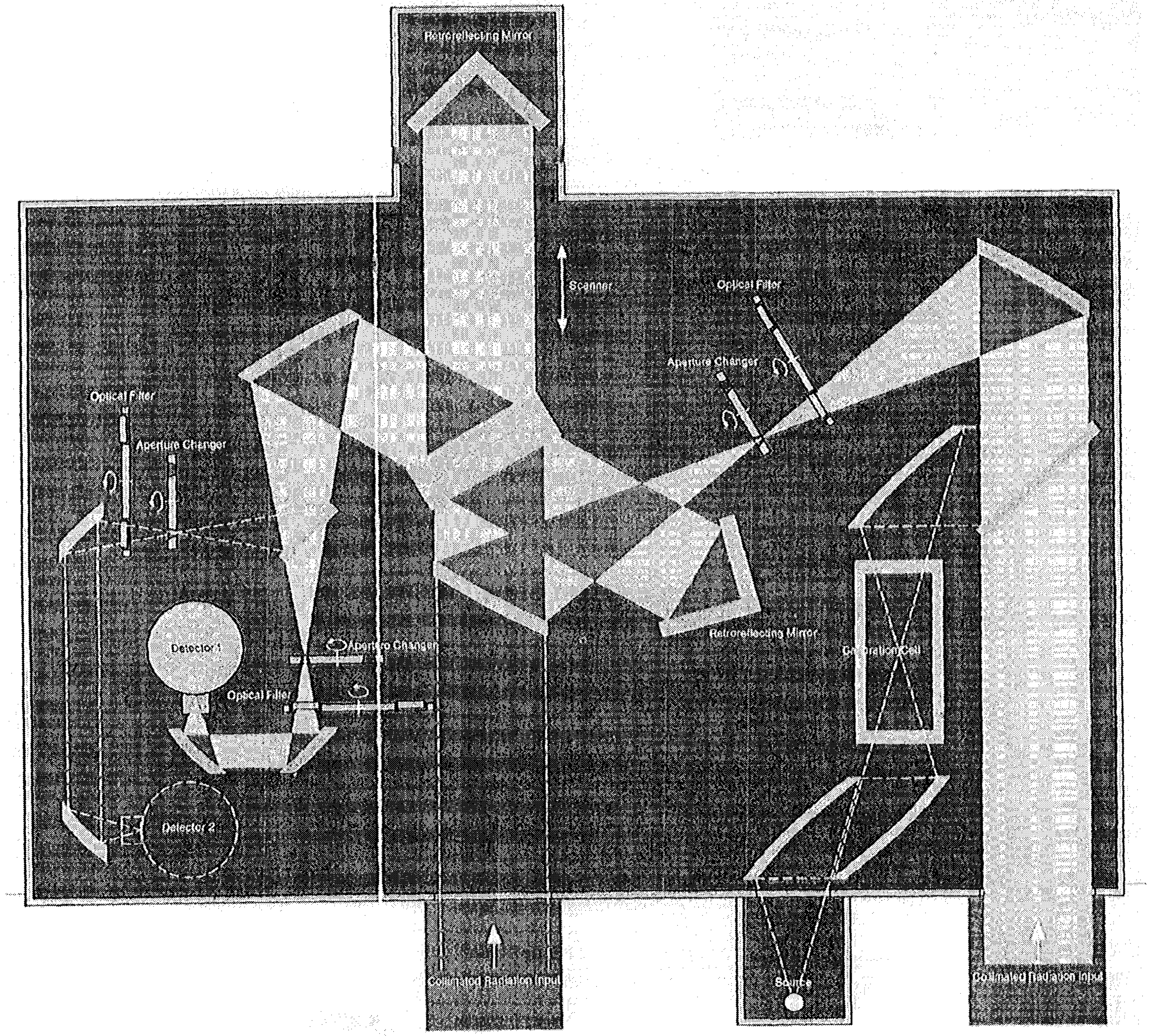
  ⇒ recording of interferogram of incident light (sun, thermal emission, ….)

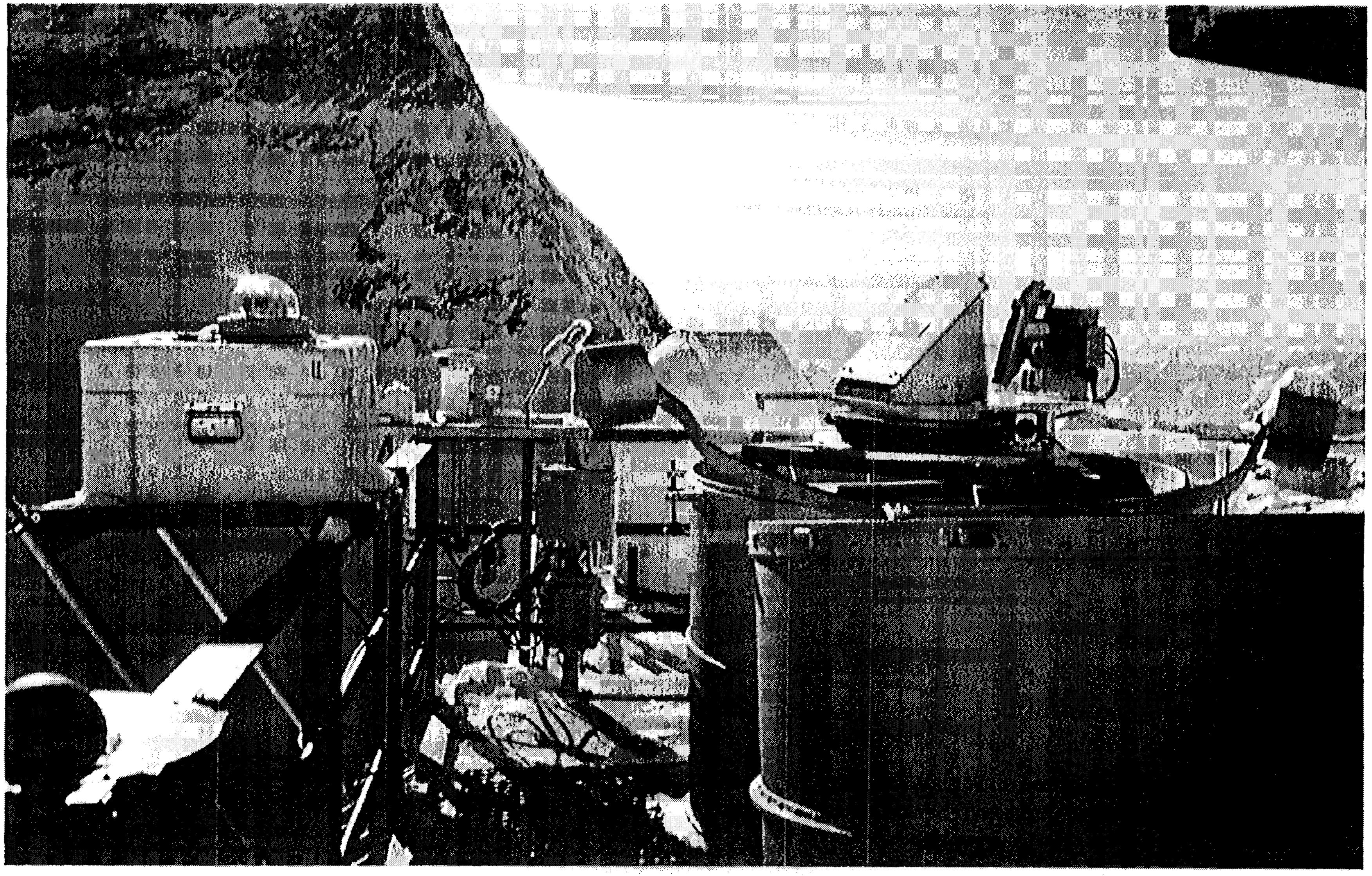
  ⇒ FFT

  ⇒ spectrum

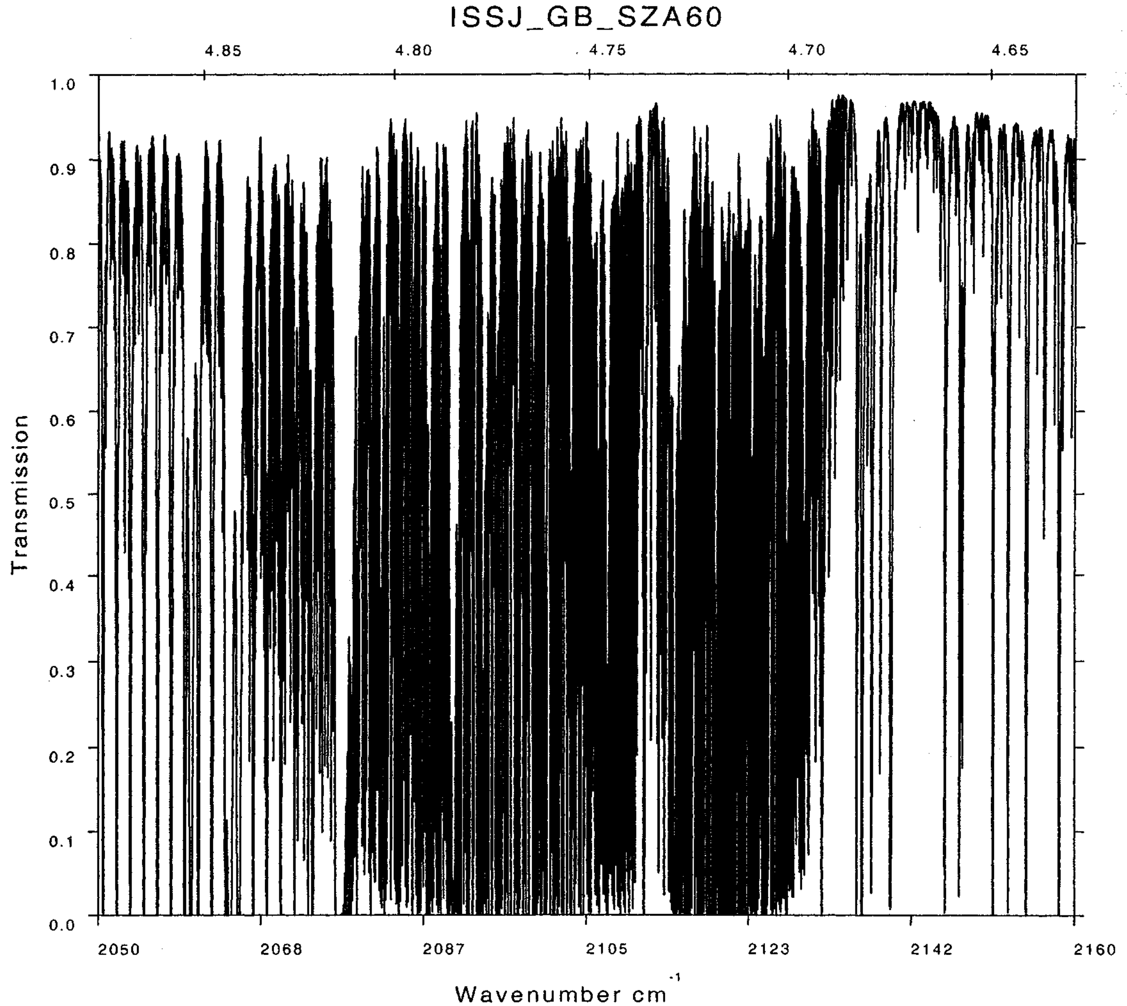
    - high spectral resolution
    - multiplex advantage

⇒ distinction of many absorption/emission signatures simultaneously

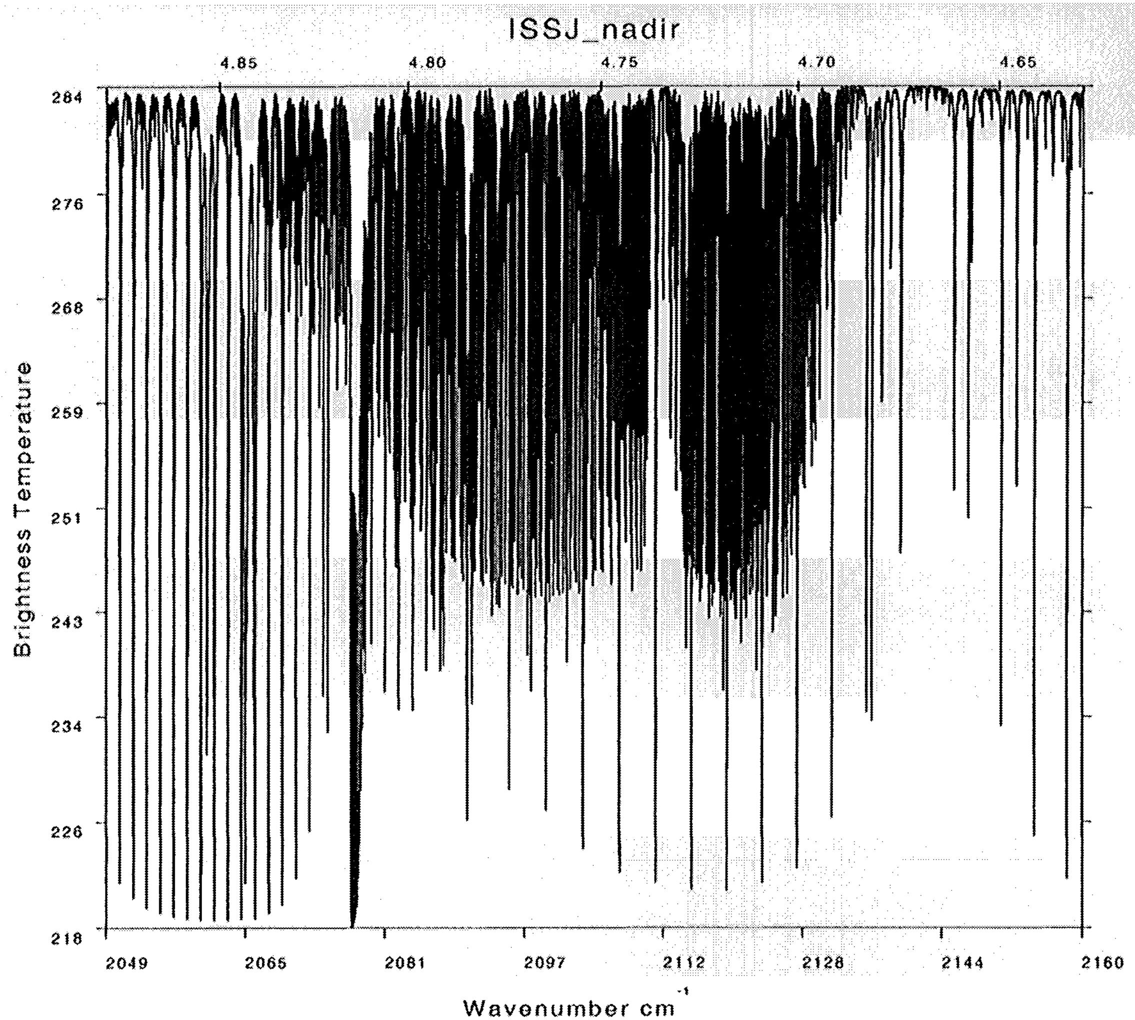

Retroreflecting Mirror
Scanner
Optical Filter
Aperture Changer
Optical Filter
Aperture Changer
Detector 1
Aperture Changer
Optical Filter
Retroreflecting Mirror
Calibration Cell
Detector 2
Collimated Radiation Input
Source
Collimated Radiation Input



Absorption ground-based spectrum



Emission nadir spectrum



FTIR atmospheric 'PRODUCTS'

- Reference gas: N_2(<1%)
- Minor constituents: CO_2 (<2%), N_2O (≤ 2%), CH_4 (≈2%), CO (≤ 4%), O_3 (≤ 5%), [H_2O]
- Halogenated trace species:

  HCl (≤ 4%), $ClONO_2$ (≈ 20%), CCl_2F_2 (≤ 4%), $CHClF_2$ (≤ 6%), HF (≤ 3%), COF_2 (≤ 20%), SF_6(≈ 30%)
- Nitrogenated trace species:

  NO(≤ 6%), NO_2 (≤ 10%), HNO_3(≈ 5%), HNO_4(monthly avg.)
- Other trace species: C_2H_2 (≈ 20%), C_2H_6 (≤ 6%), HCN (≤ 8%), OCS (≤ 8%), H_2CO (monthly avg.), [H_2CO_2, CH_3Cl, CCl_4, CCl_3F, ...]; various isotopes

(Precisions estimated for Jungfraujoch conditions)

FTIR retrieval: forward model

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

$$F(x,b) \cong f(x,b,b'); \quad \Delta f = f(x,b,b') - F(x,b)$$

$$y \cong F(x,b) + \varepsilon$$

y is the experimental measurement, x is the unknown state

ε is the experimental error term

f, F are the forward function, model, respectively

b are forward function parameters, that are in the model,

w / best estimates $\hat{b}$; some may be retrieved $\rightarrow$ included in x

b' are forward function parameters, ignored in the model

FTIR Forward Line By Line model

Solar absorption mode

RT model: Transmission $T(\tilde{v}) = I(\tilde{v}) / I_0(\tilde{v}) = \exp(-\alpha(\tilde{v}))$

with $a(\tilde{v})$ absorption coefficient:

$$\alpha(\tilde{v}) = \int_{z_0}^{\infty} dz\ l(z) \sum_i n_i(z) \sum_j S_{ij}(\tilde{v}, z) f_{ij}(\tilde{v}, z)$$

$i \rightarrow$ molecule ; $j \rightarrow$ absorption line

S_{ij} line strength / molecule ; f_{ij} *lineshape*

dependence on $z \Leftrightarrow$ dependence on P, T

Instrument model: $\tilde{T}(\tilde{v}) = T(\tilde{v}) \otimes ILS(\tilde{v})$

FTIR LBL model parameters

- Linestrength and -shape $\Rightarrow b$
  - Strength S(T) - depending on *E''*
  - Voigt lineshape is adopted,

    close to Lorentz at high pressure,

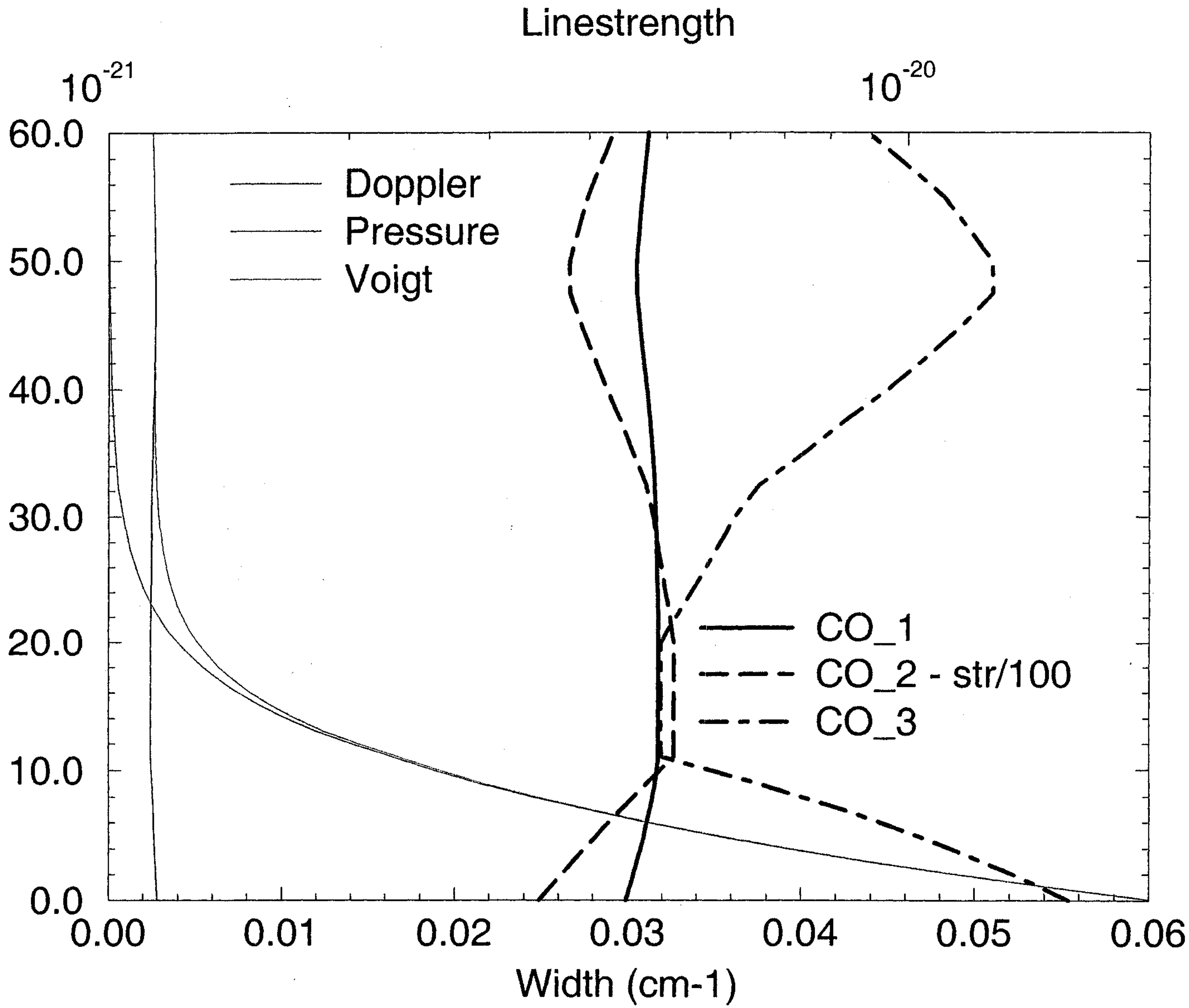
    close to Doppler at low pressure

    - *neglects* Dicke narrowing, line mixing, ... $\Rightarrow b'$

Doppler HWHM $\alpha_{\mathrm{D}} = \nu_0 \sqrt{\dfrac{2kT\ln 2}{M}}$

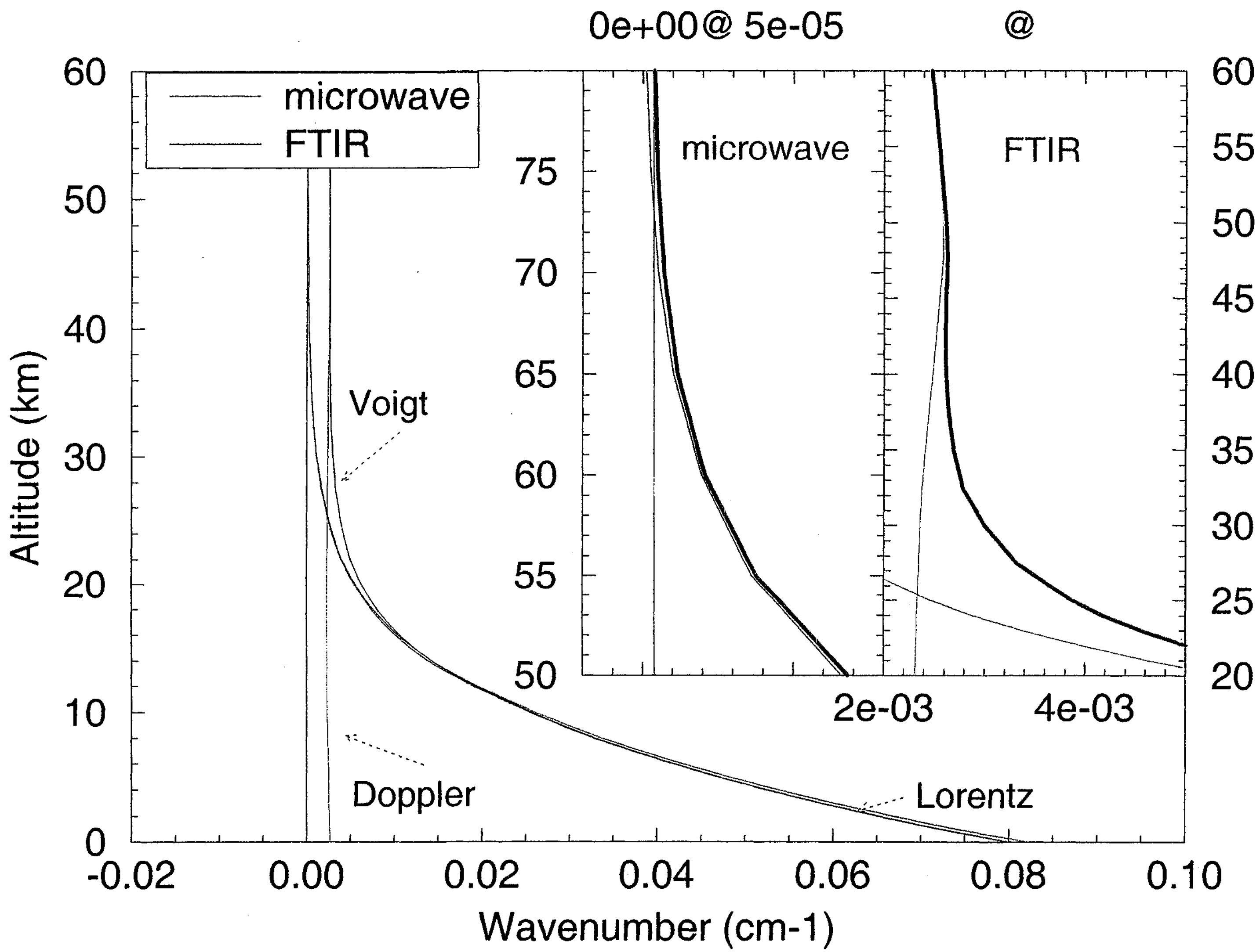
Lorentz HWHM $\alpha_L = \alpha_{L,0} (P/P_0)^m (T_0/T)^n$

$m \leq 1 \quad n: 0.5 \rightarrow 1$ (databases for $\alpha_{L,0}$ and n)



Linestrength
10^-21
10^-20
60.0
50.0
40.0
30.0
20.0
10.0
0.0
Doppler
Pressure
Voigt
CO_1
CO_2 - str/100
CO_3
0.00
0.01
0.02
0.03
0.04
0.05
0.06
Width (cm-1)

Linewidth contributions - comparison



FTIR measurement sensitivities

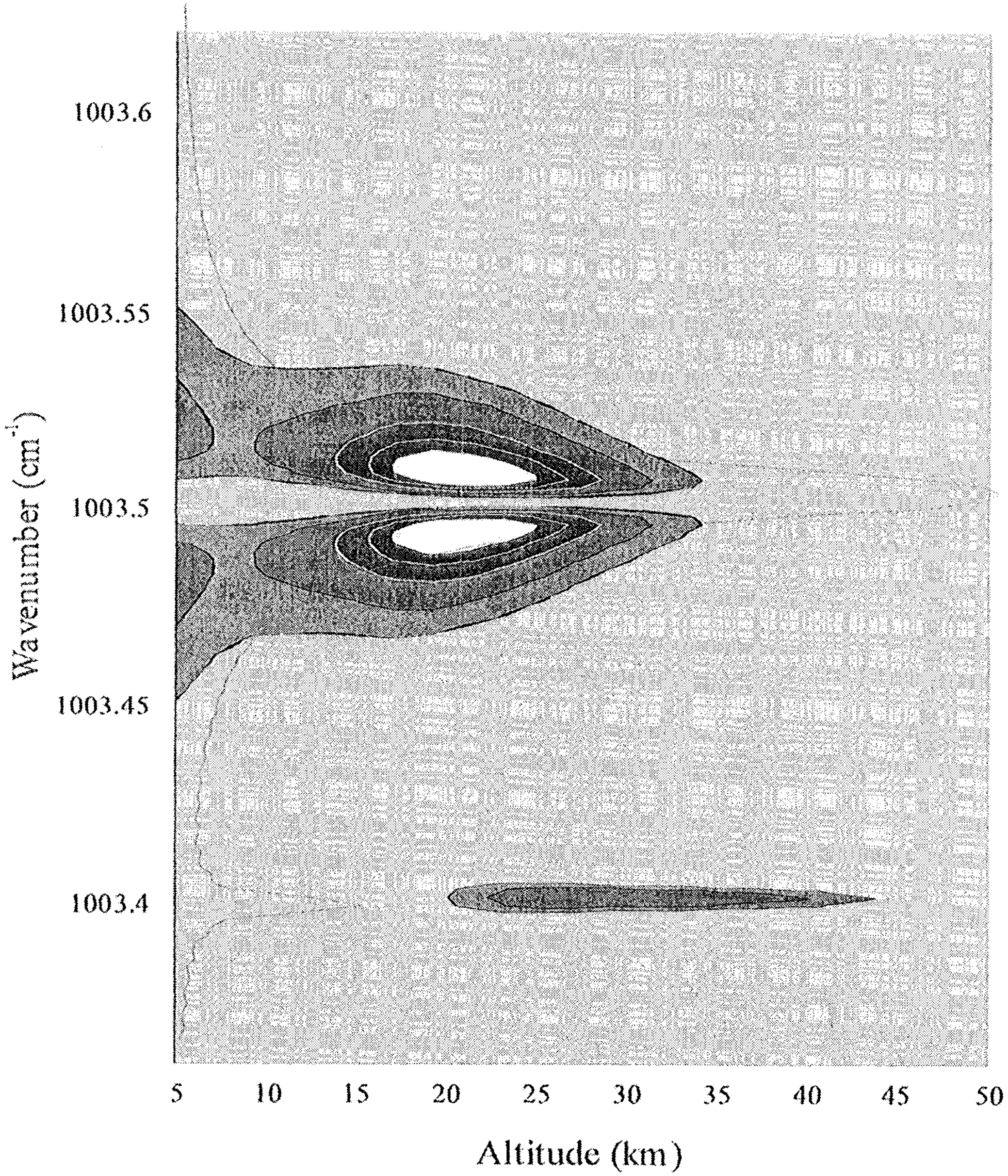
- Weighting f^{ion}: $\mathbf{K}_x = \partial \mathbf{y} / \partial \mathbf{x} \cong \partial \mathbf{F} / \partial \mathbf{x}$
  - saturated lines:

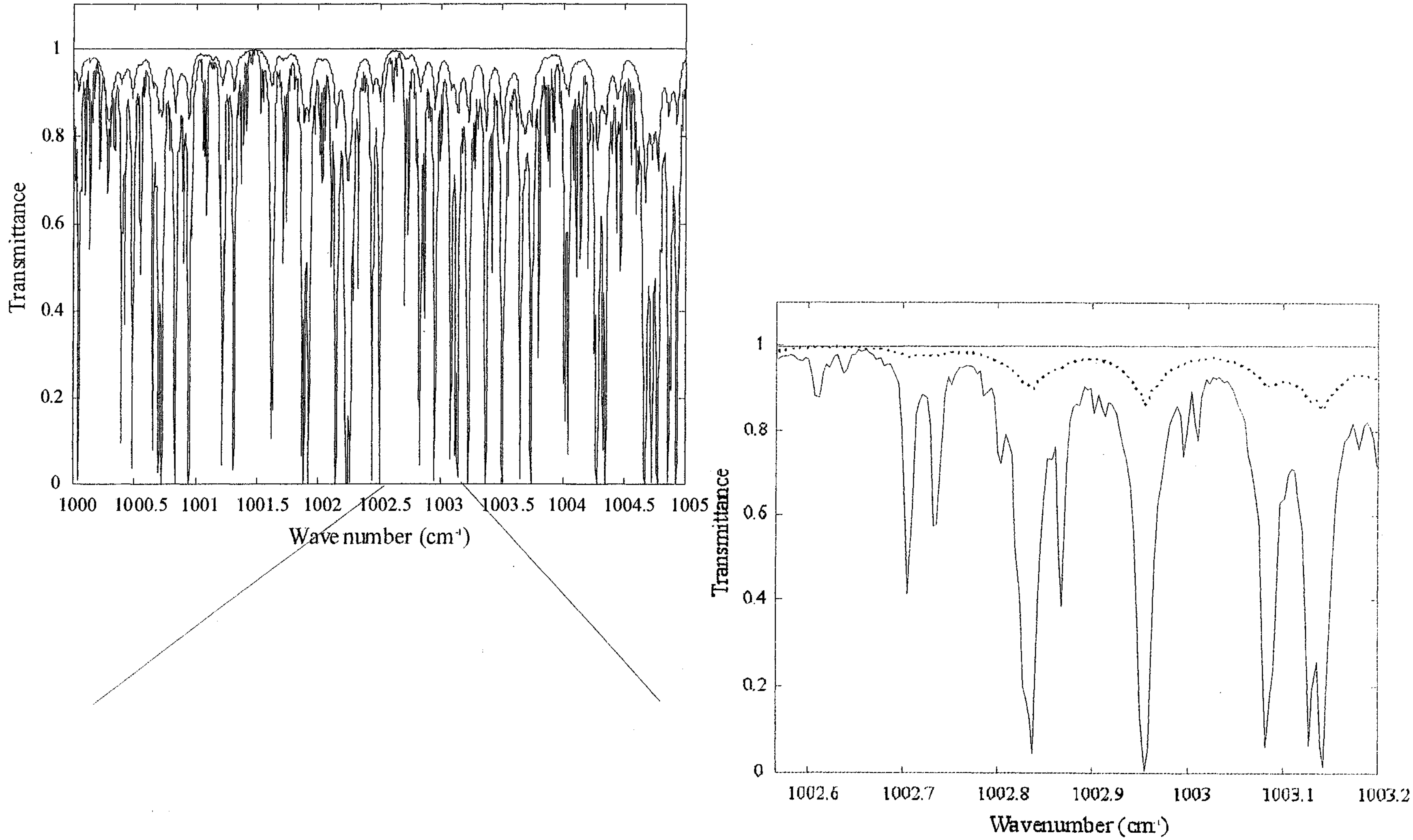
    more sensitive to tropospheric contributions,

    reduced information content as to stratosphere
  - weak lines:

    more information about the stratosphere

$$\mathbf{K}_x = \partial \mathbf{y} / \partial \mathbf{x} \cong \partial \mathbf{F} / \partial \mathbf{x}$$

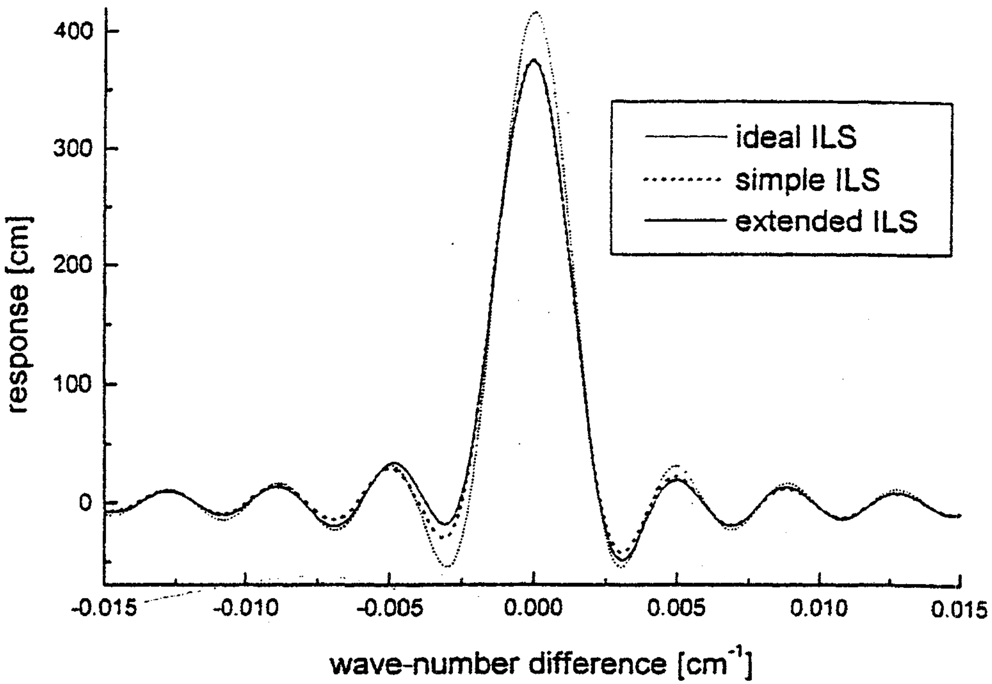



1
0.8
0.6
0.4
0.2
0
Transmittance
1000
1000.5
1001
1001.5
1002
1002.5
1003
1003.5
1004
1004.5
1005
Wave number (cm⁻¹)
1
0.8
0.6
0.4
0.2
0
Transmittance
1002.6
1002.7
1002.8
1002.9
1003
1003.1
1003.2
Wavenumber (cm⁻¹)

FTIR instrument function

- ILS $\Rightarrow \boldsymbol{b}$
  - FTS-ILS (ν): sinc ($\propto$ OPD) $\otimes$ Boxcar ($\propto \Omega$)

    $\otimes$ *EAP-function*



FTIR retrieval: Inverse Model -1

- General formulation

$$\hat{x} = R(\,F(x,b) + \Delta f\,(x,b,b') + \varepsilon,\; x_a,\; \hat{b},\; c)$$

$\hat{x}$ is the retrieval result for x, through the inverse method R

x_a and c: retrieval method parameters

x_a the a priori estimate of x

- FTIR:
  - $x \Leftrightarrow$ target concentrations (column w/ fixed profile$\rightarrow$ ... $\rightarrow$ profile), selected model par^{s};
  - $c \Leftrightarrow x_a$, S_a, $S_\varepsilon \Leftrightarrow SNR_{retr}$, convergence criterium

FTIR retrieval: Inverse Model - 2

- OEM - Non-linear case- Newtonian iteration:

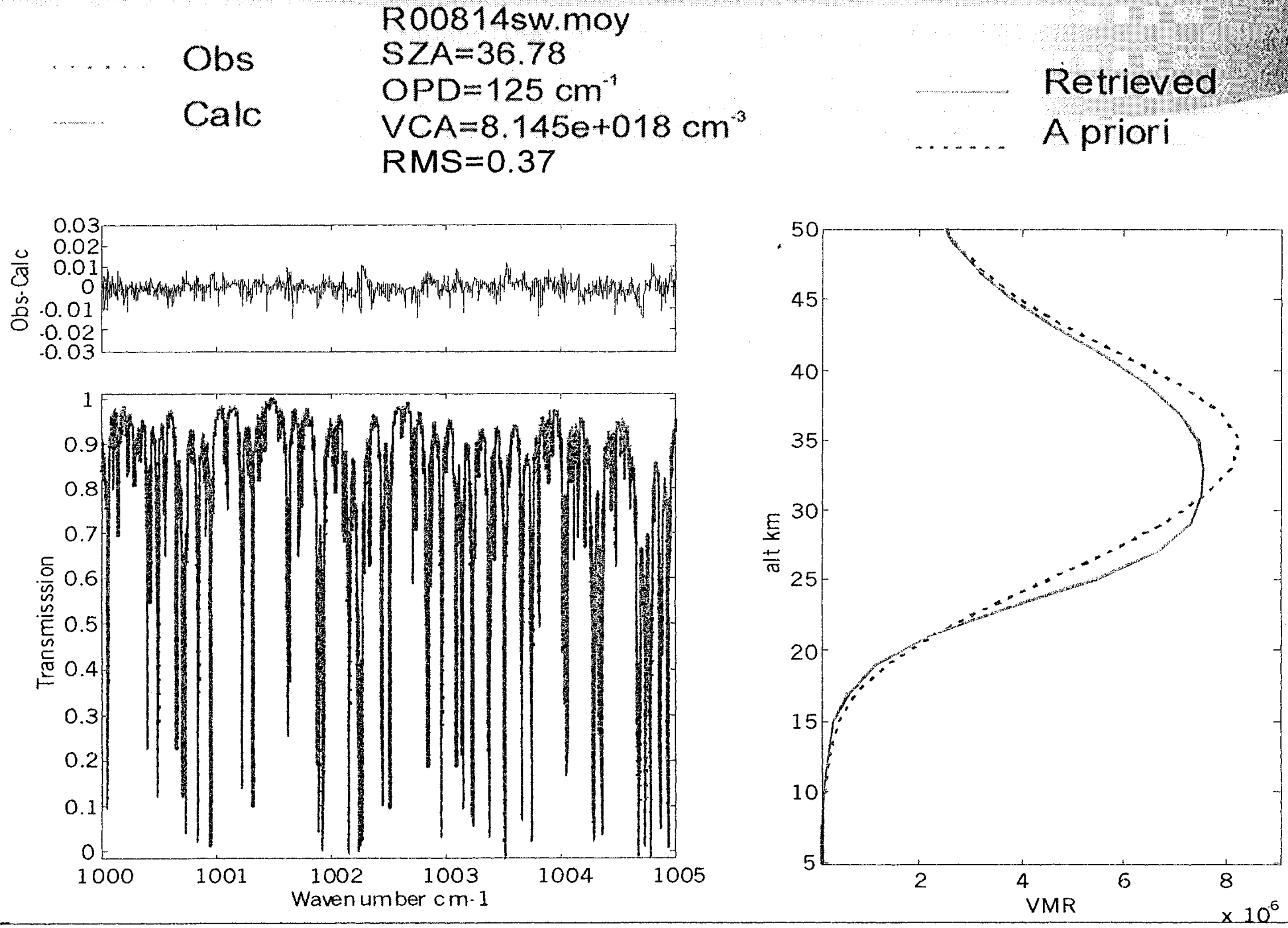
$$\hat{x} = (S_a^{-1} + K^T S_\varepsilon^{-1} K)^{-1} (K^T S_\varepsilon^{-1} y + S_a^{-1} x_a)$$

$$x_{n+1} = (S_a^{-1} + K_n^T S_\varepsilon^{-1} K_n)^{-1} \left[K_n^T S_\varepsilon^{-1} (y_m - y_n + K_n x_n) + S_a^{-1} x_a \right]$$

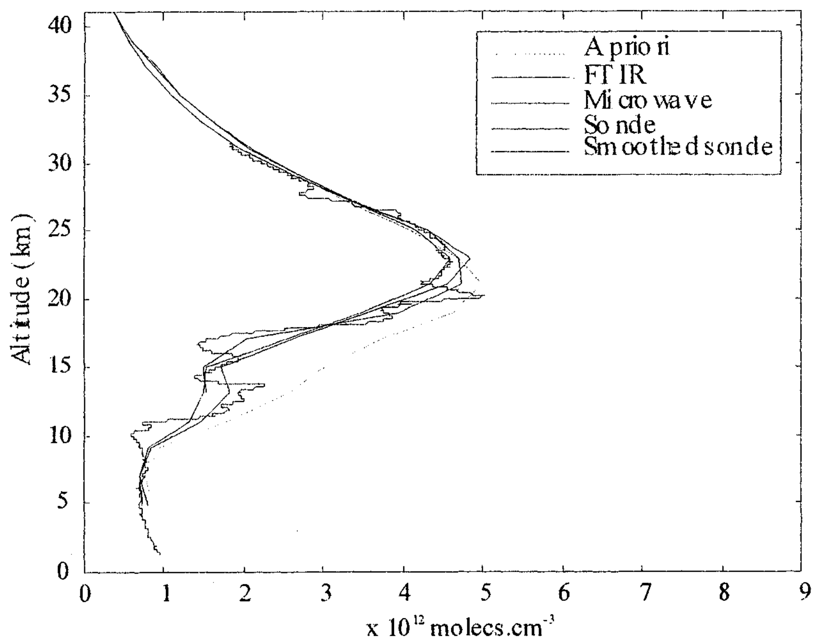
$$x_{n+1} = x_a + S_a K_n^T (K_n S_a K_n^T + S_\varepsilon)^{-1} \left[(y_m - y_n) - K_n (x_a - x_n) \right]$$

- For vertical inversion of ground-based solar absorption FTIR: *SFIT2* code, empirical implementation of OEM
  - empirical estimations of best S_ε, S_{x_a} and of covariances of all retrieved parameters (S_b)
  - best ? best fit, w/o instabilities in retrieved state = best compromise between a priori and measurement info

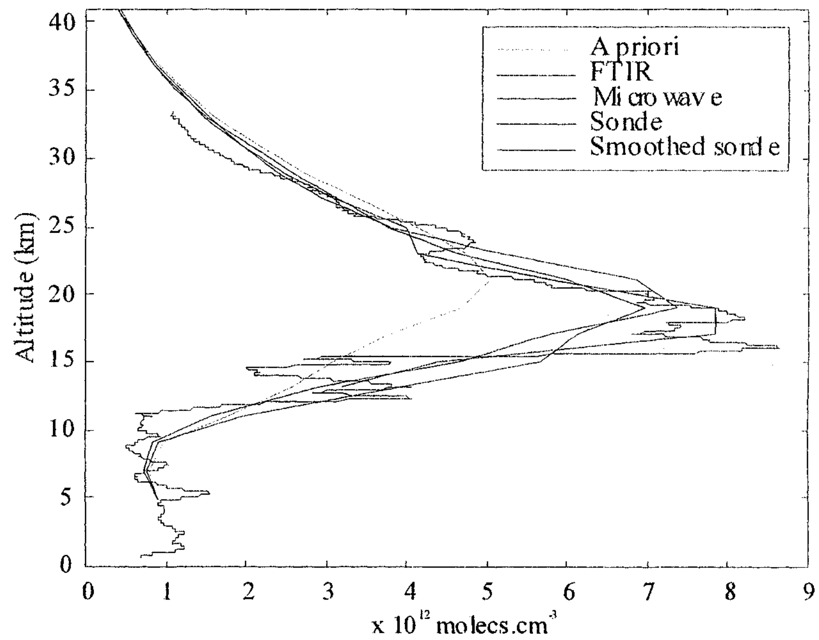
FTIR inversion: examples for O_3



FTIR inversion: examples for O_3 - 2



1999-03-12



1999-03-17

Retrieval characterisation - 1

After linearisation and re-arrangement

$$\hat{x} - x_a = R(F(x_a, \hat{b}), \hat{b}, x_a, c) - x_a \quad \text{bias} \quad \triangleright 0$$

$$+ A(x - x_a) \quad \text{smoothing}$$

$$+ G_y \varepsilon_y \quad \text{retrieval error}$$

$G_y = \dfrac{\partial R}{\partial y}$ sensitivity of retrieval to measurement

$K_x = \dfrac{\partial F}{\partial x}$ sensitivity of forward model to unknown state

(weighting function)

$A = G_y K_x$ sensitivity of retrieved to real state (averaging kernel)

Retrieval characterisation - 2

Or else

$$\hat{x} - x = (A - I)(x - x_a)$$ smoothing error

$$+ G_y K_b (b - \hat{b})$$ model parameter error

$$+ G_y \Delta f(x, b, b')$$ forward model error

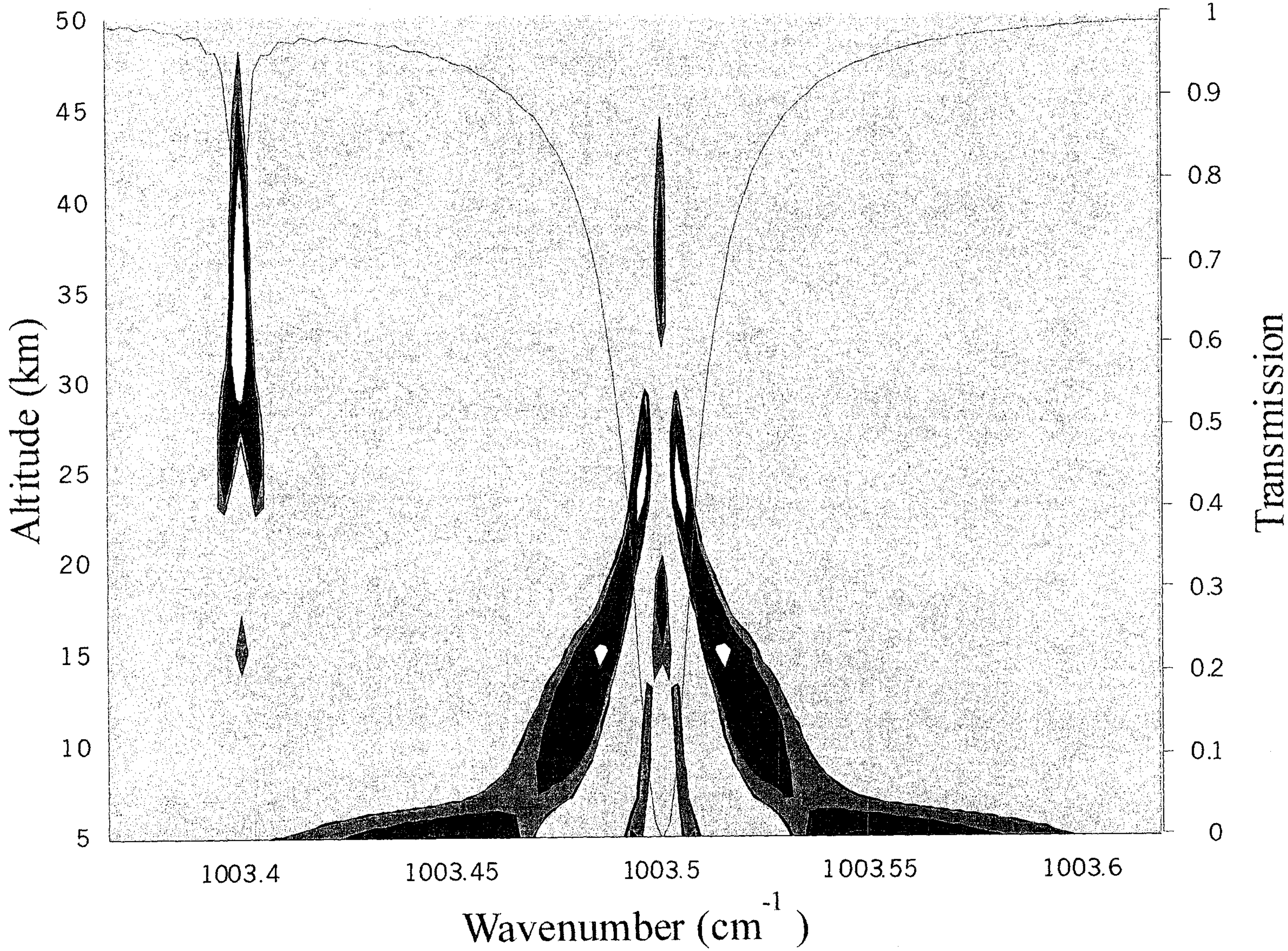
$$+ G_y \varepsilon$$ 'retrieval' (measurement) error

$$K_b = \frac{\partial F}{\partial b}$$ sensitivity of forward model to model parameters

$$S_A = (A - I) S_x (A - I)^T$$ covariance of smoothing error

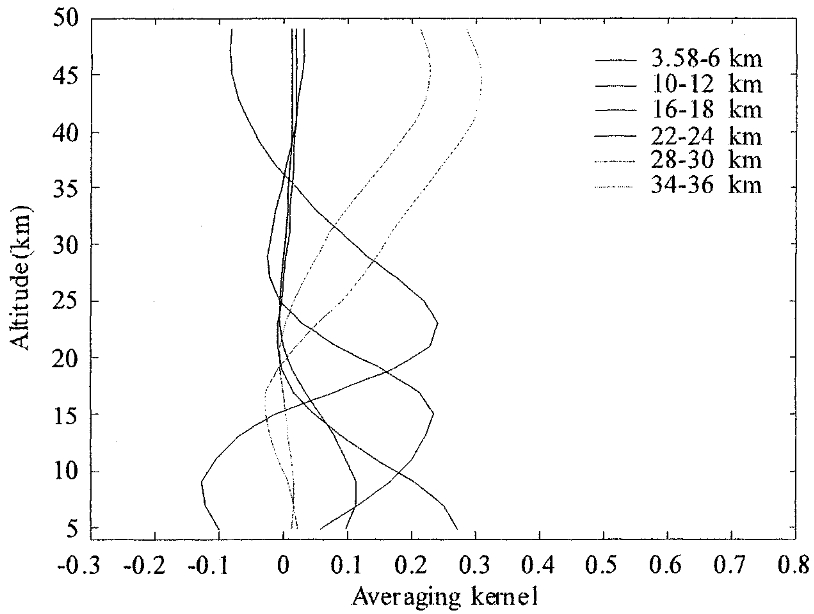
$$S_y = G_y S_\varepsilon G_y^{\ T}$$ covariance of measurement error

Contribution function $G_y = \partial\hat{\mathbf{x}}/\partial\mathbf{y} \cong \partial\mathbf{R}/\partial\mathbf{y}$

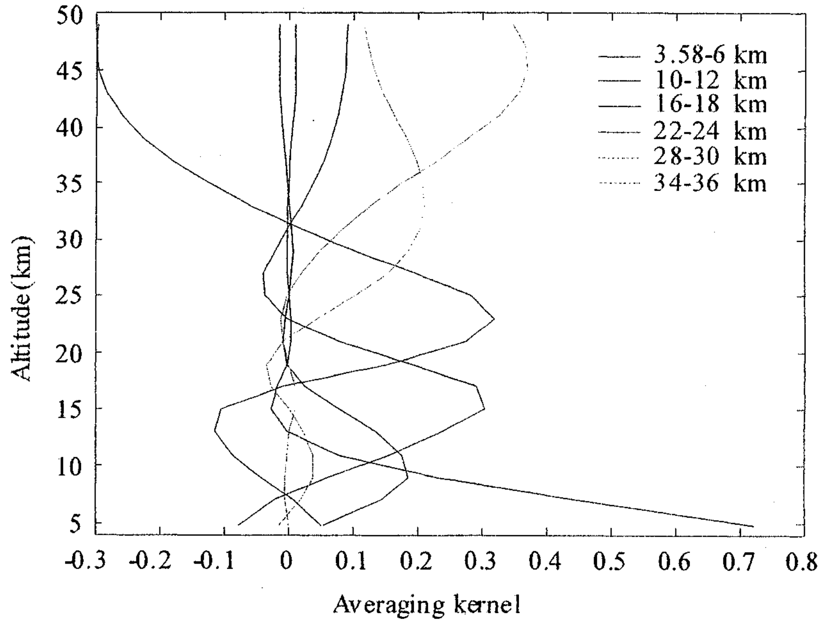


FTIR inversion: Averaging kernel

O_3



1002.6-1003.2 cm^{-1}

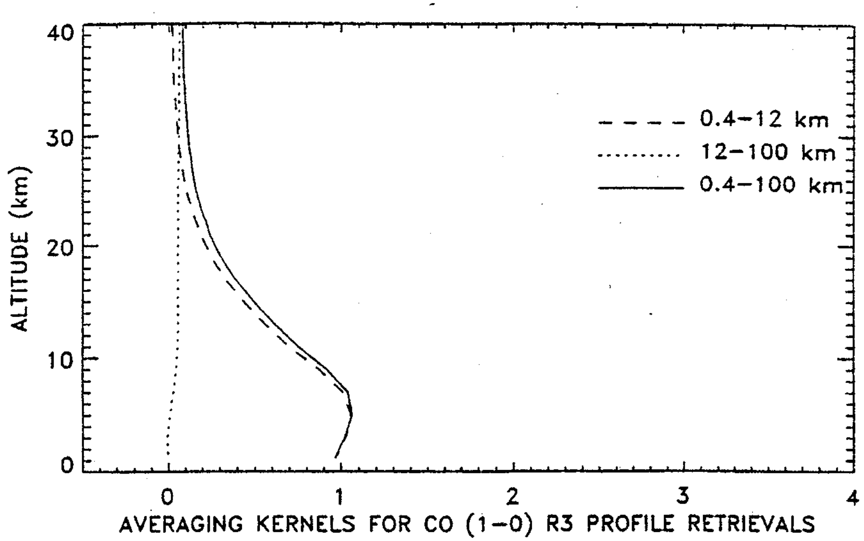


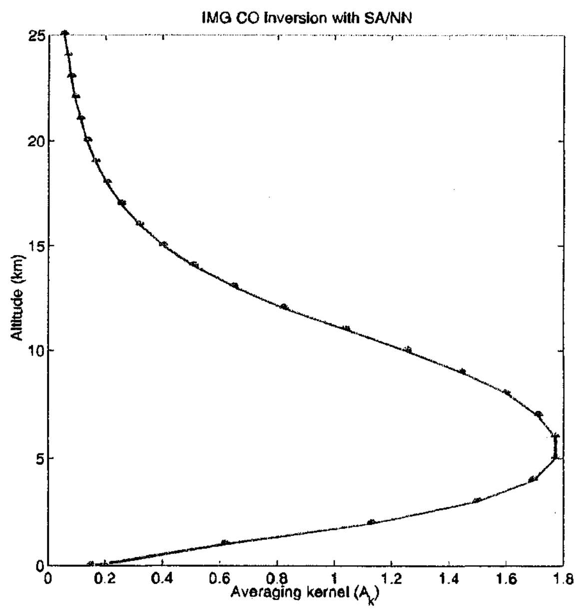
1000.0-1005.0 cm^{-1}

FTIR inversion: Averaging kernel

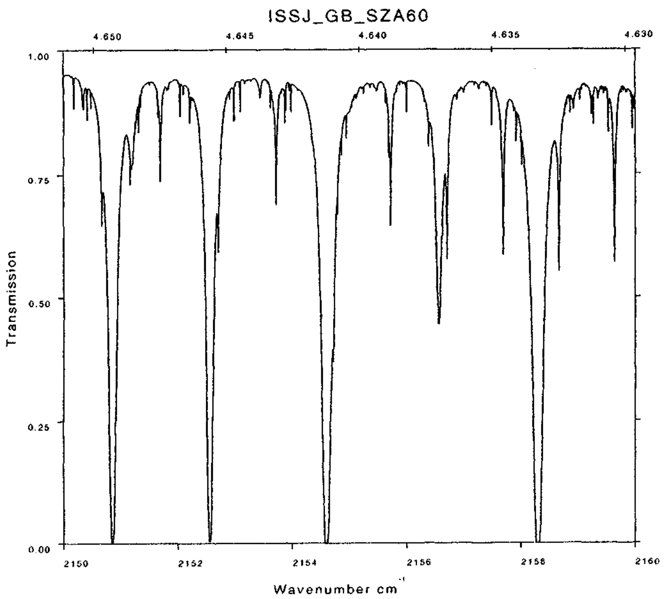
CO

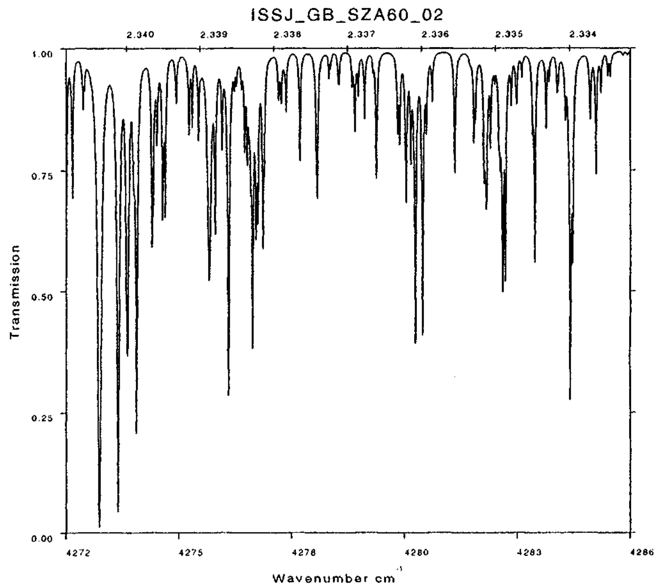
Solar absorption-GB Emission - nadir space-based

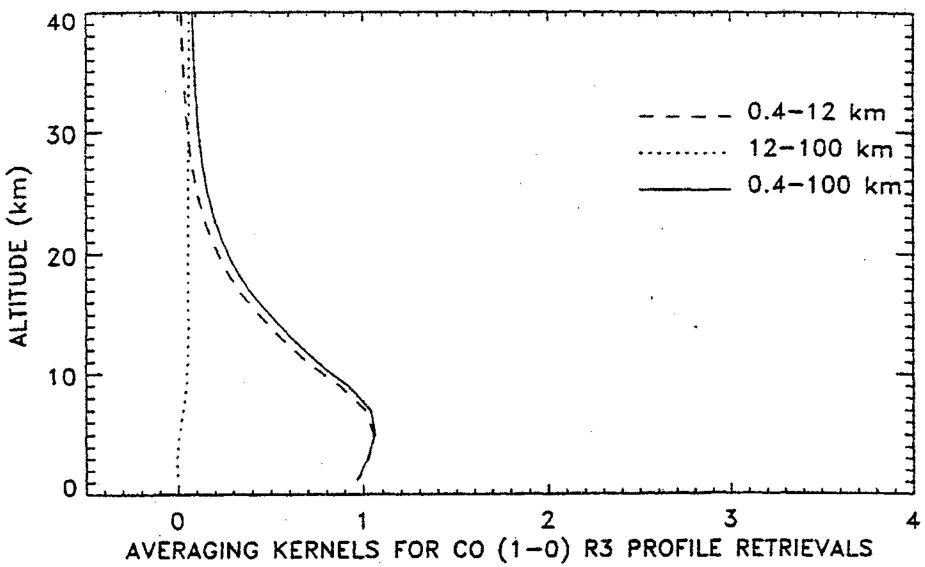


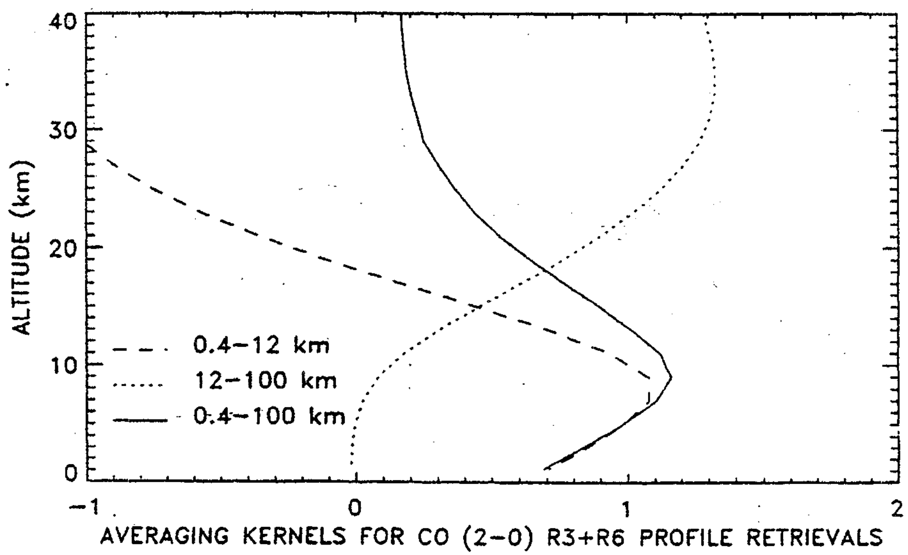


CO

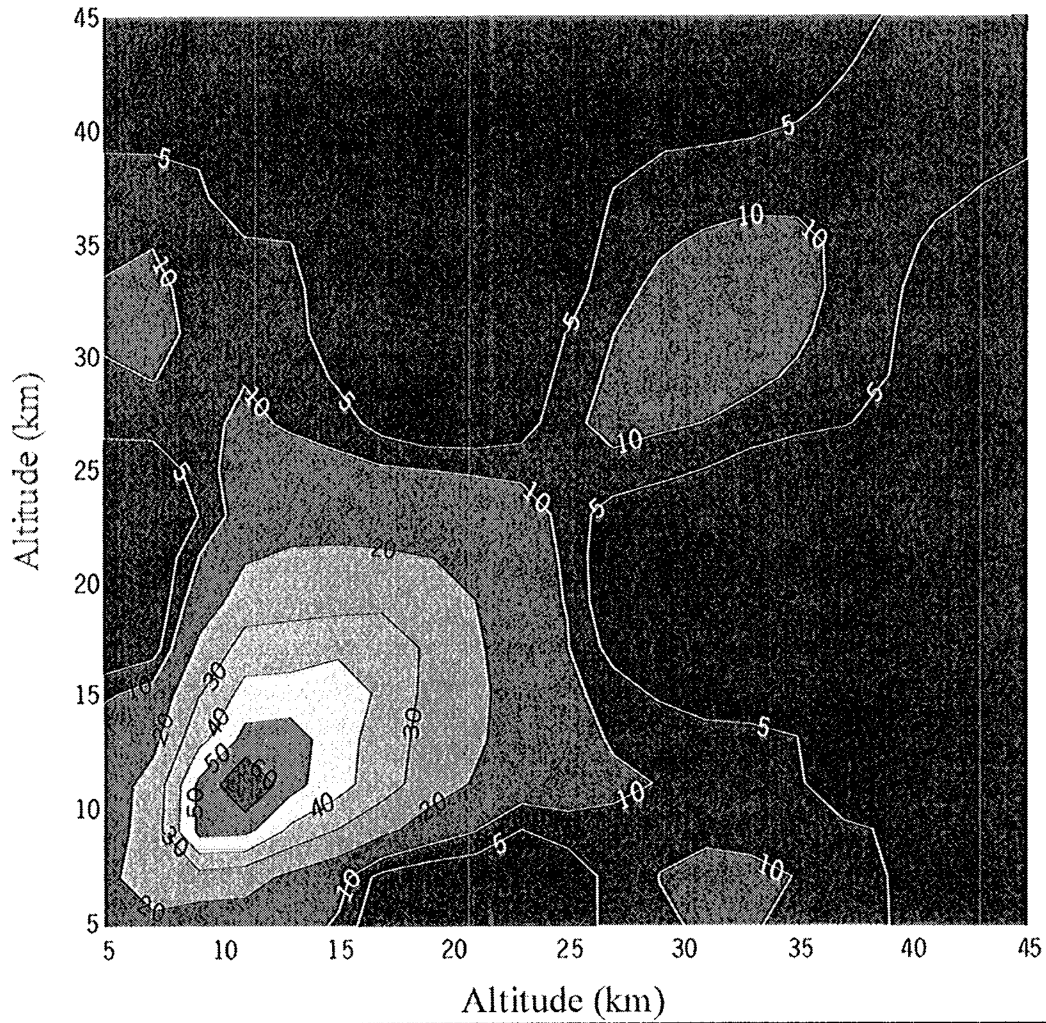

ISSJ_GB_SZA60
Transmission
Wavenumber cm⁻¹


ISSJ_GB_SZA60_02
Transmission
Wavenumber cm⁻¹


0.4–12 km
12–100 km
0.4–100 km
ALTITUDE (km)
AVERAGING KERNELS FOR CO (1–0) R3 PROFILE RETRIEVALS


0.4–12 km
12–100 km
0.4–100 km
ALTITUDE (km)
AVERAGING KERNELS FOR CO (2–0) R3+R6 PROFILE RETRIEVALS

FTIR inversion: smoothing and measurement errors - 1



$$S_A = (A - I) S_x (A - I)^T$$

$$S_y = G_y S_\varepsilon G_y^T$$

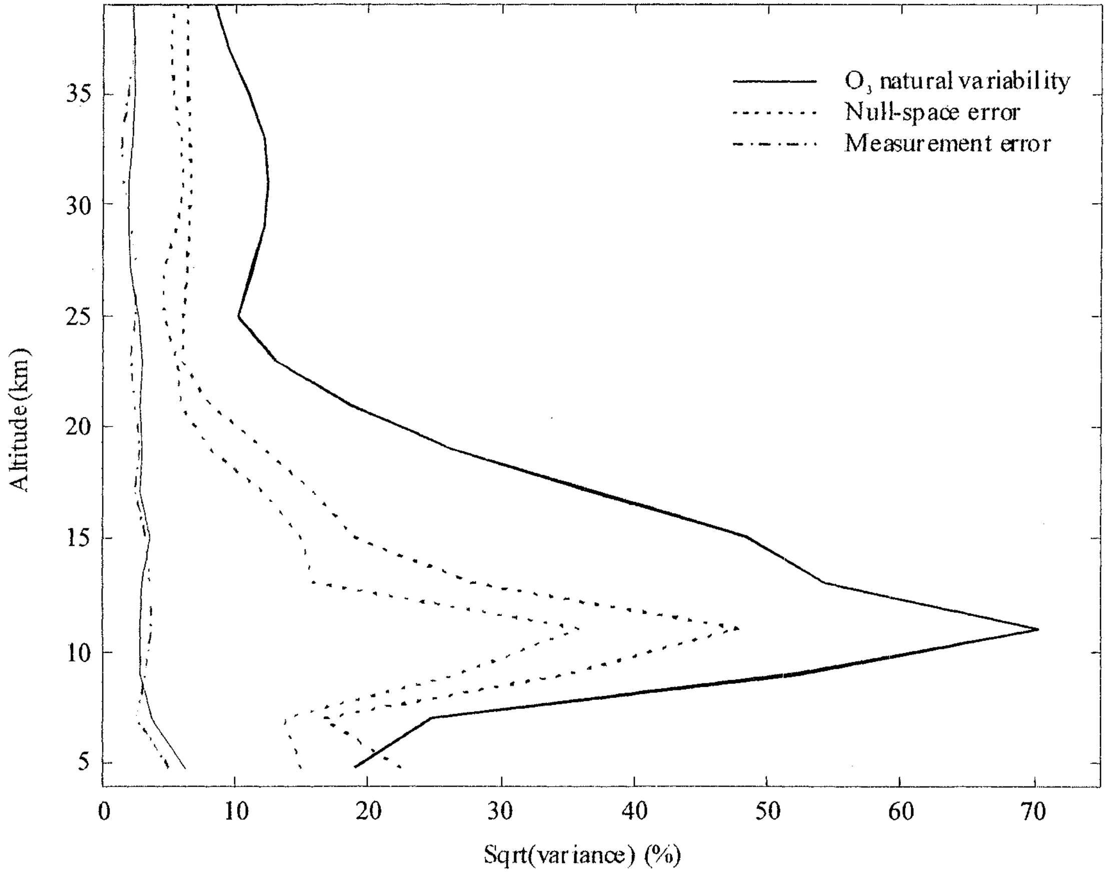
$$S_x(i,j) = \sqrt{\mathrm{cov}(x_i, x_j) / \overline{x}_i \overline{x}_j}$$

(in %);

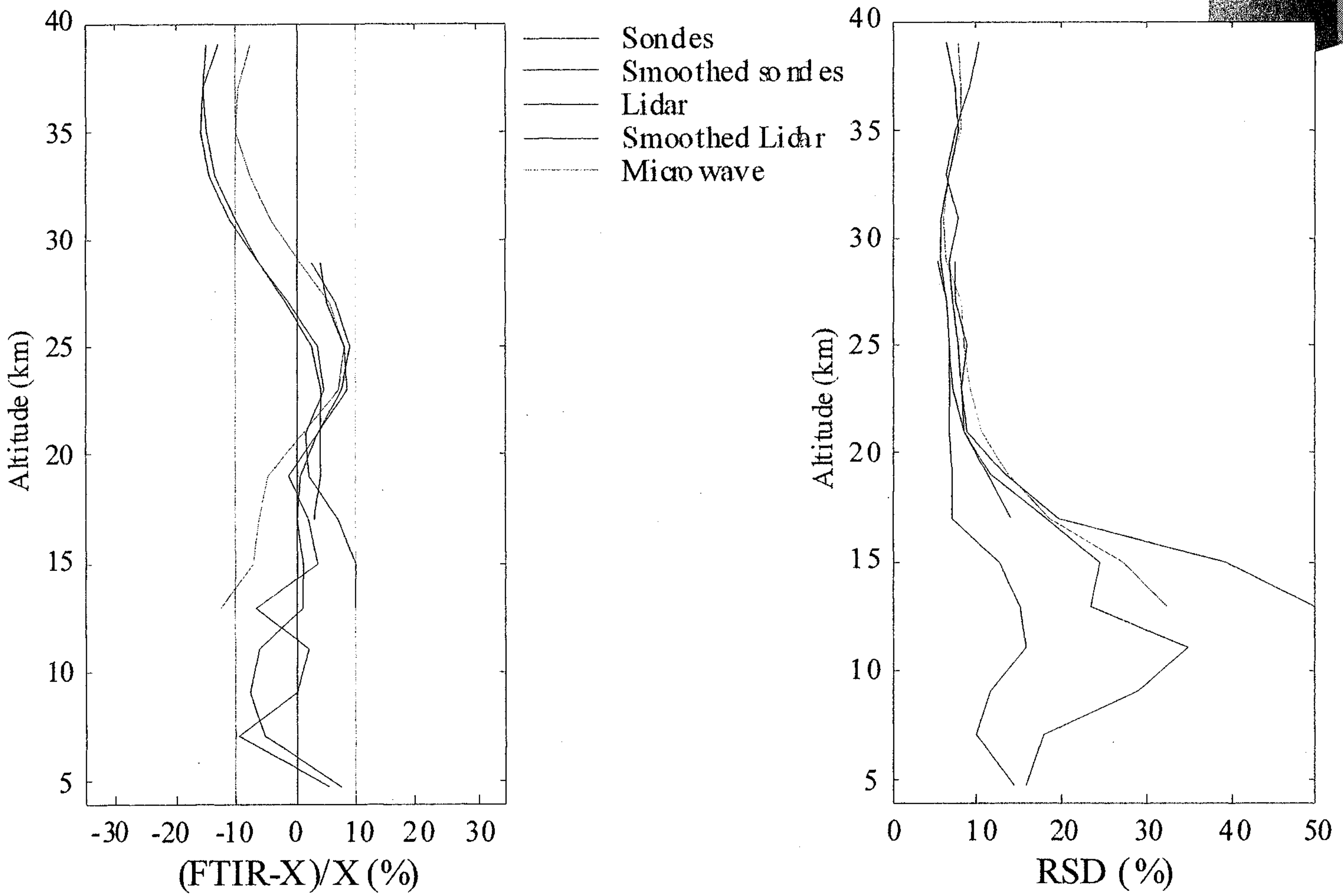
$x \equiv x_a$

FTIR inversion: smoothing and measurement errors - 2

$$S_A = (A - I) S_x (A - I)^T \qquad S_y = G_y S_\varepsilon G_y^T$$



FTIR inversion: smoothing error - 2

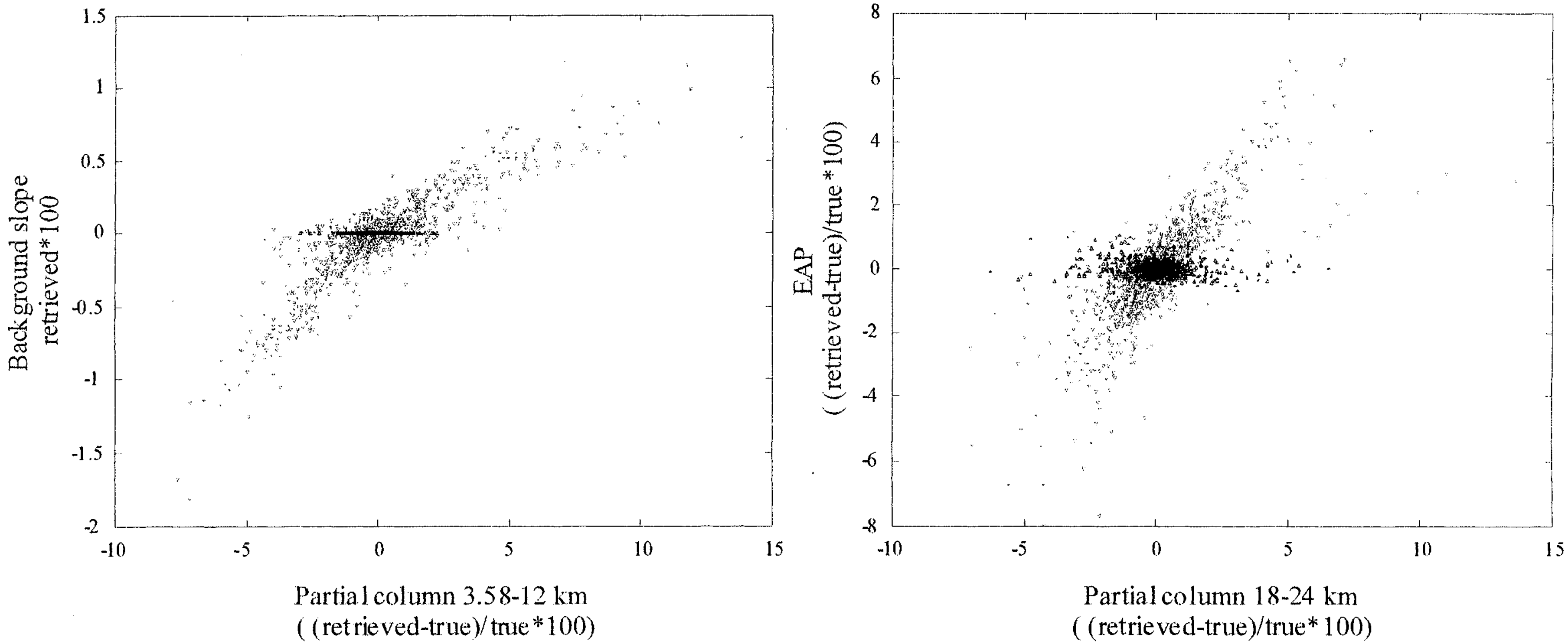


FTIR inversion: model params errors

- Spectroscopy (systematic, altitude-independent)
- P/T (random, altitude dependent)
- background slope, zero level of spectrum
- instrument parameters: EAP

estimated from Monte Carlo simulations

FTIR inversion: correlations between retrieved parameters - 1



FTIR inversion: correlations between retrieved parameters - 2

Layer	3.6-12 km		12-18 km		18-24 km		24-40 km	
Microwindow	N	B	N	B	N	B	N	B
Model parameter								
Background slope	0.9	0.1	-0.6	0.1	0.2	0.0	0.0	0.0
Effective apodization parameter	0.4	0.0	-0.5	0.2	0.8	-0.1	-0.3	0.3
Zero transmission level	0.5	-0.1	-0.5	0.3	0.7	-0.3	-0.1	0.4

Correlation coefficients between the relative errors ((retrieved-true)/true) of the retrieved partial columns and the retrieved model parameters resulting from the Monte-Carlo study (see text) for retrievals performed in the narrow microwindow (N) and in the broad microwindow (B).

FTIR inversion: total error budget

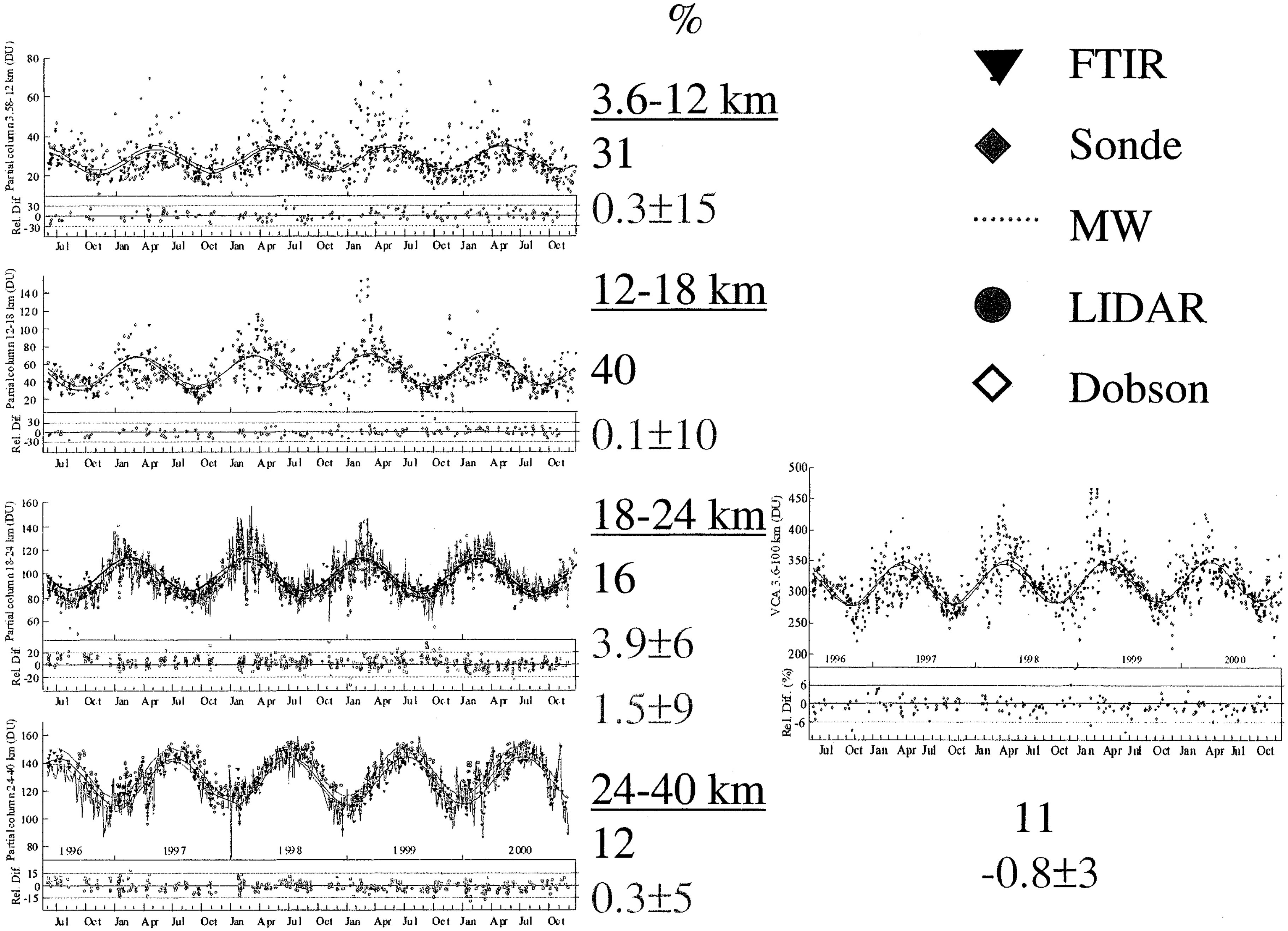
Layer	3.6-12 km	12-18 km	18-24 km	24-40 km	VCA
Systematic Error Source					
Air broadening coefficient uncertainty	4.6	1.6	0.9	-3.9	0.1
Line intensity uncertainty	2.0	2.0	2.0	2.0	2.0
EAP uncertainty	0.8	1.9	8.4	-7.9	0.6
Total systematic error	**5.1**	**3.2**	**8.7**	**9.0**	**2.1**
Random Error Source					
Temperature uncertainty	1.9	2.8	0.3	4.9	3.3
Measurement noise	1.3	2.2	1.7	1.1	0.2
Null-space error	7.8	9.2	3.7	1.6	0.2
Total random error	**8.1**	**9.9**	**4.1**	**5.3**	**3.3**

Systematic and random errors budgets (%) for the retrieval of ozone partial columns in the broad microwindow 1000 – 1005 cm^{-1}.

FTIR inversion: validation

- Comparison between FTIR retrieved profiles at the Jungfraujoch

  and correlative data, from sonde, LIDAR and microwave, from June 1996 to November 2000


%
FTIR
Sonde
MW
LIDAR
Dobson
Partial column 3.58-12 km (DU)
Rel. Dif
3.6-12 km
31
0.3±15
Partial column 12-18 km (DU)
12-18 km
40
0.1±10
Partial column 18-24 km (DU)
18-24 km
16
3.9±6
1.5±9
Partial column 24-40 km (DU)
24-40 km
12
0.3±5
VCA 3.6-100 km (DU)
Rel. Dif. (%)
11
-0.8±3
1996
1997
1998
1999
2000
Jul Oct Jan Apr Jul Oct Jan Apr Jul Oct Jan Apr Jul Oct Jan Apr Jul Oct

Conclusions

- O_3 profiles can be retrieved from GB high-resolution FTIR spectra in the 1000-1005 cm^{-1} μwindow, in 4 independent layers, incl. the troposphere, covering distinct atmospheric regimes
- The theoretical characterisation of the OEM inversion has been confirmed by a statistical comparison with independent measurements
- The inversion can cope to some extent with model and instrument uncertainties.

Conclusions

- Perspective:

  application to space-based nadir viewing FTIR experiments, like IASI/METOP-1, TES/Aura, ...