united nations educational, scientific and cultural organization

international atomic energy agency

the
abdus salam
international centre for theoretical physics

School on "Exploring the Atmosphere by Remote Sensing Techniques"
18 October - 5 November 1999

1151-19

"The ORA Experiment"

D. Fussen
Institut d'Aeronomie Spatiale de Belgique
Brussels
Belgium

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

THE ORA EXPERIMENT

acronym of **O**ccultation
RAdiometer

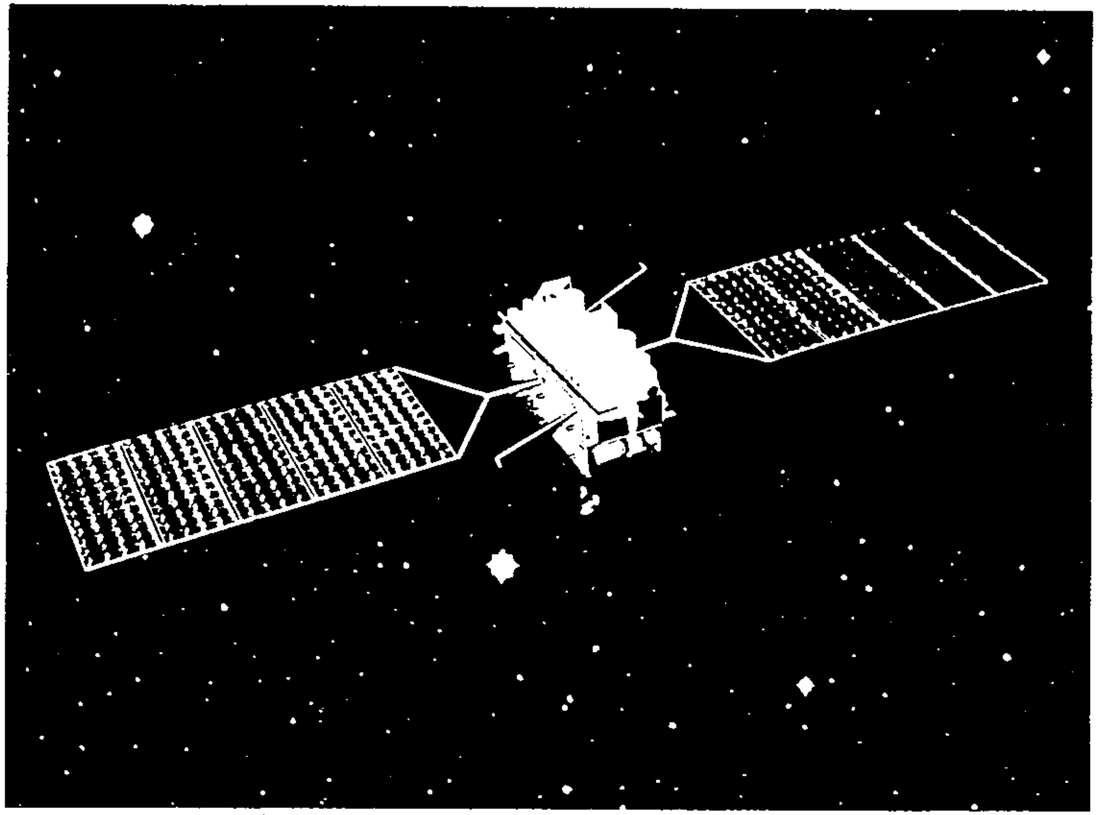
- scientific teams at the
  Belgian Institute for
  Space Aeronomy, Brussels

  instrument: Étienne ARIJS, Dennis NEVEJANS

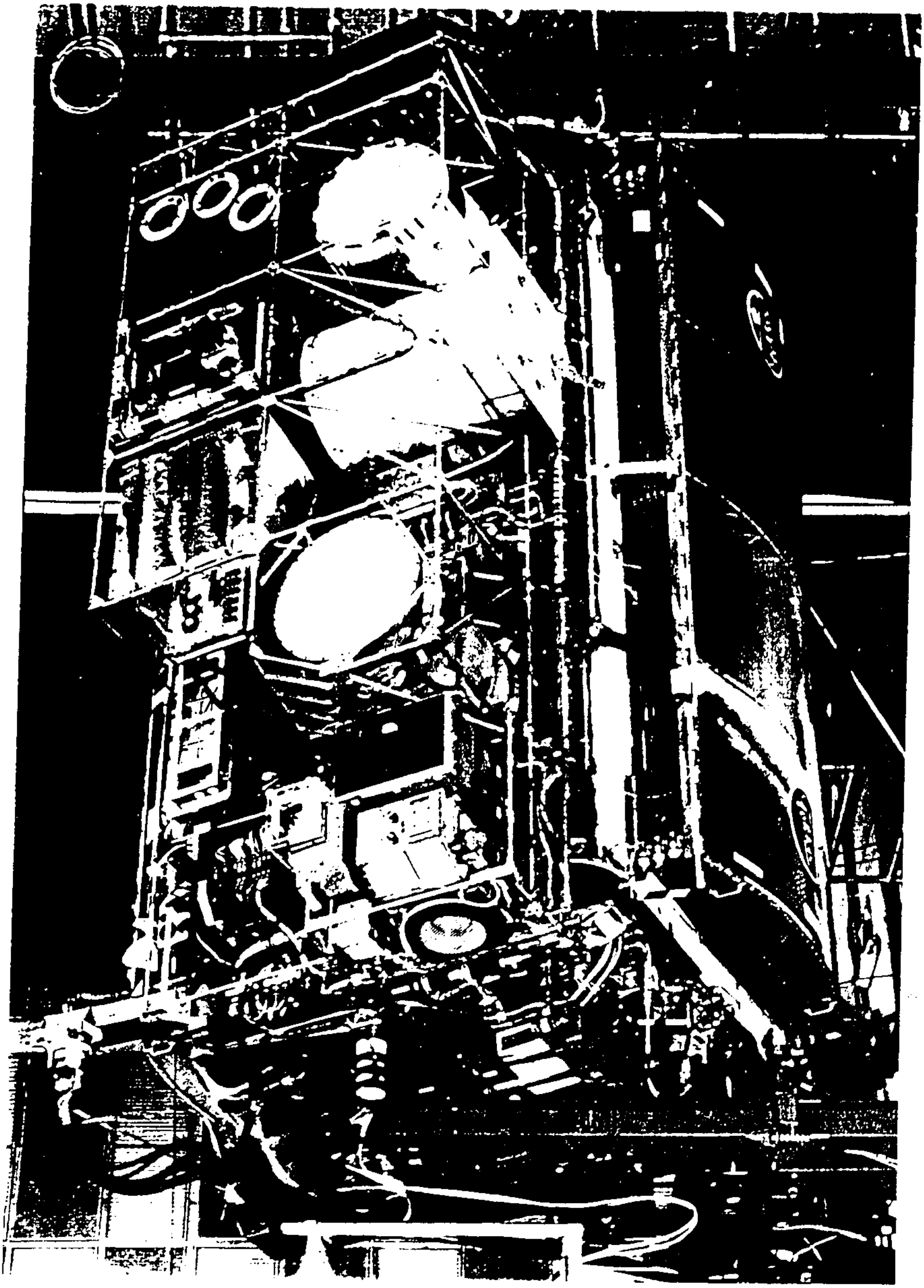
  data processing: Didier FUSSEN,
  Filip VANHELLEMONT, Christine BINGEN

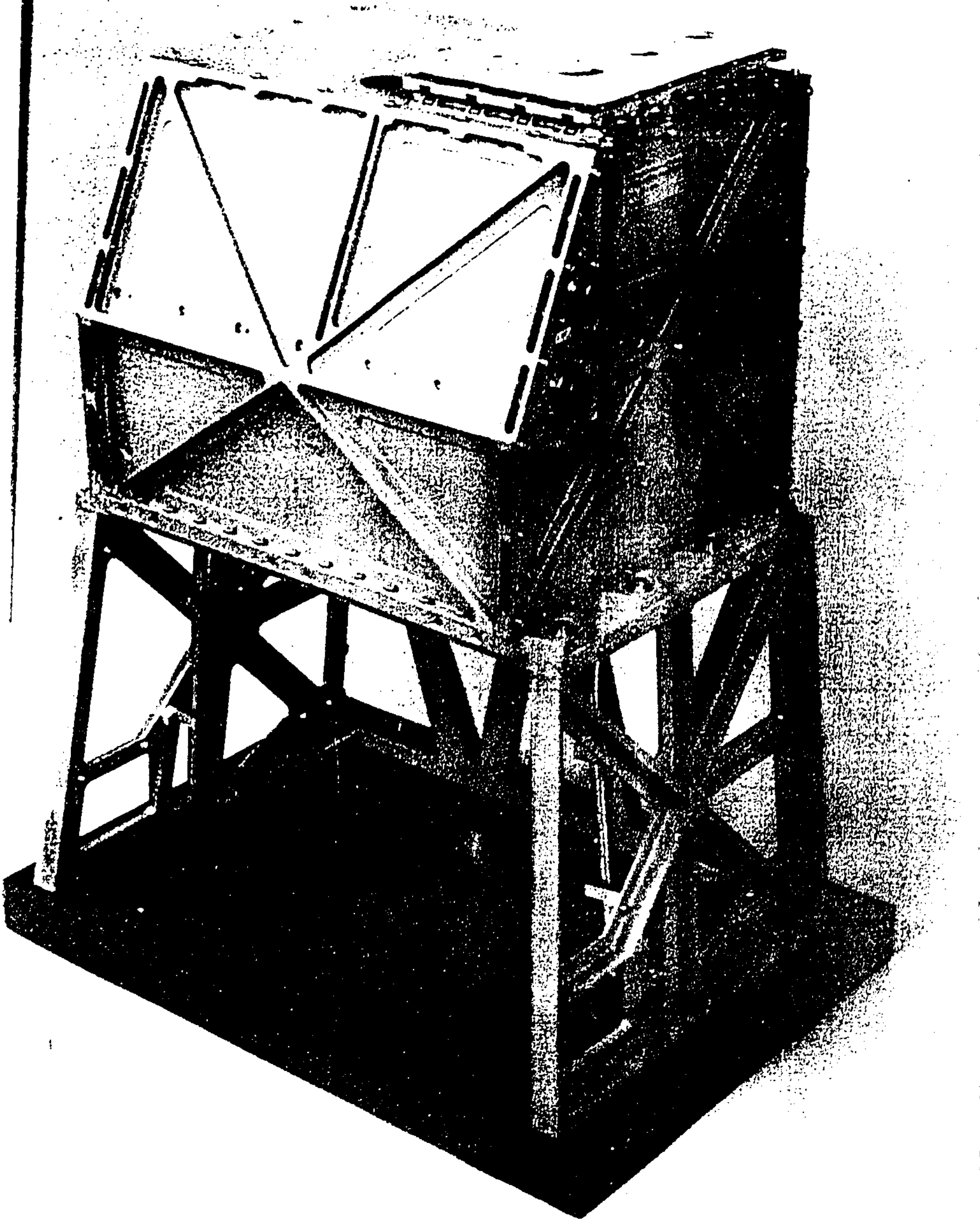
- satellite: **EU**ROPEAN
  RETRIEVABLE
  CARRIER

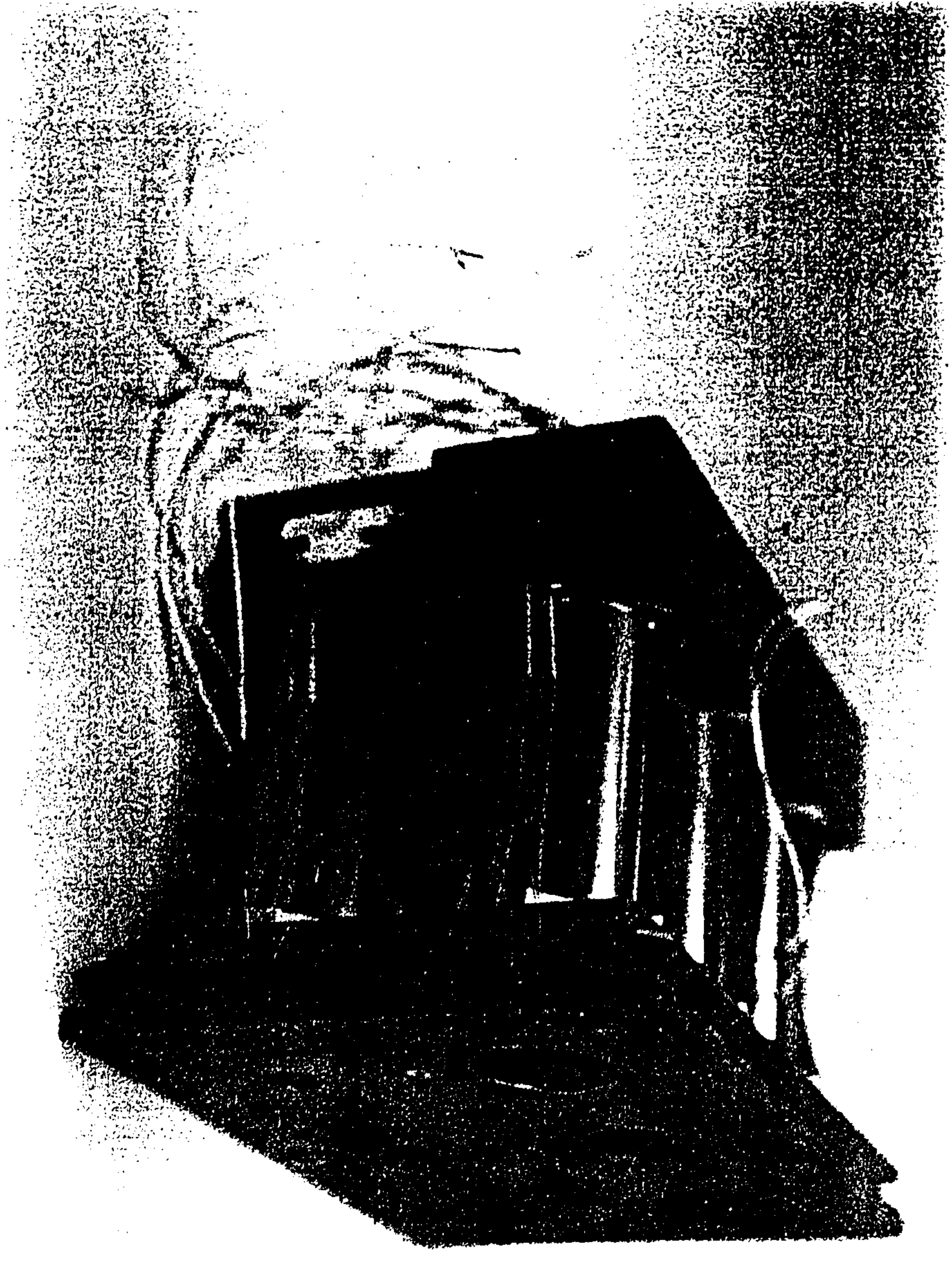
- time period: august 1992 - may 1993



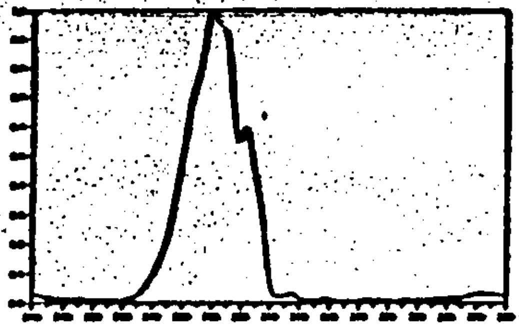
The Spacecraft



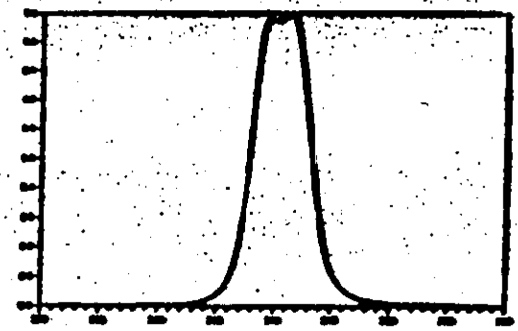




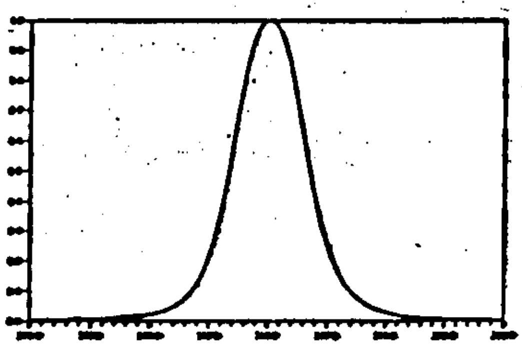
ORAlambda=3[illegible] nm transmission curve



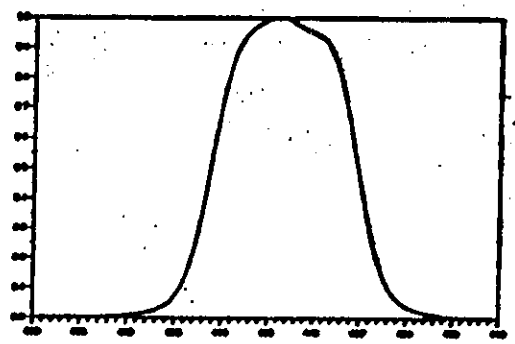
ORAlambda=340 nm transmission curve



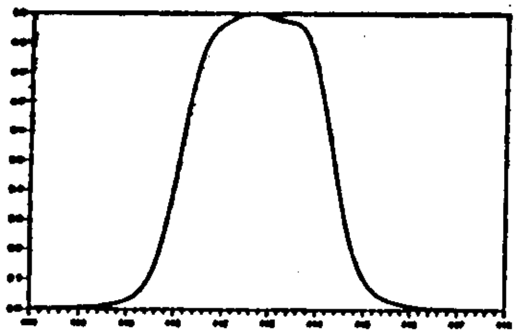
ORAlambda=385 nm transmission curve



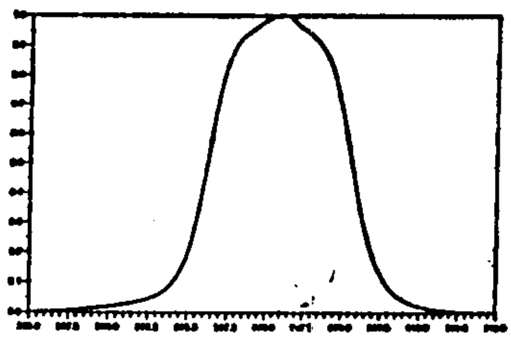
ORAlambda=435 nm transmission curve



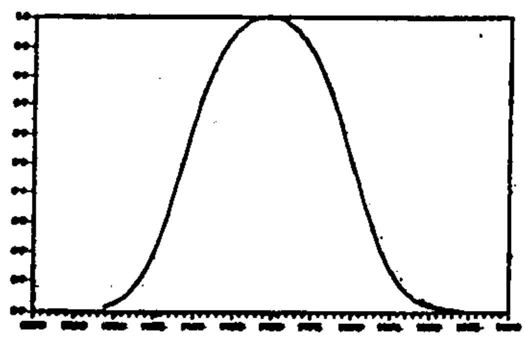
ORAlambda=442 nm transmission curve



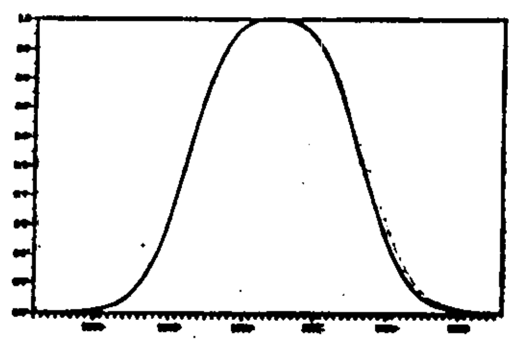
ORAlambda=600 nm transmission curve

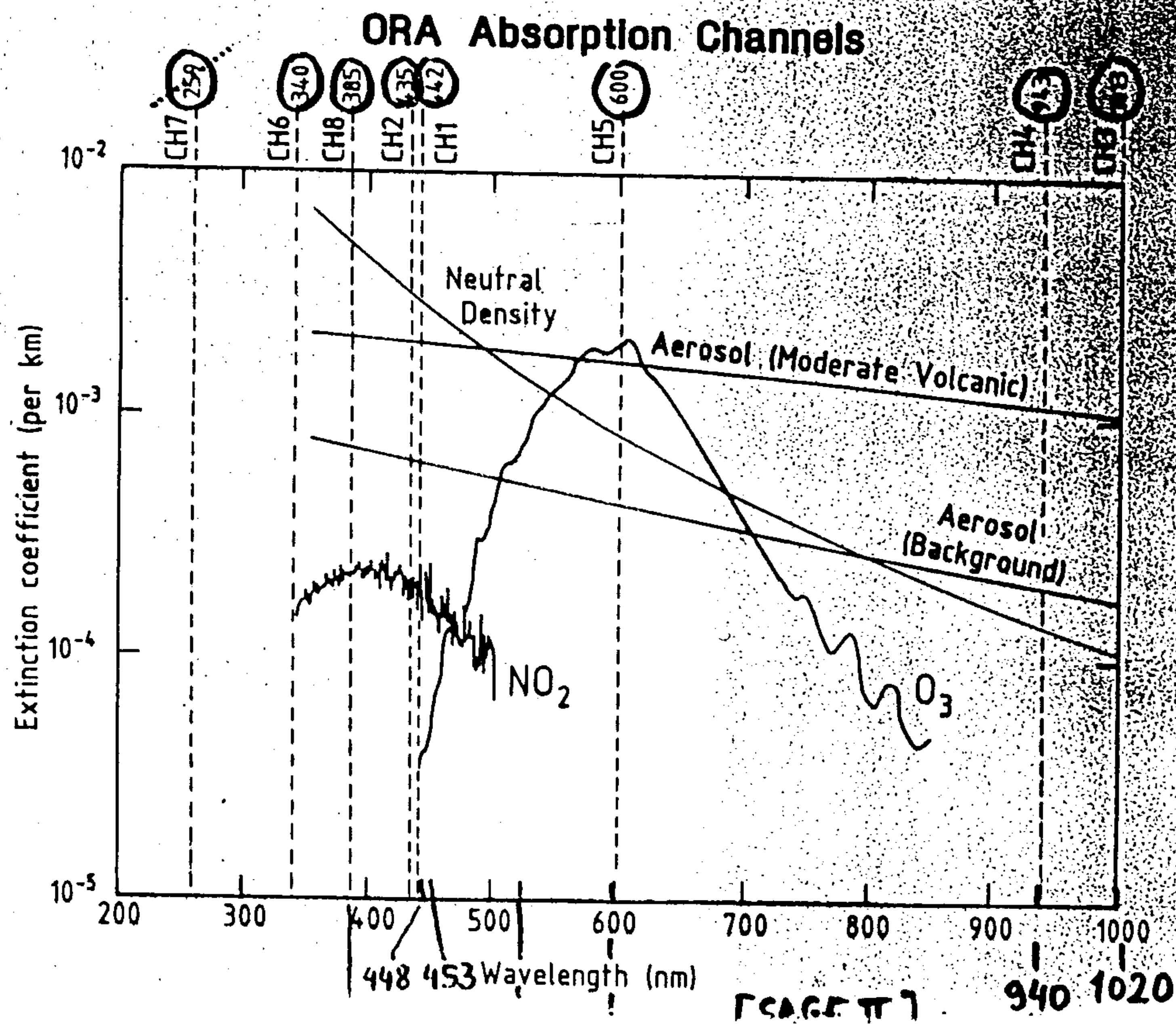


ORAlambda=943 nm transmission curve

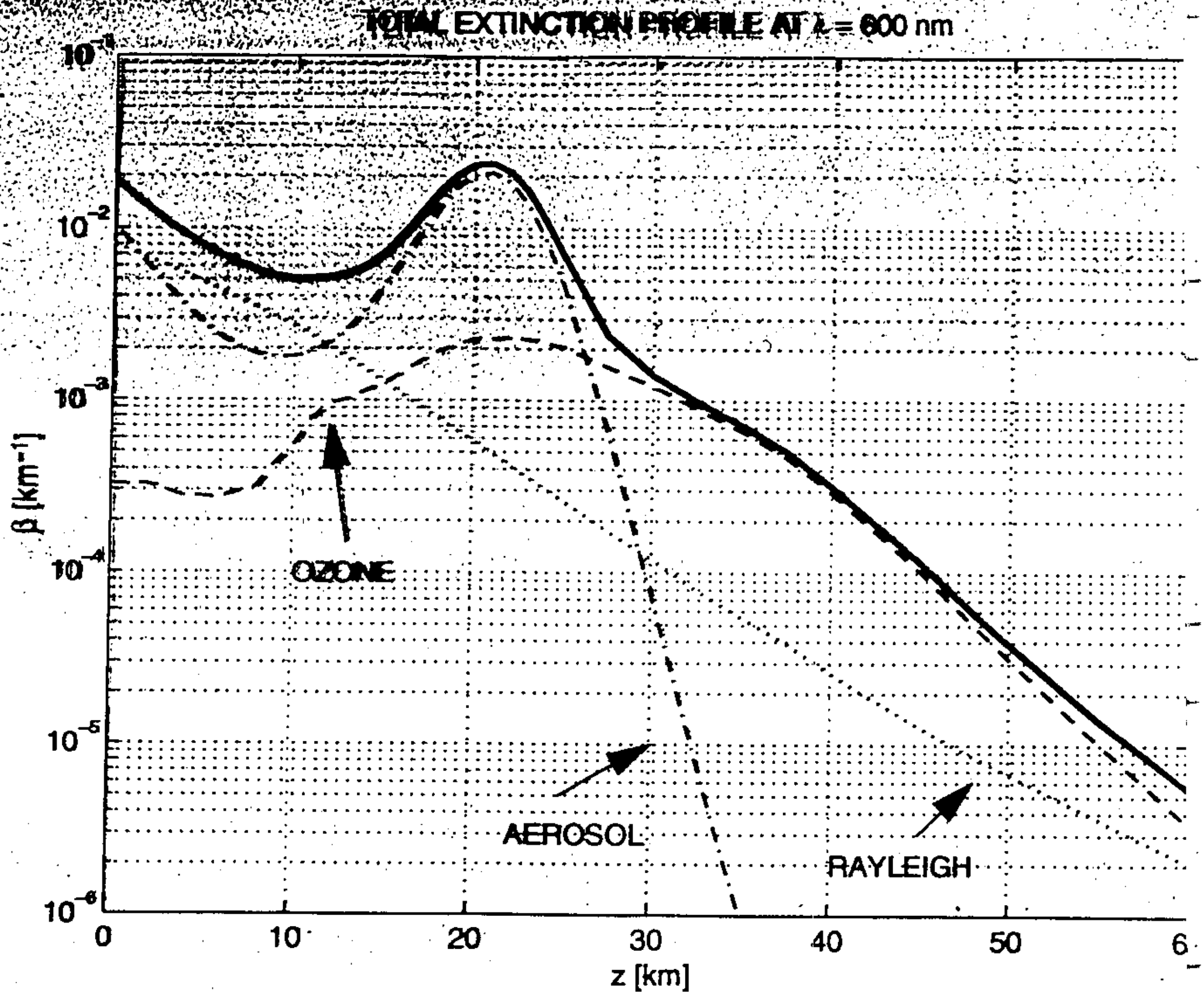


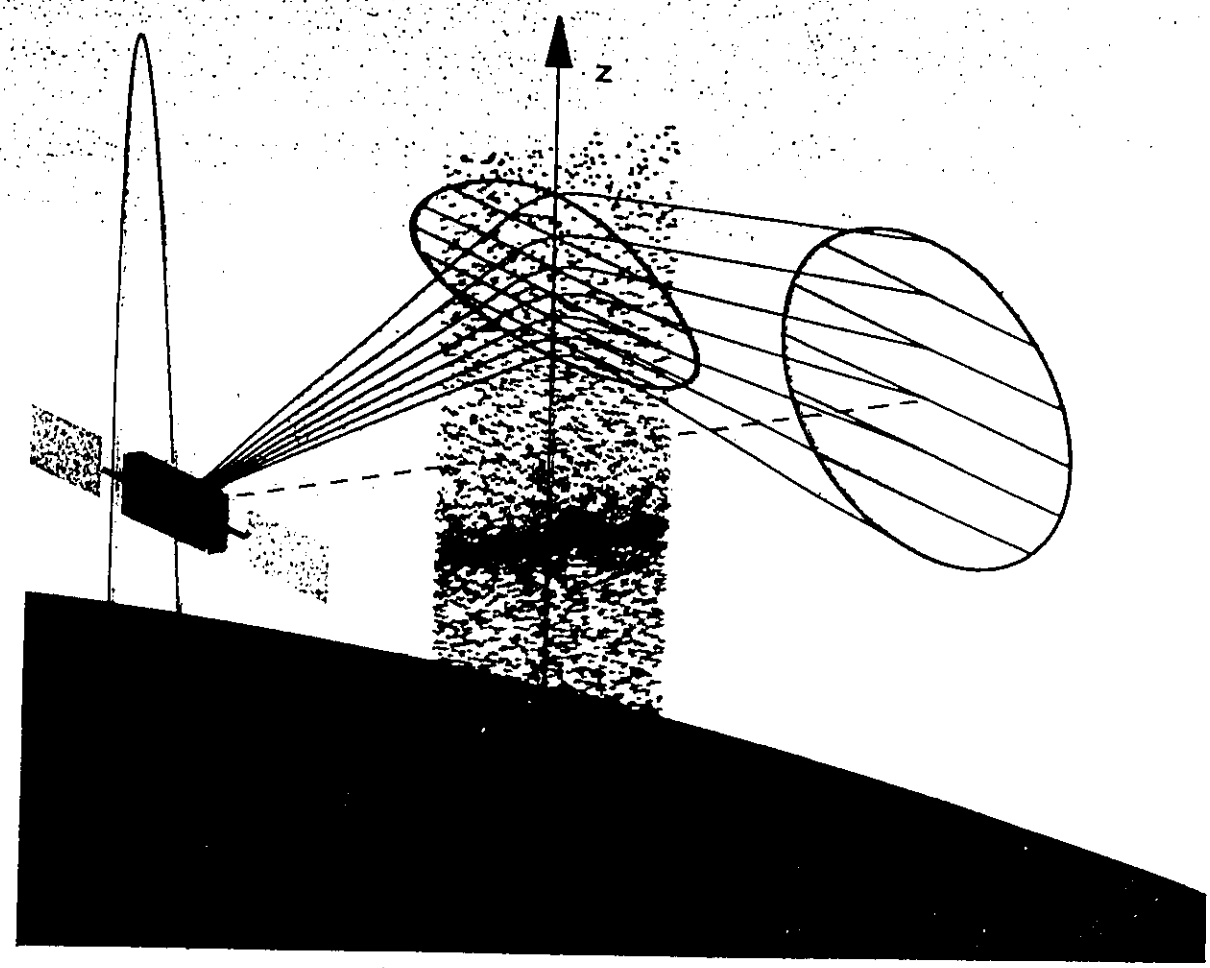
ORAlambda=1012 nm transmission curve

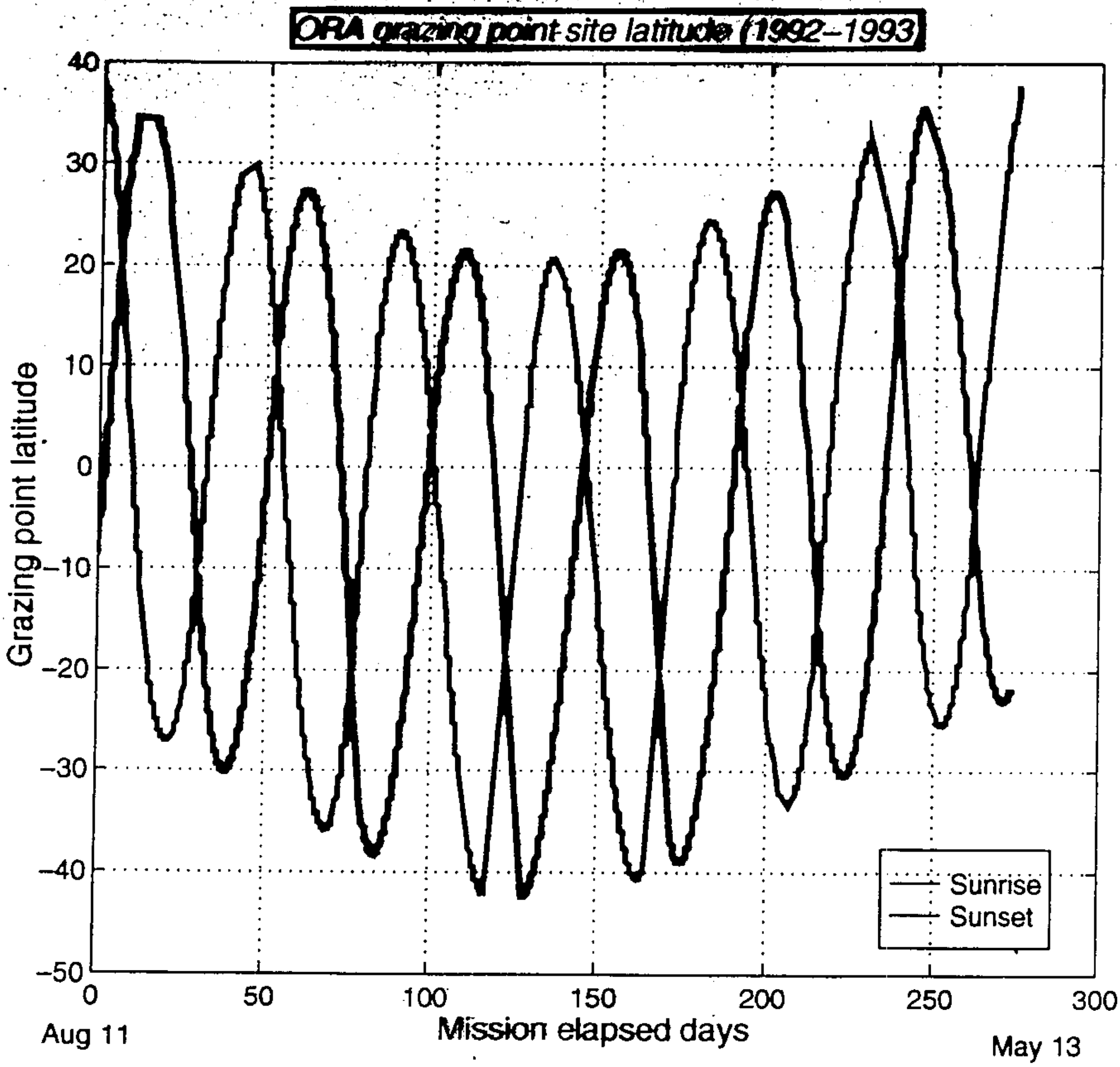




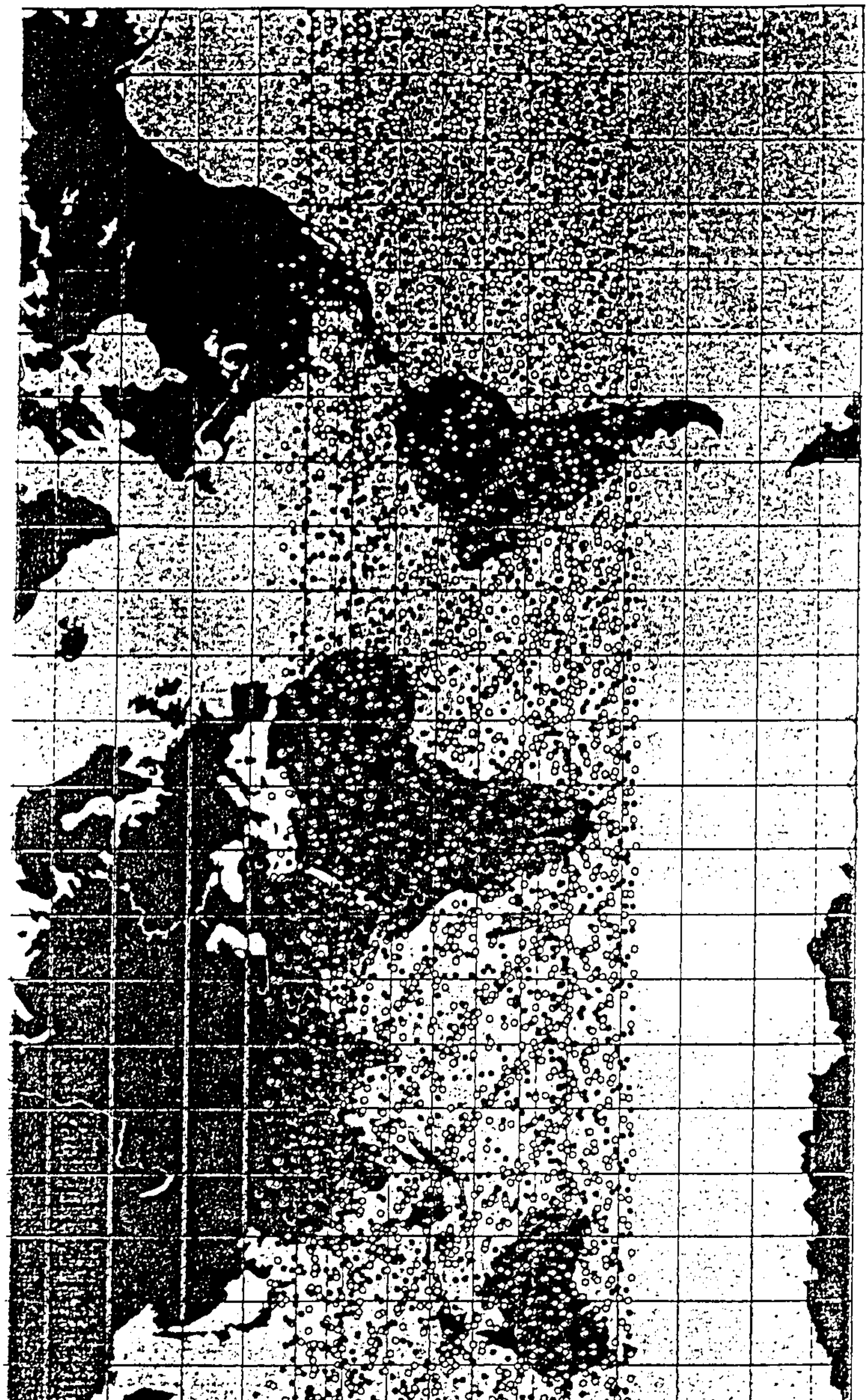
UP SUPERIEURE ⬆ OBEN


TOTAL EXTINCTION PROFILE AT λ = 600 nm
β [km⁻¹]
z [km]
OZONE
AEROSOL
RAYLEIGH

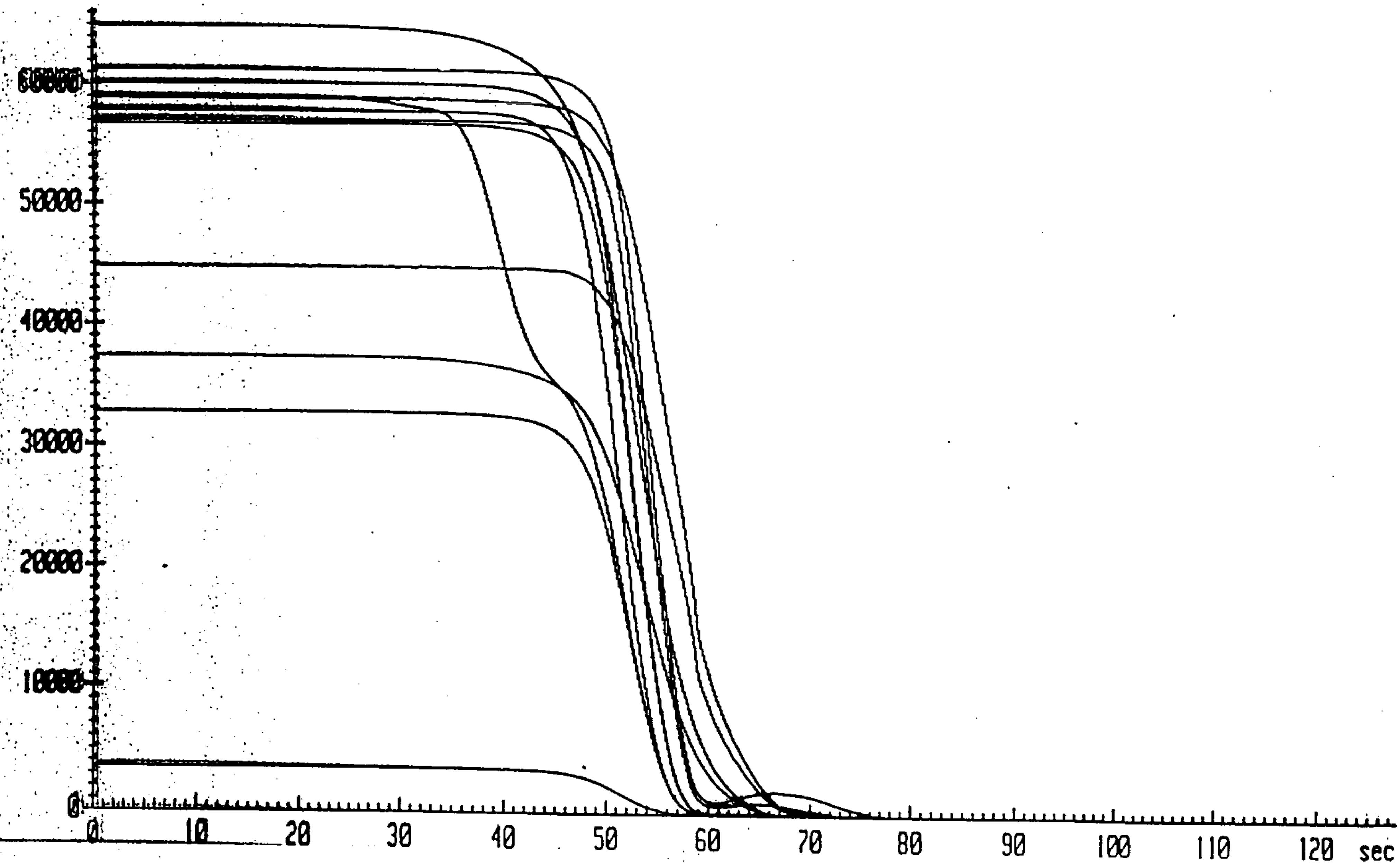

z



ORA grazing point site latitude (1992–1993)
Grazing point latitude
Mission elapsed days
Aug 11
May 13
Sunrise
Sunset
40
30
20
10
0
−10
−20
−30
−40
−50
0
50
100
150
200
250
300



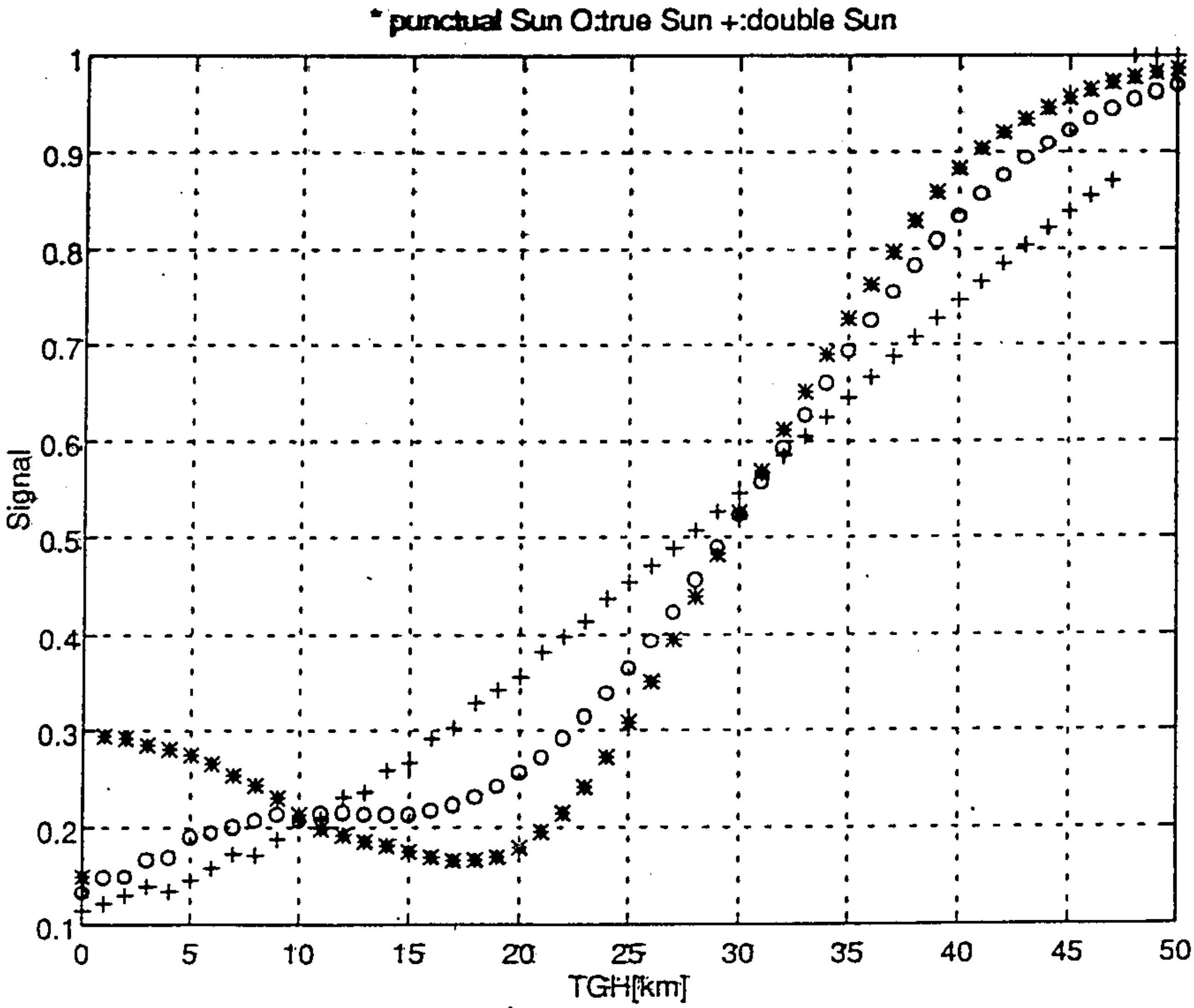
nr = 2352 , date is 10-oct-1992 16:37:09.9800282, type = SNAPSHOT
channel : 1 , 2 , 3 , 4 , 5 , 6 , 7 , 8 , 9 , 10 , 11 , 12 .
Gain : 4.7, 5.6, 4.7, 4.0, 4.0, 13.3, 9.4, 13.3, 13.3, 13.3, 5.6, 13.3
Int time : 0.142, 0.142, 0.142, 0.142, 0.142, 0.142, 0.142, 0.142, 0.142, 0.142, 0.142, 0.142

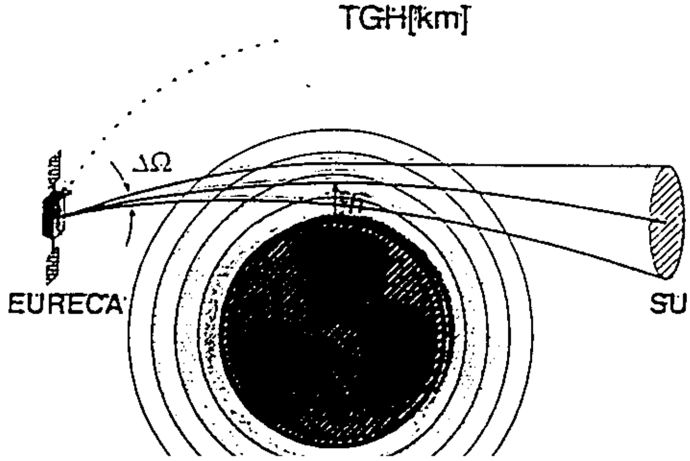


012

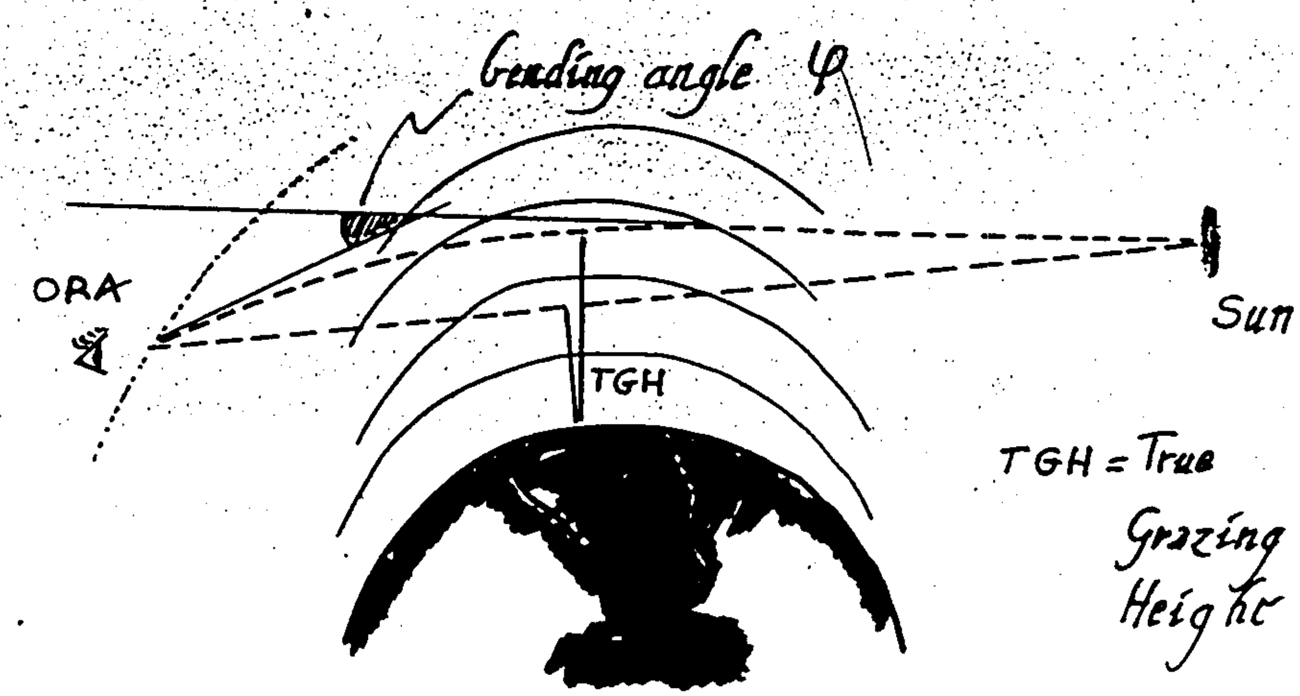
$$S_\lambda(h) = \int_{\Delta\Omega} W_\lambda(\Omega)\, e^{-\int_{s_1}^{s_2} \beta_\lambda(h(\Omega))\, ds}\, d\Omega$$

$$\beta_\lambda = \beta_\lambda^{Rayleigh} + \beta_\lambda^{Aerosol} + \beta_\lambda^{O_3} + \dots$$





OPTICAL SEGMENTS



The optical path is the solution of

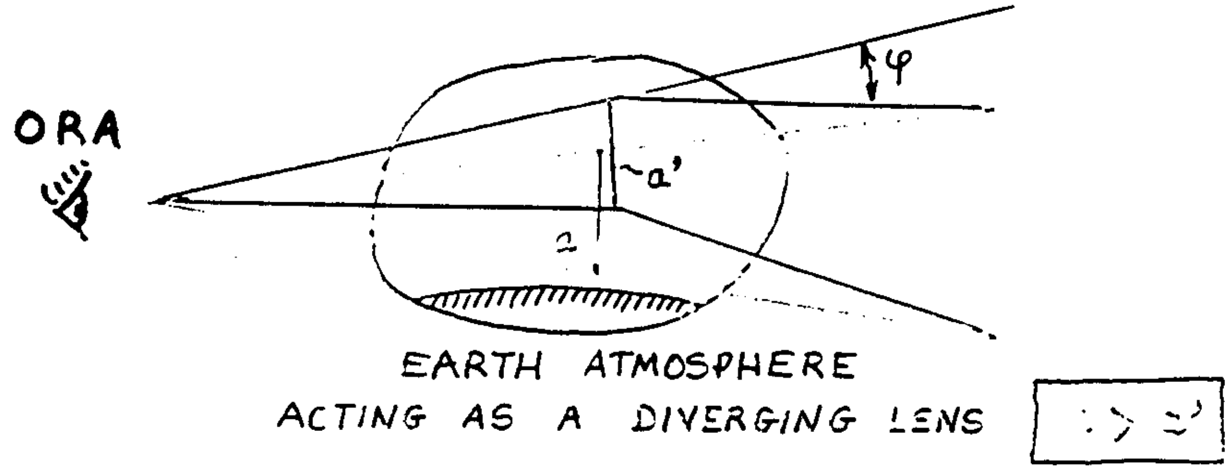
$$\frac{dr}{d\theta} = \pm \frac{r}{r_t n_t} \left[n^2(r)\, r^2 - n_t^2 r_t^2 \right]^{\frac{1}{2}}$$

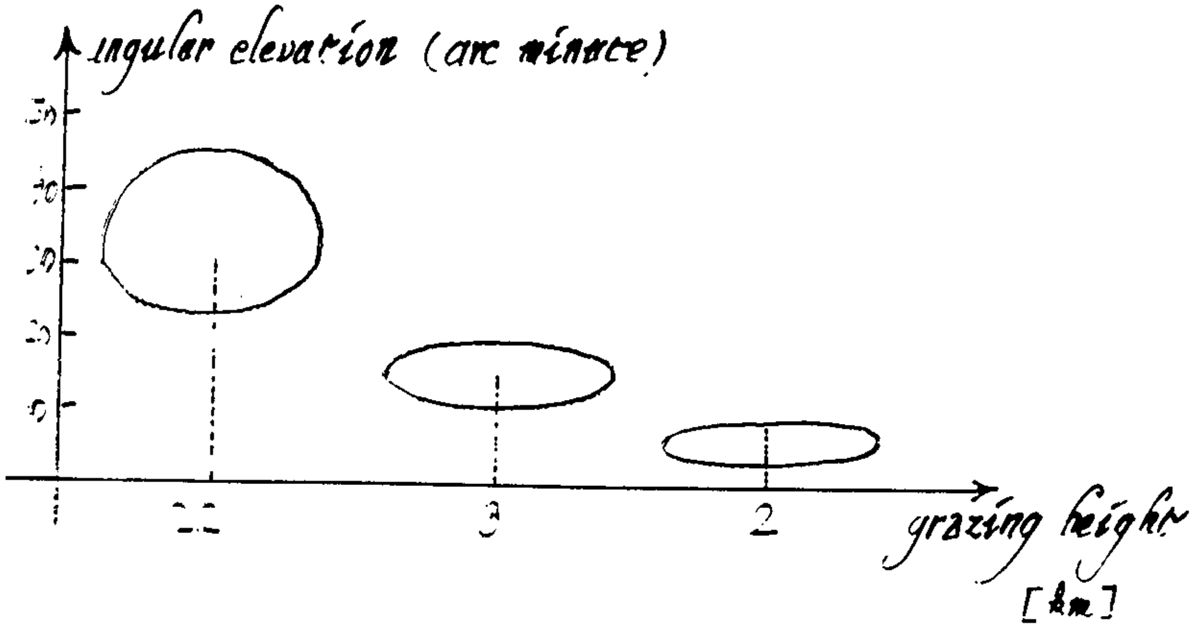
(Two points $\{r_{ORA}, \theta_{ORA}\}$, $\{r_{SUN}, \theta_{SUN}\}$)

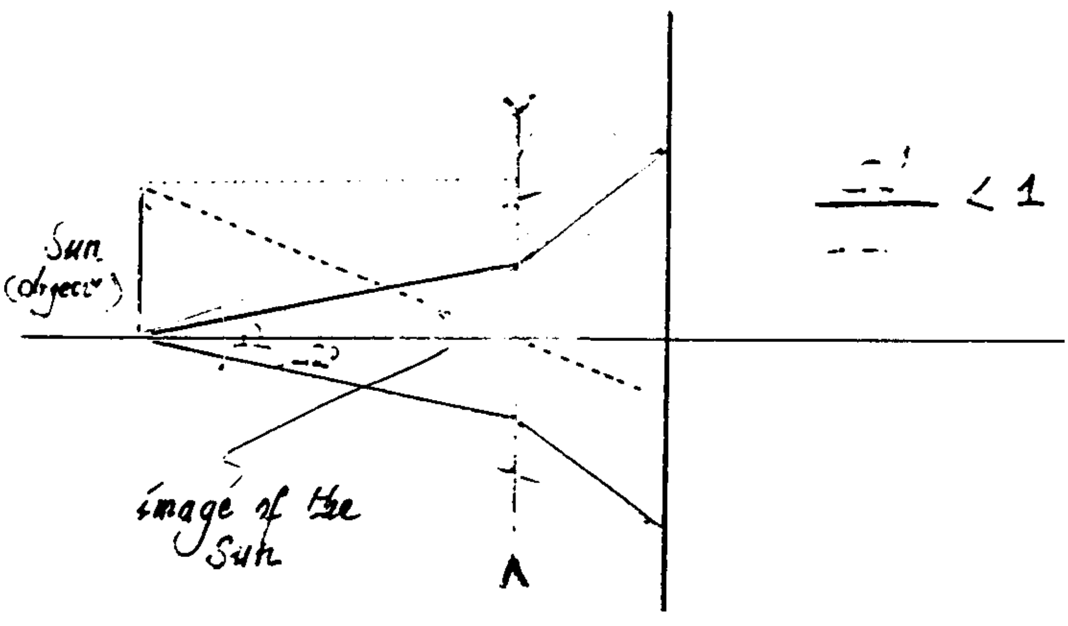
⇒ Shooting method until convergence of

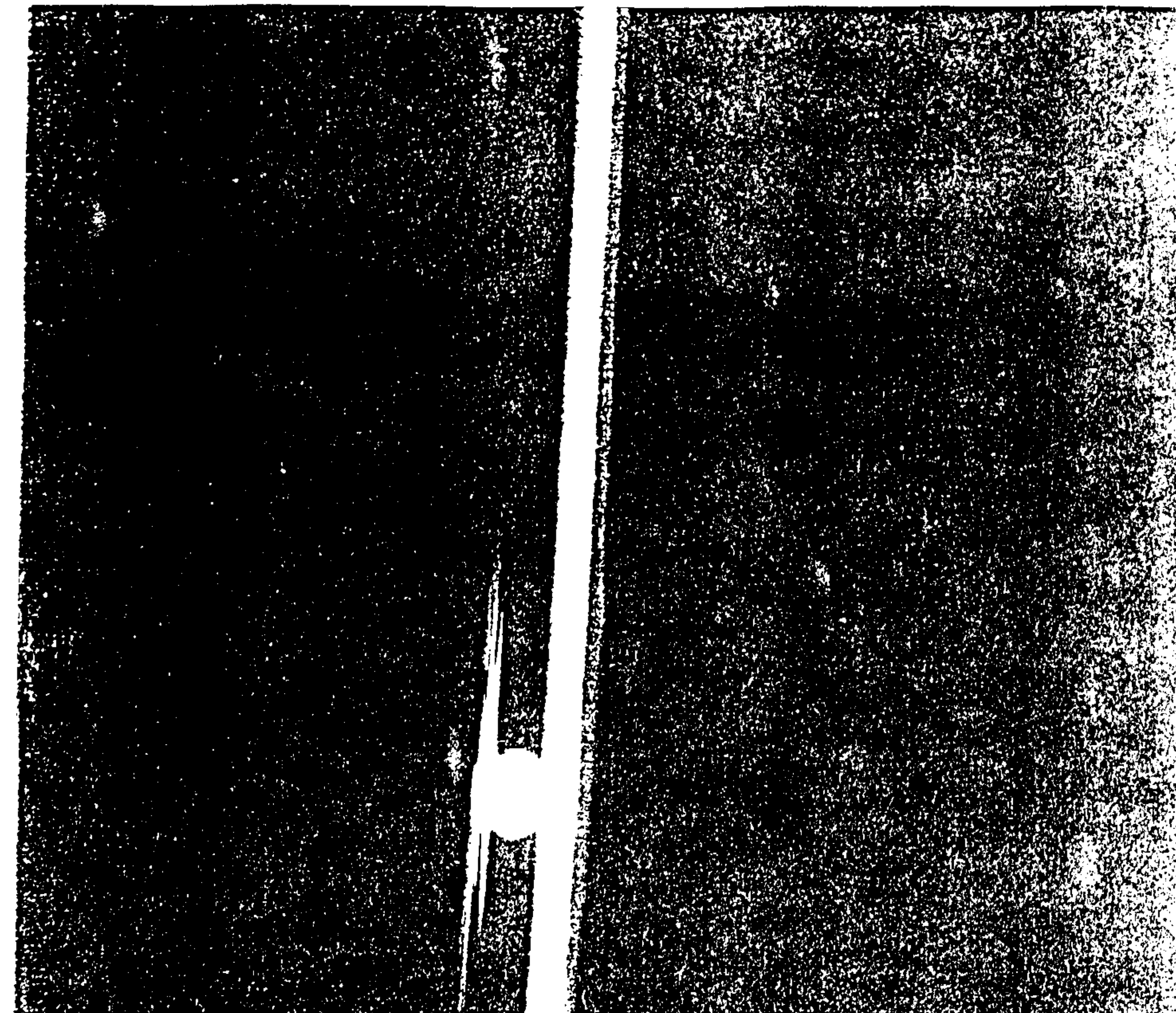
$$\left\{ \begin{array}{l} TGH \\ \varphi \\ S \end{array} \right.$$

Differential Refraction Effect

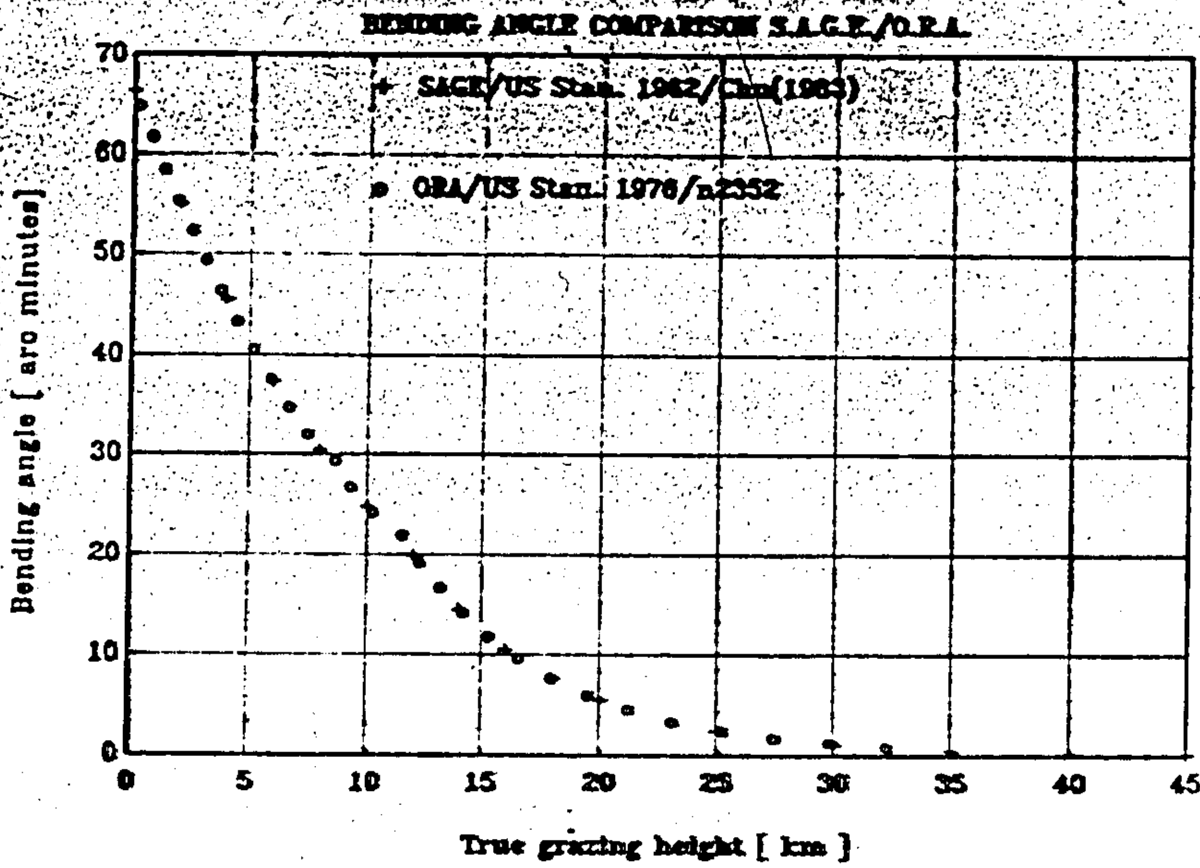


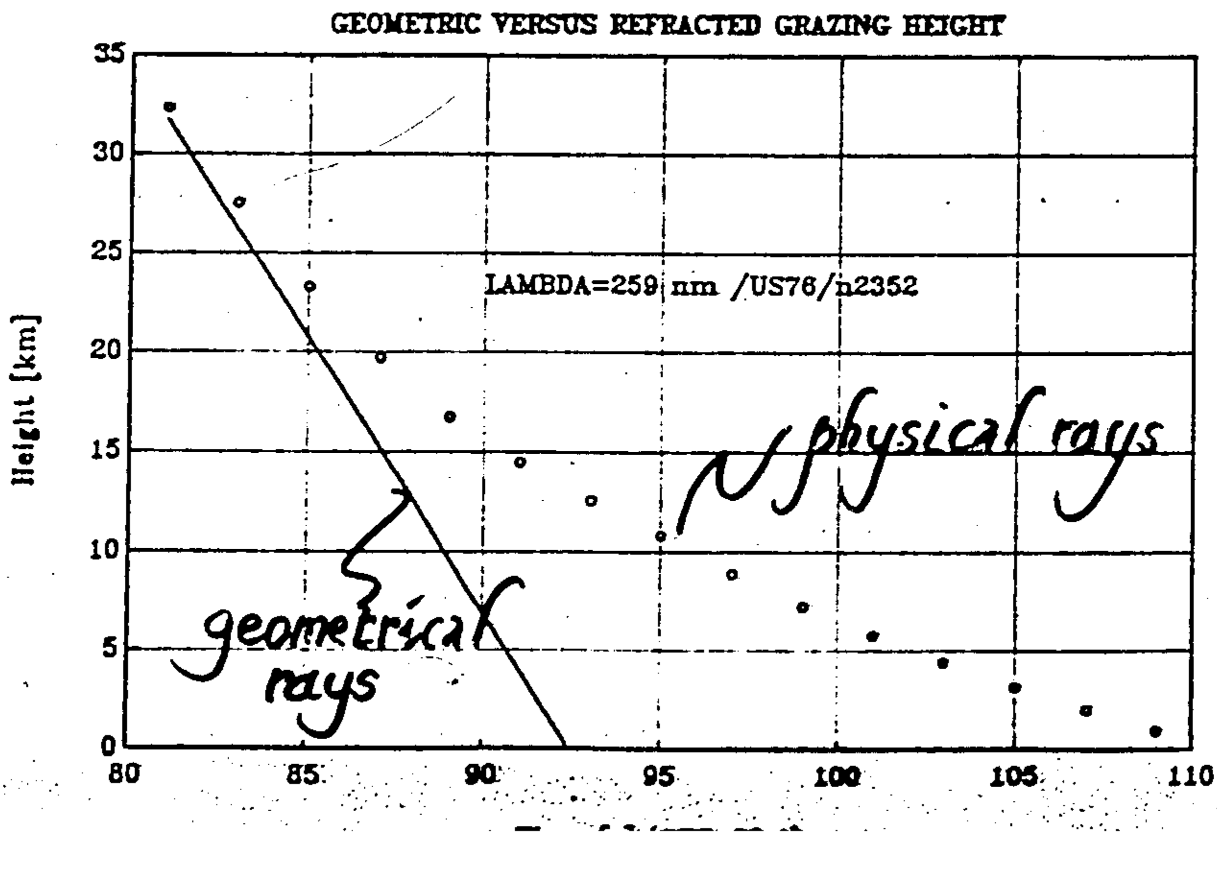




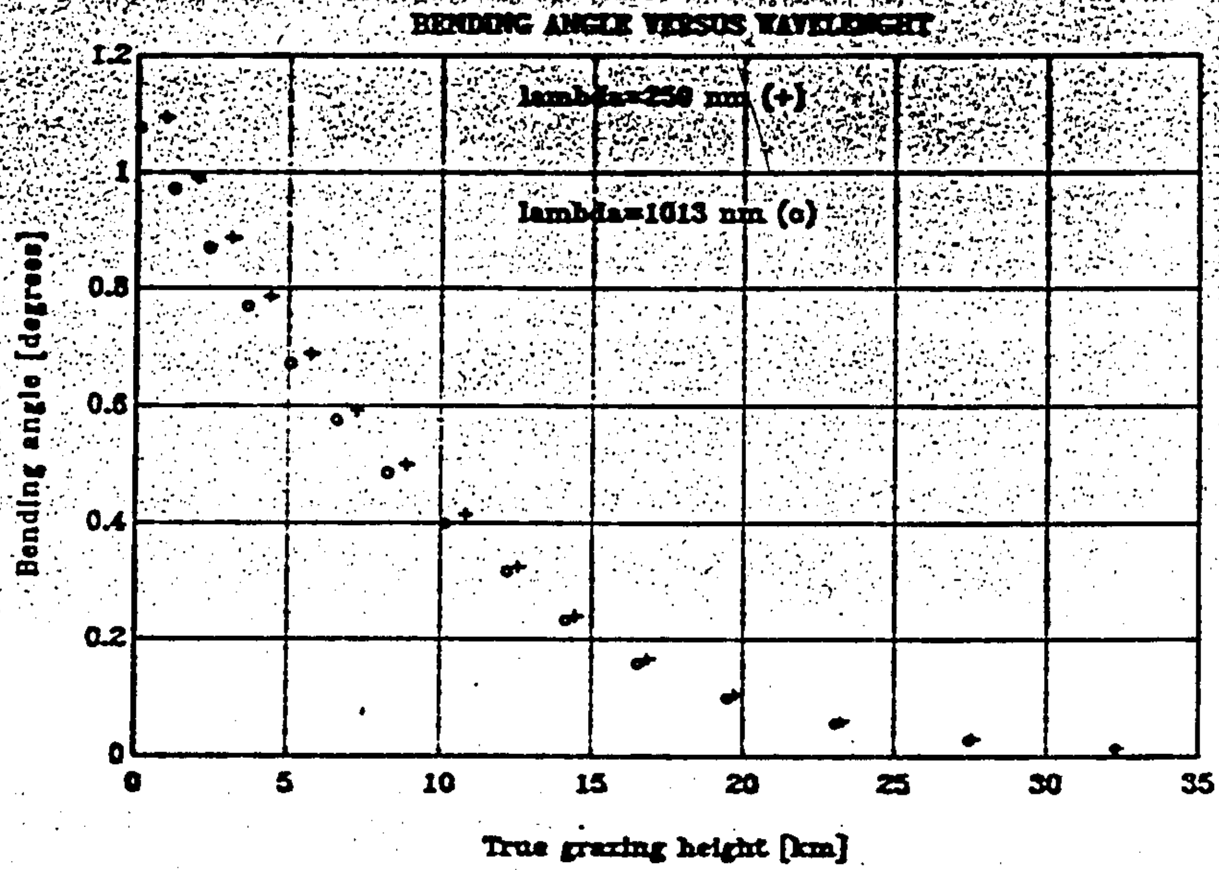


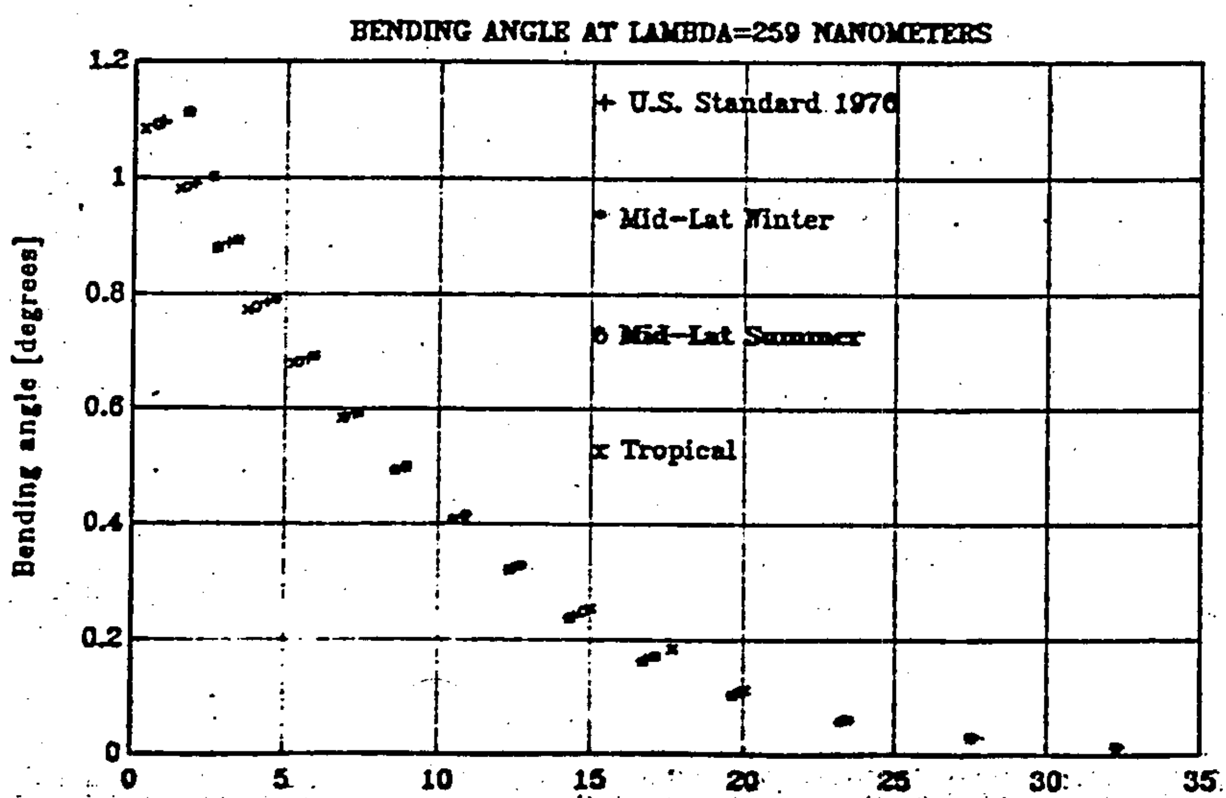
Effects of refraction



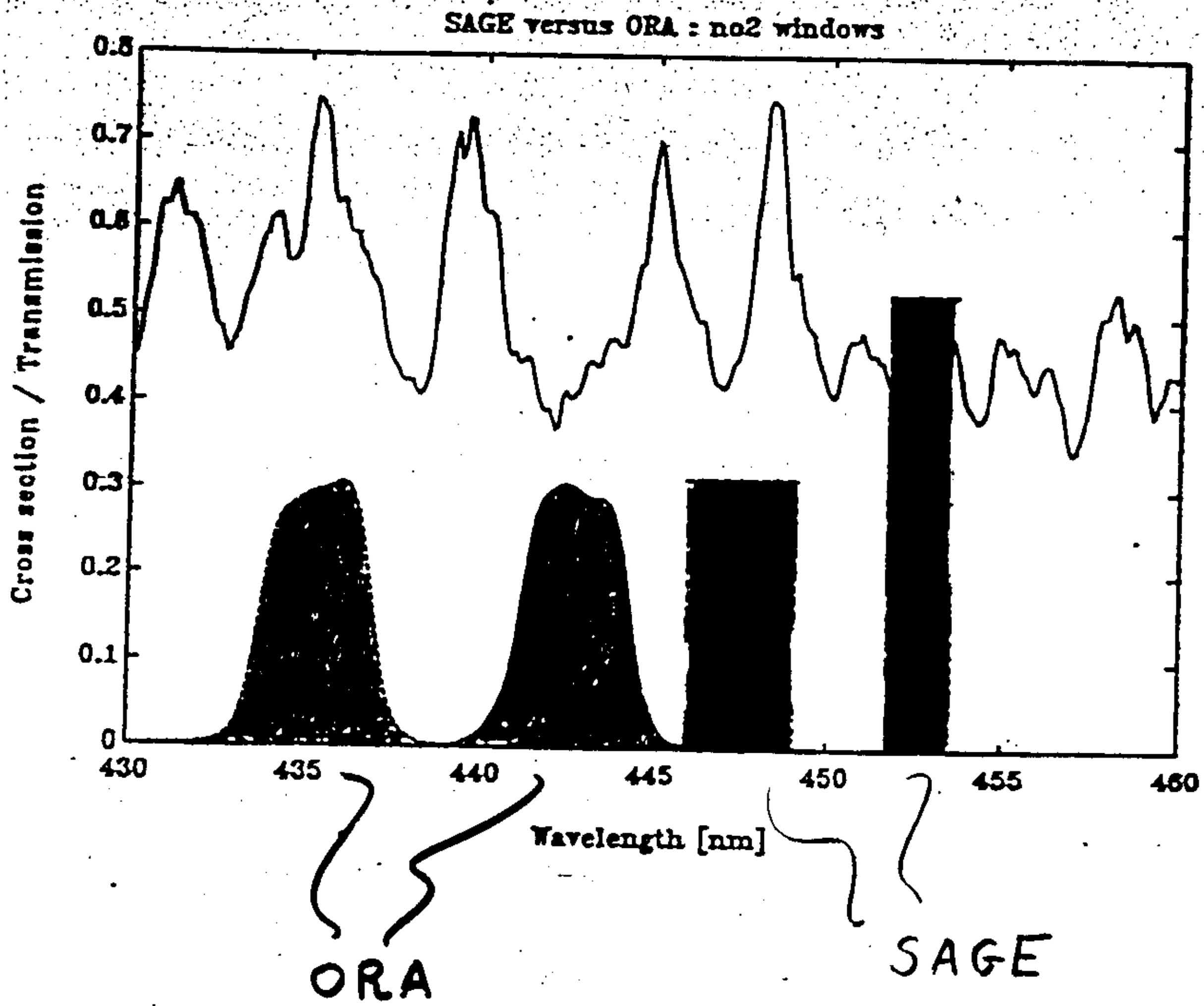


Wavelength and atmospheric dependencies





NO_2 windows



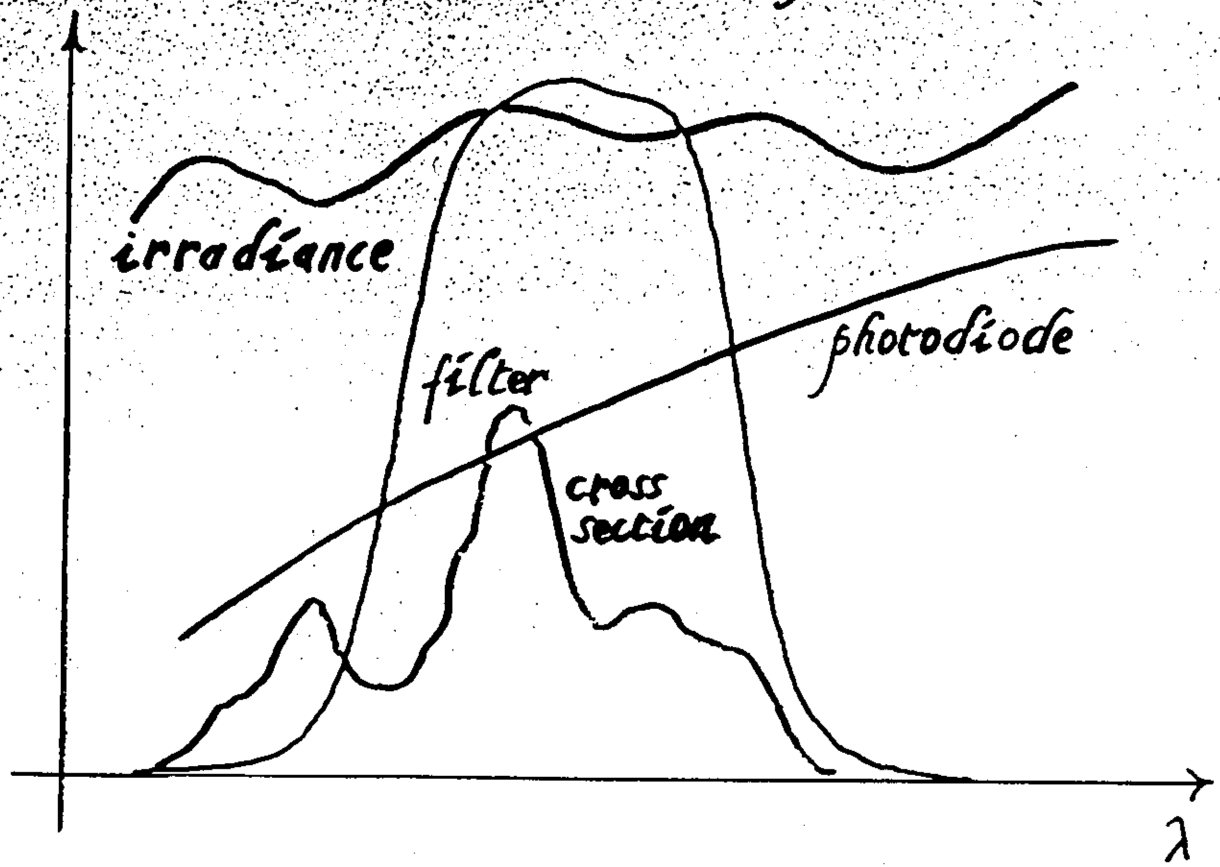
ORA: $\frac{\overline{\sigma_1}}{\overline{\sigma_2}} = 1.35$

SAGE: $\frac{\overline{\sigma_1}}{\overline{\sigma_2}} = 1.18$

Total cross section convolutions

Define $\bar{\sigma}$ as: $$\exp(-\bar{\sigma}\rho) = \int_{\lambda_1}^{\lambda_2} F(\lambda)\exp(-\sigma(\lambda)\rho)\,d\lambda$$

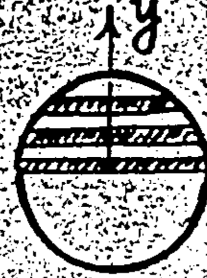
$$F(\lambda) = f(\lambda)\cdot irr(\lambda)\cdot photo(\lambda)$$

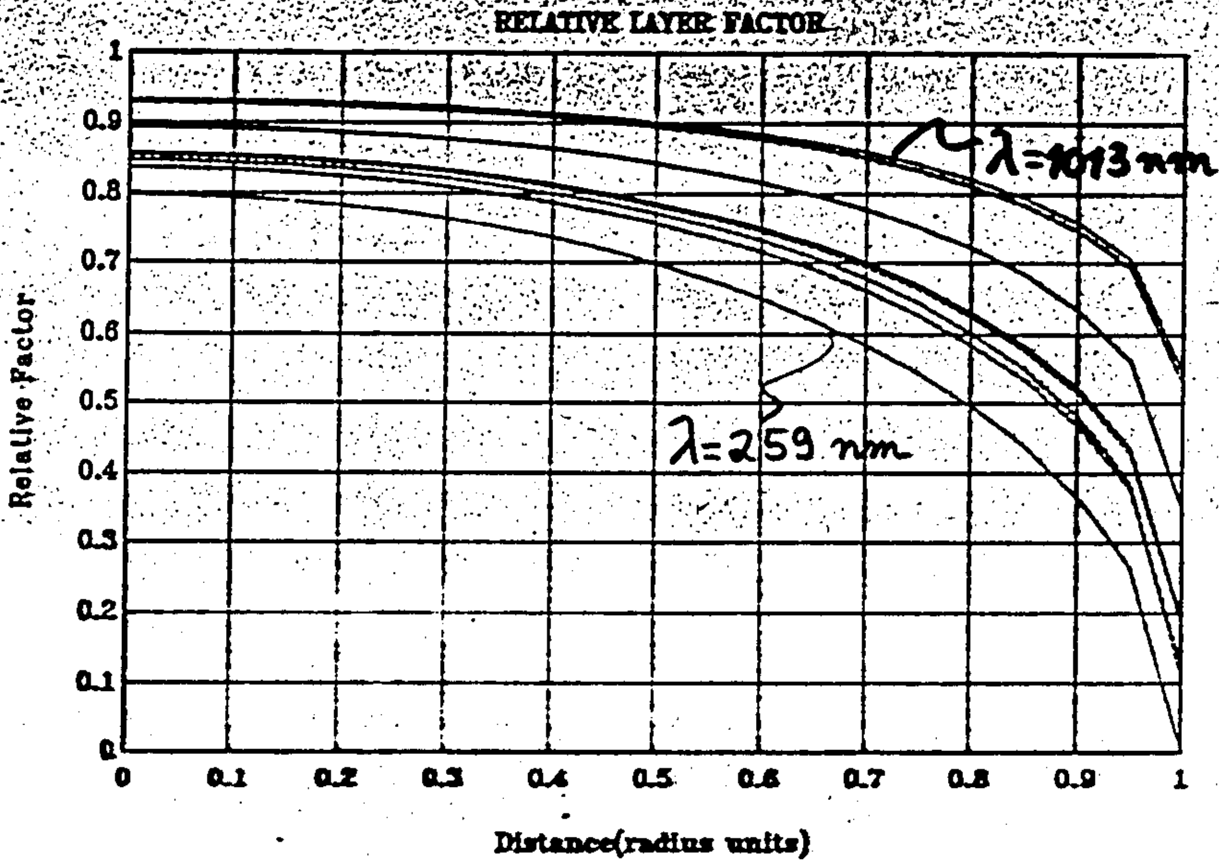


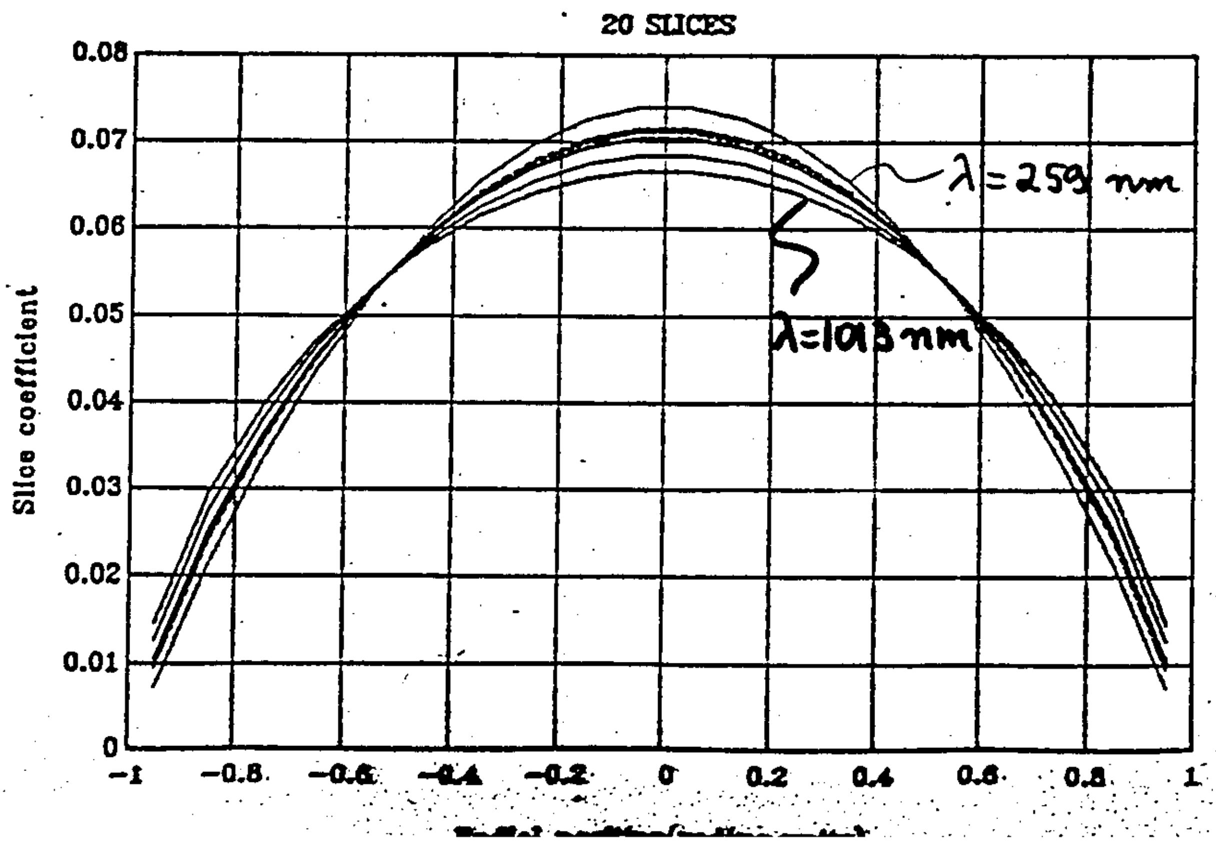
$$\bar{\sigma} = \bar{\sigma}(\rho) = -\frac{1}{\rho}\ln\int_{\lambda_1}^{\lambda_2} F(\lambda)\exp(-\sigma(\lambda)\rho)\,d\lambda$$

with: $$\int_{\lambda_1}^{\lambda_2} F(\lambda)\,d\lambda = 1$$

SOLAR LIMB DARKENING







THE INVERSION ALGORITHM

$$S_\lambda(h) = \int_{\Delta\Omega} W_\lambda(\Omega)\, e^{-\int_{s_1}^{s_2} \beta_\lambda(h(\Omega))\, ds}$$

$$\beta_\lambda = \beta_\lambda^{Rayleigh} + \beta_\lambda^{Aerosol} + \beta_\lambda^{O_3} + \cdots$$

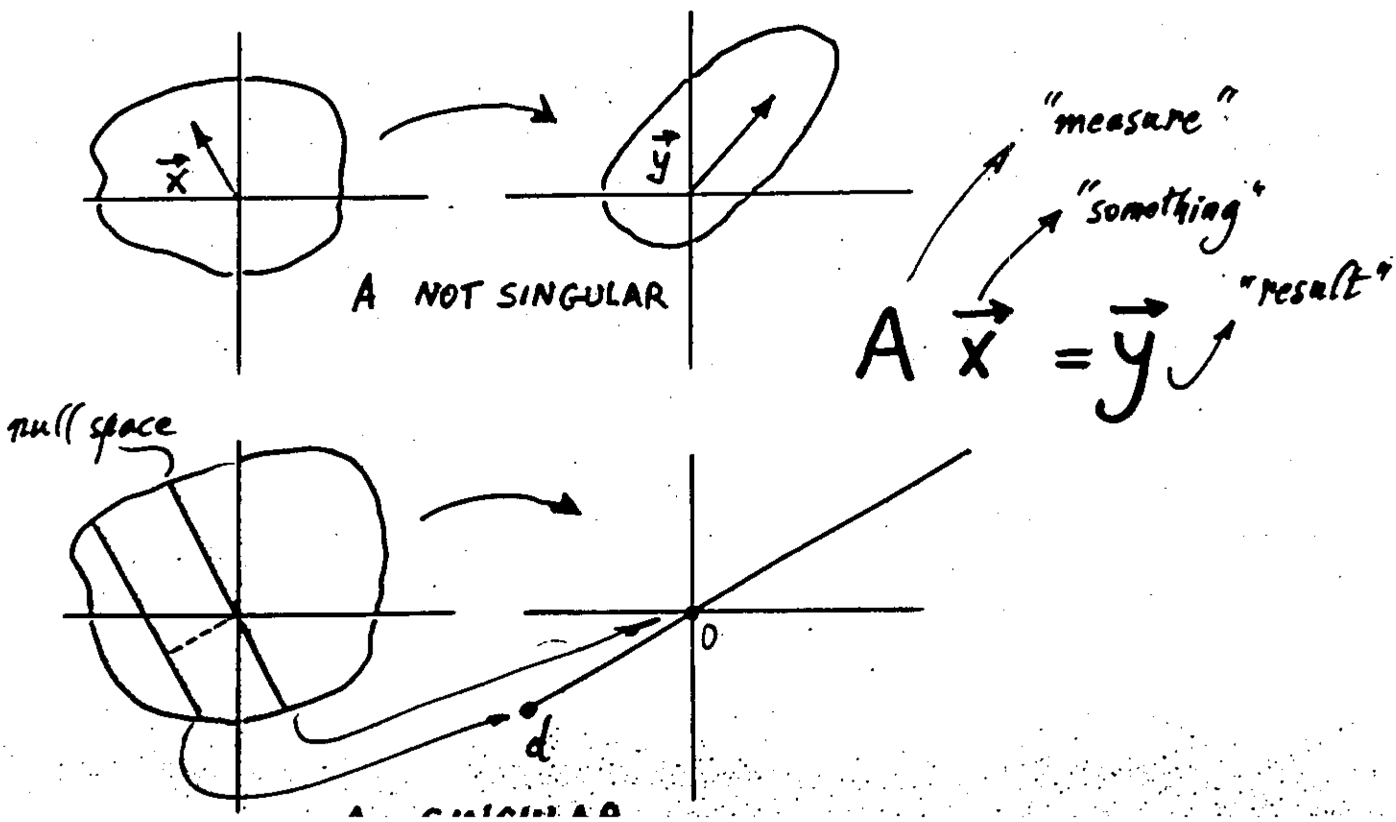
$\forall$ occultation : set of about 700 measurements $S_\lambda(h_i)$
→ choose 70 measurements ~ number of atmospheric layers

The inversion problem is basically an <u>ill-posed problem</u>

\# no hope to retrieve more informations about $\beta(h)$ than the number of measurements. ⇒ 'Spurious' fine structures.

\# Integration destroys information ! (redundance does not help you ...)

In the linear case, we have theorems...

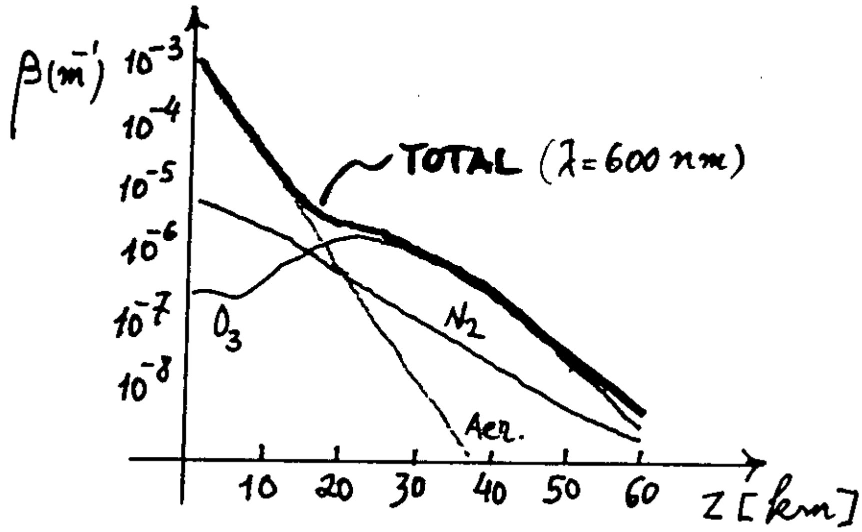


NATURAL ORTHOGONAL PROFILE EXPANSION

1) the information content of the best retrieved profile is <u>not infinite!</u>

2) iterative adjustement of the solution should be done <u>globally</u>

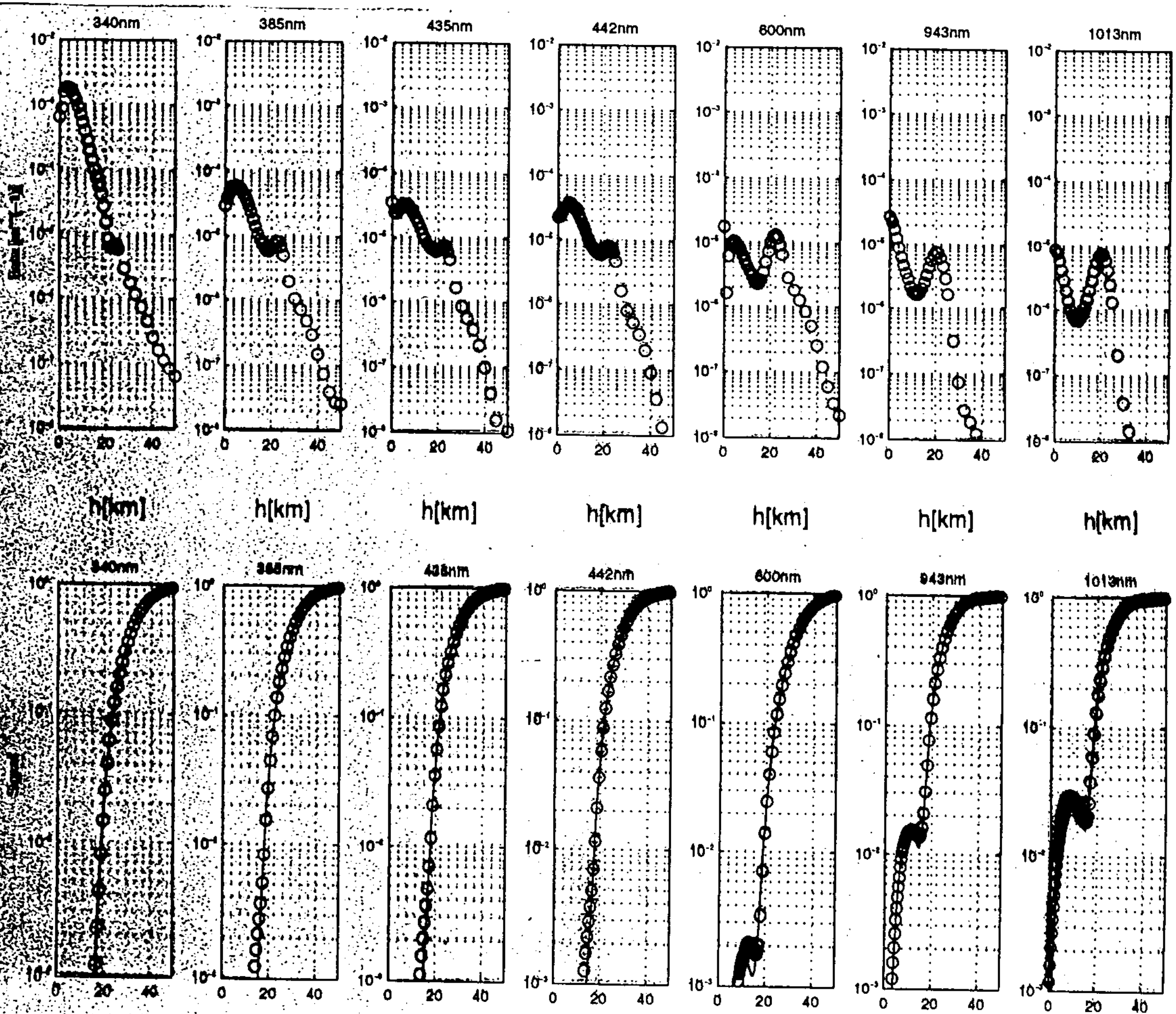
3) to preserve the constituent separation, the algorithm has to focus on <u>small scale details</u>



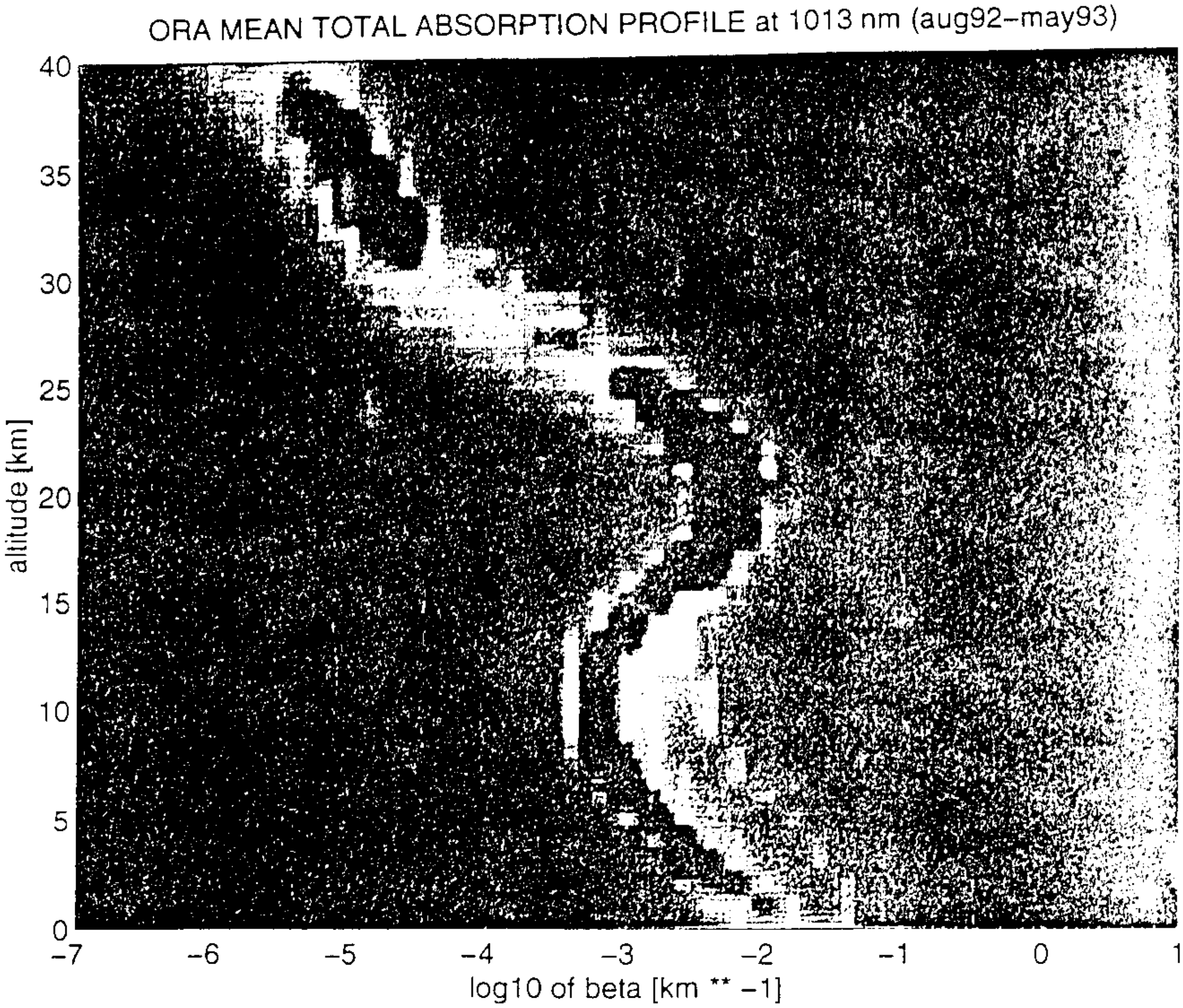
$$\boxed{\beta(z) = \beta_0(z) \cdot \sum_{k=0}^{N} \alpha_k \, |\tilde{p}_k(z)\rangle} \qquad \langle \tilde{p}_k | \tilde{p}_\ell \rangle = \delta_{k\ell}$$

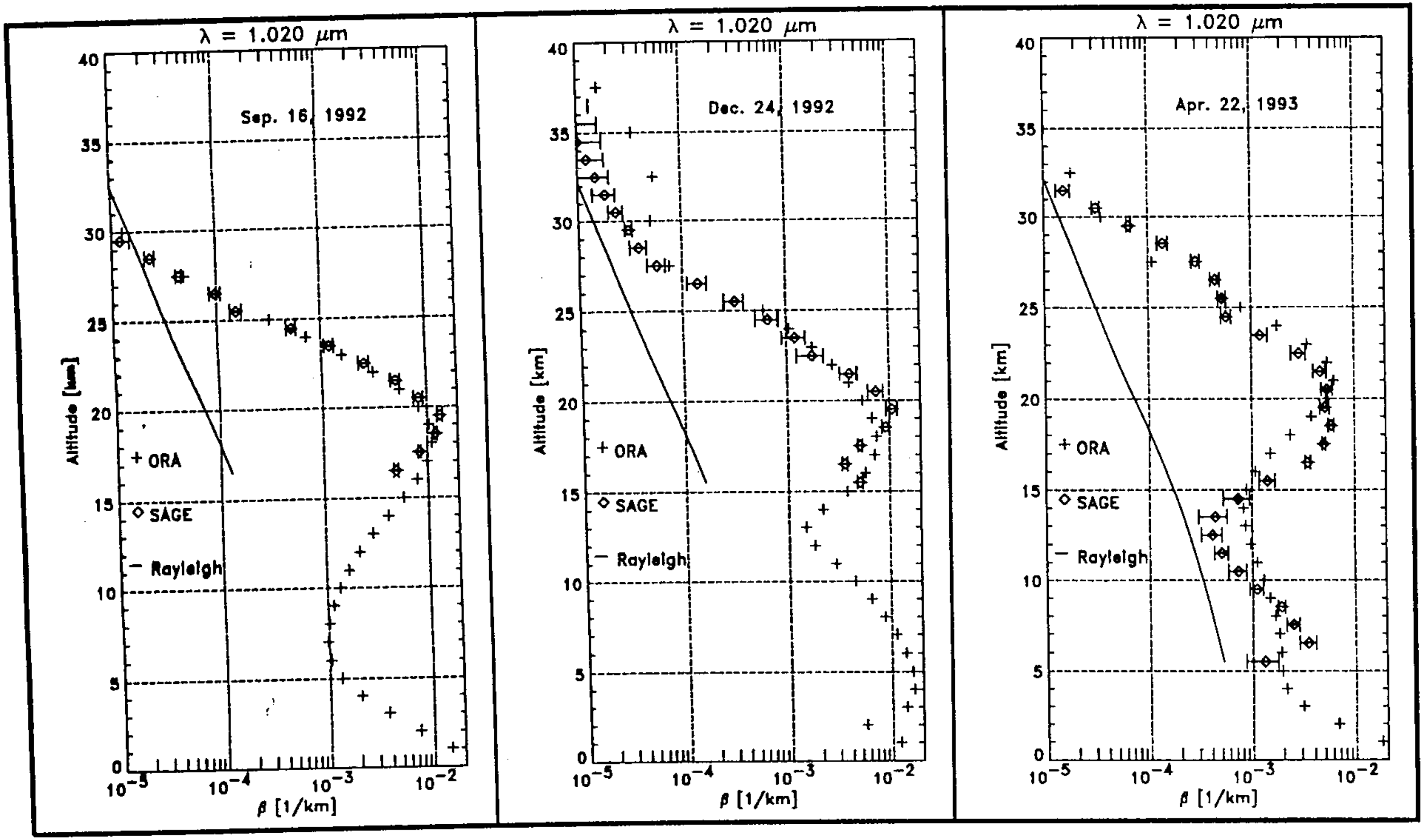
⇒ using $\beta_0(z)$ as the "measure" for the scalar product construct an orthogonal set of polynomials by STIELTJES procedure. Then solve by standard non-linear algorithm

$$\left\{ \chi^2 = \sum_i \left(\text{Signal}(i) - \text{Theory}(i; \alpha_0, \alpha_1, \ldots \alpha_N) \right)^2 \right\}_{min}$$

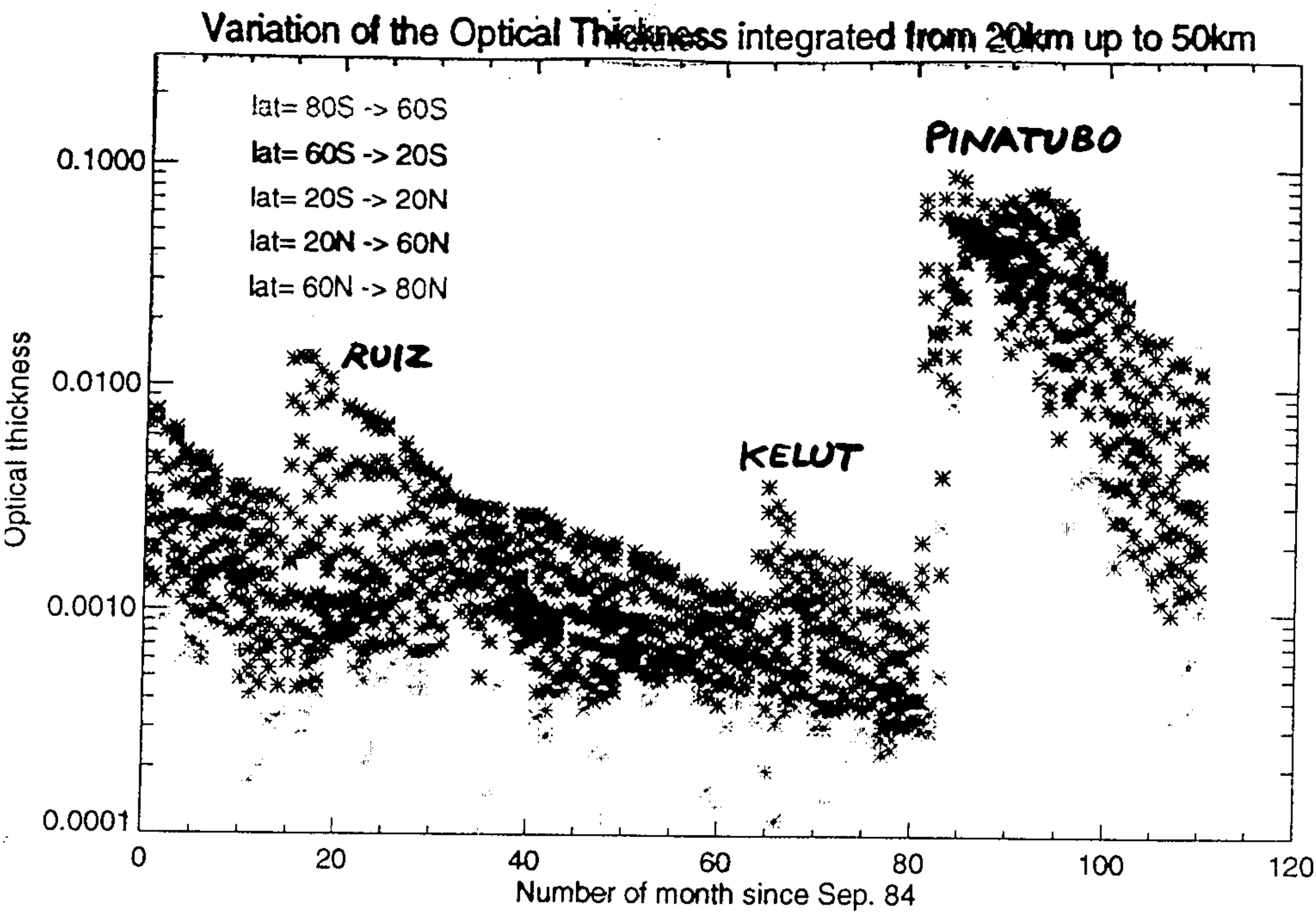


340nm
385nm
435nm
442nm
600nm
943nm
1013nm
h[km]
h[km]
h[km]
h[km]
h[km]
h[km]
h[km]
442nm
600nm
943nm
1013nm

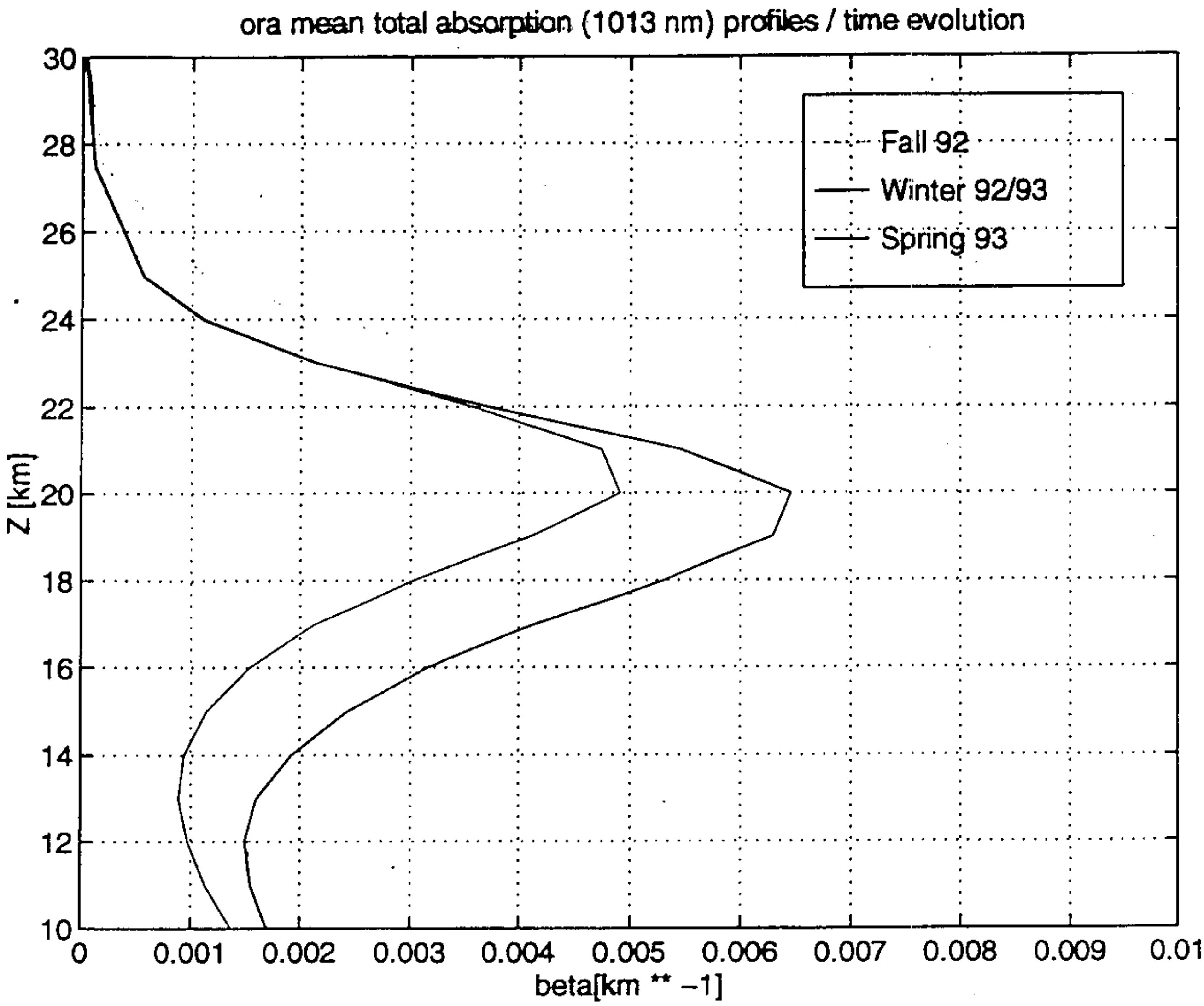

ORA MEAN TOTAL ABSORPTION PROFILE at 1013 nm (aug92–may93)
altitude [km]
log10 of beta [km ** –1]
40
35
30
25
20
15
10
5
0
–7
–6
–5
–4
–3
–2
–1
0
1

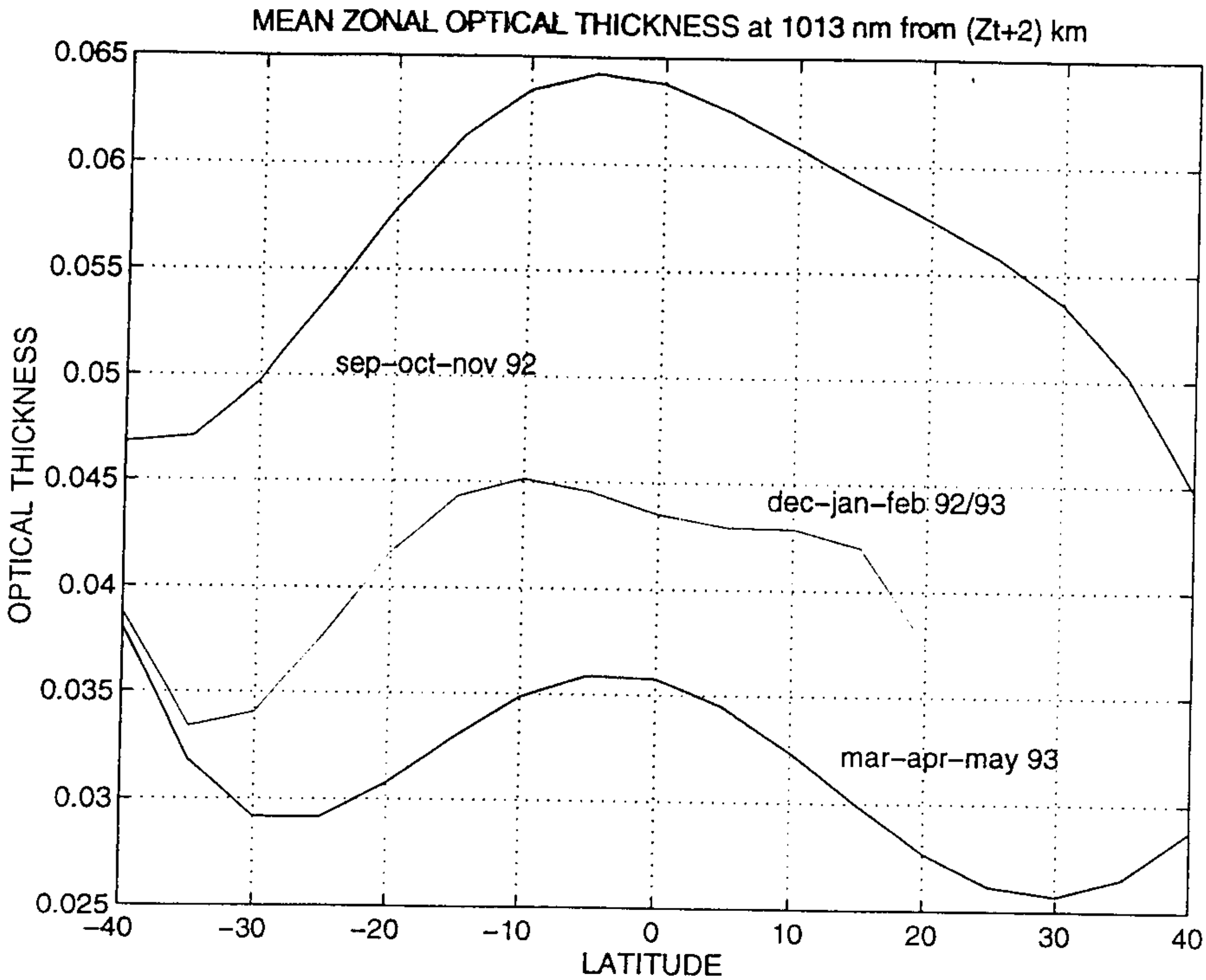


λ = 1.020 μm
Sep. 16, 1992
+ ORA
◇ SAGE
— Rayleigh
Altitude [km]
β [1/km]
λ = 1.020 μm
Dec. 24, 1992
+ ORA
◇ SAGE
— Rayleigh
Altitude [km]
β [1/km]
λ = 1.020 μm
Apr. 22, 1993
+ ORA
◇ SAGE
— Rayleigh
Altitude [km]
β [1/km]



Variation of the Optical Thickness integrated from 20km up to 50km
lat= 80S -> 60S
lat= 60S -> 20S
lat= 20S -> 20N
lat= 20N -> 60N
lat= 60N -> 80N
RUIZ
KELUT
PINATUBO
Optical thickness
0.1000
0.0100
0.0010
0.0001
0
20
40
60
80
100
120
Number of month since Sep. 84

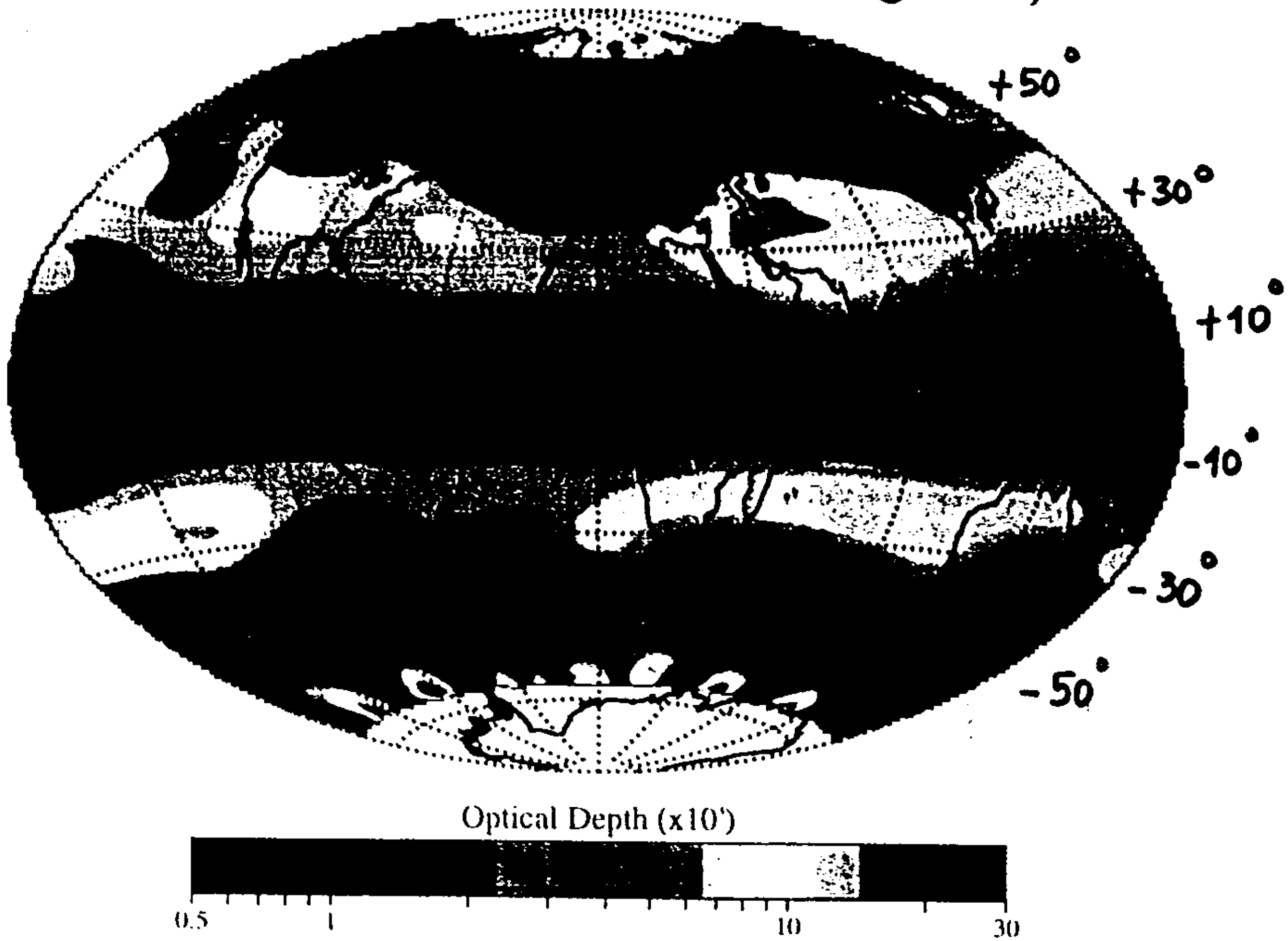

ora mean total absorption (1013 nm) profiles / time evolution
Fall 92
Winter 92/93
Spring 93
Z [km]
30
28
26
24
22
20
18
16
14
12
10
0
0.001
0.002
0.003
0.004
0.005
0.006
0.007
0.008
0.009
0.01
beta[km ** -1]



MEAN ZONAL OPTICAL THICKNESS at 1013 nm from (Zt+2) km
OPTICAL THICKNESS
0.065
0.06
0.055
0.05
0.045
0.04
0.035
0.03
0.025
sep-oct-nov 92
dec-jan-feb 92/93
mar-apr-may 93
-40
-30
-20
-10
0
10
20
30
40
LATITUDE

from "Banded structures in stratospheric aerosol distributions"
Trepte, Thomason & Kent
GRL, 21, p 2397 [Nov, 1, 1994]

SAGE, Aug 15 - Sep 24 (1993)



Main problem :
Ill-conditioning (Ill-posedness)

Example :

$$\begin{bmatrix} 1 & 2 \\ 1 & 2.01 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 3 \\ 3.01 \end{bmatrix}$$

Exact solution :

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Now : introducing 'measurement error' (5 %)

$$\begin{bmatrix} 1 & 2 \\ 1 & 2.01 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 3.15 \\ 2.86 \end{bmatrix}$$

Solution :

$$\begin{bmatrix} 61.15 \\ -29 \end{bmatrix}$$

(4753 % error on the solution !)

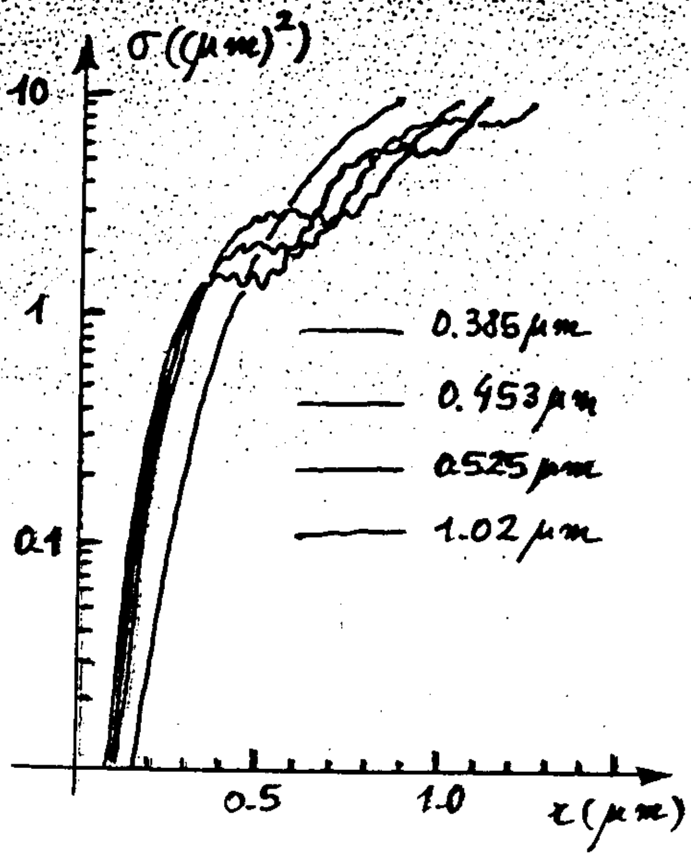
CONCLUSION :

enormous error magnification !

CAUSE :

dependence between the columns and rows of the linear system.

Aerosols...



$$\delta = \int \sigma \, n \, ds$$

but

$$\sigma = \int_0^\infty \sigma(r) N(r) \, dr$$

$\sigma(r)$ → Mie cross section; $N(r)$ → Size distribution function

REPLACE BY

$$\boxed{\delta = \int \beta_\lambda \, ds}$$

β_λ → extinction coefficient

From ab initio Mie calculations and observed unimodal size distribution, a reasonable wavelength dependency is

$$\beta_\lambda \sim \exp(c_0 + c_1 \lambda + c_2 \lambda^2)$$
or
$$c_0 + c_1 \lambda + c_2 \lambda^2$$

⇒ try to determine c_0, c_1, c_2 by correlative measurements at $\lambda_0, \lambda_1, \lambda_2 \ldots \lambda_n$!

SPECTRAL INVERSION:
Matrix equation

First: removal of Rayleigh extinction, using UKMO meteorological data.

Assumption: quadratic wavelength dependence for aerosols.

$$\beta_\lambda^A = c_0 + c_1(\lambda - \lambda_{1013}) + c_2(\lambda - \lambda_{1013})^2$$

$$\begin{bmatrix} \beta_{340}^{NO_2} & \beta_{340}^{O_3} & 1 & \Delta\lambda_{340} & (\Delta\lambda_{340})^2 \\ \beta_{385}^{NO_2} & \beta_{385}^{O_3} & 1 & \Delta\lambda_{385} & (\Delta\lambda_{385})^2 \\ \beta_{435}^{NO_2} & \beta_{435}^{O_3} & 1 & \Delta\lambda_{435} & (\Delta\lambda_{435})^2 \\ \beta_{442}^{NO_2} & \beta_{442}^{O_3} & 1 & \Delta\lambda_{442} & (\Delta\lambda_{442})^2 \\ \beta_{600}^{NO_2} & \beta_{600}^{O_3} & 1 & \Delta\lambda_{600} & (\Delta\lambda_{600})^2 \\ \beta_{1013}^{NO_2} & \beta_{1013}^{O_3} & 1 & \Delta\lambda_{1013} & (\Delta\lambda_{1013})^2 \end{bmatrix} \begin{bmatrix} x_{NO_2} \\ x_{O_3} \\ c_0 \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} \beta_{340} \\ \beta_{385} \\ \beta_{435} \\ \beta_{442} \\ \beta_{600} \\ \beta_{1013} \end{bmatrix}$$

or, for altitude z_i: $A_i \vec{x_i} = \vec{\beta_i}$

SPECTRAL INVERSION:
Total Matrix

26 altitude levels

$$\begin{bmatrix} A_1 & 0 & \cdots & 0 & \vec{s} \\ 0 & A_2 & & & \vec{s} \\ \vdots & & \ddots & \vdots & \vdots \\ 0 & & \cdots & A_{26} & \vec{s} \end{bmatrix} \cdot \begin{bmatrix} \vec{x_1} \\ \vec{x_2} \\ \vdots \\ \vec{x_{26}} \\ x_s \end{bmatrix} = \begin{bmatrix} \vec{\beta_1} \\ \vec{\beta_2} \\ \vdots \\ \vec{\beta_{26}} \end{bmatrix}$$

with straylight $\vec{s} \sim \lambda^{-4}$

$\mathbf{C_d}$: Measurement covariance matrix

$\mathbf{C_v}$: A priori covariance matrix, with altitude smoothing for every constituent ($L \sim 5$ km):

$$\sigma^2\left(z_i, z_j\right) = \sqrt{\sigma^2\left(z_i\right)\sigma^2\left(z_j\right)} \cdot \exp\left(-\left(\frac{z_i - z_j}{L}\right)^2\right)$$

$\tilde{\mathbf{x}}_\mathbf{t}$: A priori solution (from climatology)

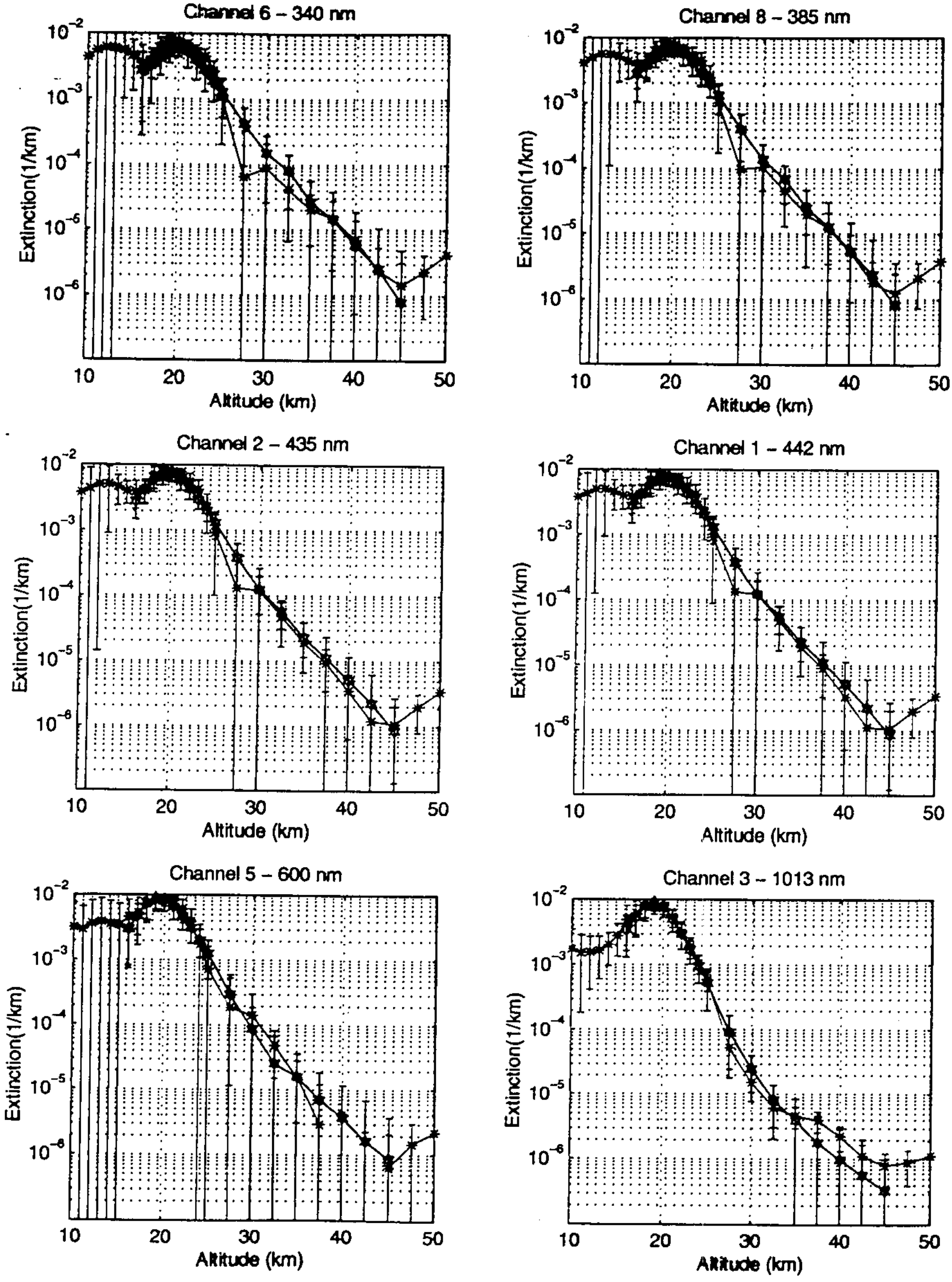
SPECTRAL INVERSION:
General Least Squares

Minimization of merit function (assuming Gaussian noise):

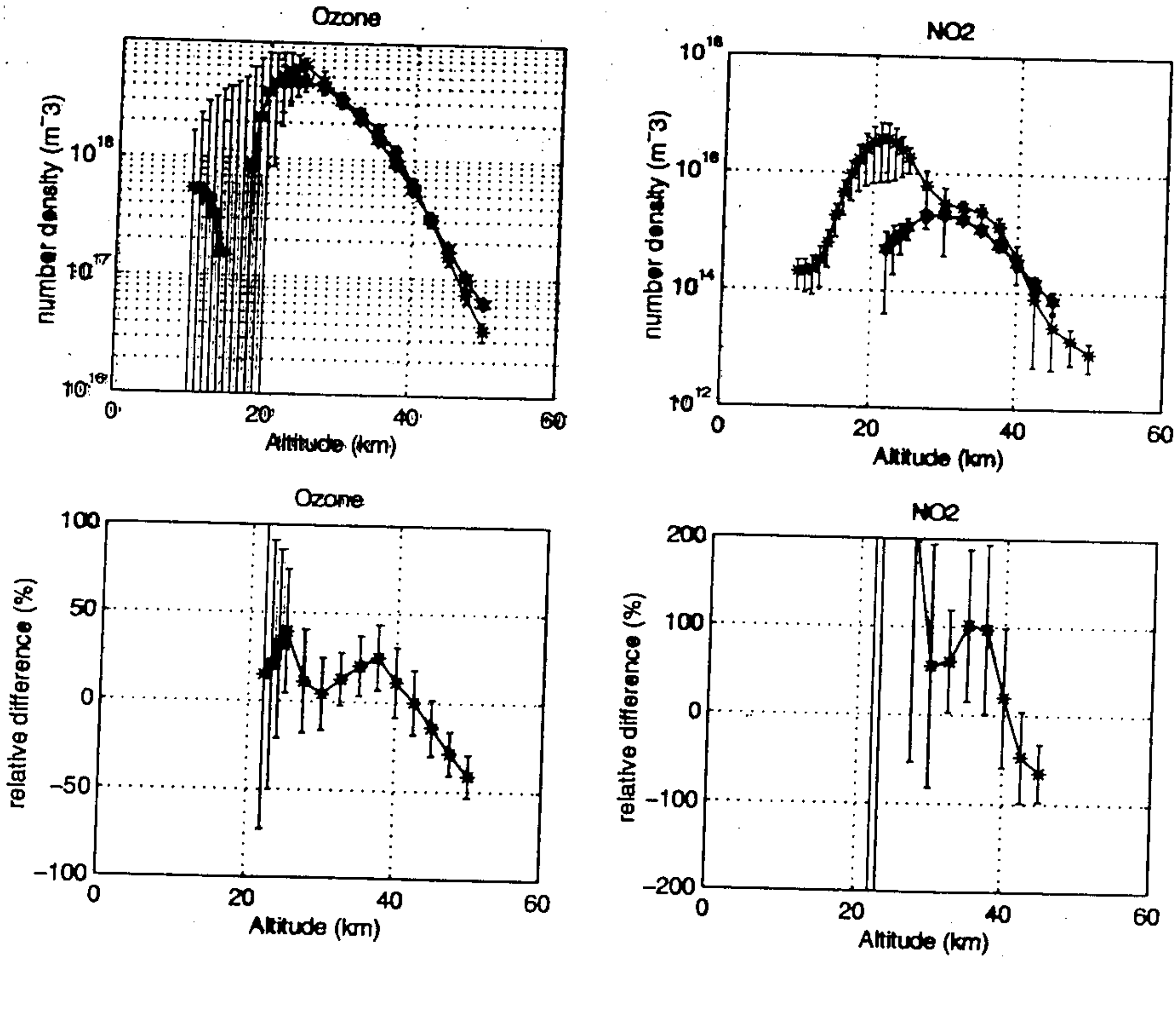
$$\langle\, A_t \vec{x_t} - \vec{\beta_t} \mid C_d^{-1} \mid A_t \vec{x_t} - \vec{\beta_t} \,\rangle$$

$$+$$

$$\langle\, \vec{x_t} - \tilde{x}_t \mid C_v^{-1} \mid \vec{x_t} - \tilde{x}_t \,\rangle$$



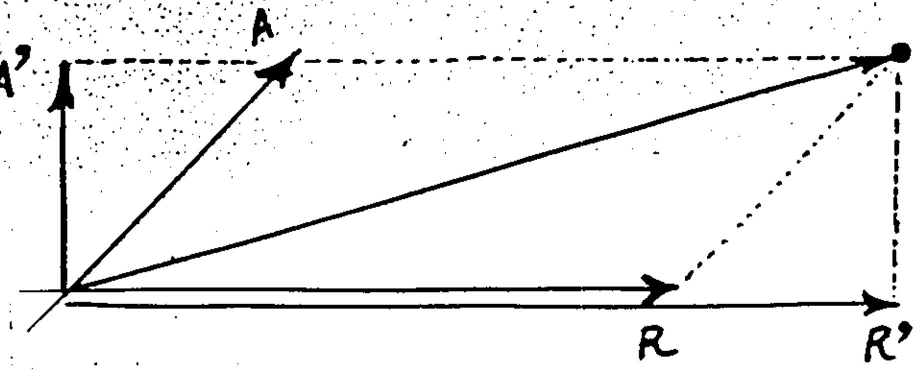
Channel 6 – 340 nm
Channel 8 – 385 nm
Channel 2 – 435 nm
Channel 1 – 442 nm
Channel 5 – 600 nm
Channel 3 – 1013 nm
Extinction(1/km)
Altitude (km)
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10
20
30
40
50


Ozone
number density (m^-3)
10^{18}
10^{17}
10^{16}
Altitude (km)
0
20
40
60
NO2
10^{18}
10^{16}
10^{14}
10^{12}
number density (m^-3)
Altitude (km)
0
20
40
60
Ozone
relative difference (%)
100
50
0
−50
−100
Altitude (km)
0
20
40
60
NO2
relative difference (%)
200
100
0
−100
−200
Altitude (km)
0
20
40
60

Kernels : orthogonality and more...

1. Rayleigh against aerosols.

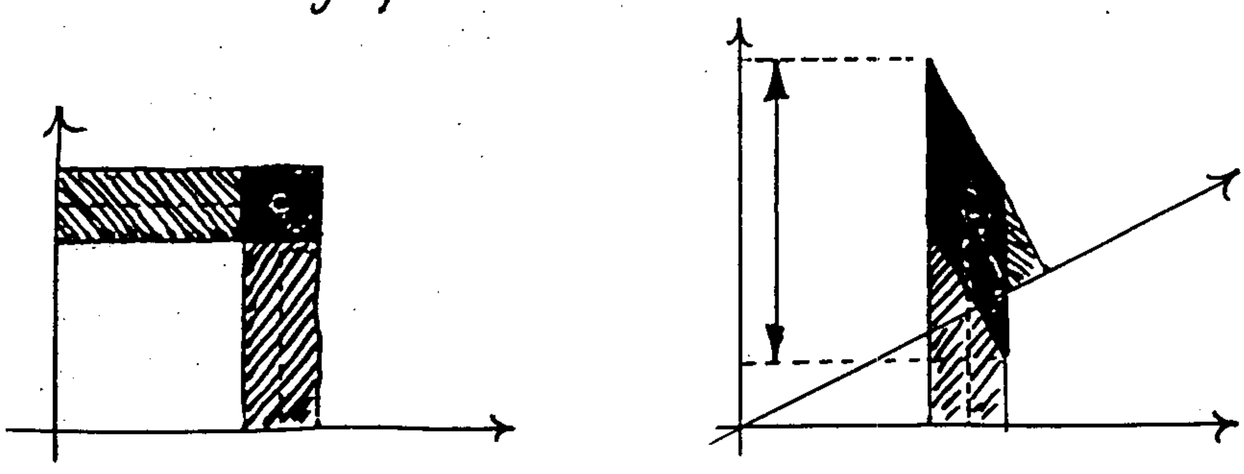
What if aerosol would behave as $1/\lambda^4$?



The direction of $\vec{A}$ is not known a priori.
It is a product of GOMOS !

⇒ some undetermination will persist...

⇒ noise amplification is unavoidable for skewed axes.



More fundamental ...

$$\beta(\lambda) = x_R \beta_R(\lambda) + x_{O_3} \beta_{O_3}(\lambda) + x_{NO_2} \beta_{NO_2}(\lambda) + \beta_{Aerosol}(\lambda)$$

with $\beta_{Aerosol} = x_0 \beta_0(\lambda) + x_1 \beta_1(\lambda) + \cdots$

$$\chi^2 = \int_{\lambda_1}^{\lambda_2} \left(M(\lambda) - \beta(\lambda) \right)^2 d\lambda$$

$$\frac{\partial \chi^2}{\partial x_i} = 0 \quad \forall_i$$

$$\begin{bmatrix} \int \beta_R^2 d\lambda & \int \beta_R \beta_{O_3} d\lambda & \int \beta_R \beta_{NO_2} d\lambda & \cdots \\ & \int \beta_{O_3}^2 d\lambda & \int \beta_{O_3} \beta_{NO_2} d\lambda & \cdots \\ \text{LL} & & \int \beta_{NO_2}^2 d\lambda & \cdots \\ & & & \end{bmatrix} \cdot \begin{bmatrix} x_R \\ x_{O_3} \\ x_{NO_2} \\ \vdots \end{bmatrix} = \begin{bmatrix} \int \beta \beta_R d\lambda \\ \int \beta \beta_{O_3} d\lambda \\ \vdots \\ \ \end{bmatrix}$$

KERNEL

$$K \vec{x} = \vec{b}$$

$$\vec{x} = K^{-1} \vec{b}$$

and also $\quad \vec{\Delta x} = K^{-1} \Delta \vec{b}$

Suppose $\beta(\lambda) = A/\lambda^4 + (\underbrace{B_0 + B_1\lambda + B_2\lambda^2}_{\text{known by God only!}})$

$M(\lambda) = a/\lambda^4 + (\underbrace{b_0 + b_1\lambda}_{\text{trial by somos people}})$

A) use of a 3 channel instrument $(\lambda_1, \lambda_2, \lambda_3)$

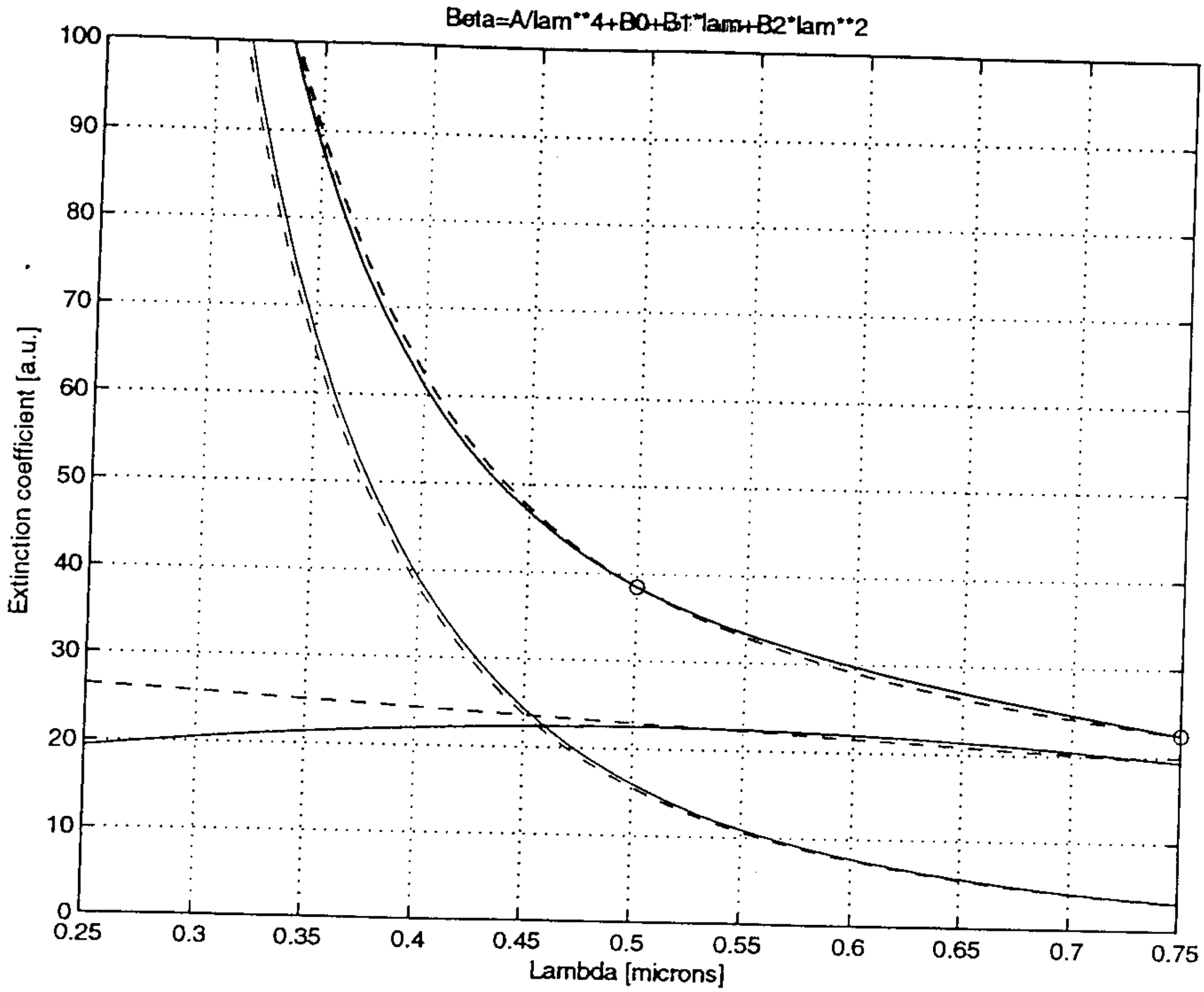
$$\left\{\begin{array}{l} \frac{a}{\lambda_1^4} + b_0 + b_1\lambda_1 = \beta_1 \\ \frac{a}{\lambda_2^4} + b_0 + b_1\lambda_2 = \beta_2 \\ \frac{a}{\lambda_3^4} + b_0 + b_1\lambda_3 = \beta_3 \end{array}\right\} \Rightarrow \begin{array}{l} a = A + \epsilon_a B_2 \\ b_1 = B_1 + \epsilon_{b_1} B_2 \\ b_0 = B_0 + \epsilon_{b_0} B_2 \end{array}$$

standard case: $A = 1 \quad B_0 = 10 \quad B_1 = 50 \quad B_2 = -50$

B_2	a	b_0	b_1	$\bar{\Delta}(\%)$
0	1	10	50	0
−50	0.958	29.4	−12.5	.01
−100	0.916	48.8	−75.0	−3.9

① The value of the retrieved aerosol coefficients should be interprited with caution!
but $b_0 + b_1\lambda \simeq B_0 + B_1\lambda + B_2\lambda^2$

② Uncertainty for aerosols leads to uncertainty for air!



Beta=A/lam**4+B0+B1*lam+B2*lam**2
Extinction coefficient [a.u.]
Lambda [microns]
100
90
80
70
60
50
40
30
20
10
0
0.25
0.3
0.35
0.4
0.45
0.5
0.55
0.6
0.65
0.7
0.75

Where does the error come from?

1. C^{-1} is an "amplifier" and a "mixer"

$C^{-1}\vec{b}$

C is a square symmetric matrix $\Rightarrow C \equiv U \Lambda U^T$

$$C^{-1} = U \Lambda^{-1} U^T$$

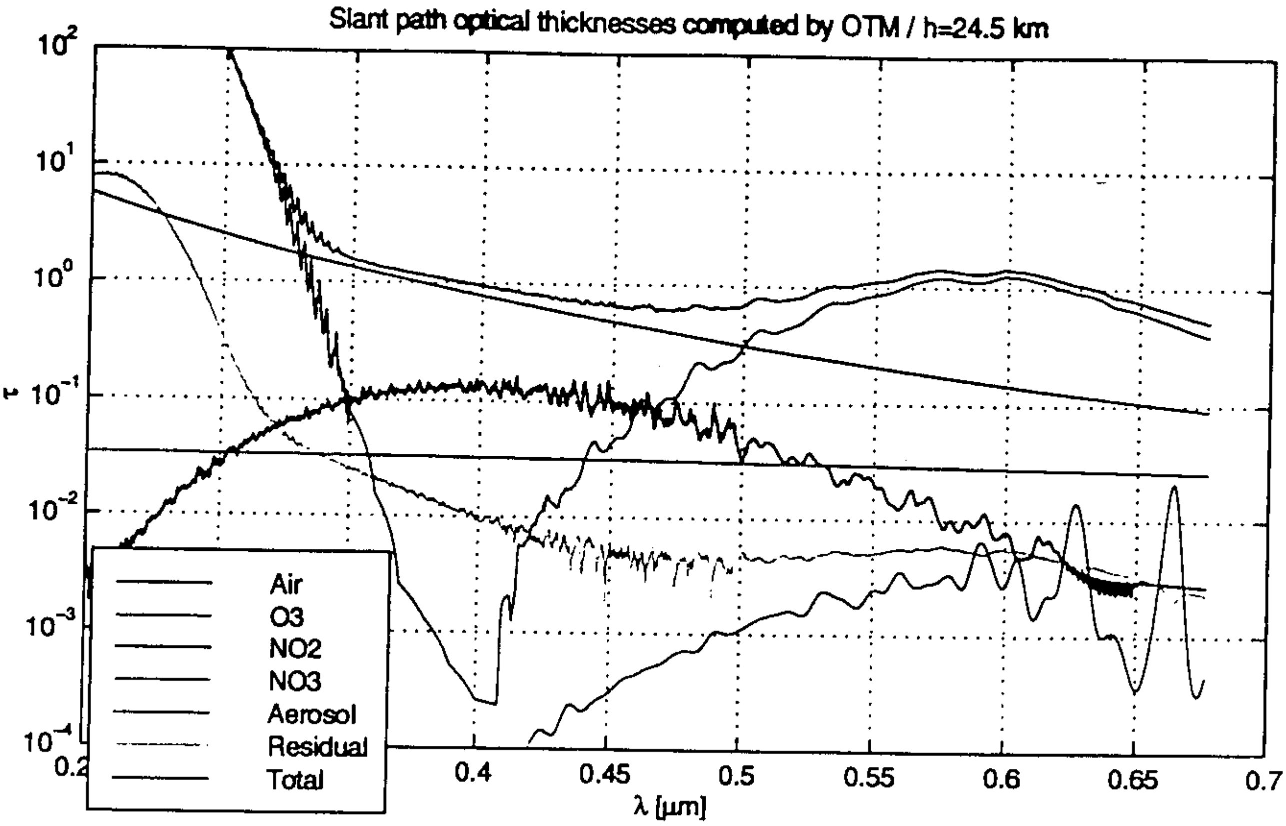
- → smallest eigenvalues are <u>dominant</u>
  - (ill-conditioning by redundancy)
  - rejection of small constituents
- → the more species, the smaller eigenvalues

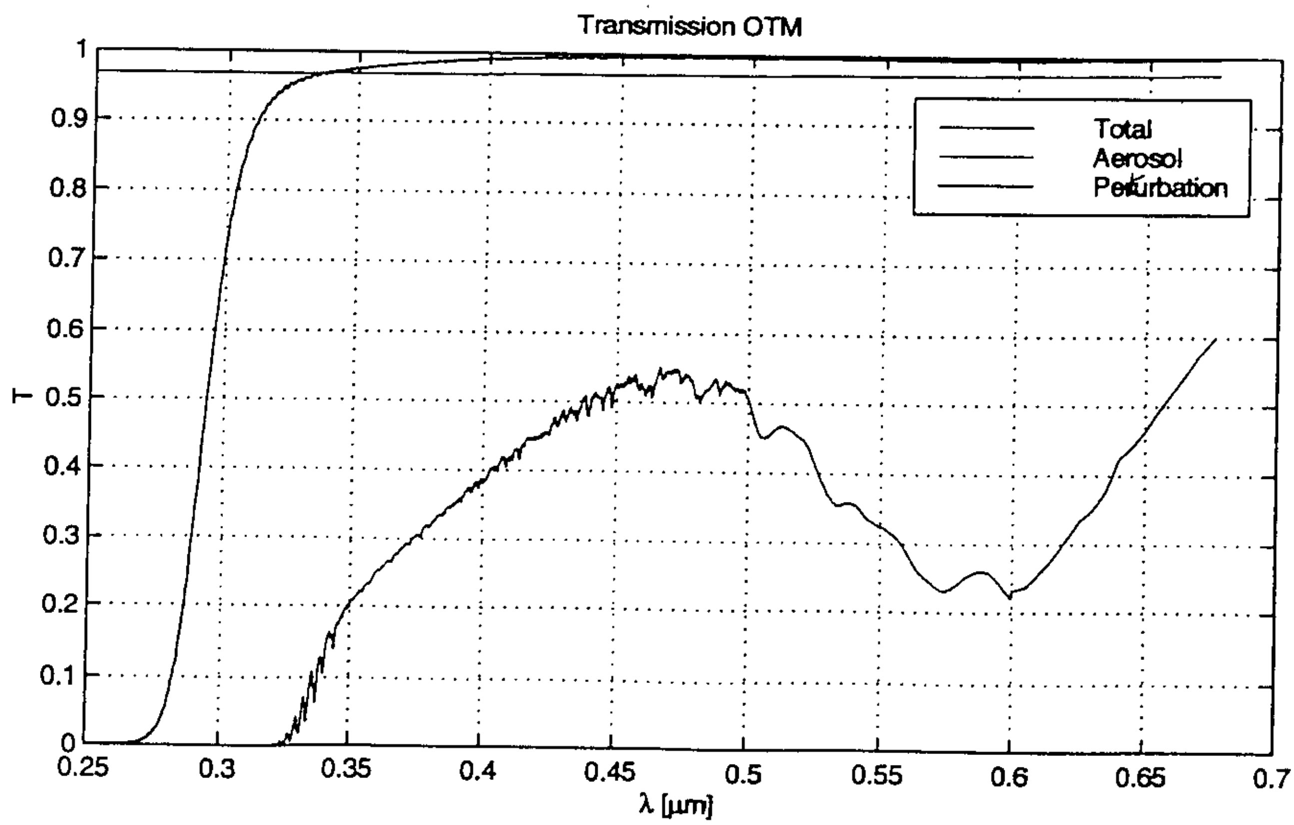
$f_{m4} = \frac{1}{\lambda^4} \quad f_{m1} = \frac{3.1}{\lambda} \quad f_0 = 16.1 \quad f_1 = 32 \cdot \lambda \quad f_2 = 64 \cdot \lambda^2$

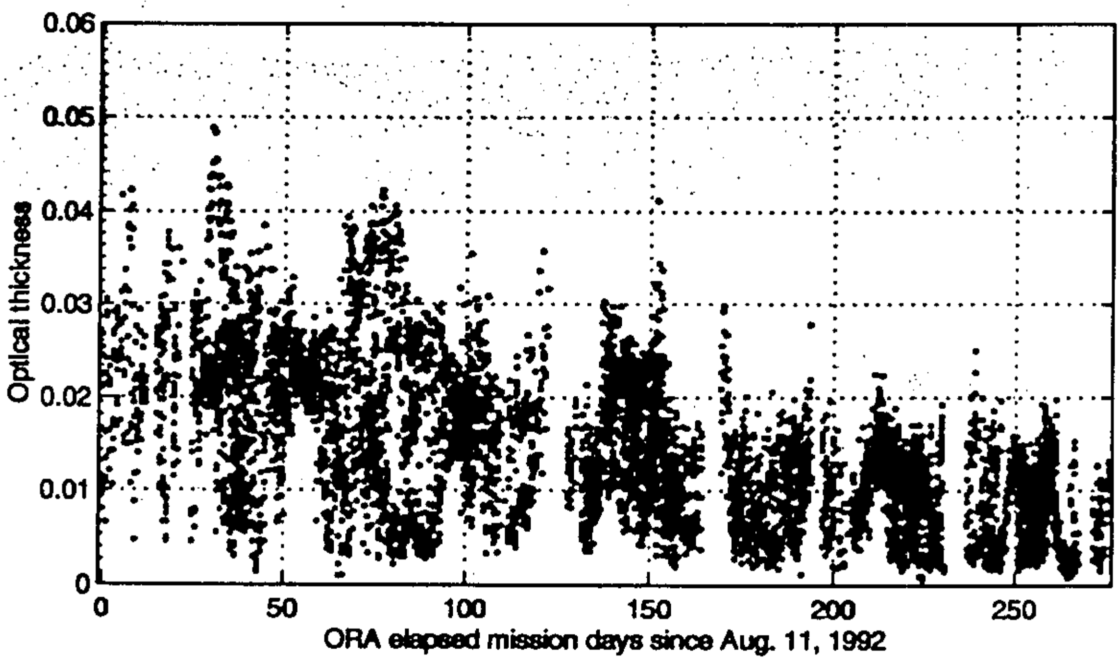
BASIS and eigenvalues		Twomey criterion $r \simeq (\lambda_{min} / \lambda_{max})^{\frac{1}{2}}$
$\{f_{m4}, f_{m1}\}$	2385 52.5	14 %
$\{f_{m4}, f_0\}$	2449 66.1	16 %
$\{f_{m4}, f_0, f_1\}$	2409 147.9 1.03	2 %
$\{f_{m4}, f_0, f_1, f_2\}$	2425 257 4.21 0.012	0.2 %

- → if C has important off-diagonal terms, C^{-1} will have too!

HOWEVER, C^{-1} IS SYMMETRIC AND <u>NOT</u> RESPONSIBLE FOR ANY BIAS

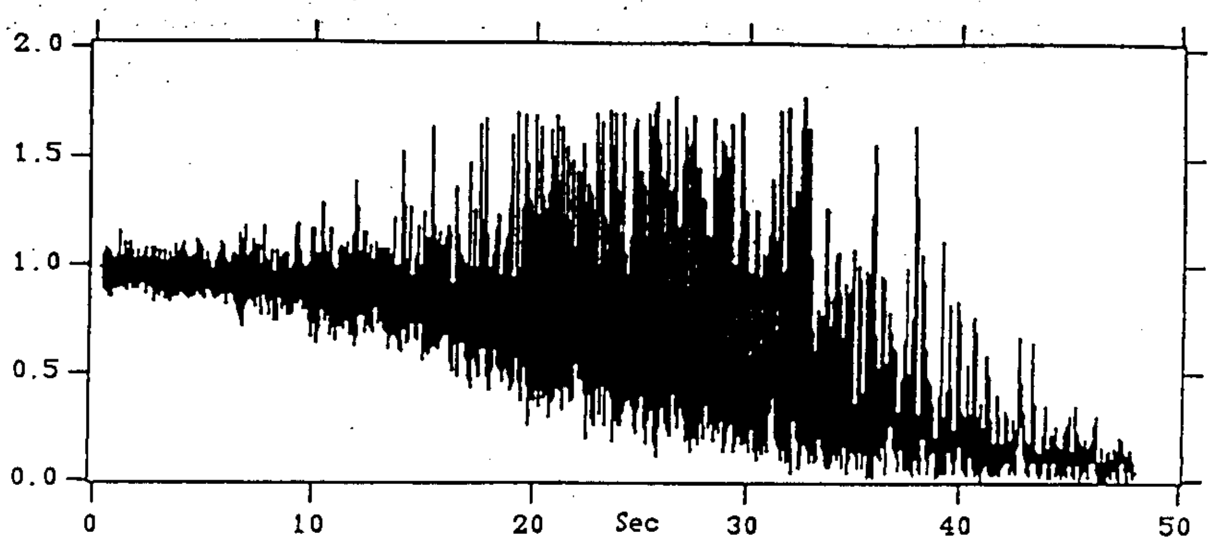

Slant path optical thicknesses computed by OTM / h=24.5 km
τ
λ [μm]
Air
O3
NO2
NO3
Aerosol
Residual
Total


Transmission OTM
T
λ [μm]
Total
Aerosol
Perturbation

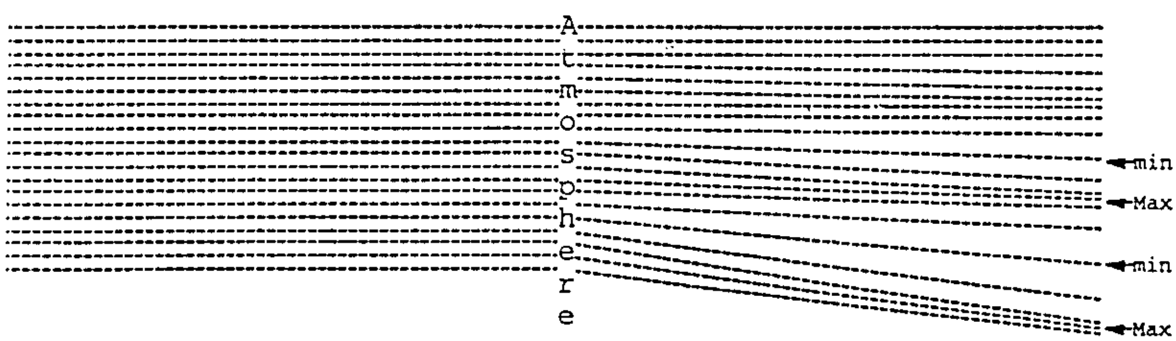


Total optical thickness @ 1.02 μm

- SAGE II
- ORA



During this measurement, altitude of the tangent point varied (non linearly) between 43.8 and 16.7 km. This measurement contains noise (mainly from photon statistics) as well as the effect of absorption and aerosols and Rayleigh diffusion, however, the optical filter was chosen in order to limit these non refractive effects. (spherical symmetry). Within this simplified geometry the refractive phenomena arise from the vertical structure as sketched below.



As the rays go deeper within the atmosphere, the mean refraction angle increases as well as the distance between "consecutive" rays at the satellite position. This general increase produces the refractive dilution.

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Tomography of the Earth's atmosphere by the spaceborne occultation radiometer ORA: Spatial inversion algorithm

Didier Fussen, Etienne Arijs, Fabienne Leclere, Dennis Nevejans and Christine Bingen
Belgian Institute for Space Aeronomy, Brussels, Belgium

APPLIED OPTICS
37, p 3121–3127, 20 May 1998

Validation of the ORA spatial inversion algorithm with respect to the Stratospheric Aerosol and Gas Experiment II data

Didier Fussen, Etienne Arijs, Dennis Nevejans, Filip Van Hellemont, Colette Brogniez, and Jacqueline Lenoble

JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 103, NO. D7, PAGES 8455–8464, APRIL 20, 1998

A critical analysis of the Stratospheric Aerosol and Gas Experiment II spectral inversion algorithm

Didier Fussen
Belgian Institute for Space Aeronomy, Brussels, Belgium