4. Retrieval – Principle and Method

4.1 SMILES observation species

4.2 Forward model development

4.3 Retrieval algorithm

4.4 Error analysis

4.5 SMILES observation capability

SMILES observations

Standard Products

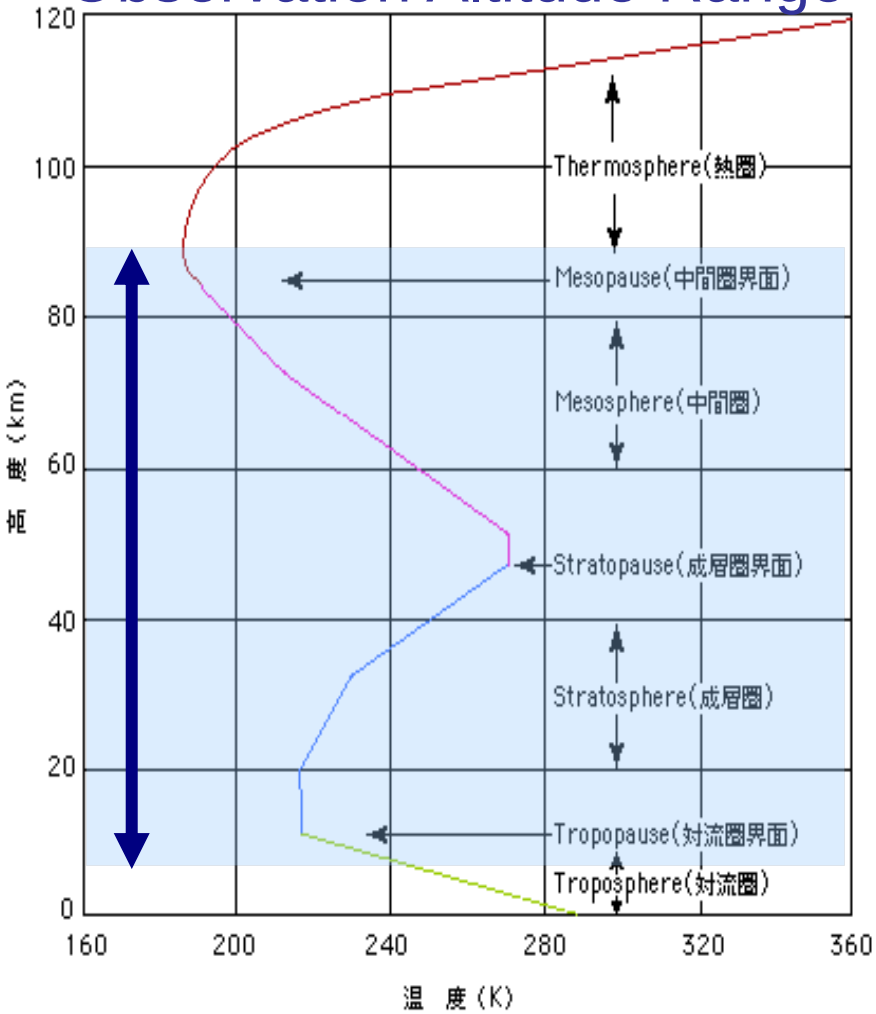
- O_3, HCl, ClO
- HO_2, HOCl
- O_3 isotopes, BrO
- HNO_3, CH_3CN

Research Products

- UT/LS region (O_3, HCl, CH_3CN)
- Upper stratosphere and lower mesosphere (O_3, HCl, HO_2)
- UTH, Cirrus Cloud
- H_2O_2
- Isotope species of HCl, and CH_3CN
- Mass-Independent Fractionation of Ozone isotopes

SMILES observation altitude range

Observation Altitude Range



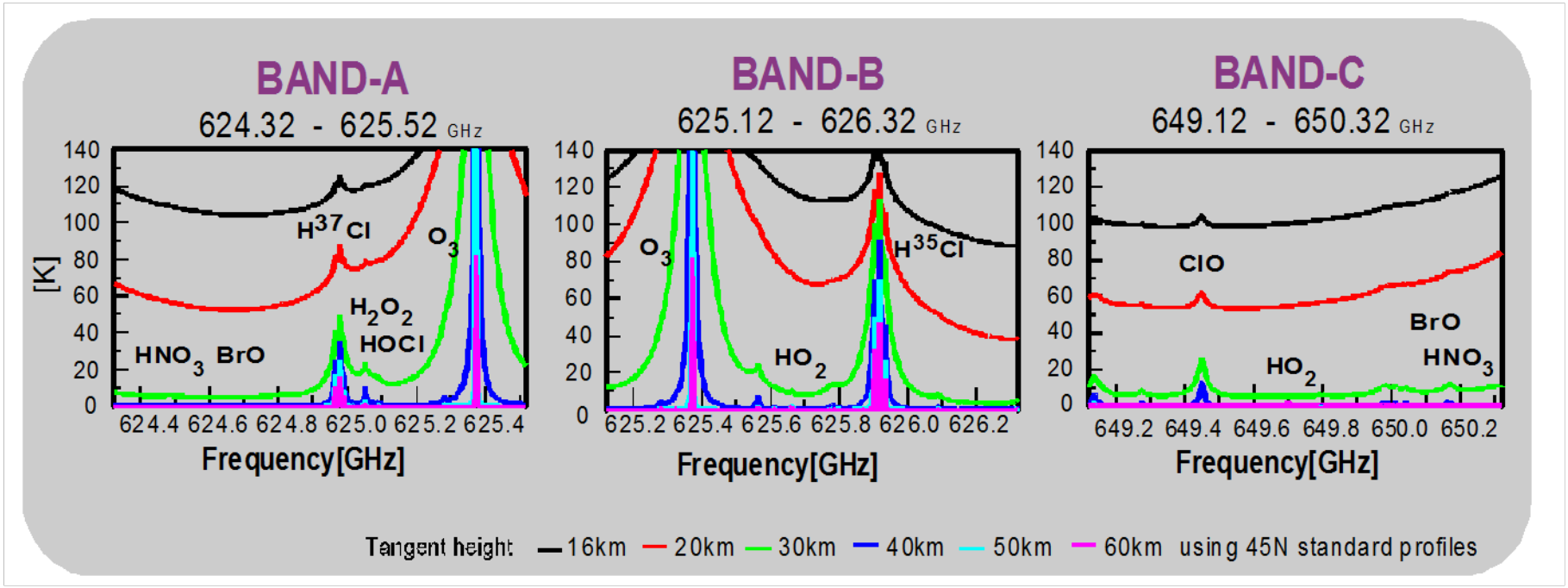
理科年表CD－ROM2004(丸善)より

Observation Species

Observation altitude range	Species
Mesosphere (medium/low SNR)	O_3, $H^{37}Cl$, $H^{35}Cl$, wind, OOO^{18} HO_2, OOO^{17}, ClO H_2O_2
Stratosphere (high SNR)	O_3, $H^{37}Cl$, $H^{35}Cl$, H_2O, ClO Temp, Pointing offset
Stratosphere (medium/low SNR)	wind, HOCl, N_2O, CH_3CN, OOO^{18}, OOO^{17} HNO_3, HO_2, BrO, H_2O_2, SO_2
UT/LS	H_2O, Ice water content, O_3

Observation frequency and spectrum

SMILES has 3 observation frequency bands.
Simulated Observation Spectrum are shown with each molecule and at each tangent height.



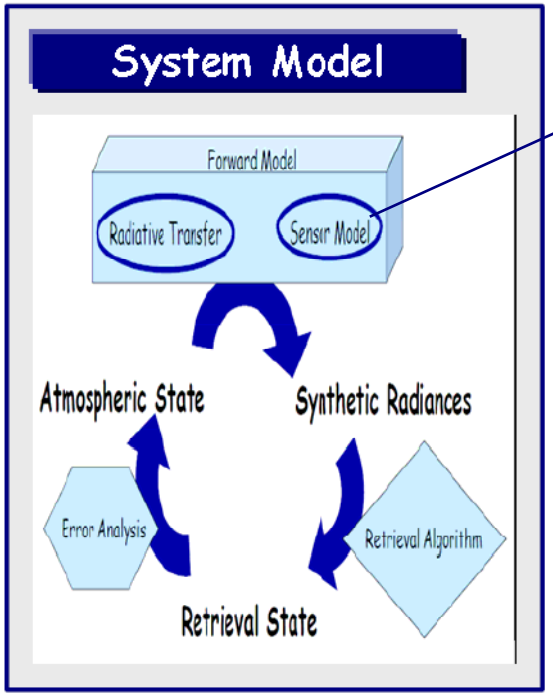
- 2 spectrometer of 1200 MHz bandwidth
- 1.8MHz resolution

Products by JEM/SMILES experiment

Processing modes	Band A	Band B	Band C
Stratospheric high SNR 10-60 km	O_3, $H^{37}Cl$, H_2O, Temp, Pointing offset	O_3, $H^{35}Cl$, H_2O, Temp, Pointing offset	H_2O, ClO
Stratospheric medium/low SNR 10-60 km	wind, HOCl, CH_3CN, OOO^{18}, HNO_3, BrO, H_2O_2, SO_2	wind, N_2O, OOO^{18}, HO_2, HNO_3, SO_2	O_3, OOO^{18}, OOO^{17}, HO_2, HNO_3, BrO
Mesospheric medium/low SNR 50-90 km	O_3, $H^{37}Cl$, wind, OOO^{18}, H_2O_2	O_3, $H^{37}Cl$, wind, OOO^{18}, HO_2, SO_2	HO_2, , OOO^{18}, OOO^{17}, ClO
UT/LS	H_2O, Ice water content, O_3		
Extremely Low SNR	H_2CO, HOBr, $ClONO_2$, OClO, ClOOCl, H_2SO4	CH_3Cl, H_2CO, HOBr, $ClONO_2$, OClO, ClOOCl	COF_2, $ClONO_2$, NO_2, OClO, ClOOCl

blue: single scan, red: daily average, green: monthly average, black: very challenging

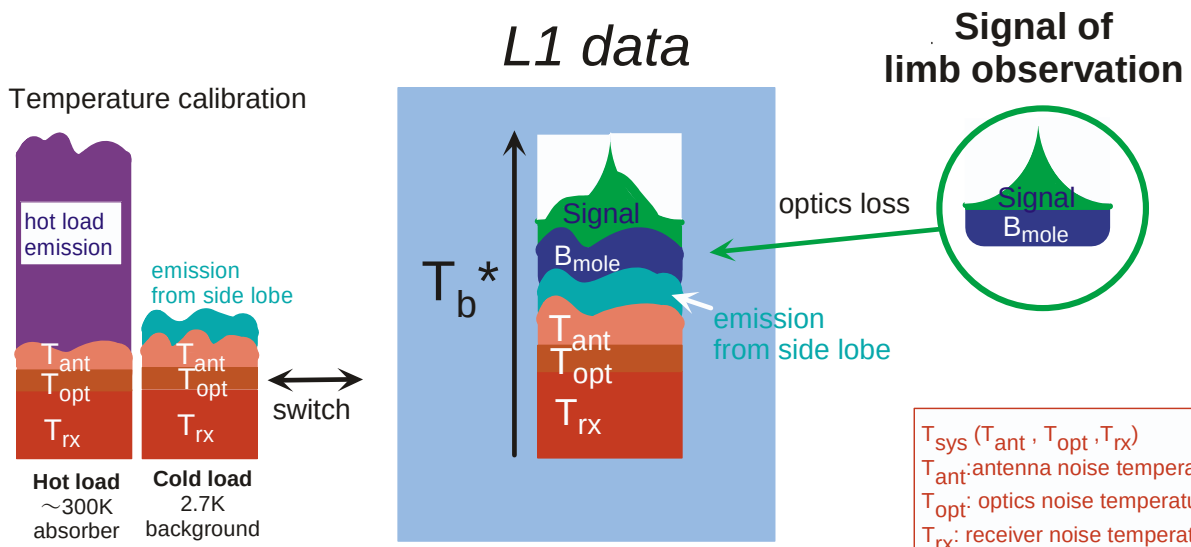
System model



Forward model
1) radiative transfer model
2) Sensor model

$$L1\ Data = S + B_{mole} + T_{sys}$$

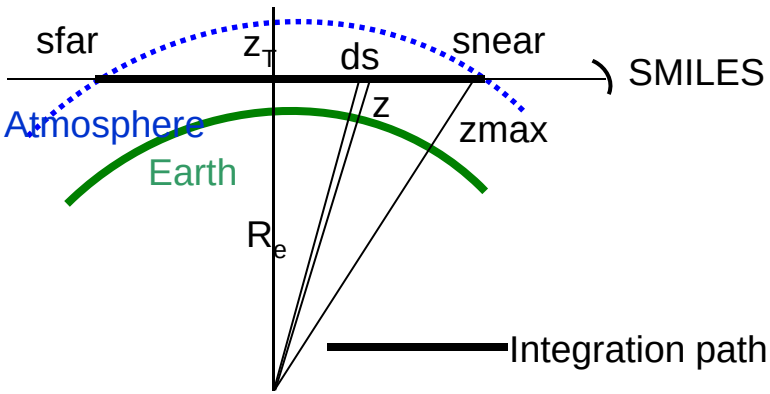
S: Signal from purpose molecule in the atmosphere
B_{mole}: Background Base line from molecules (O_3, H_2O, N_2, O_2, etc.)
T_{sys}: System noise(T_{ant}, T_{opt}, T_{rx}) + Side lobe



T_{sys} (T_{ant} , T_{opt} ,T_{rx})
T_{ant}:antenna noise temperature
T_{opt}: optics noise temperature
T_{rx}: receiver noise temperature

Radiative transfer process in the atmosphere

Limb sounding geometry (without refraction)



Radiative trans. eq. for the pencil beam

$$T_{\delta\upsilon}(s_{near}) = T_{\delta\nu}(s_{far})\exp\left\{-\int_{sfar}^{snear} k_\upsilon(s)ds\right\} + \int_{sfar}^{snear} k_\upsilon(s)T_e(s)\exp\left\{-\int_{s}^{snear} k_\upsilon(s)ds\right\}ds$$

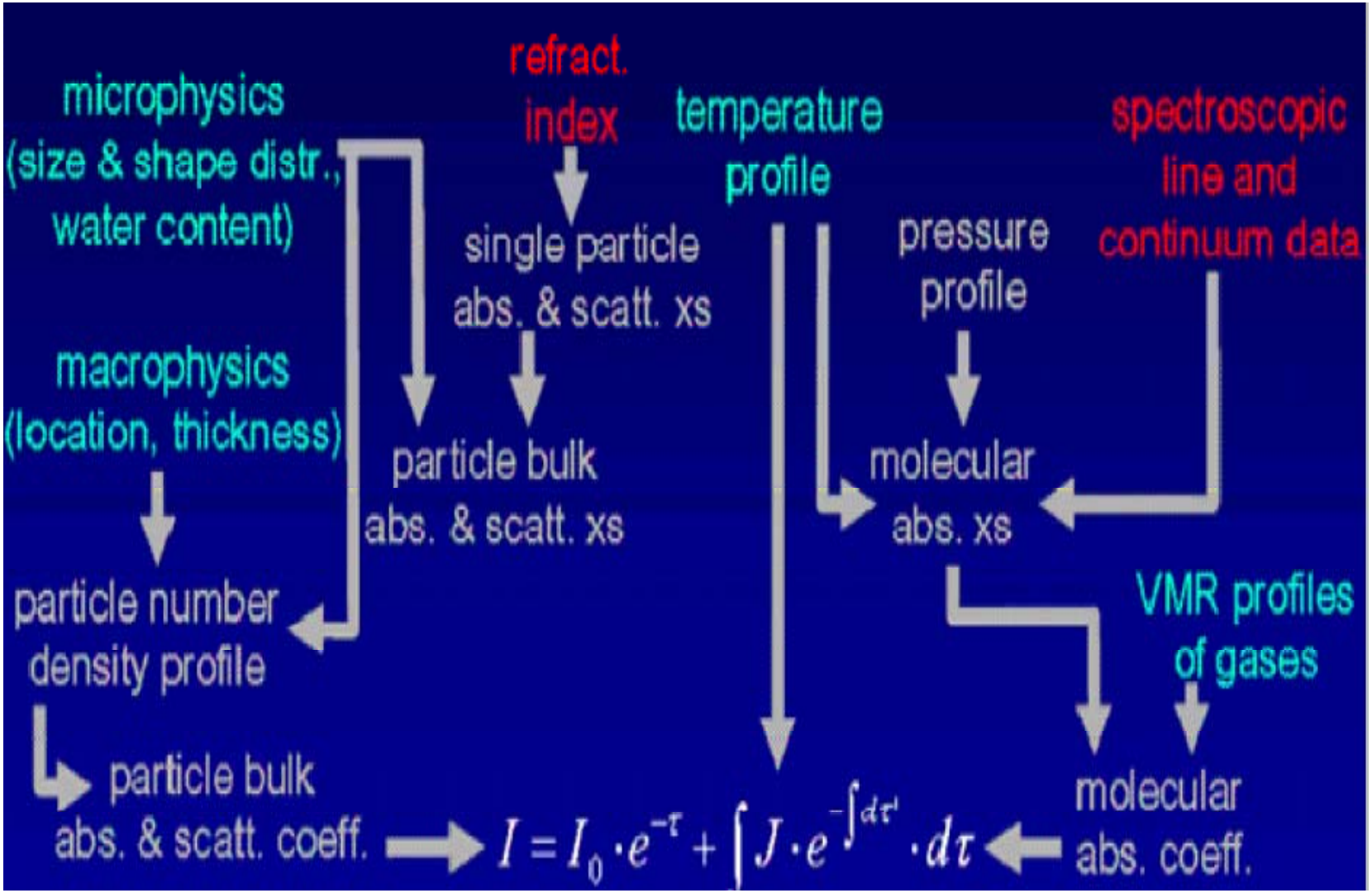
where, v is the frequency, T_e in the brightness temperature of the atmosphere
k is the line absorption for the molecular labeled by i is given by

$$k_\nu(s_i) = \sum_a \frac{x_a(s_i)P(s_i)}{kT(s_i)}\alpha_\nu^a(s_i) + k_{air}(s_i)$$

Items included

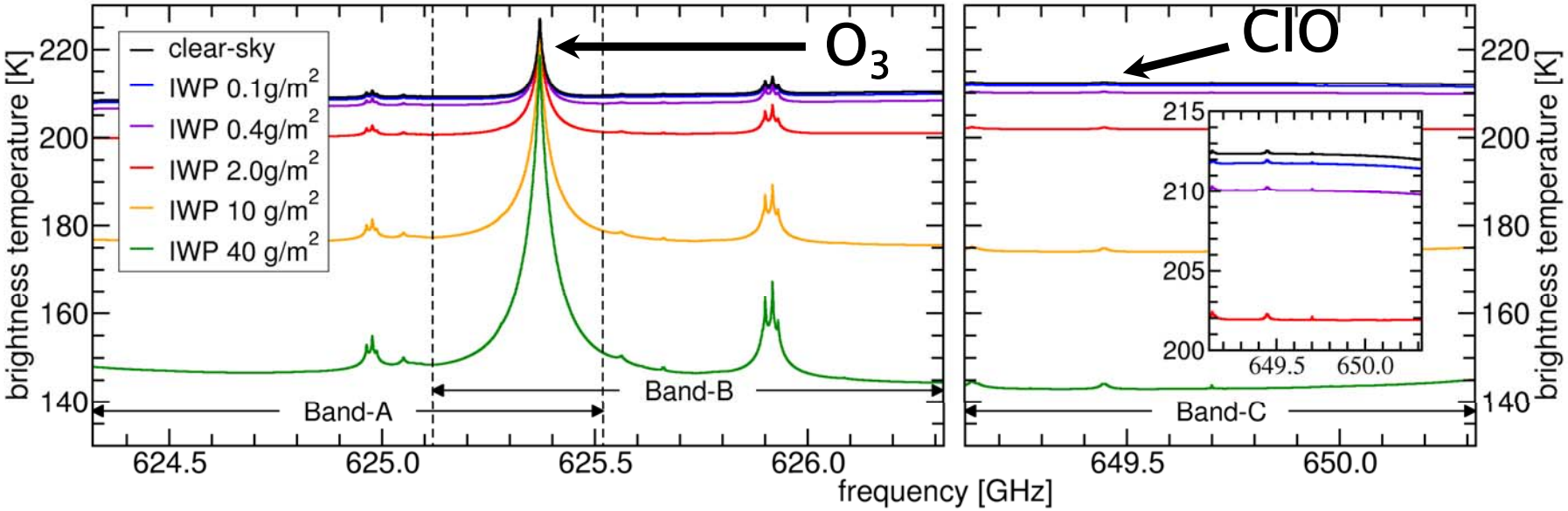
- Atmospheric Refraction is included
- Line shape function is used the Voight functions for the each pressure.
- Continuum Liebe MPM89 for operational code, SMILES continuum for research code
- 2 dimension integrals are possible for the atmospheric models in research code
- Scattering calculation included in research code

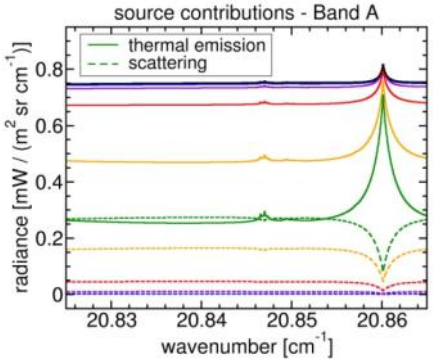
Radiative transfer calculation including cloud cases for research products



An example: Ice cloud effects in the UT/LS

An example of spectral cloud effects

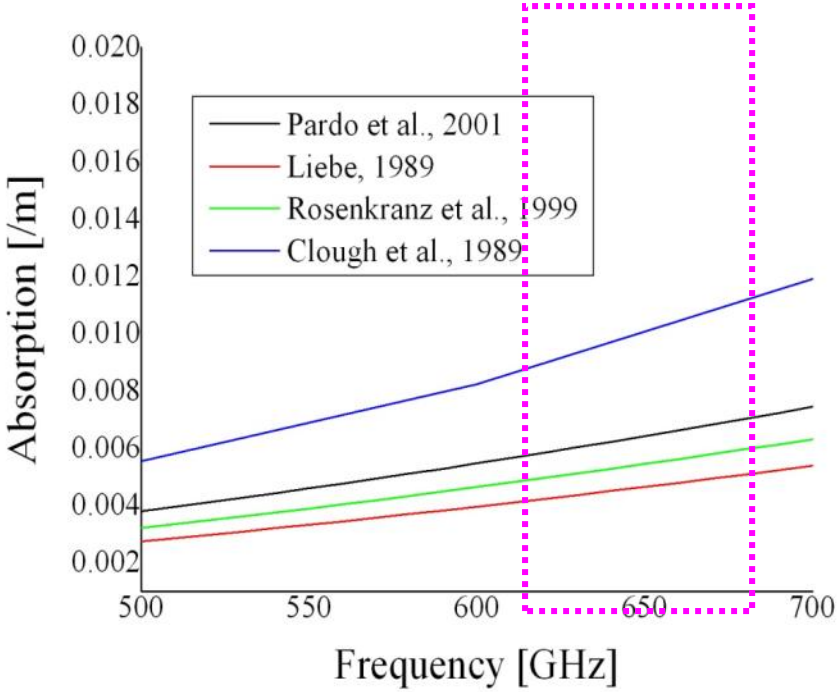




Example: Effects of cirrus in different ice water path on SMILES spectra

(SetUp: tropical standard atmosphere, cirrus 12-13km, effective size 12mm, 4km tangent altitude)

Radiative transfer calculation in the atmosphere

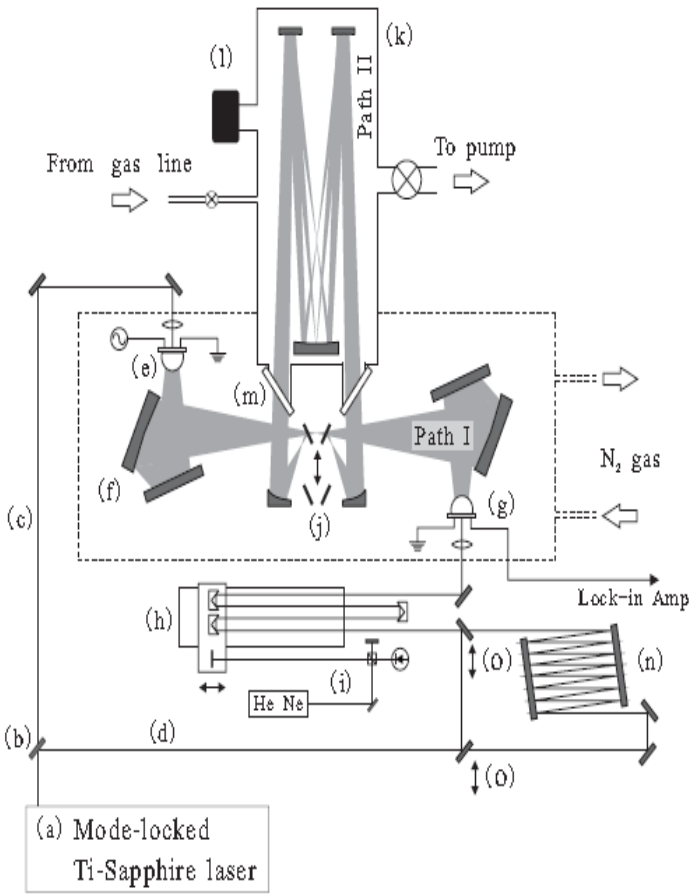


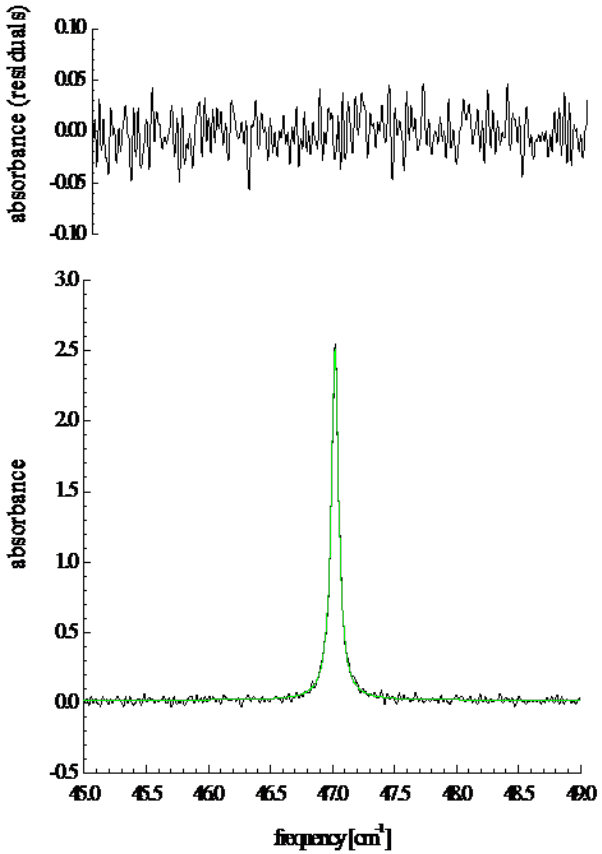
Atmospheric Continuum in SMM region

Difference of absorption of the several models are more than 50%

Continuum model applicable to SMILES

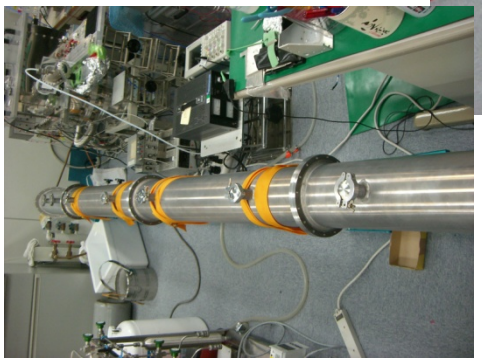
Laboratory Experiment of water vapor
TDS spectrometer + SMILES SIS spectroscopy





Continuum model applicable to SMILES

Laboratory Experiment of water vapor
TDS spectrometer + SMILES SIS spectroscopy

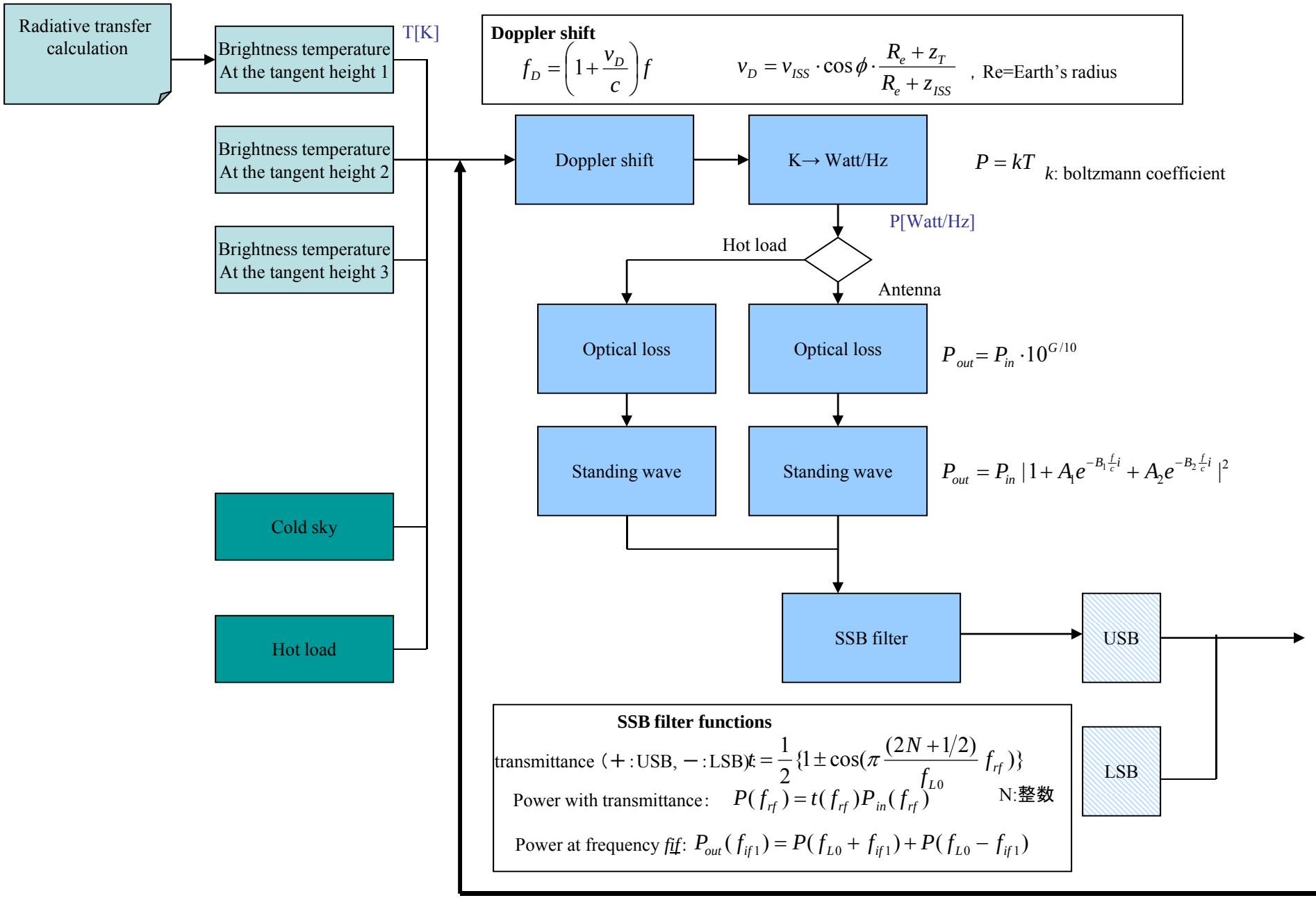


Summary of SMILES molecular spectroscopic data

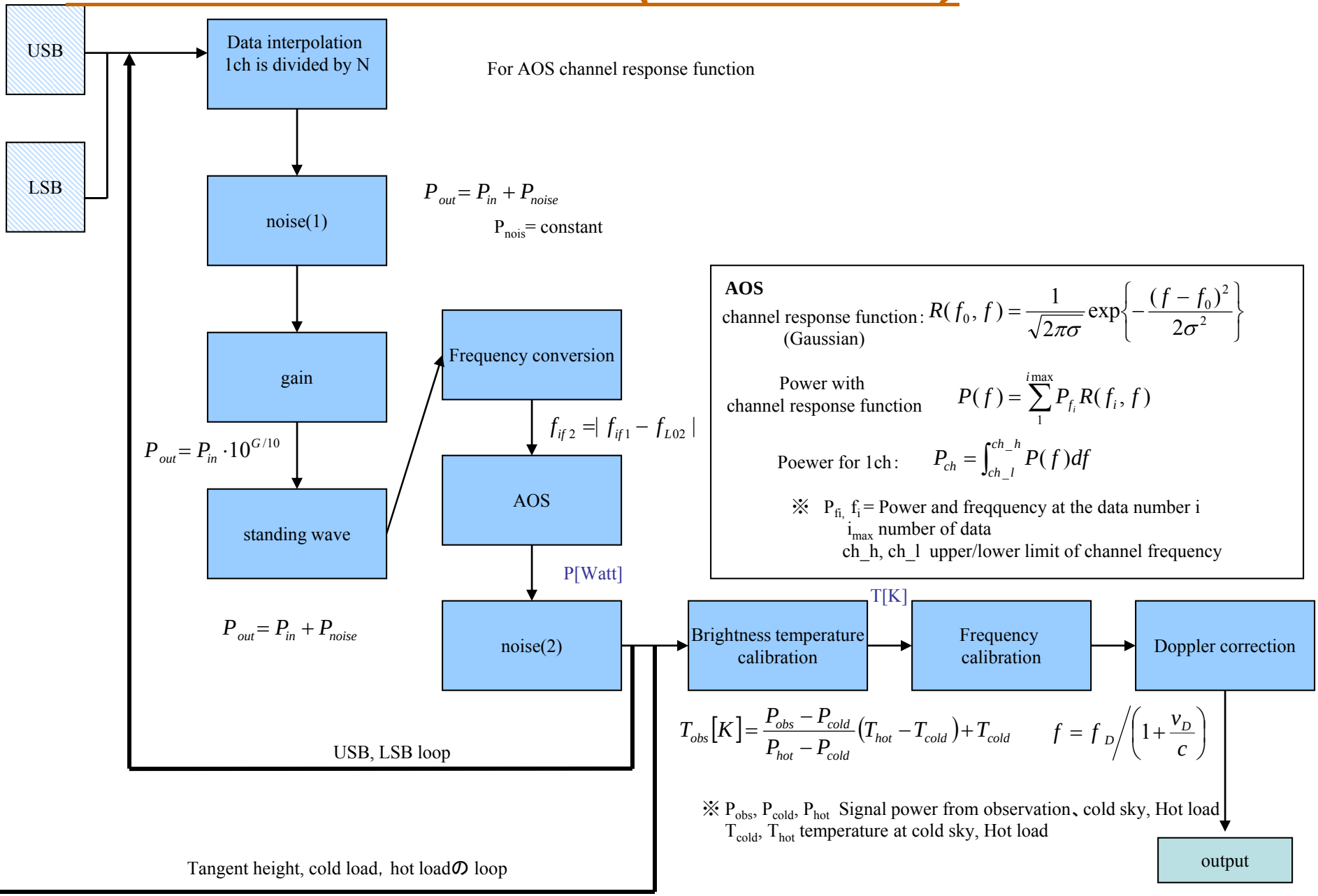
	Freq. (GHz)	γ	n	Current Accuracy	Required Accuracy by the error analysis	Priority
O_3	625.372	2.99	0.75	4%	1%	2 Yamada and Amano
	650. 732	---	---	---	1%	1
$H^{35}Cl$	625.919	3.41	0.73	4%	1%	2
	(Pressure Shift δ0(MHz/Torr)=0.146, s=0.4047, χ=0.3763) 17.8%					2
$H^{37}Cl$	624.978	---	---	---		1
ClO	649.451	2.782	0.86	3%	1%	2
HO_2	625.660	---	---	---	3%	3
	649.702	3.51	0.63	4%	3%	done Yamada and Amano
H_2O_2	625.04	3.78	---	---	3%	3
HOCl	625.076	---	---	---	3%	1
O3isotopes	Many		---	---	0.5%	1 Yamada and Amano（一部）
BrO	624.768	3.05	0.80	3%	5%	done Yamada and Amano
	650.179	3.03	0.80	3%	5%	done Yamada and Amano
HNO_3	624.484	---	---	---	3%	1
	624.776	---	---	---	3%	-
	625.345	---	---	---	3%	-
	650.288	---	---	---	3%	1
CH_3CN	624.819-	---	---	---	3%	1
	624.926	---	---	---	3%	-

Instrumental detail

Forward model development



Instrumental detail (continued)



Retrieval

Optimal Estimation Method

- Linear least-squares method, allowing « a priori » knowledge to be taken into account
- Atmospheric parameters x estimated by minimising χ^2 :

$$\chi^2 = \underbrace{[y-F(x,b)]^T \cdot S_y^{-1} \cdot [y-F(x,b)]}_{\text{measurement space}} + \underbrace{(x-x_0)^T \cdot S_{x_0}^{-1} \cdot (x-x_0)}_{\text{parameter space}}$$

y : spectral measurements
F(x,b) : forward model
b : model parameters (spectroscopy, instrument)
x_0 : « a priori » parameter vector

- Weights: Measurement and « a priori » covariance matrices S_y and S_{x_0}
- Diagnostics: Error covariance and averaging kernel matrices

Non-linear retrieval

Non-linear retrieval

iterative Levenberg-Marquardt regularisation

OEM with Levenberg-Marquardt iteration scheme:

$$x_{i+11} = x_0 + \underbrace{(K_i^T S_y^{-1} K_i + S_{x_0}^{-1} + \gamma U)^{-1} \cdot \{K_i^T S_y^{-1} \cdot}_{D_i\ :\ \text{contribution function matrix}} ([y - F(x_i, b)] + K_i [x_i - x_0]) + \gamma U [x_i - x_0]\}$$

y :	spectral measurements
$F(x,b)$:	forward model
b :	model parameters (spectroscopy, instrument)
x_i , x_0 :	parameter and « a priori » parameter vector
S_{x_0}, $S_{y,}$:	« a priori » and measurement covariance matrix
$K = (\partial F / \partial x)$:	weighting function matrix
γ :	Marquardt parameter. Convergence: $\gamma \rightarrow 0$!
U :	scaling matrix
S_b, $K_b = (\partial F / \partial b)$:	model parameter error covariance and weighting function matrices

Algorithm development for operational code

- Algorithms have been studied by NICT, Bremen university, and JAXA.

- In 2006, JAXA started the development of Operational Retrieval Code (ORC), and related algorithm studies

- Retrieval procedure based on:
  => Optimal Estimation Method
  look for a solution in the vicinity of an *a priori* value of the retrieved parameters
  => Levenberg-Marquardt iterative scheme for non linear inversion of strong lines

- Retrieved parameters:
  => Vertical distribution of the species VMR
  => Temperature distribution
  => Scan altitude offset + baseline parameters

Error estimations

Retrieval Errors : S

$$S_{total} = S_{statistic} + S_{null} + S_{model}$$

A	$= D\,K$	: averaging kernel matrix
$S_{statistic}$	$= D\,S_y\,D^T$	: statistical error
S_{null}	$= (A - U)\;S_{x_0} + (A - U)^T$	: smoothing error
S_{model}	$= (D\,K_b)\,S_b\,(D\,K_b)^T$	: model parameter error

Model parameter errors

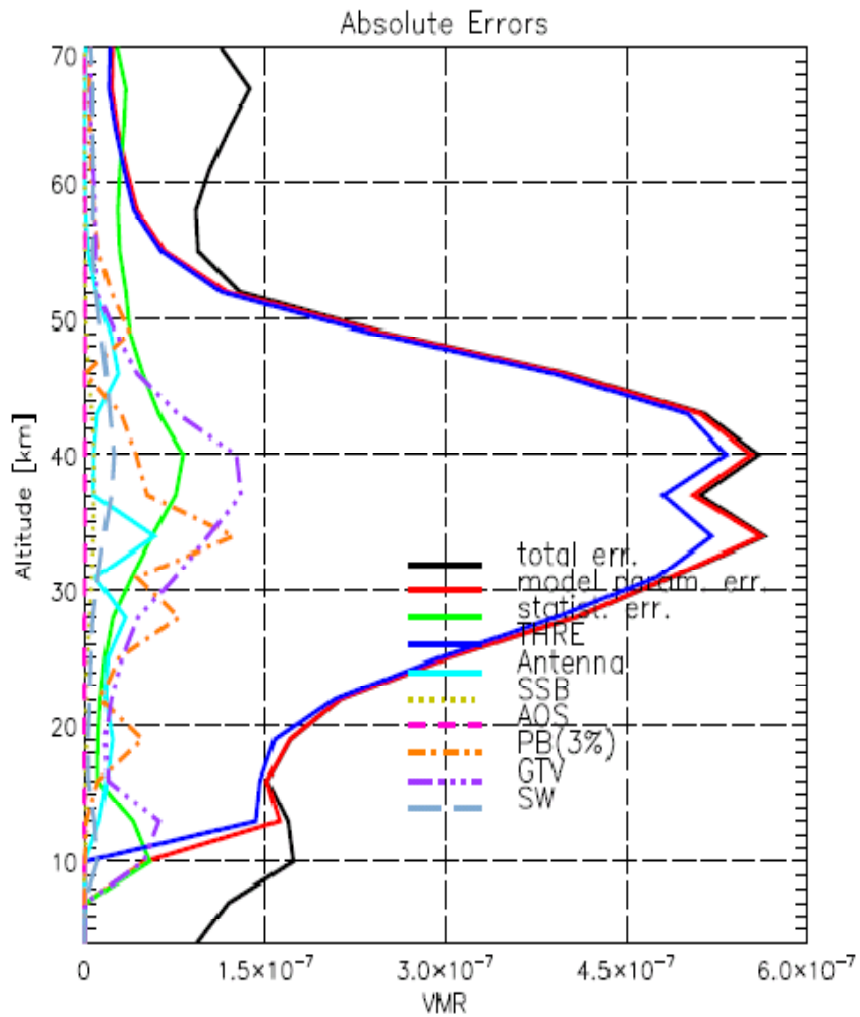
Factors in model parameter errors

1. Calibration knowledge
2. Side Band knowledge
3. Antenna Pattern knowledge
4. Pointing knowledge
5. Spectroscopic parameter knowledge
6. AOS response function knowledge

Precision and accuracy

An example for O_3

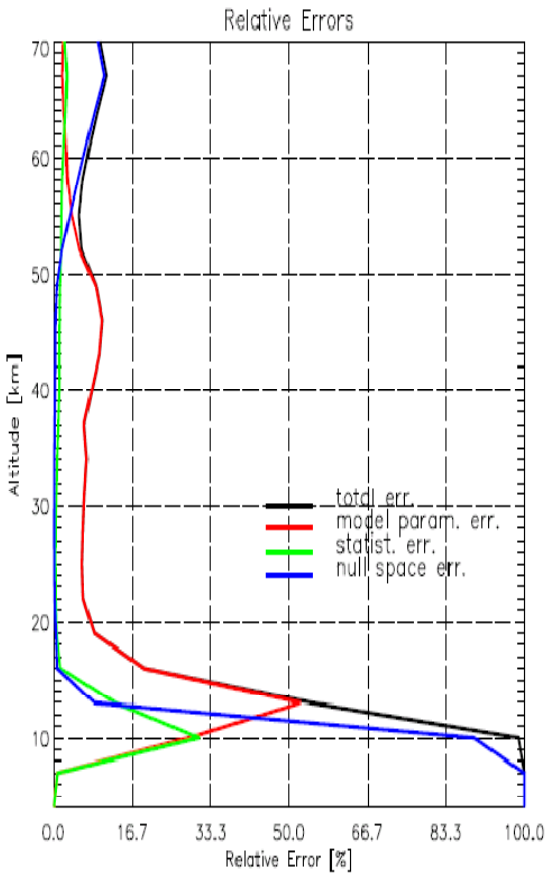
1. Calibration knowledge
   (SW: Standing wave,
   GTV: time variation of the gain)
2. Side Band knowledge
   (SSB: SSB filter ratio)
3. Antenna Pattern knowledge
   (Antenna: Antenna pattern)
4. Pointing knowledge
   (THRE: Tangent height random error)
5. Spectroscopic parameter knowledge
   (PB: Pressure broadening error)
6. AOS response function knowledge
   (AOS: error from spectrometer)



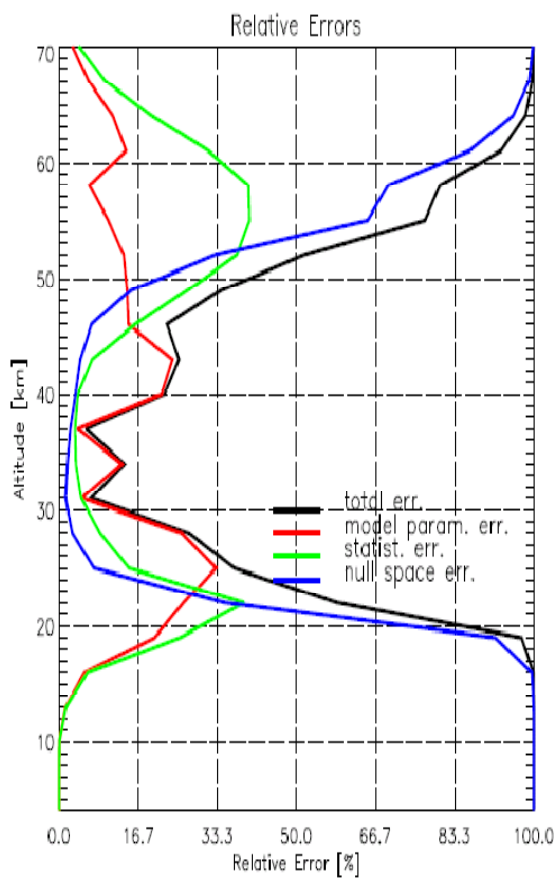
Examples for error estimations

$$S_{total} = S_{statistic} + S_{null} + S_{model}$$

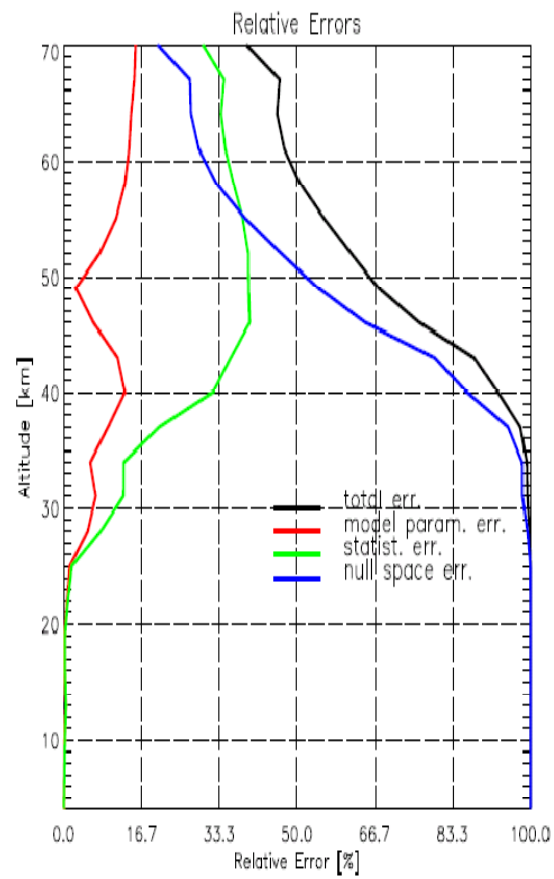
O_3



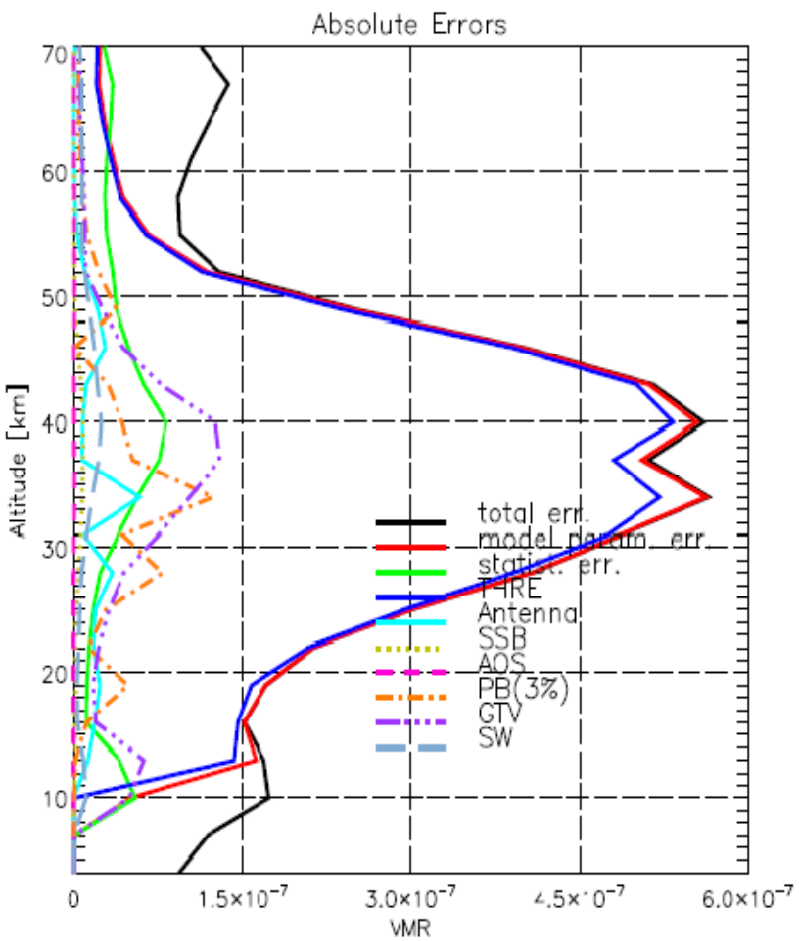
ClO



HO_2



Tangent point retrieval and its error

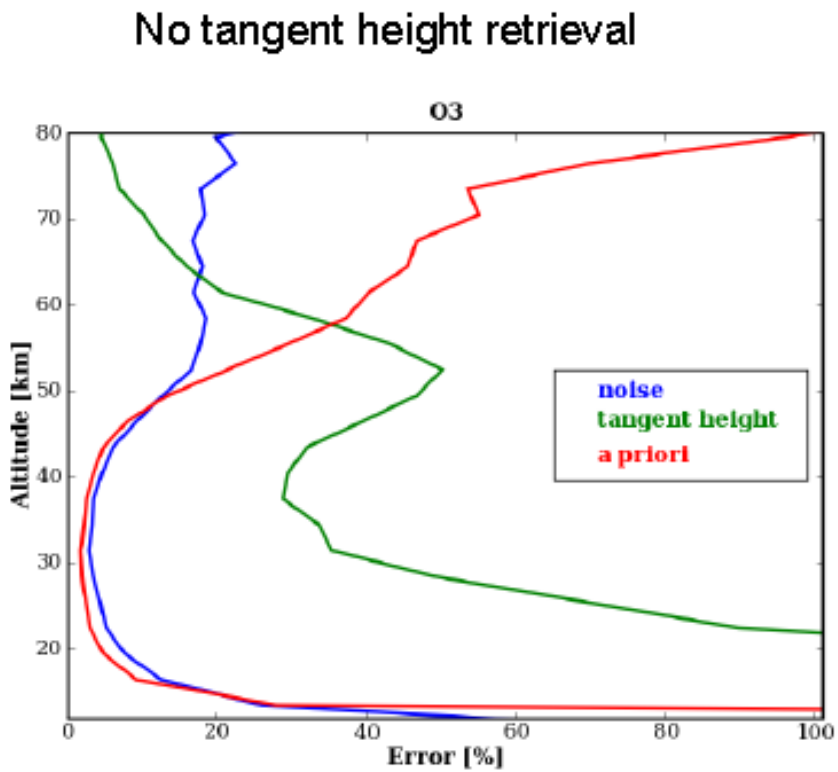


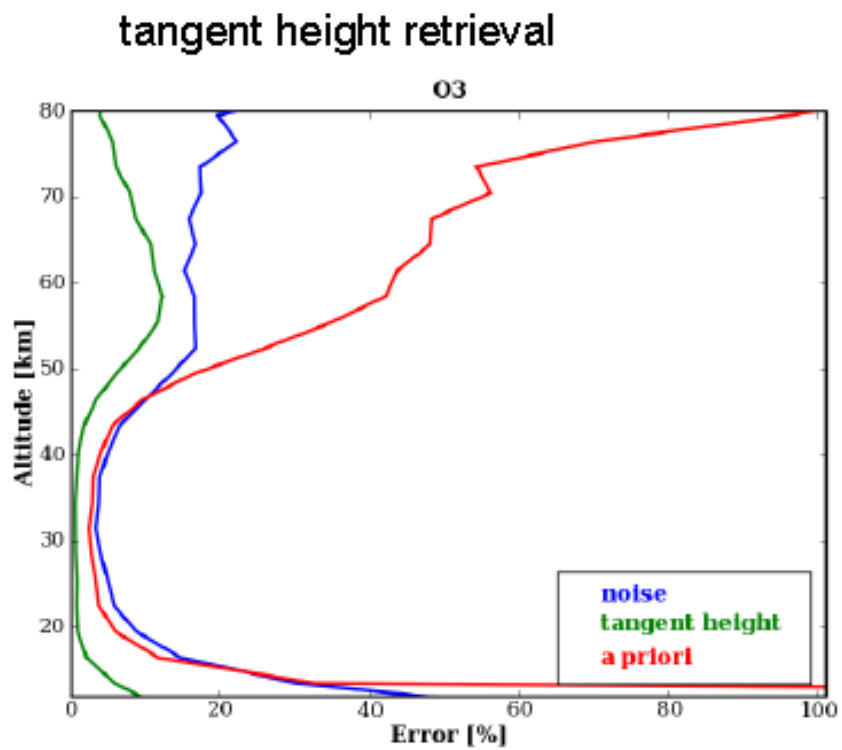
"Altitude scan off-set" can be retrieved.
→ improved to operational processing in JAXA.

"Pointing random error" is a major source of the error in O_3, HCl, and ClO retrieval.

What can we do for that?

Tangent height retrieval





- Work still in progress but first results are promising.
- Tangent height retrieval improved the retrieval error of Ozone, HCl, significantly

Ozone (mid-latitude scenario)

Observable Altitude region: 11 - 91km (tropopause 12km)
Altitude resolution: 2.1km-6.2 km

Band A

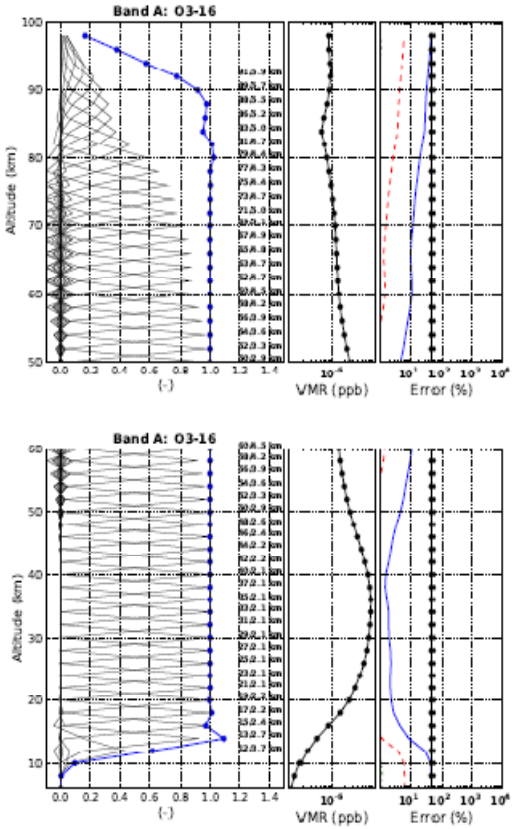


Figure 17: SMILES band A measurement capability for O3 – 16 in (top) mesospheric and (bottom) stratospheric retrieval mode assuming US Standard atmospheric conditions. (left) Averaging kernels (black) and response function (blue). Altitude and corresponding vertical resolution are given as text. (middle) A priori (= true) profile. (right) A priori error (black) and a posteriori errors for a single scan (blue), daily average (red dashed), i.e. 64 scans, and monthly average (green dash-dotted), i.e. 64*30scans. A posteriori error comprises measurement and null space error. Dots on the lines commonly denote respective tangent altitudes.

Band B

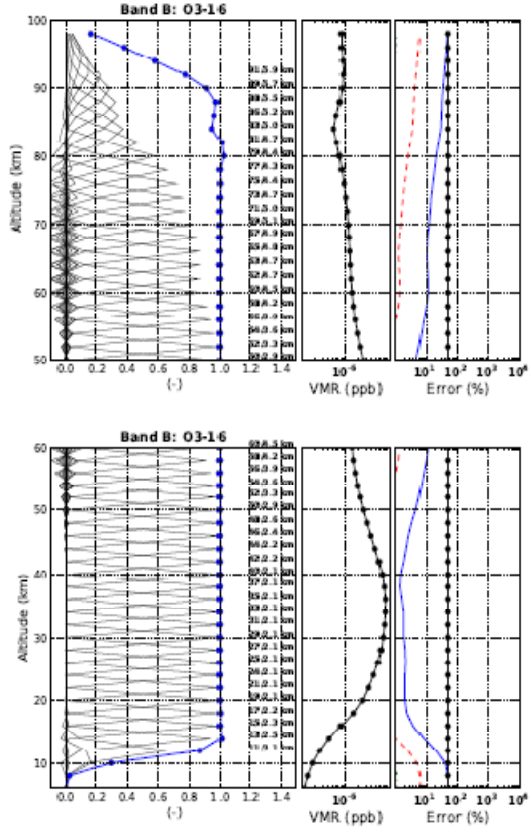
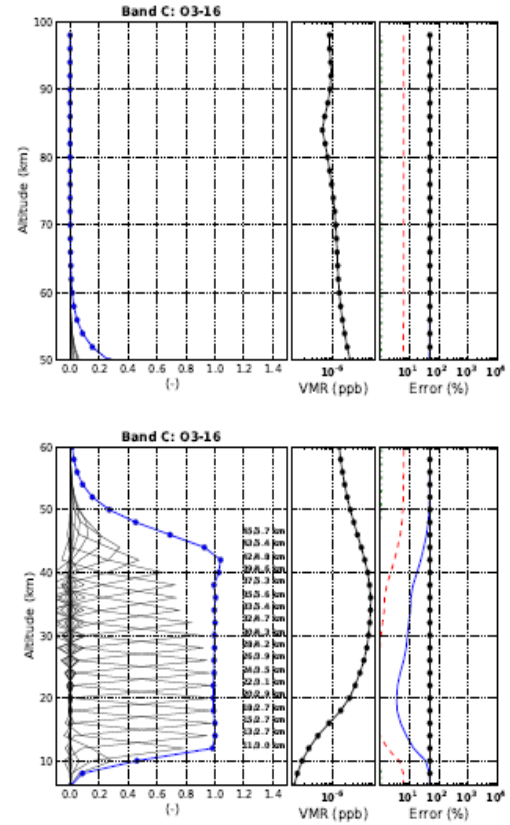


Figure 33: SMILES band B measurement capability for O3 – 16 in (top) mesospheric and (bottom) stratospheric retrieval mode assuming US Standard atmospheric conditions. (left) Averaging kernels (black) and response function (blue). Altitude and corresponding vertical resolution are given as text. (middle) A priori (= true) profile. (right) A priori error (black) and a posteriori errors for a single scan (blue), daily average (red dashed), i.e. 64 scans, and monthly average (green dash-dotted), i.e. 64*30scans. A posteriori error comprises measurement and null space error. Dots on the lines commonly denote respective tangent altitudes.

Band C



ire 50: SMILES band C measurement capability for O3 – 16 in (top) mesospheric and (bottom) tospheric retrieval mode assuming US Standard atmospheric conditions. (left) Averaging kernels ck) and response function (blue). Altitude and corresponding vertical resolution are given as . (middle) A priori (= true) profile. (right) A priori error (black) and a posteriori errors for a le scan (blue), daily average (red dashed), i.e. 64 scans, and monthly average (green dash-dotted), 64*30scans. A posteriori error comprises measurement and null space error. Dots on the lines monly denote respective tangent altitudes.

BandC ClO (mid-latitude scenario)

Observable Altitude region:

24-63km

Altitude resolution:

3.5-8.1km

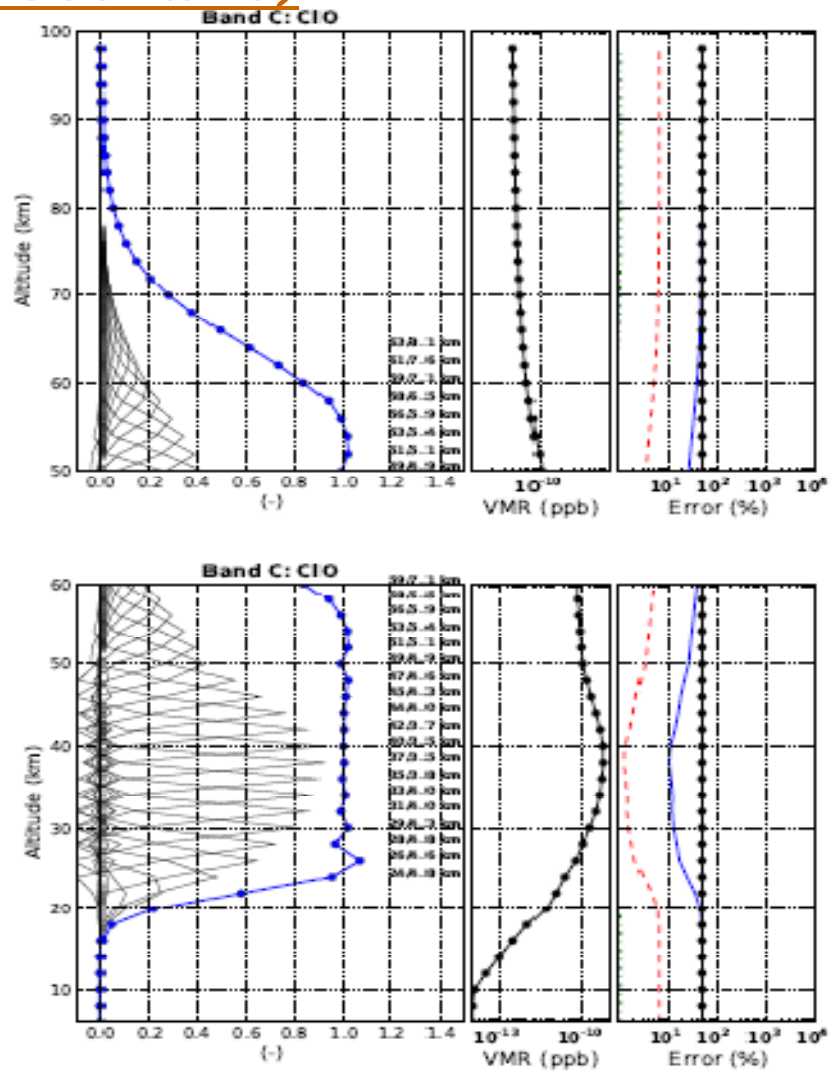


Figure 41: SMILES band C measurement capability for ClO in (top) mesospheric and (bottom) stratospheric retrieval mode assuming US Standard atmospheric conditions. (left) Averaging kernels (black) and response function (blue). Altitude and corresponding vertical resolution are given as text. (middle) A priori (= true) profile. (right) A priori error (black) and a posteriori errors for a single scan (blue), daily average (red dashed), i.e. 64 scans, and monthly average (green dash-dotted), i.e. 64*30scans. A posteriori error comprises measurement and null space error. Dots on the lines commonly denote respective tangent altitudes.

H2O (mid-latitude scenario)

Observable Altitude region: 8 - 37km (tropopause 12km)
Altitude resolution: 2.4km-5.8 km

Band A

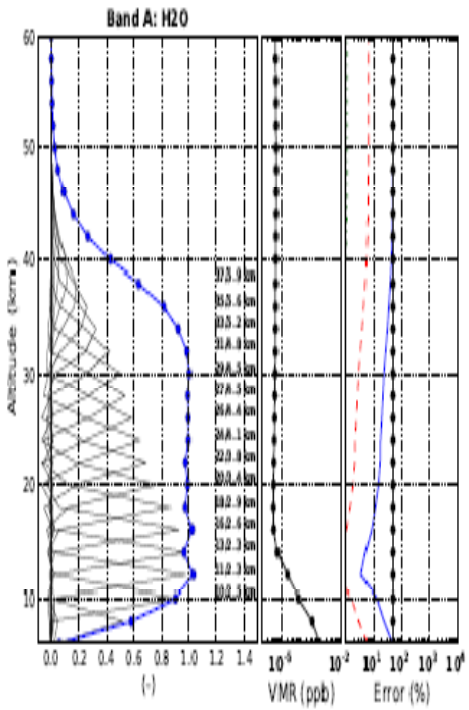


Figure 1: SMILES band A measurement capability for H_2O in (top) mesospheric and (bottom) stratospheric retrieval mode assuming US Standard atmospheric conditions. (left) Averaging kernels (black) and response function (blue). Altitude and corresponding vertical resolution are given as text. (middle) A priori (=true) profile. (right) A priori error (black) and a posteriori errors for a single scan (blue), daily average (red dashed), i.e. 64 scans, and monthly average (green dash-dotted), i.e. 64*30scans. A posteriori error comprises measurement and null space error. Dots on the lines commonly denote respective tangent altitudes.

Band B

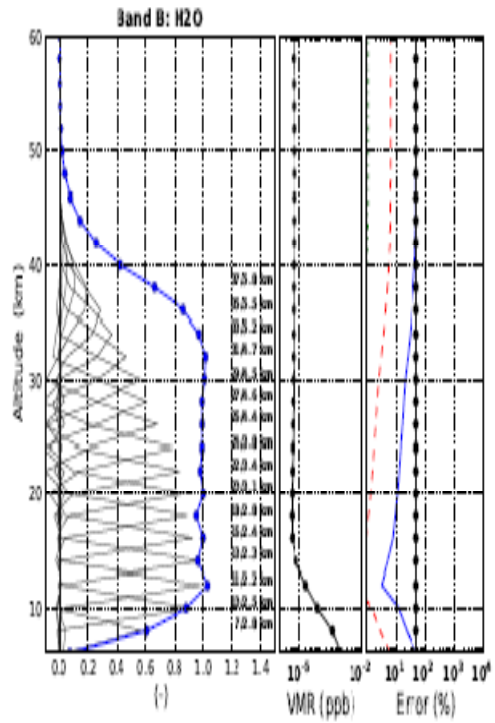


Figure 21: SMILES band B measurement capability for H_2O in (top) mesospheric and (bottom) stratospheric retrieval mode assuming US Standard atmospheric conditions. (left) Averaging kernels (black) and response function (blue). Altitude and corresponding vertical resolution are given as text. (middle) A priori (=true) profile. (right) A priori error (black) and a posteriori errors for a single scan (blue), daily average (red dashed), i.e. 64 scans, and monthly average (green dash-dotted), i.e. 64*30scans. A posteriori error comprises measurement and null space error. Dots on the lines commonly denote respective tangent altitudes.

Band C

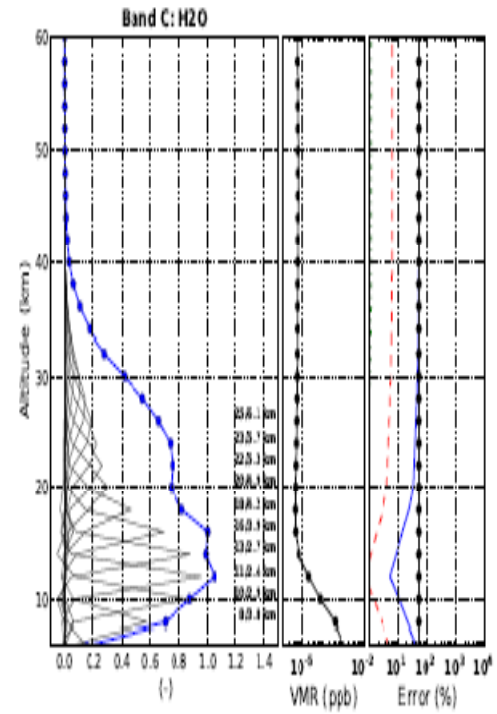
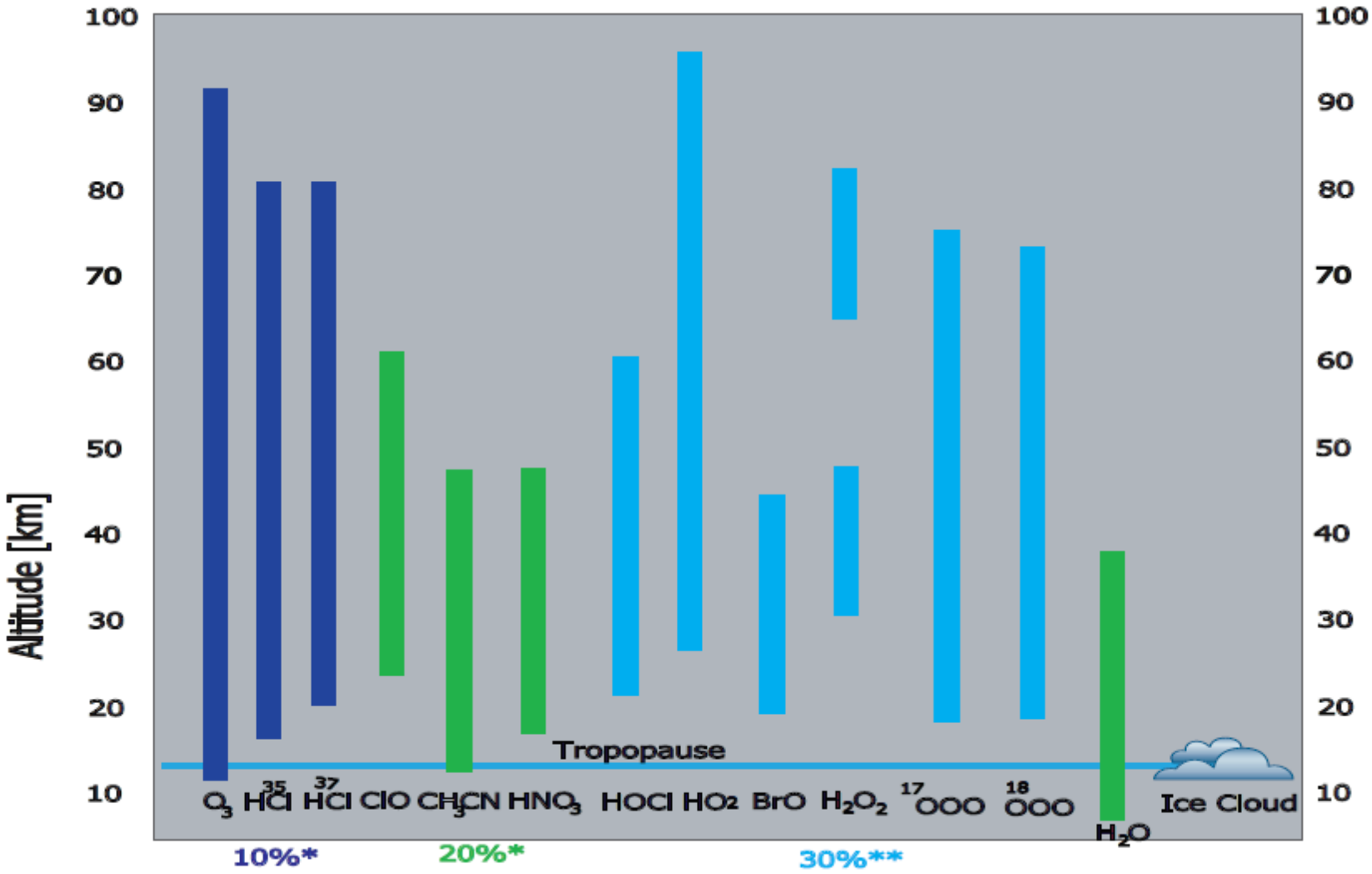


Figure 37: SMILES band C measurement capability for H_2O in (top) mesospheric and (bottom) stratospheric retrieval mode assuming US Standard atmospheric conditions. (left) Averaging kernels (black) and response function (blue). Altitude and corresponding vertical resolution are given as text. (middle) A priori (=true) profile. (right) A priori error (black) and a posteriori errors for a single scan (blue), daily average (red dashed), i.e. 64 scans, and monthly average (green dash-dotted), i.e. 64*30scans. A posteriori error comprises measurement and null space error. Dots on the lines commonly denote respective tangent altitudes.

JEM/SMILES observation



** Averaged profiles (for example, zonal mean average/ 5km altitude resolution)