The MIPAS Error Budget

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Retrieval

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Retrieval equation used for MIPAS data (IMK/IAA):

$$\hat{\boldsymbol{x}}_{i+1} = \hat{\boldsymbol{x}}_i + \left(\mathbf{K}^T \mathbf{S}_{y,\mathrm{noise}}^{-1} \mathbf{K} + \mathbf{R}\right)^{-1} \left(\mathbf{K}^T \mathbf{S}_{y,\mathrm{noise}}^{-1} \left(\boldsymbol{y} - \boldsymbol{F}(\hat{\boldsymbol{x}}_i ; \boldsymbol{b})\right) - \mathbf{R}(\hat{\boldsymbol{x}}_i - \boldsymbol{x}_{\mathrm{a}})\right)$$

$\mathbf{K}$ Jacobian matrix ($\partial y_m / \partial x_n$)
$\mathbf{S}_{\mathrm{v.noise}}$ measurement noise covariance matrix
$\boldsymbol{F}(\hat{\boldsymbol{x}}_i ; \boldsymbol{b})$ radiative transfer-forward model, incl. additional parameters $\boldsymbol{b}$
$\mathbf{R}$ regularization matrix

$$\frac{\partial \hat{\boldsymbol{x}}}{\partial \boldsymbol{x}} = \mathbf{A} = \left(\mathbf{K}^T \mathbf{S}_{y,\mathrm{noise}}^{-1} \mathbf{K} + \mathbf{R}\right)^{-1} \mathbf{K}^T \mathbf{S}_{y,\mathrm{noise}}^{-1} \mathbf{K}$$

Averaging kernel matrix

$$\frac{\partial \hat{\boldsymbol{x}}}{\partial \boldsymbol{y}} = \mathbf{G} = \left(\mathbf{K}^T \mathbf{S}_{y,\mathrm{noise}}^{-1} \mathbf{K} + \mathbf{R}\right)^{-1} \mathbf{K}^T \mathbf{S}_{y,\mathrm{noise}}^{-1}$$

Gain matrix

Error calculation (see von Clarmann et al., 2022)

$$\mathbf{S}_{x;\mathrm{meas}} = \mathbf{G}\mathbf{S}_{y;\mathrm{meas}}\mathbf{G}^T$$

$\mathbf{G}$ is available from the retrieval

$$\mathbf{S}_{x;b} = \mathbf{G}\mathbf{K}_b\mathbf{S}_{b;\mathrm{meas}}\mathbf{K}_b^T\mathbf{G}^T$$

$\mathbf{K}_b$ has to be specifically calculated

$$\Delta_{b_k}\boldsymbol{x} = -\mathbf{G}\cdot(\boldsymbol{F}_{\mathrm{perturbed}} - \boldsymbol{F}_{\mathrm{nominal}})$$

dedicated forward calculations

Error types

- systematic
- random
- „headache“
- entangled (sequential retrievals: TLOS, ozone, water vapour, . . .)

Example: spectral gain calibration error in gas retrieval

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- Gain error impacts on TLOS retrieval and gas retrieval.
- Sequential retrieval: can TLOS error due to gain be expected to cancel out?
- MIPAS has 5 spectral bands (A, AB, B, C, D)
- TLOS retrieval is done exclusively in MWs in band A
- gas retrievals possibly employ different bands (plus band A)
- There are three cases:
    1. gas MWs only from band A
    2. gas MWs from AB – D
    3. gas MWs from A plus AB - D

Note: random and systematic components of gain calib. error are essentially uncorrelated between the different bands.

In general: $\Delta_{\text{gain}}\boldsymbol{x} = -\mathbf{G}(\boldsymbol{F}_{\text{perturbed}} - \boldsymbol{F}_{\text{nominal}})$

Case 1. (gas MWs from band A only)

$$\boldsymbol{F}_{\text{perturbed}} = \left(1 + \left(\frac{\Delta y}{y}\right)_A\right) \boldsymbol{F}\left(\boldsymbol{x}; \boldsymbol{TLOS} + \Delta_{\text{gain}}\boldsymbol{TLOS}\right)$$

Case 2. (gas MWs not from band A)

$$\boldsymbol{F}_{\text{perturbed}} = (1 + \Delta \boldsymbol{y}/\boldsymbol{y})\, \boldsymbol{F}(\boldsymbol{x}).$$

direct gain error

$$\boldsymbol{F}_{\text{perturbed}} = \boldsymbol{F}(\boldsymbol{x}; \boldsymbol{TLOS} + \Delta_{\text{gain}}\boldsymbol{TLOS})$$

gain error propagation from TLOS

Case 3. (gas MWs from band A plus at least another band)

$$\boldsymbol{F}_{\text{perturbed}} = \underbrace{\left(1 + \left(\frac{\Delta y}{y}\right)_A\right)} \boldsymbol{F}\left(\boldsymbol{x}; \boldsymbol{TLOS} + \Delta_{\text{gain}}\boldsymbol{TLOS}\right)$$

Use this factor only for spectral points from band A

Level 1b error contributions (2σ)

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Table 3. Summary of the level 1b data accuracy. NL is nonlinearity. For details, see text.

			Spectral band					Correlation		
			A	AB	B	C	D	spectral	altitude	time
NESR ($nW\,cm^{-2}\,sr^{-1}\,cm$)		FR	30 (80)	16	16	3	3 (5)	–	–	–
		OR	20 (50)	10	10	2	2 (3)			
Scaling accuracy (%)	Gain noise		0.1	0.1	0.1	0.1	0.4 (1.2)	resol.[a]	full	1 day
	Gain variation		0.4 (1.5)	0.3 (1.5)	0.4 (2)	0.4 (1.2)	0.6 (1.2)	band	full	1 day
	Blackbody		0.5	0.5	0.5	0.5	0.5	high[b]	full	1 day
	NL determination		2	2	2	0.4	–	band	full[c]	weeks to years
	Cubic artifact		1 (1.5)	0.1	0.1	–	–	band[d]	full[c]	mission[e]
	Total		2.4	2.1	2.1	0.8	0.9			
Offset accuracy ($nW\,cm^{-2}\,sr^{-1}\,cm$)	Offset noise	FR	6 (20)	3	2.5	0.7	0.6 (1)	resol.[a]	full	300 s
		OR	3 (10)	2	1.5	0.4	0.15 (0.3)			700 s
	Offset drift	FR	2	1	0.5	0.1	0.05	full	full	300 s
		OR	4	2	1	0.2	0.1			700 s
	NL determination		5 (10)	1 (2)	0.5	–	–	band	full[f]	week to years
	Cubic artifact		5 (10)	–	–	–	–	band[d]	full[f]	mission[e]
	Total		9.5	3.3	2.6	0.7	0.6			
Spectral accuracy (ppm)		FR			0.14			full	full	1 day
		OR			0.27					
LOS (m)					400 (700)			full	full[f]	not known

[a] according to the spectral resolution of the calibration measurements [b] depending on spectral emissivity [c] increasing with altitude [d] highly correlated but not constant within one band [e] decreasing with time [f] decreasing with altitude

From Kleinert et al., 2018

Spectroscopy error contributions (ozone retrieval)

Table 2. 1σ uncertainties of spectroscopic O_3 data as used for this work. J and K are the upper-state rotational quantum numbers.

Isotope	Band (HITRAN ID for vibr. levels)	Intensity relative uncertainty	Broadening coeff. relative uncertainty
$^{16}O^{16}O^{16}O$	2-1, 4-1, 5-1	$0.02\,(1+J/70+K/25)$	0.035
	Other bands originating from the ground state (index = 1)	$0.03\,(1+J/60+K/20)$	0.035
	Bands originating from the lower states 2 … 5	$0.04\,(1+J/50+K/17)$	0.075
	Bands originating from the lower states 6 … 14	$0.06\,(1+J/40+K/13)$	0.15
	Bands originating from the lower states > 14	$0.10\,(1+J/35+K/11)$	0.20
Others	All	$0.03\,(1+J/60+K/18)$	0.035

From Kiefer et al., 2023, based on HITRAN16 (Gordon et al., 2017) and the MIPAS specific spectroscopy data base

Representative error calculations

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- Having an error estimation for each single MIPAS measurement geolocation is pie in the sky.
- For split-up of „headache“ errors: use a sufficient number of single geolocations
- Atmospheric conditions/illumination vary

⇒ Define representative atmospheric conditions (34), and for each of these do error calculations for 30 – 35 single geolocations

This gives a total of approx. 1000 single error calculations.

Table S1. Labels and definitions of the representative atmospheric conditions which were used to calculate the error budget. Daytime atmospheres are defined by solar zenith angles $< 90°$. Nighttime atmospheres are defined by solar zenith angles $> 95°$ for NOM observations, $> 98°$ for MA observations, and $> 100°$ for UA observations.

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representative atmosphere label	month(s) used	latitude range
Northern polar winter day	Jan, Feb	65°N – 90°N
Northern polar winter night	Jan, Feb	65°N – 90°N
Northern polar spring day	Apr	65°N – 90°N
Northern polar spring night	Apr	65°N – 90°N
Northern polar summer day	Jul, Aug	65°N – 90°N
Northern polar summer night	Jul, Aug	65°N – 90°N
Northern polar autumn day	Oct	65°N – 90°N
Northern polar autumn night	Oct	65°N – 90°N
Northern midlatitude winter day	Jan, Feb	40°N – 60°N
Northern midlatitude winter night	Jan, Feb	40°N – 60°N
Northern midlatitude spring day	Apr	40°N – 60°N
Northern midlatitude spring night	Apr	40°N – 60°N
Northern midlatitude summer day	Jul, Aug	40°N – 60°N
Northern midlatitude summer night	Jul, Aug	40°N – 60°N
Northern midlatitude autumn day	Oct	40°N – 60°N
Northern midlatitude autumn night	Oct	40°N – 60°N
Tropics day	Apr	20°S – 20°N
Tropics night	Apr	20°S – 20°N
Southern midlatitude winter day	Jul, Aug	40°S – 60°S
Southern midlatitude winter night	Jul, Aug	40°S – 60°S
Southern midlatitude spring day	Oct	40°S – 60°S
Southern midlatitude spring night	Oct	40°S – 60°S
Southern midlatitude summer day	Jan, Feb	40°S – 60°S
Southern midlatitude summer night	Jan, Feb	40°S – 60°S
Southern midlatitude autumn day	Apr	40°S – 60°S
Southern midlatitude autumn night	Apr	40°S – 60°S
Southern polar winter day	Jul, Aug	65°S – 90°S
Southern polar winter night	Jul, Aug	65°S – 90°S
Southern polar spring day	Oct	65°S – 90°S
Southern polar spring night	Oct	65°S – 90°S
Southern polar summer day	Jan, Feb	65°S – 90°S
Southern polar summer night	Jan, Feb	65°S – 90°S
Southern polar autumn day	Apr	65°S – 90°S
Southern polar autumn night	Apr	65°S – 90°S

From Funke et al., 2023

Resulting error profiles for one single geolocation

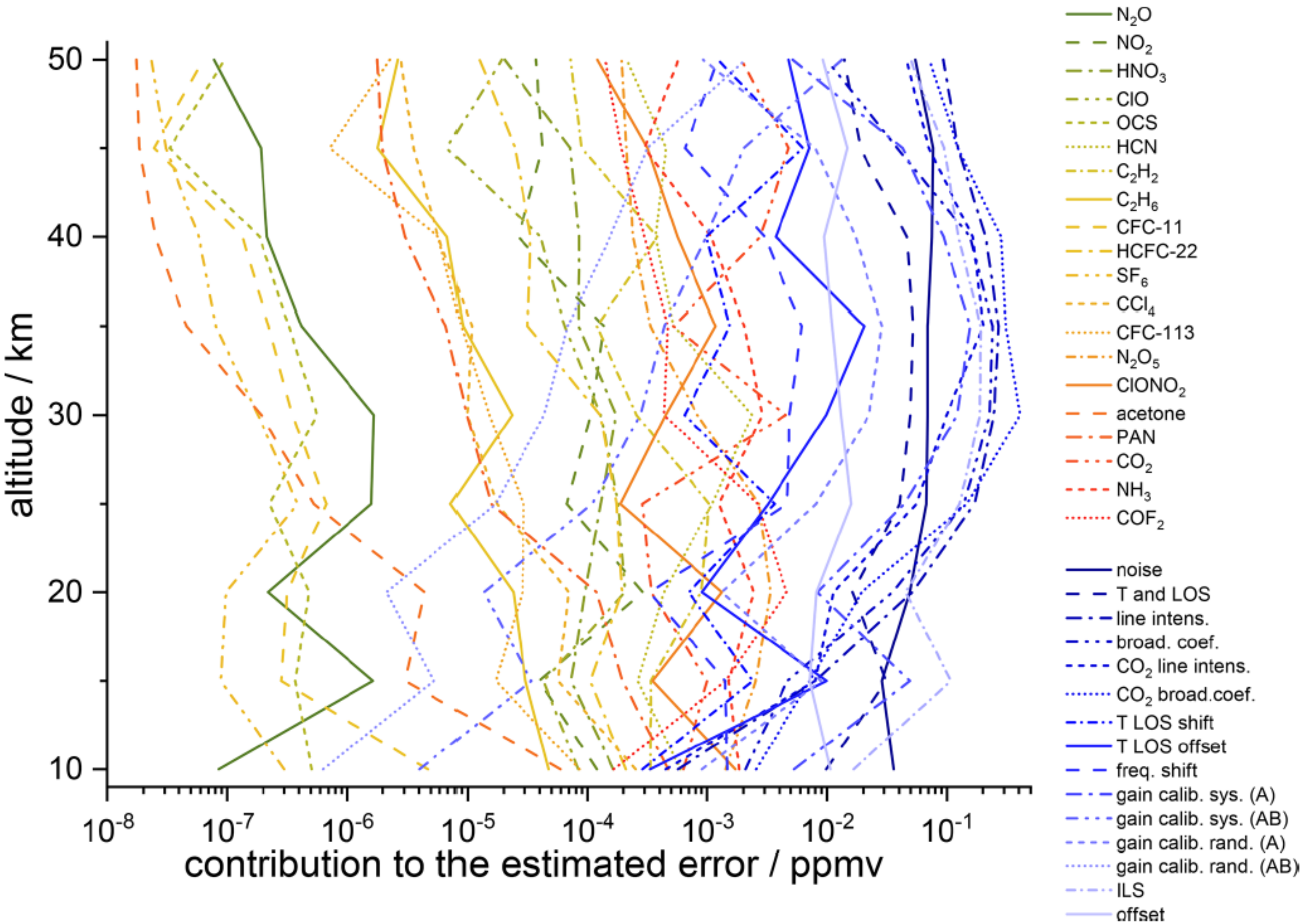
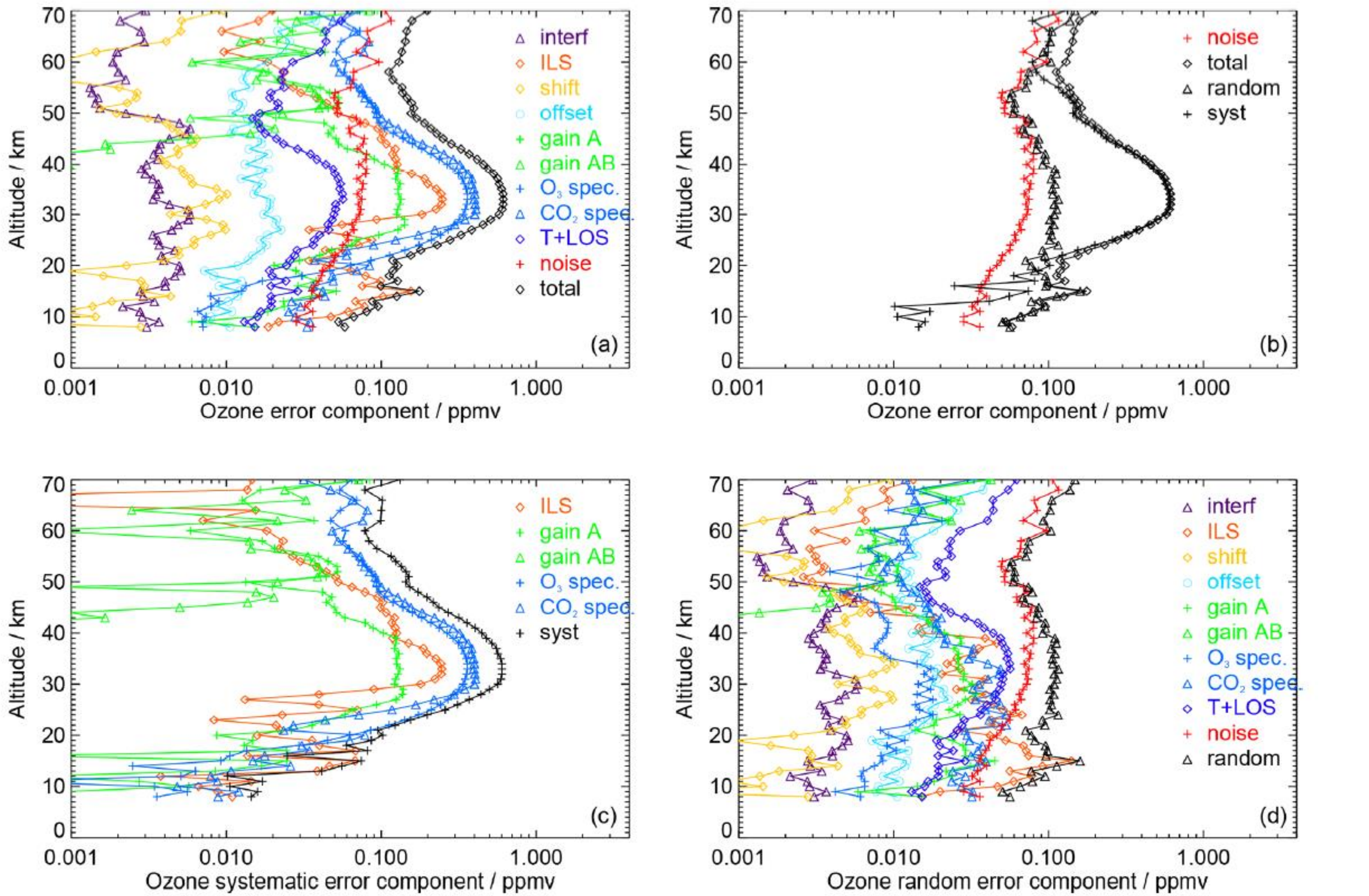


Fig. 2 from von Clarmann et al., 2022

Resulting error profiles for a repres. atmosphere

Fig. 3 from von Clarmann et al., 2022



Deliveries (Paper supplements)

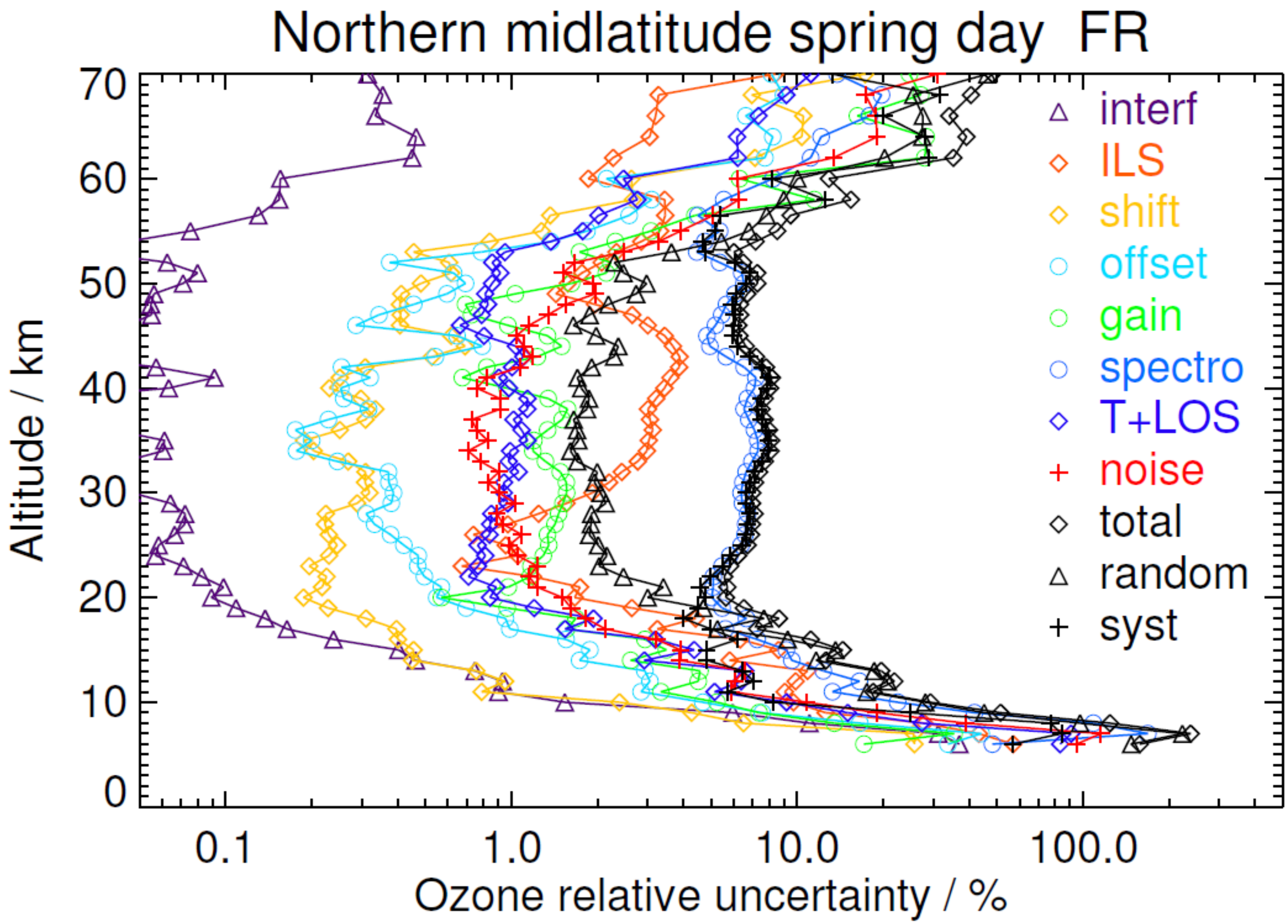


Figure S11. V8H_O3_61 Northern midlatitude spring day

Deliveries (Paper supplements)

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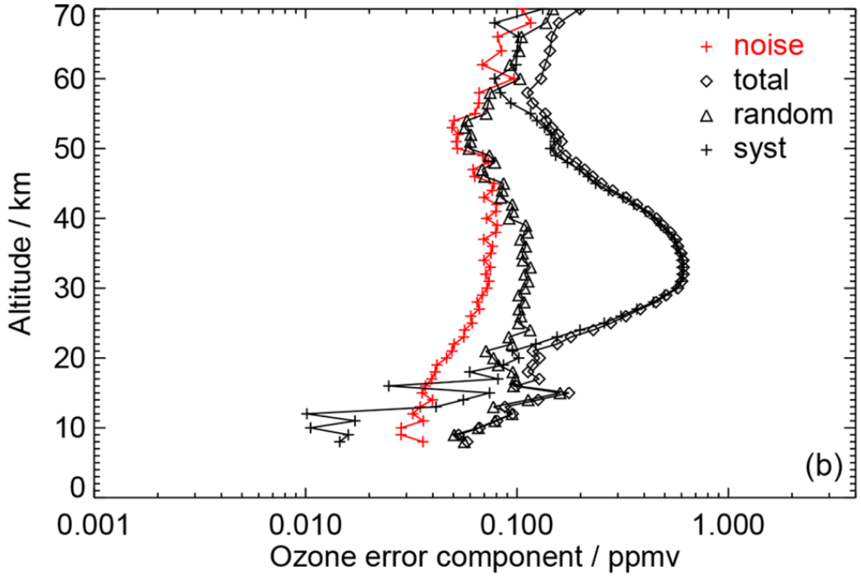
Table S12. Ozone error budget for Northern midlatitude spring day. All uncertainties are 1σ.

altitude (km)	mean target (ppmv)	interf (%)	ILS (%)	shift (%)	offset (%)	gain (%)	spectro (%)	T+LOS (%)	noise (%)	random (%)	syst (%)	total (%)
6	0.09	36.95	57.07	25.74	33.70	17.13	48.24	83.29	94.95	>100	56.86	>100
9	0.27	5.95	12.60	4.28	7.55	7.36	41.75	15.04	18.97	45.15	24.78	51.50
12	0.68	0.93	9.88	0.95	3.06	4.51	16.53	6.37	6.05	20.74	7.05	21.90
15	1.00	0.40	8.62	0.46	1.88	3.49	9.17	4.36	3.91	13.62	4.81	14.45
18	2.14	0.14	4.42	0.31	0.95	1.68	6.65	1.94	1.82	7.66	4.00	8.64
21	3.78	0.10	1.74	0.22	0.57	0.98	5.09	0.89	1.23	3.40	4.58	5.70
24	5.09	0.06	1.05	0.23	0.47	1.29	5.81	0.81	1.05	2.16	5.83	6.22
27	6.24	0.07	0.97	0.22	0.33	1.42	6.61	0.84	0.94	1.90	6.69	6.96
30	7.36	0.05	1.92	0.32	0.39	1.56	6.37	0.94	0.91	2.05	6.66	6.97
33	8.20	0.04	2.77	0.27	0.25	1.32	6.95	0.98	0.78	1.70	7.52	7.71
36	8.17	0.04	3.13	0.25	0.18	1.34	7.09	1.09	0.76	1.70	7.80	7.98
39	7.18	0.02	3.21	0.30	0.26	1.35	6.70	1.14	0.91	1.87	7.47	7.70
42	5.57	0.06	3.87	0.31	0.25	0.82	6.53	1.01	1.07	1.91	7.54	7.78
45	4.07	0.03	3.44	0.62	0.65	1.34	4.84	0.80	1.04	1.98	5.97	6.29
48	2.95	0.05	1.96	0.41	0.46	0.69	5.66	0.83	1.55	2.19	5.92	6.31
52	1.97	0.06	2.07	0.61	0.38	2.23	5.36	0.86	1.67	2.30	6.06	6.48
56	1.37	0.13	3.46	1.37	2.59	4.39	4.50	2.02	5.09	7.81	5.39	9.49
60	0.90	0.16	1.86	2.63	2.15	6.29	8.23	2.47	6.20	10.03	8.14	12.92
64	0.73	0.46	3.05	10.39	8.22	28.29	12.13	6.16	19.03	27.42	27.95	39.15
68	0.38	0.36	3.27	6.95	8.96	27.07	19.74	9.18	17.35	25.50	31.57	40.59

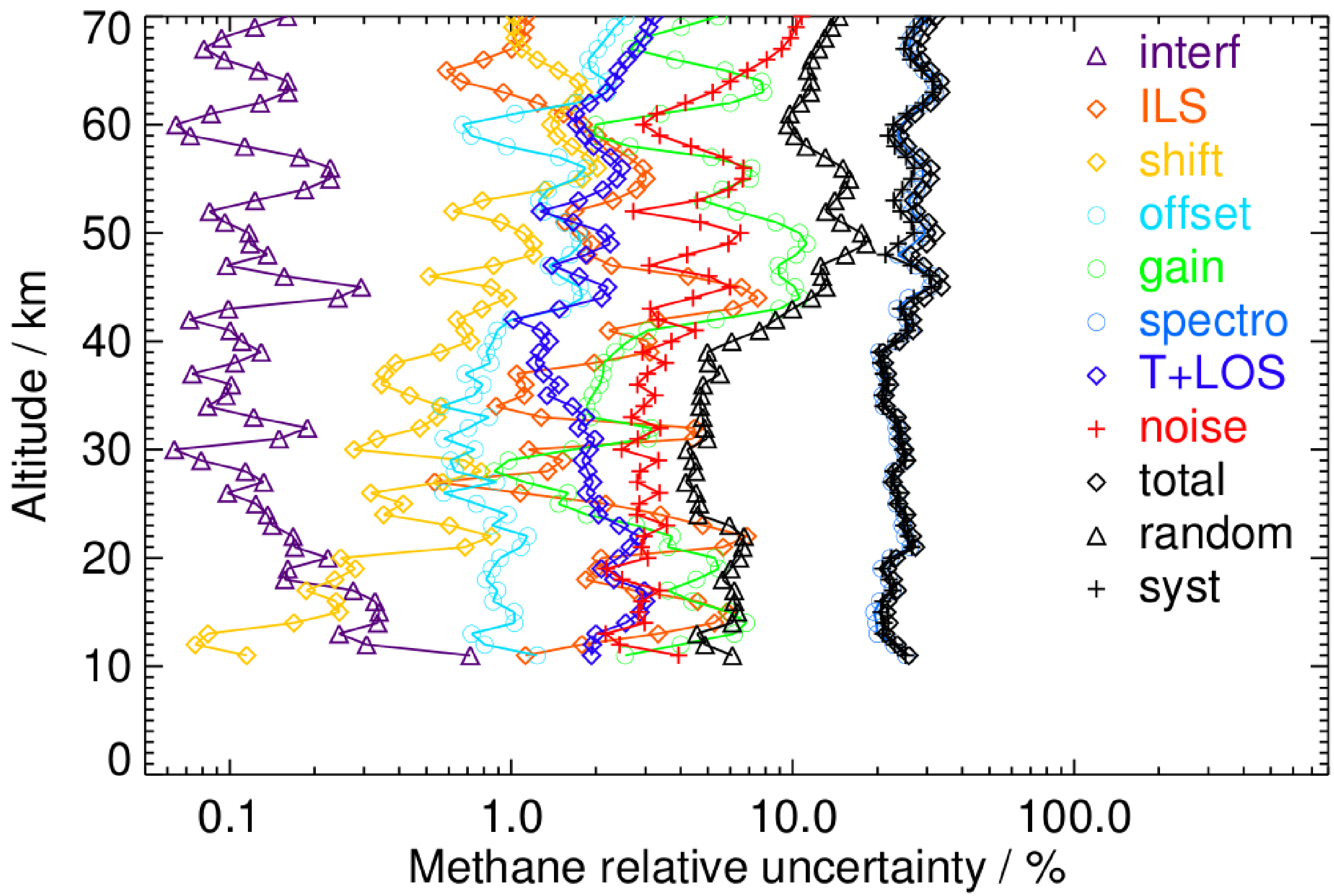
Deliveries (MIPAS data set)

In the retrieval result data files a „quasi-individual“ error budget is given:

- Noise is available for each geolocation
- The errors of multiplicative kind are scaled by the ratio of the vmrs of actual to corresponding representative gas profile.
- These, together with the additive errors from the corresponding representative atmosphere, are then used to compile the random and systematic components.



Reliablity of spectroscopic errror contributions ?



Reliablity of mean representative profiles ?