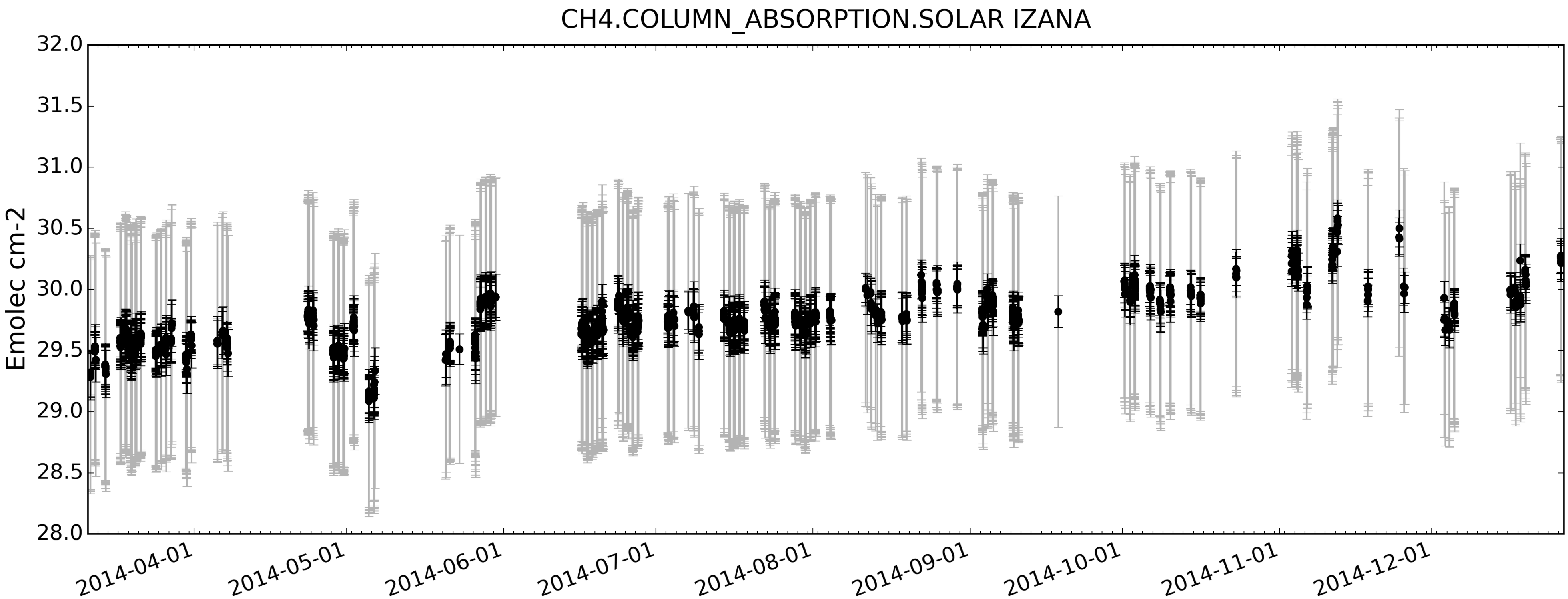
Part I. Measurement uncertainty

B. Langerock & M. De Mazière

June 2015

$\pm 3\%$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Emolec cm-2
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31.5
31.0
30.5
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29.5
29.0
28.5
28.0
2014-04-01
2014-05-01
2014-06-01
2014-07-01
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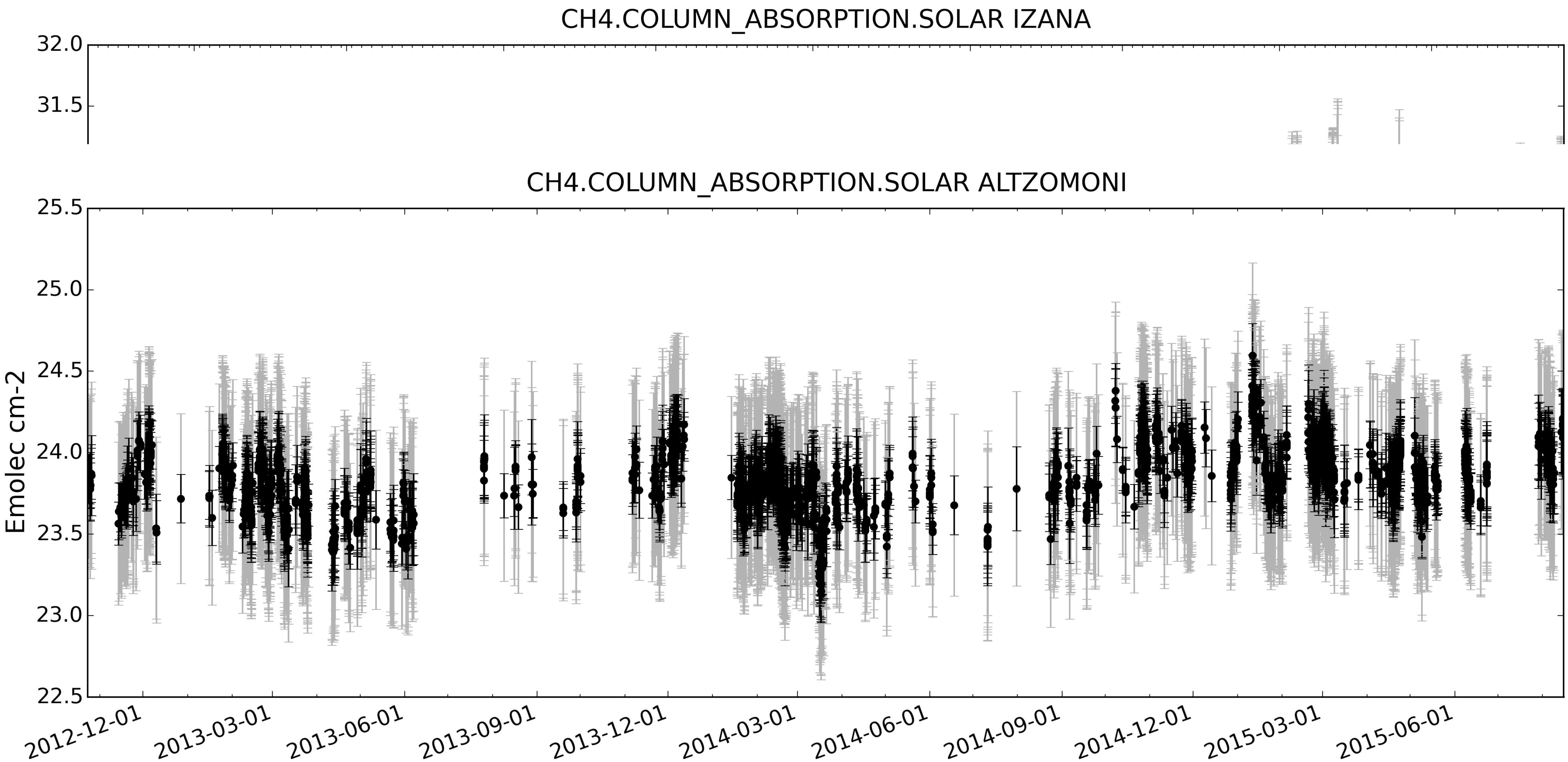
2014-11-01
2014-12-01

$\pm 3\%$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31.5
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25.5
25.0
24.5
24.0
23.5
23.0
22.5
2012-12-01
2013-03-01
2013-06-01
2013-09-01
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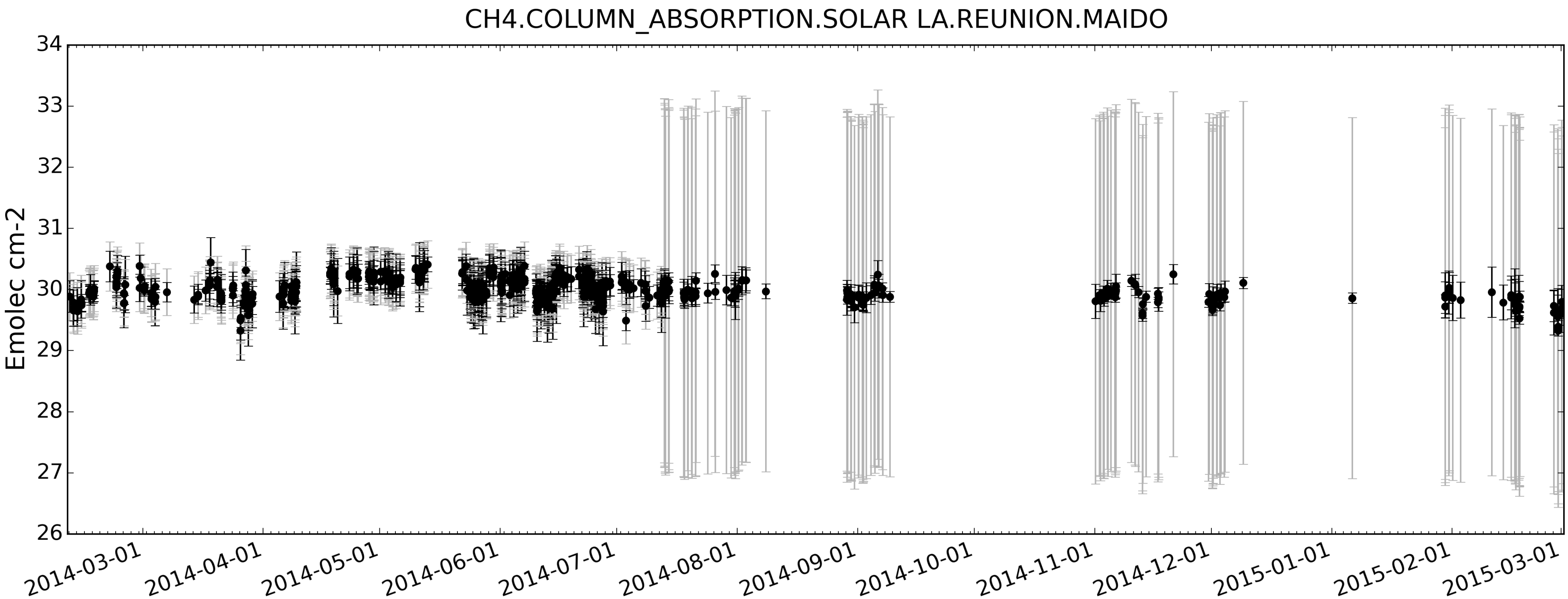
2015-06-01

$\pm10\%$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34
33
32
31
30
29
28
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26
2014-03-01
2014-04-01
2014-05-01
2014-06-01
2014-07-01
2014-08-01
2014-09-01
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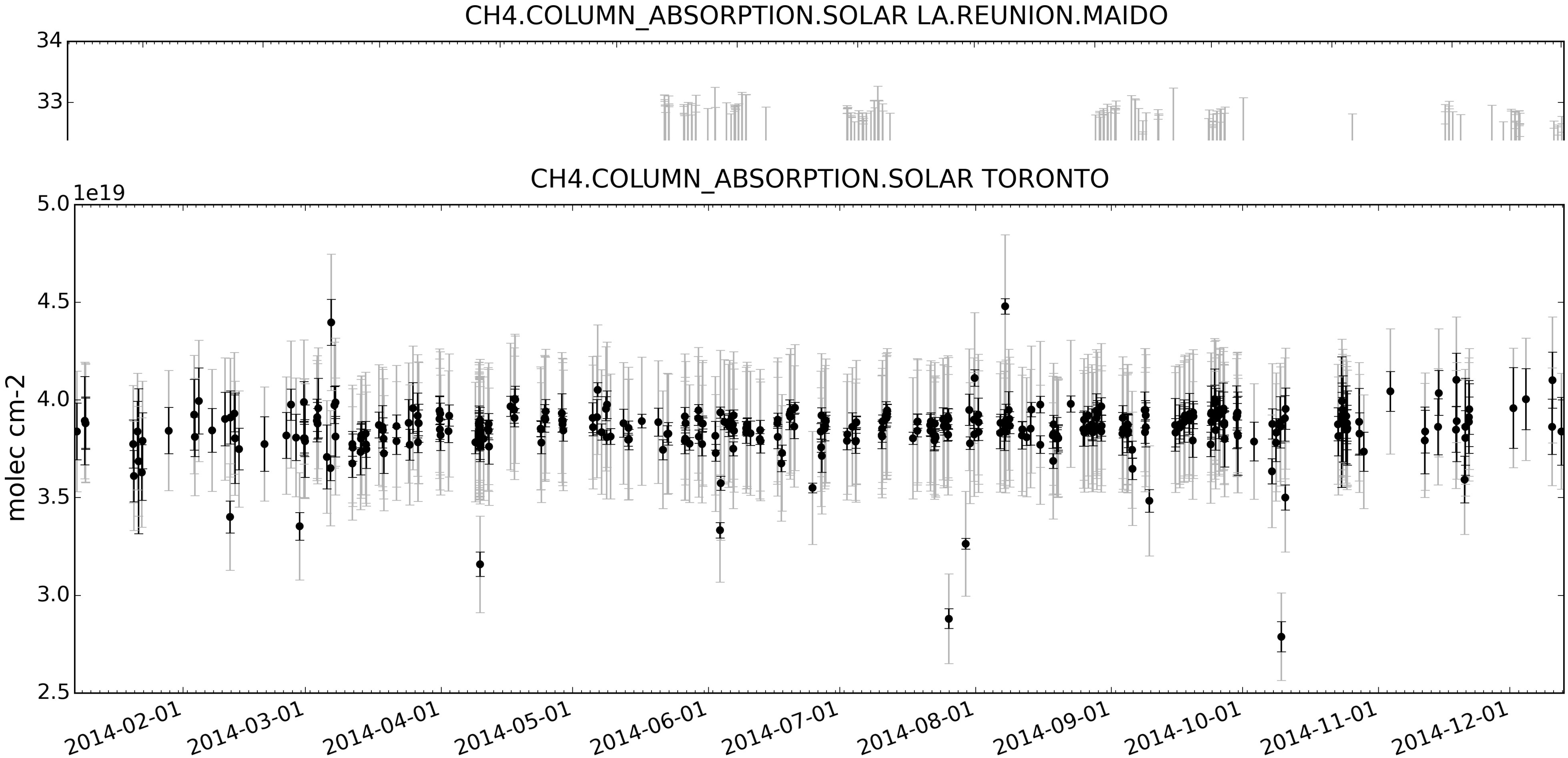
2015-02-01
2015-03-01

$\pm 10\%$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33
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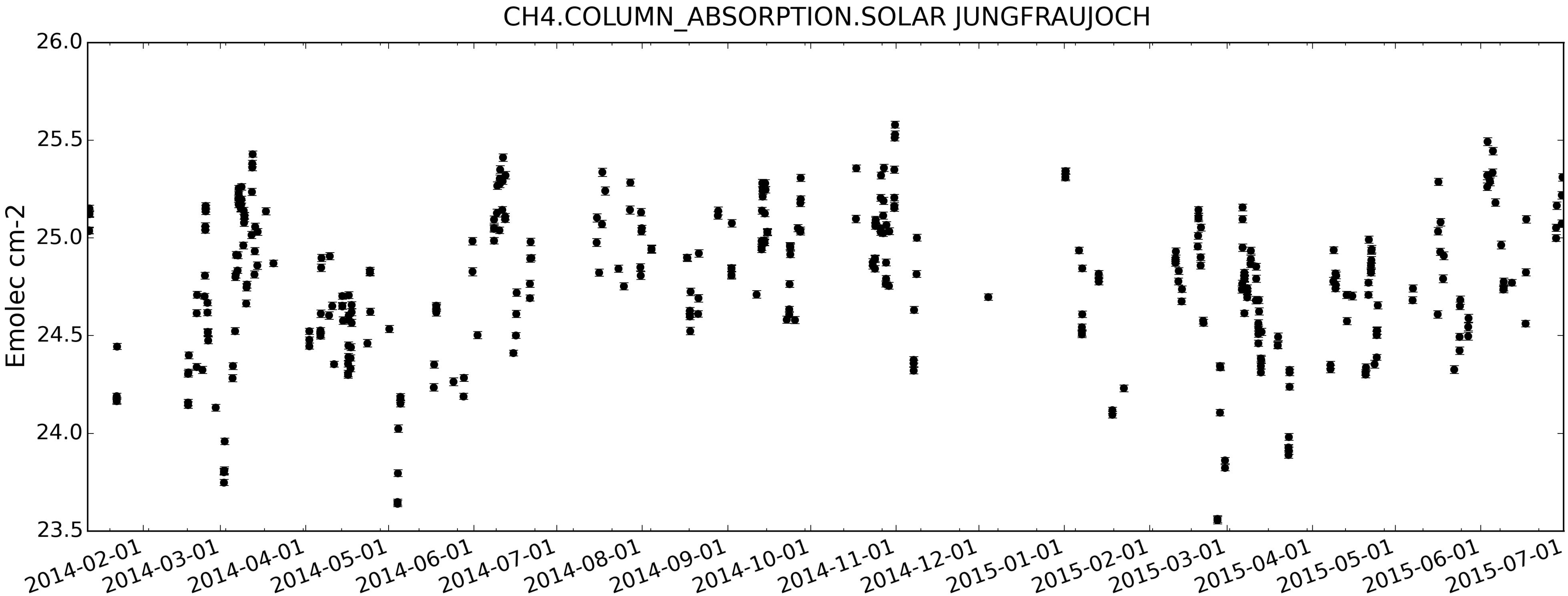
1e19
5.0
4.5
4.0
3.5
3.0
2.5
molec cm-2
2014-02-01
2014-03-01
2014-04-01
2014-05-01
2014-06-01
2014-07-01
2014-08-01
2014-09-01
2014-10-01
2014-11-01
2014-12-01

nan


CH4.COLUMN_ABSORPTION.SOLAR JUNGFRAUJOCH
Emolec cm-2
26.0
25.5
25.0
24.5
24.0
23.5
2014-02-01
2014-03-01
2014-04-01
2014-05-01
2014-06-01
2014-07-01
2014-08-01
2014-09-01
2014-10-01
2014-11-01
2014-12-01
2015-01-01
2015-02-01
2015-03-01
2015-04-01
2015-05-01
2015-06-01
2015-07-01

Definitions

cf. GUM [JCG08], P. Green 'Guide . . . ', Taylor [Tay97]

- ▷ measured quanity: temperature T, pressure P, absorbance I, . . .
- ▷ the true value of the measurand: T_t, . . . (subscript t) unknown!
- ▷ error on measurand: $\epsilon_T = (T - T_t)$ unknown!
- ▷ error is a stochastic variable with an unknown probability density function
- ▷ uncertainty is an estimate for this probability density function

mean of ϵ, covariance of ϵ, higher order moments of ϵ, . . .

Formal definition of 2 uncertainties

- **RANDOM** uncertainty is an estimate of the covariance of ϵ

  covariance = $E[(\epsilon - E[\epsilon])^2]$, or STD for scalars

- **SYSTEMATIC** uncertainty is an estimate of the mean of ϵ

  mean = $E[\epsilon]$

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Every error has a random and systematic uncertainty!

systematic uncertainty is not completely known (up to a sign)

$\rightarrow$ if it is, calibrate the measurement

How to estimate uncertainties?

cf [JCG08]

- Type A: the measurand allows repeated measurements... use textbook estimators for the uncertainty on the measurand

  the random uncertainty on **the mean** of a n times repeated measurement reduces with $\frac{1}{\sqrt{n}}$ compared to the random uncertainty on an individual measurement

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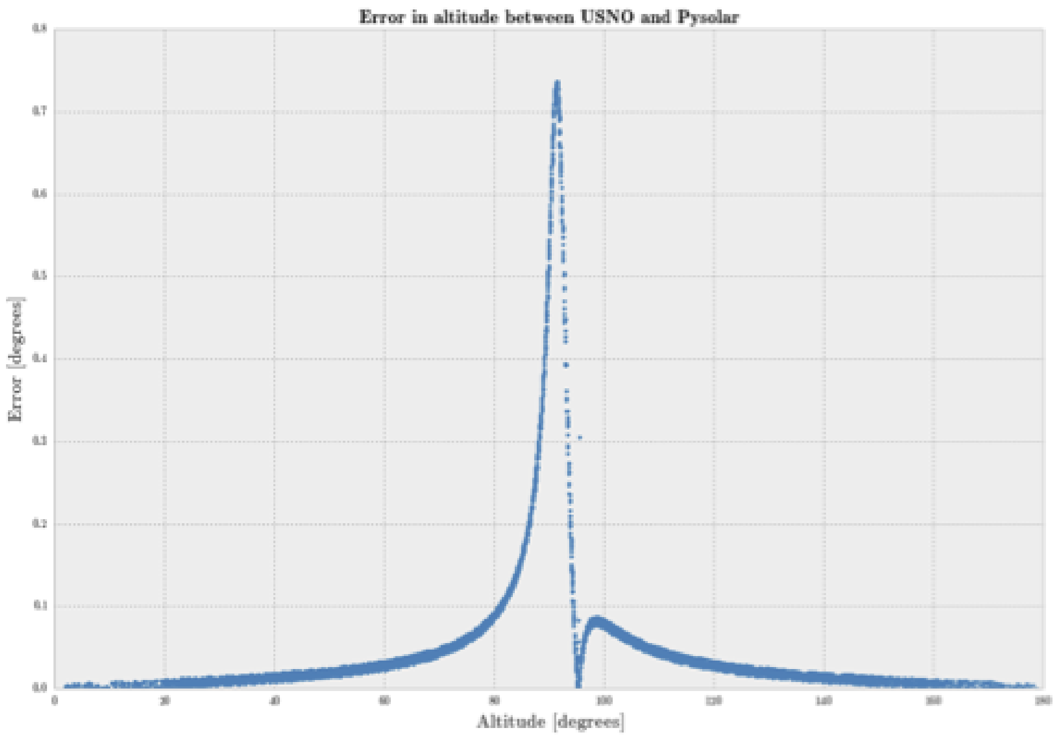
- Type B: other measurand $\rightarrow$ FTIR measurements,...

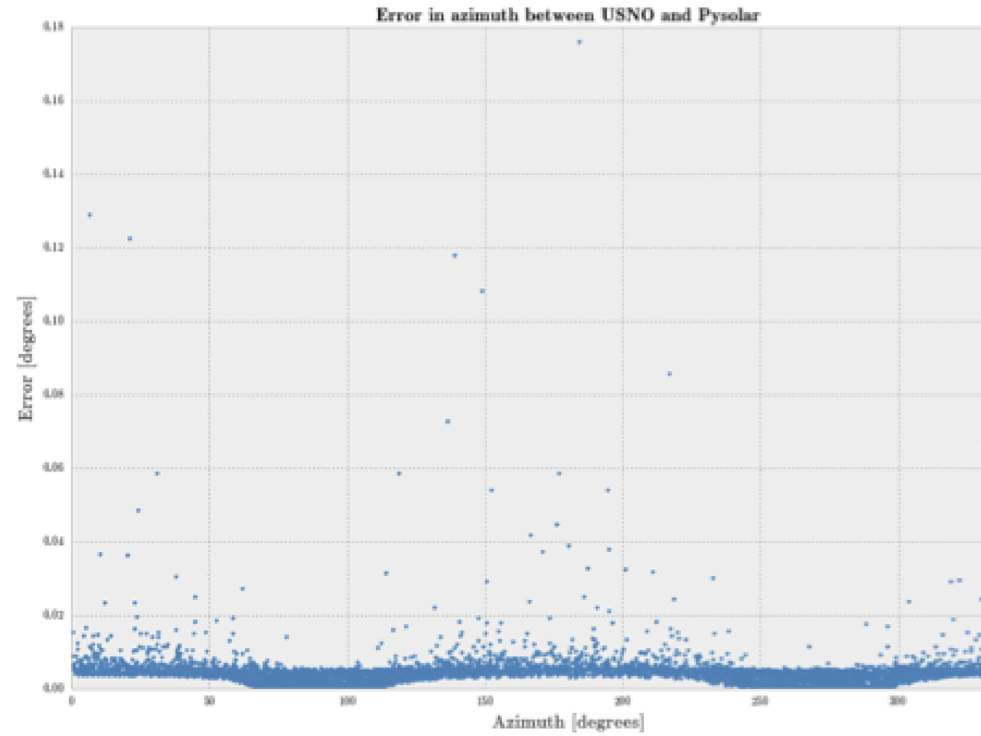
Example: solar zenith angle: numerical computation

- python library: pysolar $\rightarrow$ calculates the zenith and azimuth angle of the sun for a position+time

- the online documentation provides an estimate of the error on the computed angles:

  Compare against US Naval Observatory datapoints...
  http://aa.usno.navy.mil/data/docs/topocentric.php#notes



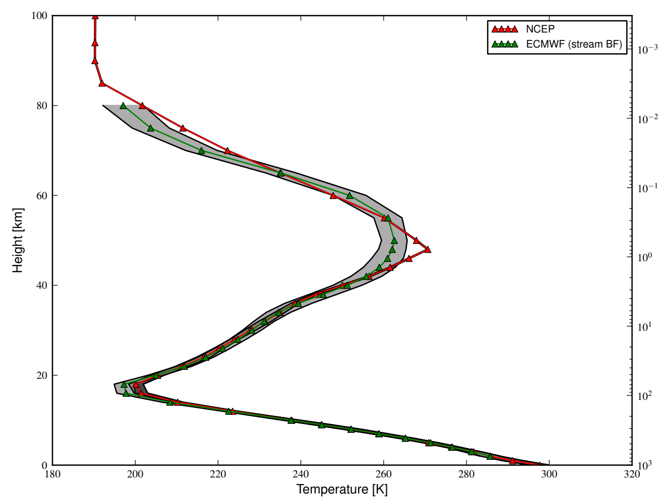


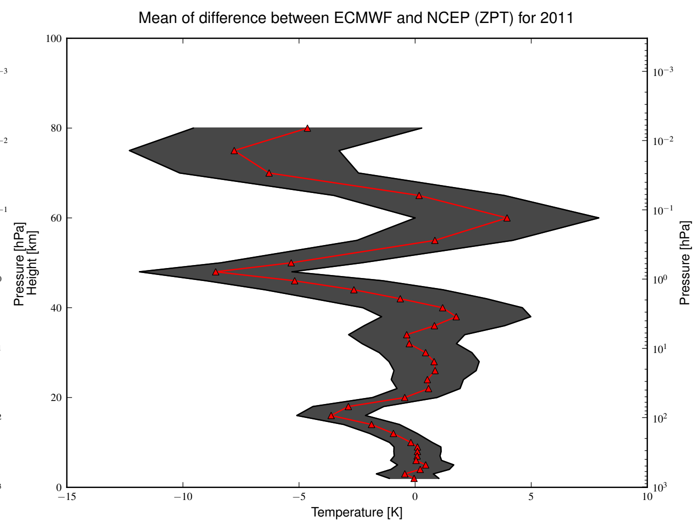
SZA error?

- Mean error: 0.0736 degrees
- Standard deviation of error: 0.124 degrees

Type B error estimates

- ▷ find an ensemble of differences
  - ▶ pysolar angles vs USNO
  - ▶ NCEP temperature profiles vs ECMWF temperature profiles
  - ▶ ...
- ▷ use standard estimators on this ensemble of differences to estimate the random and systematic uncertainty on the measurand, e.g. SZA, NCEP T, ...





Propagation of uncertainties

Why should we propagate uncertainties?

- ▷ FTIR measurement is a L1 spectrum
- ▷ FTIR target data reports O_3 concentration profiles
- ▷ the uncertainty on the O_3 profile is the **propagated** uncertainty on the measured spectrum

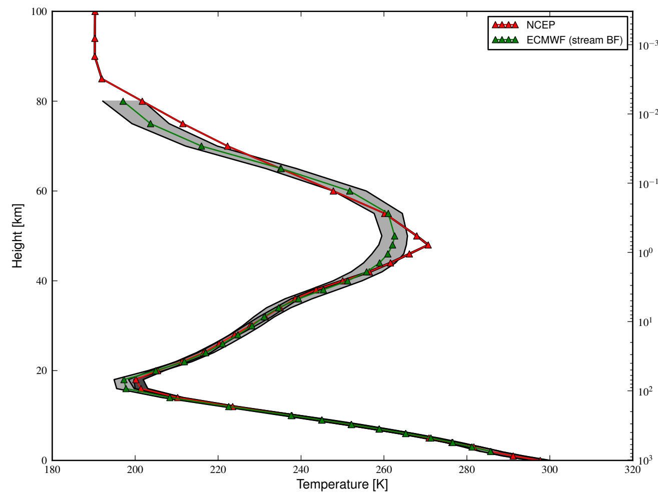
If L denotes the (linearized) transformation between the spectrum and the target profile:

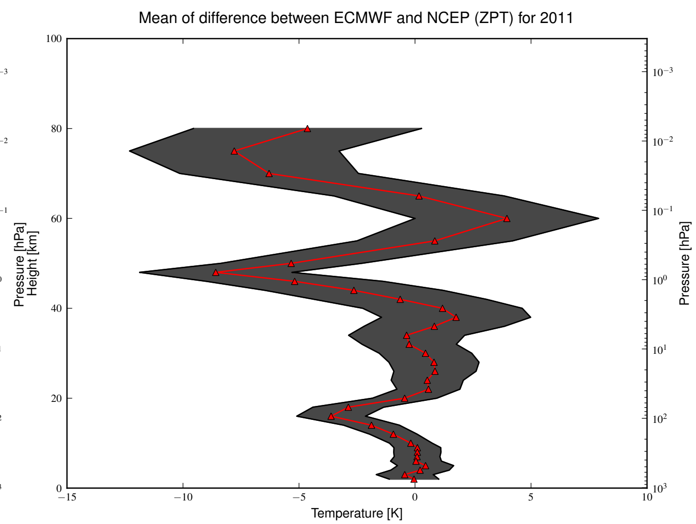
$$\text{random covariance on target} = L(\text{random covariance on source })L^*$$

Propagation of systematic uncertainties

- ▷ systematic=estimate of the mean error, but sign is missing!

- ▷ we can not mathematically propagate the unsigned mean temperature profile difference: $L|x| \neq |Lx|$





- ▷ systematic 'covariance' matrix = $E[\epsilon_T]_i E[\epsilon_T]_j$

- mathematically the systematic uncertainty matrix transforms as a covariance

- the ‘correlation’ coefficients are ±1: just enough information on sign changes to make the propagation work

  ‘the transformed syst. matrix is the syst. matrix of the transformed error’

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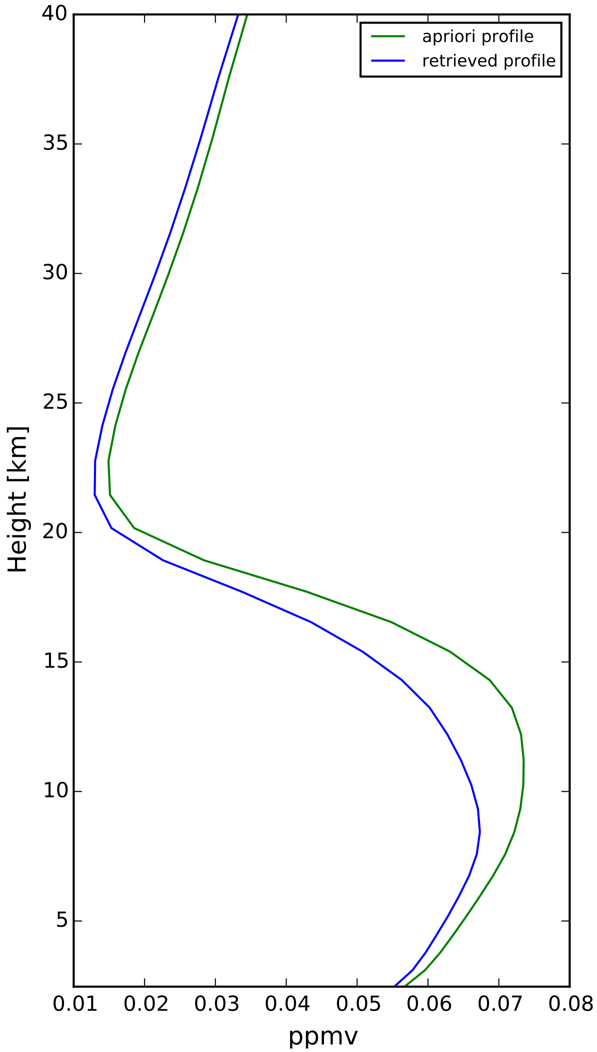
- for correct propagation, the random and systematic uncertainties should be provided as 2D matrices

FTIR reported uncertainties

- ▷ we measure L1 date, but we report concentration profiles
- ▷ the 'retrieval method' is optimal estimation: use the **measurement** to update your **best guess** on the target profile at the site
- ▷ the optimal estimation uses
  - ▶ tools from statistics
  - ▶ an iterative scheme that compares a **model spectrum** with measured spectrum

$$x_{\mathrm{FTIR}} = x_a + A(x_{\mathrm{t}} - x_a)$$



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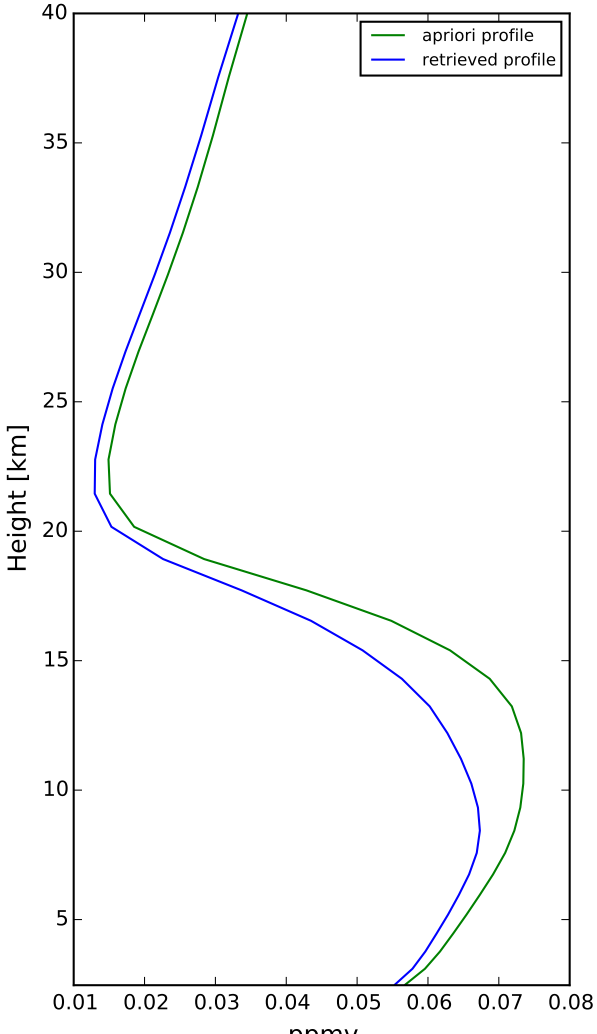

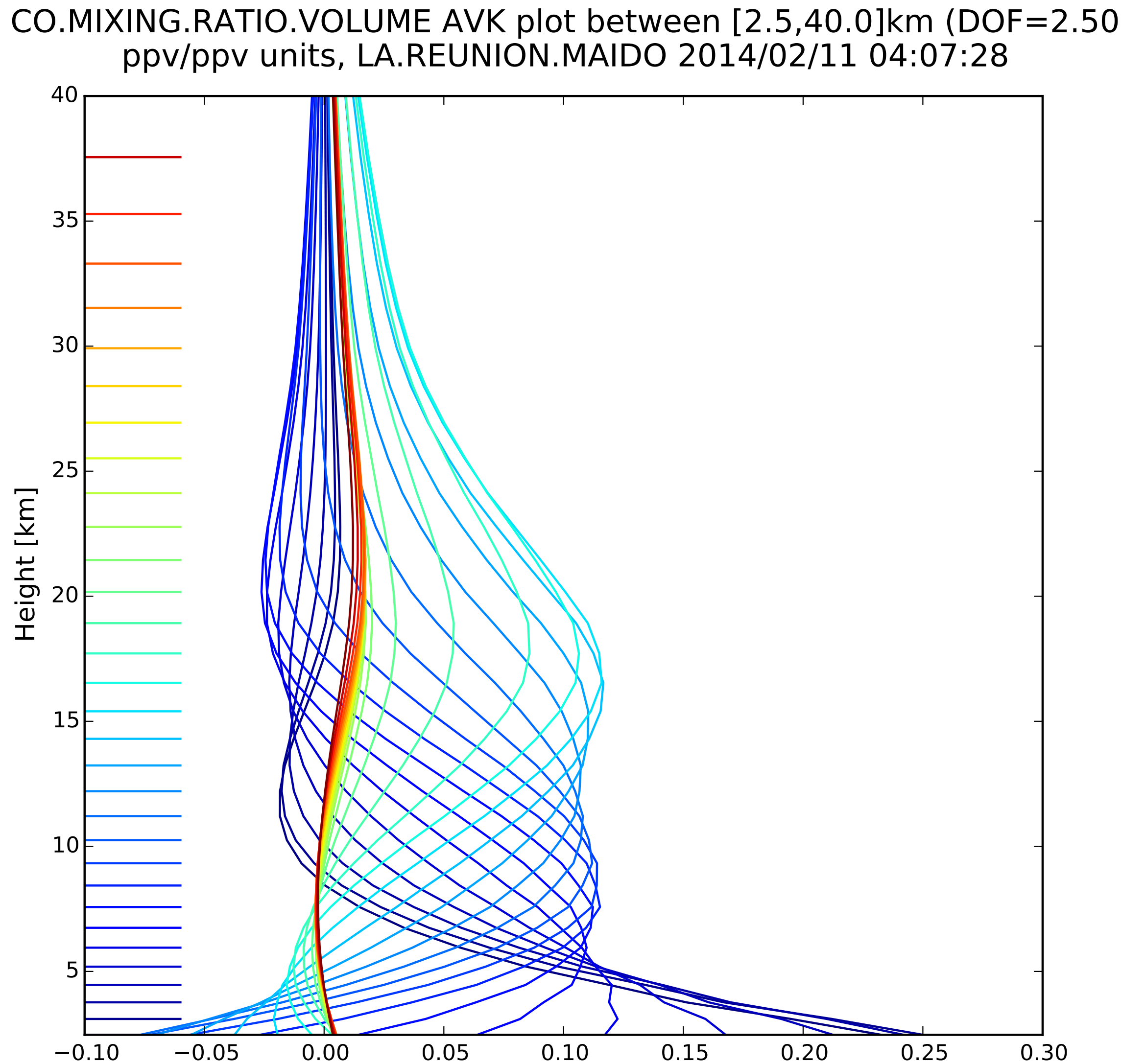

Uncertainty components

- [Rod00]:

  error on target $= (A - I_n)$ error apriori $+ G$noise $+ GK_p$error model params

- **smoothing uncertainty**: $(A - I_n)$ error apriori
- **measurement uncertainty**: Gnoise
- **model parameters uncertainties**: GK_perror model params for each parameter p (temperature, SZA, ILS, . . .)

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- other uncertainties ...

- Leading uncertainty sources: for O_3 M. Schneider ([SRH+08]), O. García ([GSR+12]), C. Vigouroux ([VDMD+08, VBC+15]), ...

Table 1. Assumed uncertainties.

error source		random	systematic
phase error		0.01 rad	–
modulation eff.		1 %	–
intensity offset		0.1 %	+0.1 %
T profile	at surface	1.7 K	−3.5 K
	rest of troposphere	0.7 K	–
	at 30 km	1 K	up to +4 K
	above 50 km	6 K	up to −12 K
solar angle		0.1°	–
line intensity		–	−2 %
pres. broad. coef.		–	−2 %

$^{\alpha}$detailed description see text

GEOMS reported uncertainties

- ▷ NDACC provides a random and systematic uncertainty
- ▷ we do not report the smoothing uncertainty!
- ▷ we expect the data user to apply the AVK to the comparable data:

elimination of the apriori in the comparison

  The purpose of a comparison=true vs ref

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$$x_{\text{FTIR}} = x_{\text{t}} +$$

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$$x_{\text{FTIR}} = x_{\text{t}} + (A - I_n)\,\text{error apriori} + G\,\text{noise} + GK_p\,\text{error model}$$

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$$x^s_{\text{ref}} = x_a + A(x_{\text{ref}} - x_a) \leftarrow \text{smooth the reference profile}$$

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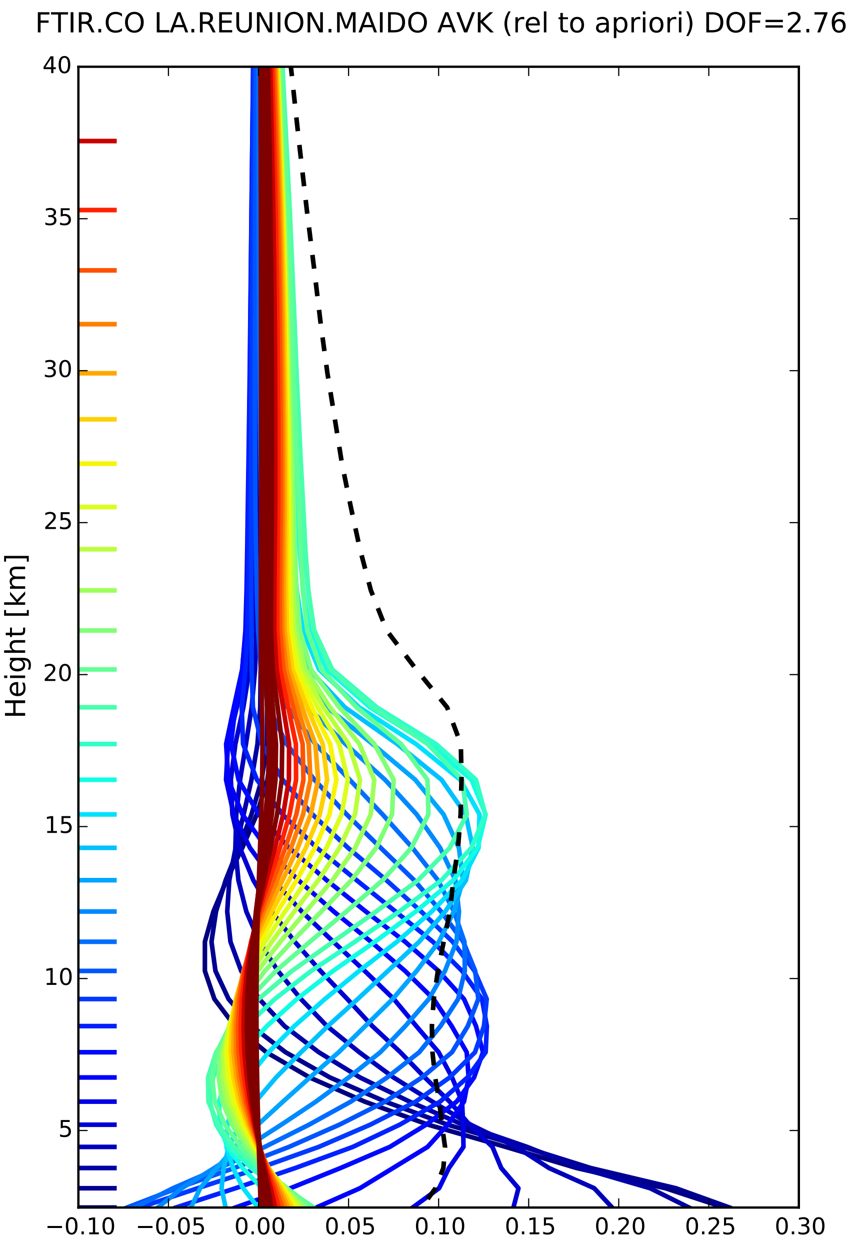
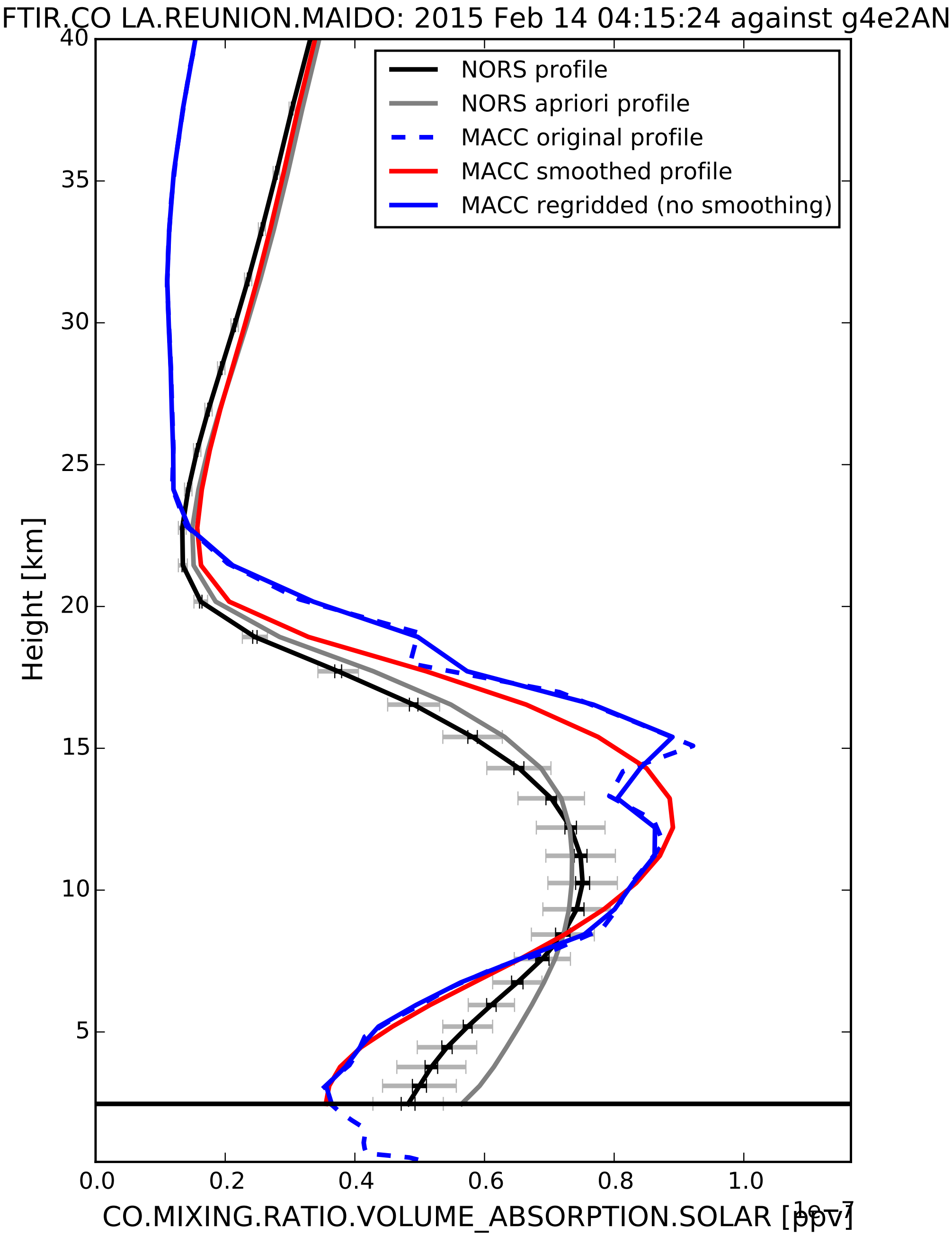
$$x_{\text{FTIR}} - x^s_{\text{ref}} = A(x_{\text{t}} - x_{\text{ref}}) + G\text{noise} + GK_p\text{error model}$$


FTIR.CO LA.REUNION.MAIDO AVK (rel to apriori) DOF=2.76
Height [km]
40
35
30
25
20
15
10
5
−0.10
−0.05
0.00
0.05
0.10
0.15
0.20
0.25
0.30


FTIR.CO LA.REUNION.MAIDO: 2015 Feb 14 04:15:24 against g4e2AN
NORS profile
NORS apriori profile
MACC original profile
MACC smoothed profile
MACC regridded (no smoothing)
Height [km]
40
35
30
25
20
15
10
5
0.0
0.2
0.4
0.6
0.8
1.0
1e−7
CO.MIXING.RATIO.VOLUME_ABSORPTION.SOLAR [ppv]

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[Tay97] J.R. Taylor. *An Introduction to Error Analysis: The Study of Uncertainties in Physical Measurements*. Physics - Chemistry - Engineering. University Science Books, 1997.

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