CH2O in Mexico City: Comparison between FTIR, MAXDOAS and Satellite

A Comparison between different remote sensing techniques with around 1 to 2 DOFS

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The questions:

- Mexico City has high CH2O columns and might be challenging for validation?
- Using retrieval with non-ideal Averaging Kernel and DOF around 1.5, how to compare?

Outline

- Maxdoas: How to test the inhomogeneity and does it affect the retrieval? (Diana's and Christina's Work)

- How to make the Kernels more similar:

  Alternative: Combination

  The normal way: AK- Smoothing

- What do we expect for the slope and correlation coefficient?

CH2O in Mexico City: datasets:

- FTIR: HR120/5 Altzomoni (since 2012)
- FTIR: Vertex 80 Mexico City at UNAM Campus
  (since 2010, with NDACC Filters since 2012)
  (*Vigouroux et al, 2018)*

- MAX-DOAS: UNAM since 2013
- *(Arrellano et al., 2016,Friedrich et al. 2019)*

- TROPOMI: data since November 2018
  15 km around the site in UNAM
  (Borsdorff et al. 2018); (Zuleica Ojeda recommendation.)

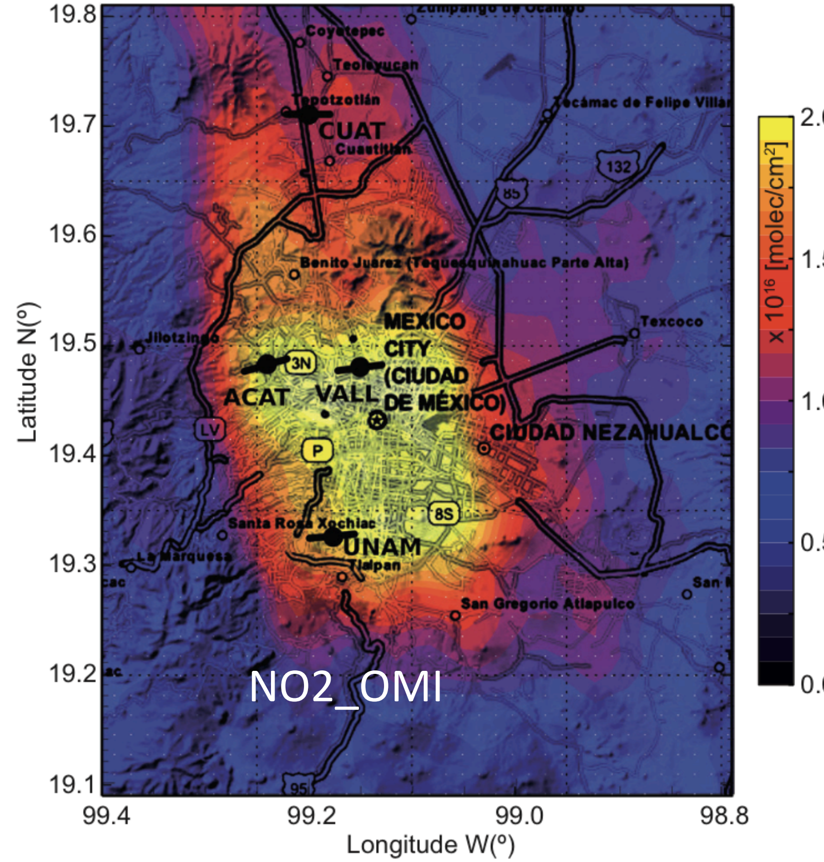
Vigouroux et al.,2018

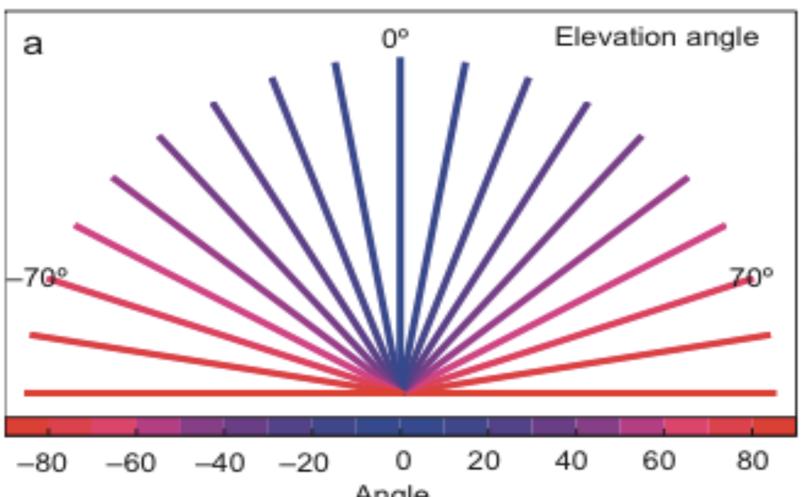
1E14

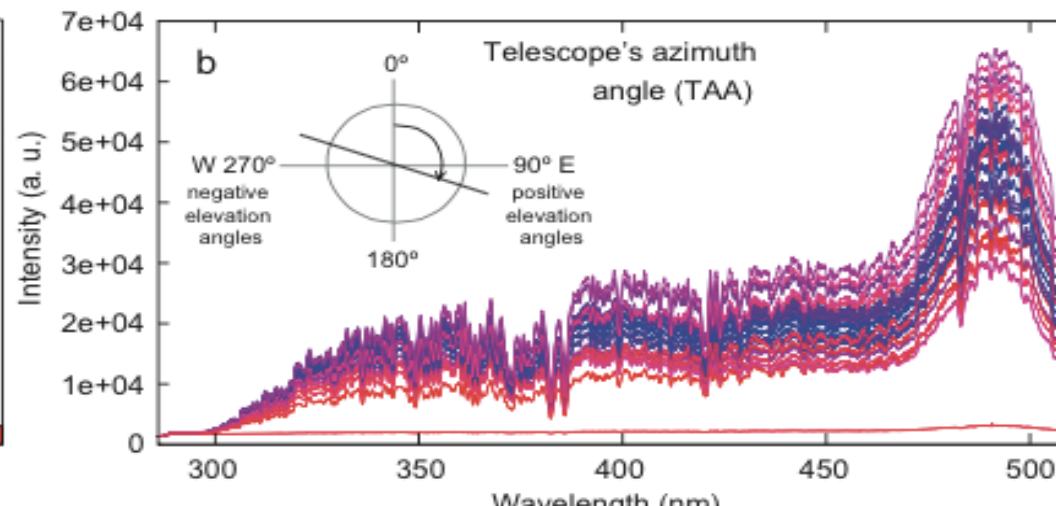
Station	DOFS	Mean TC	Rand	Smoo Rand	Total Rand	Syst	Smoo Syst	Total Syst	Diff30
Eureka	1.3	12.7	1.0	0.6	1.2 (9.3 %)	12.2 %	3.5 %	12.8 %	1.5 (11.7 %)
Ny-Ålesund	1.6	15.8	1.8	0.5	1.9 (11.7 %)	13.3 %	3.4 %	13.8 %	3.9 (24.9 %)
Thule	1.1	15.7	1.3	0.9	1.5 (9.8 %)	14.3 %	3.8 %	14.8 %	1.8 (11.7 %)
Kiruna*	1	17.5	3.5	0.8	3.6 (20.8 %)	25.6 %	8.6 %	27.1 %	0.7 (3.8 %)
Sodankyla	1.1	25.4	1.5	1.7	2.3 (9.0 %)	13.4 %	3.8 %	14.1 %	2.4 (9.3 %)
St Petersburg	1.4	59.4	2.6	2.1	3.3 (5.6 %)	13.9 %	2.4 %	14.2 %	2.8 (4.6 %)
Bremen	1.2	59.6	2.3	1.7	2.9 (4.8 %)	12.9 %	2.9 %	13.3 %	3.1 (5.2 %)
Paris*	1	73.0	5.3	1.4	5.5 (7.6 %)	16.3 %	4.6 %	17.0 %	3.3 (4.8 %)
Zugspitze*	1	12.3	2.2	0.5	2.3 (18.6 %)	20.7 %	5.8 %	21.7 %	1.0 (8.0 %)
Toronto	1.3	95.1	5.1	4.1	6.7 (7.1 %)	12.6 %	2.7 %	13.0 %	19.3 (20.4 %)
Boulder	1.1	57.6	2.6	3.9	4.7 (8.2 %)	12.7 %	2.1 %	13.0 %	5.3 (9.2 %)
Izaña*	1	20.4	3.3	0.2	3.3 (16.0 %)	20.9 %	4.4 %	21.4 %	0.8 (4.0 %)
Mauna Loa	1.1	10.1	1.4	1.0	1.8 (17.3 %)	12.5 %	3.8 %	13.1 %	1.4 (14.0 %)
Mexico City*	1.0	220.9	11.1	2.5	11.4 (5.2 %)	12.0 %	1.2 %	12.1 %	24.0 (10.9 %)
Altzomoni*	1.1	21.8	2.3	1.2	2.6 (11.7 %)	16.0 %	3.2 %	16.3 %	2.3 (10.5 %)
Paramaribo	1.5	64.3	3.4	1.3	3.6 (5.6 %)	12.2 %	3.1 %	12.7 %	11.9 (18.5 %)
Porto Velho	1.1	190.0	3.5	8.3	9.1 (4.8 %)	12.8 %	4.1 %	13.5 %	5.9 (3.1 %)
Saint-Denis	1.2	38.8	2.2	0.8	2.4 (6.1 %)	13.4 %	4.3 %	14.1 %	2.8 (7.2 %)
Maïdo	1.2	20.0	1.4	0.4	1.4 (7.3 %)	12.9 %	2.3 %	13.1 %	1.1 (5.6 %)
Wollongong	1.5	78.9	3.0	2.2	3.7 (4.7 %)	10.9 %	3.0 %	11.6 %	11.6 (15.0 %)
Lauder	1.4	25.6	1.5	0.4	1.6 (6.3 %)	12.4 %	2.6 %	12.8 %	3.6 (14.0 %)
Median	1.1	25.6	2.3	1.2	2.9 (7.6 %)	12.9 %	3.4 %	13.5 %	2.8 (9.3 %)

MAX-DOAS

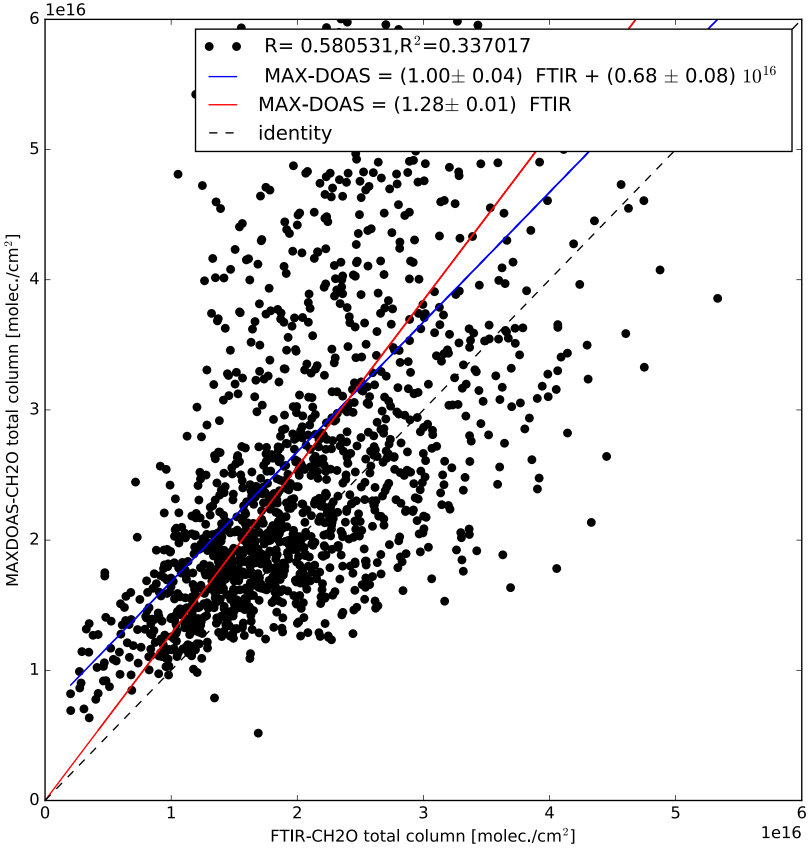
Arellano et al, 2016



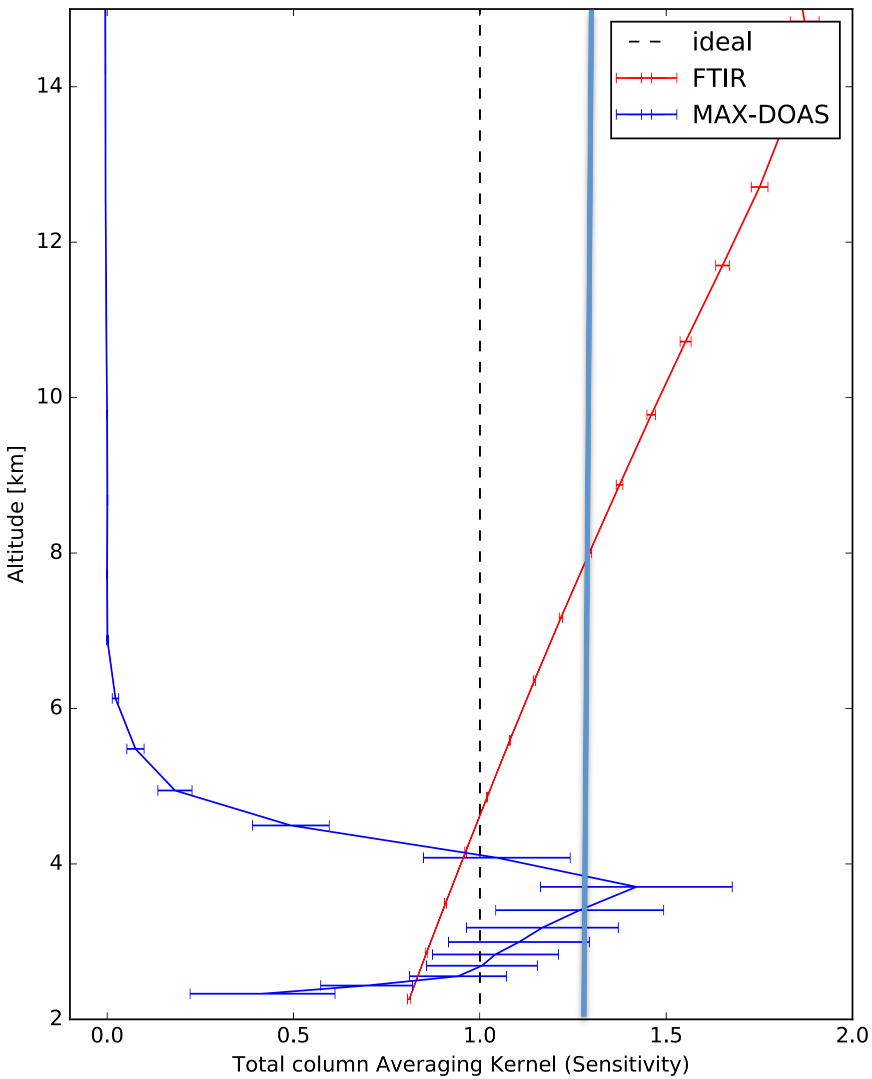




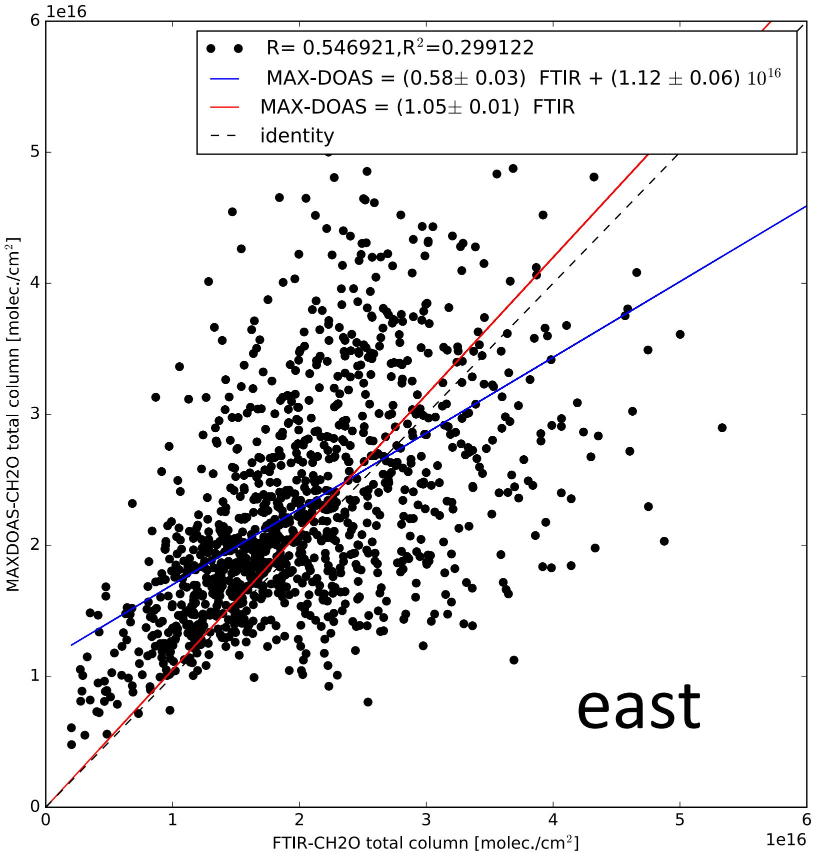
Both: 1.28



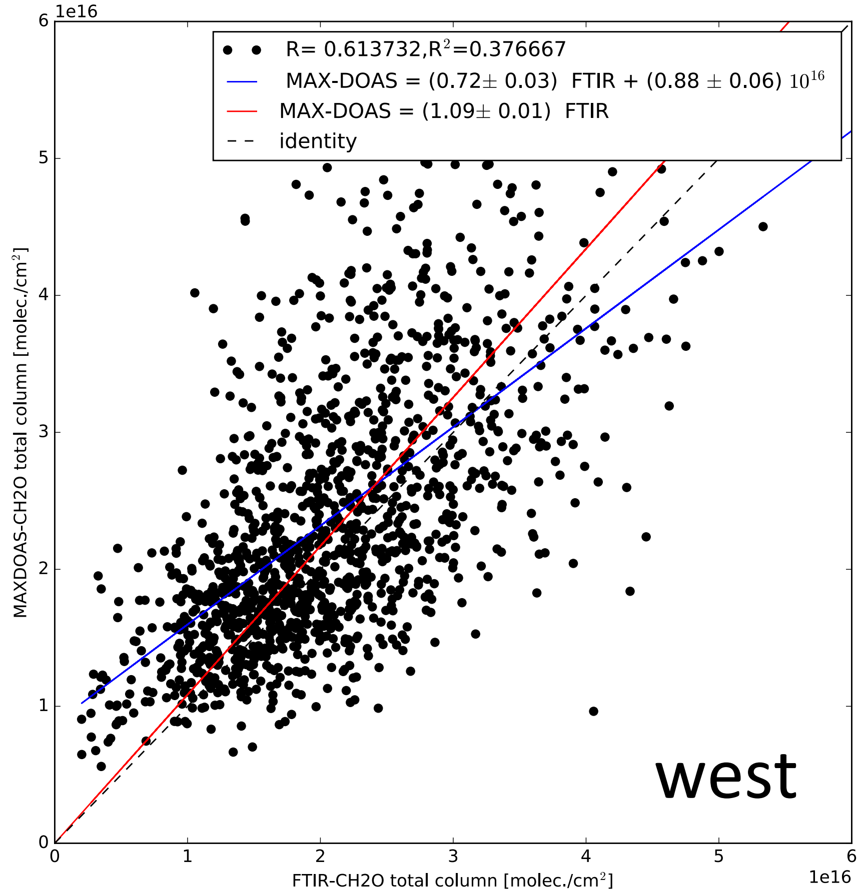
R= 0.580531,R²=0.337017
MAX-DOAS = (1.00± 0.04) FTIR + (0.68 ± 0.08) 10^16
MAX-DOAS = (1.28± 0.01) FTIR
identity
MAXDOAS-CH2O total column [molec./cm²]
FTIR-CH2O total column [molec./cm²]
1e16



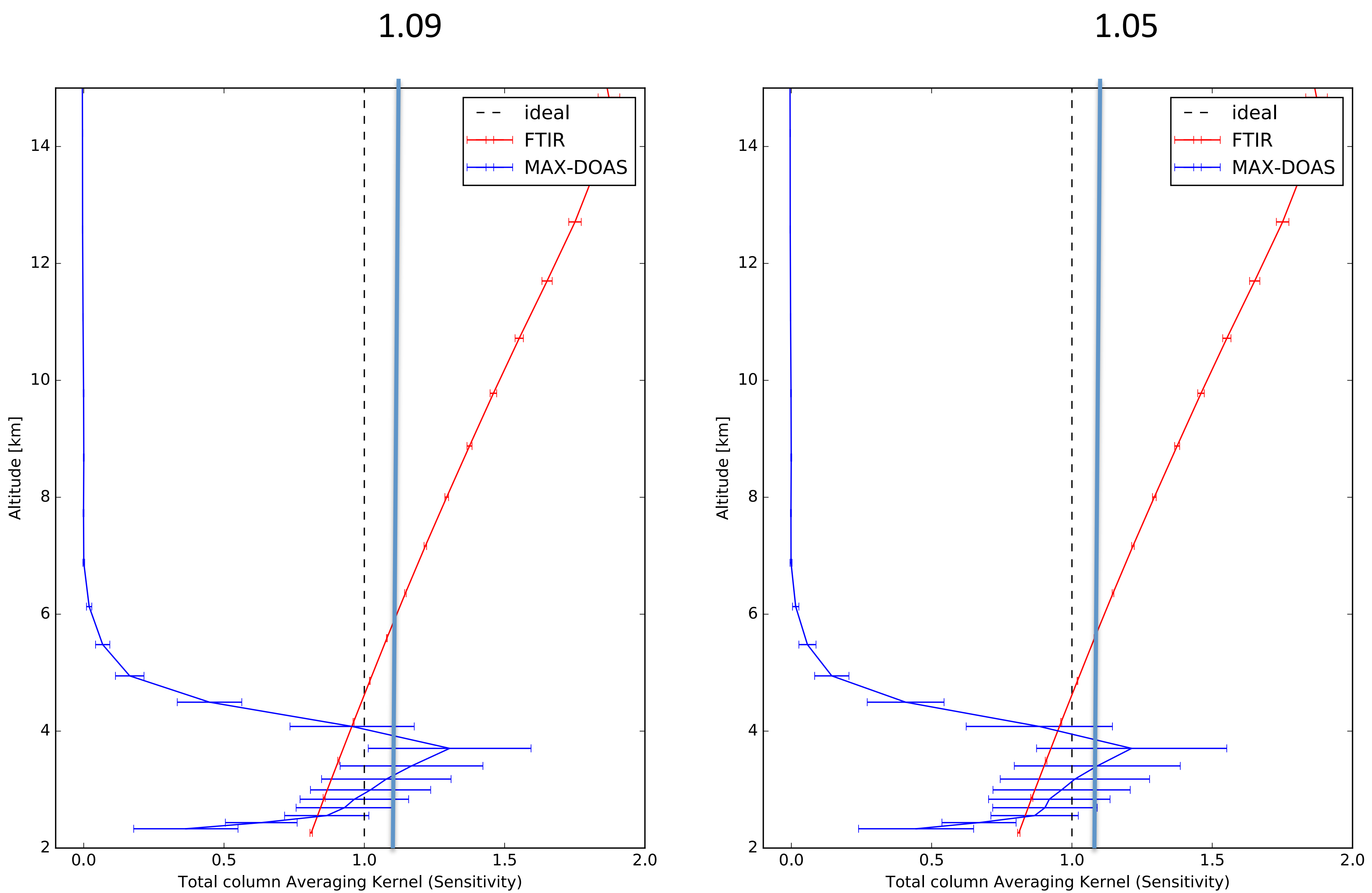
ideal
FTIR
MAX-DOAS
Altitude [km]
Total column Averaging Kernel (Sensitivity)


R= 0.546921,R²=0.299122
MAX-DOAS = (0.58± 0.03) FTIR + (1.12 ± 0.06) 10¹⁶
MAX-DOAS = (1.05± 0.01) FTIR
identity
1e16
MAXDOAS-CH2O total column [molec./cm²]
FTIR-CH2O total column [molec./cm²]
east

1.09

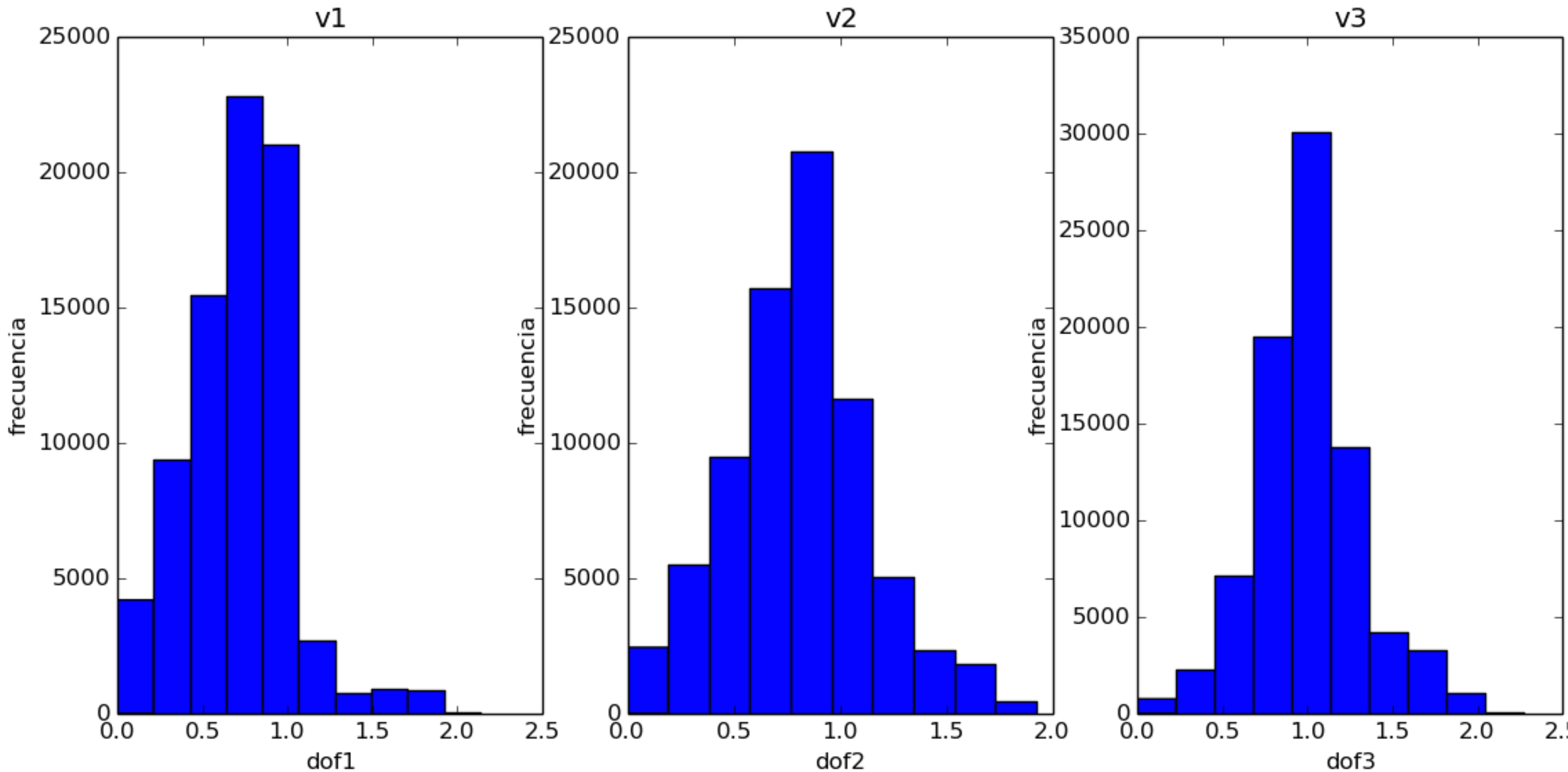

R= 0.613732,R²=0.376667
MAX-DOAS = (0.72± 0.03) FTIR + (0.88 ± 0.06) 10¹⁶
MAX-DOAS = (1.09± 0.01) FTIR
identity
1e16
MAXDOAS-CH2O total column [molec./cm²]
FTIR-CH2O total column [molec./cm²]
west

1.05



1.09
1.05
ideal
FTIR
MAX-DOAS
Altitude [km]
Total column Averaging Kernel (Sensitivity)
0.0
0.5
1.0
1.5
2.0
2
4
6
8
10
12
14

1.5


v1
v2
v3
25000
20000
15000
10000
5000
0
25000
20000
15000
10000
5000
0
35000
30000
25000
20000
15000
10000
5000
0
frecuencia
frecuencia
frecuencia
0.0 0.5 1.0 1.5 2.0 2.5
0.0 0.5 1.0 1.5 2.0
0.0 0.5 1.0 1.5 2.0 2.5
dof1
dof2
dof3

The apriori contribution

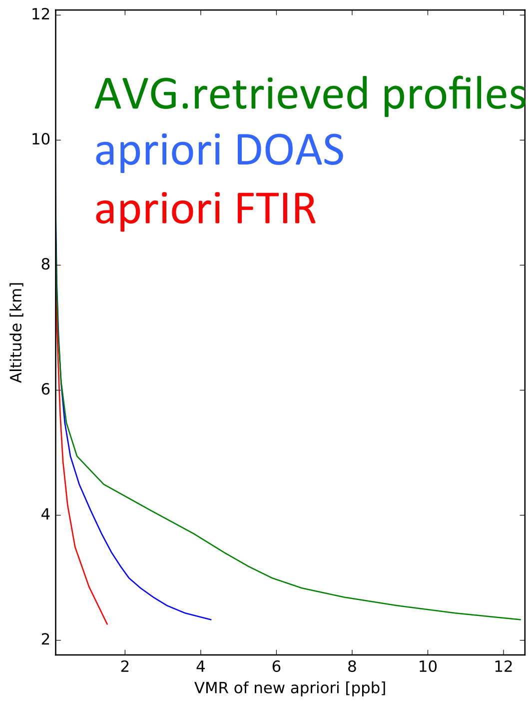
$$\hat{\vec{x}} - \vec{x}_{apr} = \mathbf{A}(\vec{x}_{true} - \vec{x}_{apr}) + \epsilon$$

$$\vec{g}^{T} \cdot (\hat{\vec{x}} - \vec{x}_{apr}) = \vec{g}^{T} \cdot \mathbf{A}(\vec{x}_{true} - \vec{x}_{apr}) + error$$

$$\hat{col} - col_{apr} = \mathbf{a}^{\mathbf{T}}(\vec{x}_{true} - \vec{x}_{apr}) + error$$

$$\hat{col} = \mathbf{a}^{\mathbf{T}}\vec{x}_{true} + (col_{apr} - \mathbf{a}^{\mathbf{T}}\vec{x}_{apr}) + error$$

$$\hat{col} = \mathbf{a}^{\mathbf{T}}\vec{x}_{true} - \underbrace{(\mathbf{a}^{\mathbf{T}} - \mathbf{1}) \cdot \vec{x}_{apr}}_{\text{apriori contribution}} + error$$



Equations from Rodgers

$$\hat{col}_{east} = \mathbf{a^T}_{east}\vec{x}_{true} + (col_{apr} - \mathbf{a^T}_{east}\vec{x}_{apr}) + error$$

$$\hat{col}_{west} = \mathbf{a^T}_{west}\vec{x}_{true} + (col_{apr} - \mathbf{a^T}_{west}\vec{x}_{apr}) + error$$

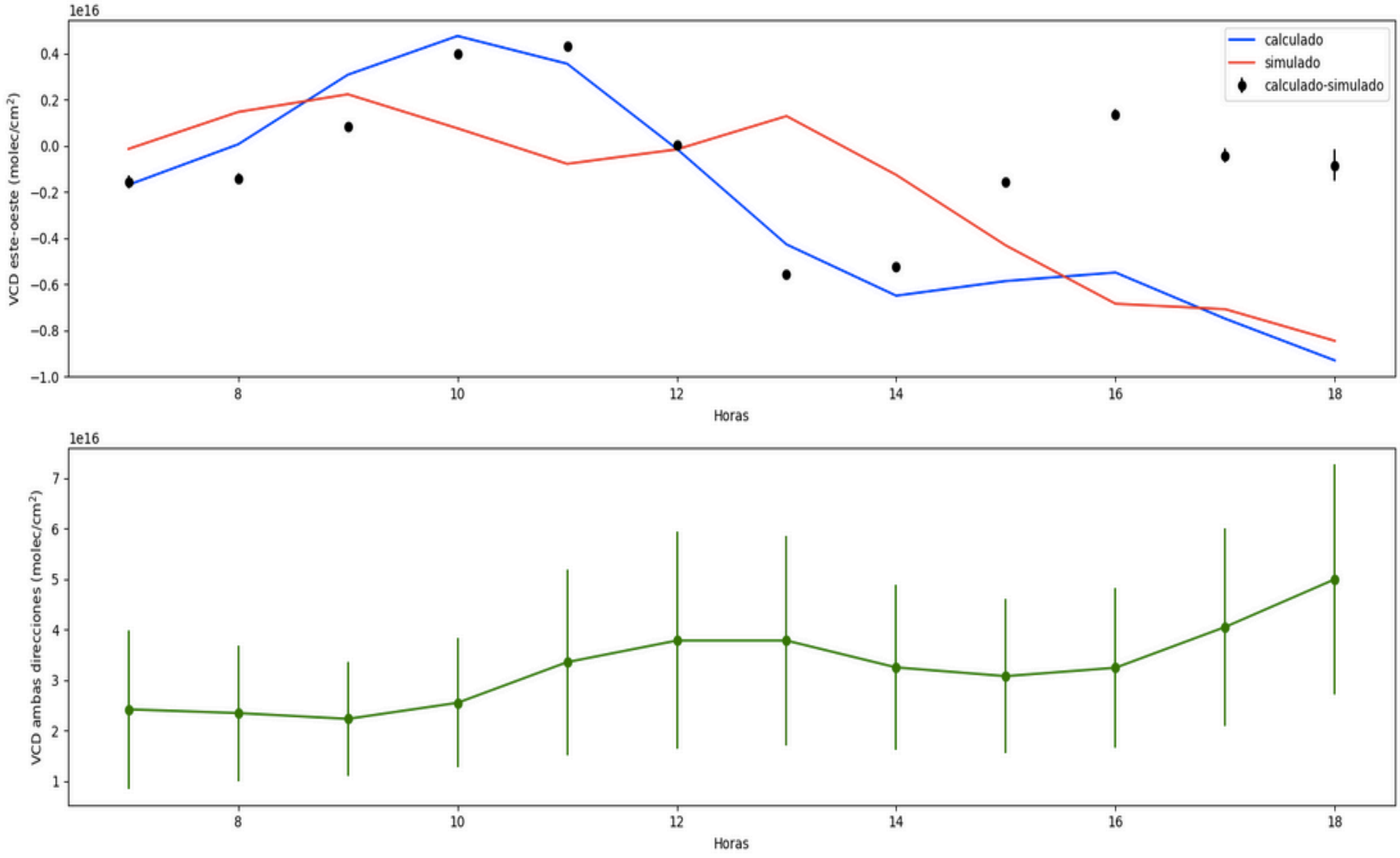
$$\hat{col}_{est} - \hat{col}_{west} = (\mathbf{a^T}_{east} - \mathbf{a^T}_{west})\vec{x}_{true} - (\mathbf{a^T}_{east} - \mathbf{a^T}_{west})\vec{x}_{apr}) +$$

$$\Delta\hat{col}_{est-west} = \underbrace{(\mathbf{a^T}_{east} - \mathbf{a^T}_{west})}_{\text{this we have}}\underbrace{(\vec{x}_{true} - \vec{x}_{apr})}_{\text{this we estimate}} + error_{random}$$

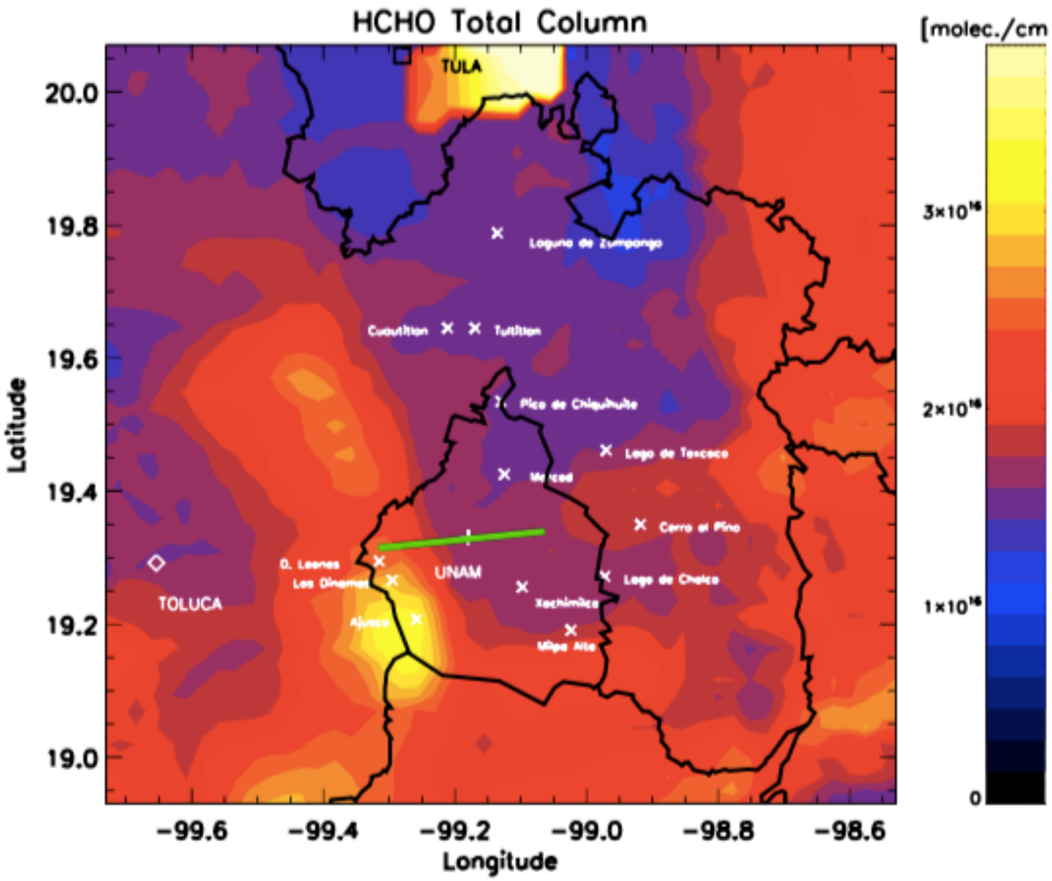
$$\underbrace{\vec{x}_{true} := \hat{\vec{x}}_{both}}_{our\ optimal\ estimation}$$

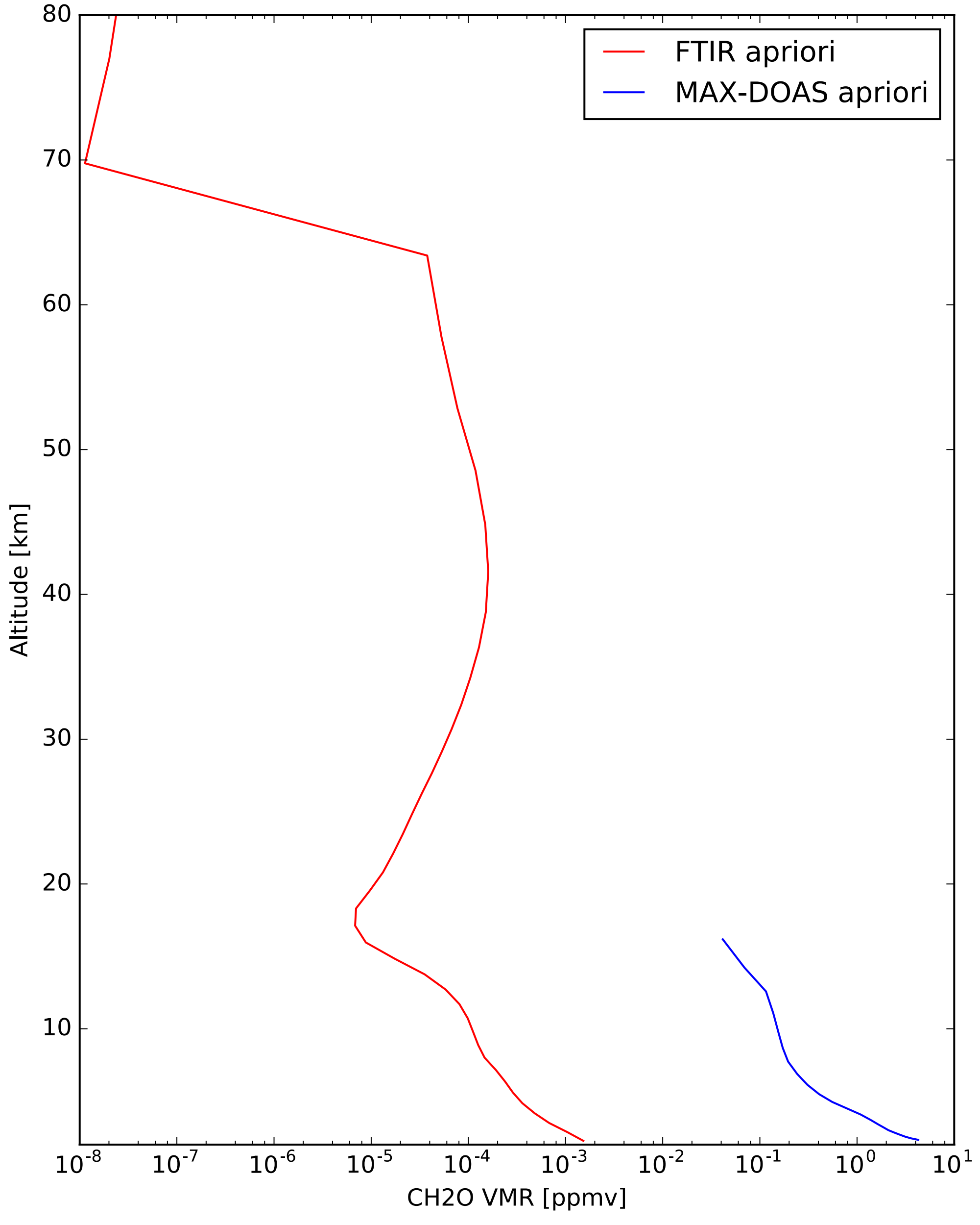
$$\Delta\hat{col}^{est-west}_{simulated} = \underbrace{(\mathbf{a^T}_{east} - \mathbf{a^T}_{west})}_{\text{this we have}}\underbrace{(\vec{x}_{both} - \vec{x}_{apr})}_{\text{this we estimate}}$$

CH2O-MAX-DOAS



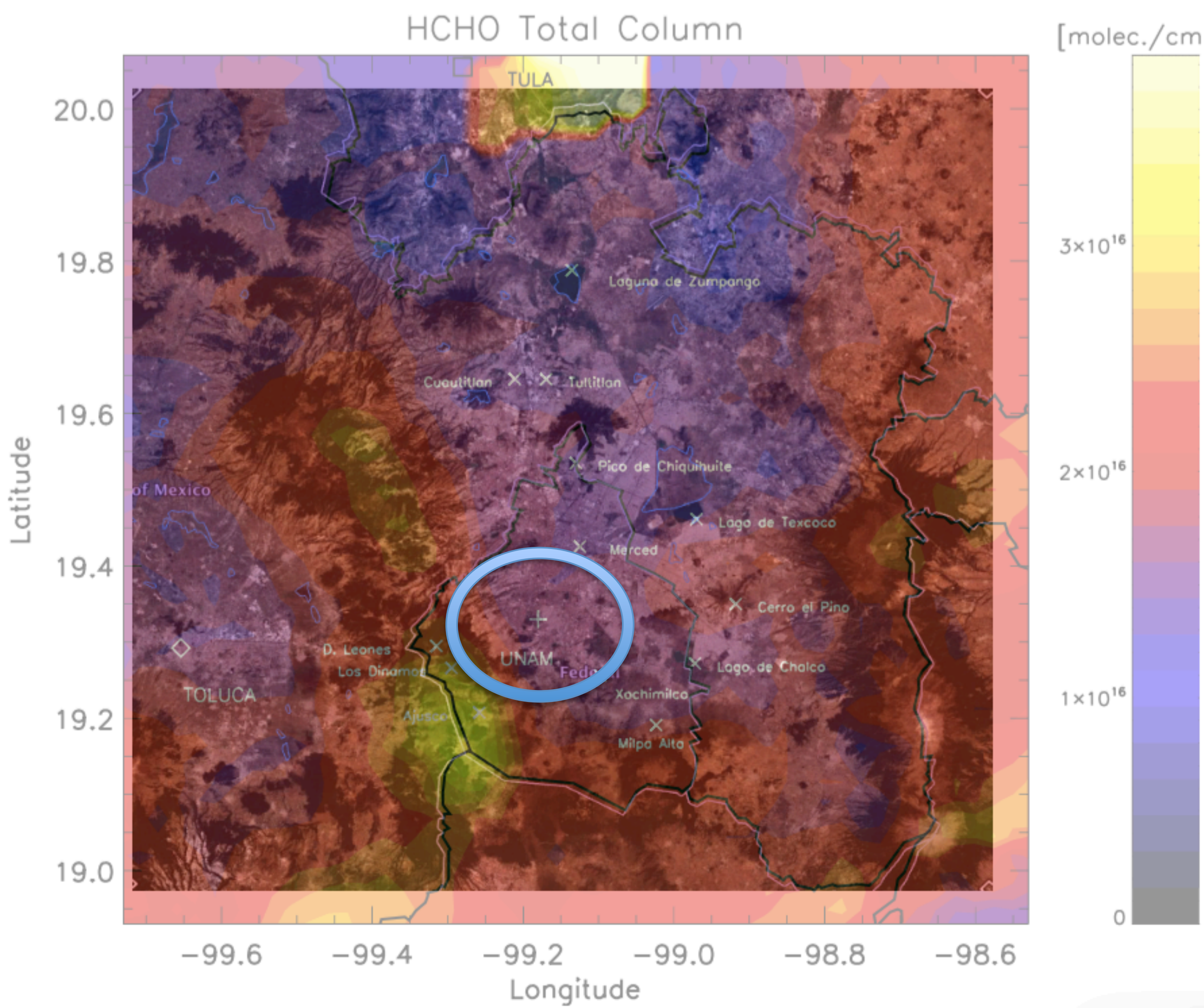
CH2O from OMI





FTIR apriori
MAX-DOAS apriori
Altitude [km]
CH2O VMR [ppmv]
80
70
60
50
40
30
20
10
10^-8
10^-7
10^-6
10^-5
10^-4
10^-3
10^-2
10^-1
10^0
10^1

Mexico City in the early afternoon



The a priori Contribution

$$\hat{\vec{x}} - \vec{x}_{apr} = \mathbf{A}(\vec{x}_{true} - \vec{x}_{apr}) + \epsilon$$

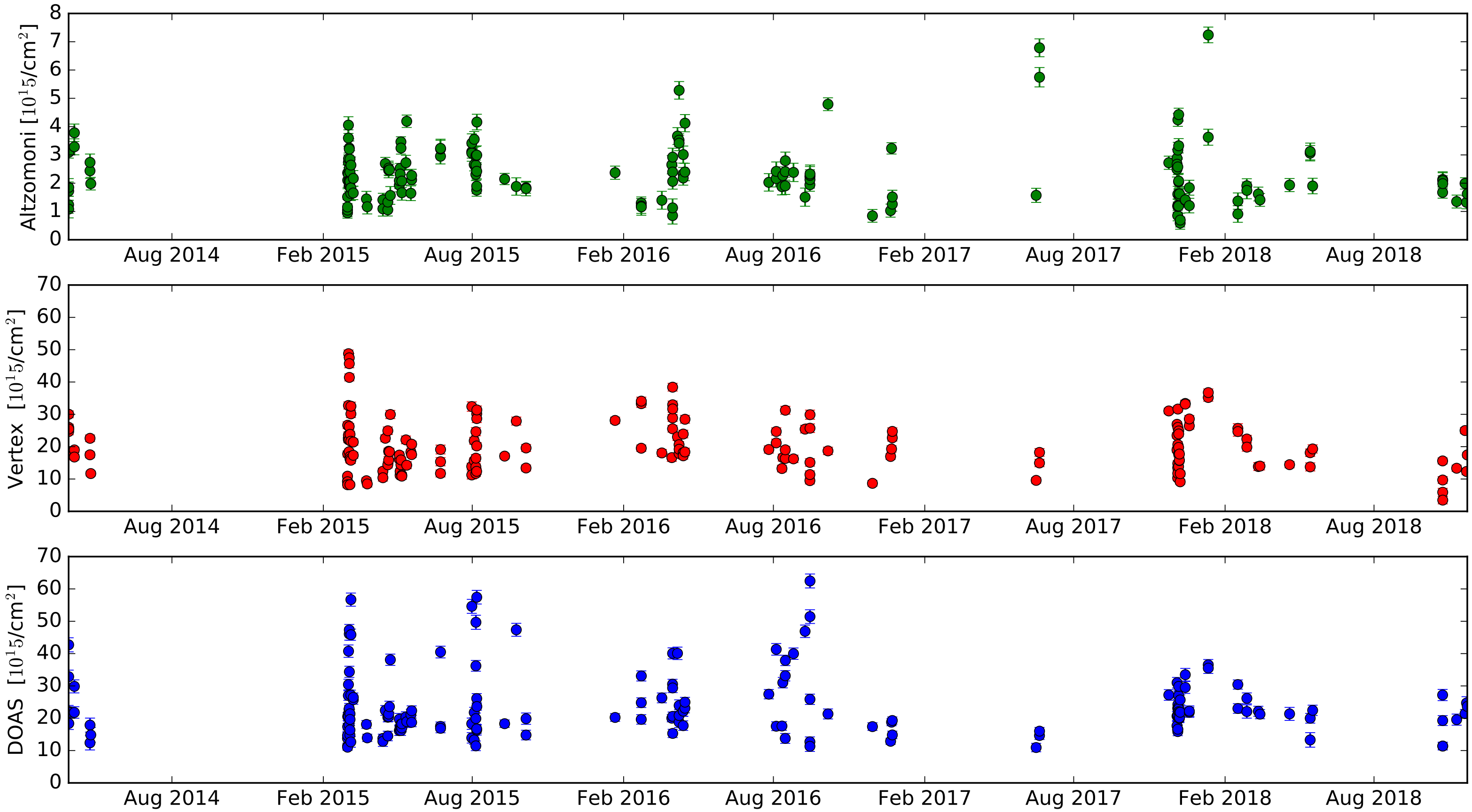
$$\vec{g}^{\,T} \cdot (\hat{\vec{x}} - \vec{x}_{apr}) = \vec{g}^{\,T} \cdot \mathbf{A}(\vec{x}_{true} - \vec{x}_{apr}) + error$$

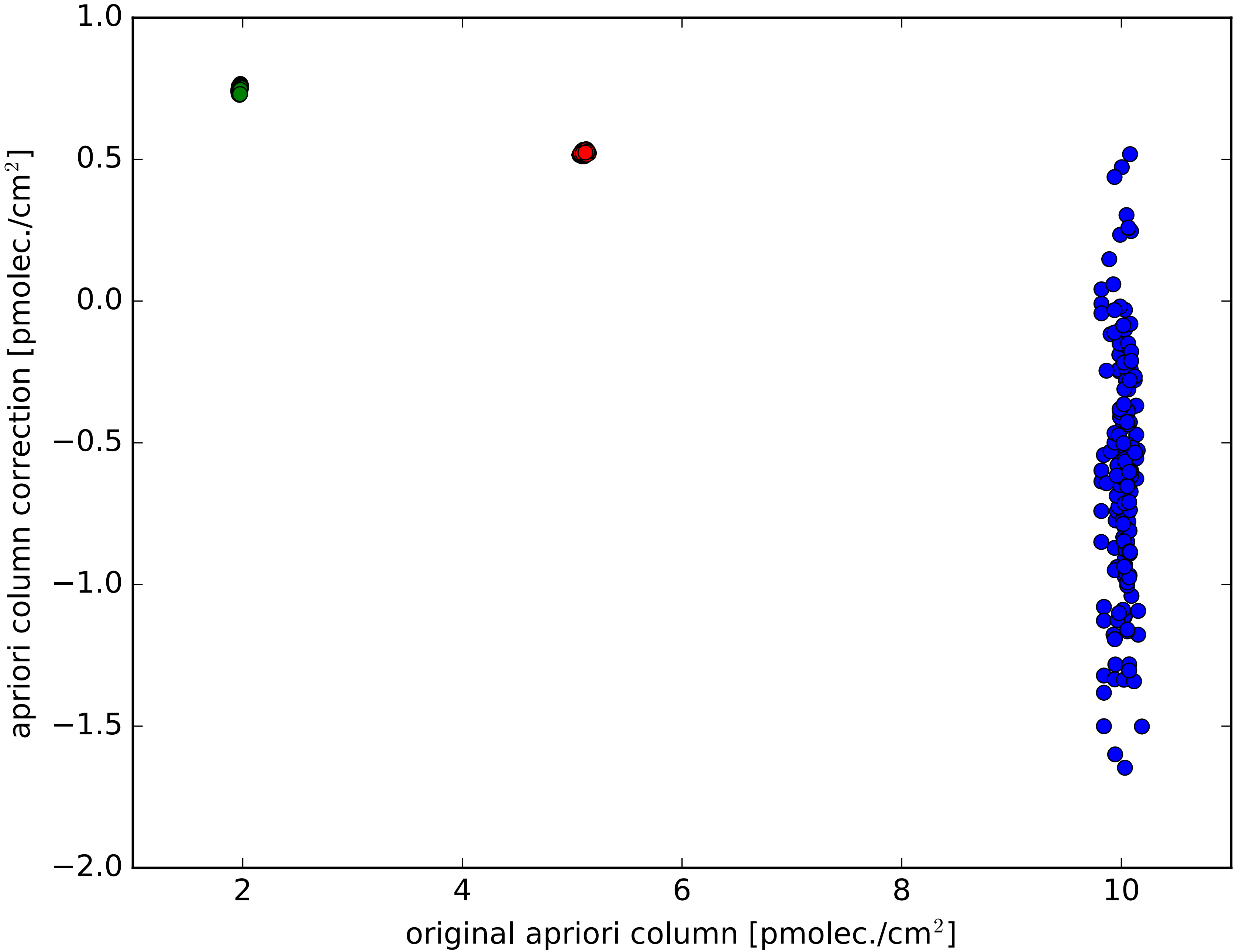
$$\hat{col} - col_{apr} = \mathbf{a}^{\mathbf{T}}(\vec{x}_{true} - \vec{x}_{apr}) + error$$

$$\hat{col} = \mathbf{a}^{\mathbf{T}}\vec{x}_{true} + (col_{apr} - \mathbf{a}^{\mathbf{T}}\vec{x}_{apr}) + error$$

$$\hat{col} = \mathbf{a}^{\mathbf{T}}\vec{x}_{true} - \underbrace{(\mathbf{a}^{\mathbf{T}} - \mathbf{1}) \cdot \vec{x}_{apr}}_{\text{apriori contribution}} + error$$

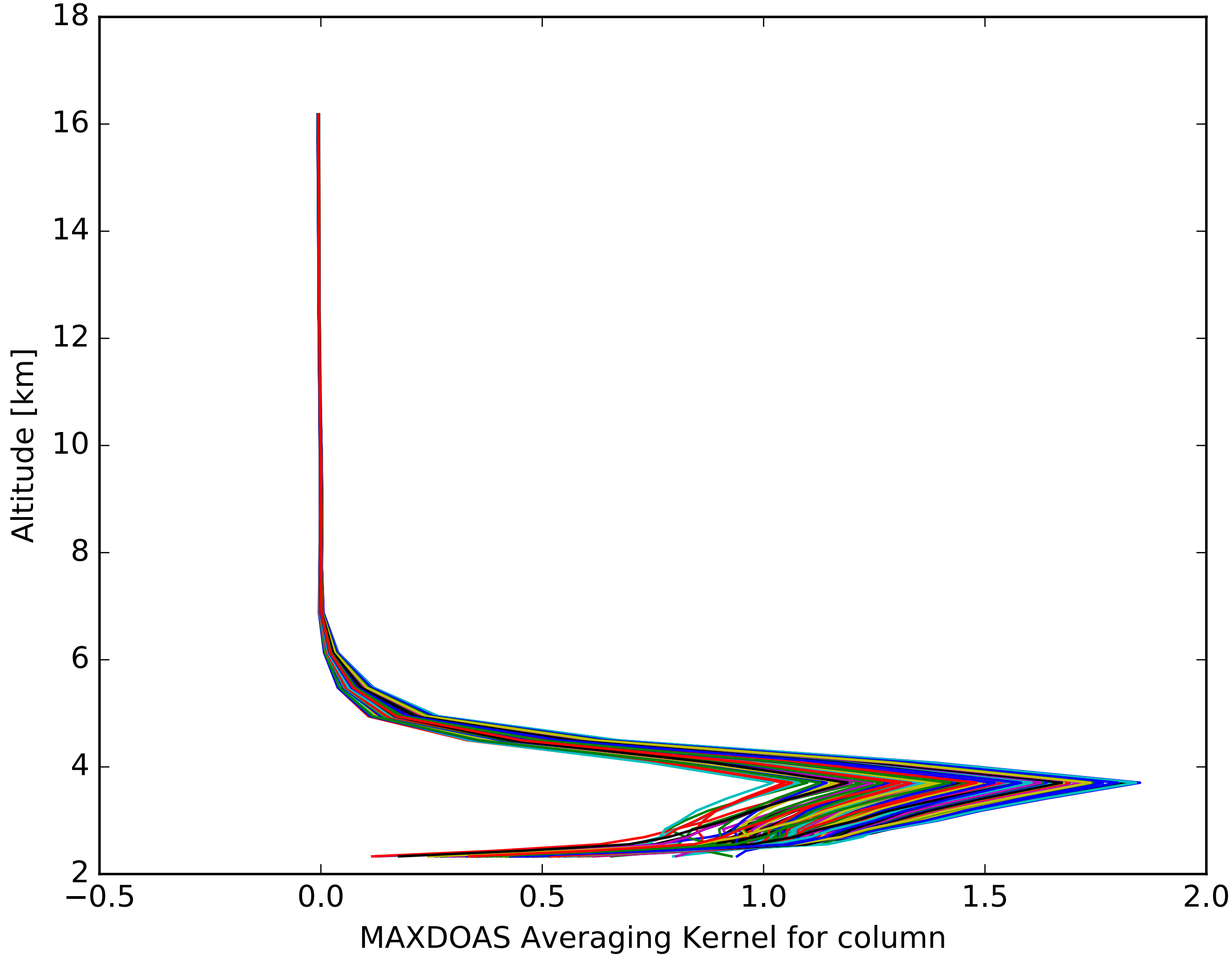
Altzomoni, Vertex, MAXDOAS hourly means



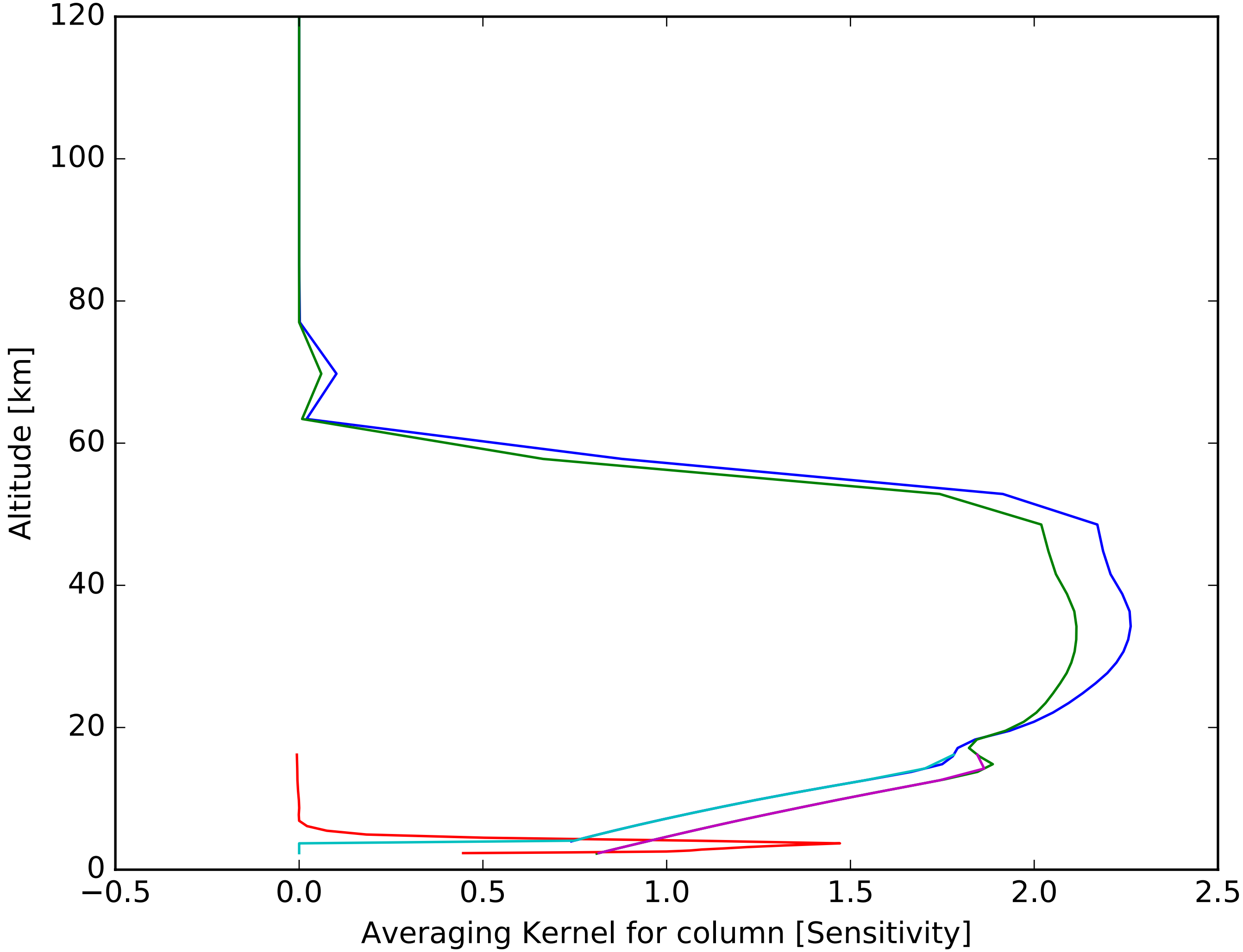


1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
2
4
6
8
10
apriori column correction [pmolec./cm^2]
original apriori column [pmolec./cm^2]

AK for vertical column

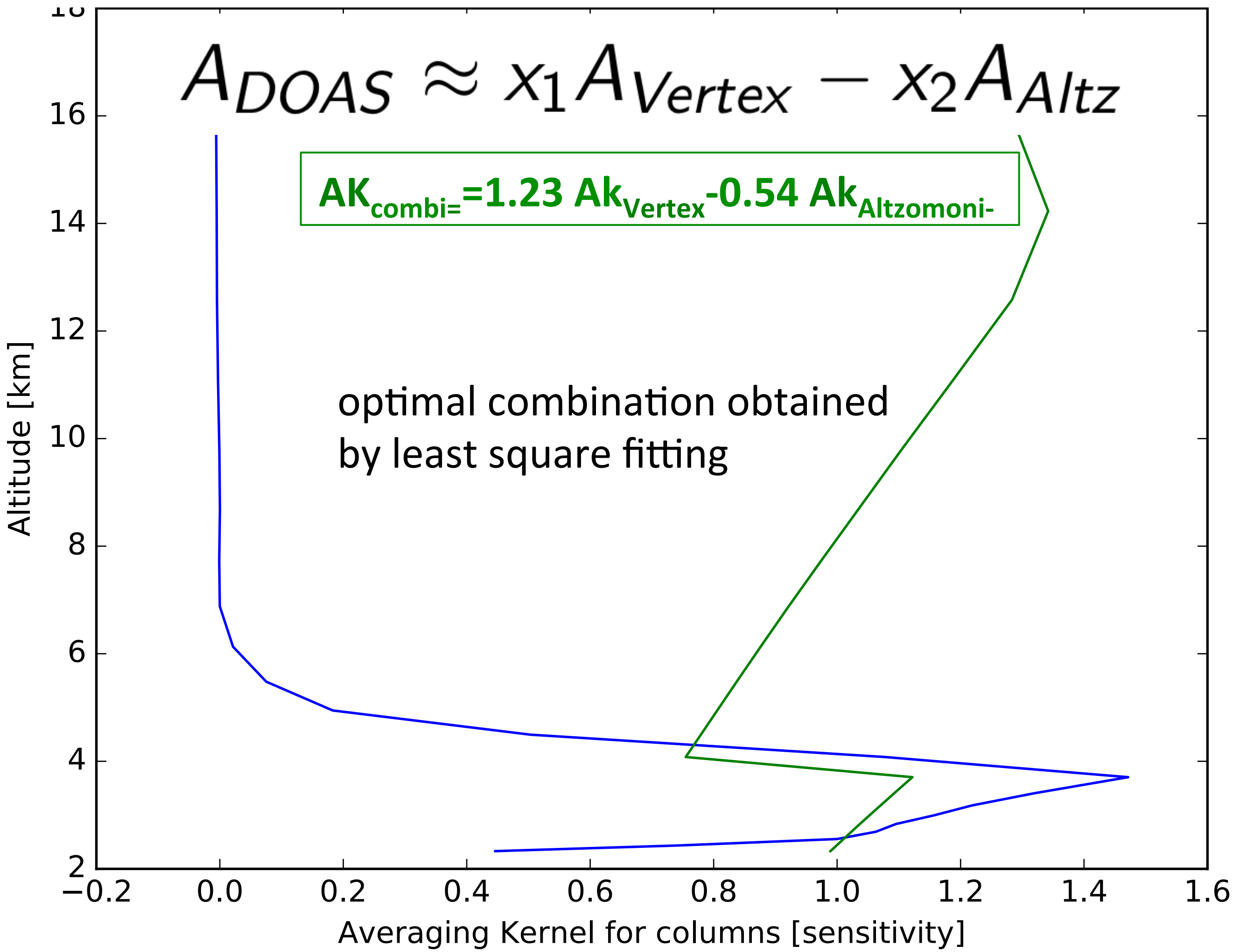


AK for vertical column



AK for vertical column

$$\left|(A_{DOAS} - x_1 A_{Vertex} - x_2 a A_{Altz}) SA (A_{DOAS} - x_1 A_{Vertex} - x_2 A_{Altz})^T\right|$$



CH2O-Vertex+Altzomoni

original
0.80 +/- 0.02 R: 0.63 R^2: 0.40
(8.2 +/-1.2) Pmolec.+ (0.51+/- 0.05) x

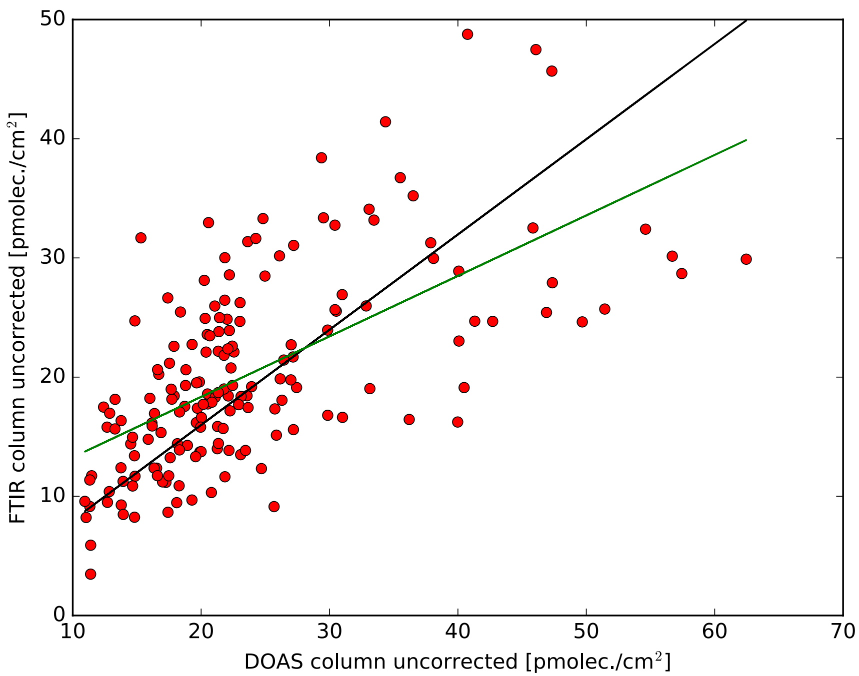
DOAS	FTIR
STD:10.1	8.1
AVG: 23.23	20.3

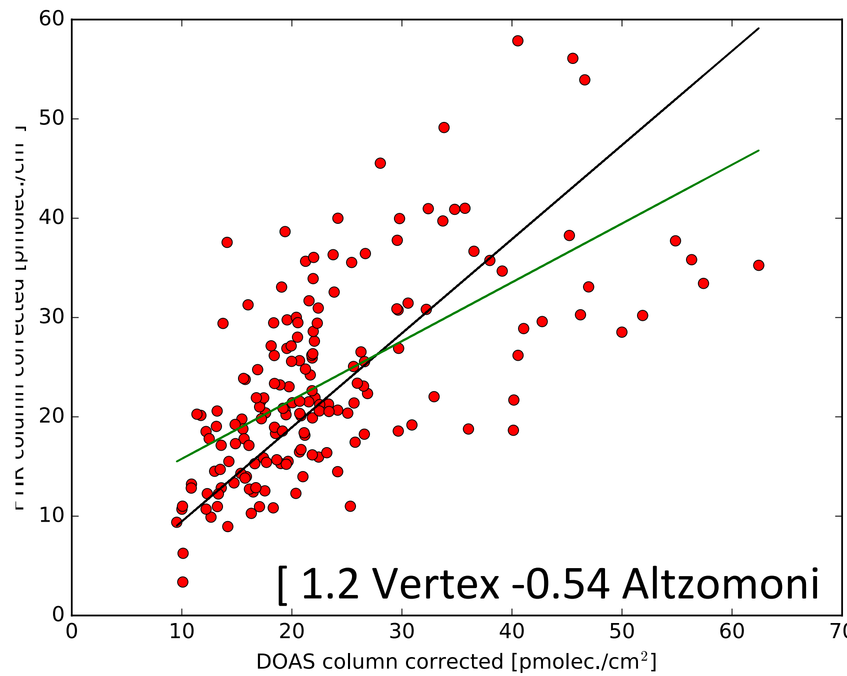
Diff: 3.54 +/- 0.61 pmolec/ cm2
(16.3 +/- 2.8) % rms: 9.2 %

0.95+/- 0.025
R: 0.63 R^2: 0.393
(9.86 +/- 1.43)Pmolec. + (0.59 +/-0.06) x

DOAS	FTIR
STD: 10.3	9.7
AVG: 23.2	23.6

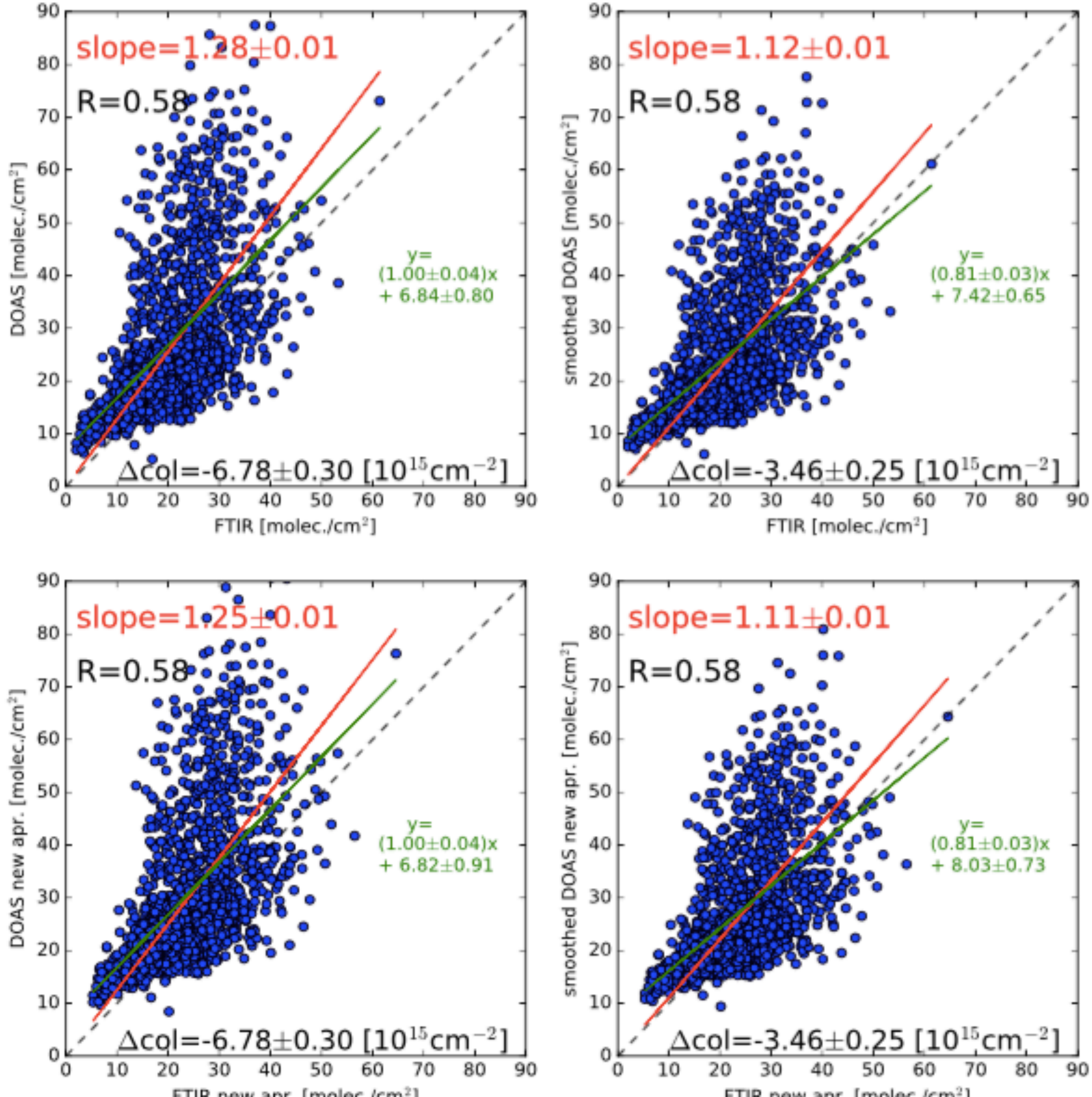
Diff: -0.38 +/- 0.66 pmolec/cm2
(-1.635 +/- 2.8) % rms: 9.2 %





direct

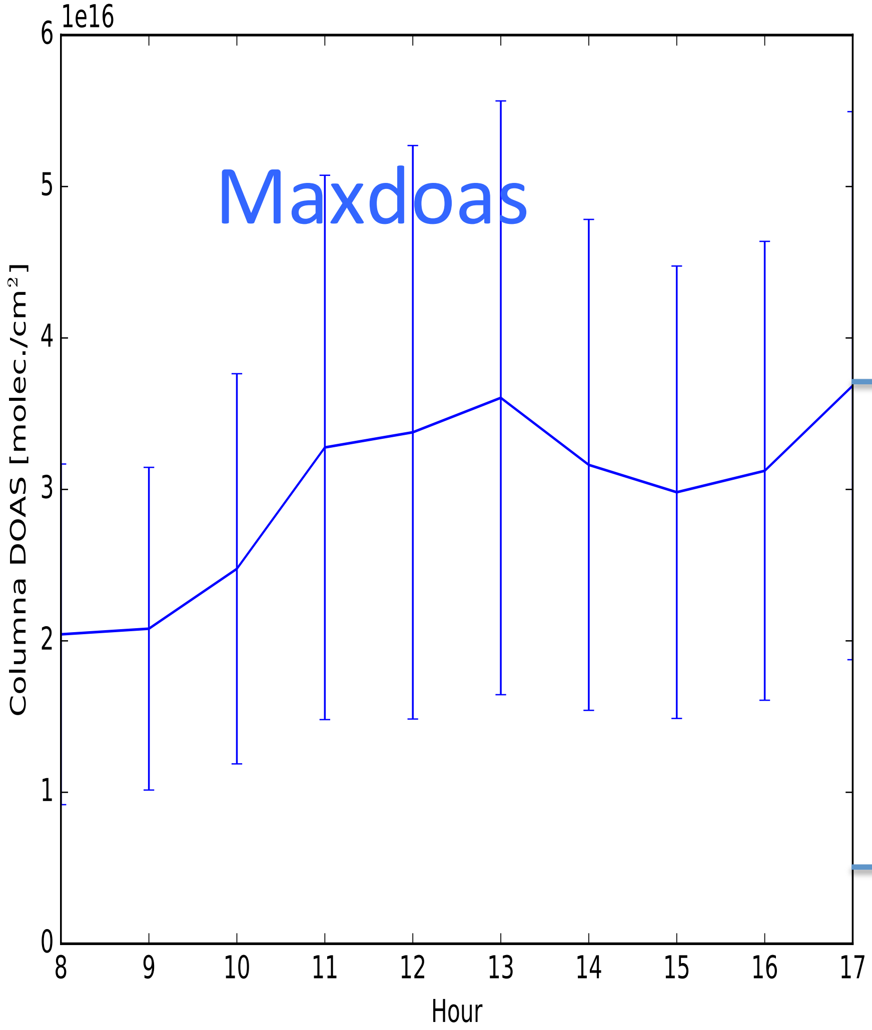
AK smooth

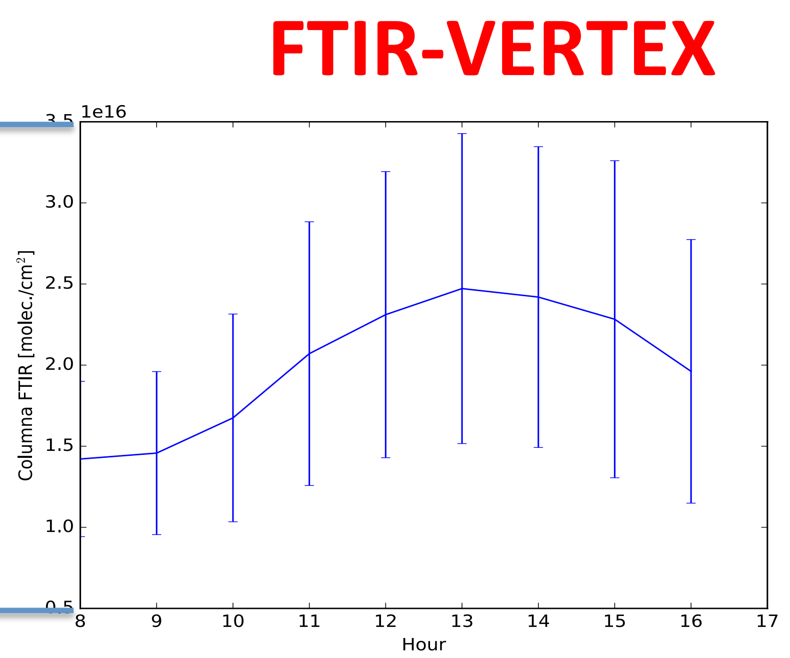


apriori corrected

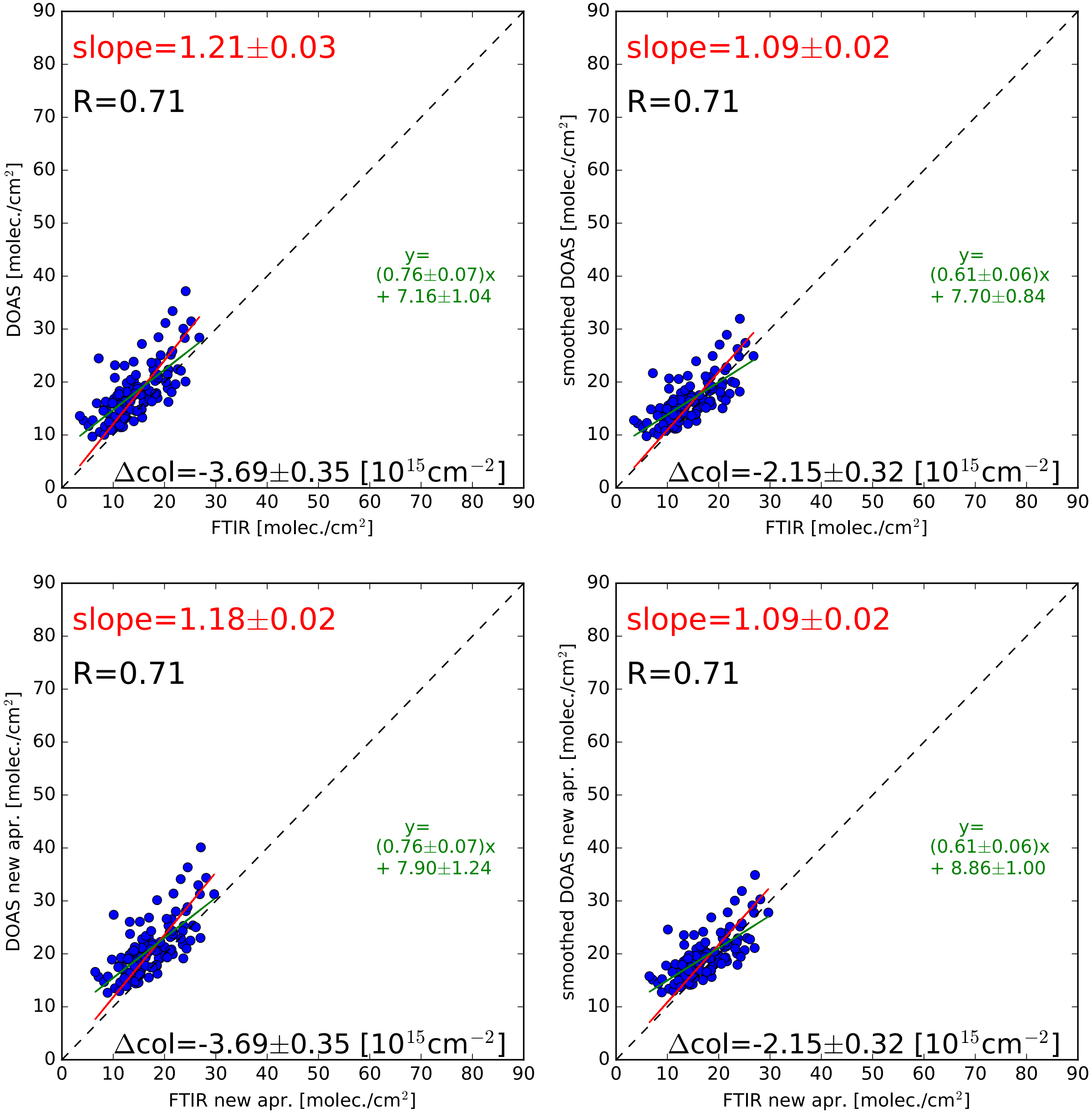
AK smoothed + apriori corrected

Comparison Vertex-DOAS



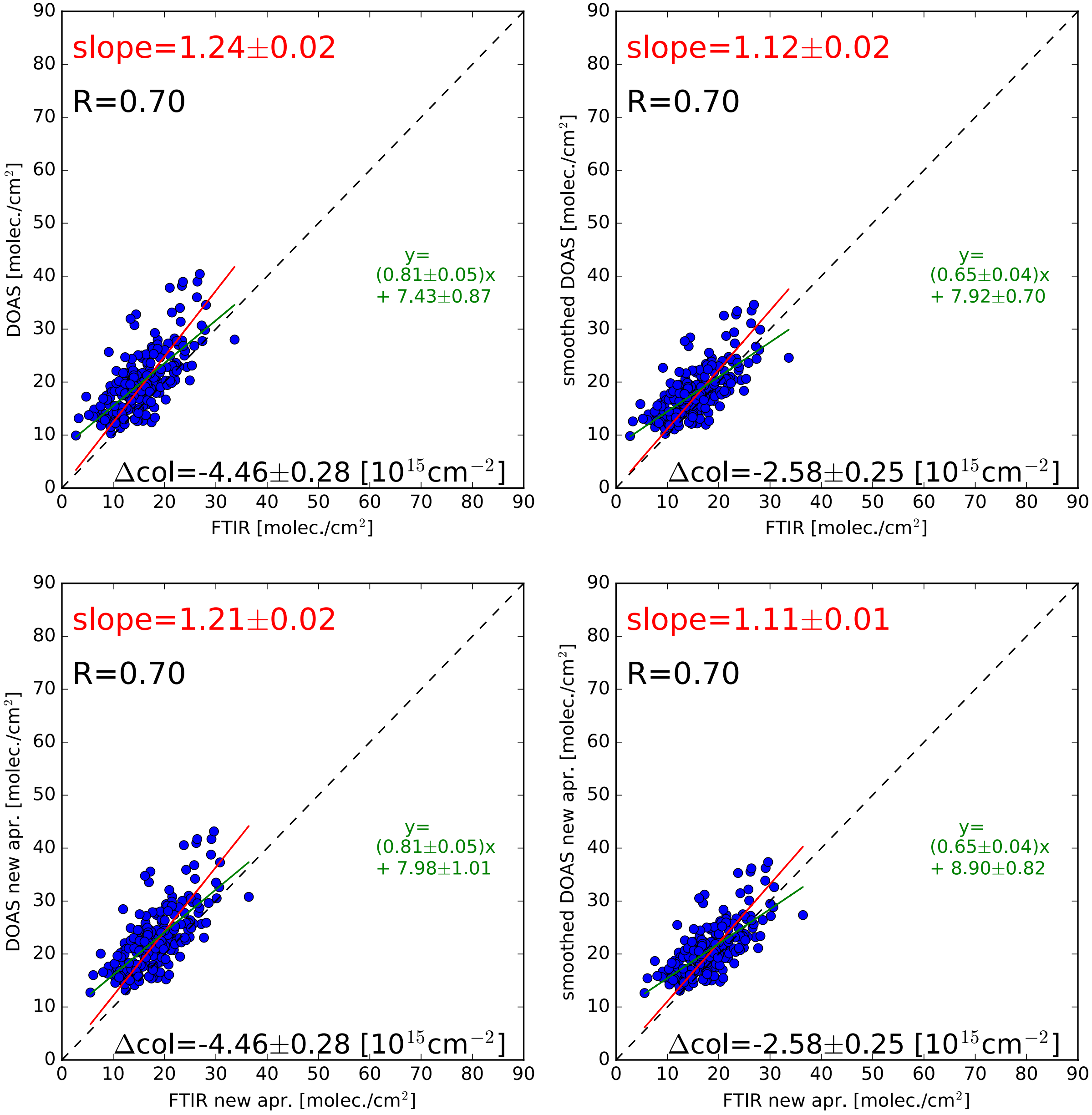


9:00 LT (UT-6)



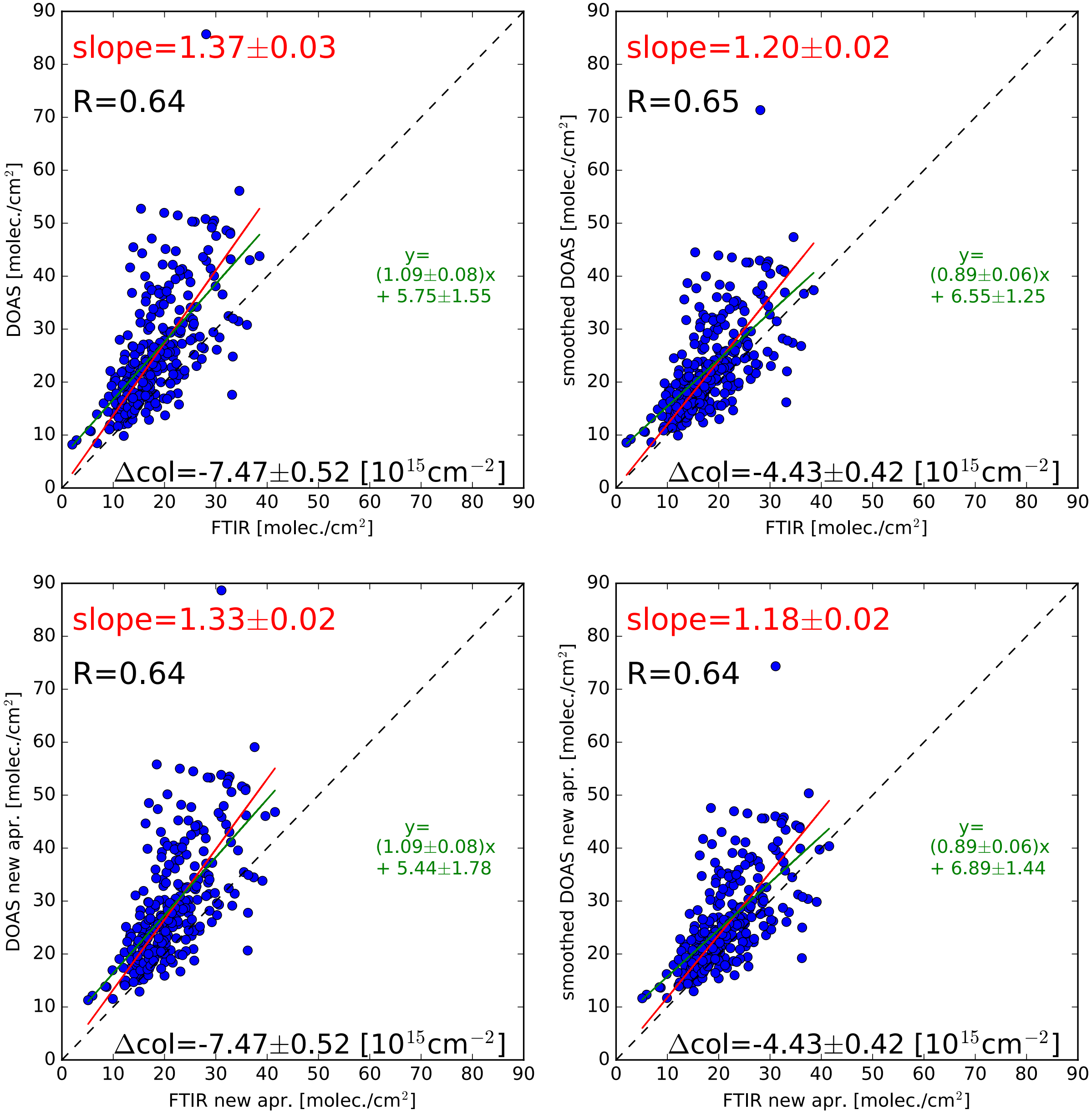
slope=1.21±0.03
R=0.71
y=
(0.76±0.07)x
+ 7.16±1.04
Δcol=-3.69±0.35 [10^15cm^-2]
DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=1.09±0.02
R=0.71
y=
(0.61±0.06)x
+ 7.70±0.84
Δcol=-2.15±0.32 [10^15cm^-2]
smoothed DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=1.18±0.02
R=0.71
y=
(0.76±0.07)x
+ 7.90±1.24
Δcol=-3.69±0.35 [10^15cm^-2]
DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]
slope=1.09±0.02
R=0.71
y=
(0.61±0.06)x
+ 8.86±1.00
Δcol=-2.15±0.32 [10^15cm^-2]
smoothed DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]

10:00 LT (UT-6)



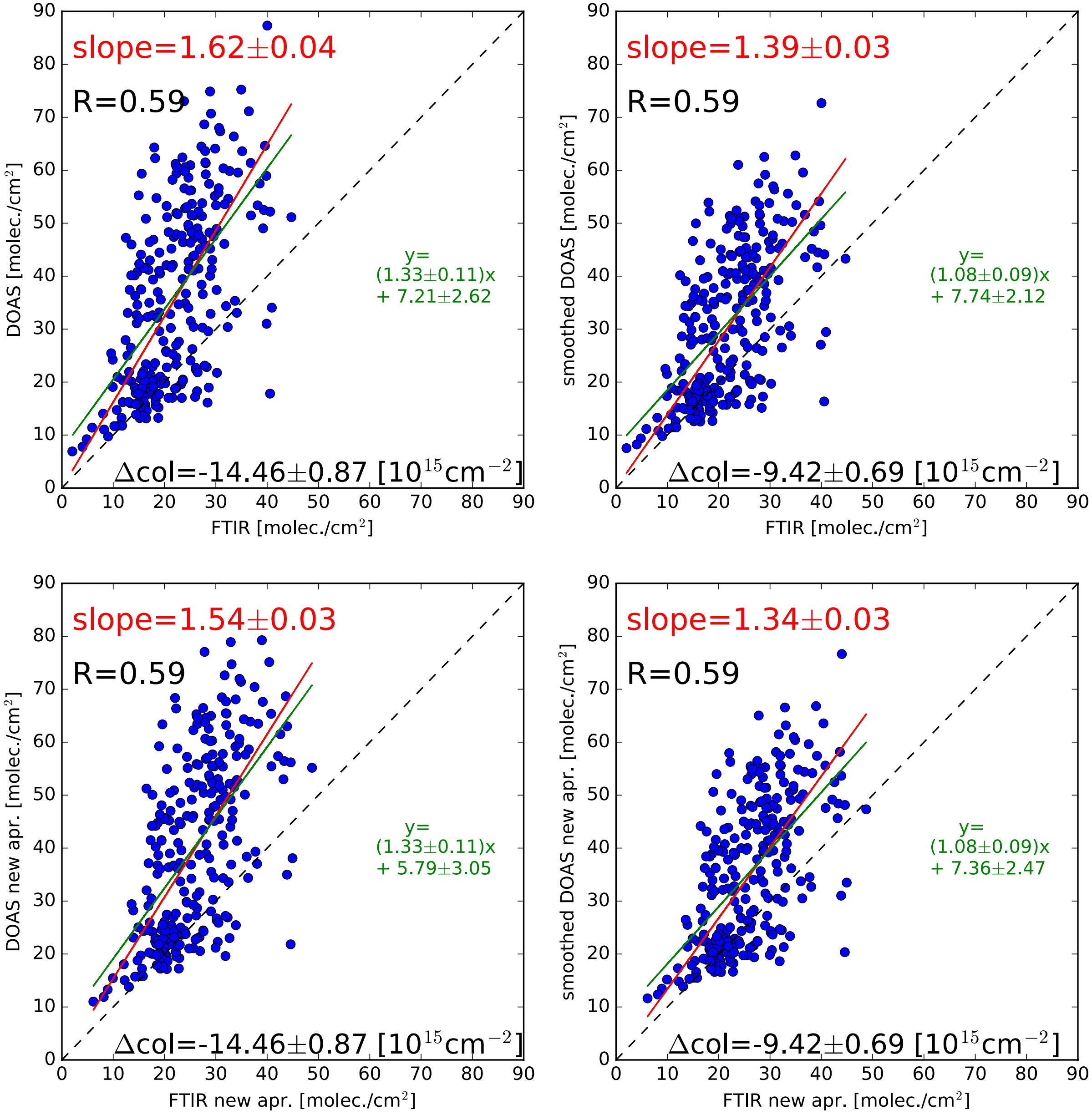
slope=1.24±0.02
R=0.70
y=
(0.81±0.05)x
+ 7.43±0.87
Δcol=-4.46±0.28 [10^15cm^-2]
DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=1.12±0.02
R=0.70
y=
(0.65±0.04)x
+ 7.92±0.70
Δcol=-2.58±0.25 [10^15cm^-2]
smoothed DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=1.21±0.02
R=0.70
y=
(0.81±0.05)x
+ 7.98±1.01
Δcol=-4.46±0.28 [10^15cm^-2]
DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]
slope=1.11±0.01
R=0.70
y=
(0.65±0.04)x
+ 8.90±0.82
Δcol=-2.58±0.25 [10^15cm^-2]
smoothed DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]

11:00LT (UT-6)

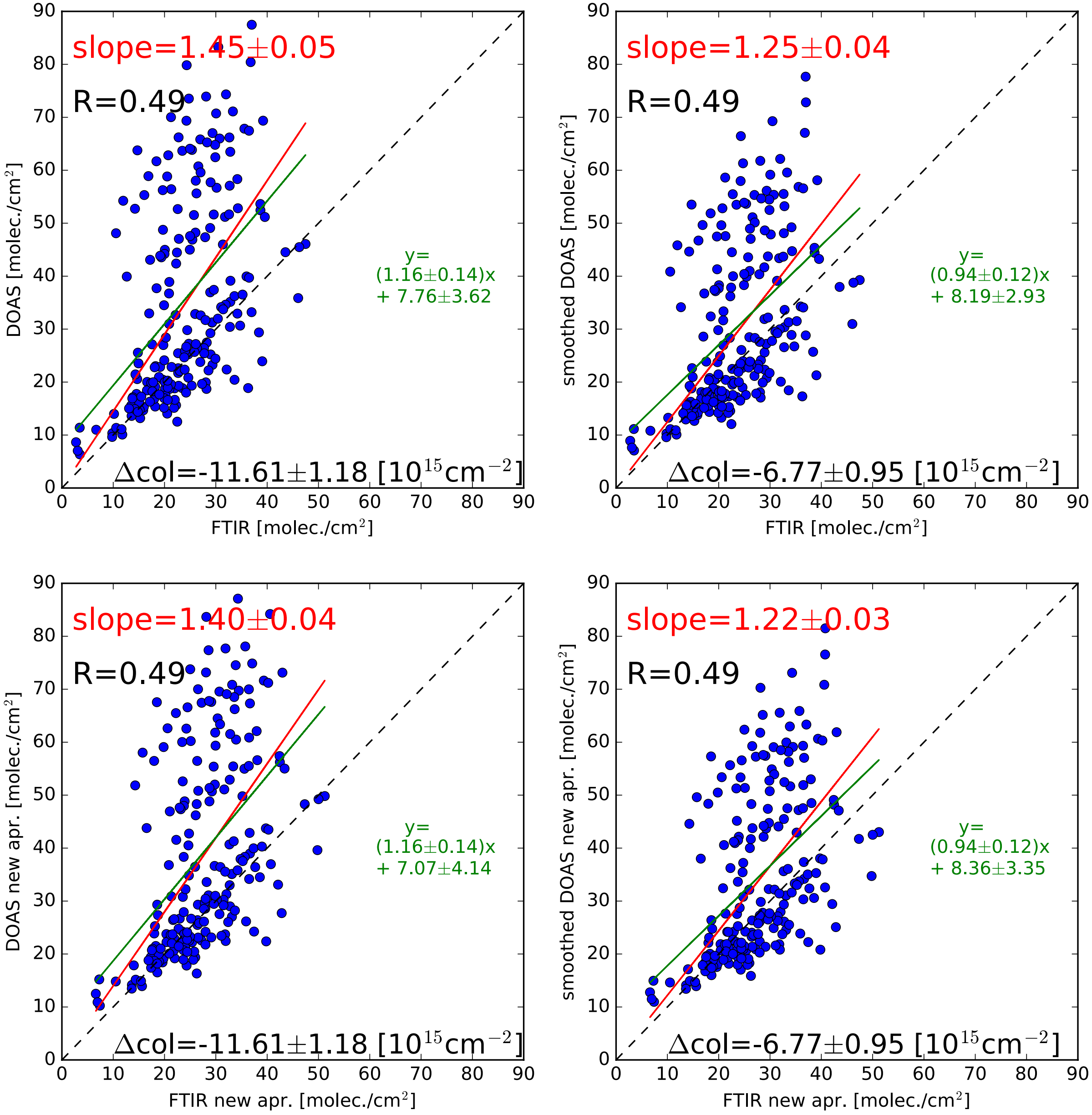


slope=1.37±0.03
R=0.64
y=
(1.09±0.08)x
+ 5.75±1.55
Δcol=-7.47±0.52 [10^15cm^-2]
DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=1.20±0.02
R=0.65
y=
(0.89±0.06)x
+ 6.55±1.25
Δcol=-4.43±0.42 [10^15cm^-2]
smoothed DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=1.33±0.02
R=0.64
y=
(1.09±0.08)x
+ 5.44±1.78
Δcol=-7.47±0.52 [10^15cm^-2]
DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]
slope=1.18±0.02
R=0.64
y=
(0.89±0.06)x
+ 6.89±1.44
Δcol=-4.43±0.42 [10^15cm^-2]
smoothed DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]

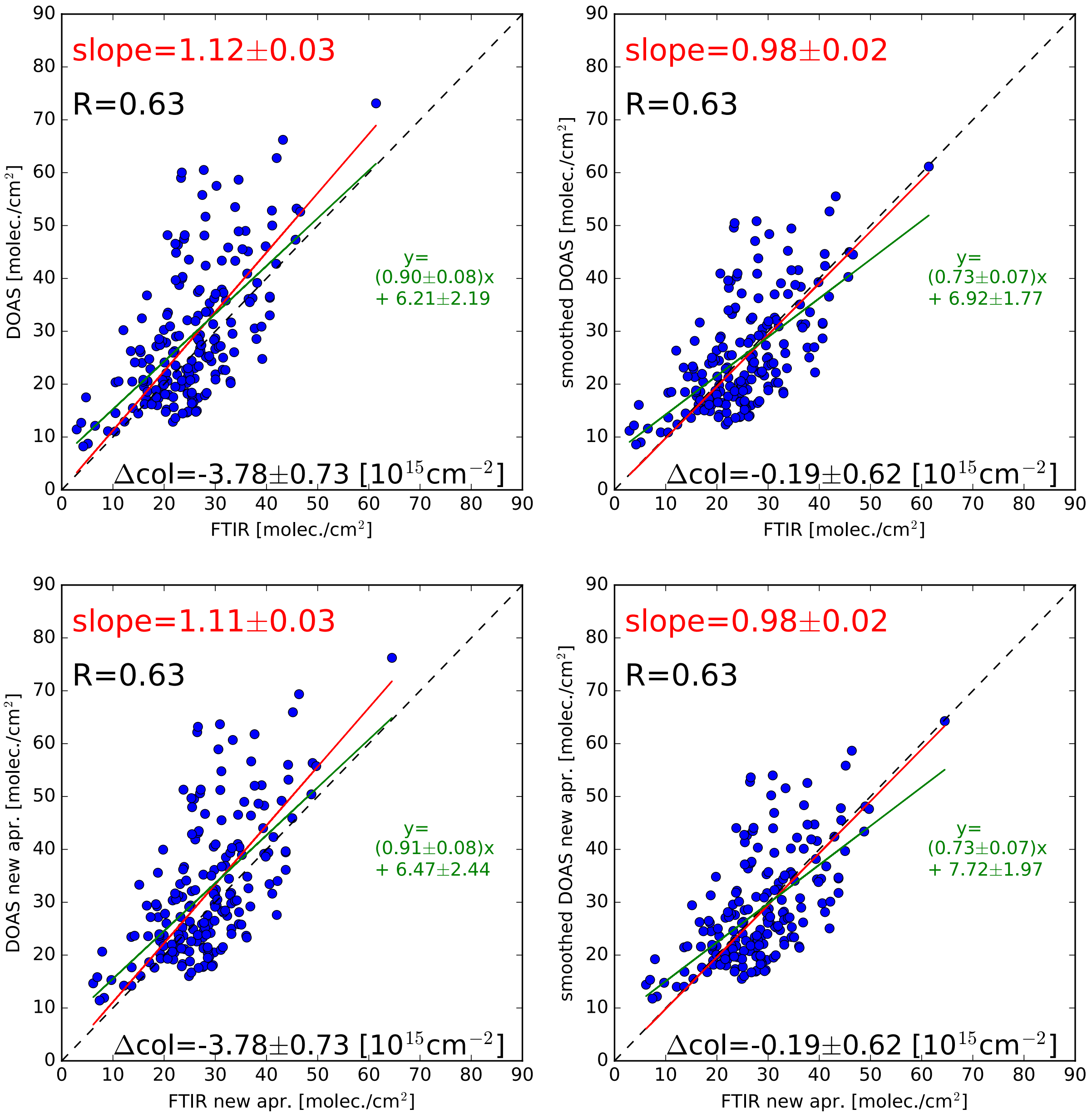
12:00LT (UT-6)


slope=1.62±0.04
R=0.59
y=
(1.33±0.11)x
+ 7.21±2.62
Δcol=-14.46±0.87 [10^15cm^-2]
DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=1.39±0.03
R=0.59
y=
(1.08±0.09)x
+ 7.74±2.12
Δcol=-9.42±0.69 [10^15cm^-2]
smoothed DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=1.54±0.03
R=0.59
y=
(1.33±0.11)x
+ 5.79±3.05
Δcol=-14.46±0.87 [10^15cm^-2]
DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]
slope=1.34±0.03
R=0.59
y=
(1.08±0.09)x
+ 7.36±2.47
Δcol=-9.42±0.69 [10^15cm^-2]
smoothed DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]

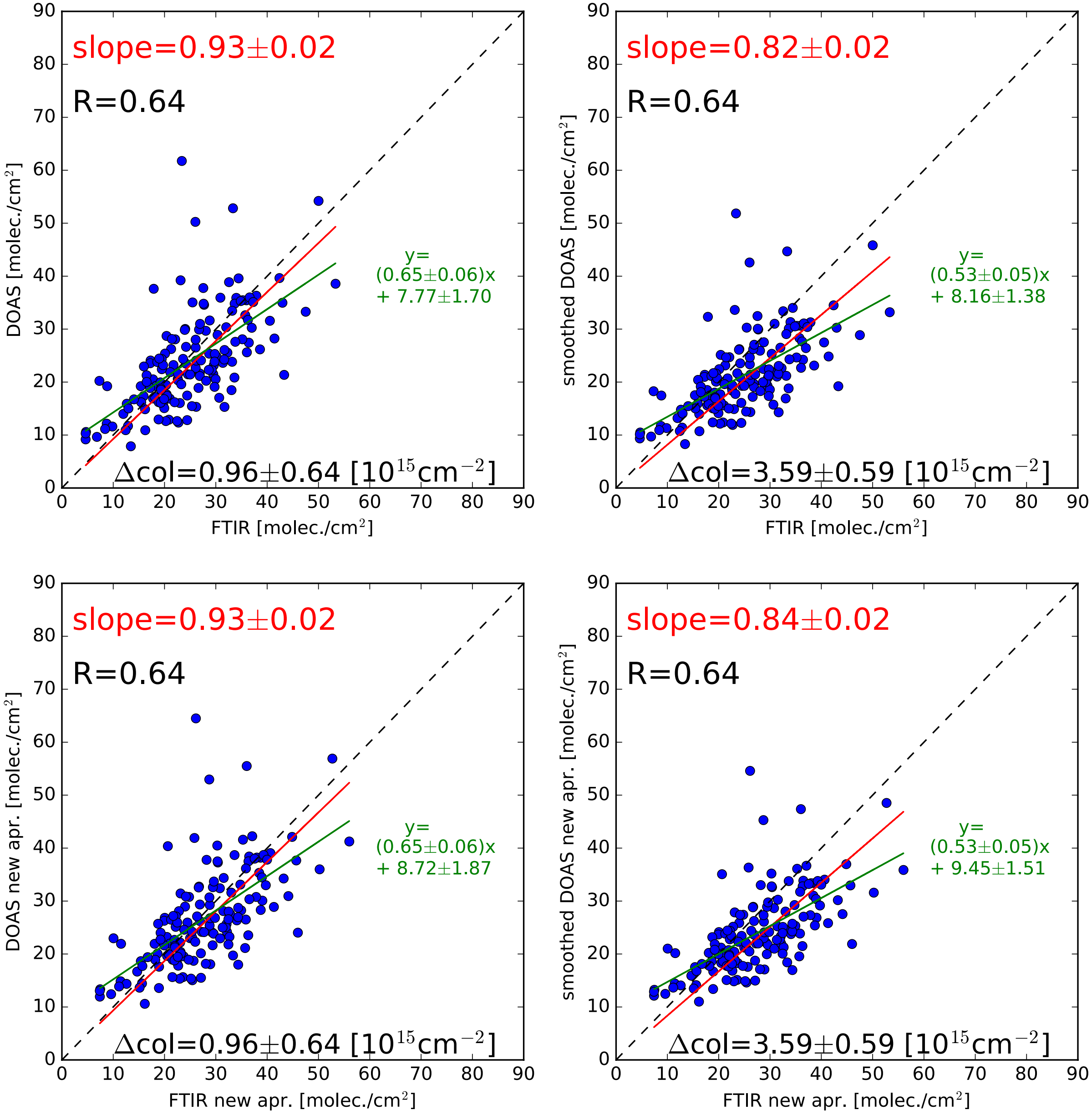
13:00LT (UT-6)


slope=1.45±0.05
R=0.49
y=
(1.16±0.14)x
+ 7.76±3.62
Δcol=-11.61±1.18 [10^15cm^-2]
DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=1.25±0.04
R=0.49
y=
(0.94±0.12)x
+ 8.19±2.93
Δcol=-6.77±0.95 [10^15cm^-2]
smoothed DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=1.40±0.04
R=0.49
y=
(1.16±0.14)x
+ 7.07±4.14
Δcol=-11.61±1.18 [10^15cm^-2]
DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]
slope=1.22±0.03
R=0.49
y=
(0.94±0.12)x
+ 8.36±3.35
Δcol=-6.77±0.95 [10^15cm^-2]
smoothed DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]

14:00LT (UT-6)

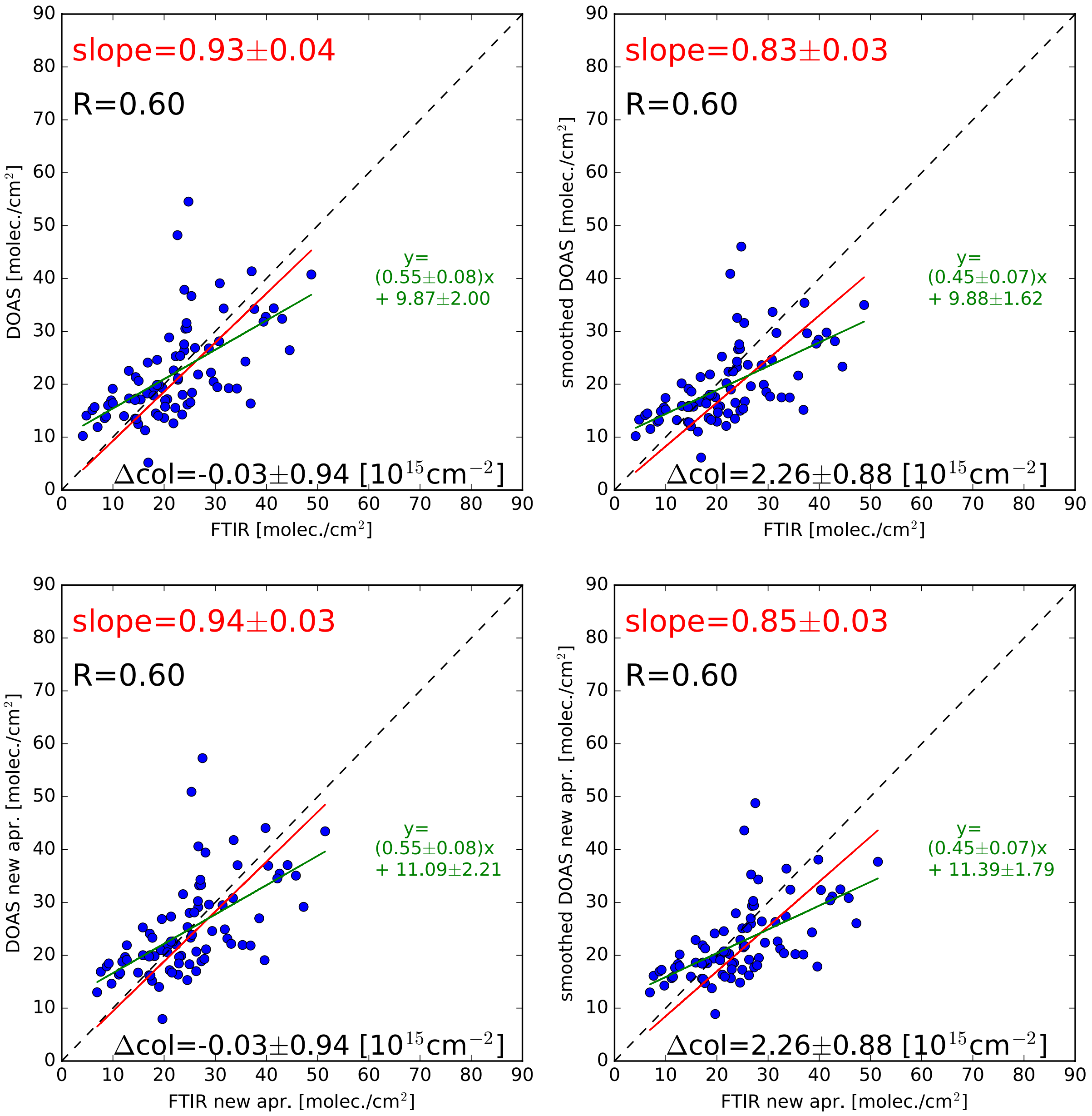

slope=1.12±0.03
R=0.63
y=
(0.90±0.08)x
+ 6.21±2.19
Δcol=-3.78±0.73 [10^15cm^-2]
DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=0.98±0.02
R=0.63
y=
(0.73±0.07)x
+ 6.92±1.77
Δcol=-0.19±0.62 [10^15cm^-2]
smoothed DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=1.11±0.03
R=0.63
y=
(0.91±0.08)x
+ 6.47±2.44
Δcol=-3.78±0.73 [10^15cm^-2]
DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]
slope=0.98±0.02
R=0.63
y=
(0.73±0.07)x
+ 7.72±1.97
Δcol=-0.19±0.62 [10^15cm^-2]
smoothed DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]

15:00LT (UT-6)



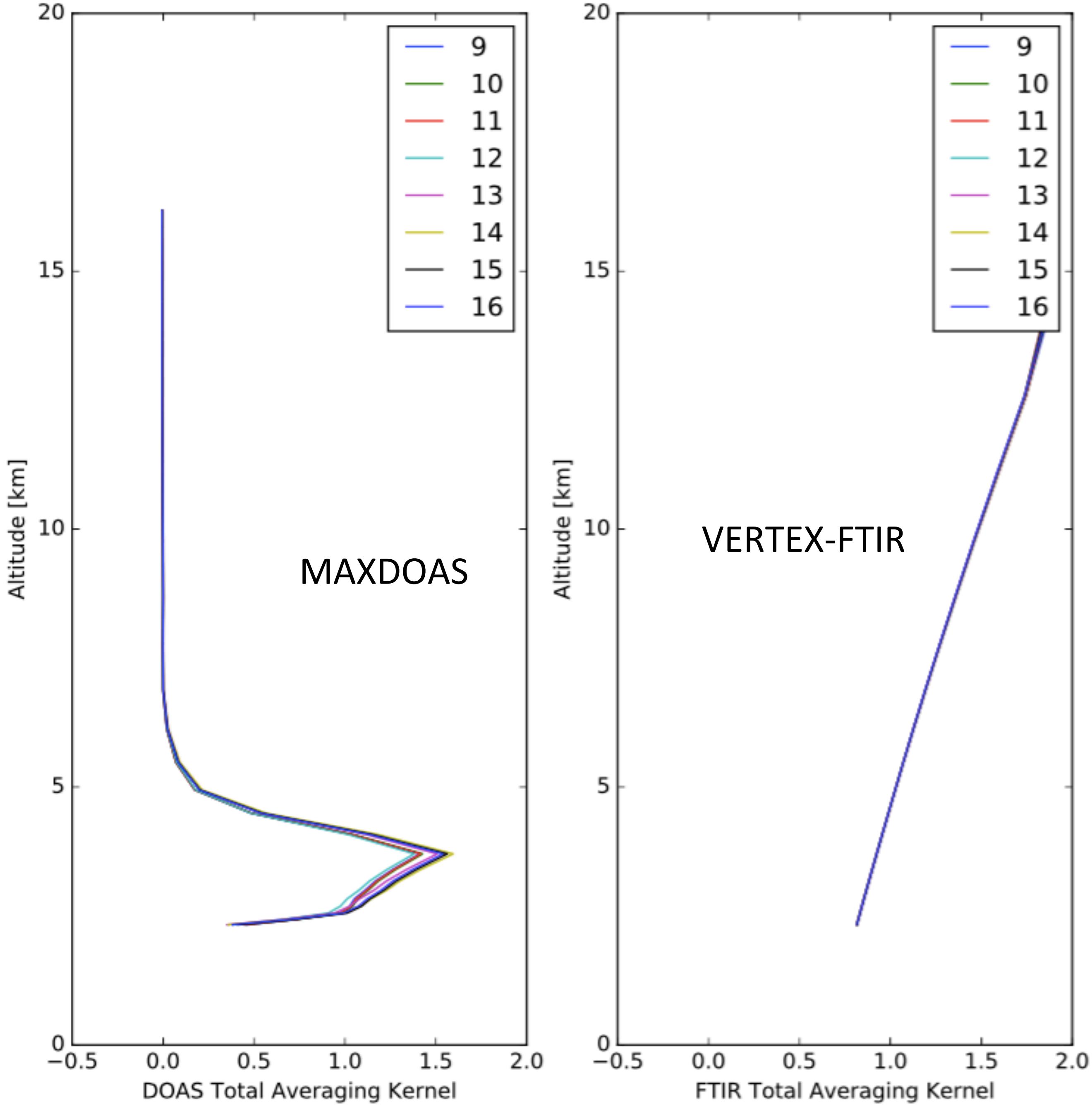
slope=0.93±0.02
R=0.64
y=
(0.65±0.06)x
+ 7.77±1.70
Δcol=0.96±0.64 [10^15 cm^-2]
DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=0.82±0.02
R=0.64
y=
(0.53±0.05)x
+ 8.16±1.38
Δcol=3.59±0.59 [10^15 cm^-2]
smoothed DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=0.93±0.02
R=0.64
y=
(0.65±0.06)x
+ 8.72±1.87
Δcol=0.96±0.64 [10^15 cm^-2]
DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]
slope=0.84±0.02
R=0.64
y=
(0.53±0.05)x
+ 9.45±1.51
Δcol=3.59±0.59 [10^15 cm^-2]
smoothed DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]

16:00LT (UT-6)



slope=0.93±0.04
R=0.60
y=
(0.55±0.08)x
+ 9.87±2.00
Δcol=-0.03±0.94 [10^15cm^-2]
DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=0.83±0.03
R=0.60
y=
(0.45±0.07)x
+ 9.88±1.62
Δcol=2.26±0.88 [10^15cm^-2]
smoothed DOAS [molec./cm^2]
FTIR [molec./cm^2]
slope=0.94±0.03
R=0.60
y=
(0.55±0.08)x
+ 11.09±2.21
Δcol=-0.03±0.94 [10^15cm^-2]
DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]
slope=0.85±0.03
R=0.60
y=
(0.45±0.07)x
+ 11.39±1.79
Δcol=2.26±0.88 [10^15cm^-2]
smoothed DOAS new apr. [molec./cm^2]
FTIR new apr. [molec./cm^2]

AKs



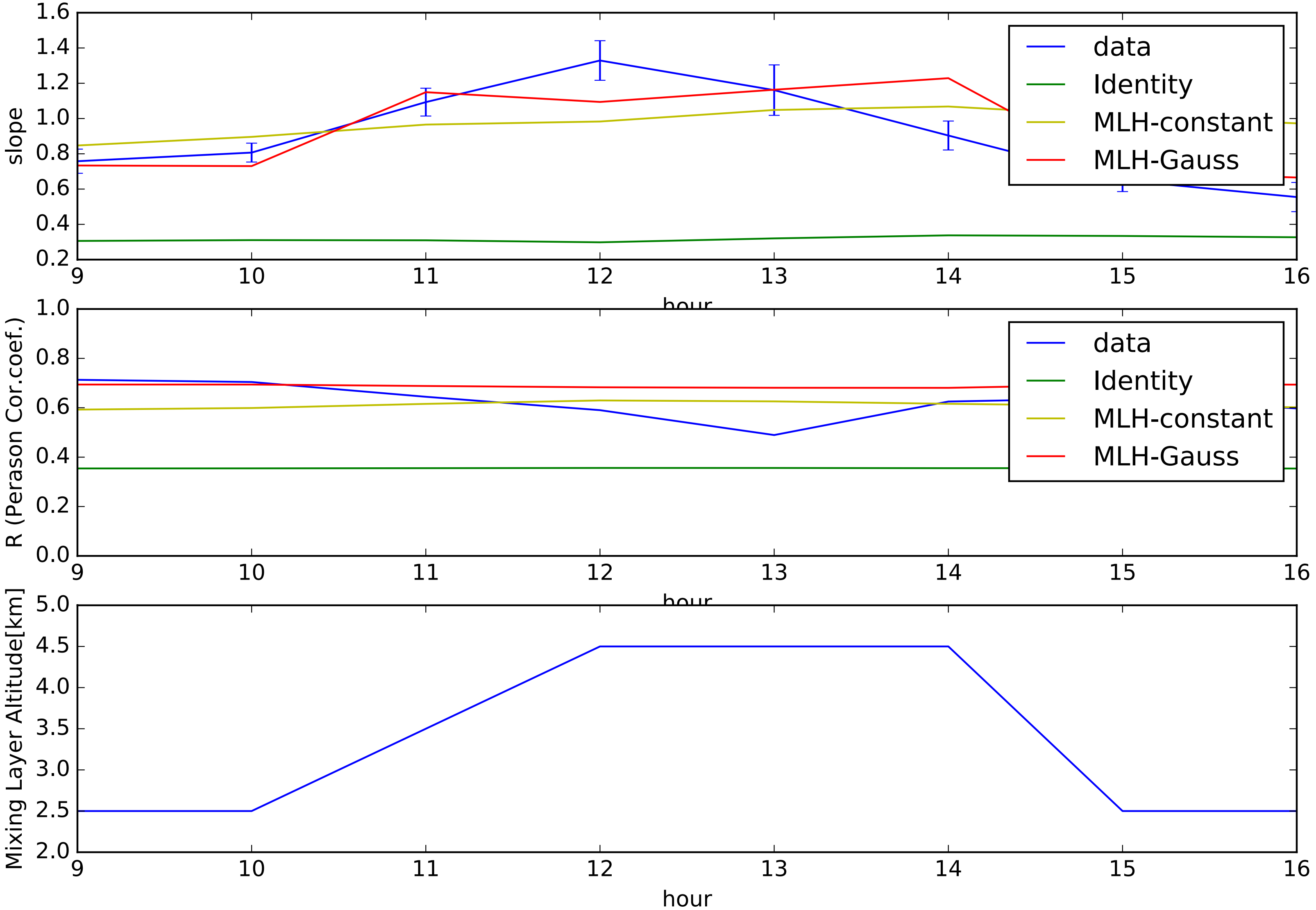
MAXDOAS
VERTEX-FTIR
Altitude [km]
DOAS Total Averaging Kernel
FTIR Total Averaging Kernel
9
10
11
12
13
14
15
16
0
5
10
15
20
−0.5
0.0
0.5
1.0
1.5
2.0

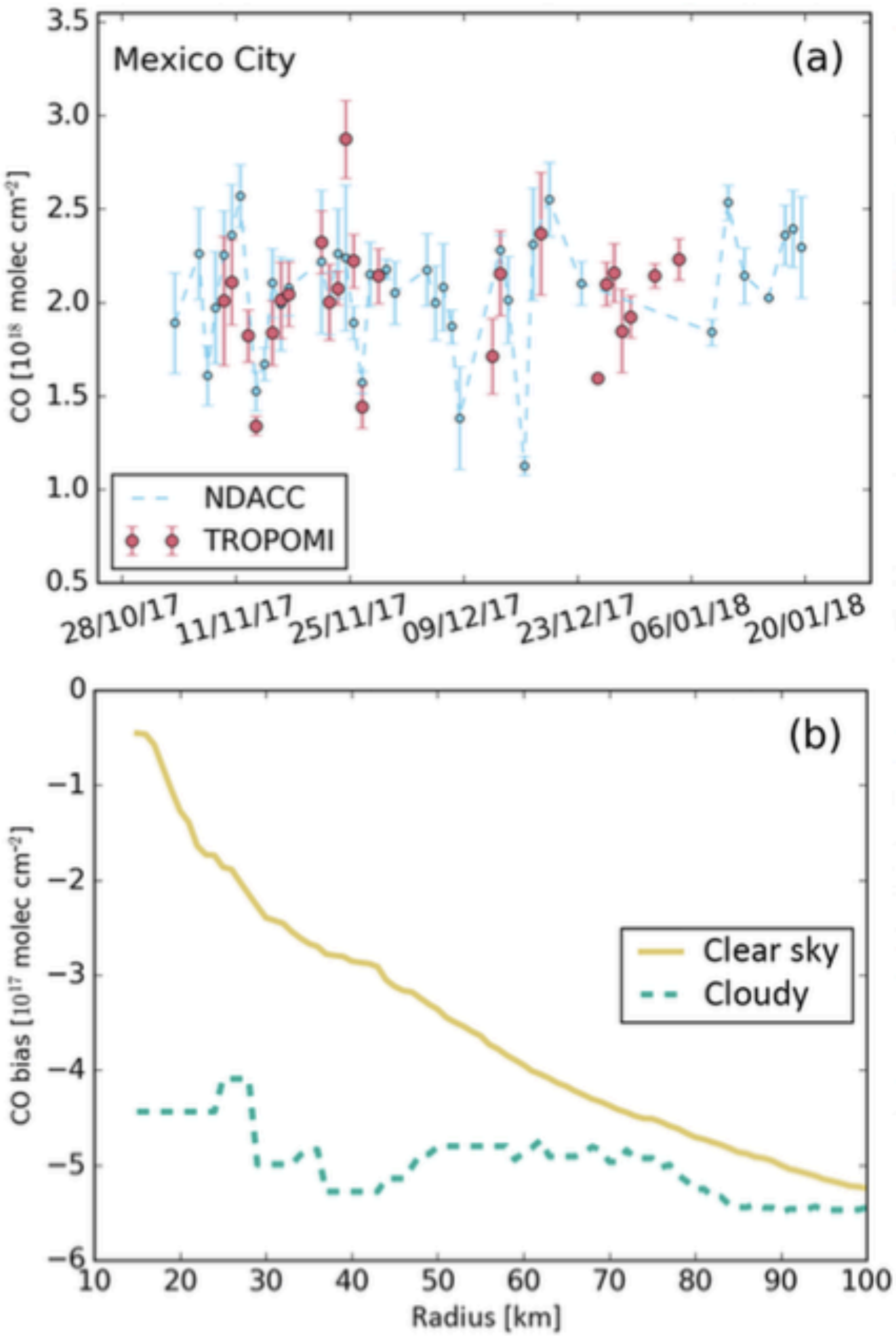
Comparison Vertex80-MAXDOAS: What should we expect?

$$Slope = \frac{\langle x|y\rangle}{\langle x|x\rangle} = \frac{\langle A_{FTIR}|Sa|A^T_{DOAS}\rangle}{\langle A_{FTIR}|Sa|A^T_{FTIR}\rangle}$$

$$R = \frac{\langle A_{FTIR}|Sa|A^T_{DOAS}\rangle}{\sqrt{(\langle A_{FTIR}|Sa|A^T_{FTIR}\rangle + \sigma^2_{FTIR}) \cdot (\langle A_{DOAS}|Sa|A^T_{DOAS}\rangle + \sigma^2_{DOAS})}}$$

Comparison with non ideal Ak's





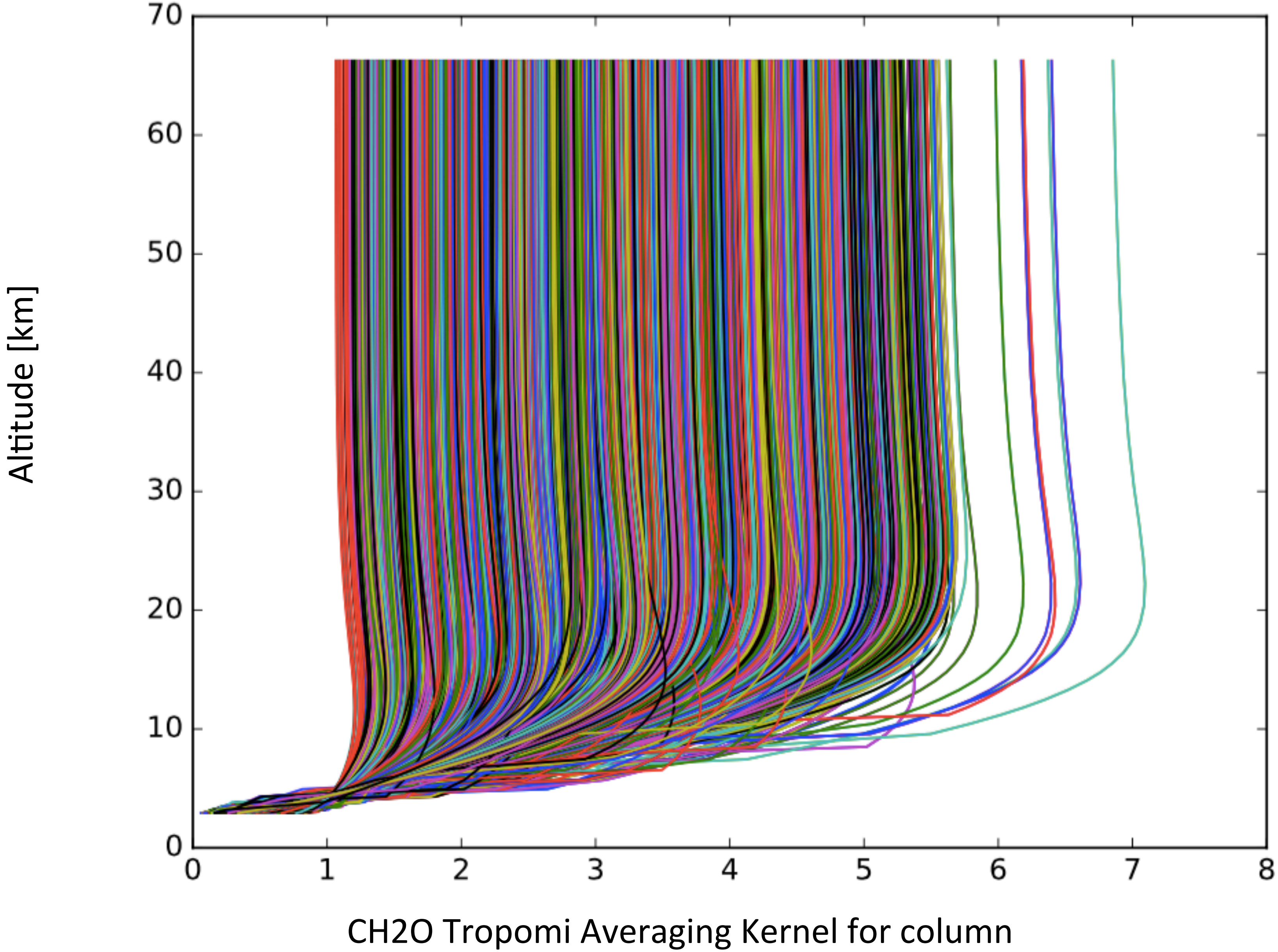
Borsdorff et al.,2018

CO-Comparison
Vertex80 and Tropomi

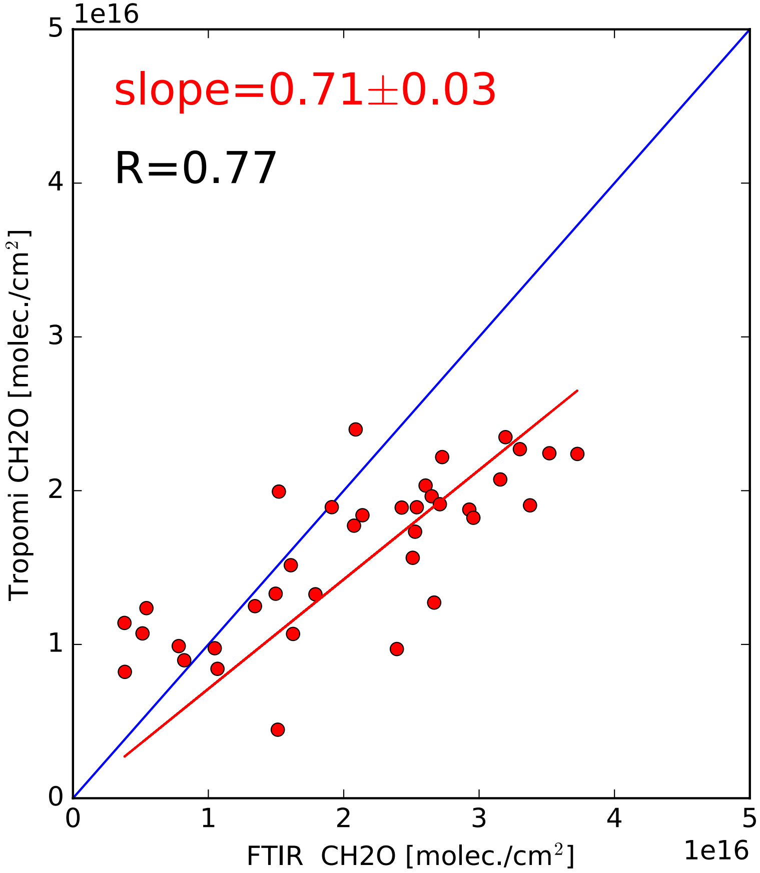
Coincidence: 15km

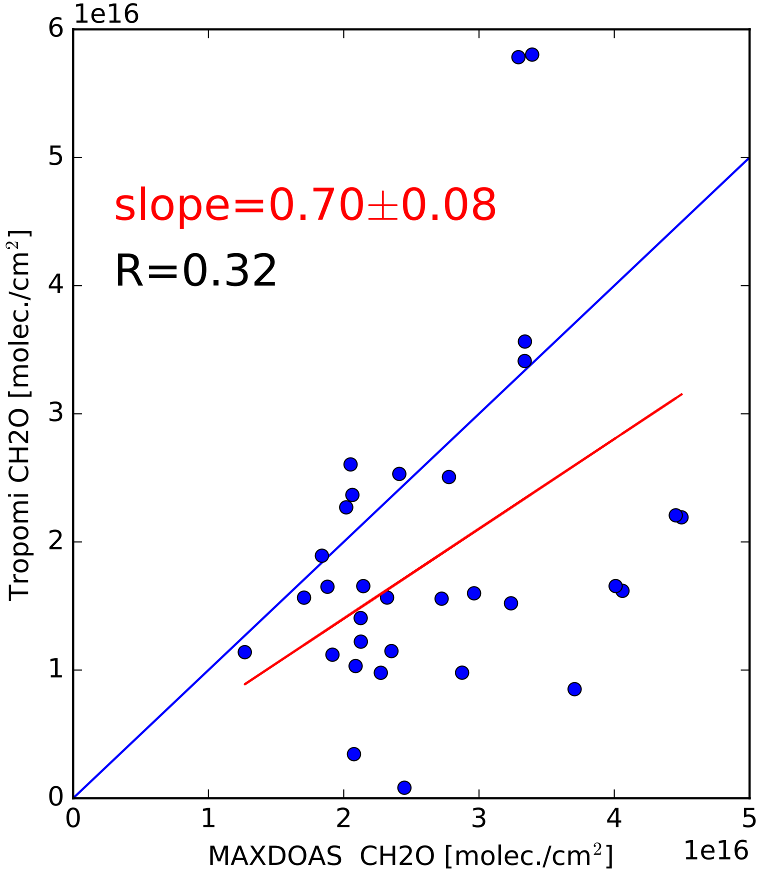
No Clouds

Cloud free CH2O Tropomi Averaging Kernel

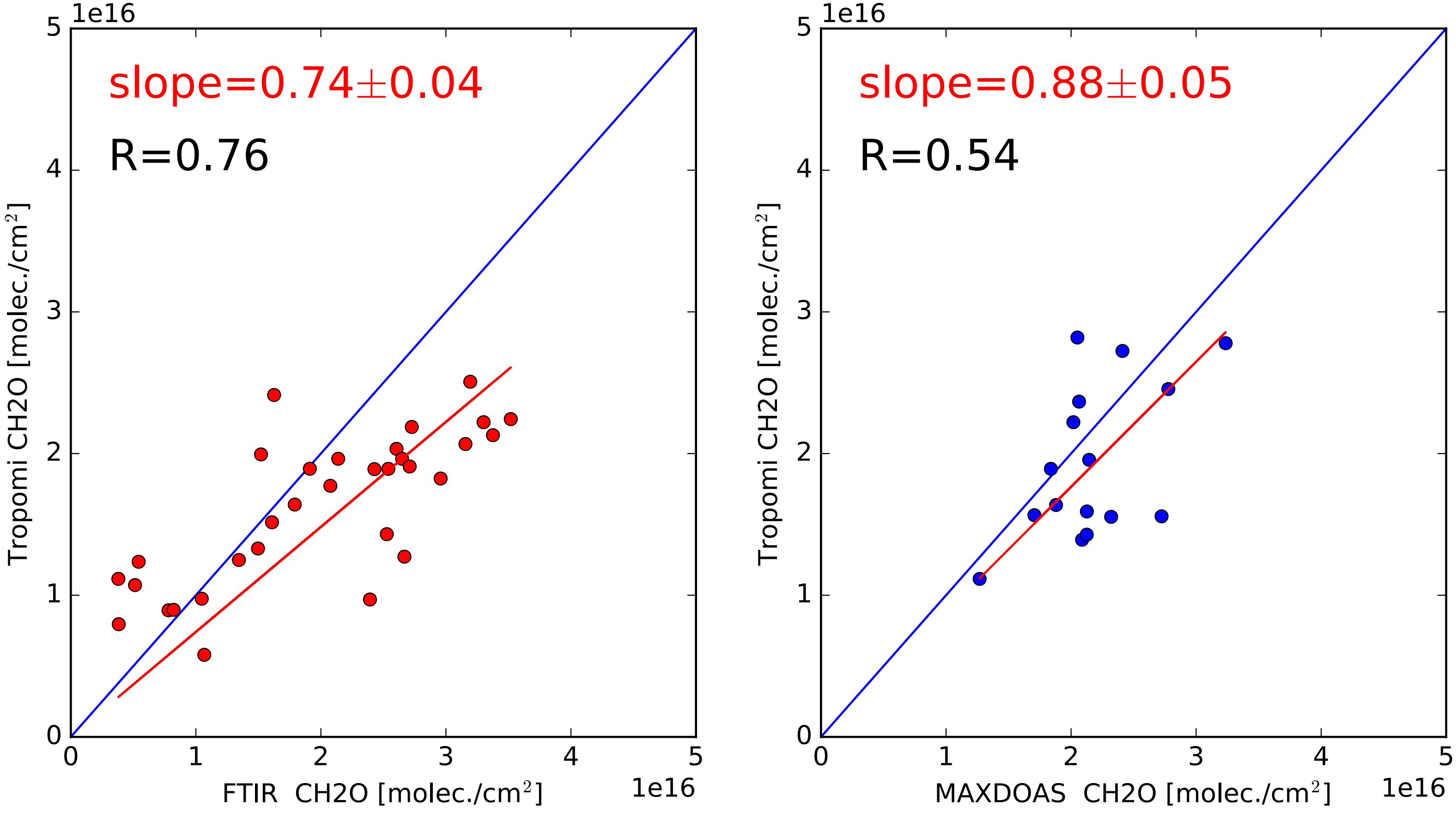


Comparison with TROPOMI: 15km





Comparison:cloud coverage <15%



Conclusion:

- CH_2O can be measured by FTIR and MAX-DOAS
- The inhomogeneity is difficult to measure, but at 13:00 there is more CH_2O in the West
- For a fair comparison it would be nice to have a good Sa –Matrix to calculate the expected slope and R.

- Tropomi comparison needs a strict coincidence criteria (Borsdorff.et al., 2018) and just very cloud-free (<15%) measurements should be taken: but then Vertex and MAXDOAS are quite consistent with TROPOMI

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