PGN products quantitative uncertainty

WP2126

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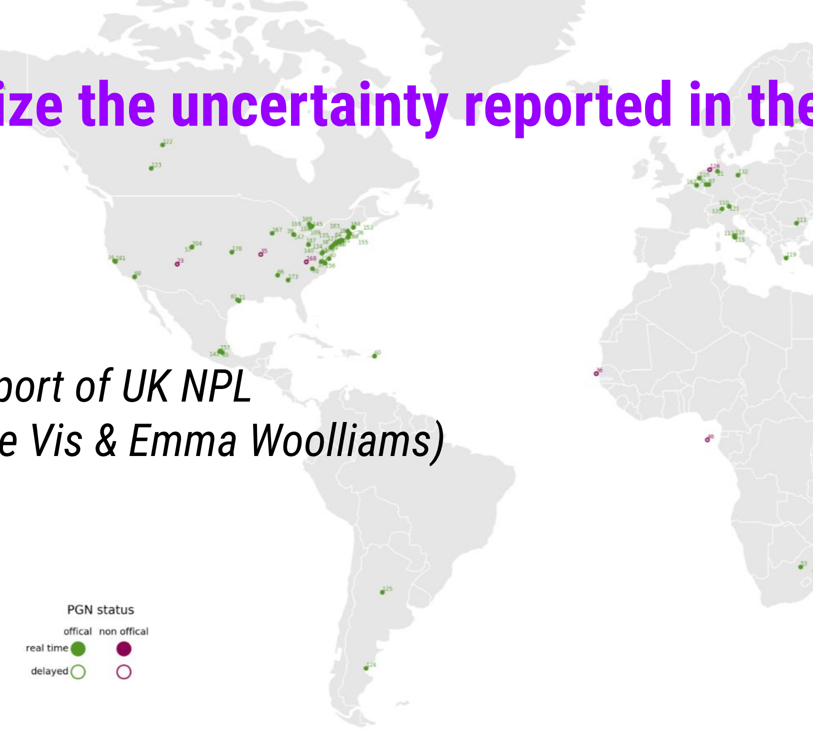
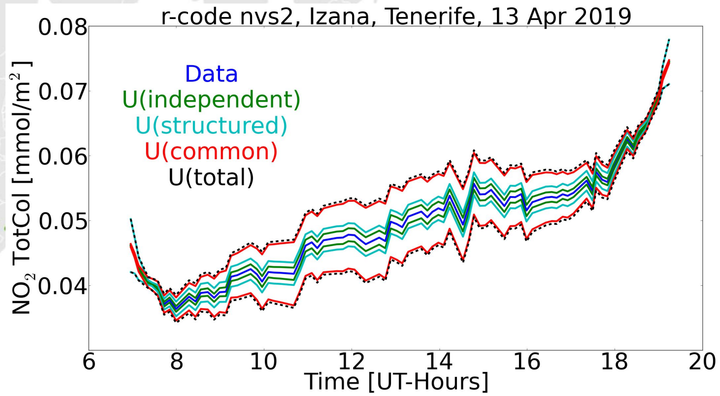
Goal of this QA4EO WP2126

Optimize the uncertainty reported in the PGN trace gas products

with support of UK NPL
(Pieter De Vis & Emma Woolliams)





20220330

61 AldineTX
168 BlacksburgVA*
20 Busan
120 Davos
122 FortMcKay
121 Innsbruck-FKS*
56 MaunaLoaHI
187 PittsburghPA
164 Seosan
193 Tsukuba
161 Xianghe
* more than one instrument

65 Altzomoni*
155 BostonMA
118 Cabauw
39 DearbornMI
23 FourCornersNM
30 Juelich
142 MexicoCity-UNAM
53 Potchefstroom*
54 Seoul
176 Tsukuba-NIES
146 Yokosuka

189 Anmyeon
57 BoulderCO
26 CambridgeMA*
104 Downsview*
199 Fukuoka
167 KenoshaWI
157 MexicoCity-Vallejo
55 QueensNY
149 Seoul-SNU
163 Tsukuba-NIES-West
191 Yongin

119 Athens-NOA
204 BoulderCO-NCAR
184 CapeElizabethME
185 EastProvidenceRI
59 GreenbeltMD*
198 Kobe
34 MountainViewCA
138 Rome-IIA
126 ShipSonne2
136 Hefei*

173 AtlantaGA*
21 Bremen
70 ChapelHillNC
169 Egbert
37 HamptonVA
11 LaPorteTX*
197 Nagoya
115 Rome-ISAC
109 StGeorge
150 Ulsan

190 Bangkok
134 BristolPA
31 CharlesCityVA
144 Eureka-PEARL
156 HamptonVA-HU
183 LondonderryNH
69 NewBrunswickNJ
117 Rome-SAP
123 StonyPlain
159 Wakkerstroom

38 BayonneNJ
112 Broadmeadows
67 Cologne
174 FairbanksAK
105 Helsinki
153 LynnMA
64 NewHavenCT
147 SWDetroitMI
182 Tel-Aviv
40 WallopsIslandVA

172 Beijing*
180 BronxNY
124 ComodoroRivadavia
60 Fajardo
66 HuntsvilleAL
186 MadisonCT
152 NyAlesund
181 SanJoseCA
194 Tokyo-TMU
140 WashingtonDC

171 Beijing-RADI
162 Brussels-Uccle
125 Cordoba
102 Fang
201 Incheon-ESC
178 ManhattanKS
51 OldFieldNY
46 SaoTome*
145 Toronto-Scarborough
177 WestportCT

132 Berlin
111 Bucharest
36 Dakar
35 ForestParkMO
110 Innsbruck
135 ManhattanNY-CCNY
166 PhiladelphiaPA
196 Sapporo*
108 Toronto-West
68 WrightwoodCA

Basic equation for total vertical column data

Differential slant column from spectral fitting

Slant column in reference (determined in calibration)

$$VC = \frac{\Delta SC + SC_{REF}}{AMF}$$

Output: Vertical column

Air mass factor (only valid for “sun free”)

Noise

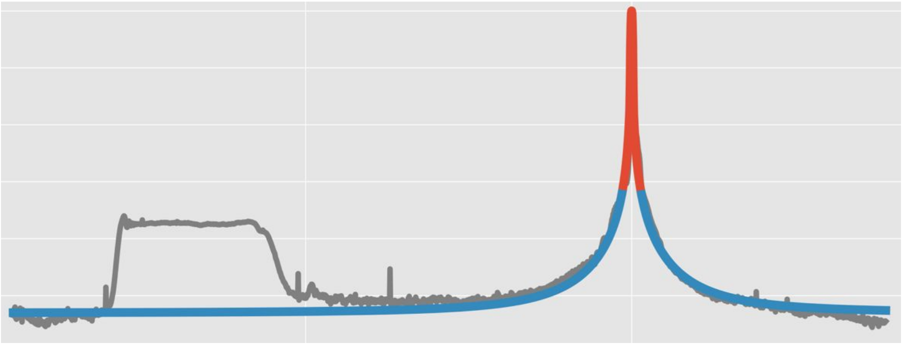
Noise

Green box:
this error source
is included in v1.8

$$VC = \frac{\Delta SC + SC_{REF}}{AMF}$$

→ *The measurement noise was the only uncertainty component already included in processor version v1.7, i.e. at the beginning of QA4EO.*

L1 corrections



Noise

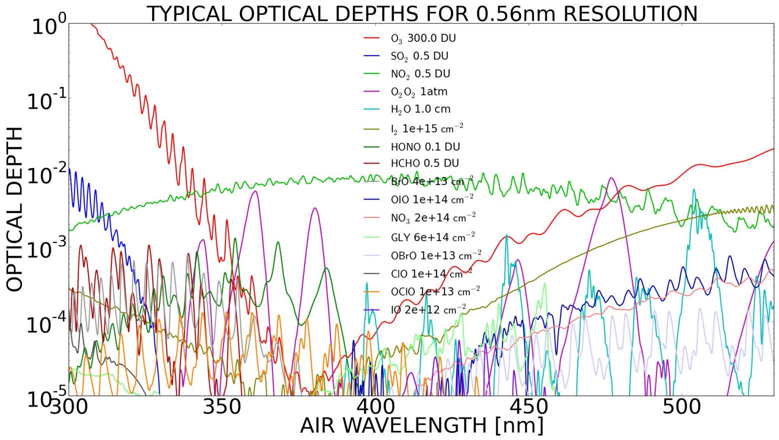
Impact of L1 corrections (linearity, stray light, etc.)

Red box: this error source is not yet included

$$VC = \frac{\Delta SC + SC_{REF}}{AMF}$$

→ While this component is not explicitly included in processor, it will partially captured by the "Structured-discrepancy" uncertainty output, which is planned for v1.9

Cross section source



Noise

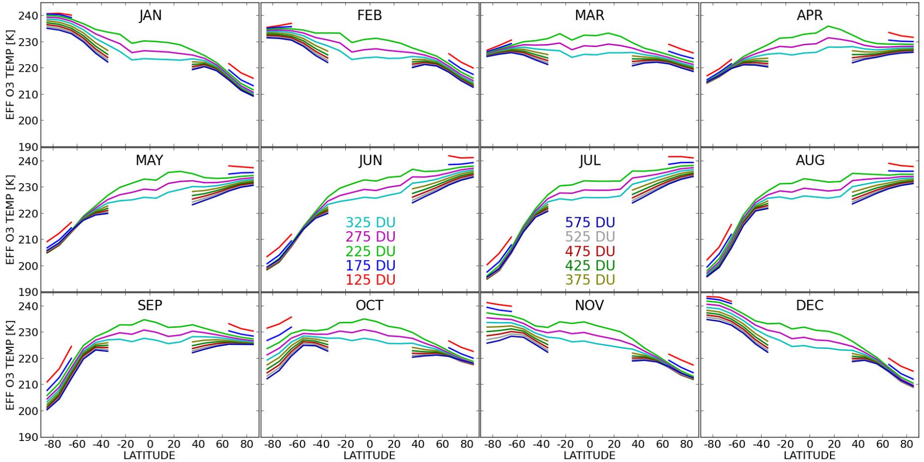
Impact of L1 corrections (linearity, stray light, etc.)

Choice of cross sections

$$VC = \frac{\Delta SC + SC_{REF}}{AMF}$$

→ ***No plans to include this uncertainty yet***

Effective gas temperature



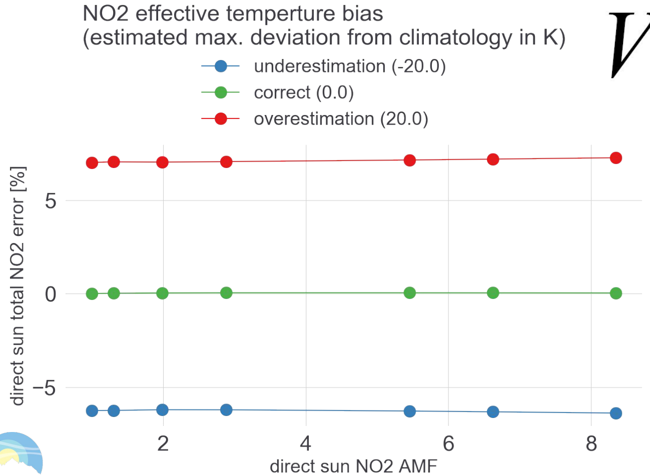
Noise

Impact of L1 corrections (linearity, stray light, etc.)

Choice of cross sections

Effective temperature used in spectral fitting

$$VC = \frac{\Delta SC + SC_{REF}}{AMF}$$



→ Included in v1.8, i.e. at the end of phase 1 of QA4EO (Dec 2021)

Algorithm error

Noise

Algorithm error

Impact of L1 corrections (linearity, stray light, etc.)

"What error does the spectral fitting algorithm using pre-convoluted cross sections cause on the data?"

Choice of cross sections

Effective temperature used in spectral fitting

$$VC = \frac{\Delta SC + SC_{REF}}{AMF}$$

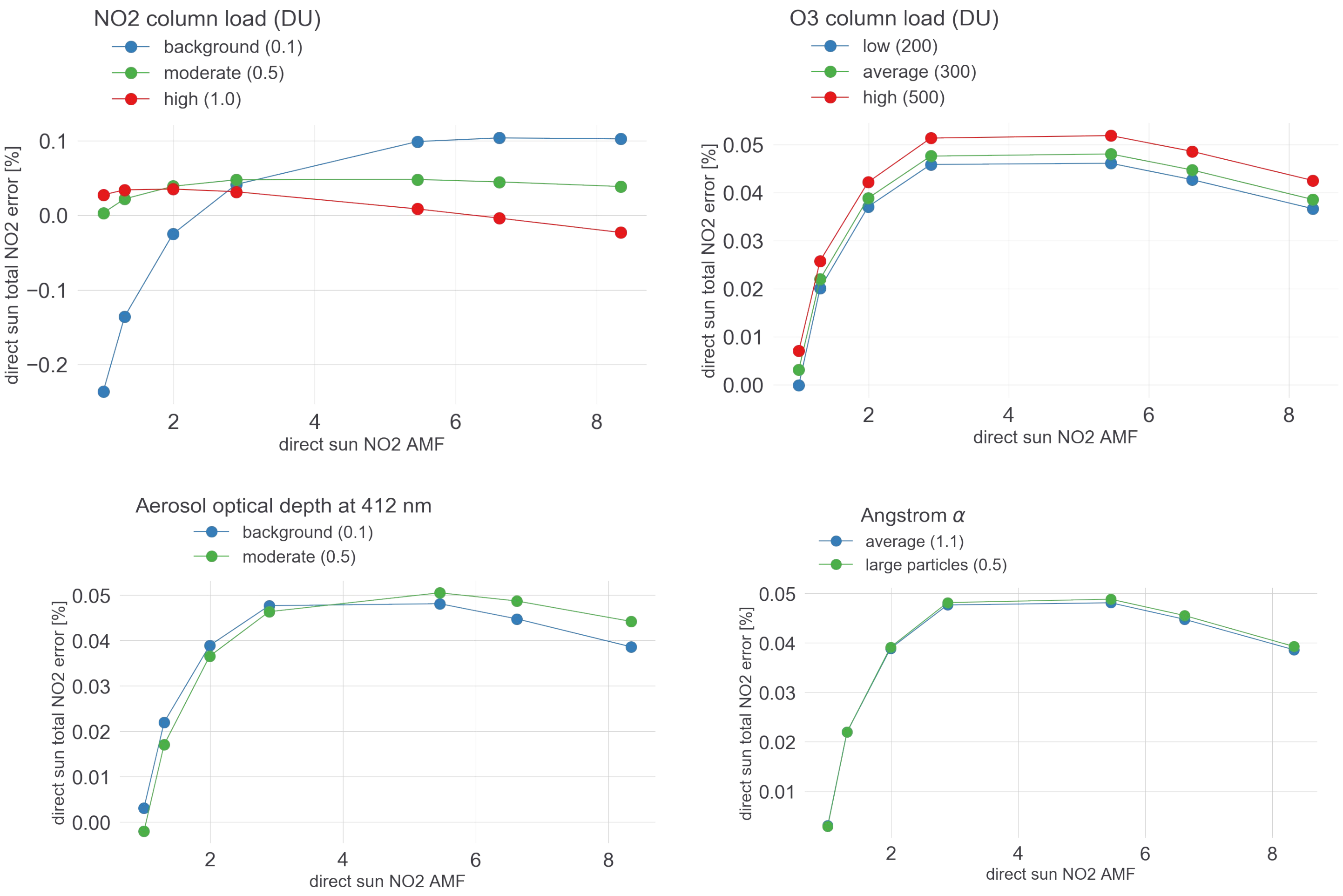
→ ***While this component is not explicitly included in processor yet, it will partially captured by the "Structured-discrepancy" uncertainty output, which is planned for v1.9***

→ ***Evaluated for NO2 total columns using simulations***

Algorithm error

→ Impact of trace gas columns and aerosols on NO2 data negligible

→ This does not necessarily need to be the same for other products (e.g. HCHO, SO2)



Discrepancy error

Noise

Algorithm error

Impact of L1 corrections (linearity, stray light, etc.)

Discrepancy error

Choice of cross sections

"Whenever the measured (extraterrestrial) spectrum does not fit to the given reference spectrum"

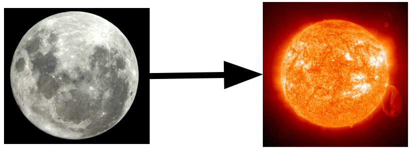
Effective temperature used in spectral fitting

$$VC = \frac{\Delta SC + SC_{REF}}{AMF}$$

→ Evaluated for NO2 using simulations

Orange box: this error source will be included in v1.9

Discrepancy error possible reasons



1. The reference is not taken from the instrument itself (extraterrestrial spectrum from literature).
2. Different optics have been used, e.g. when the reference obtained from direct sun data is used for direct moon or sky radiance measurements.
3. Instrumental changes, either long term ("sensitivity drift" from optical degradation) or short term ("unwanted spectral signal" arising from pointing inaccuracies, dirty entrance window, etc.).

→ 1 and 2 would cause an additional contribution to the common uncertainty.

→ The combination of all these effects is planned to be quantified in v1.9 as “Structured-discrepancy uncertainty” U_{SD}. The reason it is "structured" is that we cannot separate the short-term effects from the common effects.

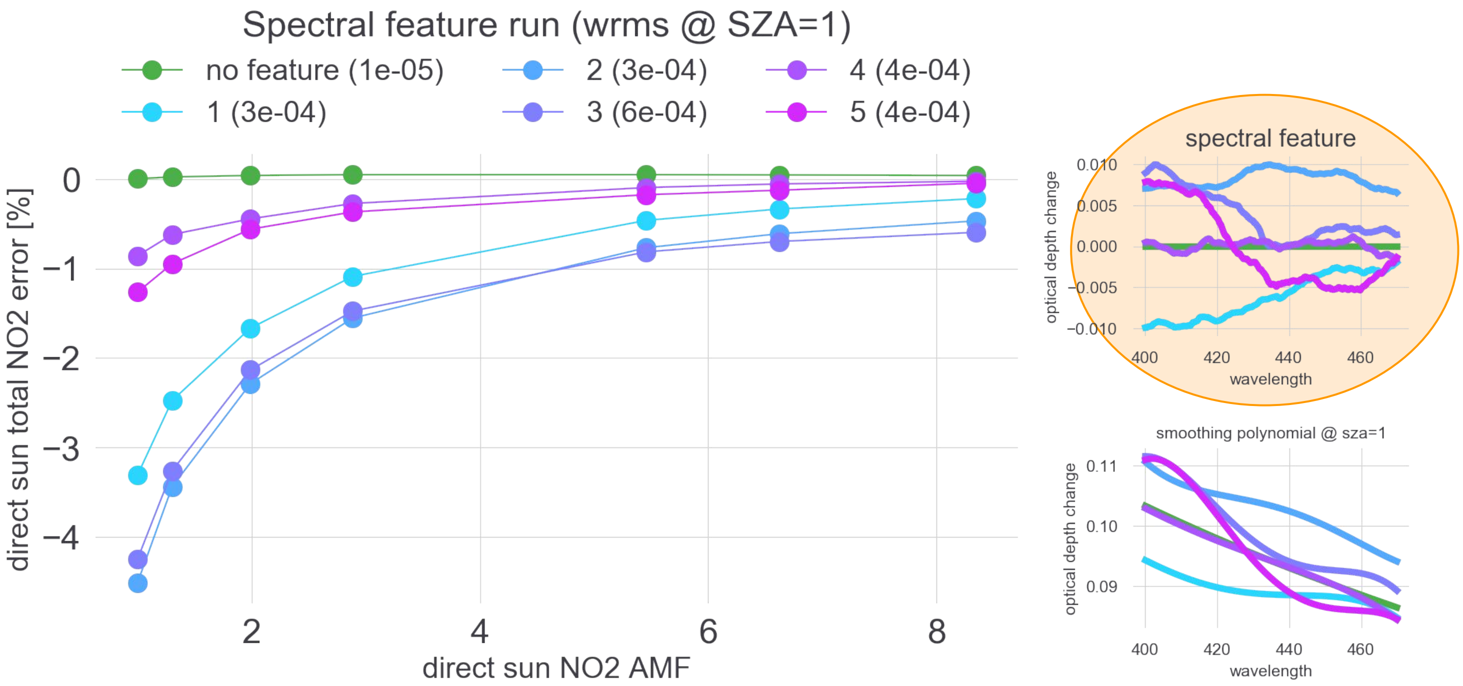
→ We will make use of the weighted RMS (wrms) of the residuals to quantify this uncertainty:

$$U_{SD}(X_j) = U_I(X_j) \cdot \sqrt{\left(\frac{\text{wrms}}{\text{wrmse}}\right)^2 - 1}$$

Discrepancy error simulations

→ Used “structured noise” to simulate the discrepancy error

→ We believe that the simulated errors agree with what we observe in the measurements



Field calibration uncertainty

Noise

Algorithm error

Impact of L1 corrections (linearity, stray light, etc.)

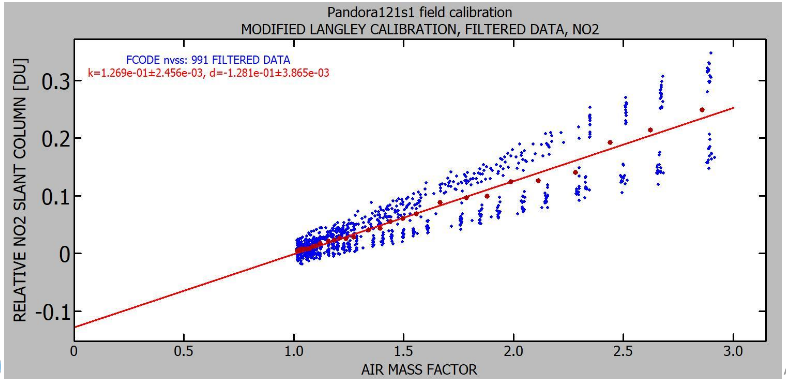
Discrepancy error

Choice of cross sections

Field calibration uncertainty (selection of days, statistical approach etc.)

Effective temperature used in spectral fitting

$$VC = \frac{\Delta SC + SC_{REF}}{AMF}$$



→ Included in v1.8, i.e. at the end of phase 1 of QA4EO (Dec 2021)

Effective height

Noise

Algorithm error

Impact of L1 corrections (linearity, stray light, etc.)

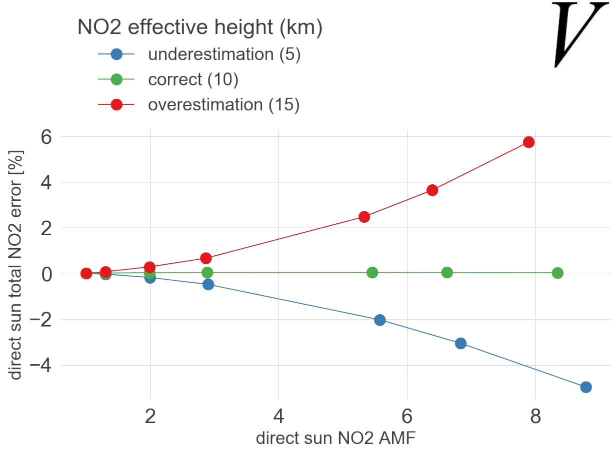
Discrepancy error

Field calibration uncertainty (selection of days, statistical approach etc.)

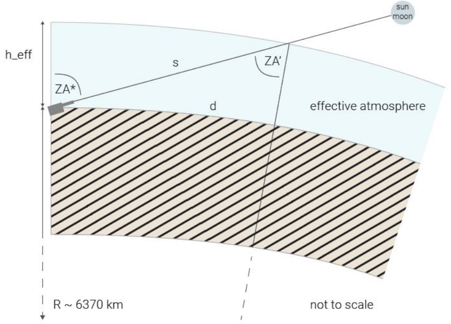
Choice of cross sections

Effective temperature used in spectral fitting

$$VC = \frac{\Delta SC + SC_{REF}}{AMF}$$



→ *Included in v1.8*



Impact of effective height

PGN Uncertainty All Components

Noise

Algorithm error

Impact of L1 corrections (linearity, stray light, etc.)

Discrepancy error

Choice of cross sections

Field calibration uncertainty (selection of days, statistical approach etc.)

Effective temperature used in spectral fitting

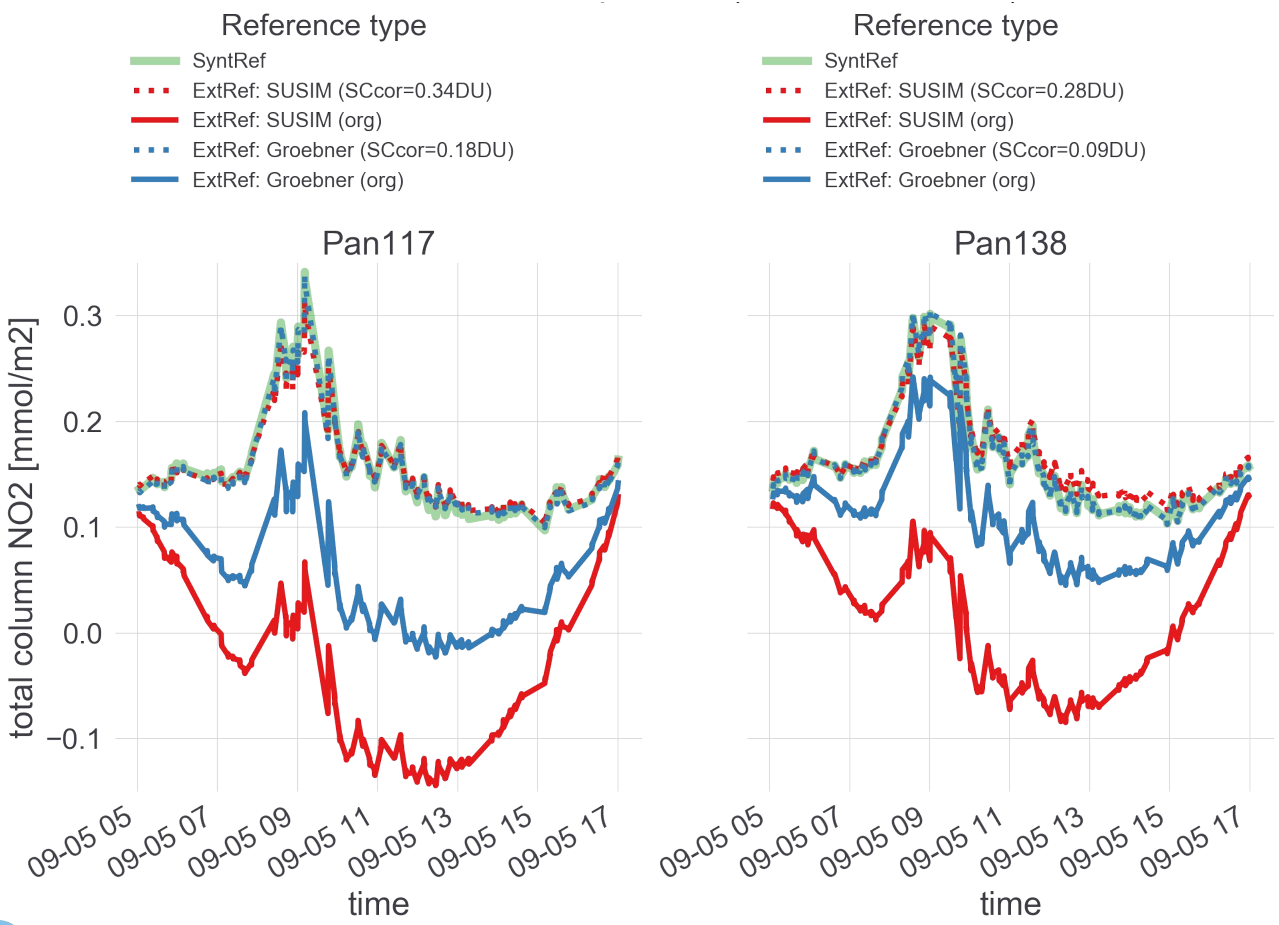
$$VC = \frac{\Delta SC + SC_{REF}}{AMF}$$

Output:
Independent uncertainty
Common uncertainty
Total uncertainty

Impact of effective height

Retrieving NO2 columns using an extraterrestrial (ET) reference instead of the “usual” synthetic reference

Residual NO2 absorption features in reference spectra?

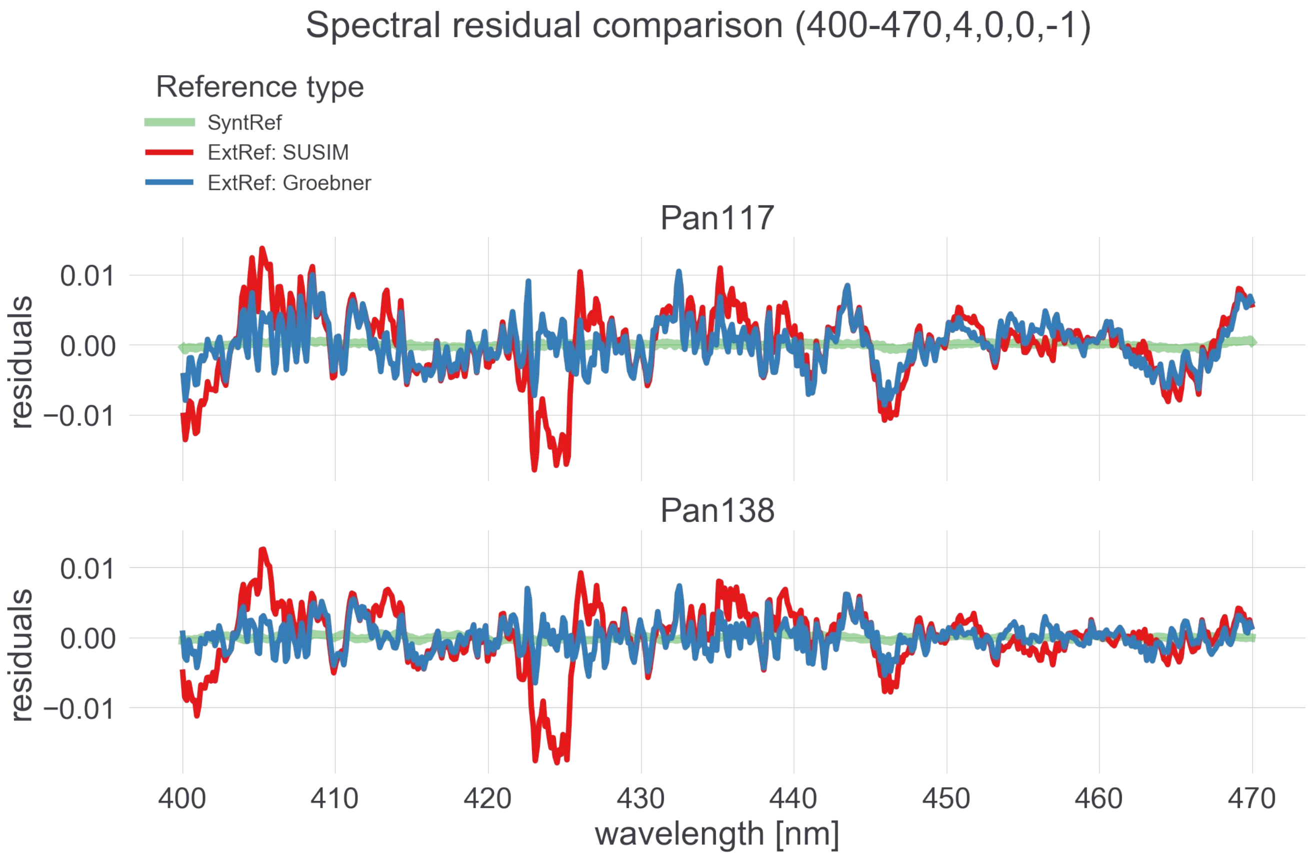


Here:

“SUSIM”= Kurucz+SUSIM

“Groebner”= Kurucz+Gröbner

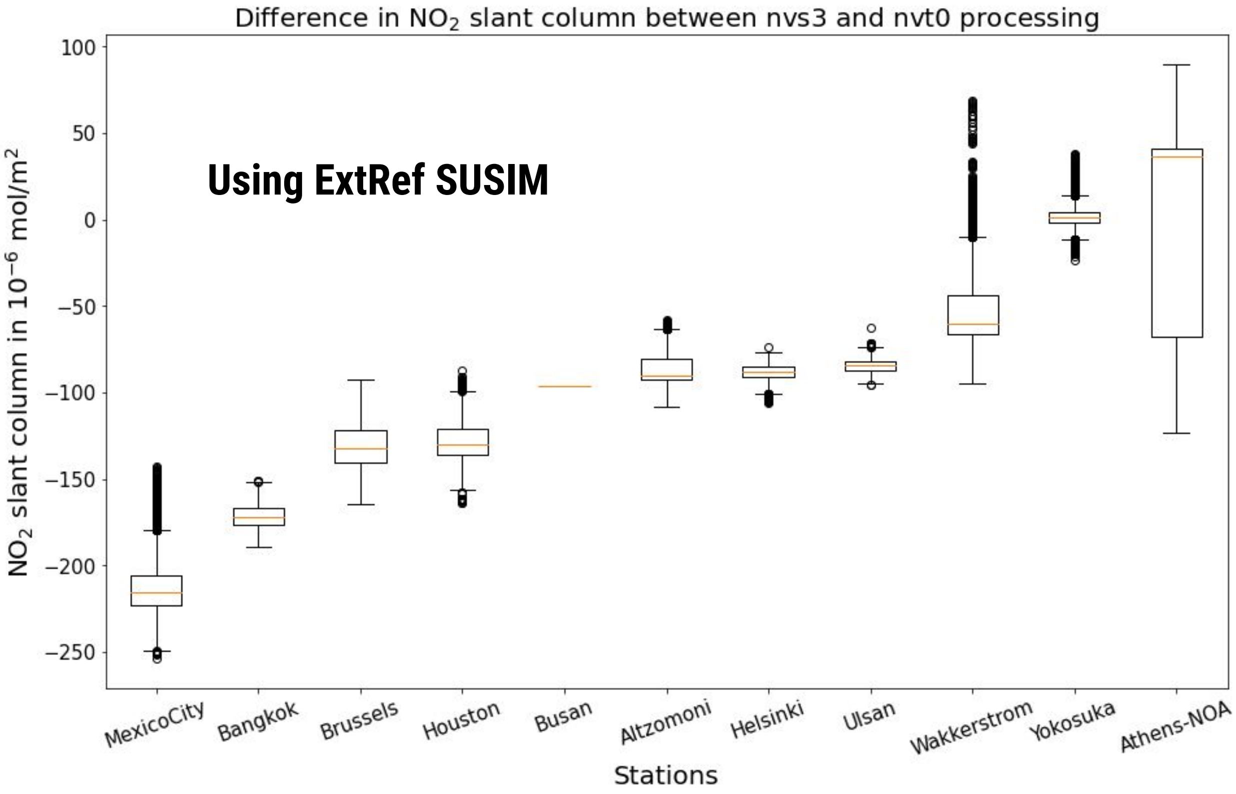
Residual NO2 absorption features in reference spectra



The difference in the ET spectra causes a difference in the retrieved NO2.

→ We suspect a residual NO2 column amount included in both ET spectra, which makes sense since both state that they have not been corrected for NO2.

Difference total NO2 using ext. reference to operational NO2



The difference to the “true” NO2 column amount is a combination of:

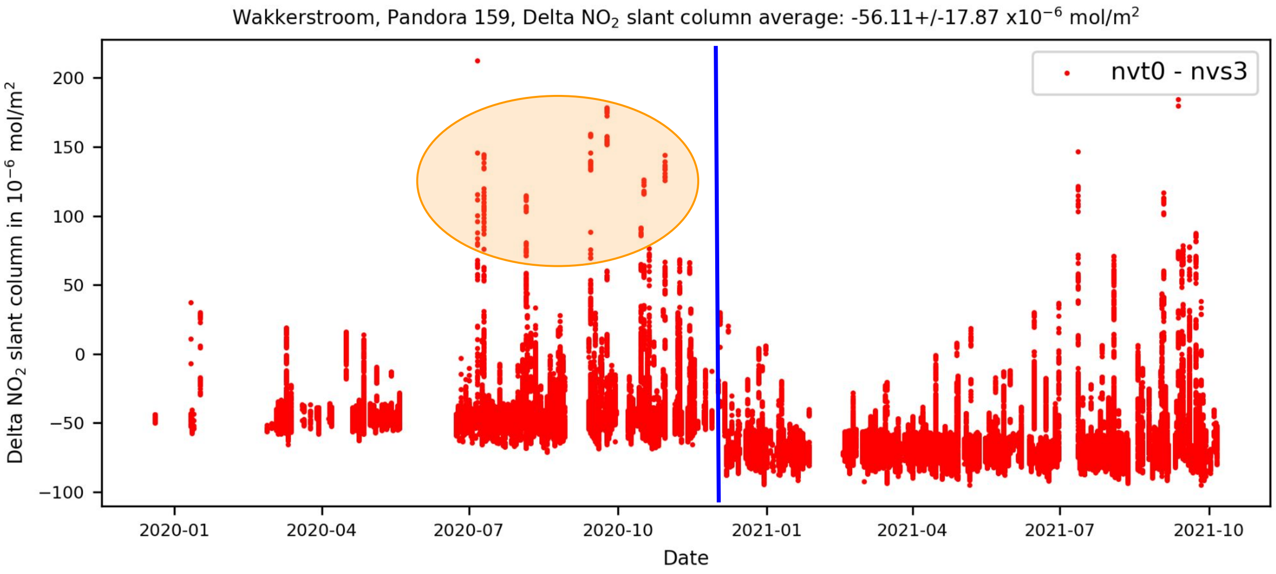
- NO2 column in ET spectrum
- Discrepancy error specific to each instrument

There seems to be a cluster around 1e-4mol/m2~0.22DU

Practical use of ET retrieval

A time series of the differences shows some SZA effects ("outliers" at high SZAs), but more importantly can reveal changes of the instrument sensitivity.

→ ET retrieval "jumps" when the instrument changes
→ Operational retrieval introduces a new "validity period" to be correct



Conclusions

- Several new uncertainty components have been introduced in processor version v1.8.
- The so-called algorithm and discrepancy errors were simulated and analyzed for NO2 columns:
  - The algorithm error is negligible. This does not necessarily need to be the same for other products (e.g. HCHO, SO2)
  - The discrepancy error is significant. It will be included in v1.9.
- NO2 retrievals using ET spectra from literature differ from the truth for two reasons:
  - We believe the ET spectra include NO2.
  - Each instrument has its own specific discrepancy error
- NO2 retrievals using ET spectra are a very useful tool to track the instrument stability.