Task 3.4:

Sensitivity Analysis of Ozone Retrieval

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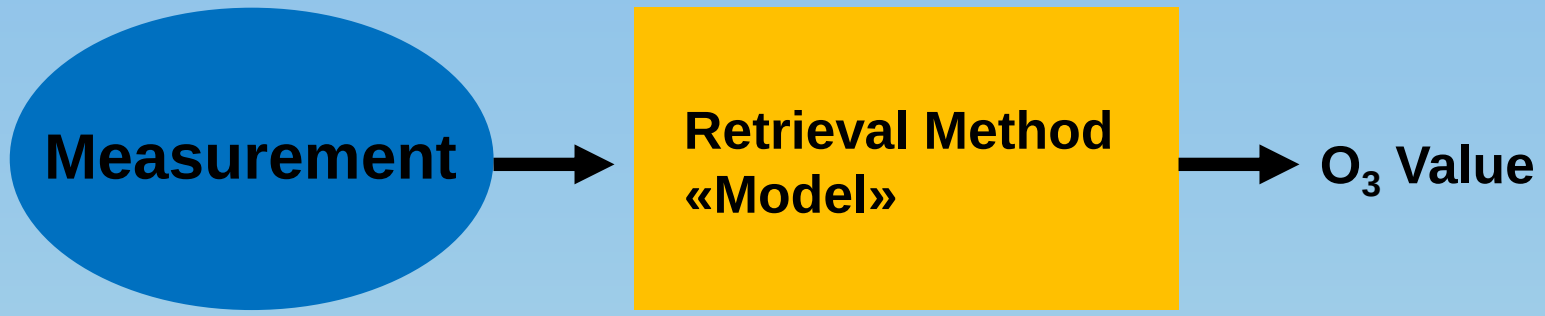
for final IRS2016 presentation with

Julian Gröbner, Mario Blumthaler, Omar El Gawhary, Petri Kärhä, Ingo Kröger, Alberto Redondas and Mark Weber

The European Metrology Research Programme (EMRP) is jointly funded by the EMRP participating countries within EURAMET and the European Union.

Uncertainty Ozone Retrieval



Uncertainty of **measurement**: + Uncertainty of **model**: = Uncertainty of **O_3 value**

Metrology (Physics)

Physics: Beer-Lambert law

$$I_\lambda = I_\lambda^0 e^{-\tau_\lambda m}$$

$$\log I_\lambda = \log I_\lambda^0 - \tau_\lambda^R m_R - \tau_\lambda^{O3} m_{O3} - \tau_\lambda^{SO2} m_{SO2} - \tau_\lambda^{aod} m_{aod}$$

Today: **multispectral measurements** from e.g. array spectroradiometer

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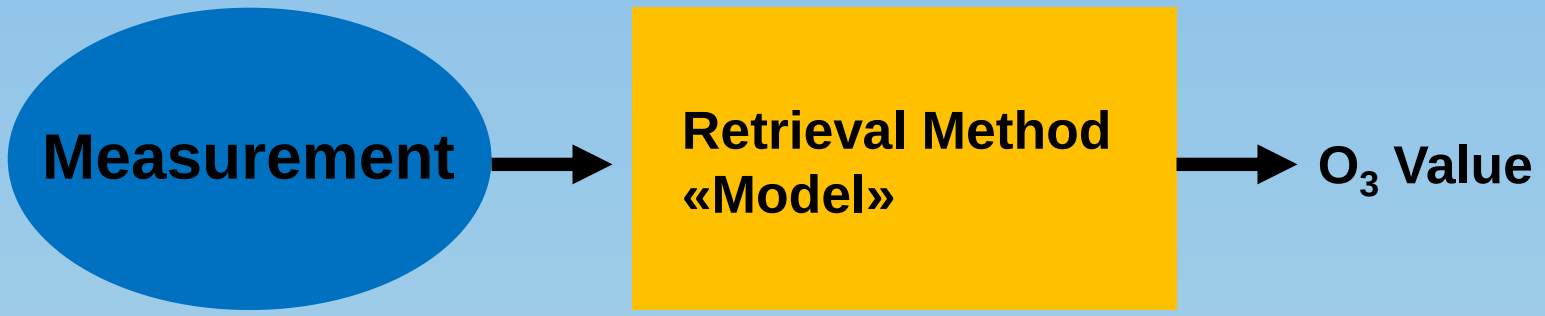

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Metrology (Physics)

- Wavelength uncertainty
- Bandpass (FWHM)
- Uncertainty of calibration
- Sensitivity of the detector: NEI: Noise equivalent irradiance
- Spectral resolution: sampling of spectrum (wavelength)

Physics: Beer-Lambert law

- selected wavelength range
- selected cross-section
- selected atmospheric temperature
- computational uncertainty (used functions)
- extraterrestrial spectrum
- air mass range

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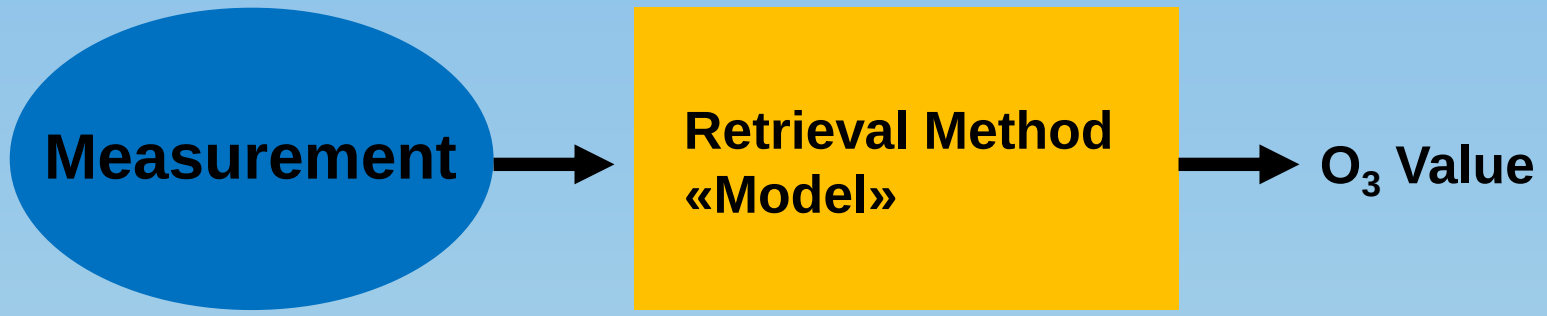

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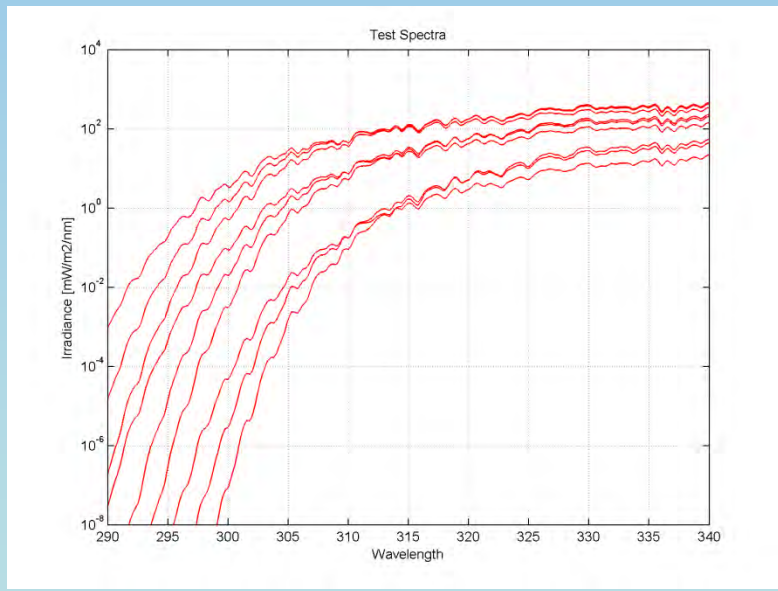
Dependencies between **measurement** uncertainties and **model** uncertainties

Procedure

1. **Generating spectrum (PMOD-model)** between 290– 340 nm with known parameters:
   - FWHM=0.1 nm, sampling Resolution 0.01 nm
   - Cross-section -> Bremen
   - Temperature of atmosphere (one layer): -45°
   - Pressure: 1023 mbar
   - For 9 atmospheric conditions in terms of Ozone, Airmass and Aerosols Optical Depth (AOD) -> **Test-Conditions**

Ozone = [350,250,450,355,255,455,352,252,452];
Airmass = [1.2,1.2,1.2,2.1,2.1,2.1,4,4,4];
AOD = [1.4,2.4,0.5,1.4,2.4,0.5,1.4,2.4,0.5];



2. **Retrieving ozone with a least square fit of the used model**
   - Unknown atmospheric parameters: Ozone, Aerosols (alpha and beta)
   - Variation of the uncertain parameters

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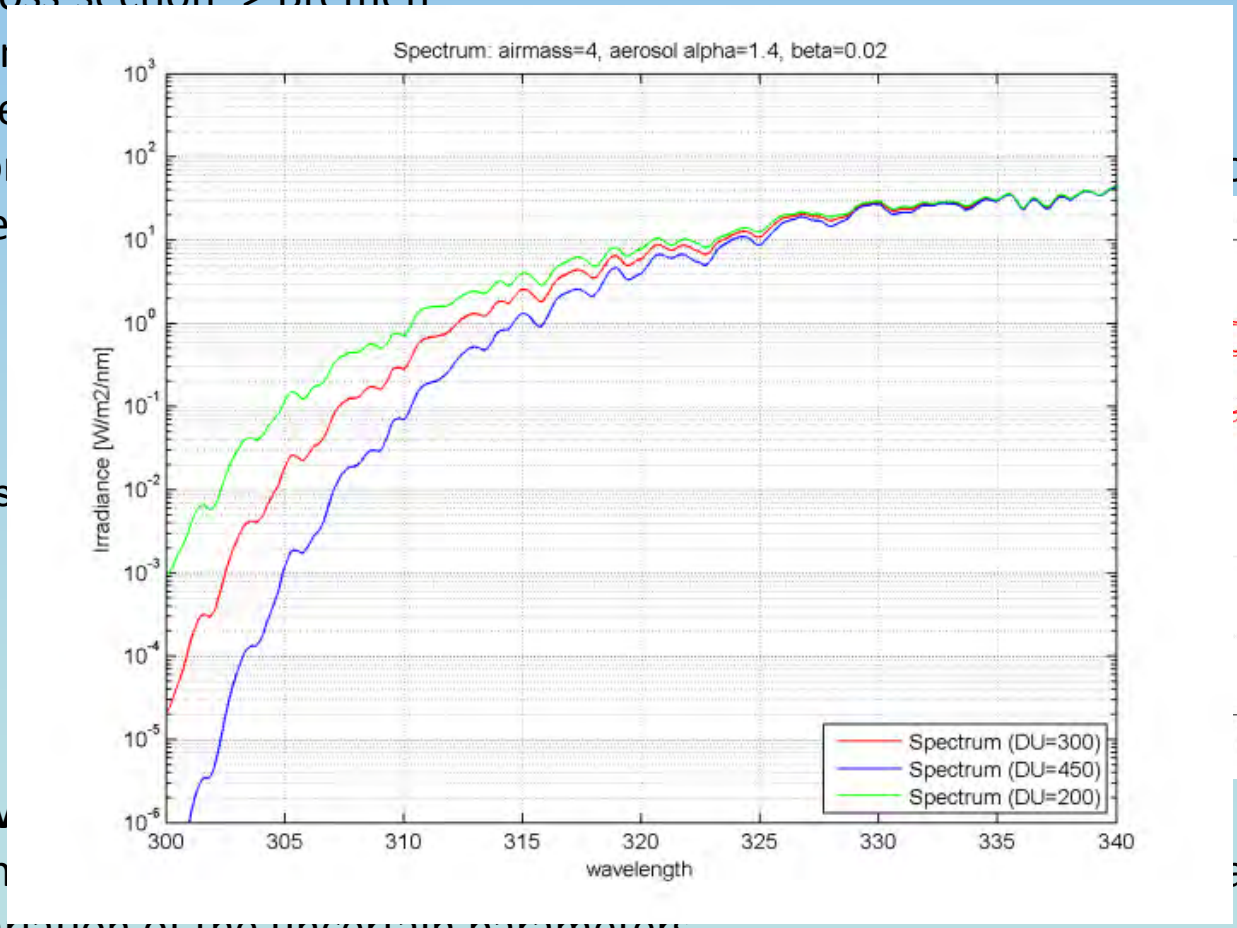

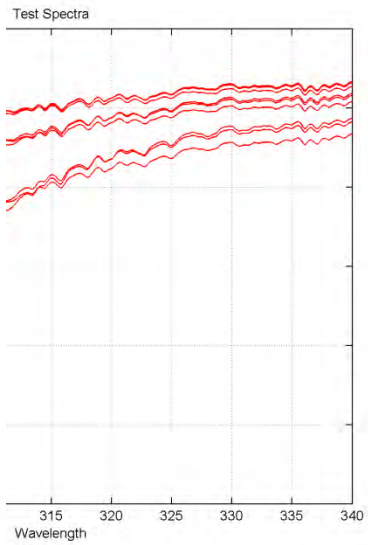

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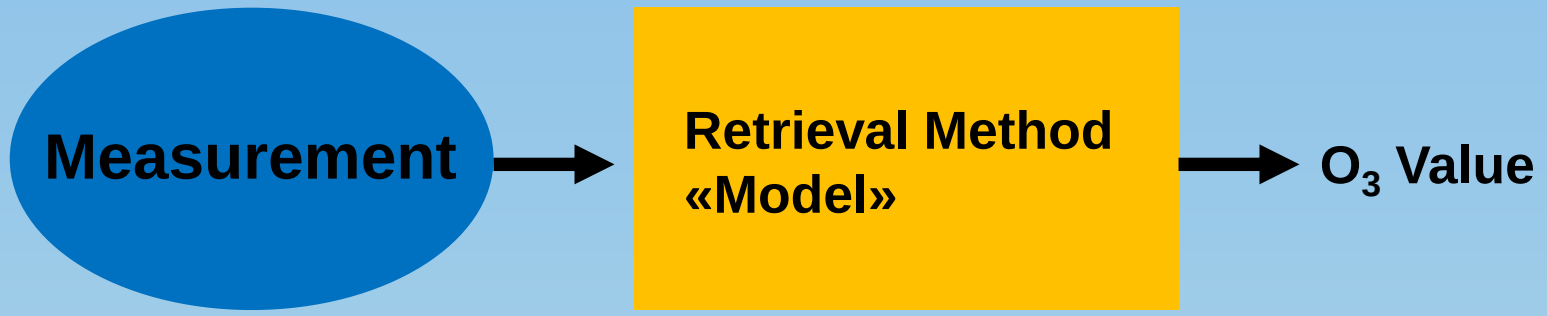
Uncertainty Ozone Retrieval



Uncertainty of **measurement**: + Uncertainty of **model**: = Uncertainty of **O_3 value**

Metrology (Physics)

- Wavelength uncertainty
- Bandpass (FWHM)
- Uncertainty of calibration
- Sensitivity of the detector: NEI: Noise equivalent irradiance
- Spectral resolution: sampling of spectrum (wavelength)

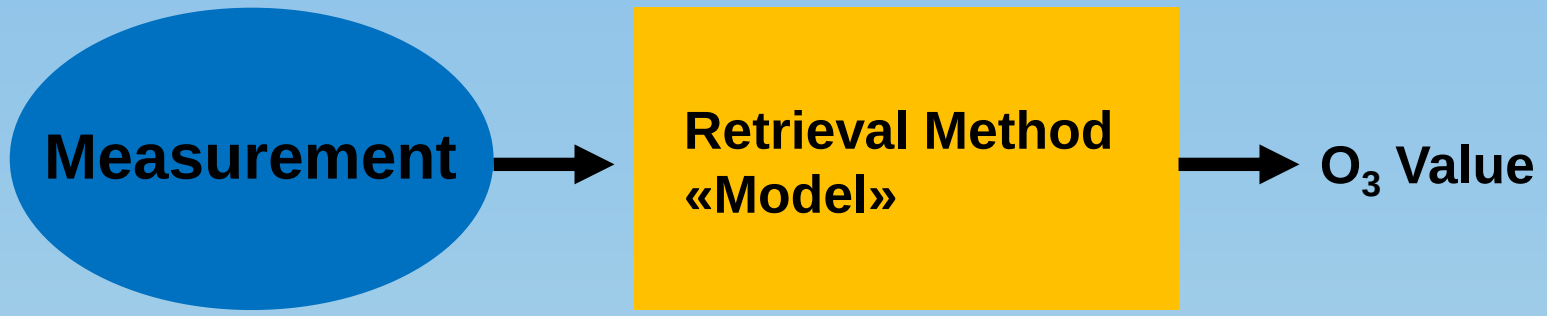
Physics: Beer-Lambert law

- selected wavelength range
- selected cross-section
- selected atmospheric temperature
- computational uncertainty (used functions)
- extraterrestrial spectrum
- air mass range

- **Uncertainty < 0.00001,**
- **=> Retrieval works well.**

(Matlab: lsqnonlin – trust region reflective similar Levenberg-Marquardt))

Uncertainty Ozone Retrieval



Uncertainty of **measurement**:

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+

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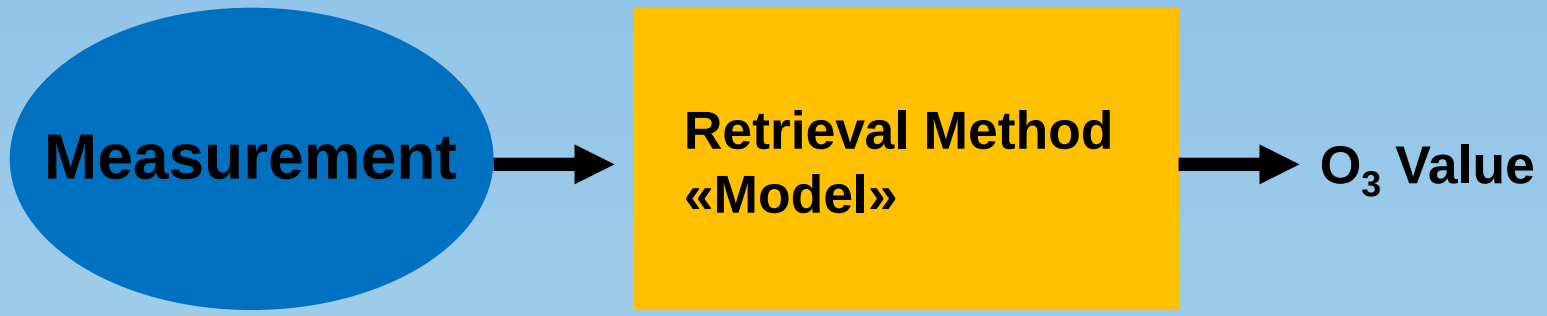
- **Uncertainty < 0.003** in the extreme case of
  - Wavelength range: 320 – 340 nm
  - FWHM=2.0 nm
  - Resolution=1.0 nm

Uncertainty Ozone Retrieval



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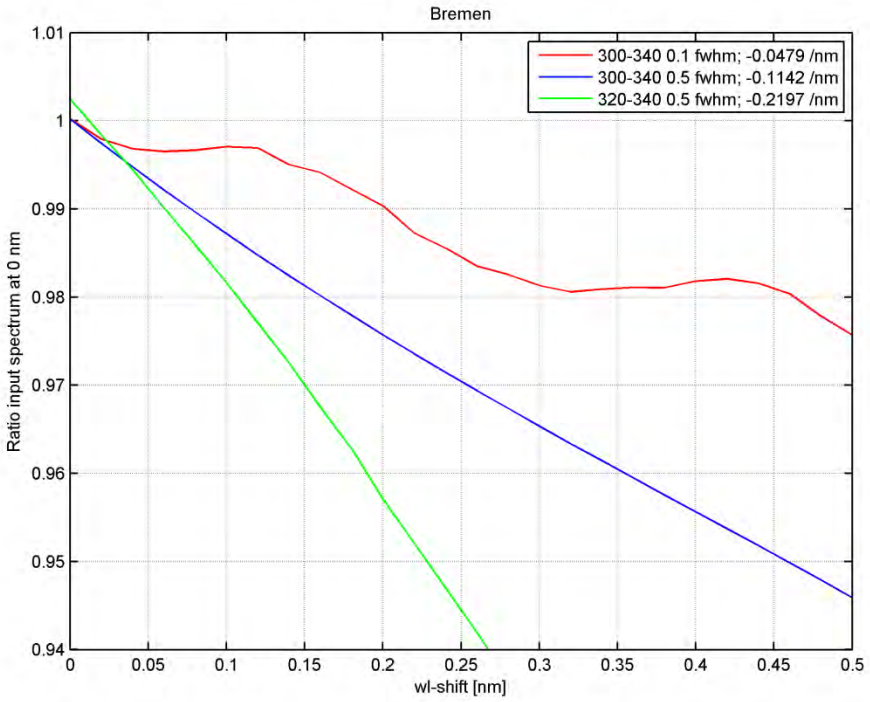
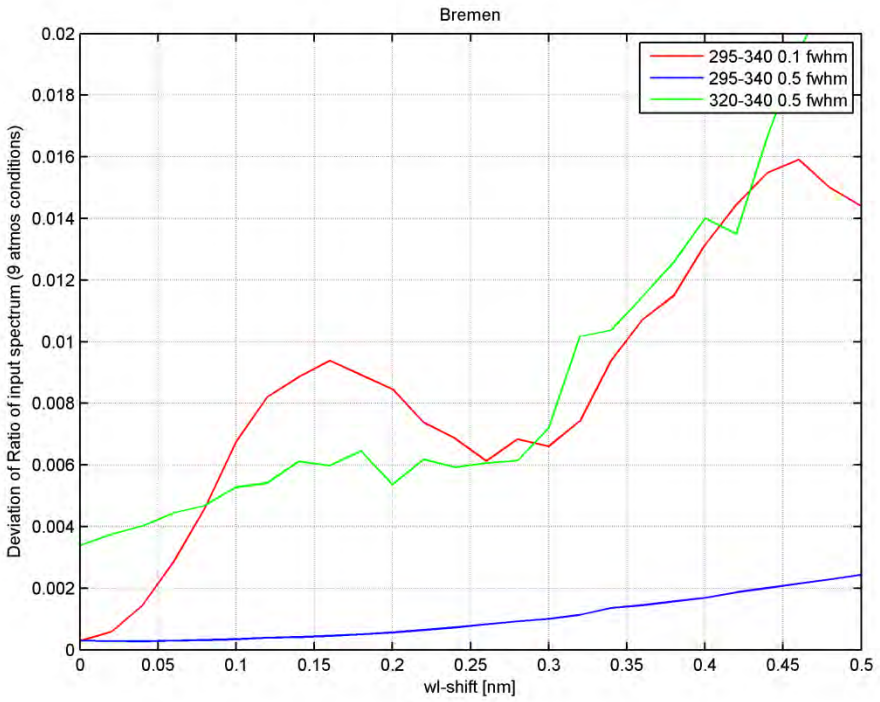
Wavelength uncertainty & FWHM





Conclusion:

- max. 0.22 uncertainty / nm wl shift
- Narrow FWHM and using the entire spectrum reduces uncertainty.

Uncertainty Ozone Retrieval

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Measurement → **Retrieval Method «Model»** → **O_3 Value**

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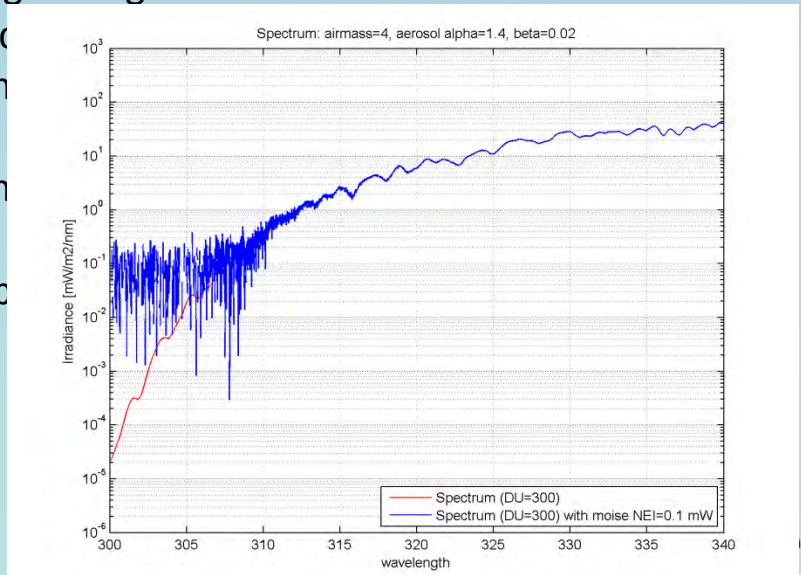
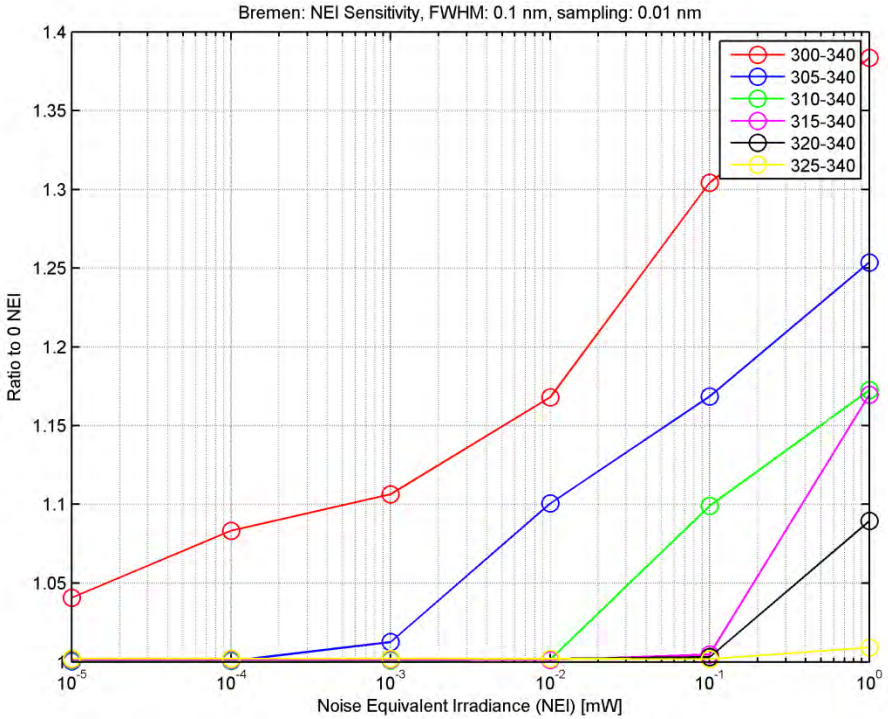
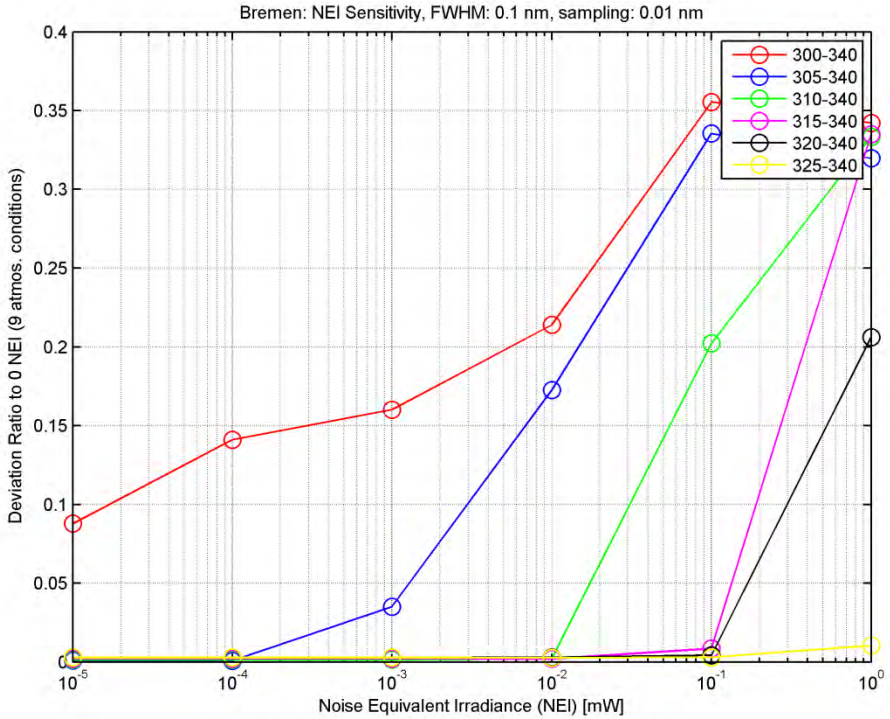


NEI & Wavelength Range

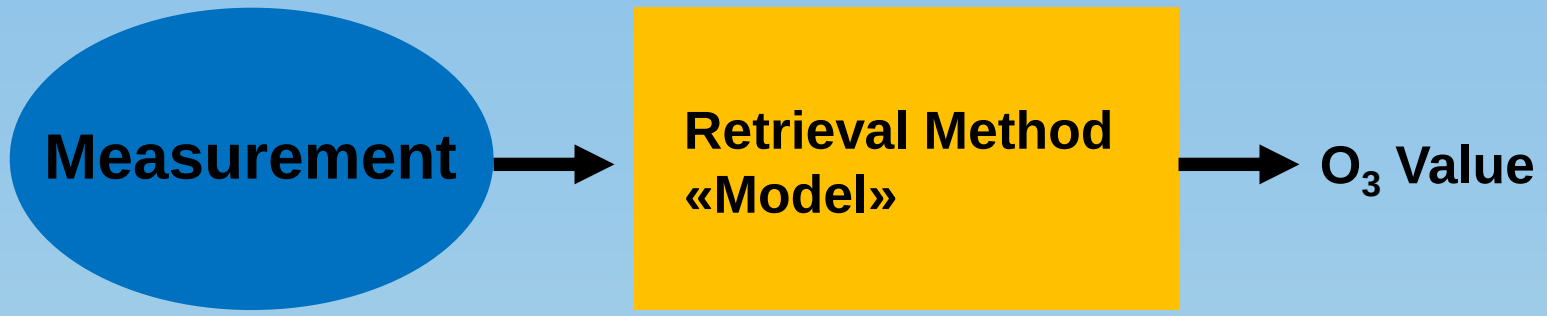




Conclusion:

- NEI significantly limits the range of selectable wavelength ranges:
- Results above are similar for different FWHM and resolutions
- **Comprehensive noise reduction did not work!**

Uncertainty Ozone Retrieval



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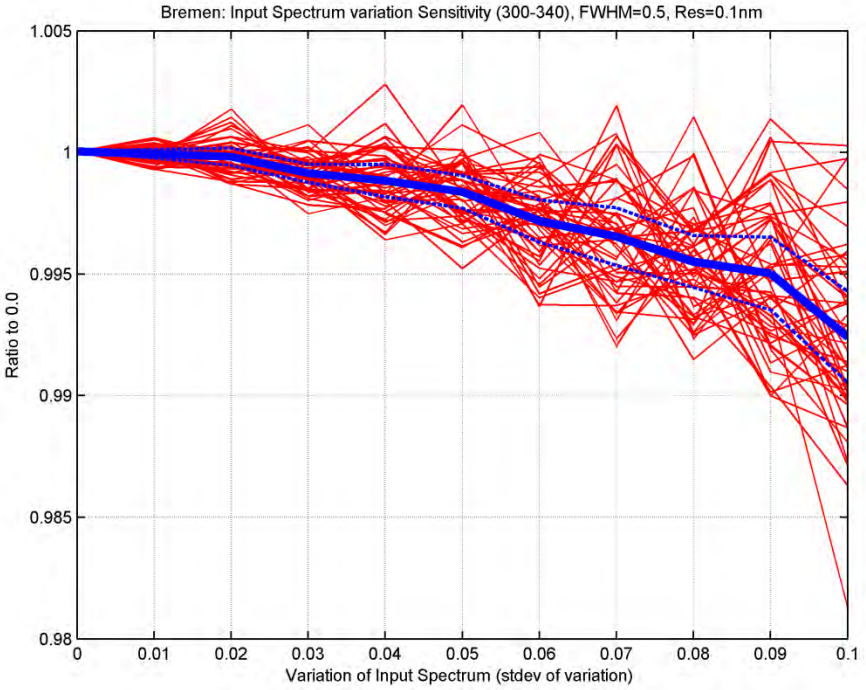
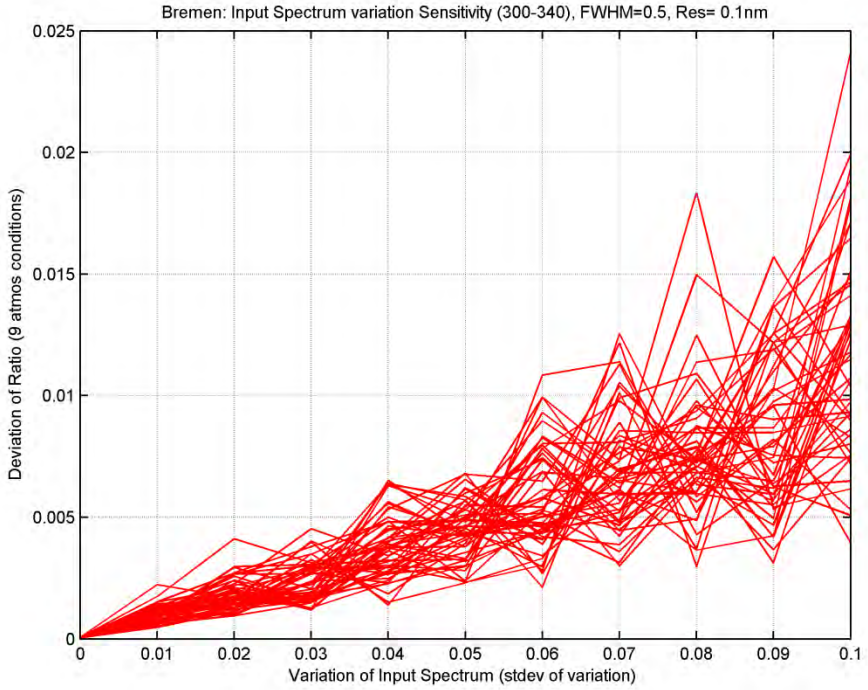
Uncertainty of calibration

- Adding white noise (gaussian) to the input Spectrum: factor instead of absolute value as for the NEI.

300 – 340 nm
FWHM=0.5 nm





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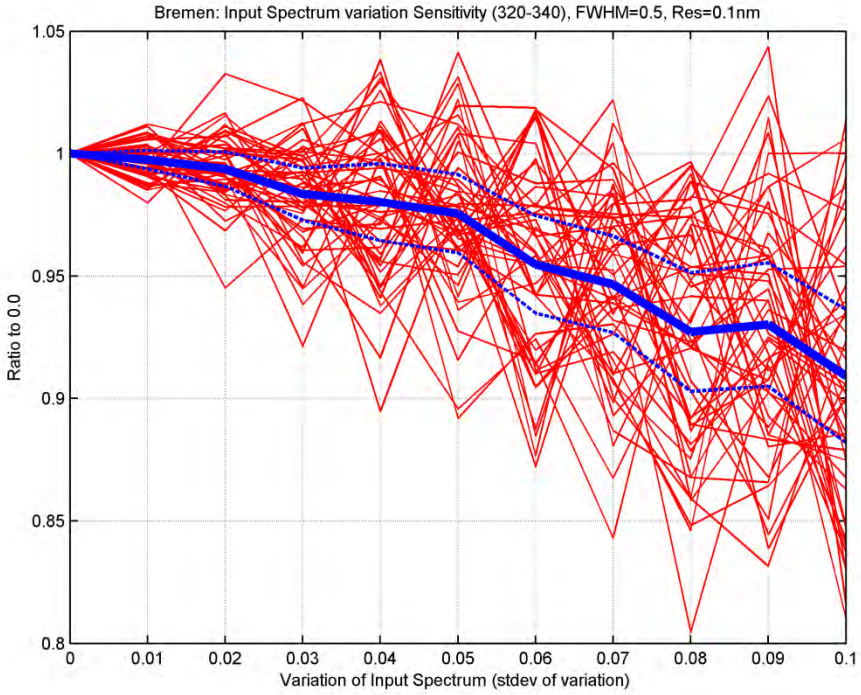
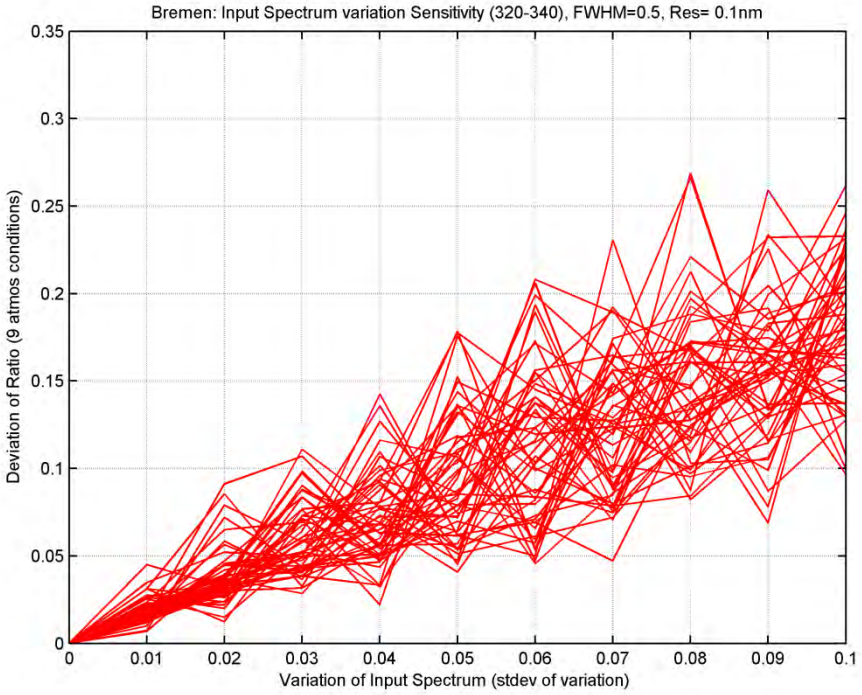
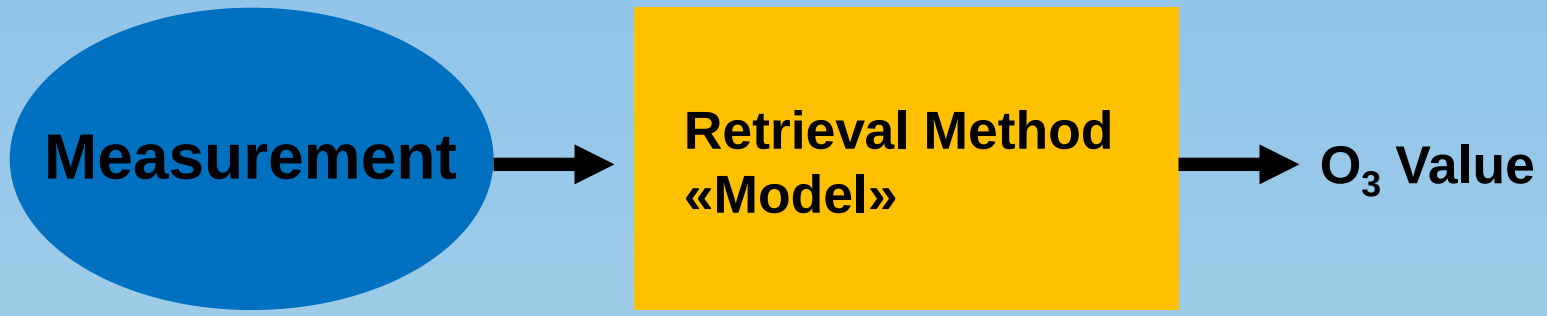




Conclusion:

- Random noise of input spectrum increases uncertainty linearily (at 320-340)
- A factor of 10 less at 300 – 340 nm
- Slight dependence on resolution
- No effect with constant factor of input spectrum

Uncertainty Ozone Retrieval



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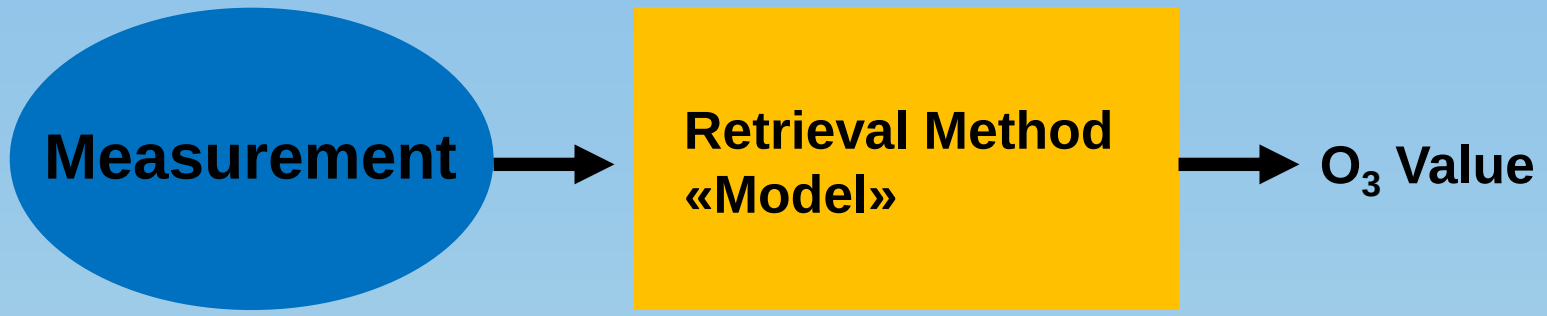
Bremen – PaurBass
(@T=-45°C & -30°C)

300-340 nm: 1.004+/-0.001
310-340 nm: 1.002+/-0.001
320-340 nm: 1.009+/-0.006

Bremen – Brion @ T=-45°

300-340 nm: 0.999+/-0.001
310-340 nm: 1.011+/-0.001
320-340 nm: 1.004+/-0.002

Uncertainty Ozone Retrieval



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Bremen – PaurBass
(@T=-60°C)
300-340 nm: 1.018+/-0.002
310-340 nm: 0.997+/-0.001
320-340 nm: 1.016+/-0.003

Bremen – PaurBass
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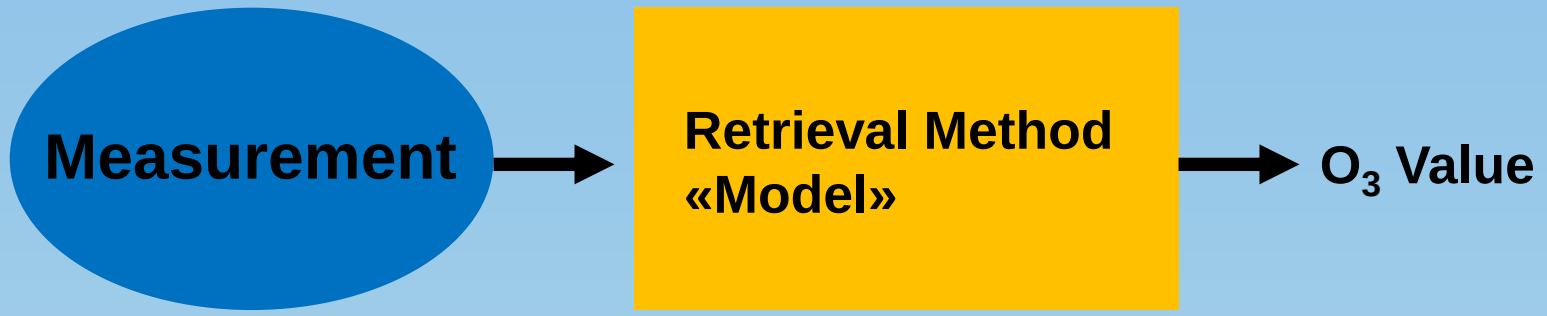

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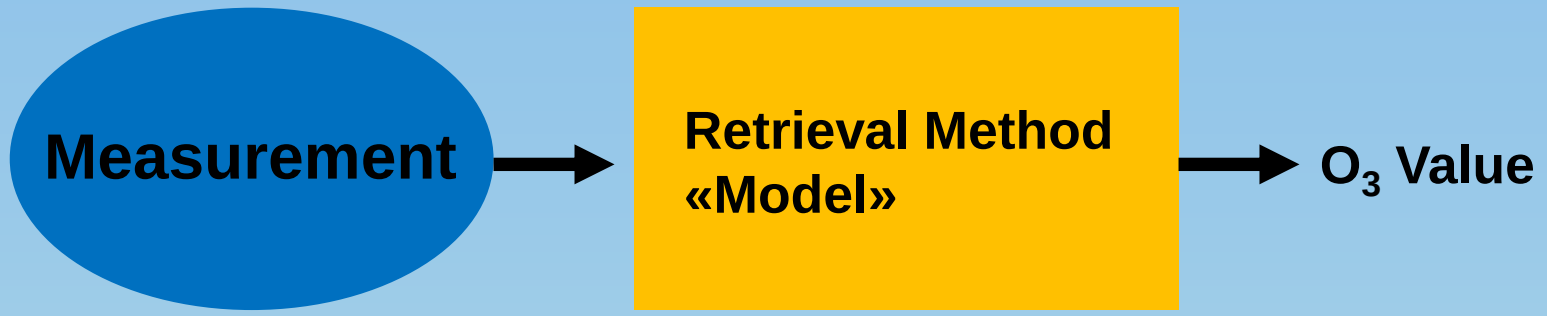

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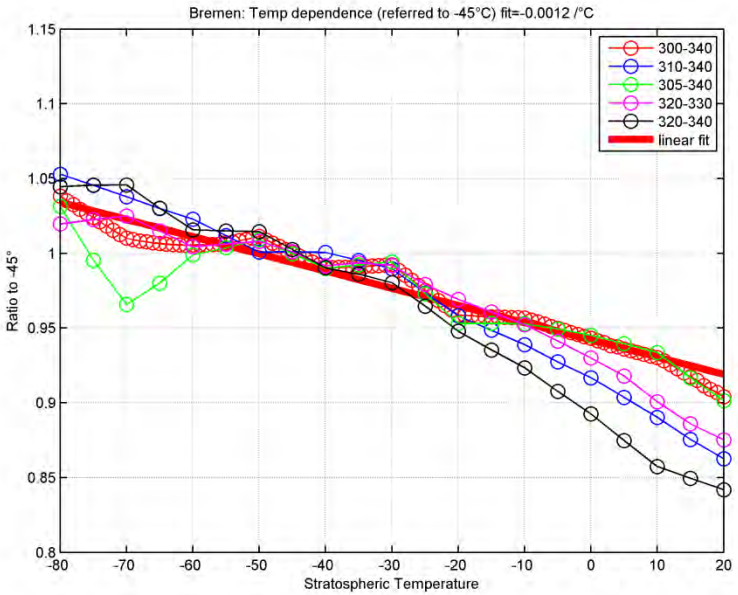
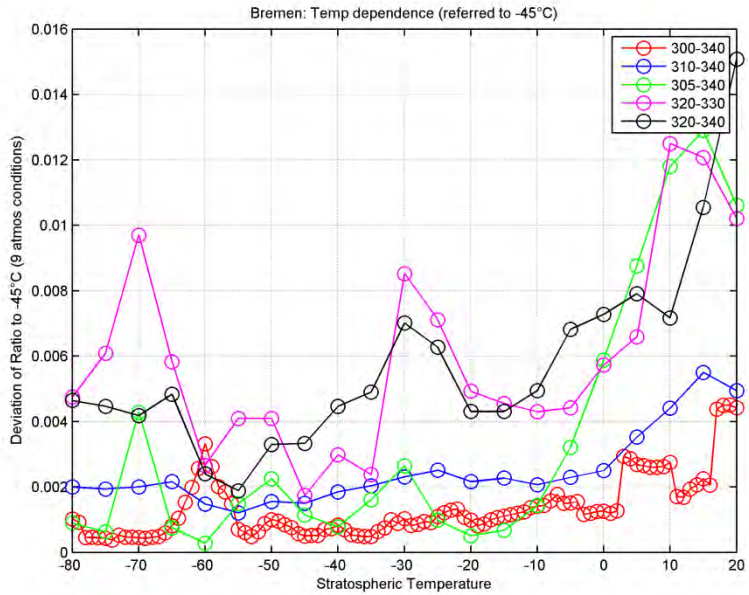
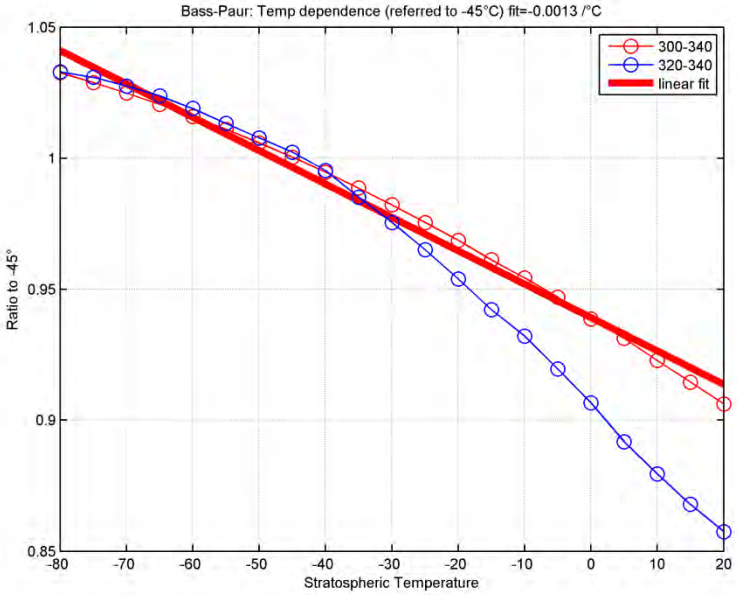
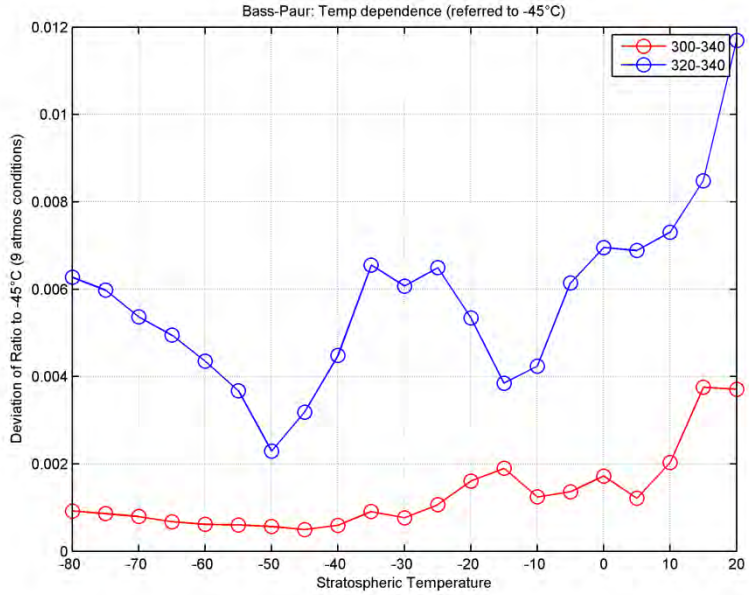
X-section & Temperature & WL

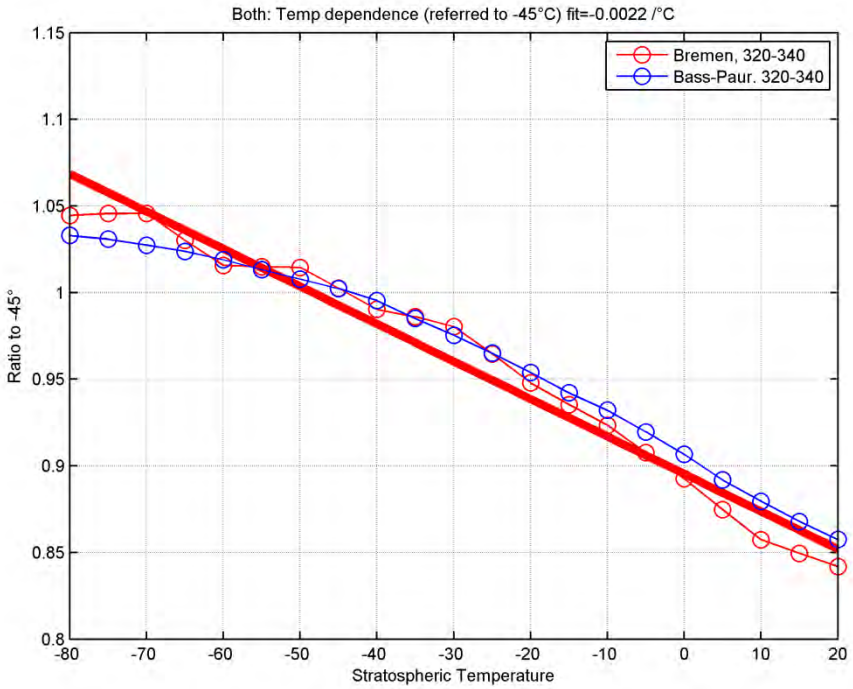


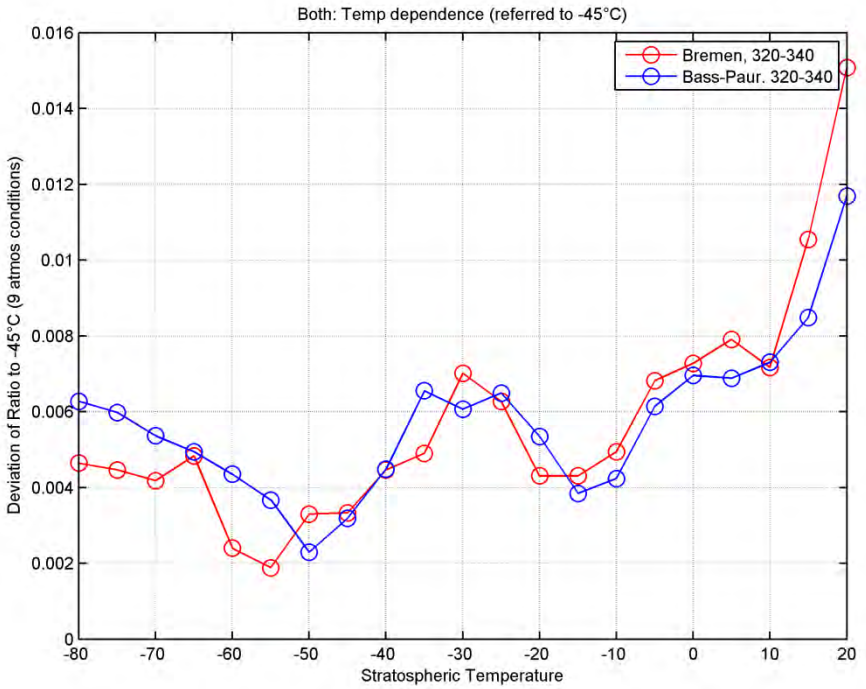






X-section & Temperature & WL

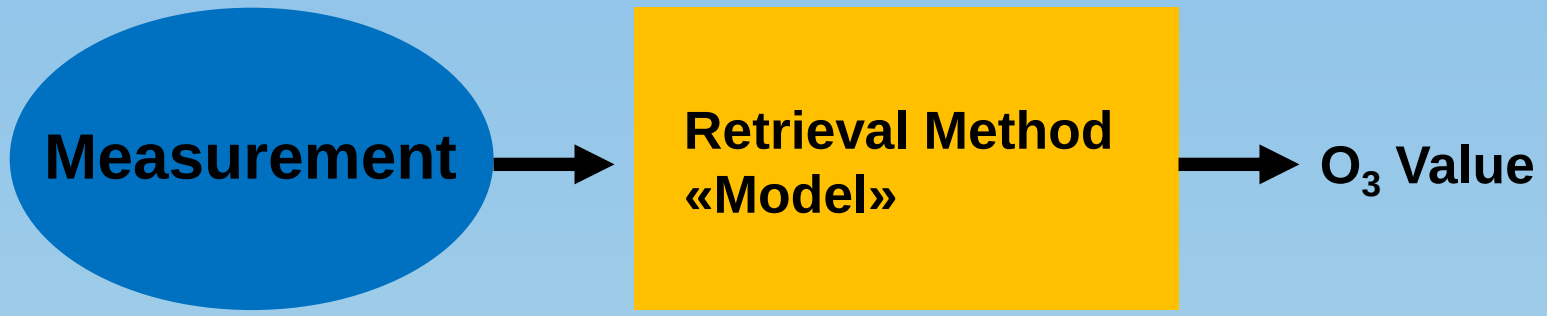




Conclusion (WL-Range between 320 – 340):

- **Uncertainty of** about 0.0025 / °C (atmospheric temperature)
- Uncertainty of about max. 0.7% when using either Bremen of Baur-Pass
- **Note:** Temperature retrieval from spectral analyis was not possible

Uncertainty Ozone Retrieval



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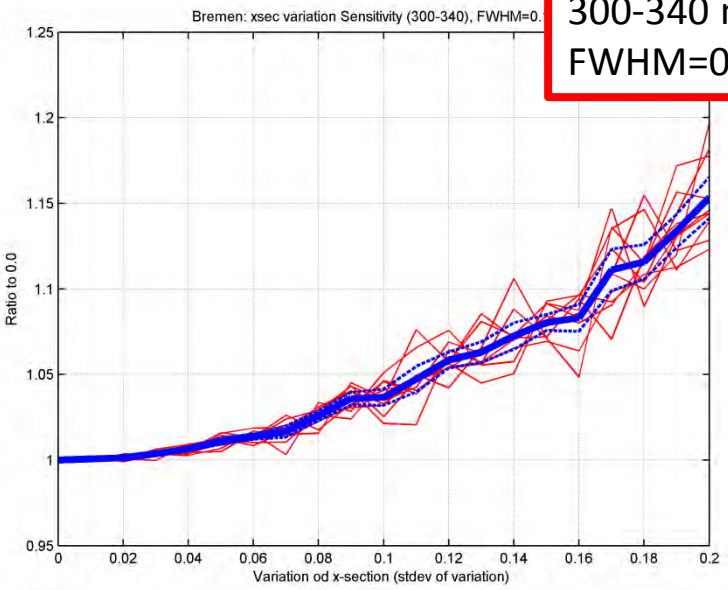
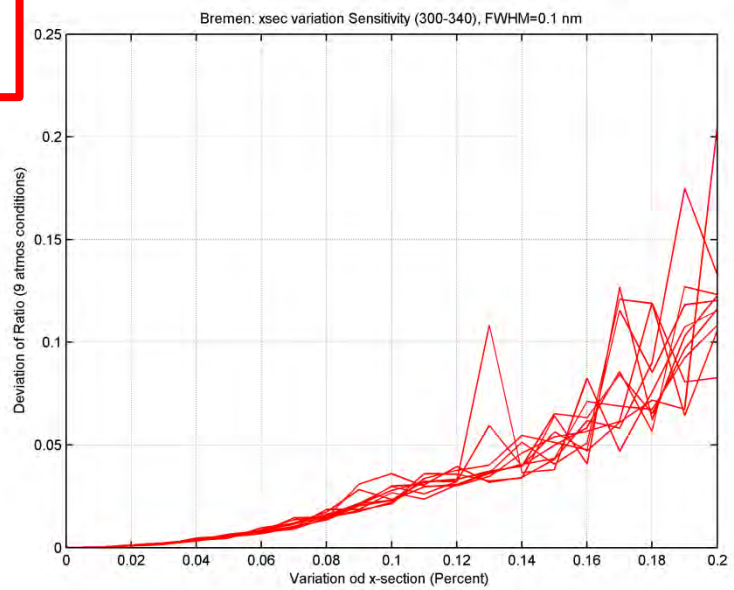
Variation of X-section

- Adding white noise (gaussian) to the x-section

300-340 nm
FWHM=0.1 nm





320 – 340 nm
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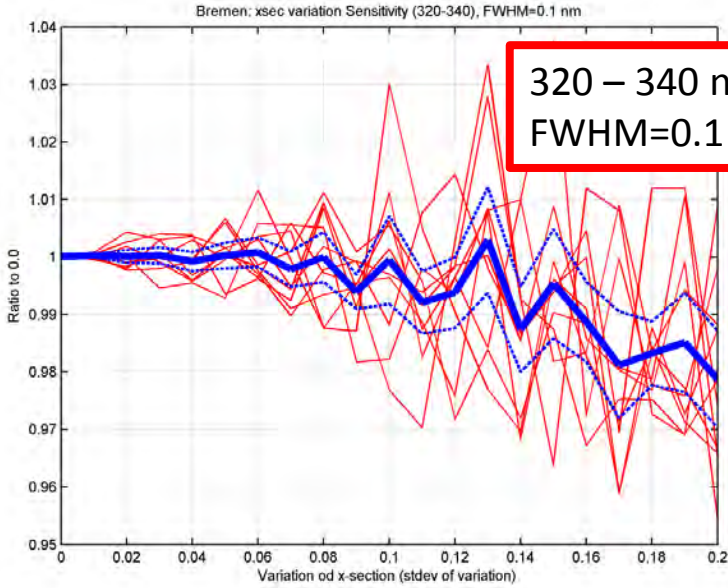

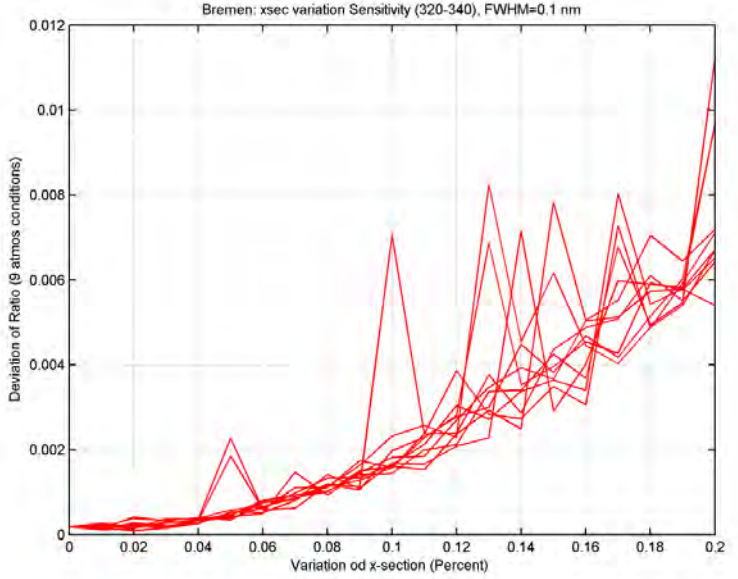

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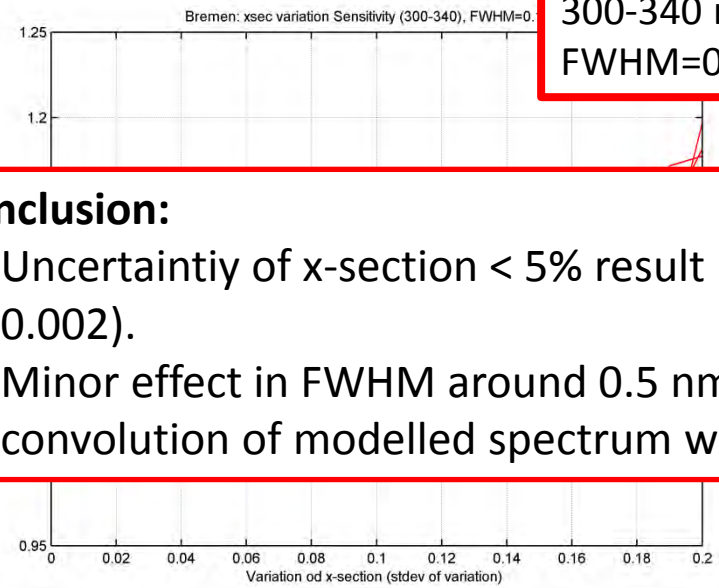
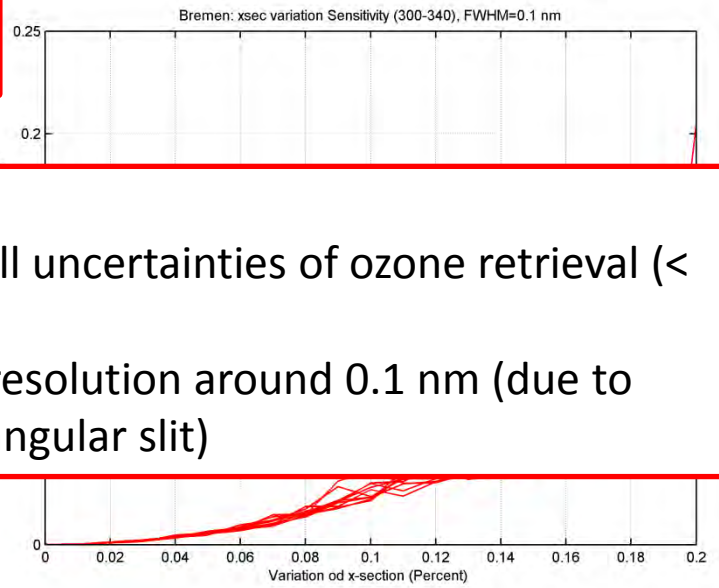
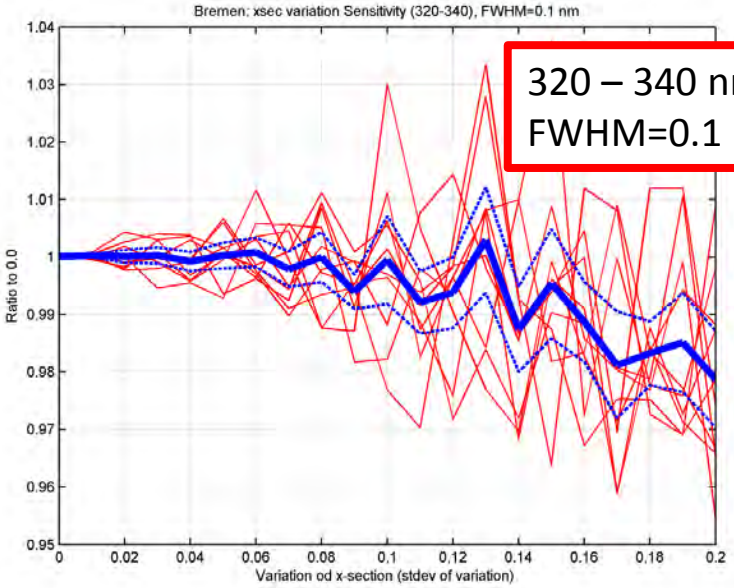


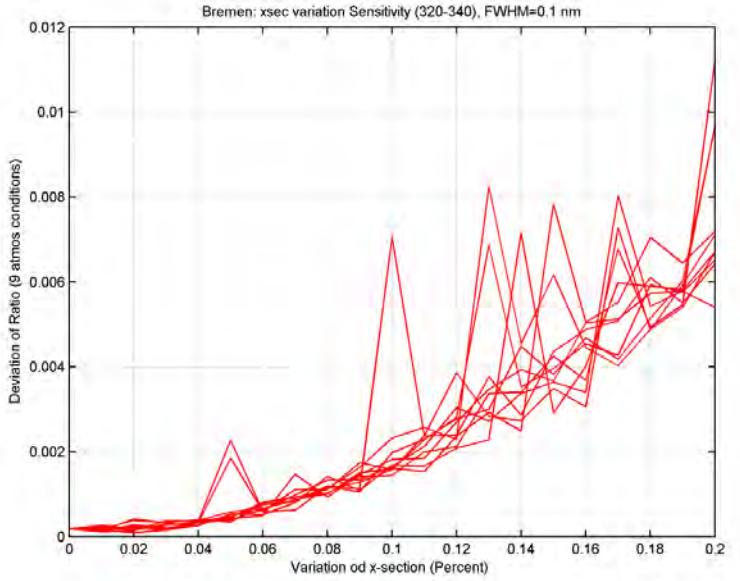


Conclusion:

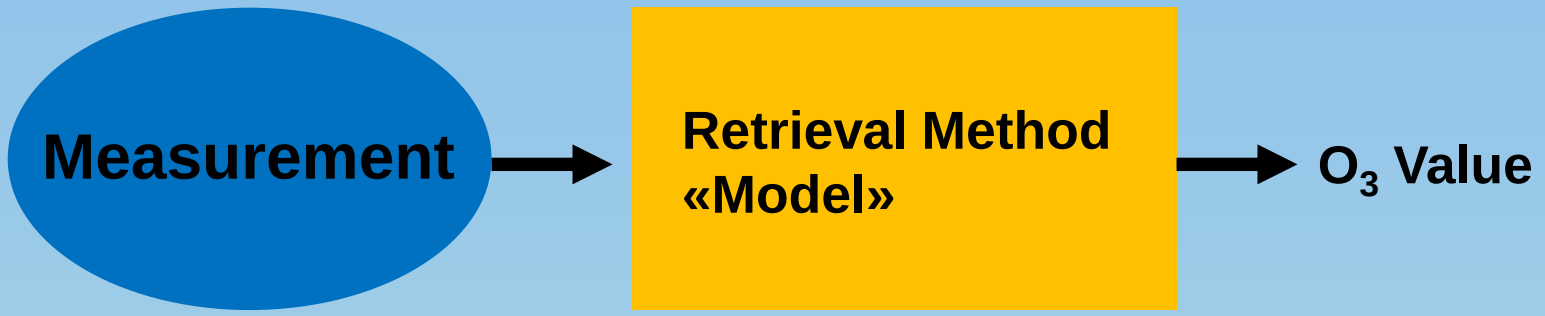
- Uncertaintiy of x-section < 5% result in small uncertainties of ozone retrieval (< 0.002).
- Minor effect in FWHM around 0.5 nm and resolution around 0.1 nm (due to convolution of modelled spectrum with triangular slit)

320 – 340 nm
FWHM=0.1 nm





Uncertainty Ozone Retrieval



Uncertainty of **measurement**: + Uncertainty of **model**: = Uncertainty of **O_3 value**

Metrology (Physics)

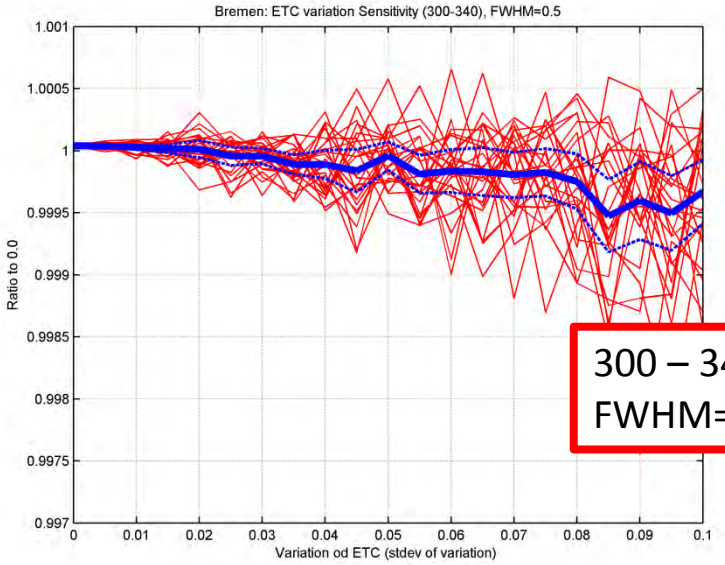
- Wavelength uncertainty
- Bandpass (FWHM)
- Uncertainty of calibration
- Sensitivity of the detector: NEI: Noise equivalent irradiance
- Spectral resolution: sampling of spectrum (wavelength)

Physics: Beer-Lambert law

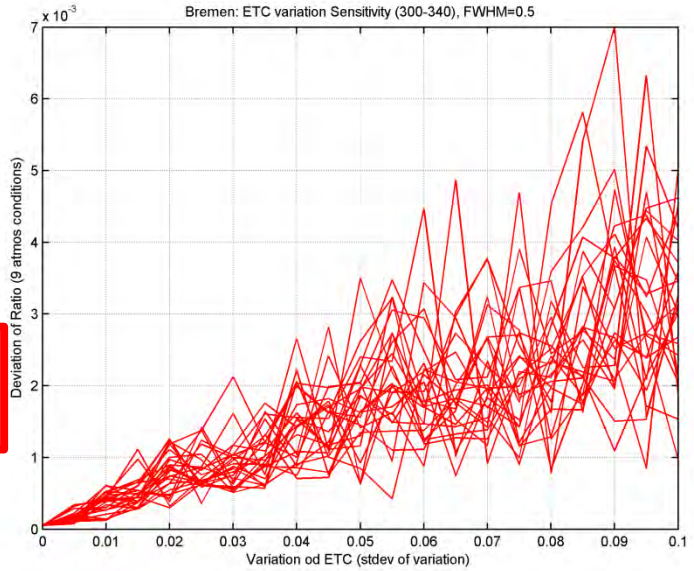
- selected wavelength range
- selected cross-section
- selected atmospheric temperature
- computational uncertainty (used functions)
- extraterrestrial spectrum
- air mass range

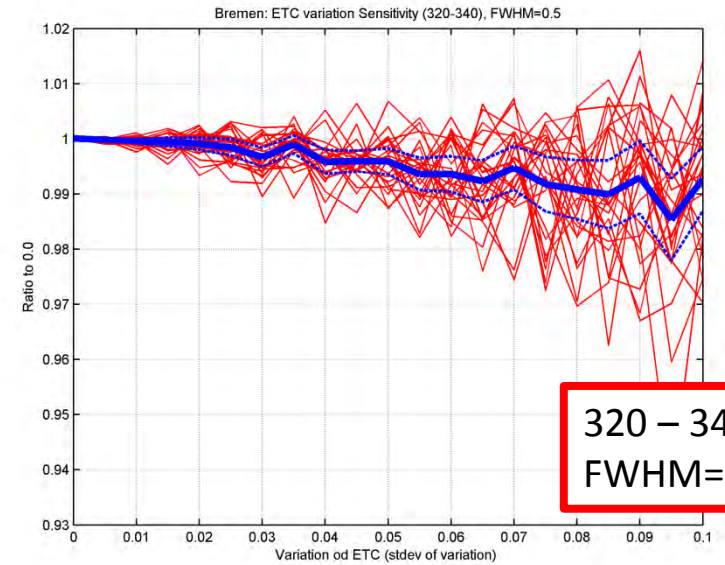
Variation of Extraterrestrial Spectrum

- Adding white noise (gaussian) to the ETC



300 – 340 nm
FWHM=0.5 nm





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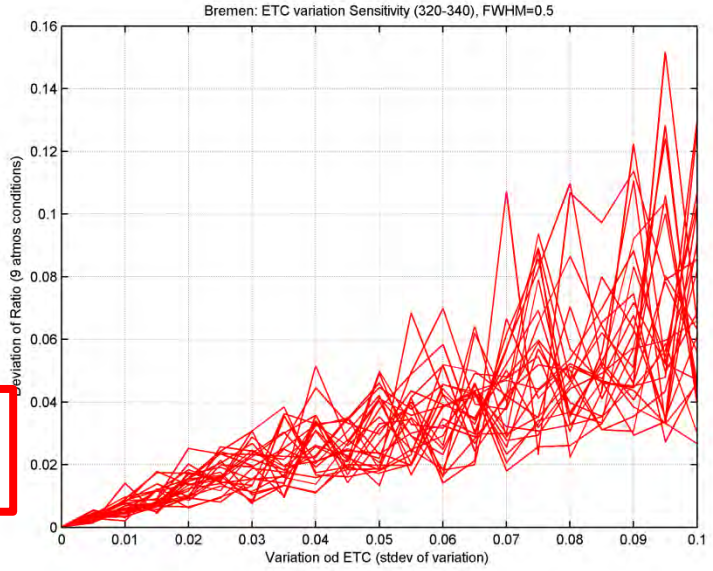

Variation of Extraterrestrial Spectrum

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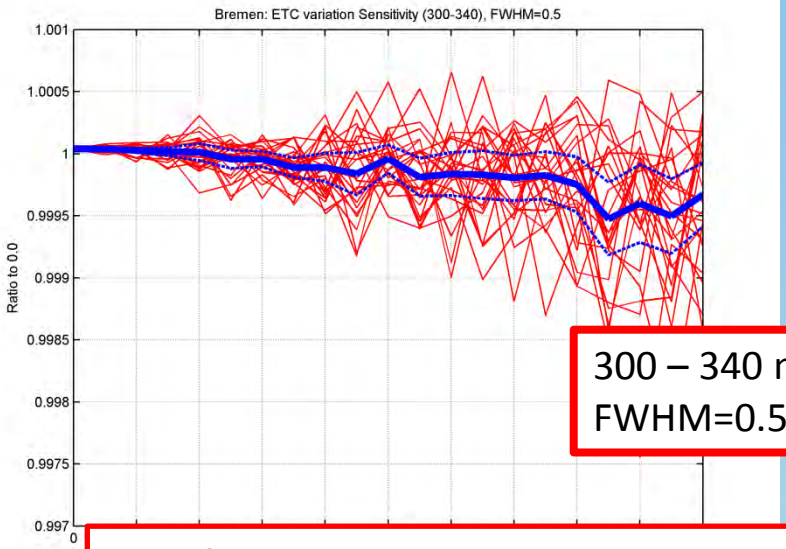
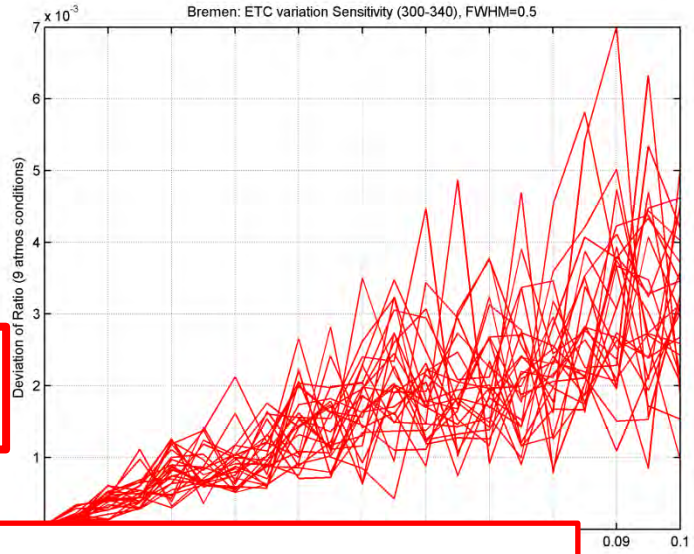
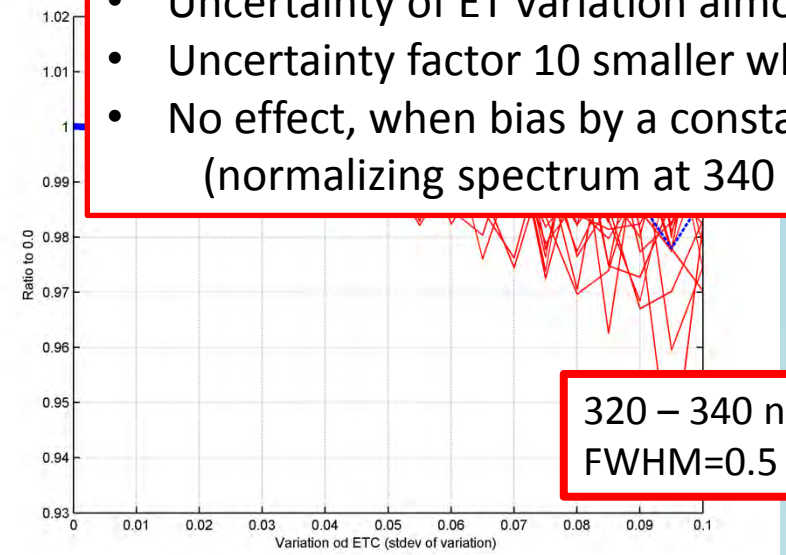


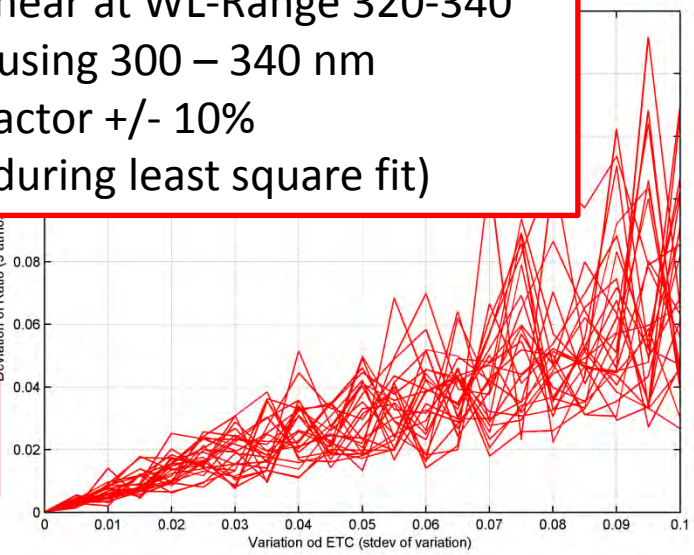


300 – 340 nm
FWHM=0.5 nm

Conclusion:

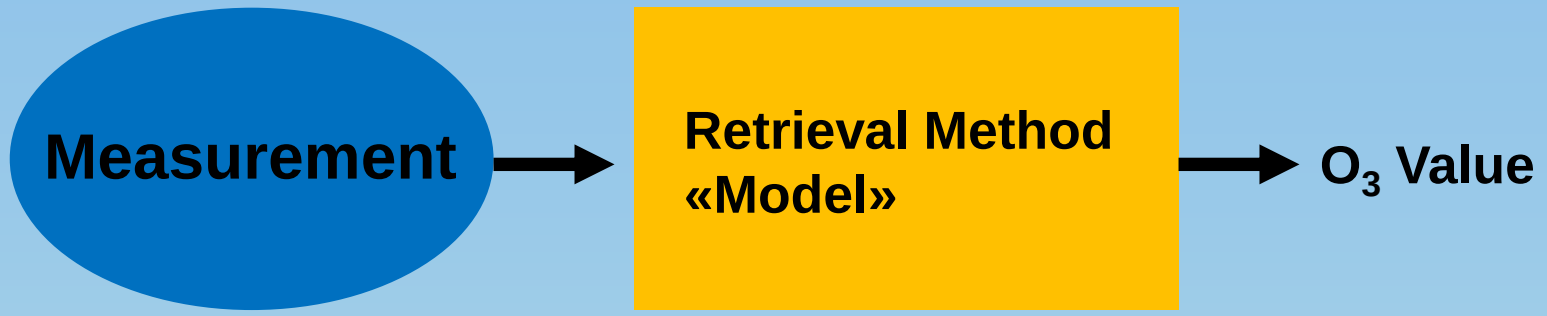
- Uncertainty of ET variation almost linear at WL-Range 320-340
- Uncertainty factor 10 smaller when using 300 – 340 nm
- No effect, when bias by a constant factor +/- 10%
  (normalizing spectrum at 340 nm during least square fit)





320 – 340 nm
FWHM=0.5 nm

Uncertainty Ozone Retrieval



Uncertainty of **measurement**: + Uncertainty of **model**: = Uncertainty of **O_3 value**

Metrology (Physics)

- Wavelength uncertainty
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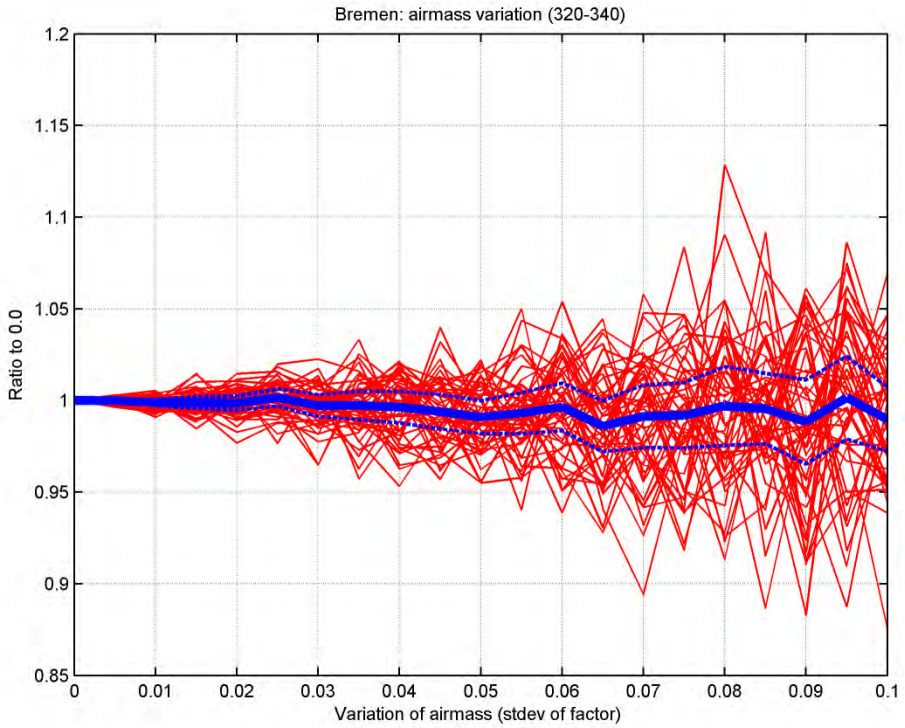
- Uncertainty of calibration
- Sensitivity of the detector: NEI: Noise equivalent irradiance
- Spectral resolution: sampling of spectrum (wavelength)

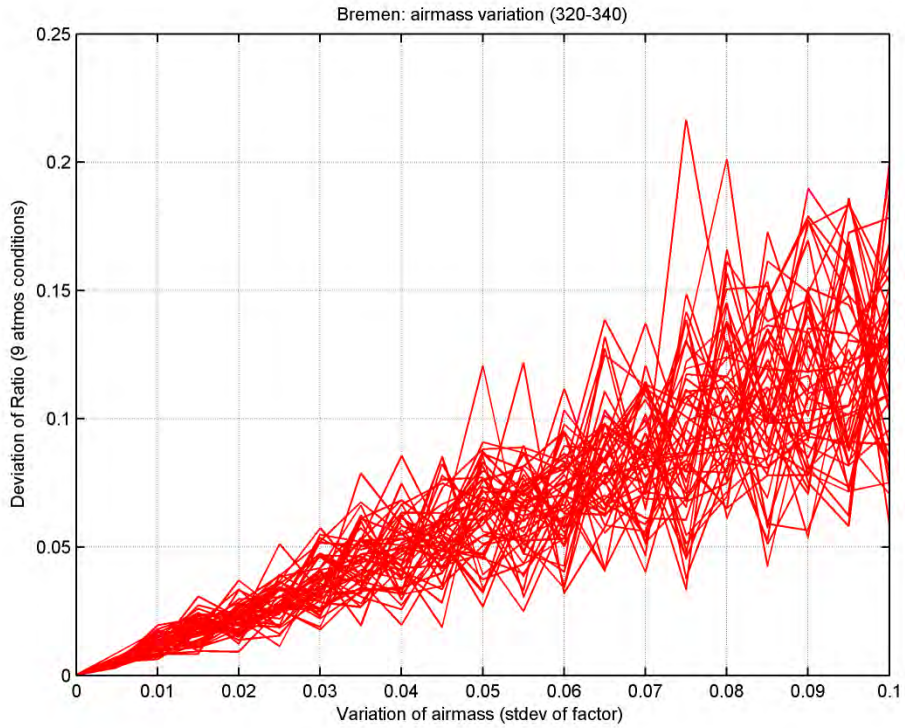
Physics: Beer-Lambert law

- selected wavelength range
- selected cross-section
- selected atmospheric temperature
- computational uncertainty (used functions)
- extraterrestrial spectrum
- air mass range

Variation of Airmass

- Adding gaussian noise to the airmass





Conclusion:

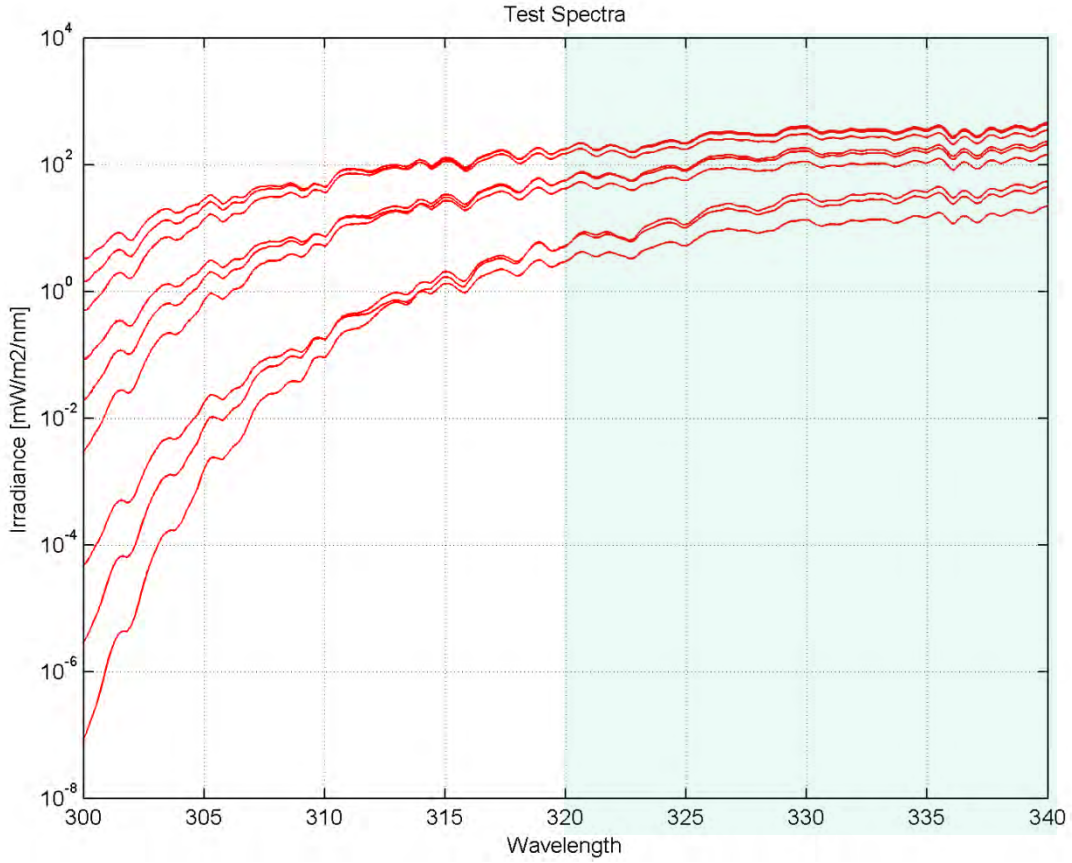
- Uncertaintiy of air mass uncertainty is linear with the ozone retrieval uncertainty.
- No depending on WL-Range, FWHM or Resolution.

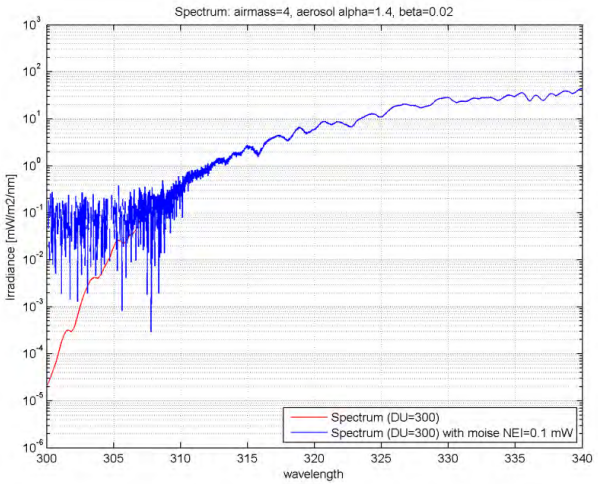
$$\log I_\lambda = \log I_\lambda^0 - \tau_\lambda^R m_R - \tau_\lambda^{O3} m_{O3} - \tau_\lambda^{SO2} m_{SO2} - \tau_\lambda^{aod} m_{aod}$$

Summary

- NEI = Noise equivalent irradiance is the most relevant factor for the uncertainty of total ozone retrieval using multispectral measurements.

Why? NEI limits the range of usable wavelength range => a smaller rang of wavelength reduced the dynamic range of the analysed spectrum.





Summary

	300-340 nm	320-340 nm	Remark
WL uncertainty	0.11 ± 0.004% / nm	**0.21 ± 0.02**% / nm	Depending on FWHM
X-section (Bremen- PB)	1.004 ± 0.001	**1.009 ± 0.0067**	
Bremen: Atmos.T uncertainty	0.0012 ± 0.002 / °C	**0.0021 ± 0.008**/°C	
BP: Atmos.T uncertainty	0.0013 ± 0.001/°C	**0.0018 ± 0.01**/°C	
Xsec variation (Bremen)	<0.005 at 0.1 variation	<0.005 at 0.1 variation	Depending on FWHM
ETC variation (PMOD)	<0.003 at 0.5 variation	**~0.03 at 0.5** variation	Constant factor-> no effect
Air Mass Variation	~0.05 at 0.5 variation	~0.05 at 0.5 variation	Linear
Spectrum uncertainty (calibration)	0.005 at 0.05 variation	**0.05 at 0.05** variation	Depending Resolution

Variation of ALL

Procedure:

a) **Settings** (Avantes Array Spectroradiometer – AVOS2): FWHM: 0.5 nm, Spectral resolution: 0.15 nm

b) **Generated Spectrum**: T-Atmos.=-45°C, x-section=Bremen, ETC=PMOD;

c) Variation of:

- **Wavelength Uncertainty**: 0.05 nm. Randomly selected from Normaldistribution with 0.05 nm standard deviation
- **Random selection of x-section** (Bremen and Baur-Pass)
- Random selection of **atmospheric temperature** of x-section between -60°C and -30°C
- Adding gaussian noise to **x-section** (standard deviation=0.05 of applied factor)
- Adding gaussian noise to **extraterrestrial spectrum** (stdev =0.05 of applied factor)
- Adding gaussian noise to **input spectrum** (stdev =0.05 of applied factor)

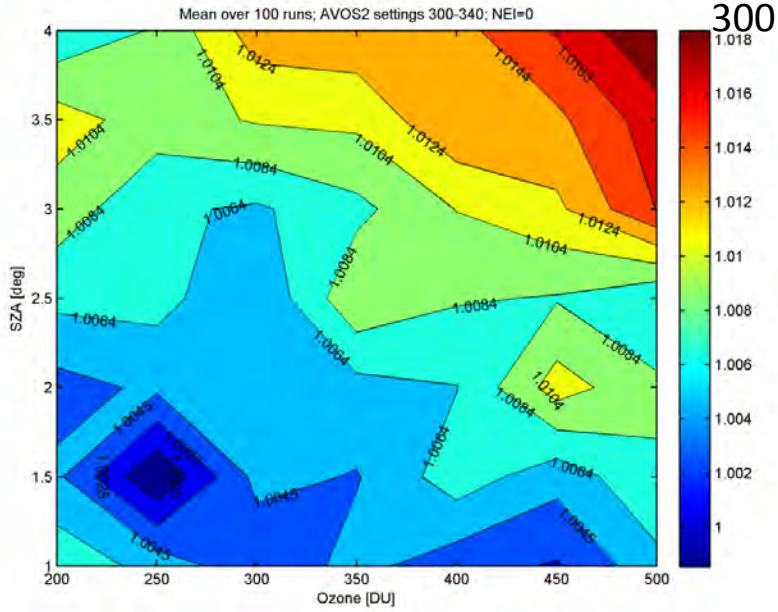
d) No variation of: Air mass

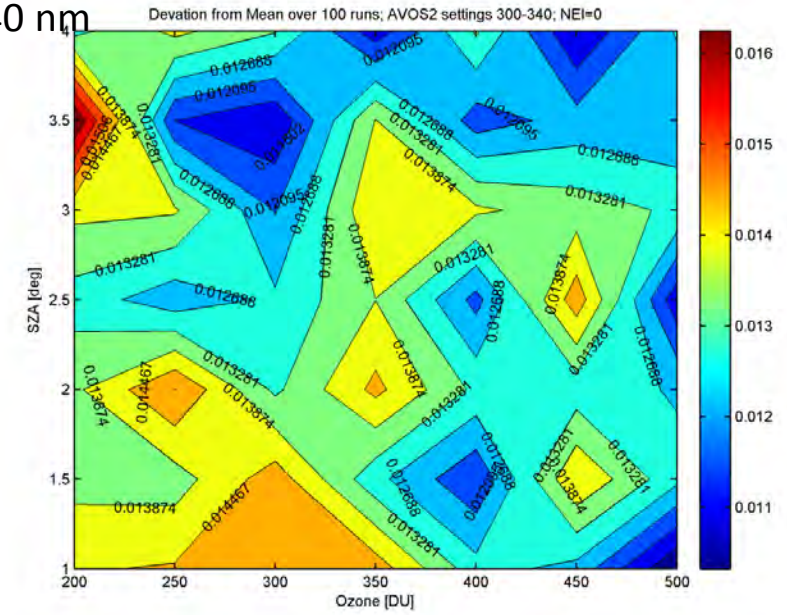
e) Atmosphere: **different ozone and airmass** (fixed aerosols)

f) **Ensemble runs** (100); calculating **mean and standard deviation of all runs**

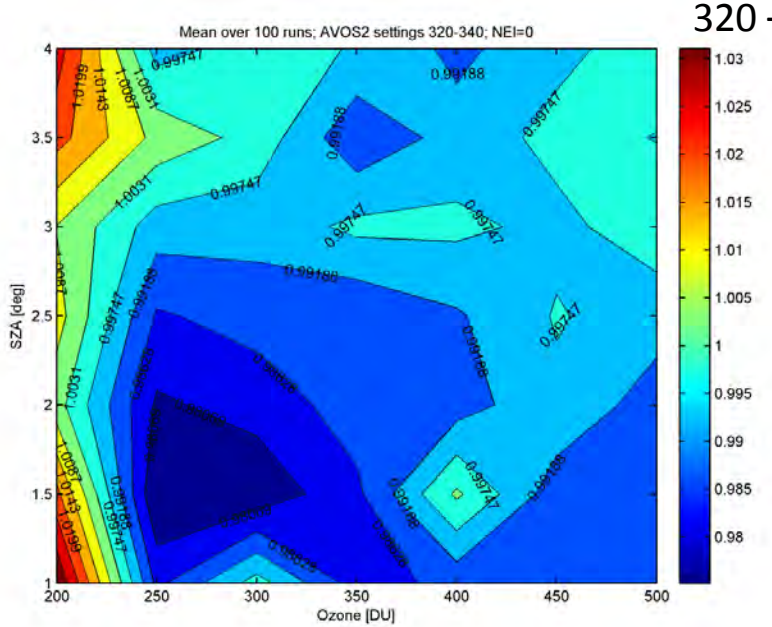
Variation of ALL; NEI=0!

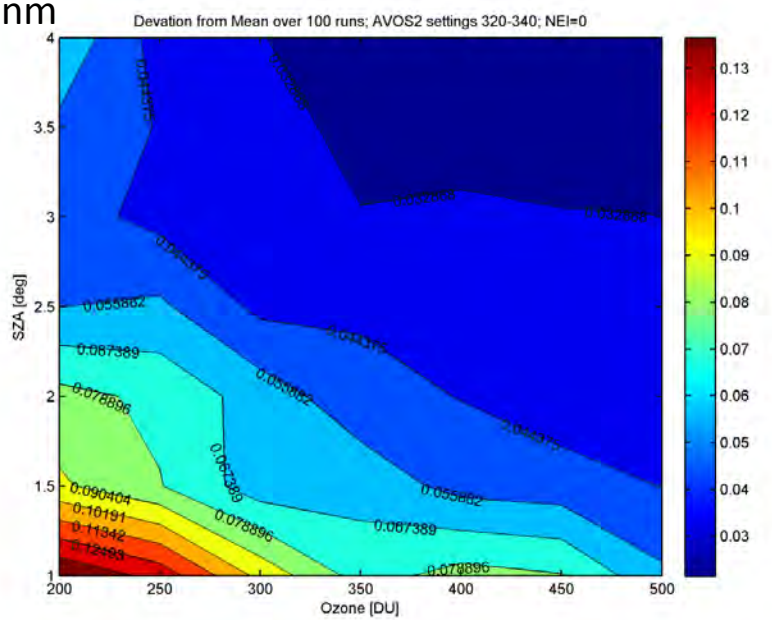
300 – 340 nm





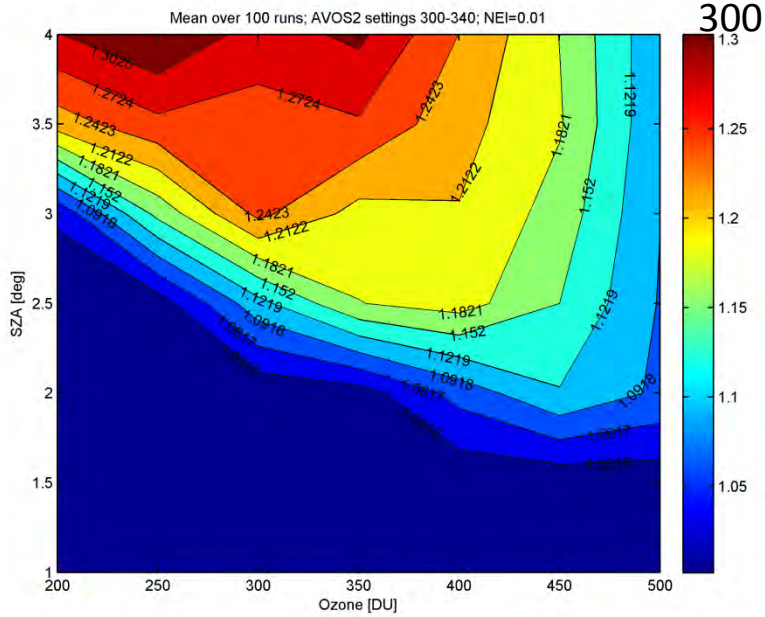
320 – 340 nm

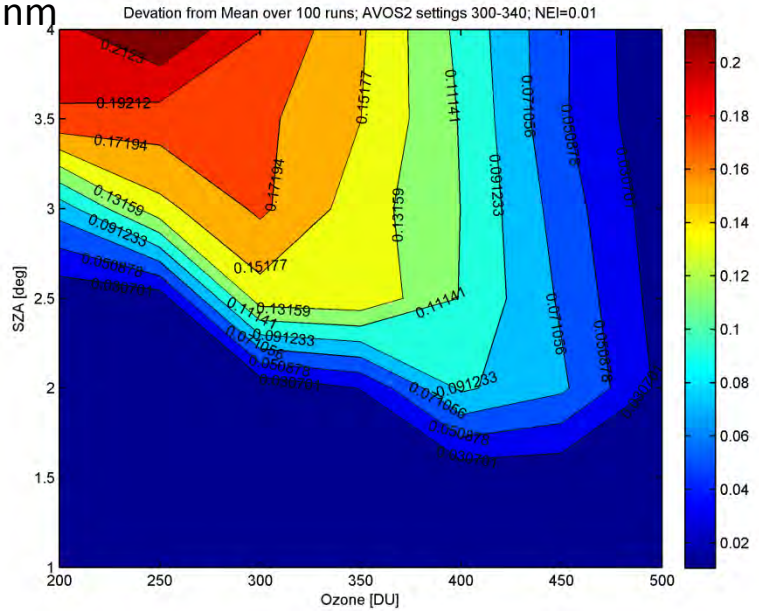




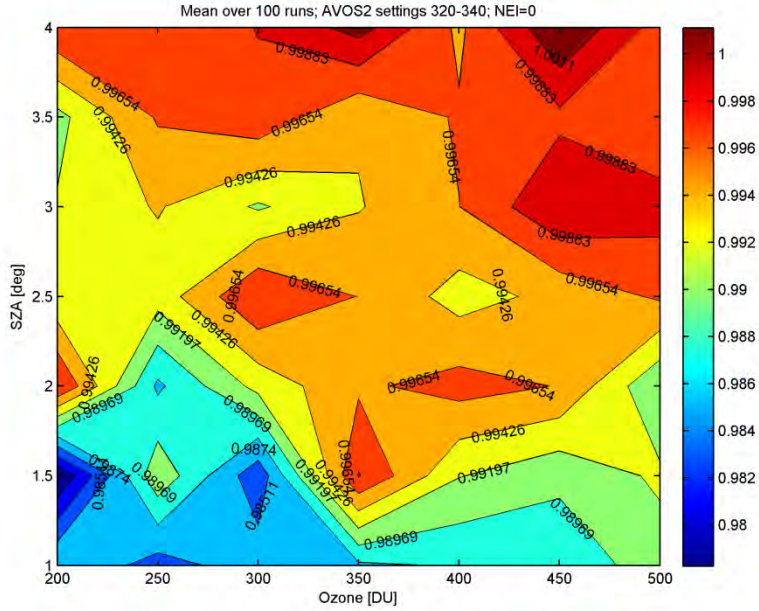
Variation of ALL; NEI=0.01!

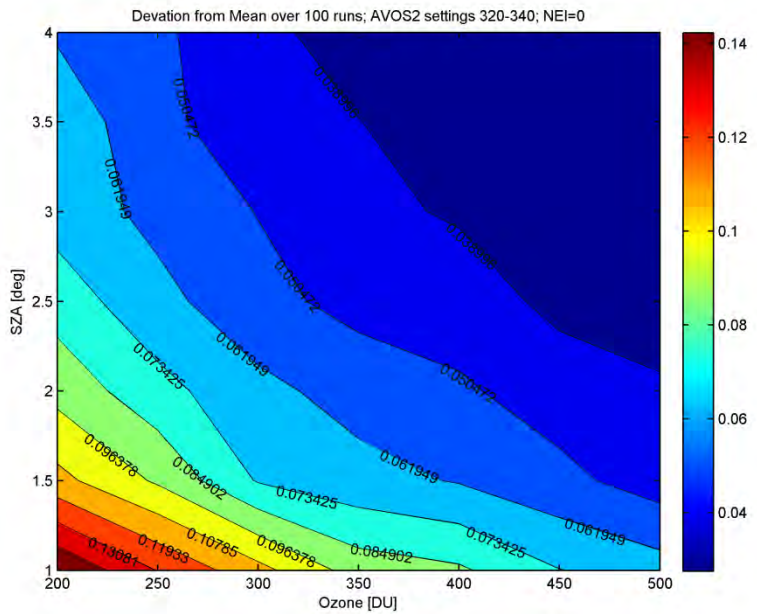
300 – 340 nm





320 – 340 nm





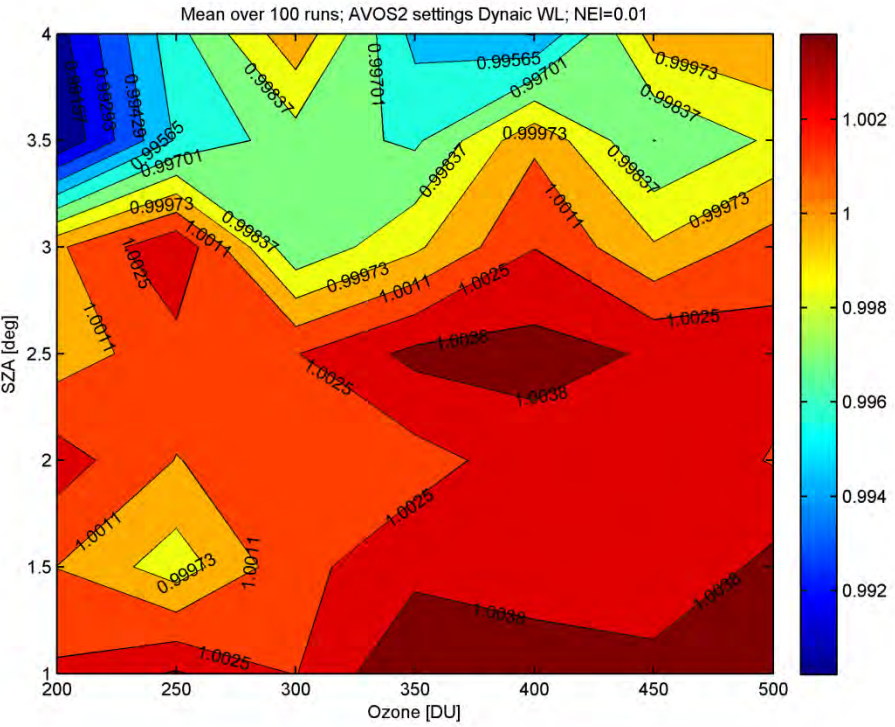
Variation of ALL; Dynamic WL

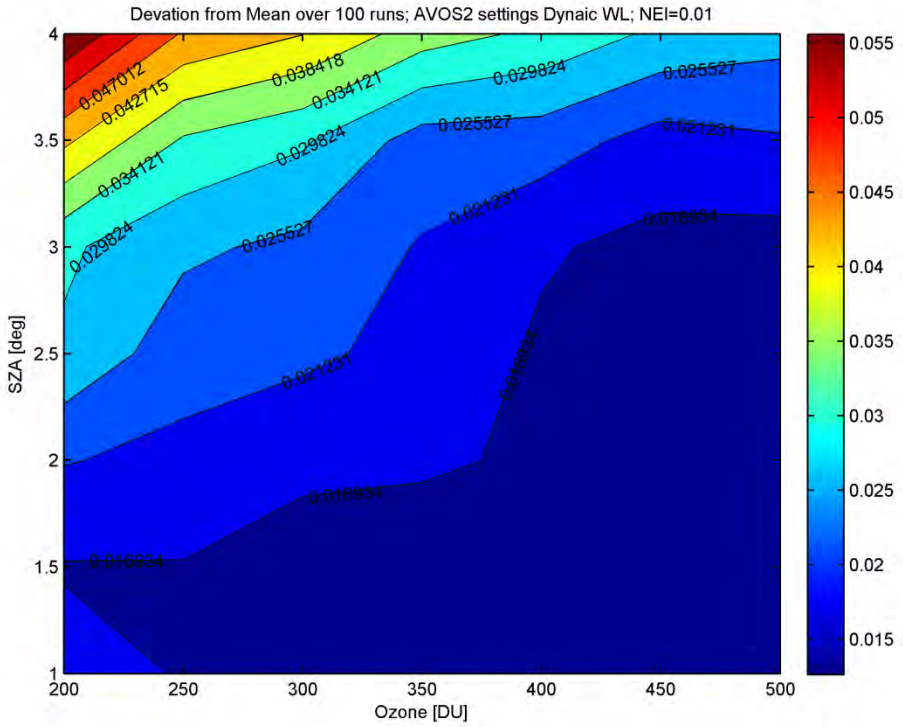
- Select WL-Range depending on airmass (solar zenith angle)

Here with NEI=0.01, linear dependency:

airmass=**1**; WL-Range **[300 340];** airmass=**2**; WL-Range **[306 340];**

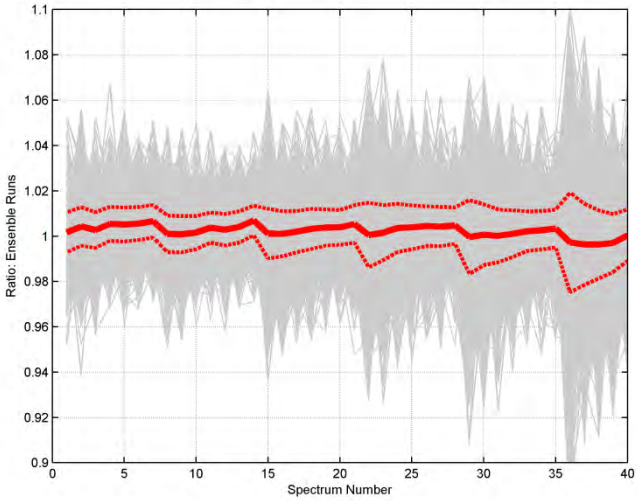
airmass=**3**; WL-Range **[313 340];** airmass=**4**; WL-Range **[320 340];**

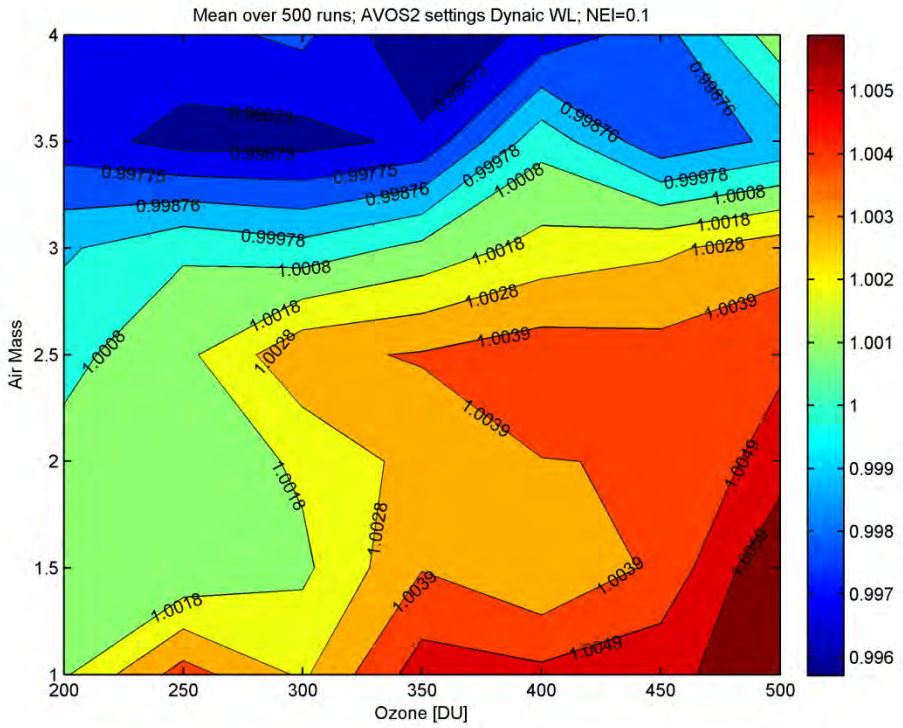


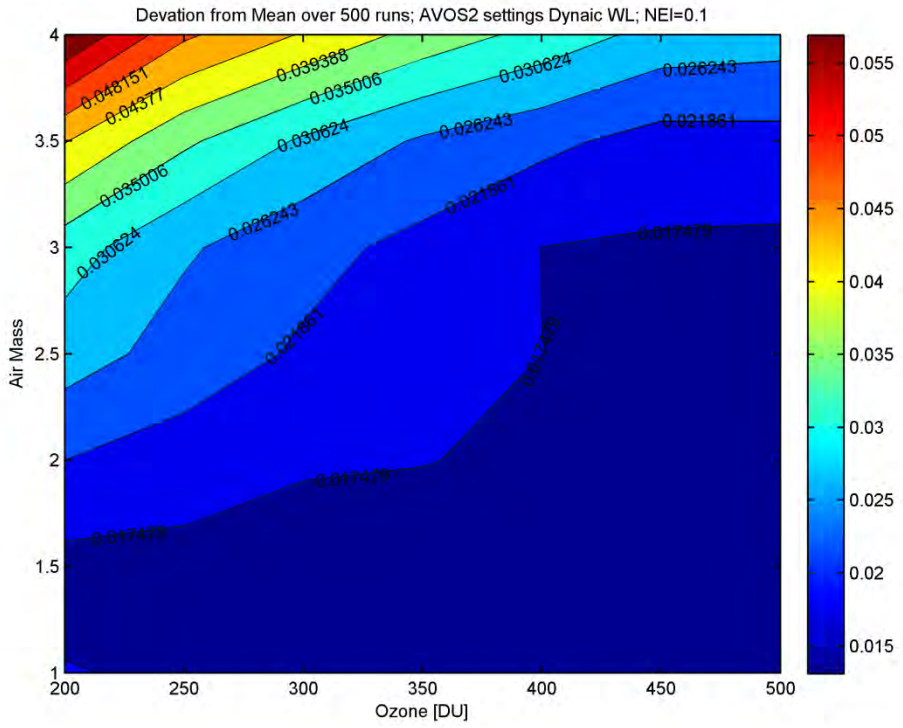


Variation of ALL; Dynamic WL

- **NEI=0.1!**

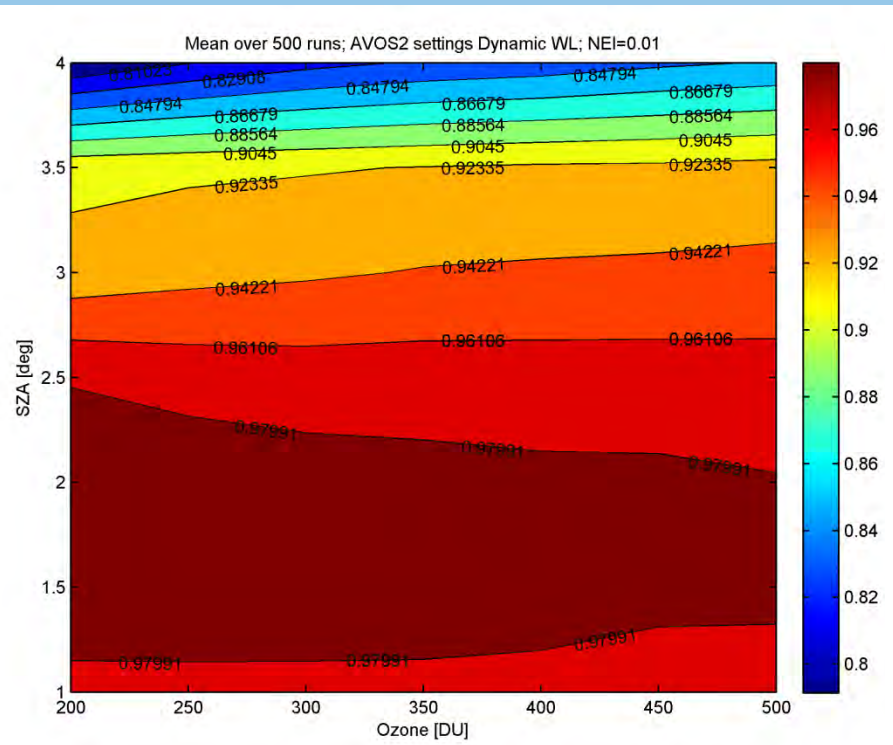


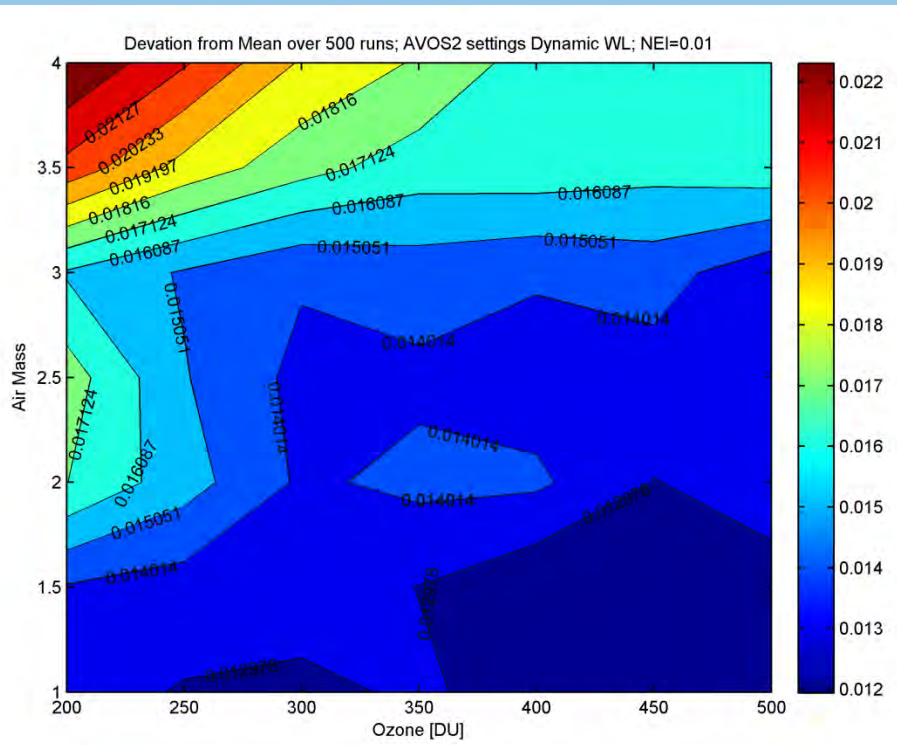




Variation of ALL; Dynamic WL

- **With “Noise-Reduction-Trick”** -> more finetuning with real data





Conclusions

Overall uncertainty of ozone retrieval by multispectral measurements depends mainly on;

- Selected **wavelength range** for the retrieval between 300-340 nm (full spectrum results in less uncertainty)
- NEI = **Noise equivalent Irradiance** => impact on selection of usable wavelength range
- **Wavelength uncertainty**
- **Atmospheric conditions** (Airmass, slightly of Ozone content)
- Random variation of input spectrum

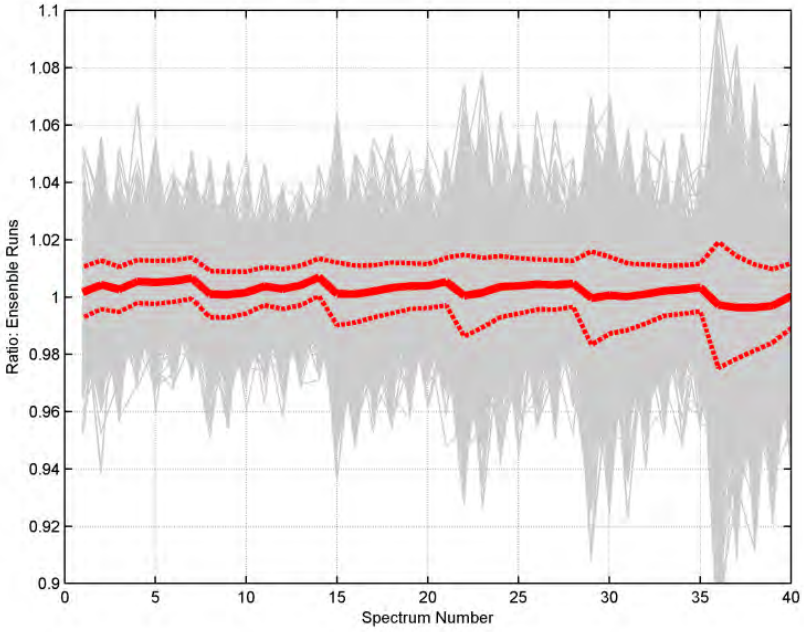
Minor contributions for the overall uncertainty are from:

- Selected **X-sections**; Variations of X-section
- Variation of **extraterrestrial spectrum**
- **Stratospheric Temperature**
- **Bandpass** (except in combination with wavelength shift)
- **Resolution** (regarding white noise of input spectrum)

Conclusions

Analysis / software can be used for:

- Further **optimizing the retrieval method** for a specific instrument (fine tuning).
- **Choosing specification** of a new commercial instrument or optimal design of a new instrument.
- **Indicate** (reduce) **of the uncertainty** of the ozone measurement using the ensemble runs of retrieval.



Conclusions

Thanks for your suggestions