A Modeling and Simulation Study for the GeoXO Atmospheric Composition Instrument (ACX):

System Level SO_2 and O_3 Retrieval Performance as a Function of SNR

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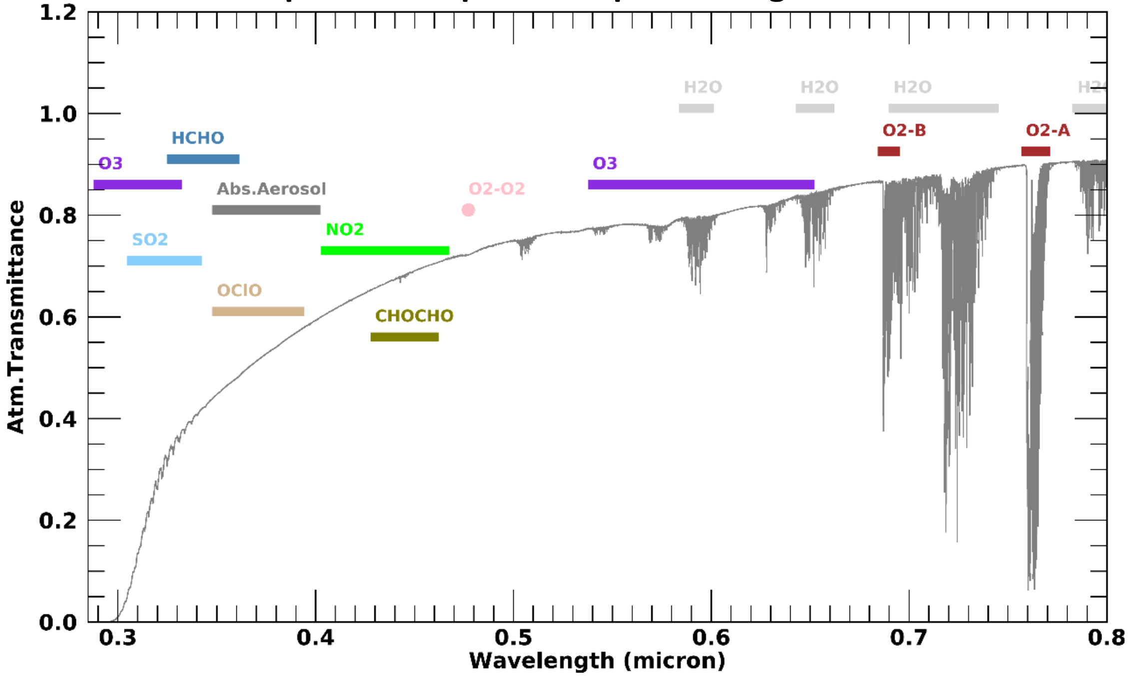
NOAAs Geostationary and Extended Observations (GeoXO) ACX Introduction

ACX: observations of air pollutants to improve air quality monitoring and mitigate health impacts from severe pollution and smoke events

- Enhance NOAA’s current capabilities to monitor hourly variation in pollutants
- Enhance NOAA’s air quality forecasting capabilities (pollution alerts, regulatory guidance, reduced health impacts)

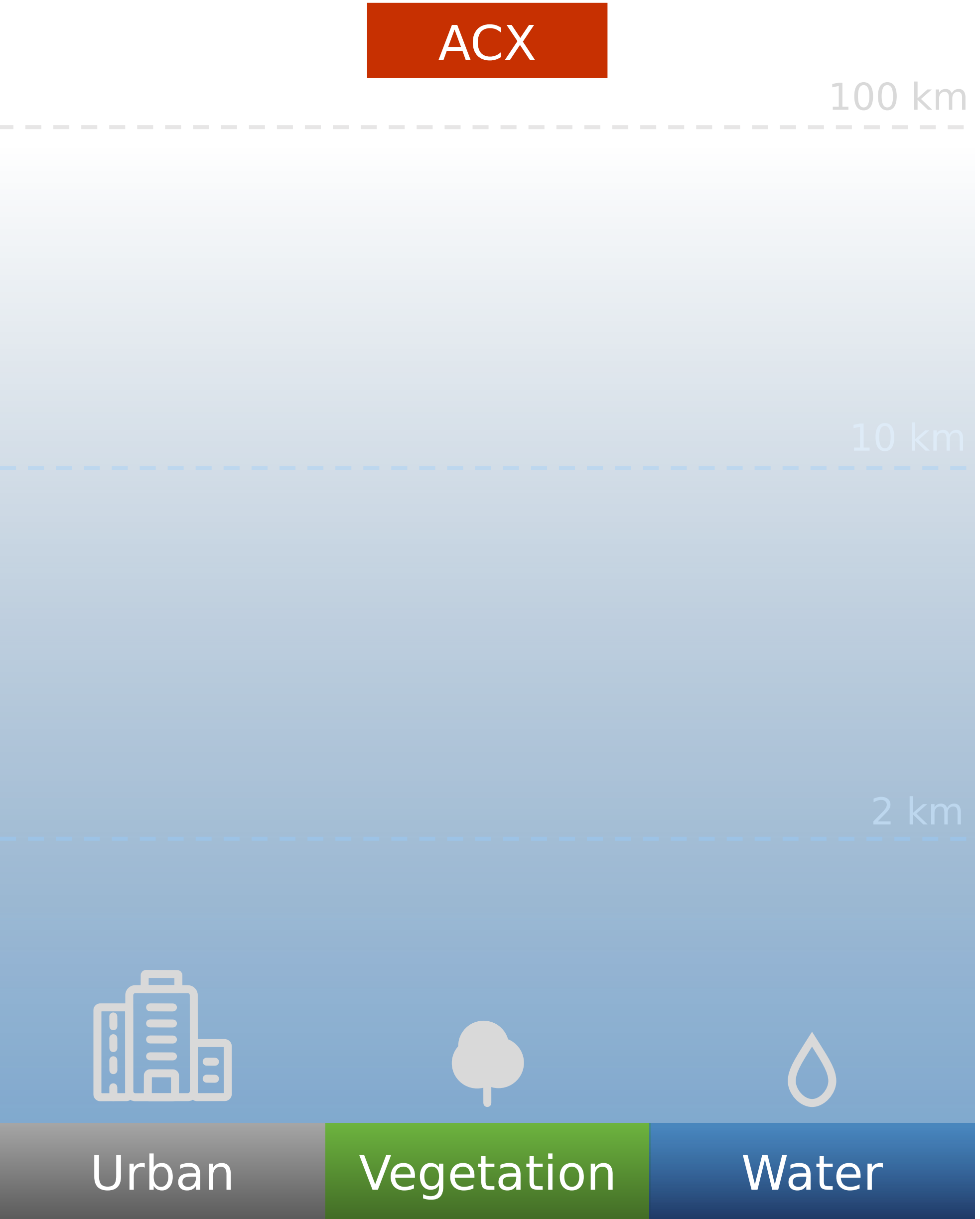
Atmospheric Composition Spectral Regions of Interest



Planned ACX Instrument	
Spectral Resolution	0.6 nm
Spectral Sampling	0.2 nm
Spectral Range	300 – 500 nm; 540 – 740 nm
Temporal Revisit	60 min
Spatial Resolution	25 km^2 at nadir

https://www.nesdis.noaa.gov/next-generation/geostationary-extended-observations-geoxo

ACX Performance Assessment



Translate instrument specifications to science performance metrics

Stratospheric + Composition

Tropospheric Composition

Boundary Layer Composition

Surface Reflect

Objective:

Assess instrument performance considerations through end-to-end physics based imaging system & scene modeling & simulation to inform decision making.

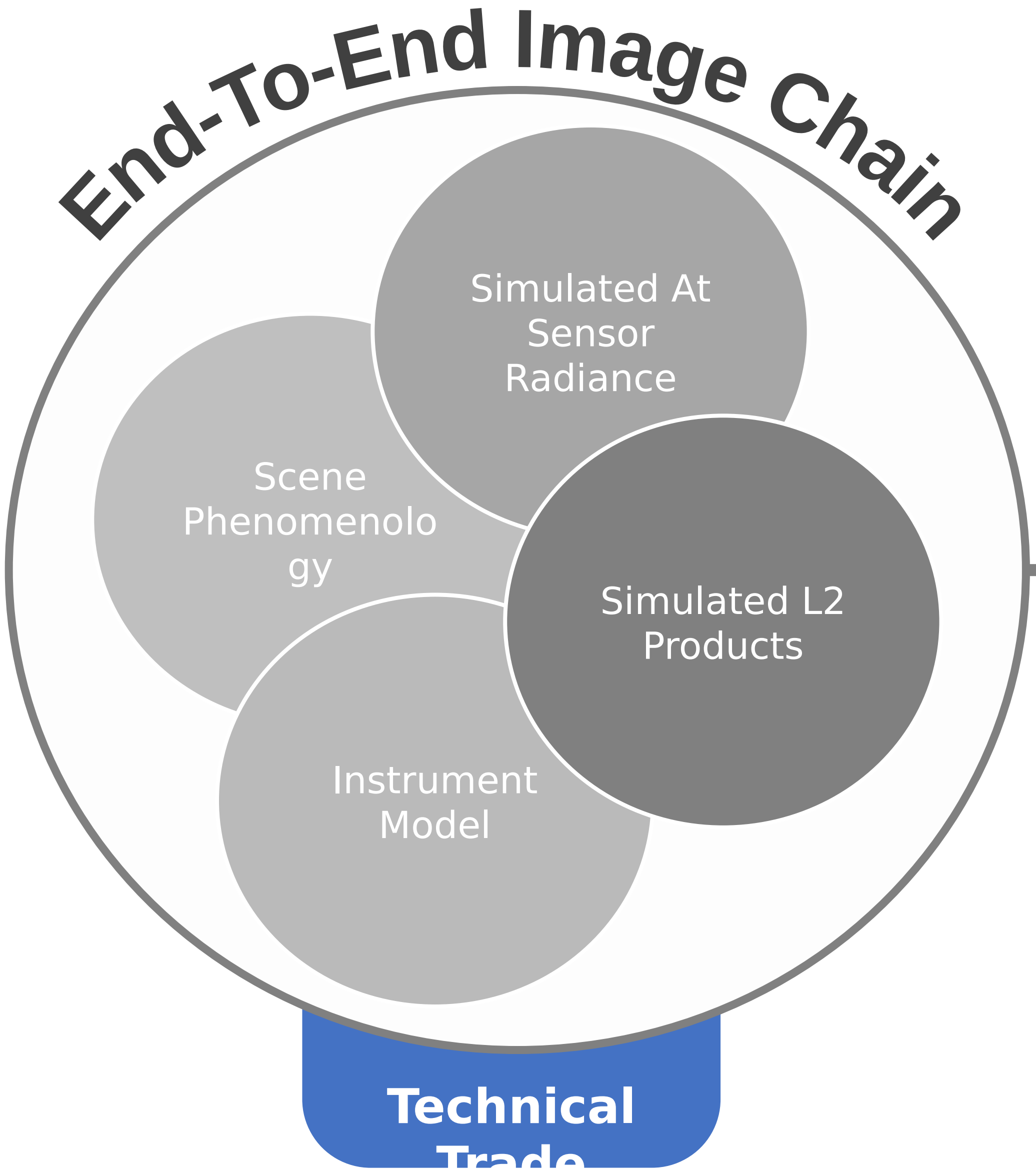
Investigate the impacts of simulated ACX SNR specification on trace gas retrieval performance

- Previously studied NO_2 (420 – 450 nm)
  [EUMETSAT 2021]
- This study investigates SO_2 and O_3 retrievals (approx. 300 – 350 nm)

NO_2
O_3
SO_2

[reference]

Utility of the Instrument Performance Assessment Simulations

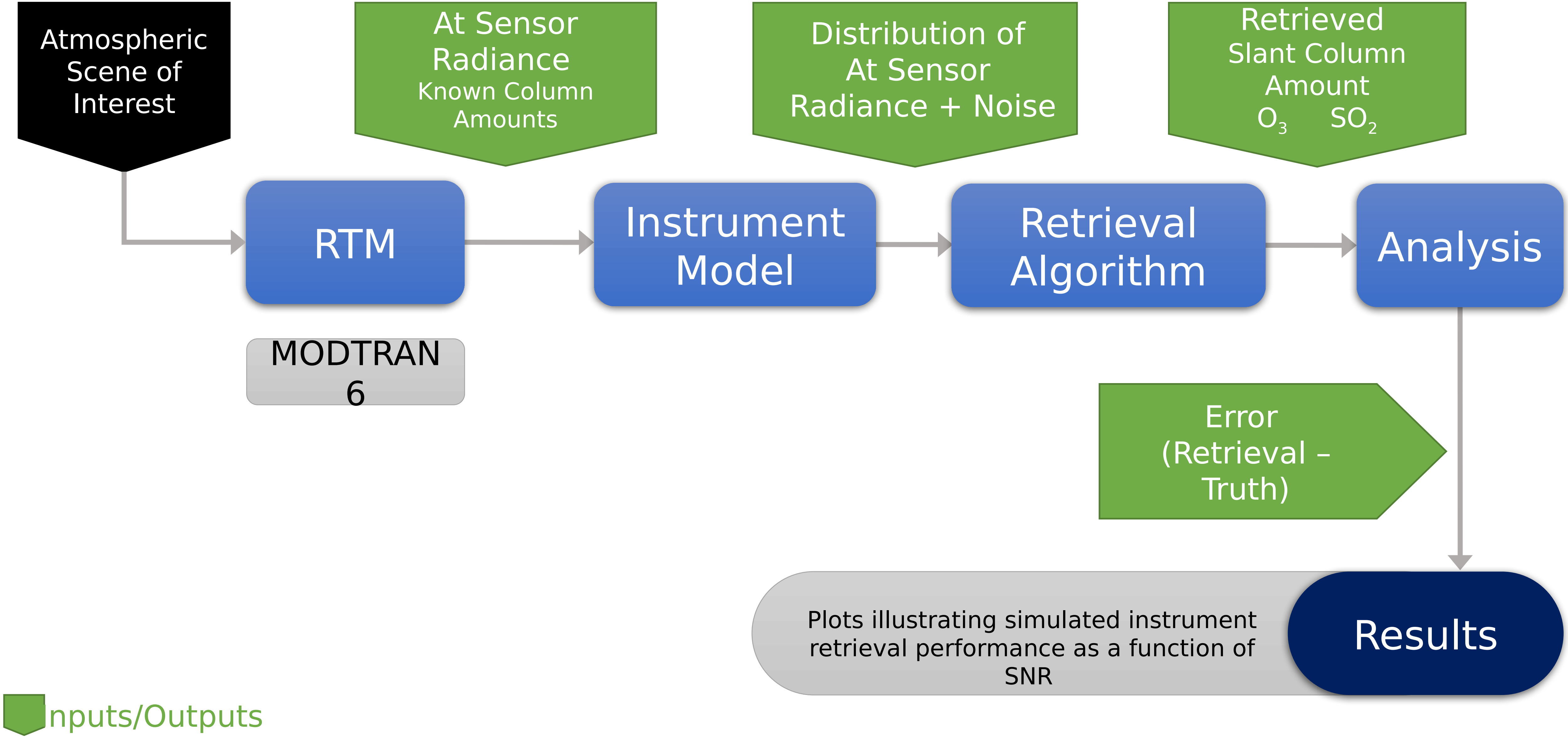


Objective:
Assess instrument performance considerations through end-to-end physics based imaging system & scene modeling & simulation

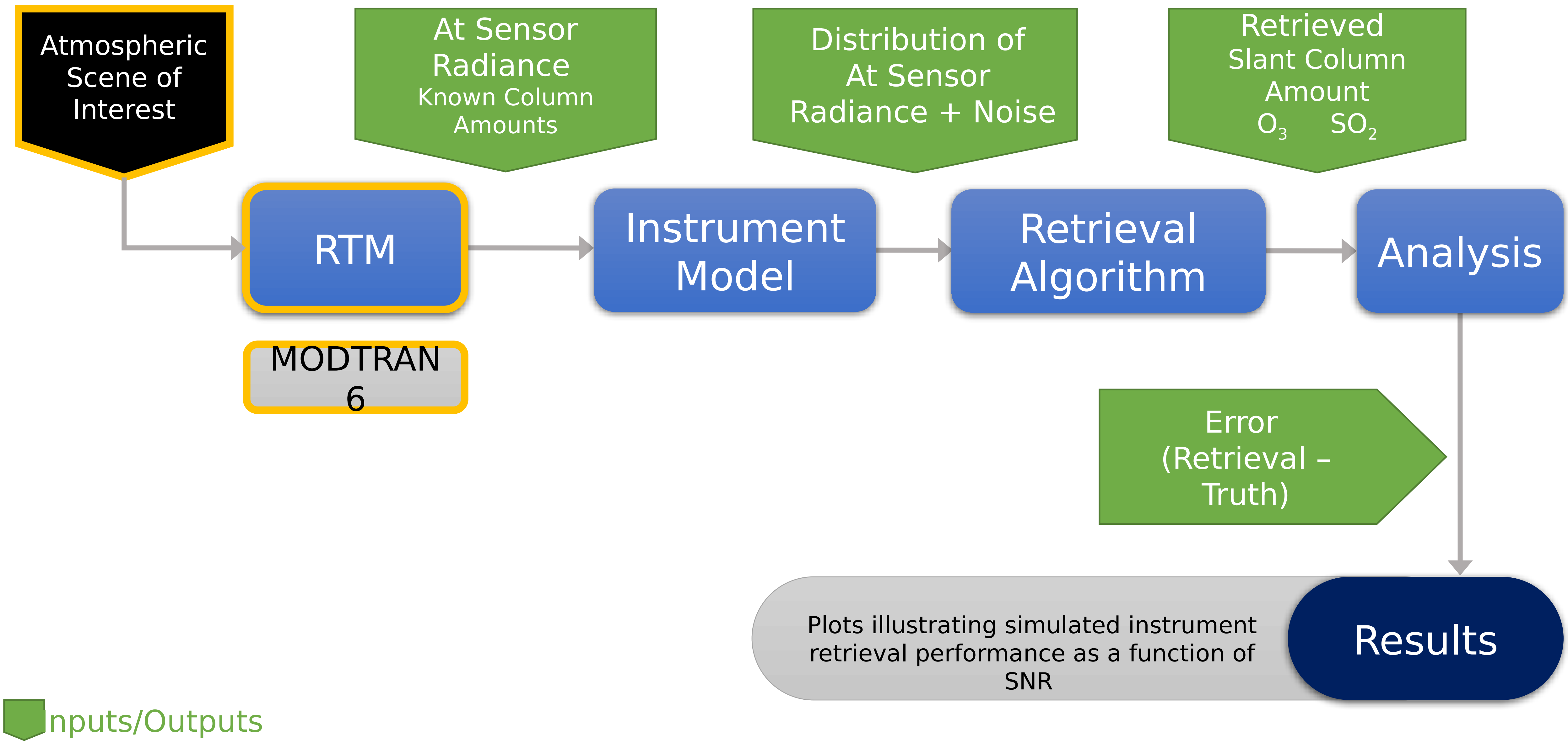
ACX Quantitative Analysis to Inform Decision Makers

Framework designed to rapidly facilitate various quantitative instrument performance assessment trade studies against engineering and science applications

Modeling & Simulation Framework



Modeling & Simulation Framework



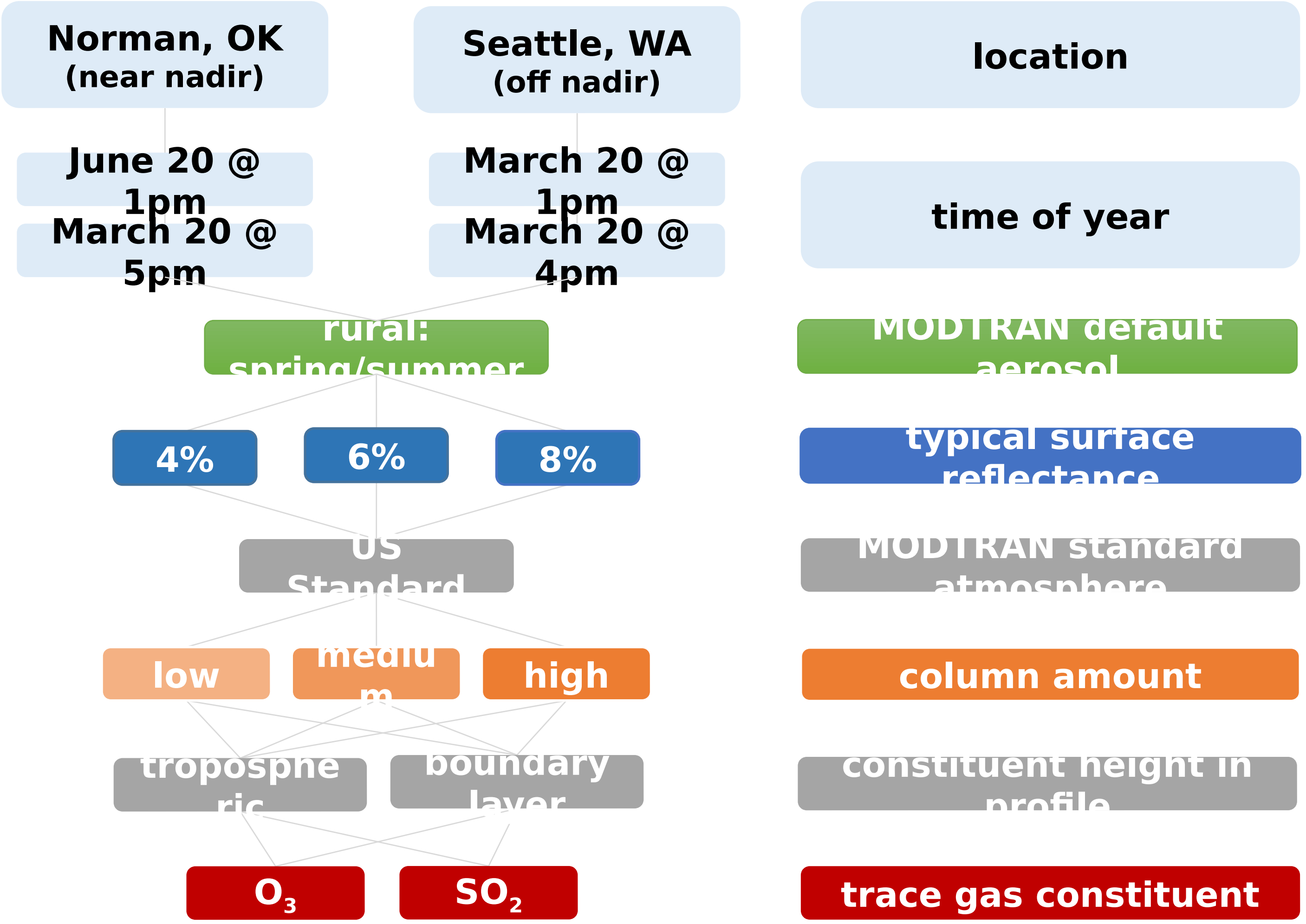
ACX SNR Performance Assessment – Scene Sc[…]s

Atmospheric Scene of Interest

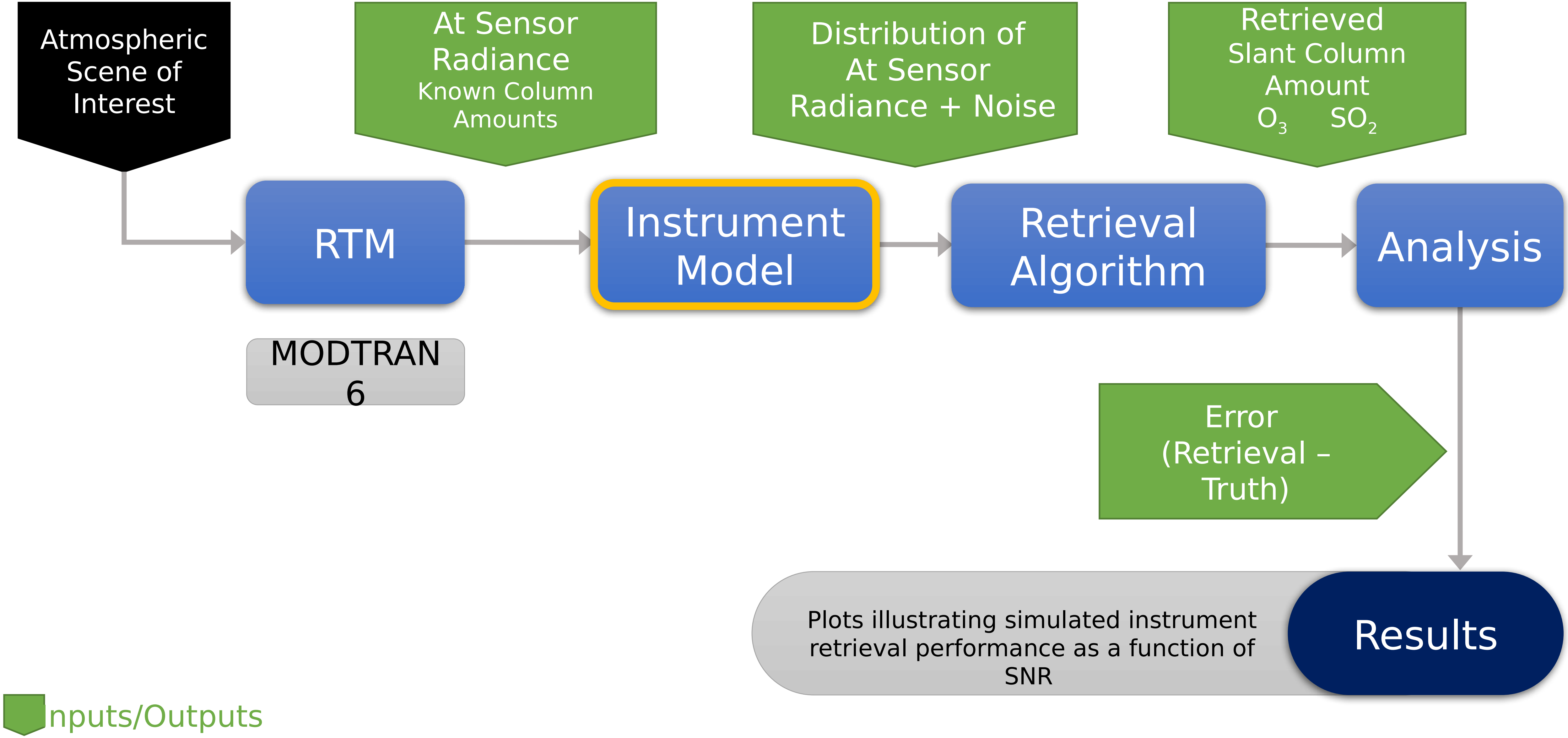
RTM

Accounts for the variability of concentration amount for a given standard atmosphere under typical surface and aerosol conditions with varying view geometry and solar conditions from GEO-central orbital location (105°W)

72 scene simulations were generated for each trace gas to span the bounding cases of observation conditions



Modeling & Simulation Framework

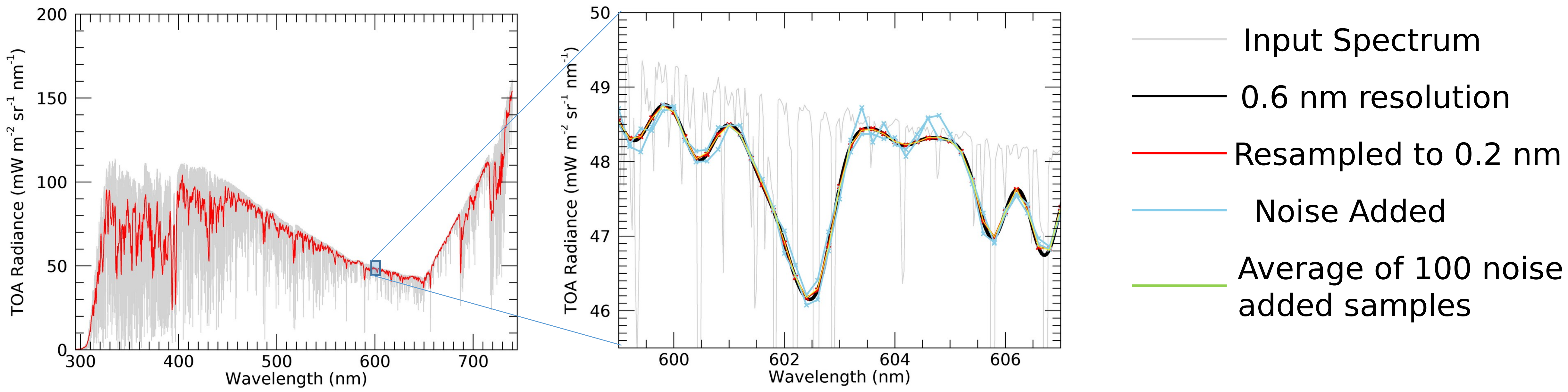


ACX Noise Simulation

Instrument Model

The ACX instrument model consists of the following steps:

1) The MODTRAN output spectra are convolved with a gaussian simulating the instrument spectral response function, resulting in a 0.6 nm spectral resolution
2) The degraded resolution spectrum is resampled to the expected instrument sampling of 0.2 nm/pix
3) Noise is added to achieve varying SNR as described below



ACX Instrument Response Model

Instrument Model

- Realistic baseline instrument parameters are used for setting up the tool
  - Follows current GeoXO ACX Performance Operational Requirement Document (PORD) specifications
  - Special thanks to Xiong Lu and Kelly Chance for assistance in this process
- Can be updated as the ACX instrument evolves

Instrument Parameters	
	spectral radiance at instrument resolution
	detector area
$\approx \pi/(2f\#)^2$	solid angle of acceptance of instrument
	integration time
	wavelength
	spectral interval per pixel
	optical system transmittance, combined with grating efficiency
	detector quantum efficiency
	Bit depth
	Read-out noise
	Dark current

ACX SNR Simulations – 10 Levels Assessed

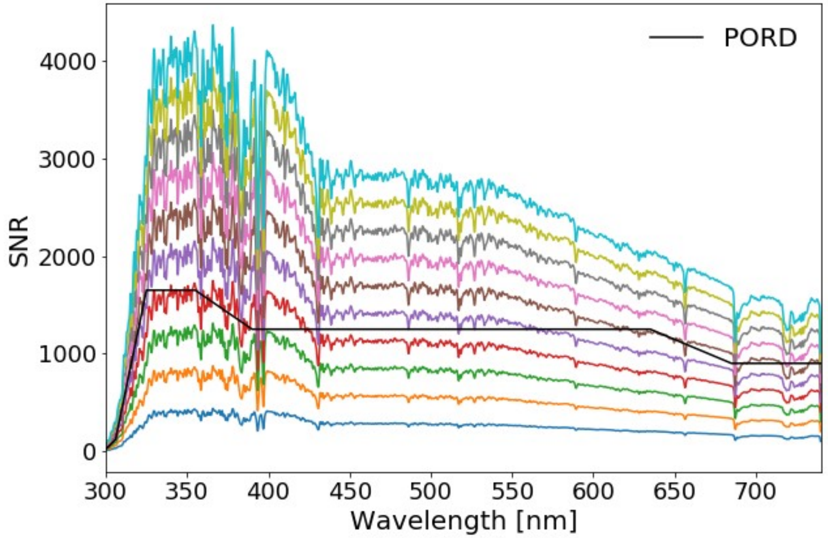
Instrument Model

For each spectrum, 1000 implementations for 10 different SNR levels are generated

- Each increasing SNR level decreases the noise by factors of 1 through 10, corresponding to averaging 1 - 100 samples
- 1000 random normally distributed noise implementations are generated for each SNR level

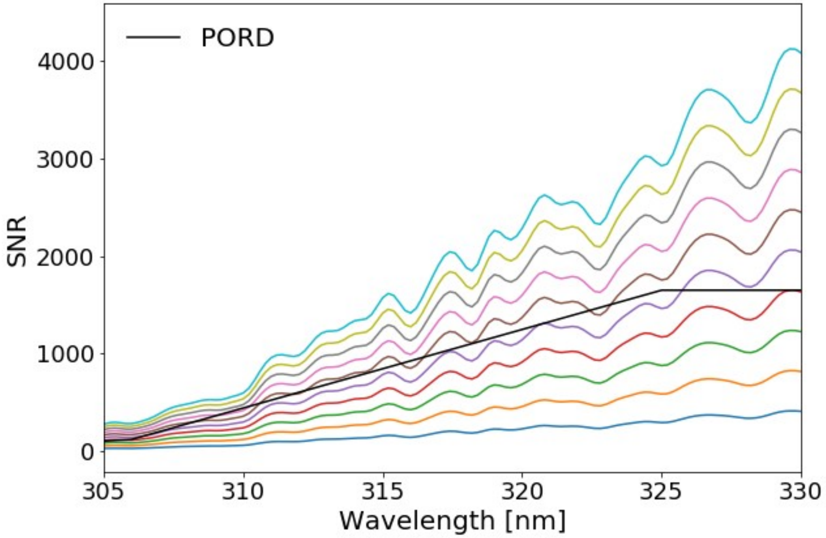
Note that the SNR values are calculated using nominal radiance defined in PORD

ACX Wavelength Range



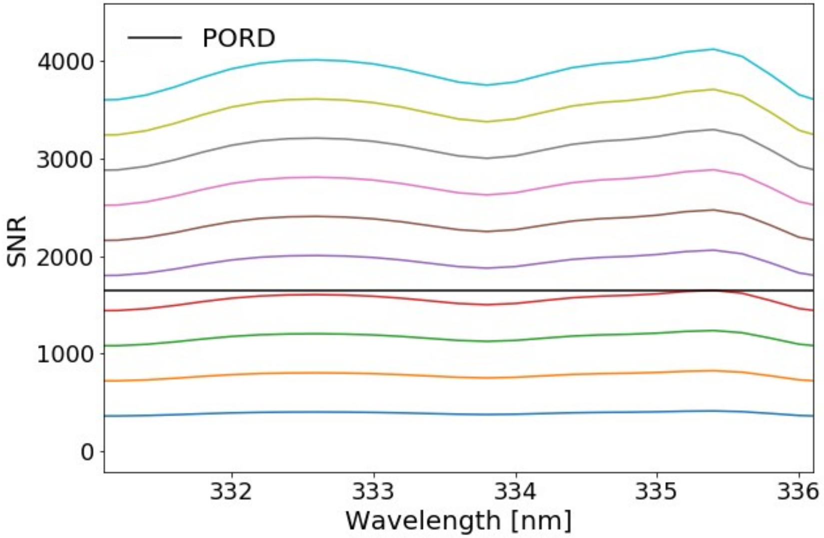
300 – 740 nm

SO_2 Retrieval Range



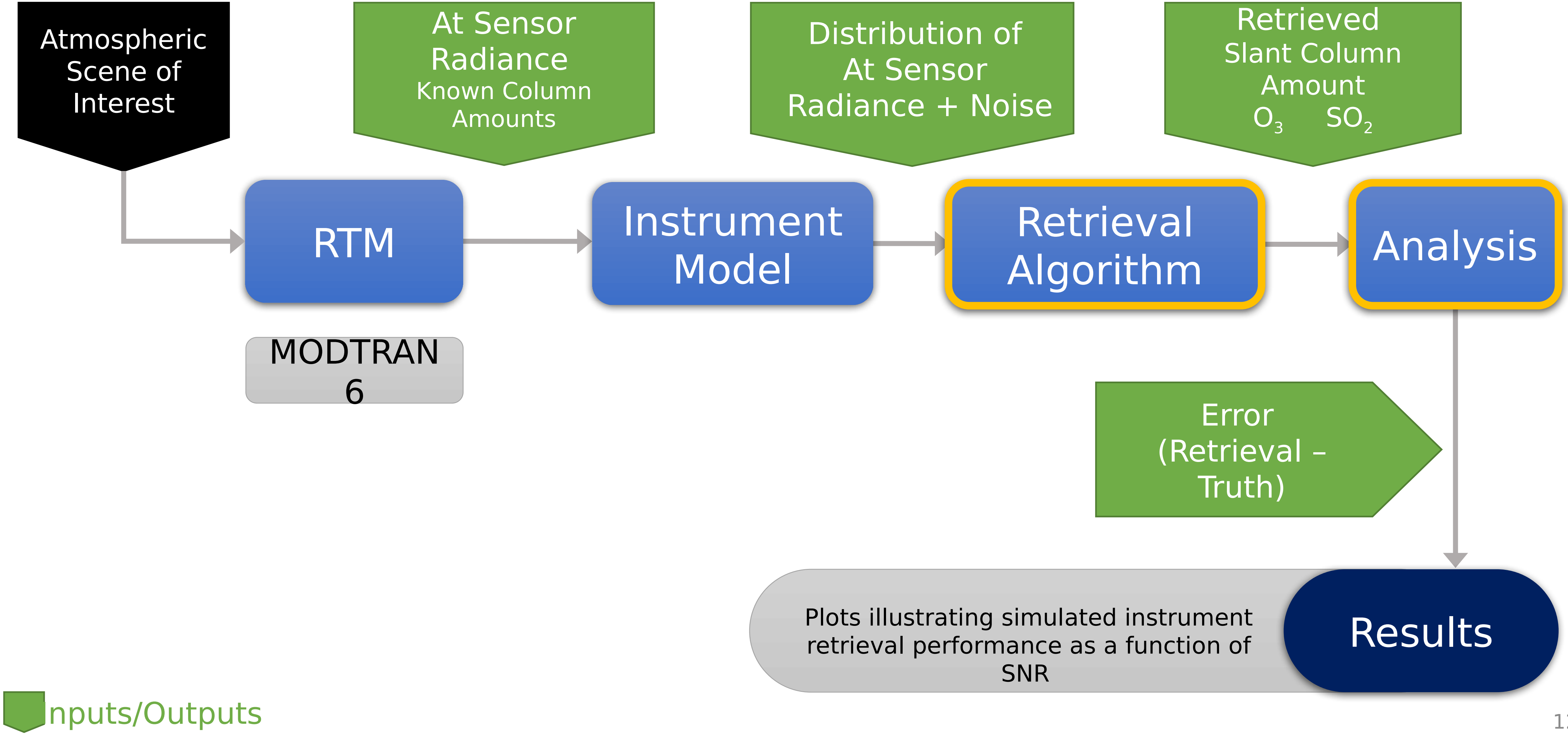
305 – 330 nm

O_3 Retrieval Range



331.1 – 336.1 nm

Modeling & Simulation Framework



Simulated ACX Retrieval Algorithms and A

Retrieval Algorithm | Analysis

Physical retrieval of concentration amount derived via comparison to a “Truth” LUT

Predicted at sensor radiance distribution as a function of SNR of known atmospheric concentrations
- **Concentration Amount:** Low, Medium, High
- Constrained Atmospheric Cases ***at a given SNR level***
- ***Fixed at a single view geometry***

Searched for Best →

Truth LUT
- **Concentration Amount:** none through extreme amount in finite step sizes
- ***NO Noise Included***
- ***Fixed at a single view geometry***

Compute retrieval concentration amount error (retrieval – truth):
- **Computation:** determine error as the standard deviation of (retrieval – truth) for each SNR
- **Output:** Illustrates the simulated instrument retrieval performance as a function of SNR and physical parameters of the scene simulated

Retrieval Algorithm: Constrained Energy Minimi

Step 1 – Build Look Up Table (**LUT**)
Result: Observed reflectance for a realistic range of known constituent amounts

RTM

Solar Model

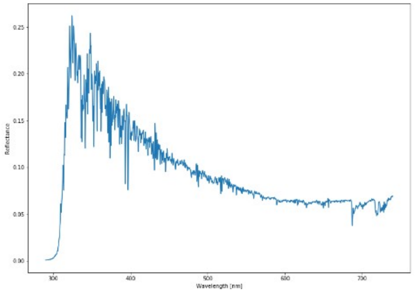
Scene Inputs
•Aerosol
•Surface Type
•Time of Day
•Location
•Atm. Profiles
(Known Total Column Amount,)

Solar Model

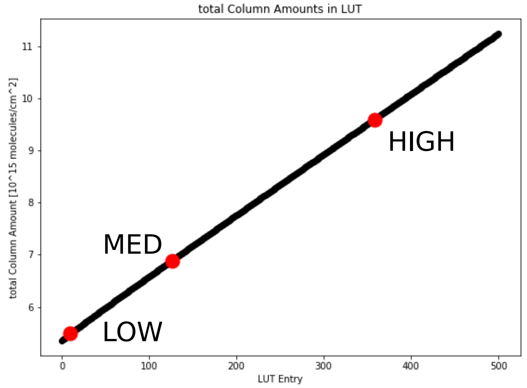
Radiance
NO_2, No Noise

$$\rho = \frac{L \pi r_{sun}^2}{E_{sun} \cos(\theta_{zen})}$$

Reflectance
NO_2, No Noise



α	Reflectance Spectra
0.0002	[0.00104251, 0.00102242, 0.00100026, ..., 0.06951616, 0.0693598, 0.0690303]
...	
BKGRND	
...	
MED	
...	
...	
HIGH	
...	
0.0004	



Step 2 – Calculate mean and inverse covariance matrix of spectra from noise model
Result: m and **S**$^{-1}$

Radiance
HIGH NO_2, SNR 1270

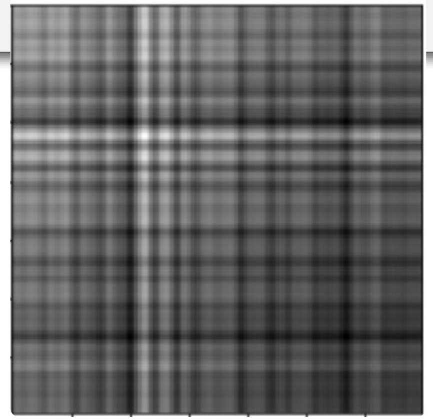
Radiance
HIGH NO_2, SNR 1530

10 SNR Levels

1000 implementations

Radiance
HIGH NO_2, SNR 3820

Inverse Covariance



Retrieval Algorithm: Constrained Energy Minimi

Retrieval Algorithm | Analysis

Step 3 – For each spectra, x … use constrained energy minimization (CEM) to determine slant column amount
Result: Retrieved amount for each observed spectra

Radiance
HIGH NO_2, SNR 1100

Radiance
HIGH NO_2, SNR 1400

10 SNR Levels

Radiance
HIGH NO_2, SNR 4500

Reflectance = Radiance / Solar Model

ctanc e
HIGH NO_2, SNR 1800

For each spectra … **x = observed spectra**

α	t
0.0002	[0.00104251, 0.00102242, 0.00100026, …, 0.06951616, 0.0693598 , 0.0690303]
…	
BKGRND	
…	
MED	
…	
…	
HIGH	
…	
0.0004	

Calculate CEM value for every spectra, t, in LUT

CEM(**x**)

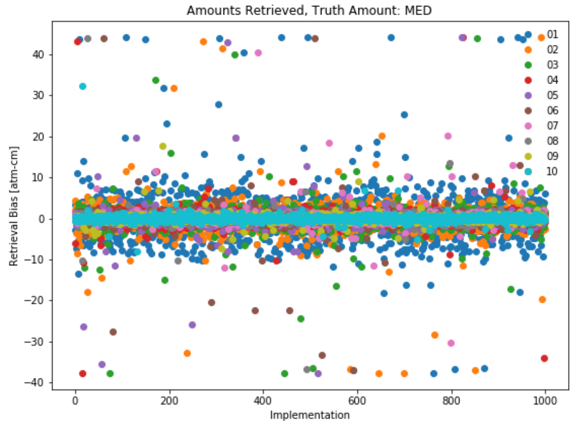
CEM Values
0.24
…
--0.5
…
0.74
…
…
1.001
…
0.664

Search LUT for CEM Value closest to 1

0.000360

from that LUT entry is retrieved value

Step 4 – For each SNR level, calculate bias and standard deviation (predicted error) from 1000 implementations
Result: Expected error for this SNR



- Bias and standard deviation of 1000 implementations gives retrieval error
- Repeat for each SNR level to plot as a function of SNR
- Repeat with a new scene to plot as a function of constituent amount

END RESULT

Baseline Retrieval and Analysis Framework For This Effort

RTM → **Instrument Noise Model** → **Retrieval Algorithm** → **Analysis**

Solar Model

Scene Inputs
•Aerosol
•Surface Type
•Time of Day
•Location
•Atm. Profiles
(Known Total Column Amount)

Radiance
HIGH NO_2, No Noise

Instrument Inputs
•Detector Specs
•Optical System Transmittance
•Detector Quantum Efficiency
•Bit-Depth
•Read-out Noise
•Dark Current

Radiance
HIGH NO_2, SNR 1270

Radiance
HIGH NO_2, SNR 1530

10 SNR Levels

Radiance
HIGH NO_2, SNR 3820

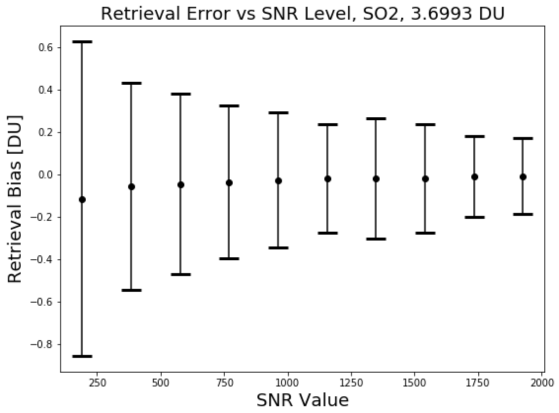
1000 implementations

Predicted **Slant Column Amount** for each spectra output from instrument noise model
- 10 SNR levels
- 1000 implementations per SNR level
- Constrained Energy Minimization (CEM) compares each observed spectra to a LUT with known constituent amounts

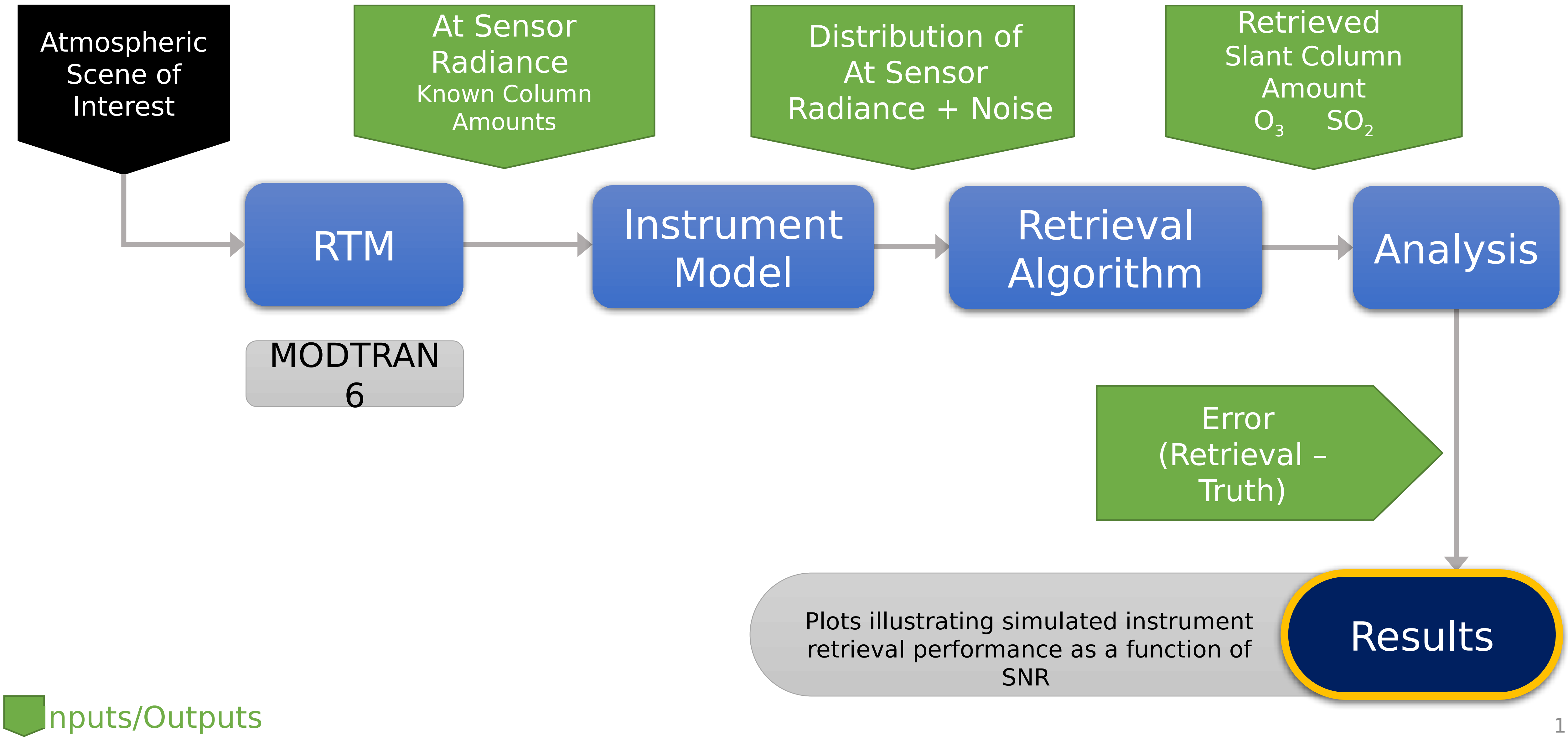
CEM(x)

Note: Analysis based on a DOAS-like approach; results may vary with other operational approaches

- Calculate bias and standard deviation of 1000 implementations to determine retrieval error
- Repeat for each SNR level
- Repeat for each constituent amount



Modeling & Simulation Framework



ACX SO_2 Modeling Scenarios

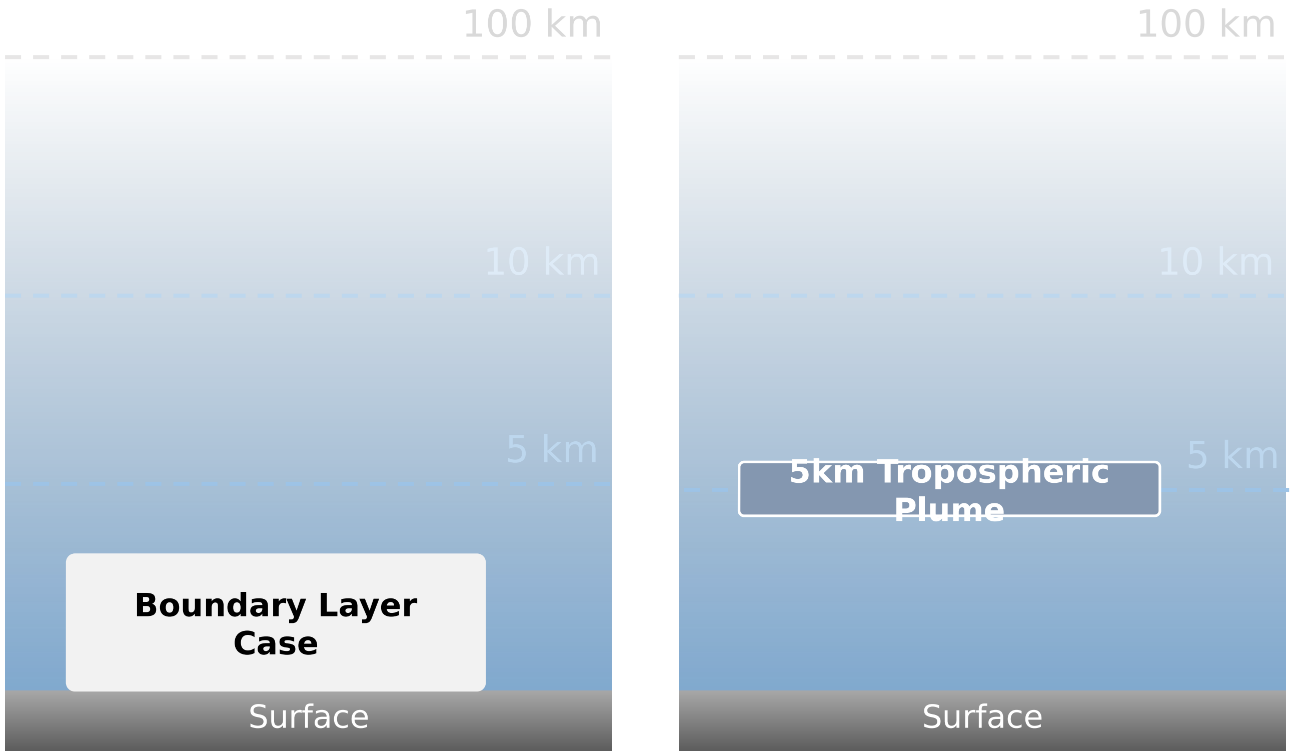
Two modeling scenarios:

- Boundary layer case: SO_2 injected into the atmosphere from 0 – 3 km (anthropogenic pollution)
  - Three amounts of SO_2 (Low, Medium and High)
- 5 km tropospheric plume: SO_2 injected into 1 km of the atmosphere at 5 km altitude (outgassing volcano)
  - Three amounts of SO_2 (Low, Medium and High)

Different viewing geometries result in different slant column amounts for the same amount of SO_2

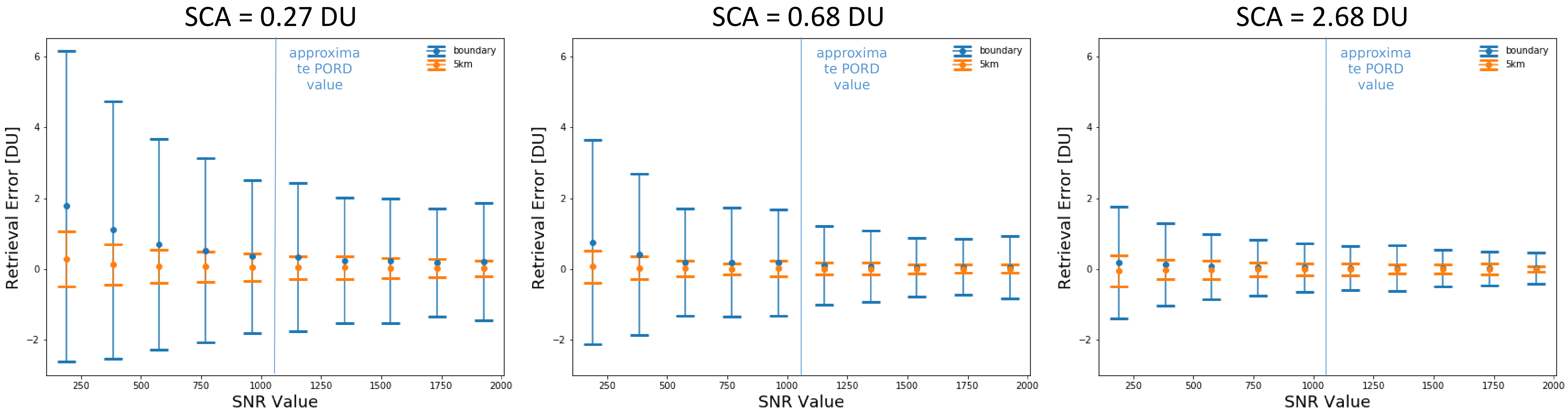
		Norman, OK (near-nadir)	Seattle, WA (oblique)
	SO_2 Injected*	Slant Column Amount (SCA)	
Low	0.2 DU	0.27 DU	0.37 DU
Medium	0.5 DU	0.68 DU	0.94 DU
High	2.0 DU	2.68 DU	3.70 DU

* SO_2 was injected to US standard atmospheric profile
Oblique viewing results in larger SCAs than near-nadir viewing



ACX Simulated Boundary Layer Case vs Tropospheric Plume

- Each data point and error bars: (mean ± 1 σ) of 1000 simulations
- Norman, OK: June 20, 2021 @ 1 pm (closer to nadir viewing)
- Retrieval results improve for greater amounts of SO_2 in profile
- Retrieval performance with a tropospheric plume outperforms retrieval performance for the boundary layer case



ACX Simulated Boundary Layer Case vs Tropospheric Plume

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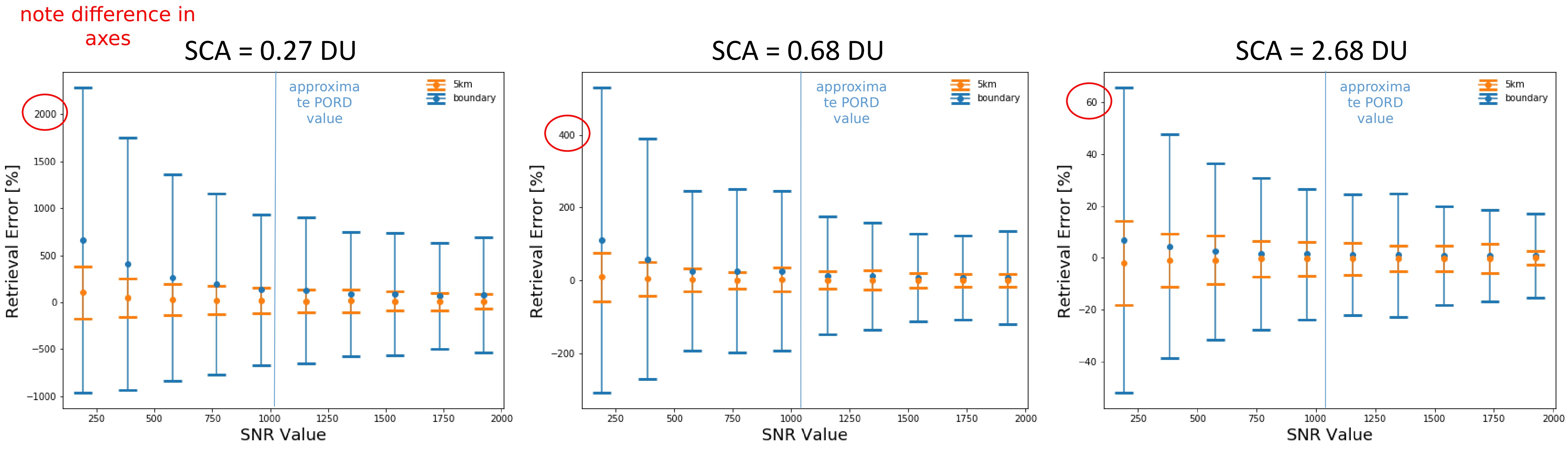
- Norman, OK: June 20, 2021 @ 1 pm (closer to nadir viewing)
- Retrieval results improve for greater amounts of SO_2 in profile
- Retrieval performance with a tropospheric plume outperforms retrieval performance for the boundary layer case
- Results as a percentage of slant column amount show that boundary layer cases have extremely



Similar results were found for the Seattle, WA: March 20, 2021 @ 1pm (backup slides)

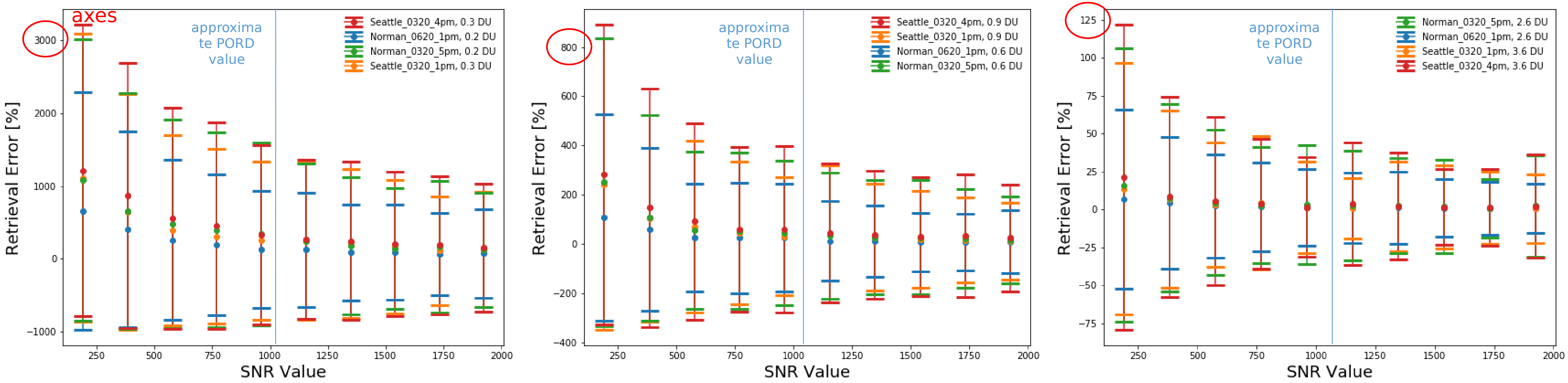
ACX Simulated View Geometries and Solar Zenith Angle

- Each data point and error bars: (mean ± 1 σ) of 1000 simulations
- All location, date and time combinations with SO_2 added to the bo
- Retrieval results improve for greater amounts of SO_2 in profile
- Retrievals errors decrease as solar zenith angle decreases in mos

Location	Date	Local Time	SZA
Norman, OK	June 20	1 pm	13.63°
Norman, OK	March 20	5 pm	58.72°
Seattle, WA	March 20	1 pm	47.55°
Seattle, WA	March 20	4 pm	59.12°

Boundary Layer Case

note difference in axes



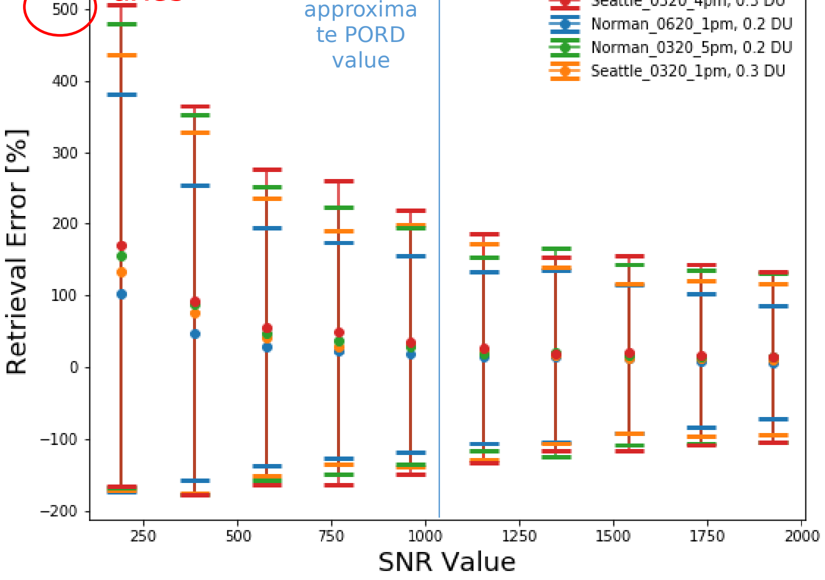
ACX Simulated View Geometries and Solar Zenith Angle

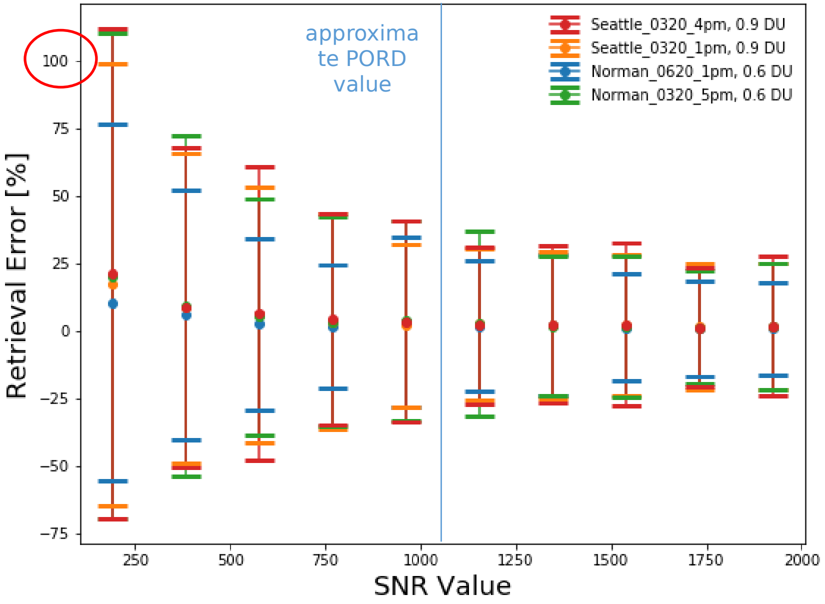
- Each data point and error bars: (mean ± 1 σ) of 1000 simulations
- All location, date and time combinations with SO_2 added @ 5km a
- Retrieval results improve for greater amounts of SO_2 in profile
- Retrievals errors decrease as solar zenith angle decreases in mos

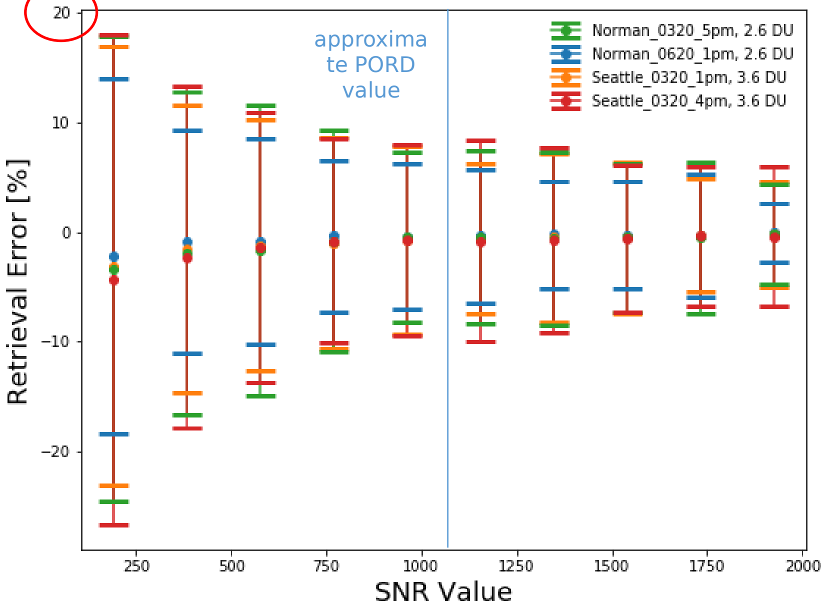
Location	Date	Local Time	SZA
Norman, OK	June 20	1 pm	13.63°
Norman, OK	March 20	5 pm	58.72°
Seattle, WA	March 20	1 pm	47.55°
Seattle, WA	March 20	4 pm	59.12°

5 km Tropospheric Plume

note difference in axes





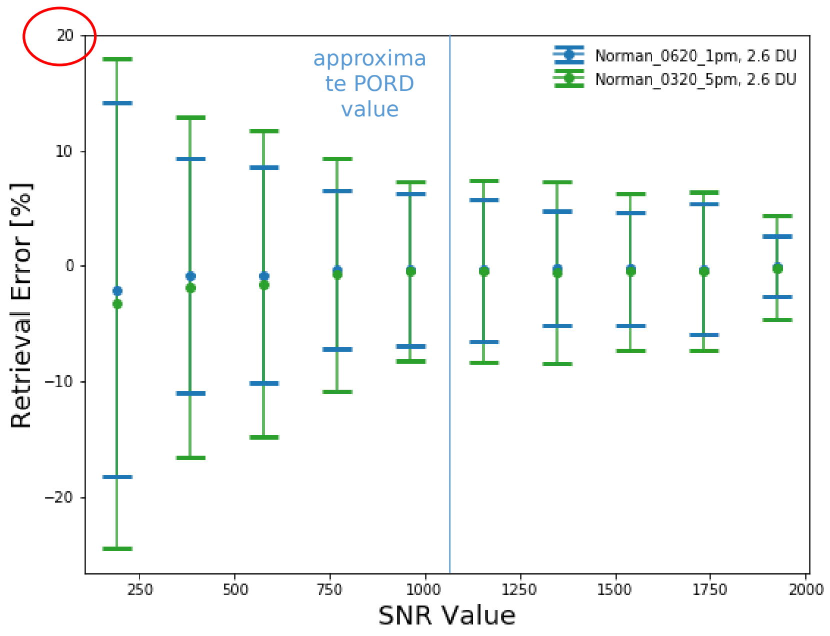


ACX Simulated View Geometries and Solar Zenith Angle

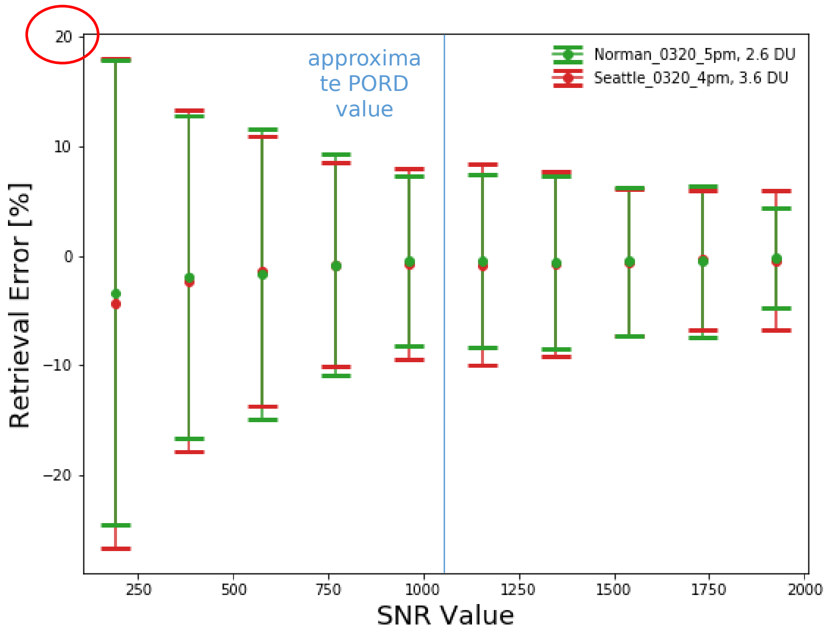
- Each data point and error bars: (mean ± 1 σ) of 1000 simulations
- See variation in retrieval performance with changes in solar zenit
- Same location and SCA but different date and time – different res
- Different locations and SCA with similar SZA – similar results
- This illustrates the SZA impact on simulated retrieval performance

Location	Date	Local Time	SZA
Norman, OK	June 20	1 pm	13.63°
Norman, OK	March 20	5 pm	58.72°
Seattle, WA	March 20	1 pm	47.55°
Seattle, WA	March 20	4 pm	59.12°

13.63° vs 58.72° SZA



58.72° vs 59.12 ° SZA



ACX O_3 Modeling Scenarios

Two modeling scenarios:

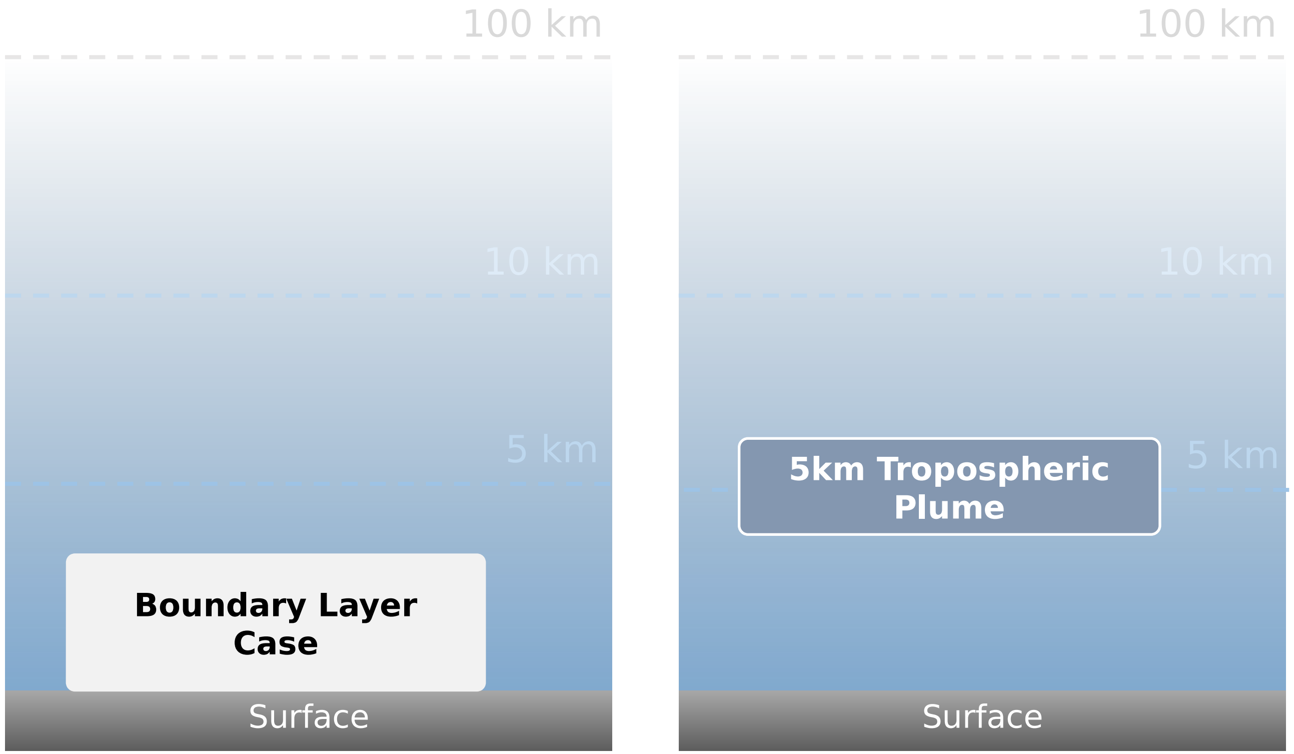
- Boundary layer case: O_3 injected into the atmosphere from 0 – 3 km (smog)
  - Three amounts of O_3 (Low, Medium and High)
- 5 km tropospheric plume: O_3 injected into 2 km of the atmosphere at 5 km altitude (photochemical reactions)
  - Three amounts of O_3 (Low, Medium and High)

Different viewing geometries result in different slant column amounts for the same amount of O_3

Note: There are multiple O_3 operational retrieval algorithms; this study utilizes a DOAS-like approach

		Norman, OK (near-nadir)	Seattle, WA (oblique)
	O_3 Injected*	Slant Column Amount (SCA)	
Low	50 DU	476 DU	653 DU
Medium	60 DU	489 DU	671 DU
High	70 DU	503 DU	690 DU

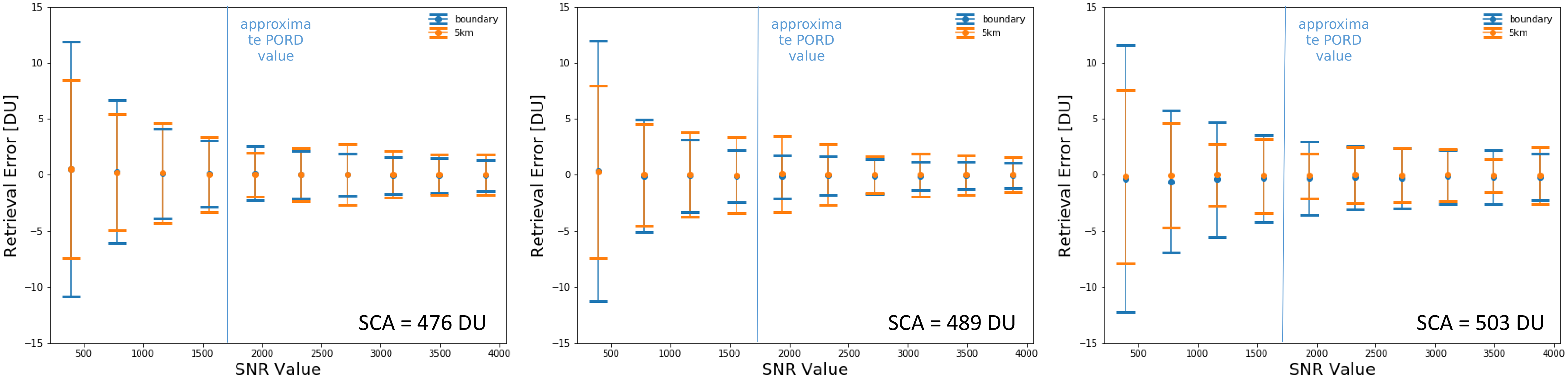
* O_3 was injected to US standard atmospheric profile
Oblique viewing results in larger SCAs than near-nadir viewing



ACX Simulated Boundary Layer Case vs Tropospheric Plume

- Each data point and error bars: (mean ± 1 σ) of 1000 simulations
- At near-nadir viewing and small SZA, retrieval performance is comparable for O_3 injected into the boundary layer and at 5 km in the troposphere

Norman, OK: June 20, 2021 @ 1pm (near-nadir viewing, SZA = 13.63°)



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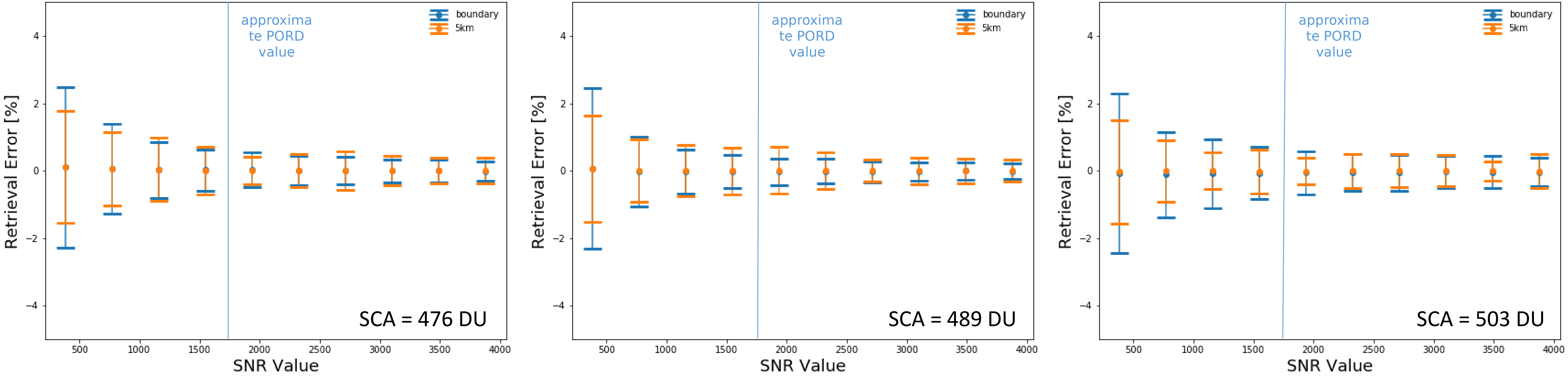
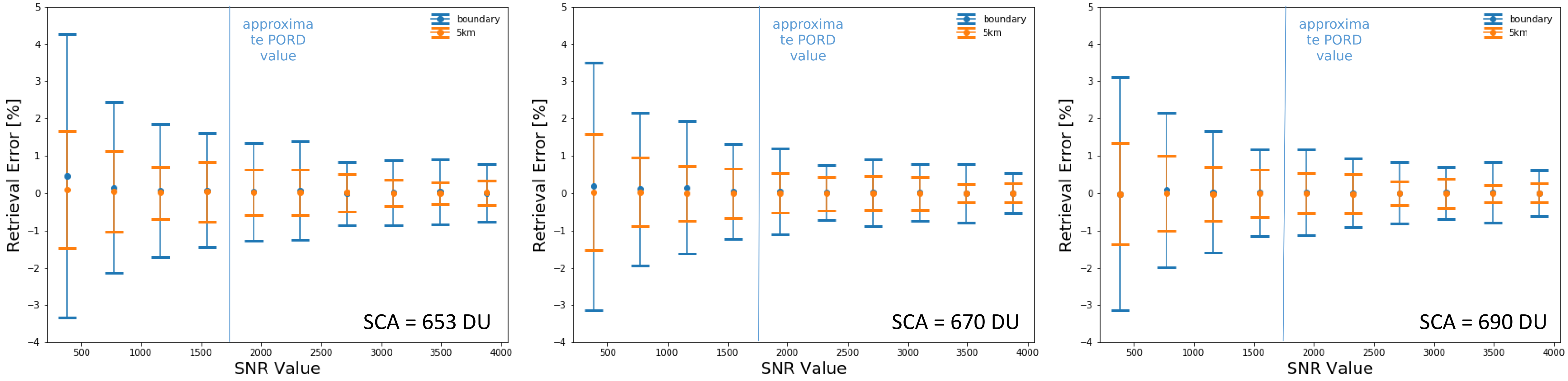


Note that retrieval bias as a percentage is small because O_3 slant column amounts are large due to an increased amount of O_3 in the stratosphere

ACX Simulated Boundary Layer Case vs Tropospheric Plume

- Each data point and error bars: (mean ± 1 σ) of 1000 simulations
- At near-nadir viewing and small SZA, retrieval performance is comparable for O_3 injected into the boundary layer and at 5 km in the troposphere
- At oblique viewing and larger SZA, retrieval performance is better for O_3 injected at 5 km in the troposphere compared to O_3 injected in the boundary layer

Seattle, WA: March 20, 2021 @ 1pm (oblique viewing, SZA = 47.55°)



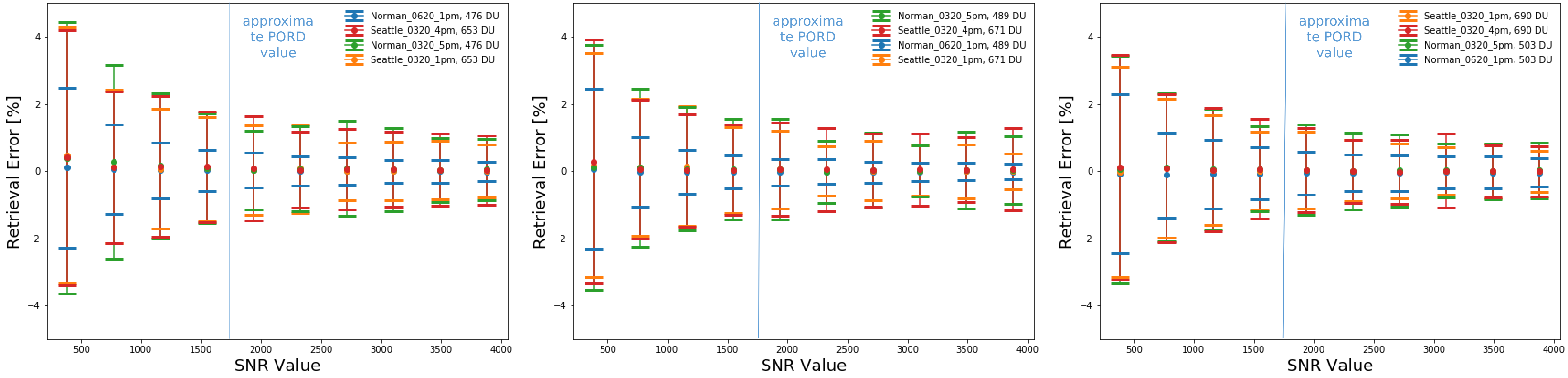
Note that retrieval bias as a percentage is small because O_3 slant column amounts are large due to an increased amount of O_3 in the stratosphere

ACX Simulated View Geometries and Solar Zenith Angle

- Each data point and error bars: (mean ± 1 σ) of 1000 simulations
- All location, date and time combinations with O_3 added to the boundary layer
- Retrieval performance is comparable for all view geometries and solar zenith angles simulated when O_3 is injected into the boundary layer, with the exception of near-nadir viewing on the summer solstice near solar noon (improved retrieval performance

Location	Date	Local Time	SZA
Norman, OK	June 20	1 pm	13.63°
Norman, OK	March 20	5 pm	58.72°
Seattle, WA	March 20	1 pm	47.55°
Seattle, WA	March 20	4 pm	59.12°

Boundary Layer Case



ACX Simulated View Geometries and Solar Zenith Angle

- Each data point and error bars: (mean ± 1 σ) of 1000 simulations
- All location, date and time combinations with O_3 added @ 5 km altitude
- Retrieval performance is comparable for all view geometries and solar zenith angles simulated with O_3 injected at 5 km in the troposphere

Location	Date	Local Time	SZA
Norman, OK	June 20	1 pm	13.63°
Norman, OK	March 20	5 pm	58.72°
Seattle, WA	March 20	1 pm	47.55°
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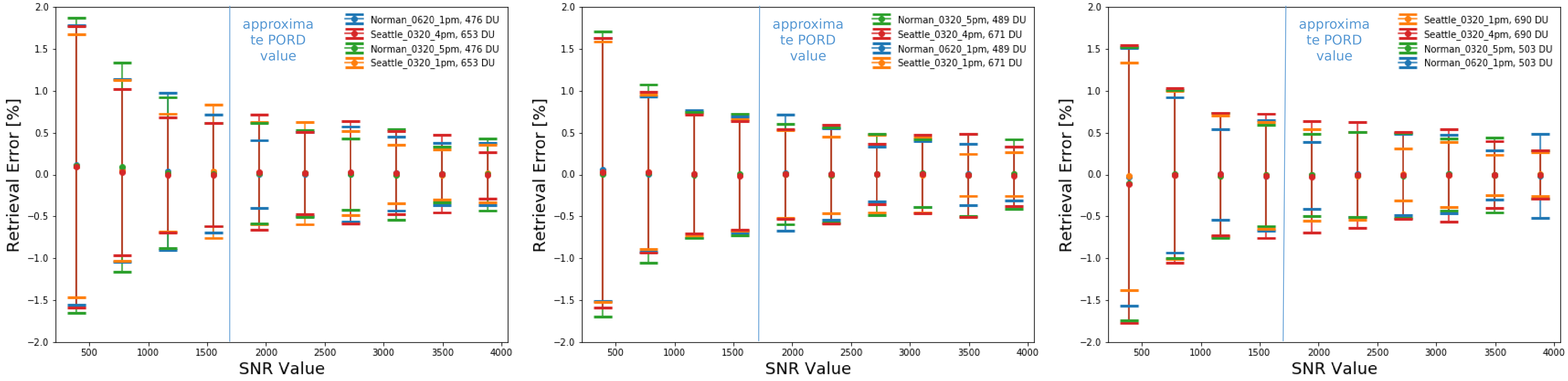
5 km Tropospheric Plume



Summary and Conclusions

- An end-to-end physics based imaging system and scene modeling & simulation capability has been further developed in support of the GeoXO program to conduct quantitative instrument performance assessments and trade studies of the ACX system
- This work investigated the impacts of simulated ACX SNR specifications on trace gas retrieval performance:
  - » Previously studied NO_2 (420 – 450 nm) [EUMETSAT 2021]
  - » This study investigated SO_2 and O_3 retrievals (approx. 300 – 350 nm)

Simulated ACX SO_2 Retrievals Summary

- Retrieval uncertainty decreased as the slant column amount of SO_2 increased
- Retrieval performance for a tropospheric plume outperforms retrieval performance for the boundary layer case
- Retrievals errors decrease as solar zenith angle decreases in most cases

Simulated ACX O_3 Retrievals Summary

- Retrieval performance is better for O_3 injected at 5 km in the troposphere compared to O_3 injected in the boundary layer
  - » Exception is near-nadir viewing on the summer solstice near solar noon
- Retrieval performance is comparable for most view geometries and solar zenith angles simulated
  - » Exception is boundary layer O_3 injection with near-nadir viewing on the summer solstice near solar noon (improved retrieval performance)

Conclusions:

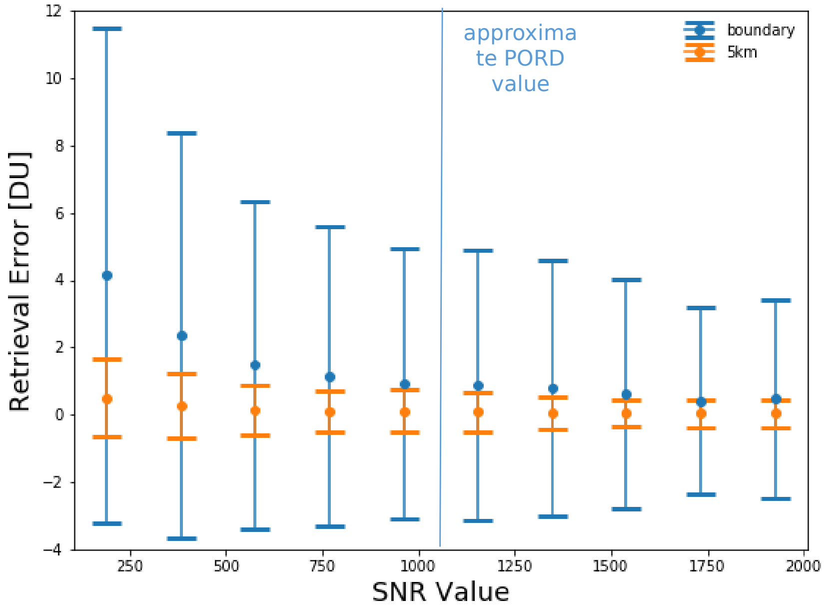
- Retrieval of SO_2 and low amounts of O_3 in the boundary layer were found to be challenging regardless of SNR
- Retrieval errors did not vary greatly with changes in SNR (up to 50%) for O_3 and large amounts of SO_2 at higher altitudes in the troposphere; performance for these scenarios was acceptable within this range of SNR values

Backup

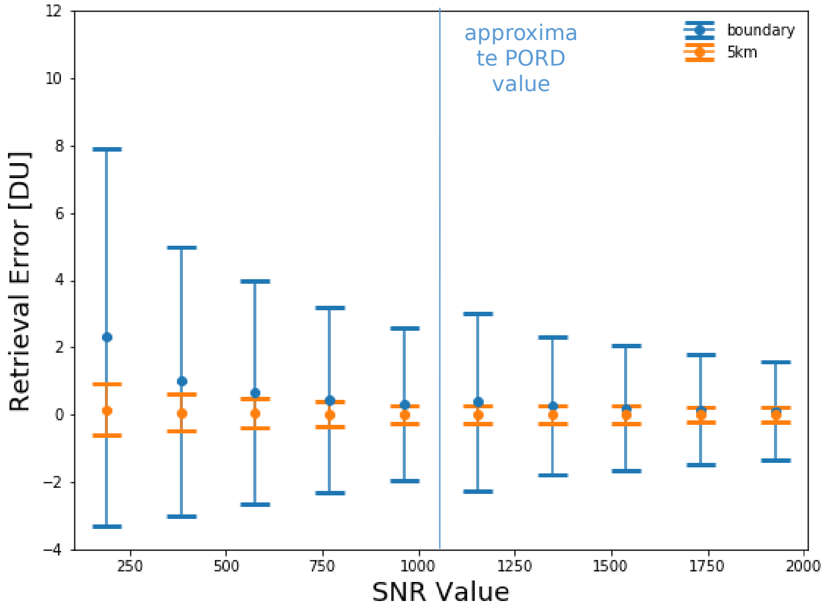
Boundary Layer Case vs Tropospheric Plume

- Each data point and error bars: (mean ± 1 σ) of 1000 simulations
- Seattle, WA: March 20, 2021 @ 1 pm (off-nadir viewing)
- Retrieval results improve for greater amounts of SO_2 in profile
- Retrieval performance with a tropospheric plume outperforms retrieval performance for the boundary layer case

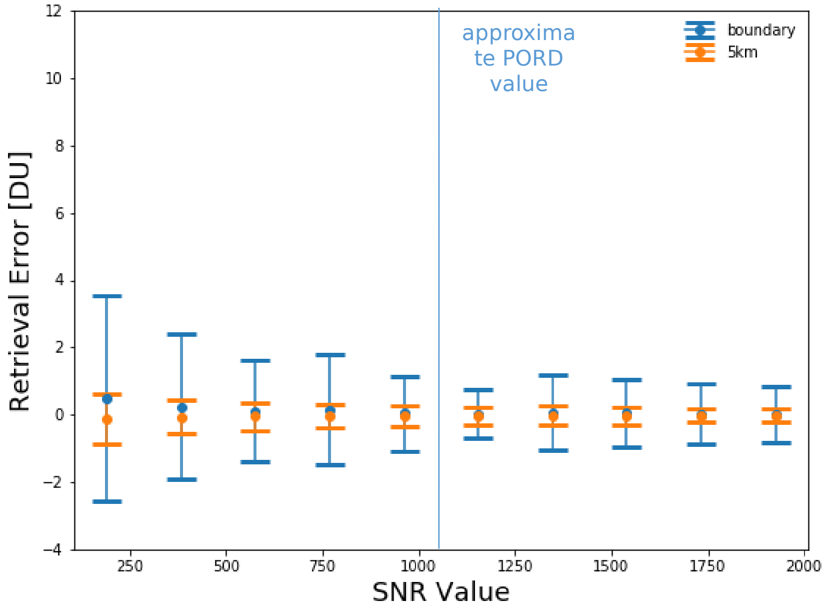
SCA = 0.37 DU



SCA = 0.94 DU



SCA = 3.70 DU

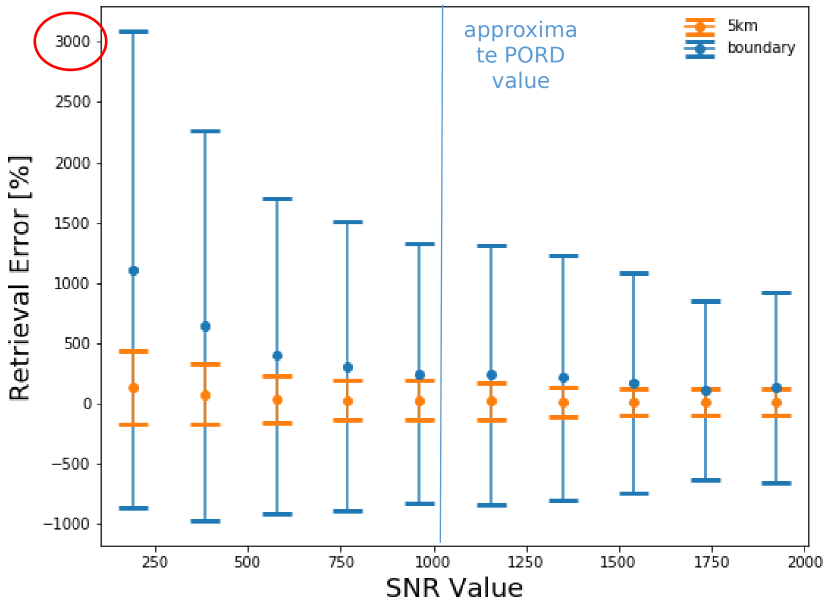


Boundary Layer Case vs Tropospheric Plume

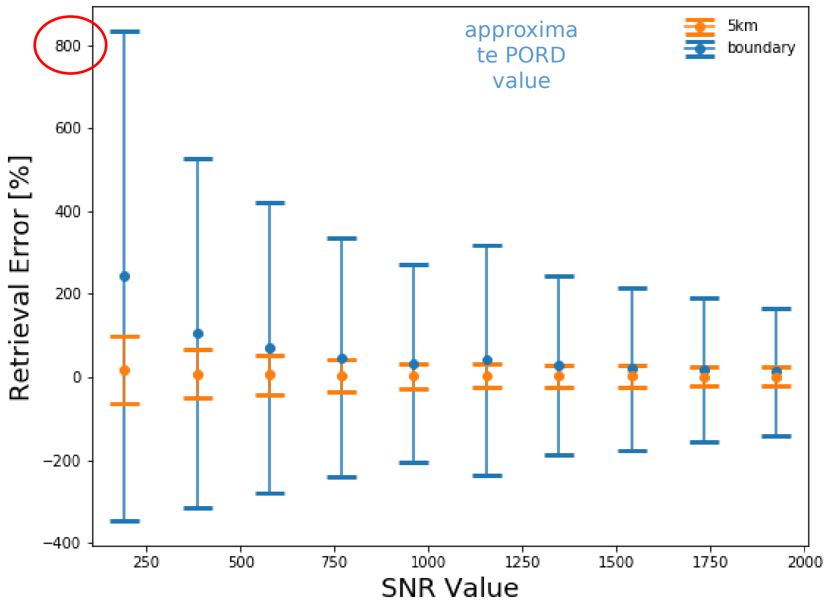
- Each data point and error bars: (mean ± 1 σ) of 1000 simulations
- Seattle, WA: March 20, 2021 @ 1 pm (off-nadir viewing)
- Retrieval results improve for greater amounts of SO_2 in profile
- Retrieval performance with a tropospheric plume outperforms retrieval performance for the boundary layer case
- Results as a percentage of slant column amount show that boundary layer cases have extremely

note difference in axes

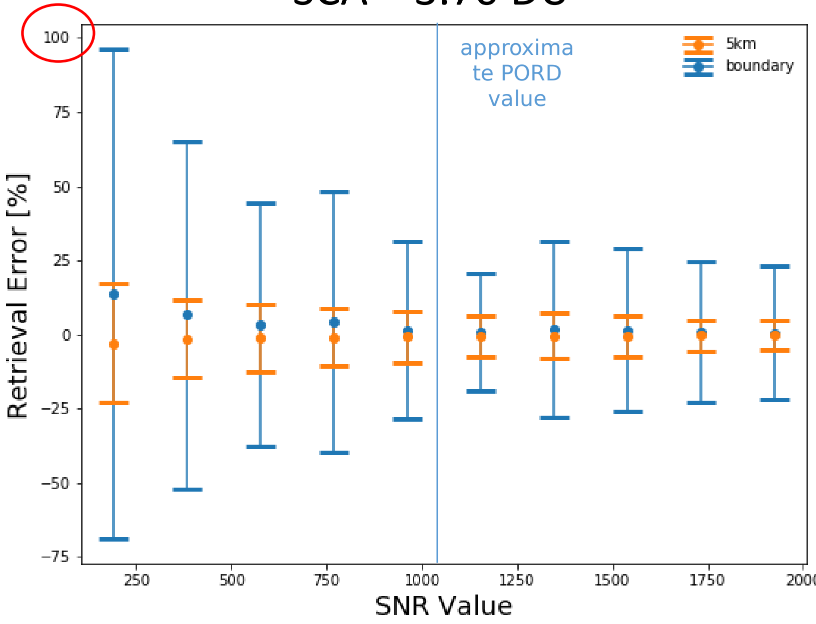
SCA = 0.37 DU



SCA = 0.94 DU



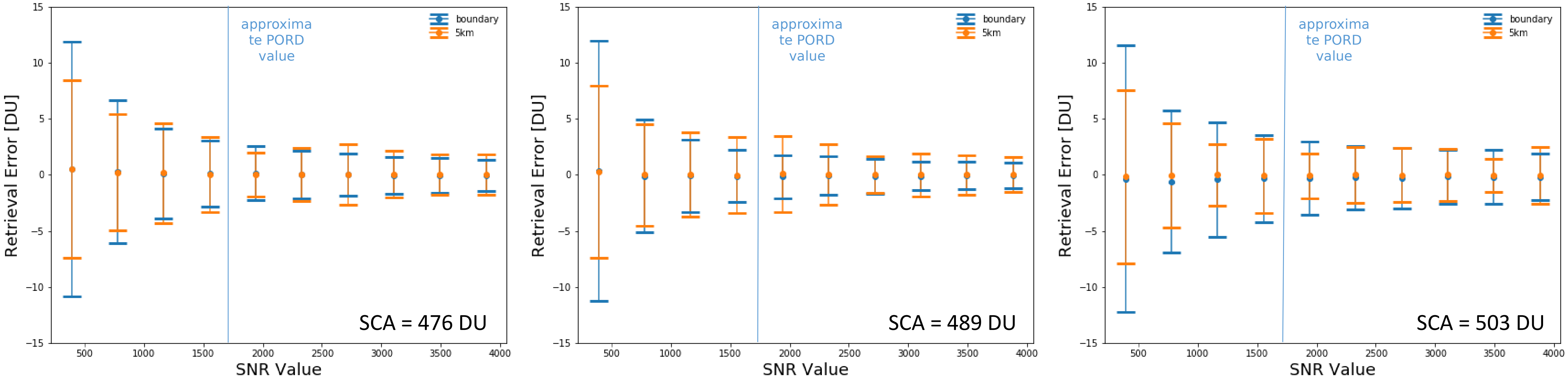
SCA = 3.70 DU



Boundary Layer Case vs Tropospheric Plume

- Each data point and error bars: (mean ± 1 σ) of 1000 simulations
- At near nadir viewing and small SZA, retrieval performance is comparable for O_3 injected into the boundary layer and at 5 km in the troposphere

Norman, OK: June 20, 2021 @ 1pm (closer to nadir viewing, SZA = 13.63°)



Boundary Layer Case vs Tropospheric Plume

- Each data point and error bars: (mean ± 1 σ) of 1000 simulations
- At near nadir viewing and small SZA, retrieval performance is comparable for O_3 injected into the boundary layer and at 5 km in the troposphere
- At off-nadir viewing and larger SZA, retrieval performance is better for O_3 injected at 5 km in the troposphere compared to O_3 injected in the boundary layer

Seattle, WA: March 20, 2021 @ 1pm (off-nadir viewing, SZA = 47.55°)