Physics-based emulation of at-sensor radiances as a tool for novel SIF retrieval schemes

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DLR

Motivation

- SIF retrieval requires accurate modeling of surface, atmospheric and sensor effects.
- Radiative transfer modeling is routinely used but is slow.
- This is an obstacle for novel SIF retrieval methods:
  - limited scope of look-up tables computed offline (e.g., fixed atmosphere conditions);
  - impractible integration into retrieval methods (e.g., semi-supervised schemes).

- Our work: Fast and accurate physics-based emulator of at-sensor radiances for SIF retrieval.
  - Spectral range: O_2-A absorption band (740–780 nm).
  - HyPlant: airborne, limited coverage, spatial resolution of ~1 m, spectral resolution of ~0.25 nm.
  - DESIS: space-based, global coverage, spatial resolution of 30 m, spectral resolution of ~3.5 nm.

- Publications:
  - Pato et al, Physics-Based Machine Learning Emulator of at-Sensor Radiances for Solar-Induced Fluorescence Retrieval in the O_2-A Absorption Band, IEEE JSTARS, Vol. 17, 2024
  - Pato et al, Simulation framework for solar-induced fluorescence retrieval and application to DESIS and HyPlant, RSE, Vol, 330, 2025

Motivation: DESIS

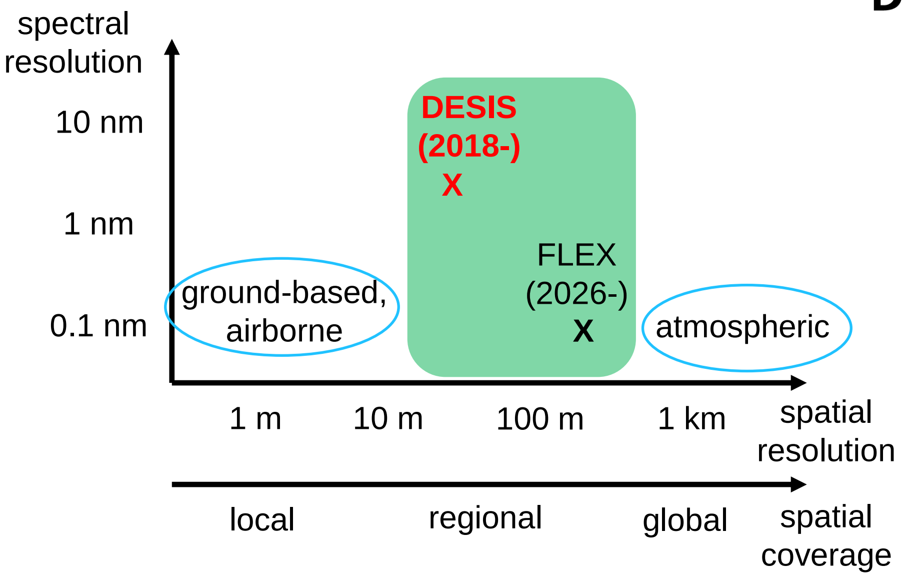
Current status of SIF measurements:

- High spectral resolution instruments provide either high spatial resolution (ground-based, airborne) or large spatial coverage (space-based).
- Moderate spectral resolution instruments fill in the gap.

DESIS advantages for SIF:

- Regional coverage around the globe possible.
- Different hours of day for same site (ISS orbit).
- Large archive of data available.
- DESIS SIF retrieval (30 m) is possible and provides intermediate step between FLEX and ground-based and airborne data.

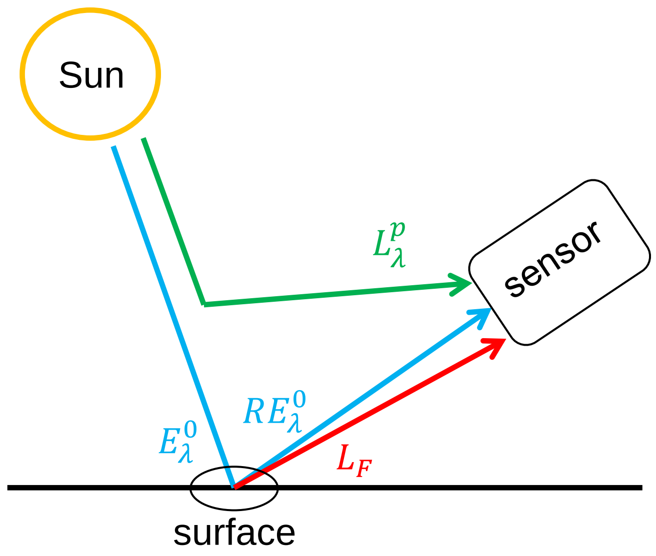
[see poster by Jim Buffat and talk by Juliane Bendig, Tue 16:15]



DESIS specification	
Spectral range	420 – 1000 nm
Number of spectral bands	235
Spectral sampling distance	2.5 nm
Spectral full width at half maximum	3.5 nm
Spectral accuracy	0.5 nm
Signal-to-noise ratio	>150
Orbit type, altitude and inclination	ISS, 400 km, 51.64°
Local time and revisit time	variable
Ground sampling distance	30 m
Product size	30 km x 30 km

[see talk by Emiliano Carmona, Thu 11:30]

Simulation framework



- At-sensor radiance model: $L_s = L_p + \frac{E_g^0 \rho T^\uparrow}{\pi(1-\rho S)} + L_F T^\uparrow$.
- Spectral range around O_2-A band: 740–780 nm.
- Atmosphere+geometry: radiative transfer with MODTRAN6 or libRadtran 2.0.6.
- Surface: reflectance and fluorescence parametric models.

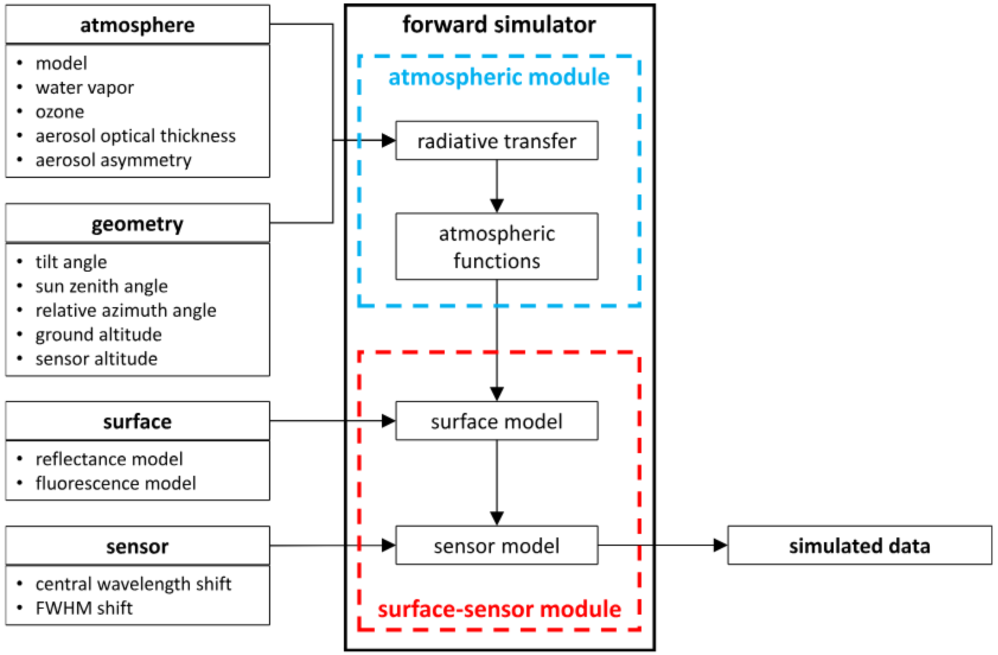
$$\rho(\lambda) = \rho_{740} + s(\lambda - \lambda_1) + \frac{s(e-1)}{2(\lambda_2-\lambda_1)}(\lambda - \lambda_1)^2$$

$$L_F(\lambda) = F_{737} \exp\left(-\frac{(\lambda-\lambda_F)^2}{2\sigma_F^2}\right) \qquad \lambda_F = 737\ \mathrm{nm},\ \sigma_F = 20\ \mathrm{nm}$$

- Sensor: based on expert DESIS and HyPlant knowledge.

$$\mathrm{CW}_b' = \mathrm{CW}_b + \delta_{\mathrm{CW}} \qquad \mathrm{FWHM}_b' = \mathrm{FWHM}_b + \delta_{\mathrm{FWHM}}$$

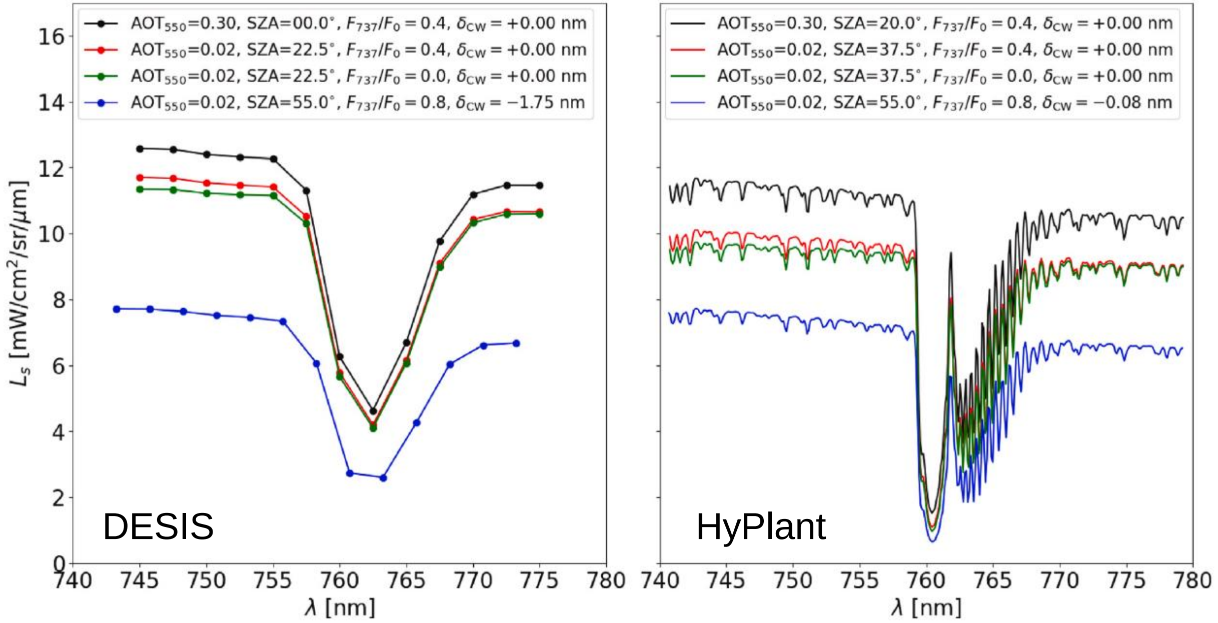
- Note: Other specialized simulation codes exist, but we opted to design a dedicated tool for our needs.



[Pato et al, RSE, Vol, 330, 2025]

Simulated datasets

- Key parameters and ranges set after sensitivity analysis.
- Sampling: uniform grid (UG), random (R), Halton (H).
- Dataset: ~4–6 M samples over 12–13 input dimensions.
- Simulation time: 1–4 min/sample (dominated by MODTRAN6 or libRadtran run time).

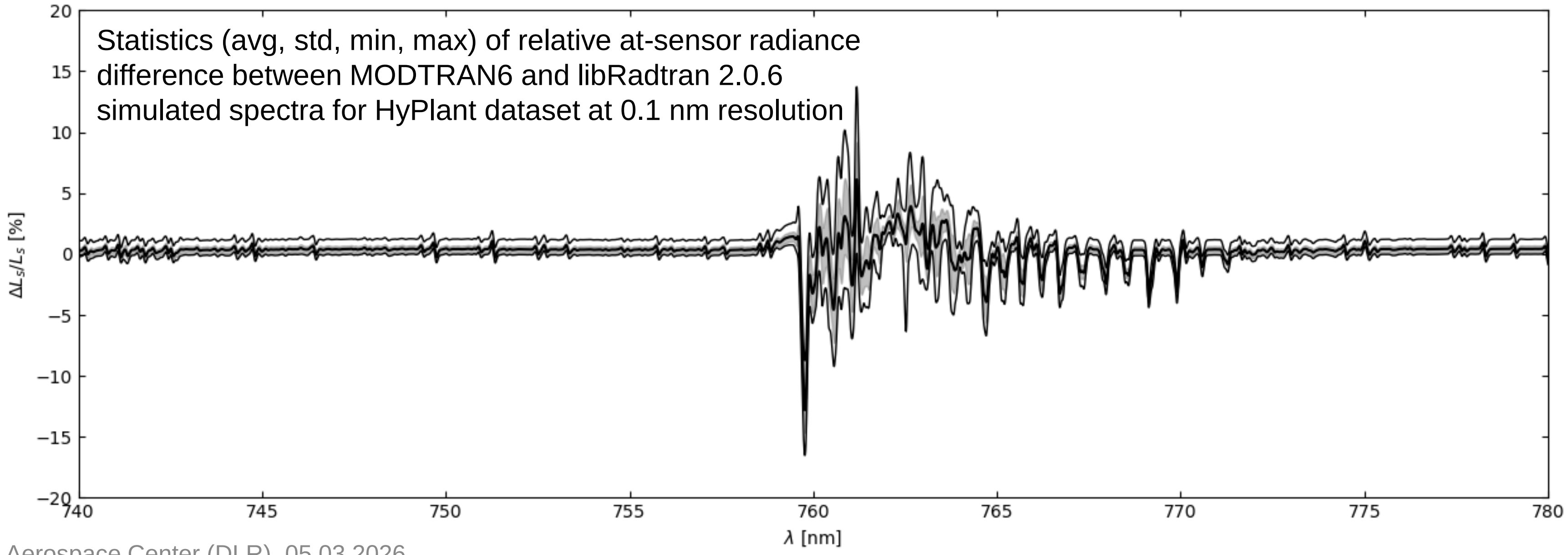


Specification		DESIS	HyPlant
Atmosphere	H_2O [cm]	0.3−5.0	0.3−3.0
	AOT_{550} []	0.02−0.30	0.02−0.30
Geometry	TA [°]	0−25	0−20
	SZA [°]	0−55	20−55
	RAA [°]	0−180	0−180
	h_{gnd} [m]	0−600	0−300
	h_{sen} [km]	100	0.659−0.691
Surface	ρ_{740} []	0.05−0.60	0.05−0.60
	s [nm^{-1}]	0−0.012	0−0.012
	e []	0−1	0−1
	F_{737}/F_0	0−0.8	0−0.8
Sensor	δ_{CW} [nm]	[−1.75, +1.25]	[−0.080, +0.080]
	δ_{FWHM} [nm]	[−0.3, +0.3]	[−0.040, +0.040]
Input dimensions		12	13
Number of bands		13	349
Number of samples		4.3×10^6	6.3×10^6
- uniform grid		1×10^6	3×10^6
- random		3×10^5	3×10^5
- Halton		3×10^6	3×10^6

[adapted from Pato et al, IEEE JSTARS, Vol. 17, 2024 and Pato et al, RSE, Vol. 330, 2025]

Simulated datasets: a word of caution

- High-resolution spectra simulated with MODTRAN6 and libRadtran 2.0.6 differ by up to 20% at the O_2-A absorption band for the “same” input (“same” from the point of view of an average user). It is not clear which of the two versions is more “correct”.
- Both SW include absorption lines from HITRAN, but at different times and with different treatments.
- Atmosphere and aerosols are in principle the same, but likely treated internally slightly differently.
- **Key point:** SIF retrieval with high-resolution data should be aware of RT systematic differences.



Emulator learning

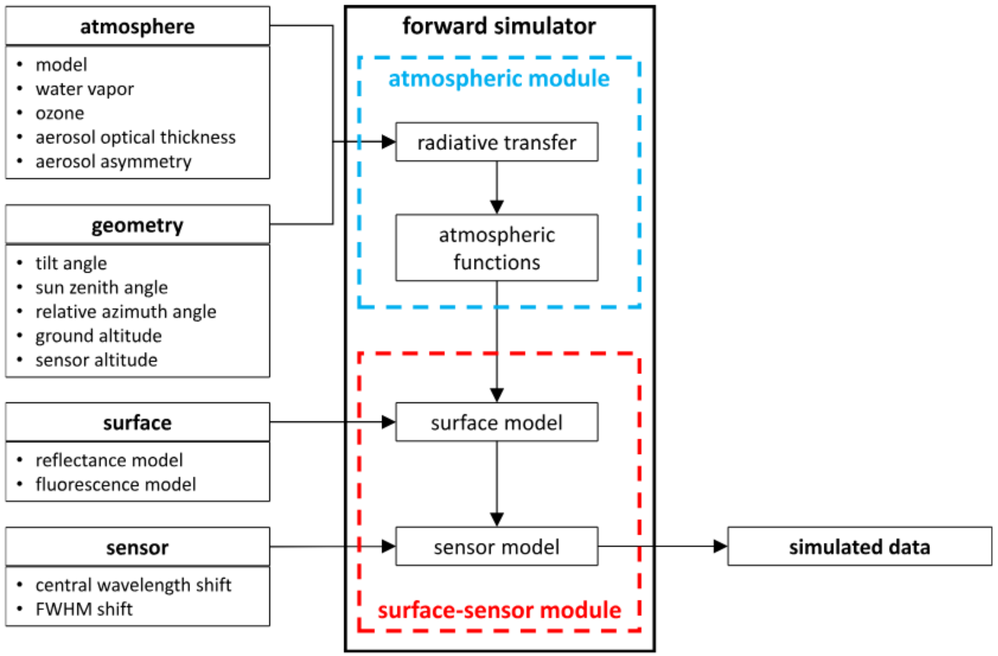
- Aim: Emulate physics-based simulator with machine learning (ML) model.
- Regression in high dimensions: $L_s = F(x)$

  $F: \mathbb{R}^{12} \rightarrow \mathbb{R}^{13}$ for DESIS, $F: \mathbb{R}^{13} \rightarrow \mathbb{R}^{349}$ for HyPlant

  learn emulator $\hat{F} \approx F$ using simulated data
- Simple ML models as emulators: polynomials, neural networks (NN), kernel ridge regression (KRR), Gaussian process regression (GPR), k nearest neighbors (kNN) and support vector regression (SVR).
- Training/validation/test split:

DESIS:	4×10^6	2×10^5	9×10^4
HyPlant:	6×10^6	2×10^5	9×10^4

- Question: Can a fast and accurate emulator be learned to replace the physics-based simulator for use in SIF retrieval?



[adapted from Pato et al, RSE, Vol, 330, 2025]

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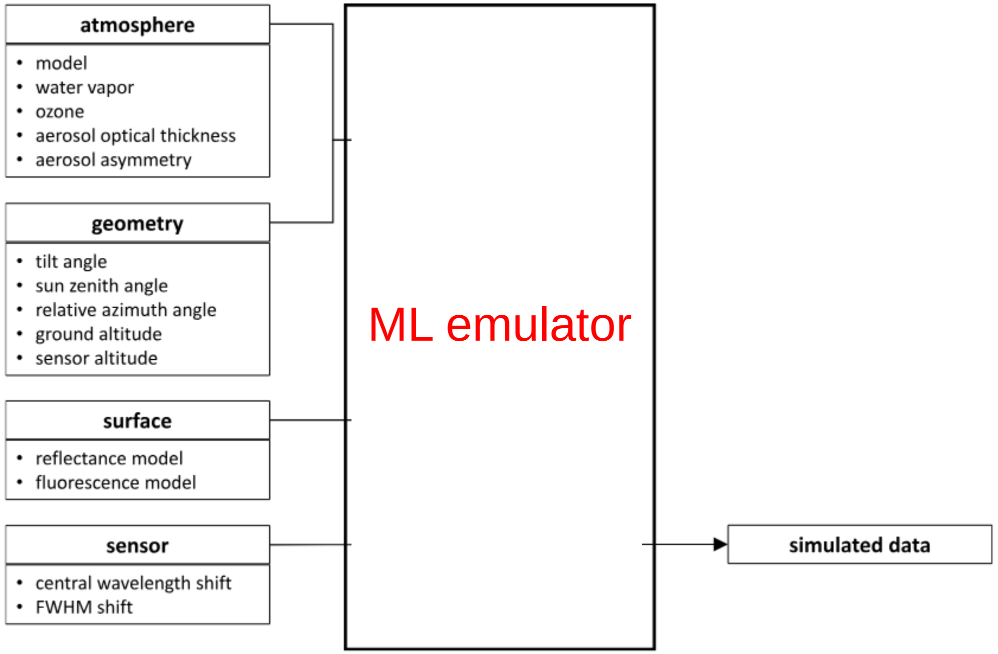


[adapted from Pato et al, RSE, Vol, 330, 2025]

Emulator learning: different models

[adapted from Pato et al, IEEE JSTARS, Vol. 17, 2024]

Performance parameter	DESIS							
	OLS	P2	P4	P5	N2	N3	KRR	GPR
Test set MAE [mW/cm^2/sr/μm]	0.77	0.17	0.011	0.0032	0.040	0.037	0.043	0.039
Total training time	1.6 s	19 s	1.8 min	1.2 min	1.2 h	1.2 h	1.1 min	2.7 s
Prediction time per sample	0.06 μs	1.1 μs	11 μs	28 μs	56 μs	45 μs	0.1 ms	0.2 ms

Performance parameter	HyPlant							
	OLS	P2	P4	P5	N2	N3	KRR	GPR
Test set MAE [mW/cm^2/sr/μm]	0.59	0.092	0.0027	0.0013	0.027	0.020	0.018	0.025
Total training time	1.7 min	45 s	1.3 min	1.5 min	2.0 h	2.2 h	6.3 s	13 s
Prediction time per sample	1.3 μs	2.2 μs	17 μs	47 μs	44 μs	43 μs	72 μs	0.7 ms

SIF accuracy goal (740–780 nm):
$L_0 = (0.04 - 0.4)\ \mathrm{mW/cm^2/sr/\mu m}$
(for $F_{737} = 0.4\ \mathrm{mW/cm^2/sr/\mu m}$)

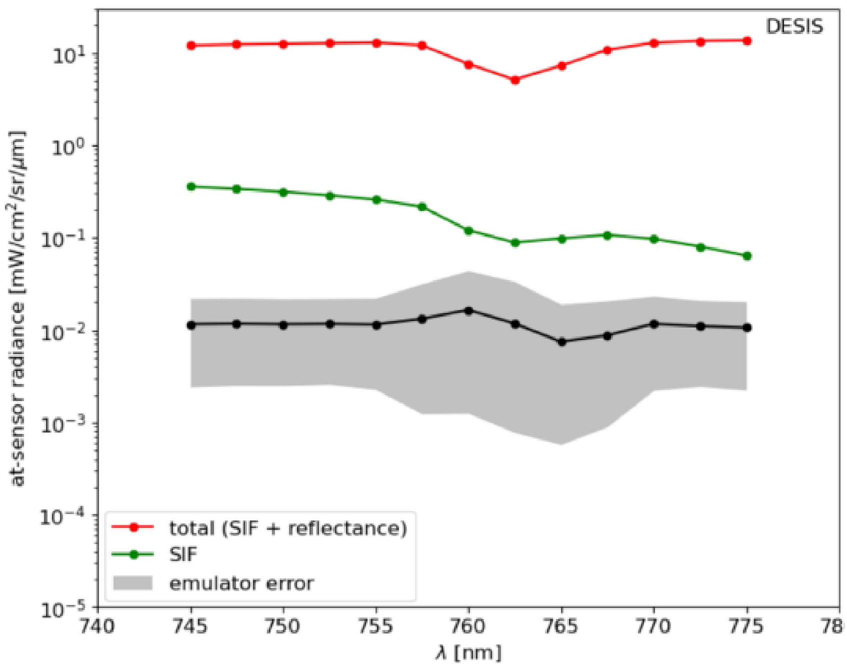
physics-based simulation time:
1–4 min per simulated spectrum

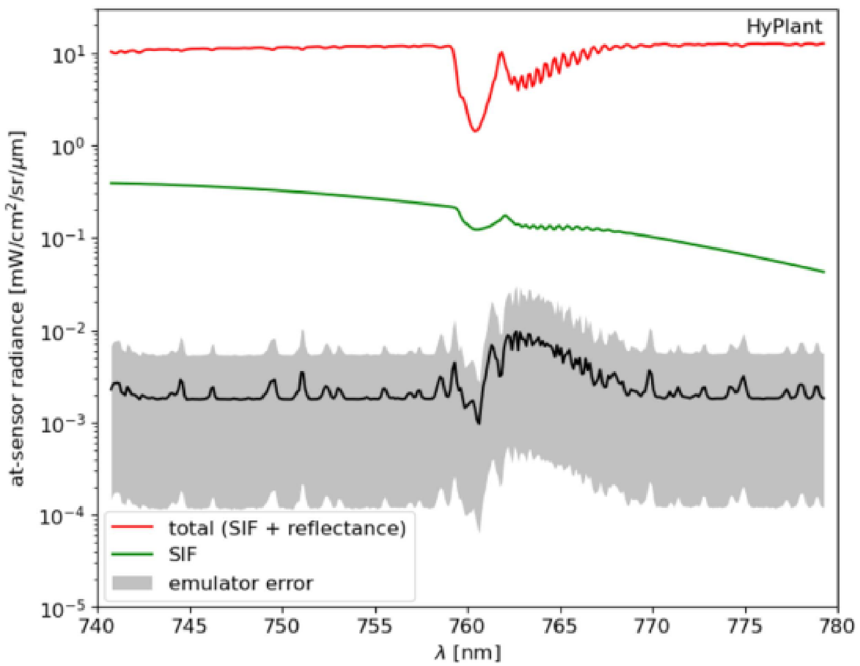
- Accuracy assessment:
  - Linear models, 2nd degree polynomials (P2), kNN and SVR show poor results.
  - NN, KRR and GPR have accuracies similar to the SIF signal.
  - Polynomials of degree 4 or higher (P4, P5) surpass SIF accuracy goal.
- A fourth degree polynomial (P4) is both accurate and fast and provides an excellent baseline emulator.
- Note: P4 is “simple” but not necessarily “small” (24 k parameters for DESIS, 831 k for HyPlant).
- Conclusion: Simple ML models are adequate to emulate full-fledged simulation in our case study.

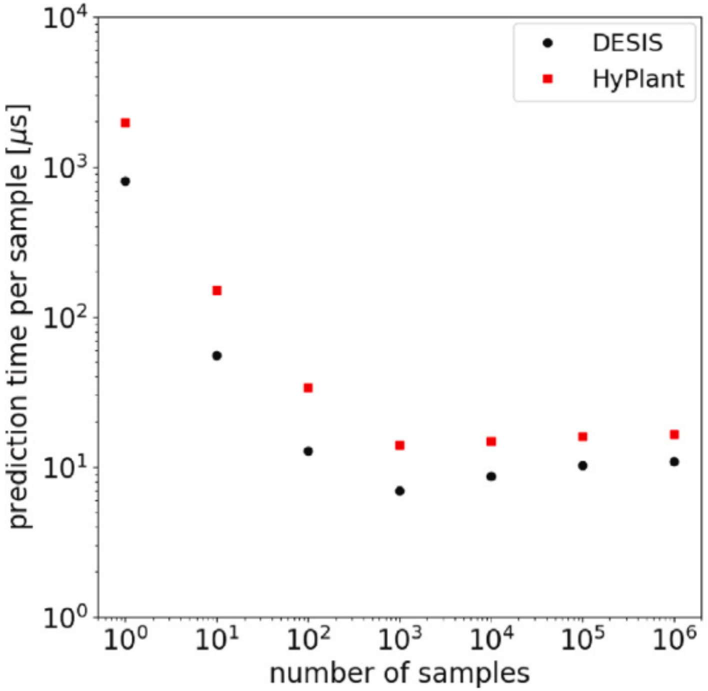
Emulator learning: baseline

Performance of baseline emulator (P4):

- Accuracy: 10% of SIF signal or better (wrt simulation)
- Speed: up to 10^7 times faster than simulation, single sample: 1–2 ms, in bulk: 10–20 µs
- There is room for improvement: Accuracy can be improved (factor ~2-3) at the price of speed or scope.



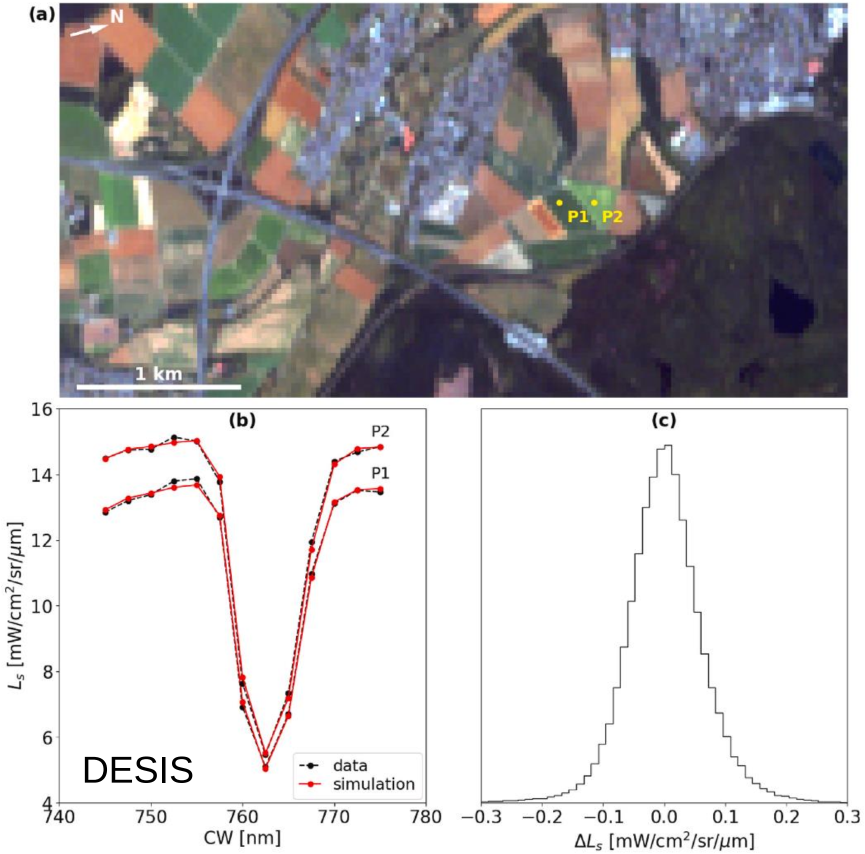


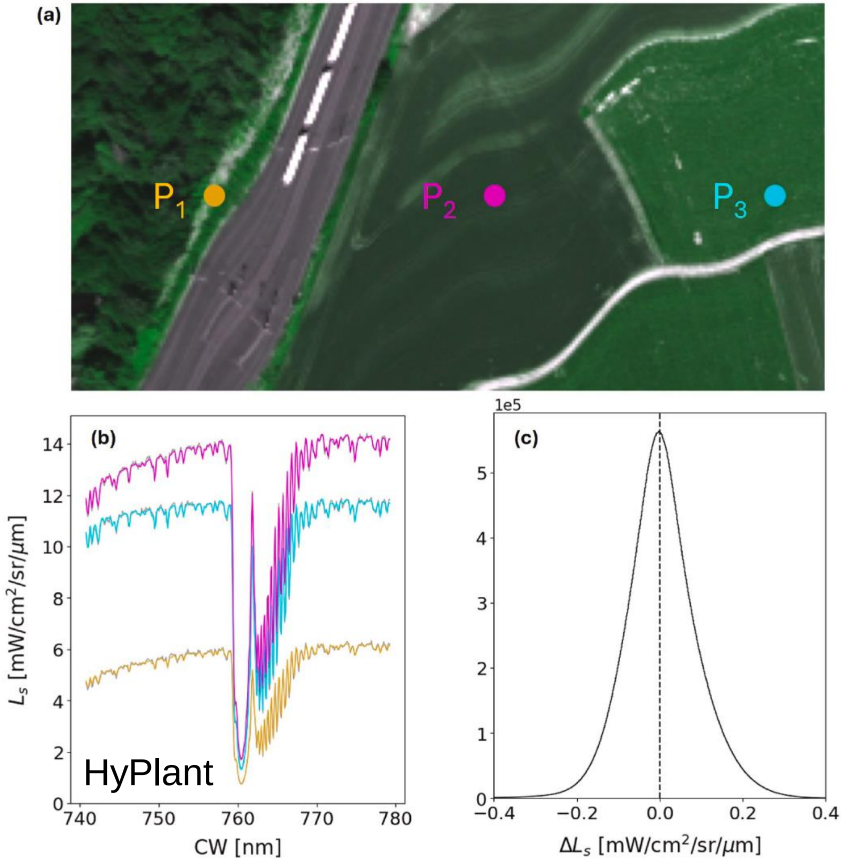


[adapted from Pato et al, IEEE JSTARS, Vol. 17, 2024 and Pato et al, RSE, Vol. 330, 2025]

Comparison to real data

- Emulators accurately reproduce DESIS and HyPlant measurements for a diverse range of surfaces.
- This demonstrates realistic nature of our simulations.

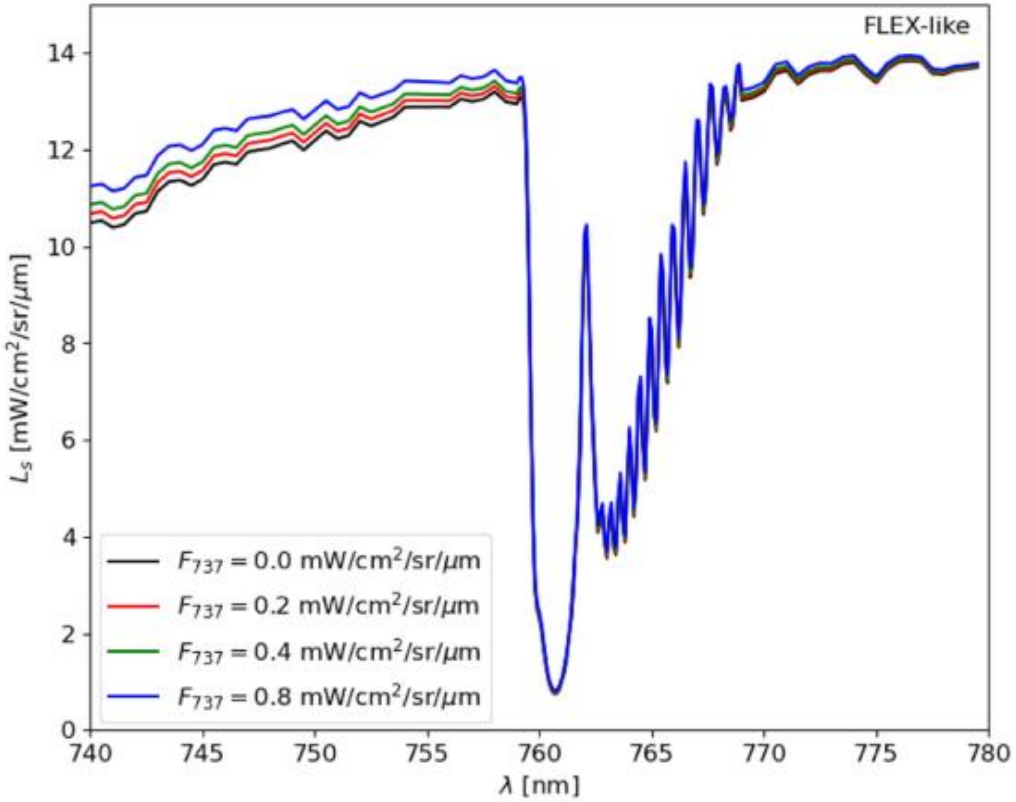




[adapted from Pato et al, RSE, Vol, 330, 2025]

Outlook

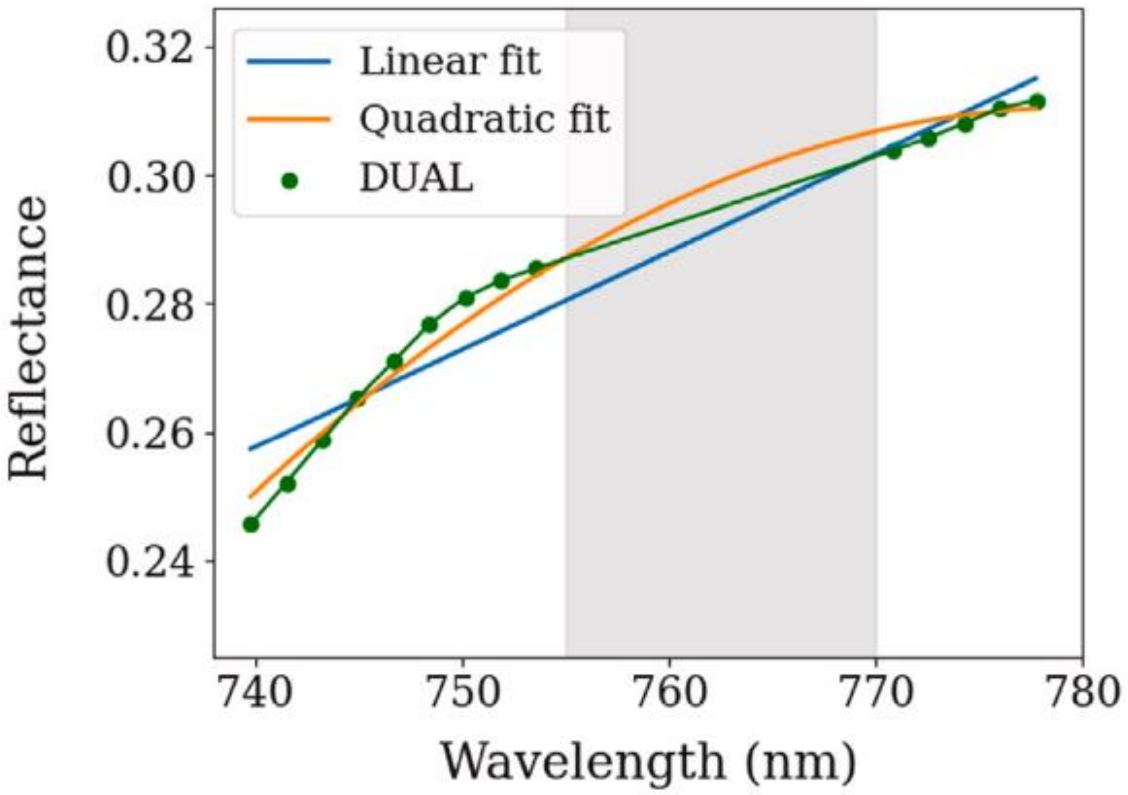
- Emulator applications (not easily possible with physics-based simulations):
  - fast and accurate online simulation step in SIF retrieval methods [see poster by Jim Buffat];
  - large tailored datasets for training or performance assessment;
  - aid uncertainty estimation.
- Scope of our work: DESIS and HyPlant at the O_2-A band.
- But it is possible to extend the work to:
  - other sensors, including FLEX (see plot);
  - other spectral ranges, e.g. O_2-B band (more work needed).

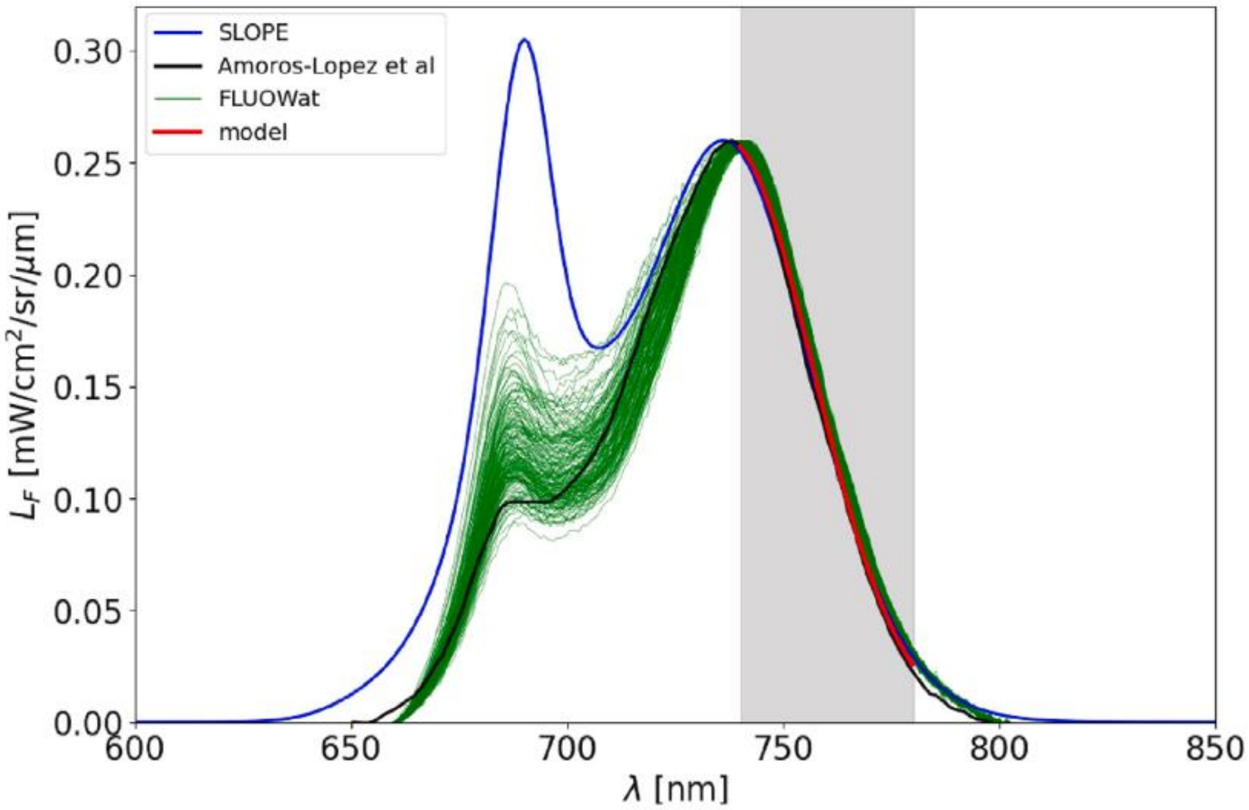


[Pato et al, IEEE JSTARS, Vol. 17, 2024]

BACKUP SLIDES

Reflectance and fluorescence models





[Pato et al, RSE, Vol, 330, 2025]

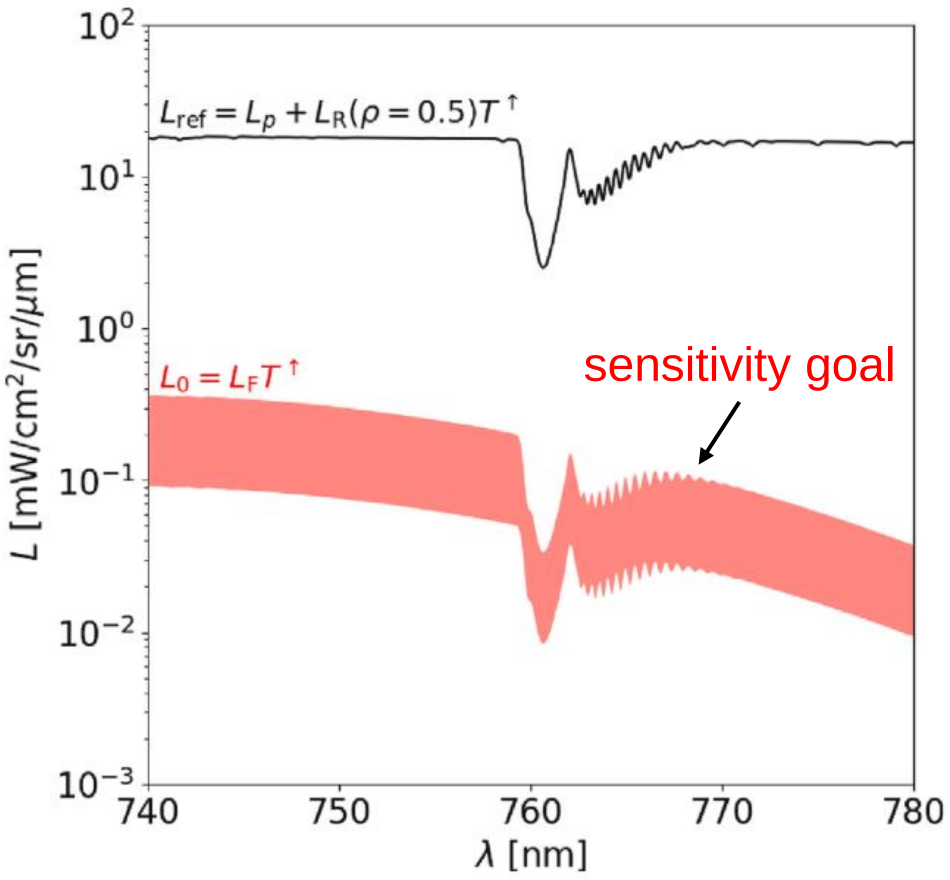
Simulated datasets

Parameter		Sensitivity analysis	DESIS DB	HyPlant DB
Atmosphere	model	mid-latitude summer, tropical	mid-latitude summer, tropical	mid-latitude summer
	H_2O [cm]	0.3–5.0	0.3–5.0	0.3–3.0
	O_3 [DU]	200–500	332	332
	AOT_{550} []	0.05–0.50	0.02–0.30	0.02–0.30
	aerosol model	rural, maritime, desert, urban, none	rural	rural
Geometry	TA [°]	0–15	0–25	0–20
	SZA [°]	0–45	0–55	20–55
	RAA [°]	0–180	0–180	0–180
	h_{gnd} [m]	0–4000	0–600	0–300
	h_{sen} [km]	0.001–100	100	0.659–0.691 agl
Surface	ρ_{740} []	0.00 – 0.60	0.05 – 0.60	0.05 – 0.60
	s [nm^{-1}]	0 – 0.0008	0 – 0.012	0 – 0.012
	e []	1	0 – 1	0 – 1
	F_{737}/F_0	0 – 0.8	0 – 0.8	0 – 0.8
Sensor	δ_{CW} [nm]	[−1.00, +1.00]	[−1.75, +1.25]	[−0.080, +0.080]
	δ_{FWHM} [nm]	[−0.25, +0.15]	[−0.3, +0.3]	[−0.040, +0.040]

DB	Specification	DESIS DB			HyPlant DB		
ATM	Input space	6d			7d		
	Sampling	UG	R	H	UG	R	H
	Nr. samples	2×3^6	2×10^3	2×10^4	3^7	10^3	10^4
SENSOR	Input space	6d			6d		
	Sampling	UG	R	H	UG	R	H
	Nr. samples	2×3^6	300	300	2×3^6	300	300
Total samples		2×10^6	6×10^5	6×10^6	3×10^6	3×10^5	3×10^6

[Pato et al, RSE, Vol, 330, 2025]

Sensitivity analysis: goal and radiative transfer

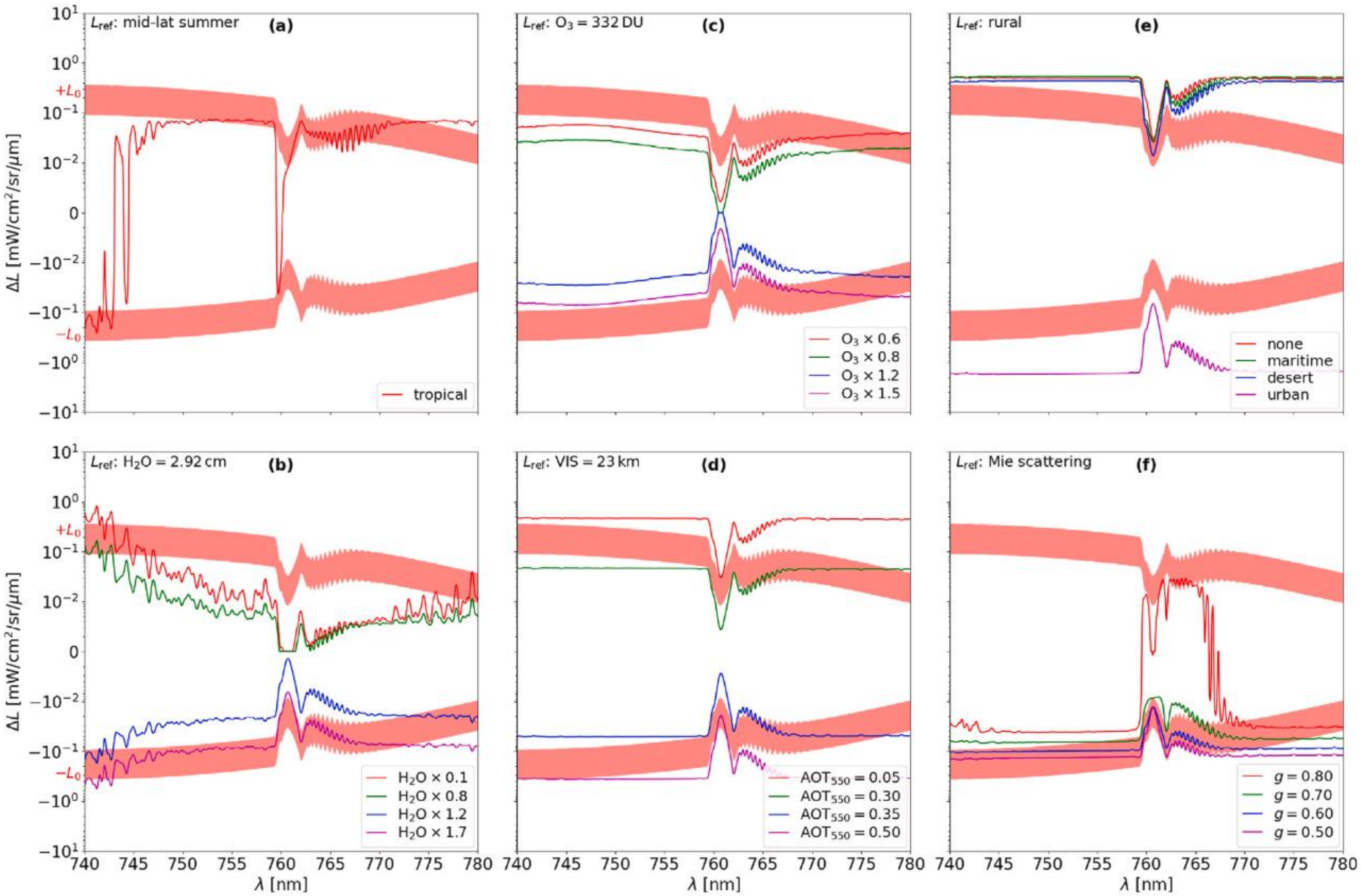


radiative transfer configurations

Case	Model	Resolution	Multiple scattering	Run time
00	correlated-k (fast)	1.0 cm^{-1} / –	Isaacs scaled (8S)	00:02
A1	line-by-line	0.1 cm^{-1} / 100	DISORT (8S)	09:13
B2	correlated-k (slow)	0.1 cm^{-1} / –	DISORT (8S)	01:40
B3	correlated-k (fast)	0.1 cm^{-1} / –	DISORT (8S)	00:59
B4	band model	0.1 cm^{-1} / –	DISORT (8S)	00:09
C2	line-by-line	0.1 cm^{-1} / 50	DISORT (8S)	04:34
C3	line-by-line	0.1 cm^{-1} / 20	DISORT (8S)	01:55
C4*	line-by-line	0.1 cm^{-1} / 10	DISORT (8S)	00:57
C5	line-by-line	0.1 cm^{-1} / 5	DISORT (8S)	00:30
C6	line-by-line	0.1 cm^{-1} / 3	DISORT (8S)	00:20
C7	correlated-k (slow)	1.0 cm^{-1} / –	DISORT (8S)	00:20
C8	correlated-k (slow)	5.0 cm^{-1} / –	DISORT (8S)	00:05
D2	line-by-line	0.1 cm^{-1} / 100	Isaacs scaled (8S)	failed
D3	correlated-k (slow)	0.1 cm^{-1} / –	Isaacs scaled (8S)	00:07
D4	correlated-k (fast)	0.1 cm^{-1} / –	Isaacs scaled (8S)	00:06
D5	line-by-line	0.1 cm^{-1} / 100	None	00:05

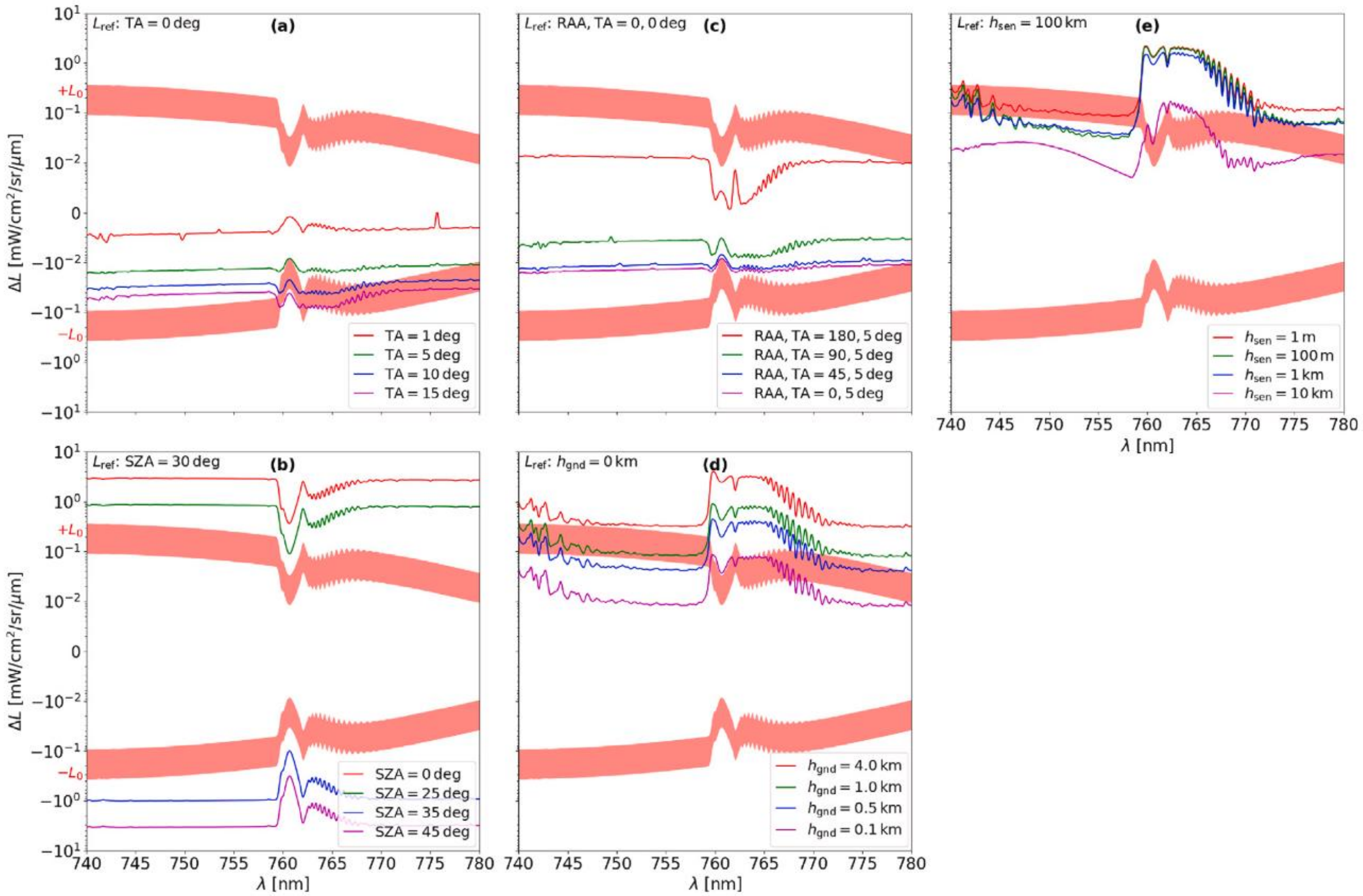
[Pato et al, RSE, Vol, 330, 2025]

Sensitivity analysis: atmosphere



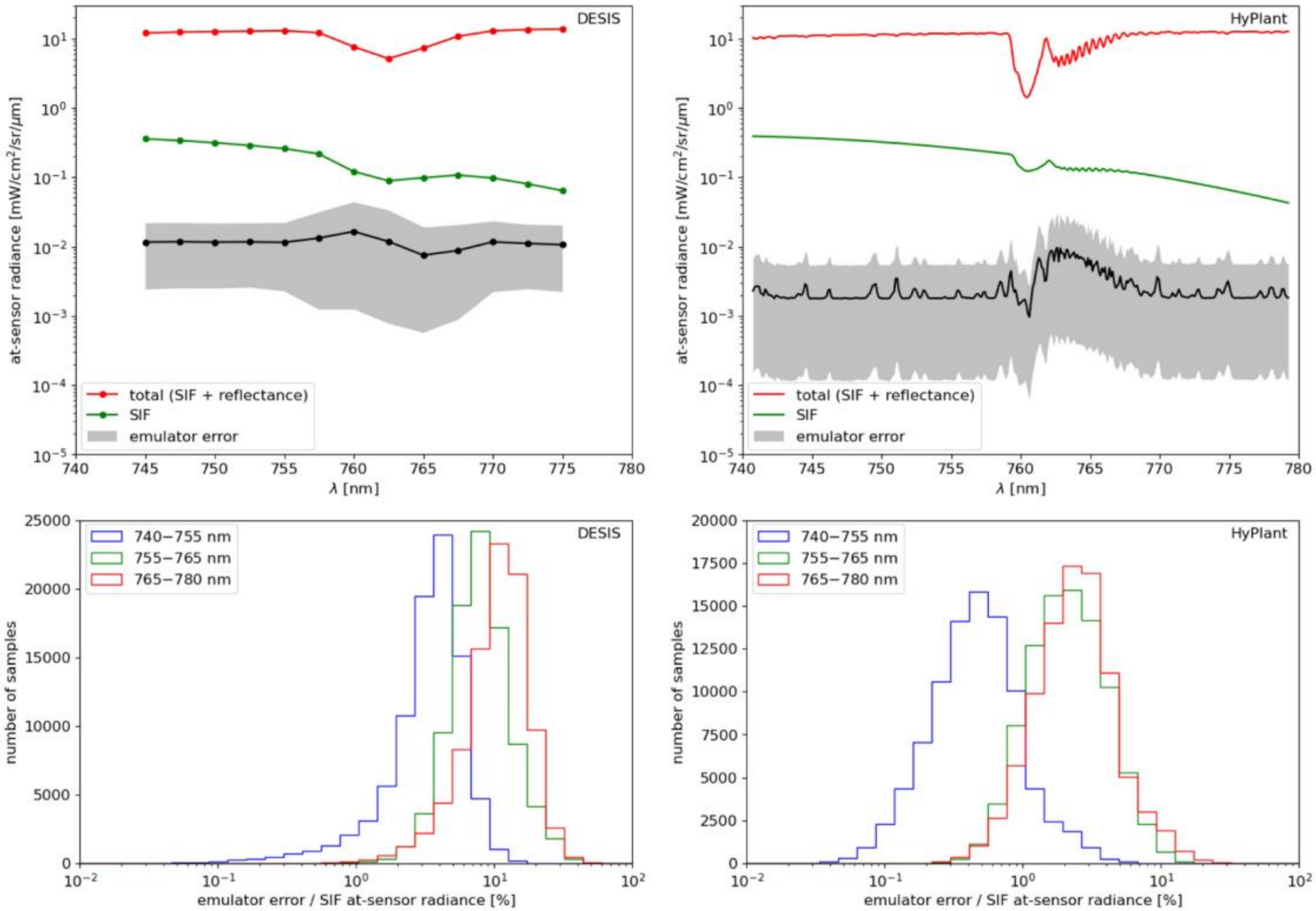
[Pato et al, RSE, Vol, 330, 2025]

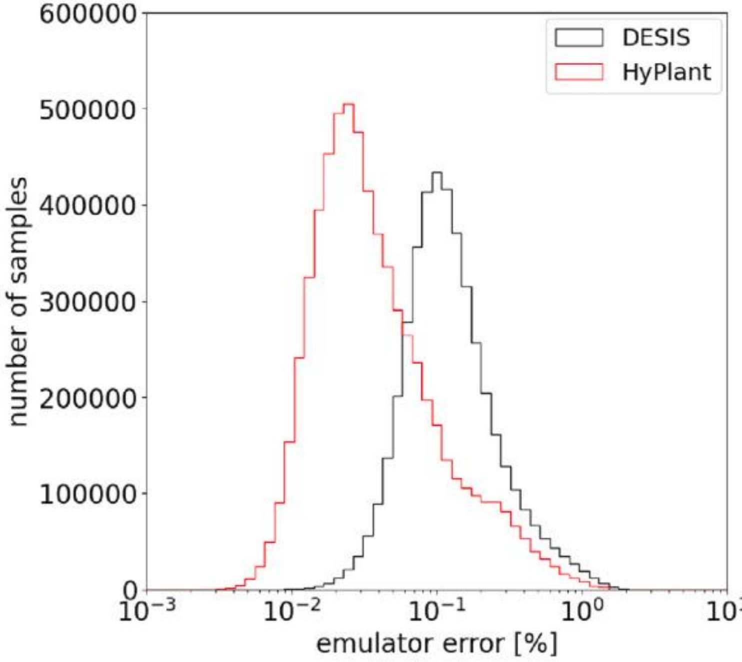
Sensitivity analysis: geometry



[Pato et al, RSE, Vol, 330, 2025]

P4 emulator performance

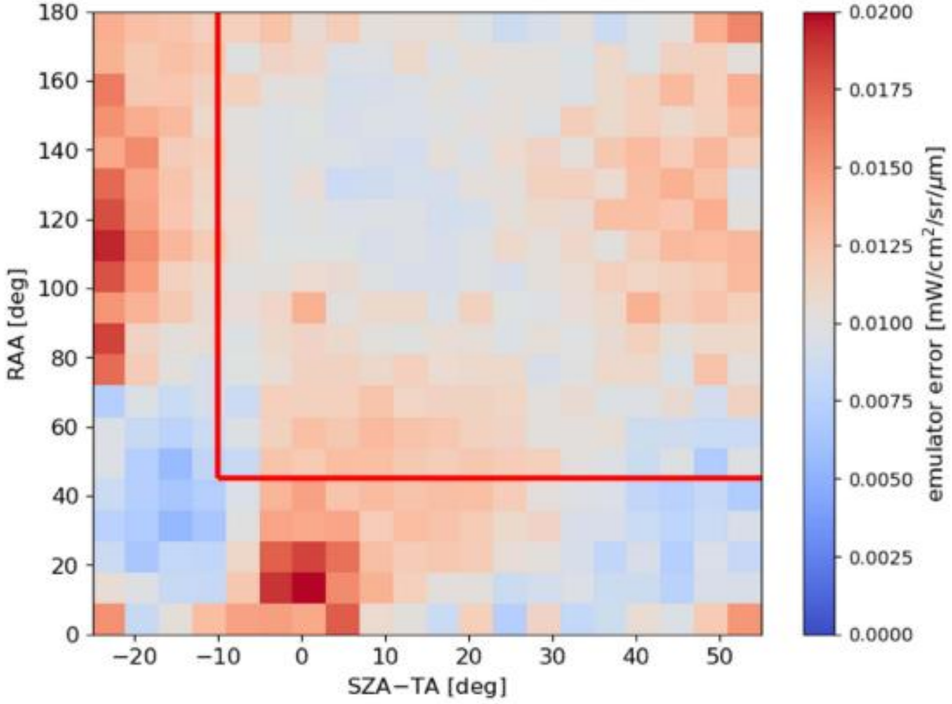




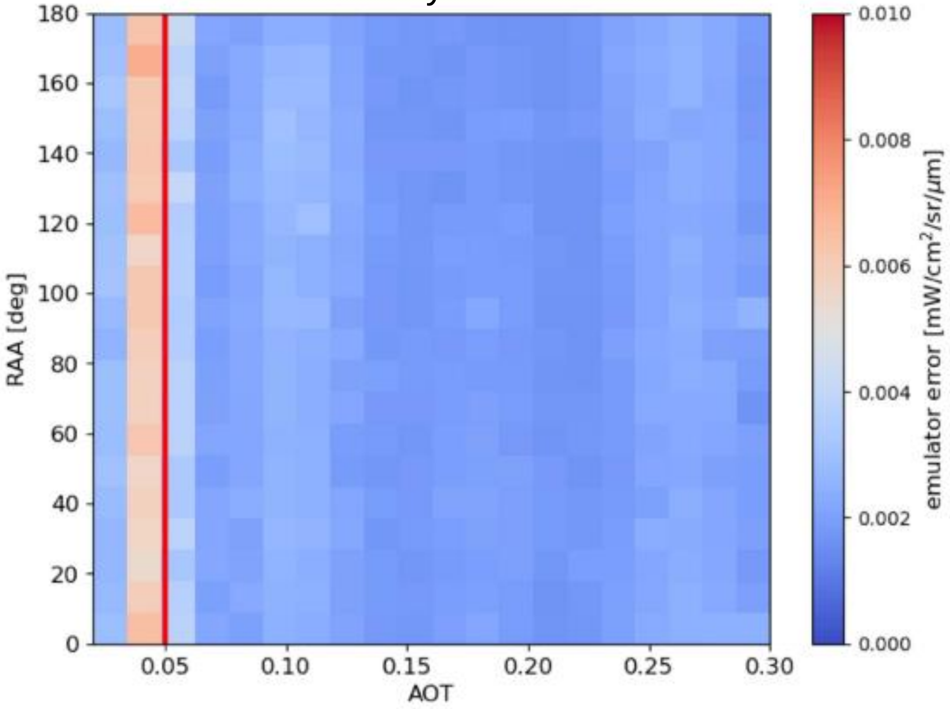
[Pato et al, IEEE JSTARS, Vol. 17, 2024, Pato et al, RSE, Vol, 330, 2025]

P4 emulator performance

DESIS



HyPlant



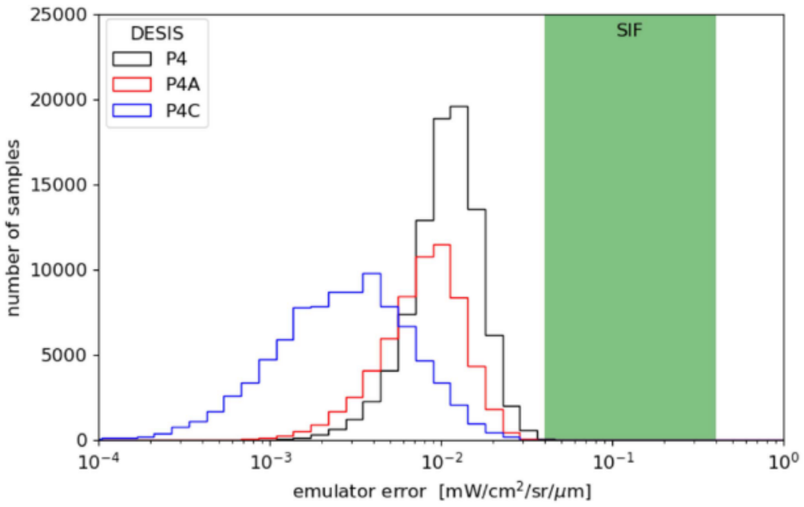
[adapted from Pato et al, IEEE JSTARS, Vol. 17, 2024]

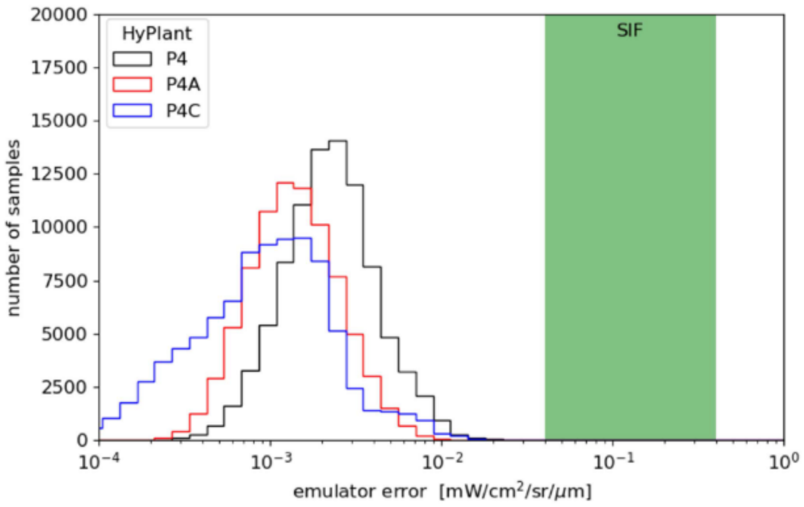
Emulator baseline improvements

There is room for improvement over baseline emulator (P4):

- Accuracy can be improved by a factor 2-3 at the price of prediction time or scope.
- Strategies: limit input space (P4A), bandwise training (P4B), learn atmospheric functions (P4C).

Performance parameter	DESIS				HyPlant			
	P4	P4A	P4B	P4C	P4	P4A	P4B	P4C
Test set MAE [$mW/cm^2/sr/\mu m$]	0.011	0.0087	0.011	0.0037	0.0027	0.0017	0.0027	0.0014
Total training time	1.8 min	1.9 min	24 min	2.1 s	1.3 min	1.4 min	8.6 h	3 s
Prediction time per sample	11 μs	11 μs	0.1 ms	6 ms	17 μs	17 μs	4 ms	173 ms

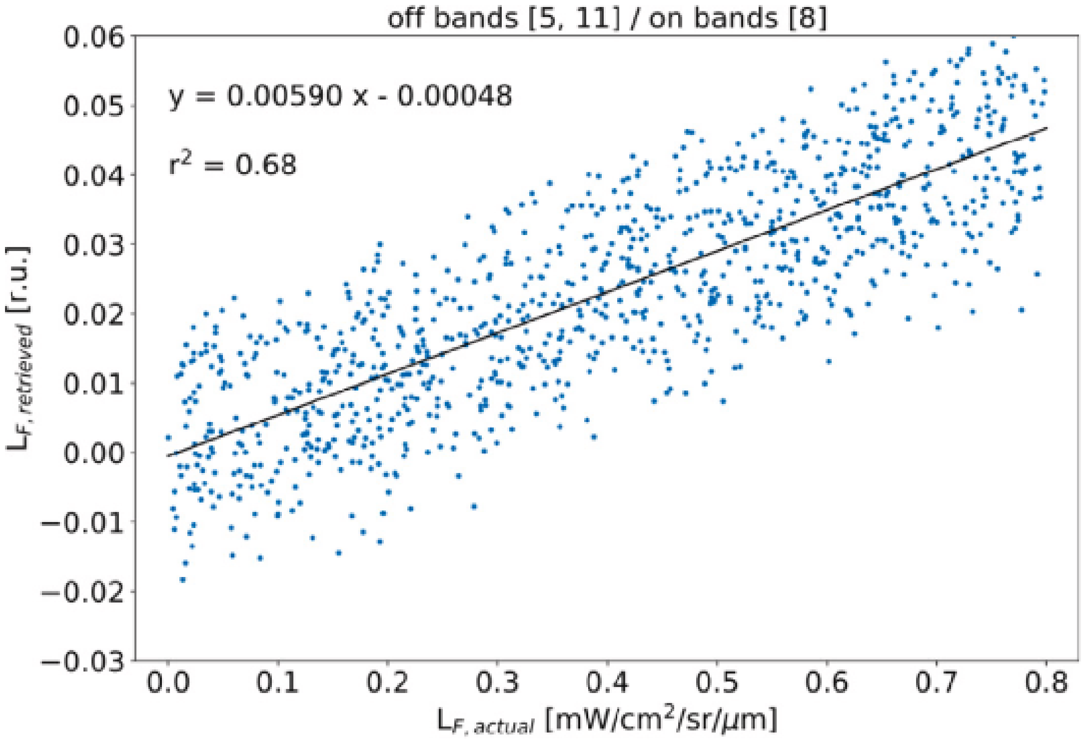




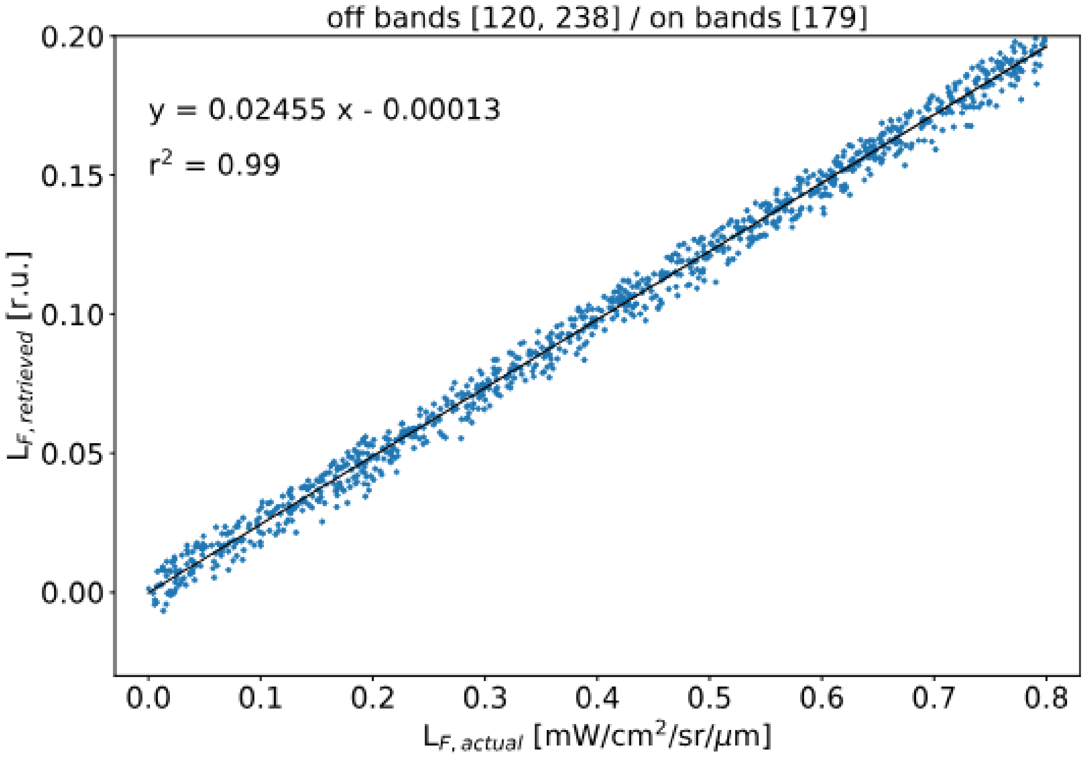
[Pato et al, IEEE JSTARS, Vol. 17, 2024]

3FLD SIF retrieval performance

DESIS



HyPlant



[adapted from Pato et al, RSE, Vol, 330, 2025]