On the relationships between solar-induced fluorescence and net photosynthesis of the canopy: a SCOPE modeling study

Jochem Verrelst[(1)], Juan Pablo Rivera[(1)], Christiaan van der Tol[(2)], Federico Magnani[(3)], Gina Mohammed[(4)], Jose Moreno[(1)]

[(1)] Image processing Laboratory (IPL), University of Valencia, Spain
[(2)] University of Twente, Netherlands
[(3)] University of Bologna, Italy
[(4)] P&M Technologies, Sault Ste Marie, Ontario, Canada

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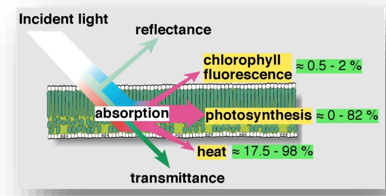
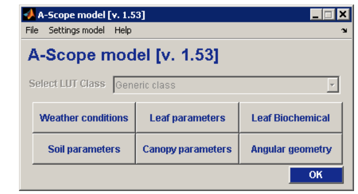
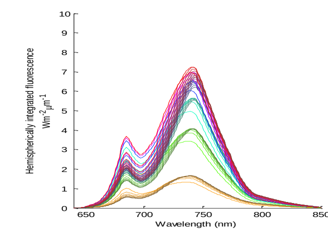
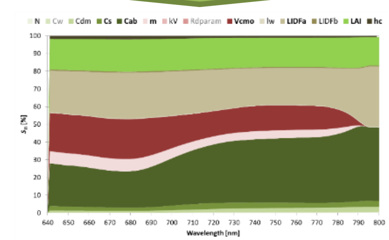
Outline:

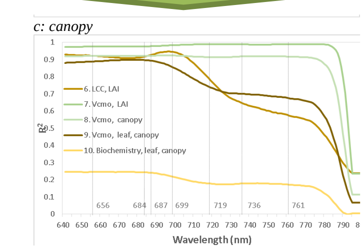
- Background
  - Sun-Induced Fluorescence (SIF)
  - How to relate SIF to photosynthesis?
  - SCOPE v.1.53 & Automated SCOPE (A-SCOPE)
- Global Sensitivity Analysis (GSA) SCOPE
  - Variance-based GSA
  - GSA results: what drives canopy-leaving SIF?
- Relating SIF with photosynthesis (NPC)
  - Simulating canopies with increasing complexity
  - Single band/multiple bands regression results
- Conclusions



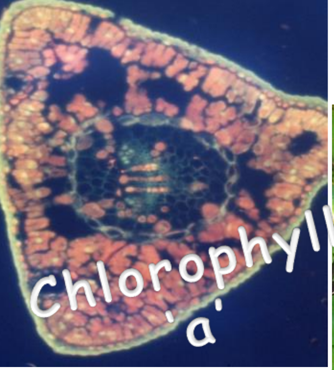


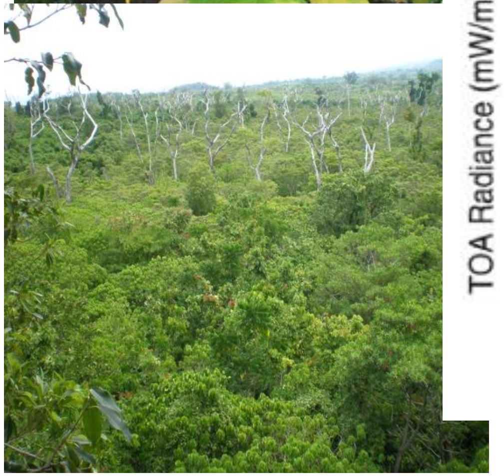


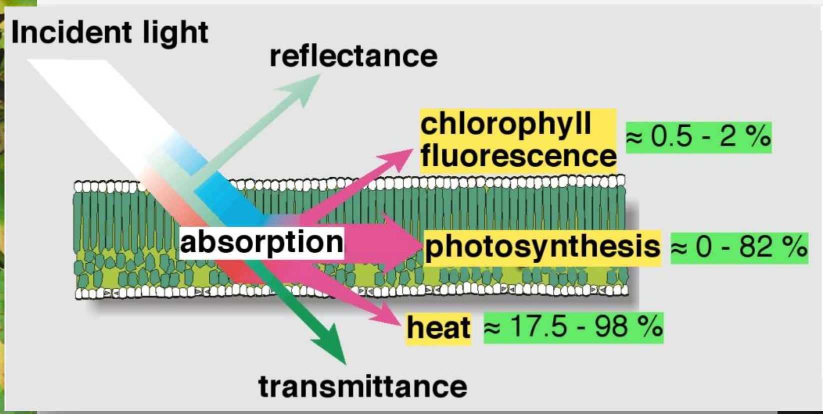


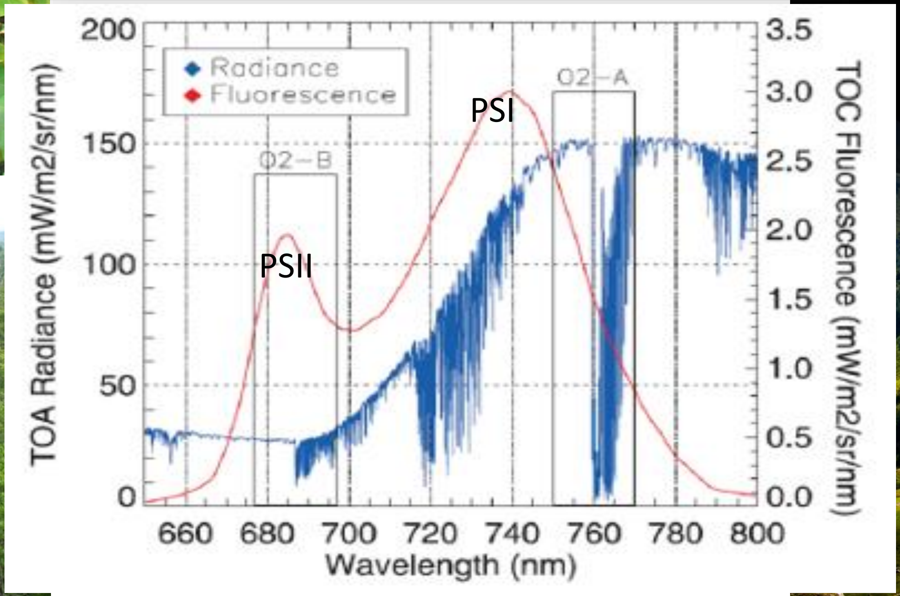


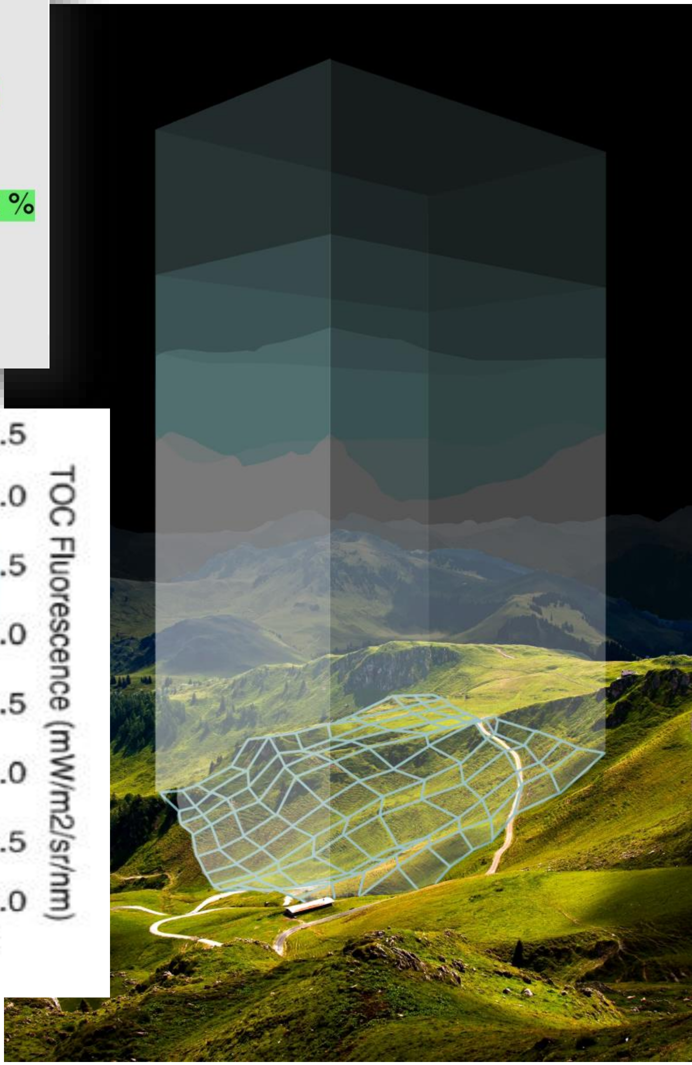
Sun-induced fluorescence from space

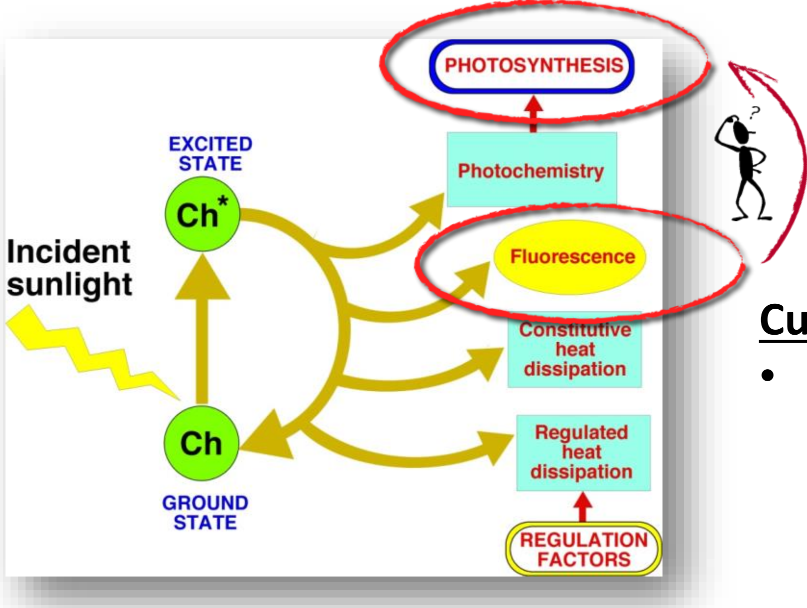












The challenge:

How to relate fluorescence to photosynthesis?

Current approach:

- **Top-down**: linking fluorescence (SIF) retrievals to photosynthesis (e.g. GPP) by means of a regression function.

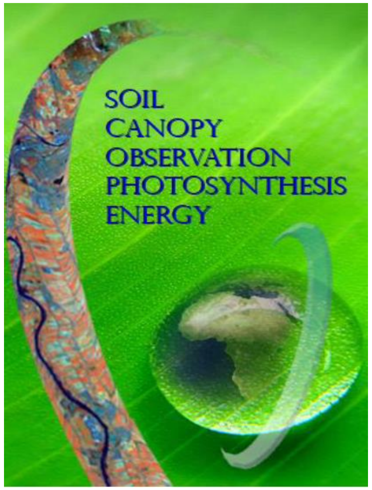
Limitations top-down approaches:

- Impact of varying biophysical variables not taken into account (**leaf, structure, micro-meteorology**).
- Current approaches use **only one SIF retrieval band, typically in second emission peak (PSI)**
- **Mostly linear regression** functions used

Towards improved understanding of canopy-leaving SIF – photosynthesis dynamics:

- The impact of photochemistry/leaf/canopy/micro-meteorology variables on SIF: **A global sensitivity analysis (GSA)**
- The predictive ability of the full SIF profile towards **net photosynthesis of the canopy (NPC): regression analysis (SIF-NPC)**

A modelling study



SCOPE (C. van der Tol & W. Verhoef)

- **SCOPE** (**Soil-Canopy-Observation of Photosynthesis and the Energy Balance**) is a **energy-balance RTM.**
- SCOPE enables to evaluate effects of observation geometry, vegetation structure, leaf physiology and climate on RS observations (**optical, thermal, and chlorophyll fluorescence**).

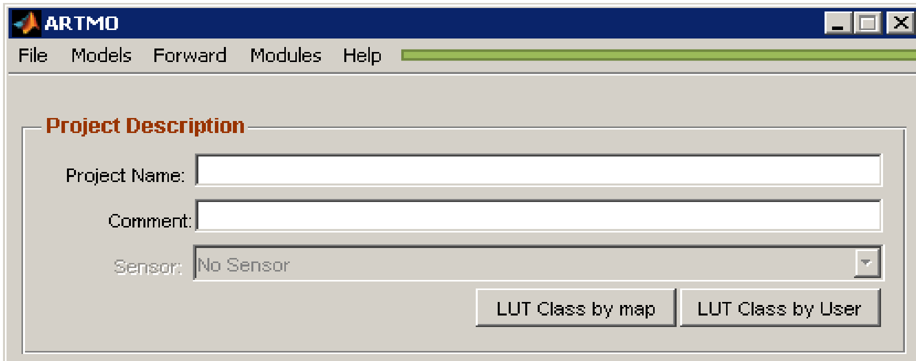
As part of esa **FLEX Photosynthesis Study (PS)**, SCOPE underwent various improvements (from v1.34 to **v1.53** and currently v. 1.60):

- Leaf optical model **FLUSPECT** to calculate **the irradiance to fluorescence conversion matrices**.
- **Separate fluorescence spectra for PSI and PSII**. **Hemispherically integrated fluorescence** added as output.
- Coupling with **MODTRAN output files**.
- Biochemistry sub-models:
  1. **Empirical** calibration of Pulse Amplitude Modulation (PAM) to the relative light saturation of photosynthesis as measured with gas exchange measurements and modeled with under typical diurnal conditions (referred to as the **TB12 model**) and during drought (referred to as **TB12-D**). (C. Van der Tol & J. Berry)
  2. **Mechanistic photosynthesis and fluorescence model** according to Von Caemmerer (2000) and developments by F. Magnani (2014) , referred as **MD12** model.

A GUI toolbox has been developed for intuitive and automated running and visualizing of simulations: A-SCOPE

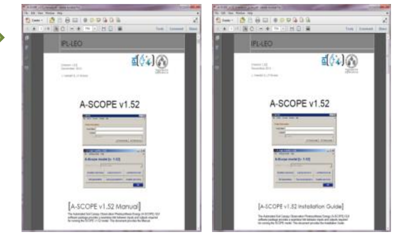
A-SCOPE v1.53

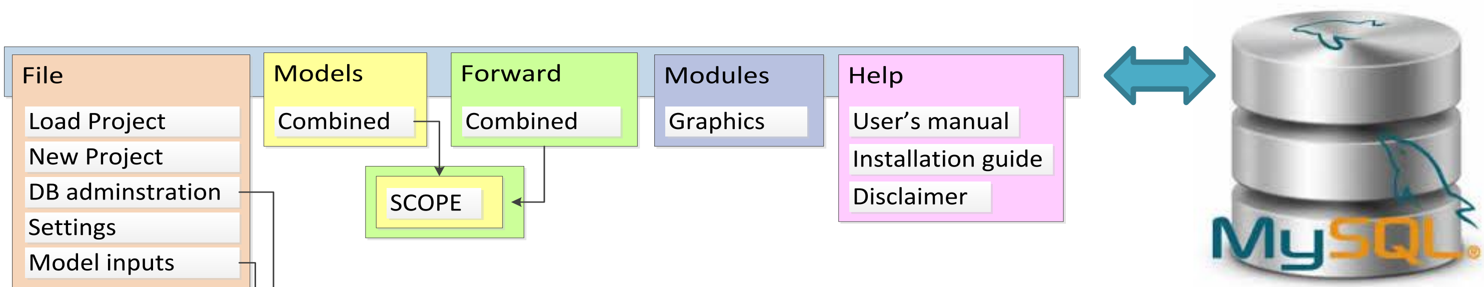
A scientific GUI toolbox encompassing SCOPE v1.53 and processing tools

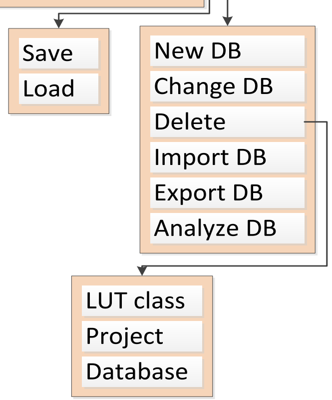


manual

Installation guide

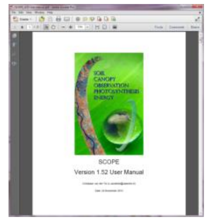


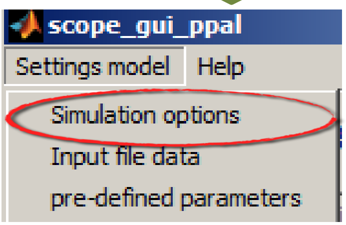


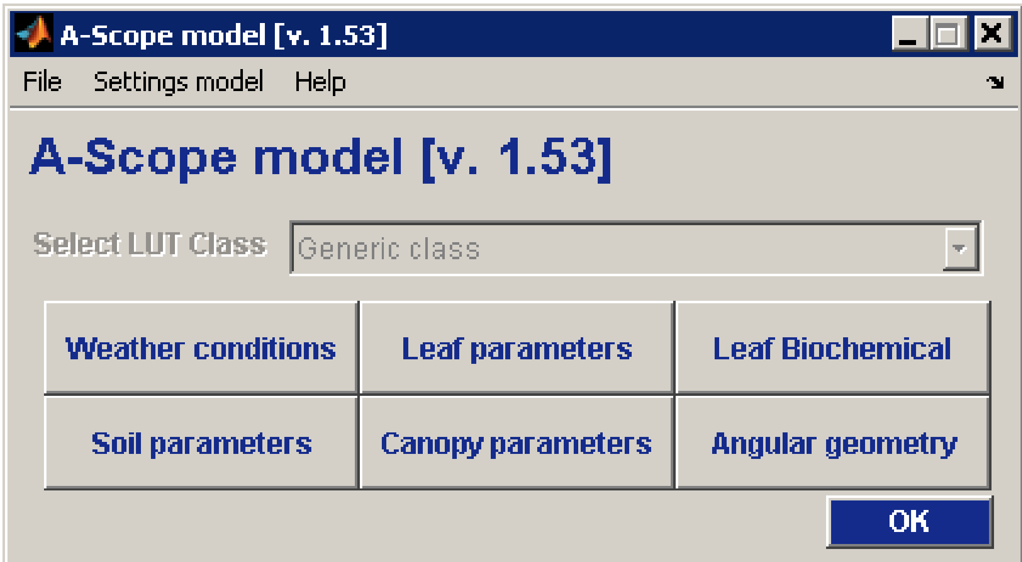


- **The running of SCOPE largely automated through interfaces.**
- **Enables to generate a large amount of simulations**
- **Input, output and metadata stored in MySQL running underneath.**
- **Outputs can be visualized and exported.**

A-SCOPE main module







Most important module is "**Leaf Biochemical**". This module is dynamic depending on the selected model in:

Settings → Simulation options:

- **TB12-drought (TB12-D)**
- **TB12**

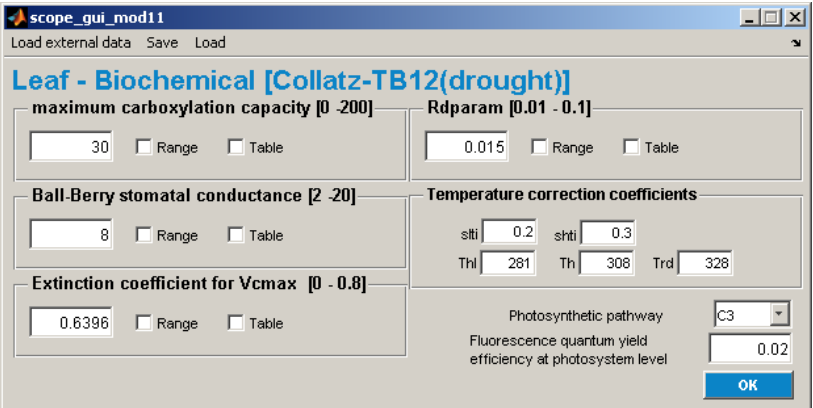
empirical

- **MD12**

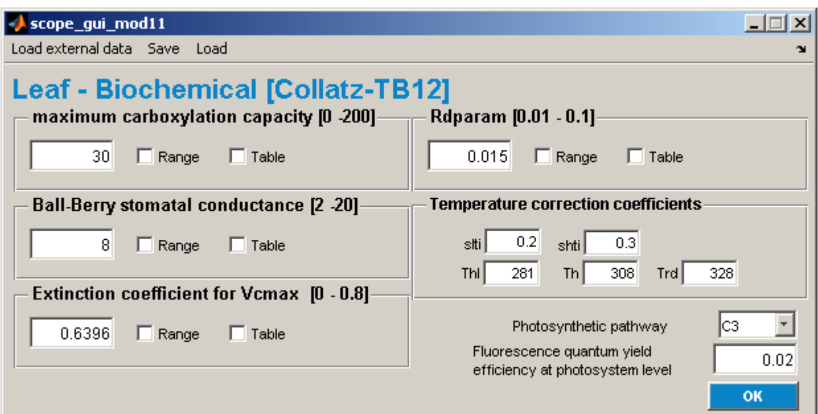
mechanistic

3 Biochemical models implemented

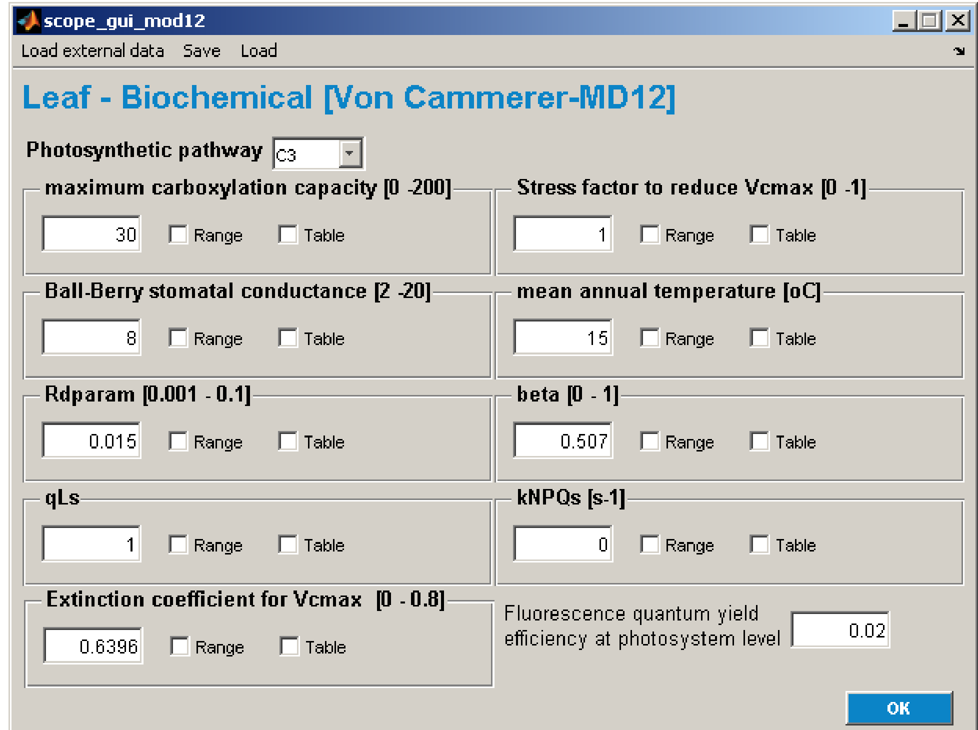
Collatz-TB12-D (drought) - *empirical*



Collatz-TB12) - *empirical*



Von Caemmerer-MD12) - *mechanistic*

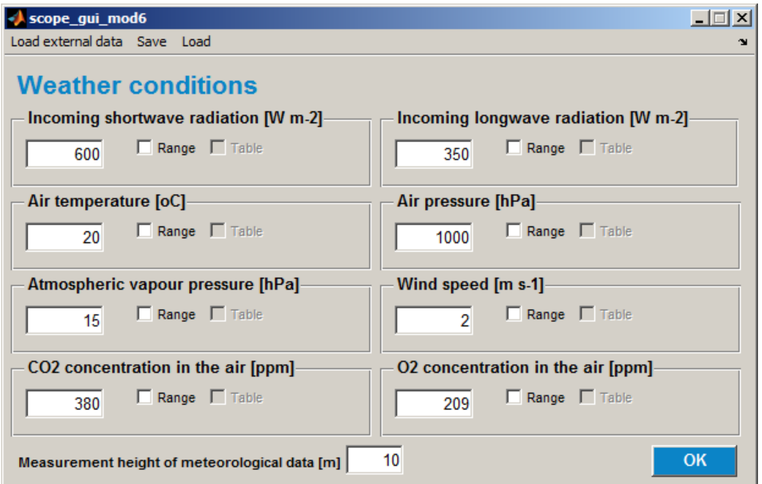


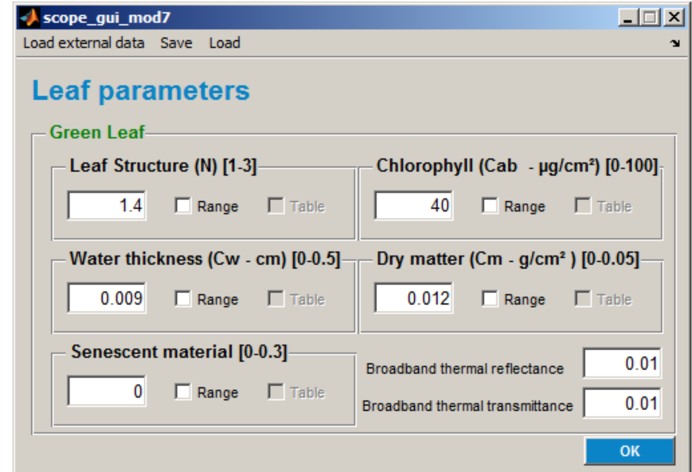
- **V_{cmo}: maximum carboxylation capacity: indicator of photothetic capcity**

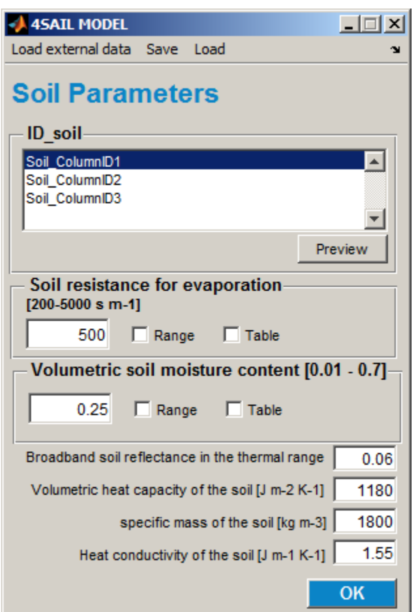
MD12 (Porcar-Castell, 2011):

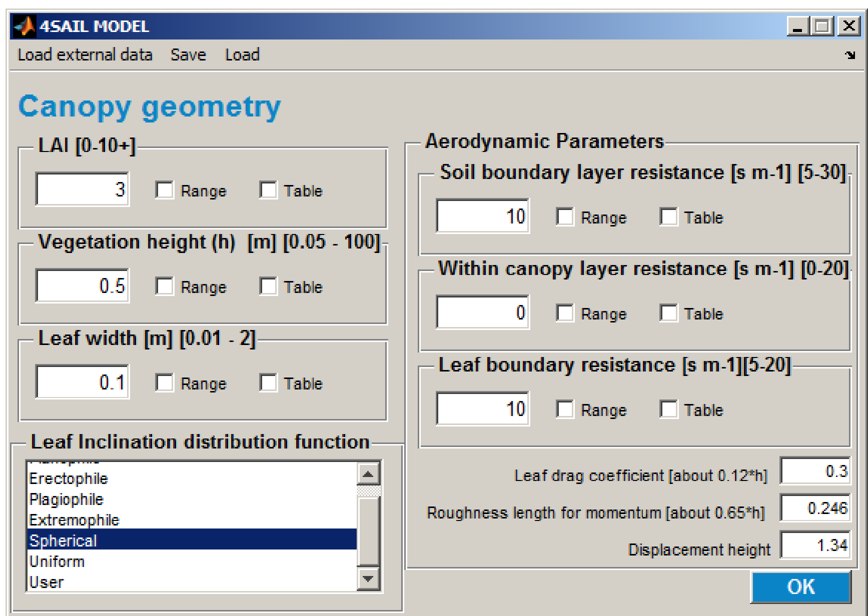
- **qLs: fraction of functional reaction centres**
- **kNPQs: rate constant of non-photochemical quenching**

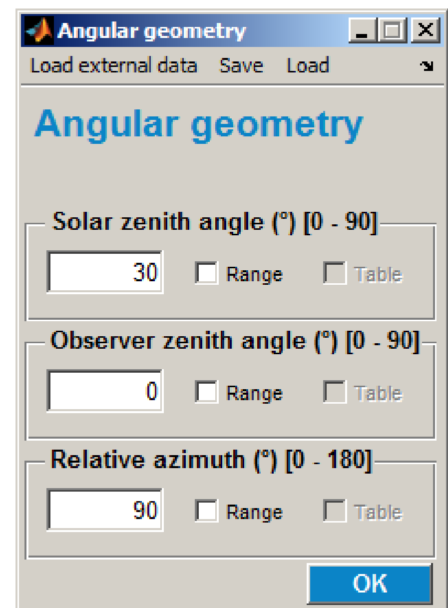
A-SCOPE v1.53 modules



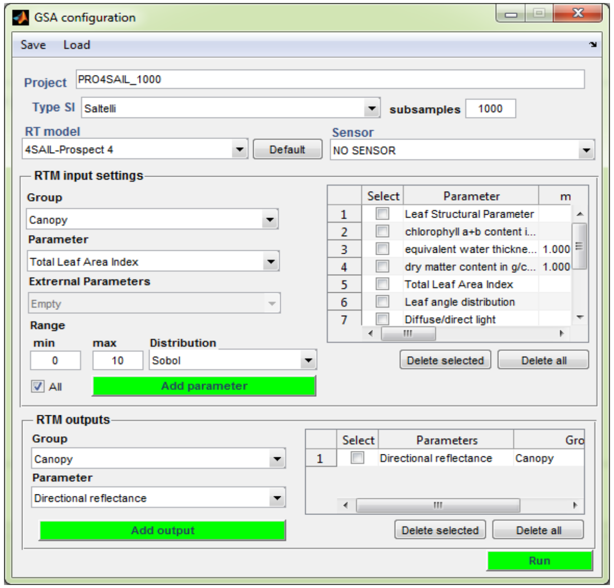








Global sensitivity analysis (GSA) toolbox



GSA Saltelli et al., 2010:

• ***First*** **order sensitivity**:

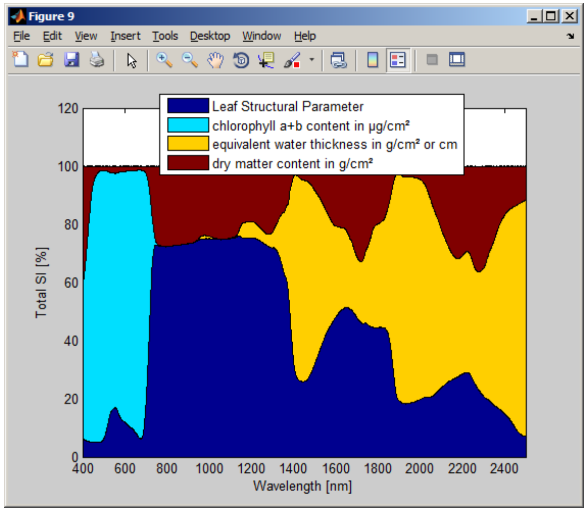
$$S_i = \frac{\frac{1}{n}\sum_{j=1}^{n} f(B)_j \left(f\left(A_B^i\right)_j - f(A)_j \right)}{\mathrm{Var}(L)}$$

• ***Total*** **sensitivitiy**:

$$S_{Ti} = \frac{\frac{1}{2n}\sum_{j=1}^{n} \left(f(A)_j - f\left(A_B^i\right)_j \right)^2}{\mathrm{Var}(L)}$$

PROSPECT-4 validity check

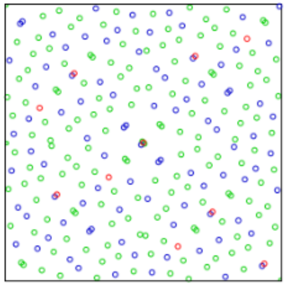
S_{TI} - normalized



GSA delivers consistent analysis. ☺

Sample distribution:

Sobol quasi-random sampling sequence (LPTAU)

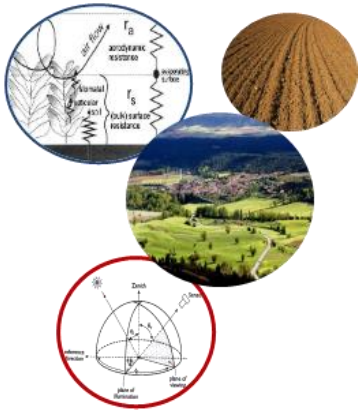


Total # of samples= ($N_{variabls}$ +2)*#sample distribution

Saltelli, A., Annoni, P., 2010, How to avoid a perfunctory sensitivity analysis, *Environmental Modeling and Software,* **25**, 1508-1517.

GSA SCOPE experimental setup:

1. <u>**Vegetation SCOPE GSA**</u> study: **varying only vegetation SCOPE variables (biochemical, leaf optical, canopy)**



2. <u>**Full SCOPE GSA**</u> study: **Varying all SCOPE variables (vegetation, soil, micrometeorological, aerodynamic)**

<u>Setup:</u>

- **2000** samples per variable according to Sobol' quasi-random sampling technique.
- Only normalized $\boldsymbol{S_{Ti}}$ shown (expressed as %).

SCOPE input variables & boundaries

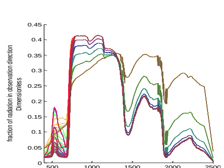
Vegetation only

Variable	Interpretation	Unit	min	max	default
Leaf optical					
N	Mesophyll Structural parameter in Prospect	[–]	1	2.5	1.4
Cw	Water content in Prospect	g/cm^2	0	0.1	0.009
Cdm	Dry matter content in Prospect	g/cm^2	0	0.05	0.012
Cs	Senescence factor Prospect	[–]	0	0.9	0
Cab	Chlorophyll content in Prospect	μg/cm2	0	80	40
Leaf biochemical					
m	Ball-Berry stomatal conductance parameter	[–]	2	20	8
kV	extinction coefficient for Vcmo in the vertical		0	0.8	0.64
Rdparam	Respiration = Rdparam*Vcmo		0.001	0.03	0.015
Vcmo	maximum carboxylation capacity		0	200	30
Leaf biochemical (MD12 only)					
Tyear	mean annual temperature	ºC	8	20	15
beta	fraction of photons partitioned to PSII		0	1	0.507
stressfactor	optional input: stress factor to reduce Vcmo		0	1	1
kNPQs	rate constant of sustained thermal dissipation		0	10	0
qLs	fraction of functional reaction centres		0	1	1
Canopy					
lw	Leaf width	m	0.01	0.1	0.1
LIDFa	LIDF parameter a, which controls the average leaf slope	[–]	– 1	1	-0.35
LIDFb	LIDF parameter b, which controls the distribution's bimodality	[–]	– 1	1	-0.15
LAI	Leaf area index	m^2m^2	0	7	3
hc	Canopy height	m	0.1	2	1

All SCOPE

Variable	Interpretation	Unit	min	max	default
Soil parameters					
rss	Soil resistance for evaporation	[200-5000 s m -1]	200	5000	500
SMC	Volumetric soil moisture content	[0.01-0.7]	0.01	0.7	0.25
Aerodynamic					
rbs	Soil boundary layer resistance	s m-1	5	30	10
rwc	Within canopy layer resistance	s m-1	0	20	0
rb	Leaf boundary resistance	S m-1	5	20	10
micrometeorologic					
p	Air pressure	[hPa]	300	1090	970
u	Wind speed	[m s-1]	0	50	2
Oa	O_2 concentration in the air	[ppm]	0	220	209
ea	Atmospheric vapour pressure	[hPa]	0	150	15
Ca	CO_2 concentration in the air	[ppm]	50	1000	380
Ta	Air temperature	[ºC]	-10	50	20
Rin	Incoming shortwave radiation	[W m-2]	0	1400	600
Rli	Incoming longwave radiation	[W m-2]	0	400	300
Geometry					
VZA	Viewing zenith angle	degree	0	10	0
RAA	Relative azimuth angle	degree	0	180	0
SZA	Sun zenith angle	degree	0	60	30

Outputs: *R*



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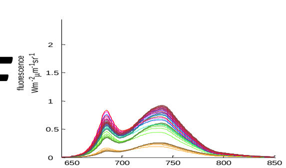
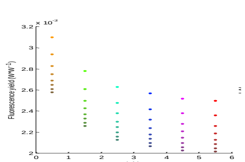
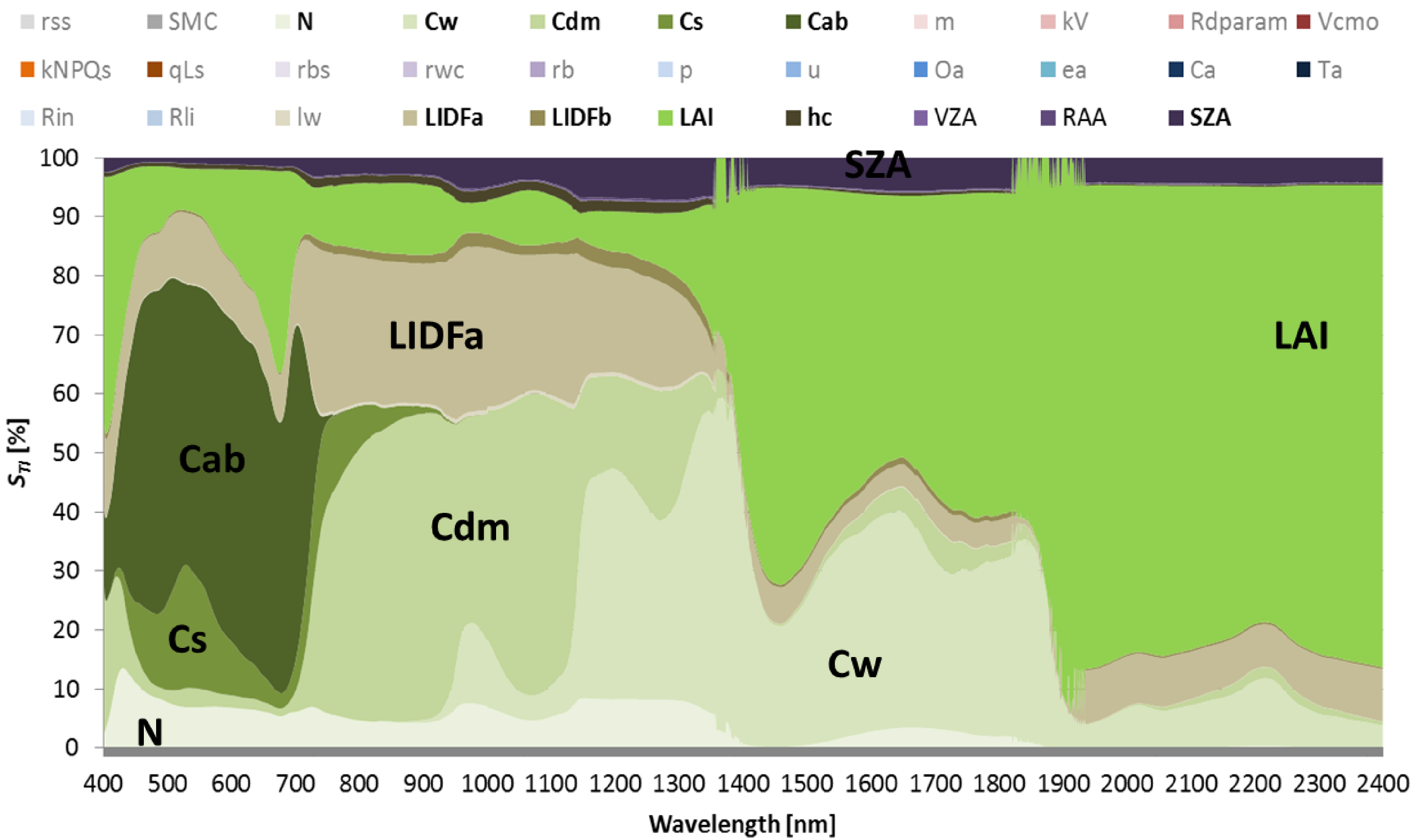


F products



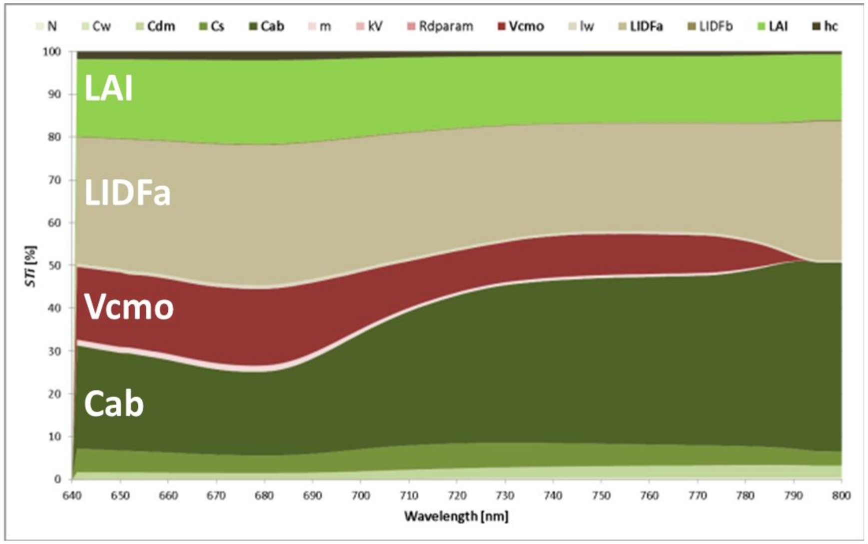
PROOF of concept GSA SCOPE: Reflectance



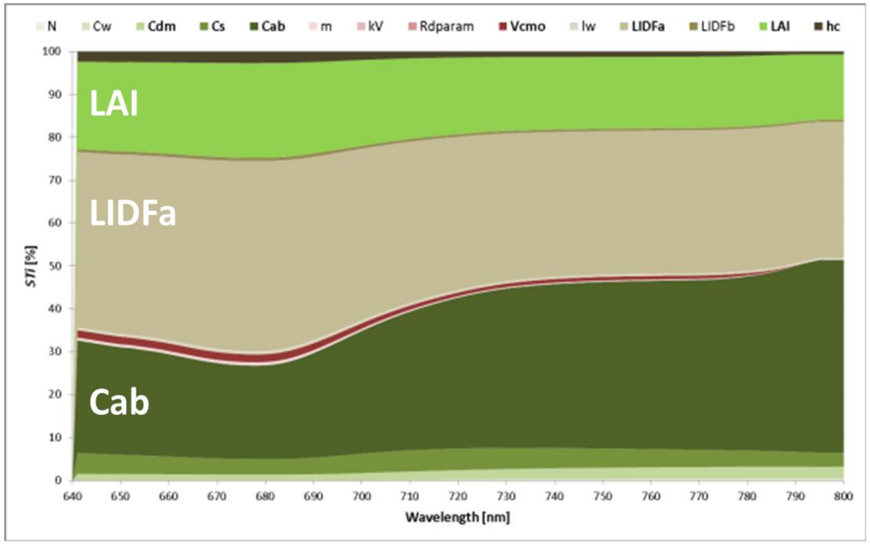
Reflectance results are consistent with PROSAIL and shows consistency of GSA analysis

GSA fluorescence: SCOPE vegetation for different biochemical models

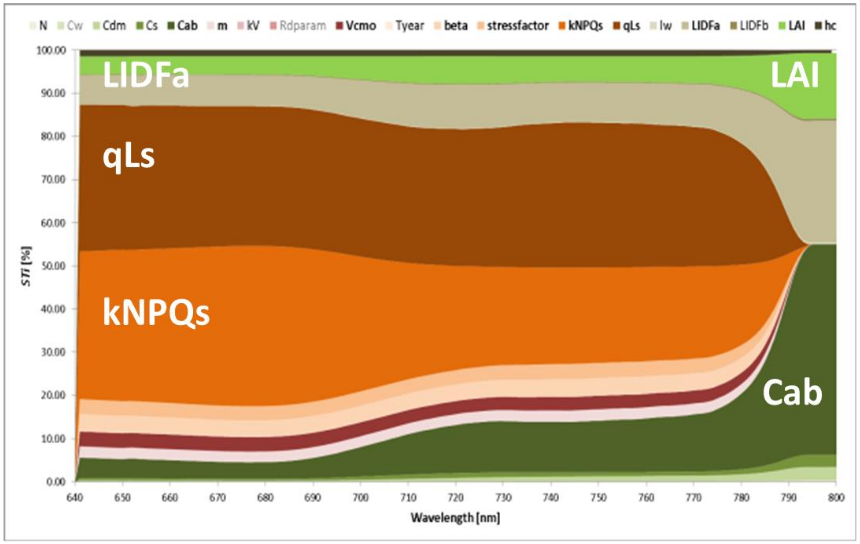
TB12-D



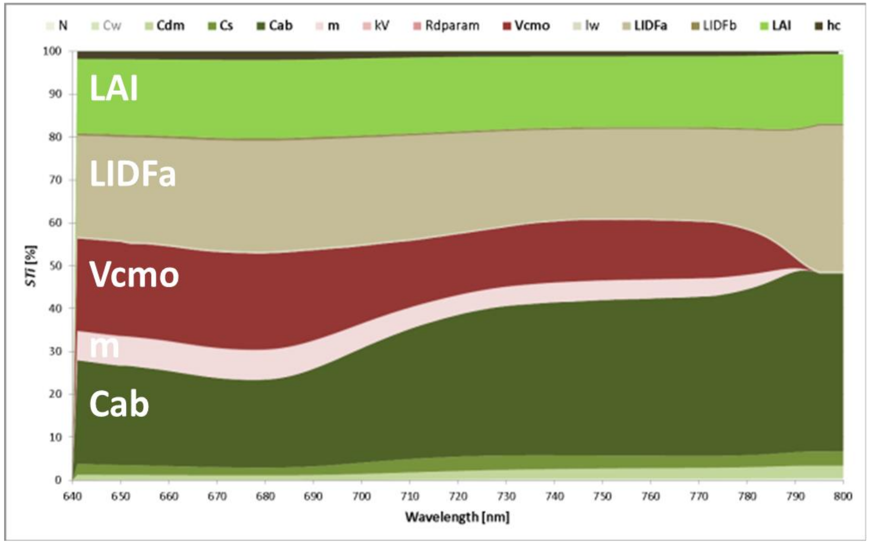
TB12



MD12

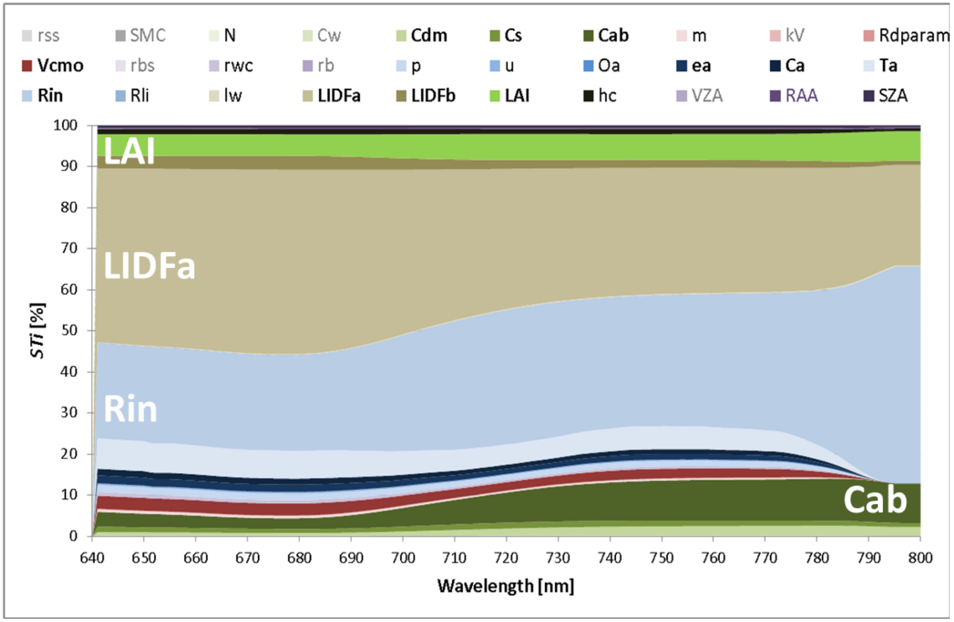


MD12 without MD12-specific vars

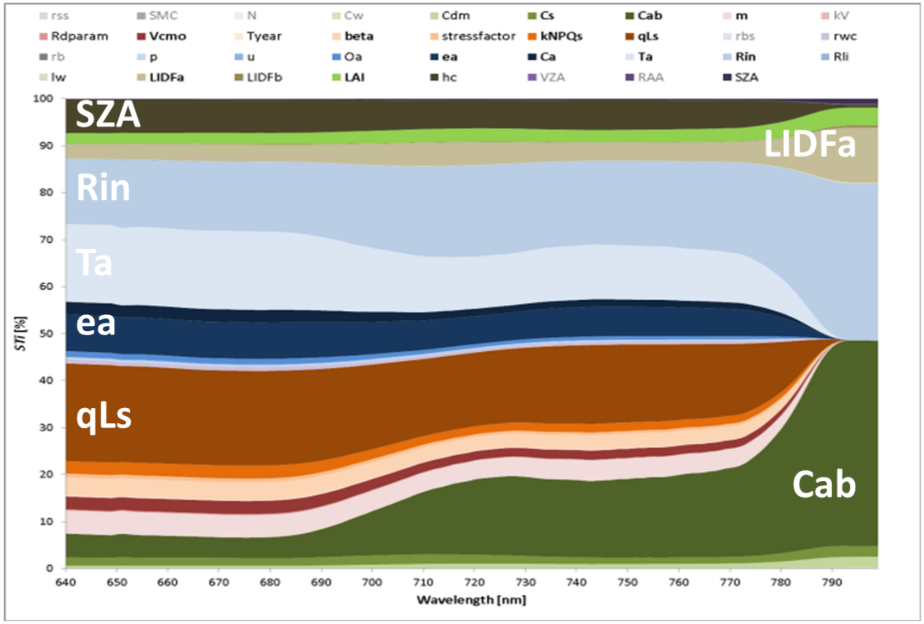


GSA fluorescence: all SCOPE variables

TB12-D



MD12



- **Essentially the same patterns as with vegetation variables only were revealed**, but these variables are **now suppressed due to the added influence of driving micrometeorological variables**.
- **V_{cmo}** contributed about ~**2.1%** to the full SIF signal, with slightly more relevance in the first peak than in the second.
- Results suggest that **in heterogeneous conditions over 97% of the canopy SIF variability is not due to variations in the photosynthetic machinery (V_{cmo})**, it is due to **leaf, canopy and micrometeorological effects** and their interactions.

Implications for SIF interpretation

- **More information directly related to photosynthesis (V_{cmo}) is to be found within the first emission peak (SIF_{red}).**

- Variations in **leaf chlorophyll content**, **vegetation structural** and **micrometeorological variables are mostly driving canopy-leaving SIF variability**, and so govern its spatial patterns. **Unbiased SIF interpretation towards photosynthesis can only be achieved by quantifying these variables.**

Having identified the driving variables, the question now is:

How strongly can canopy-leaving SIF be related to net photosynthesis of the canopy (NPC, also related to GPP)?

Requires a multi-scale regression analysis.

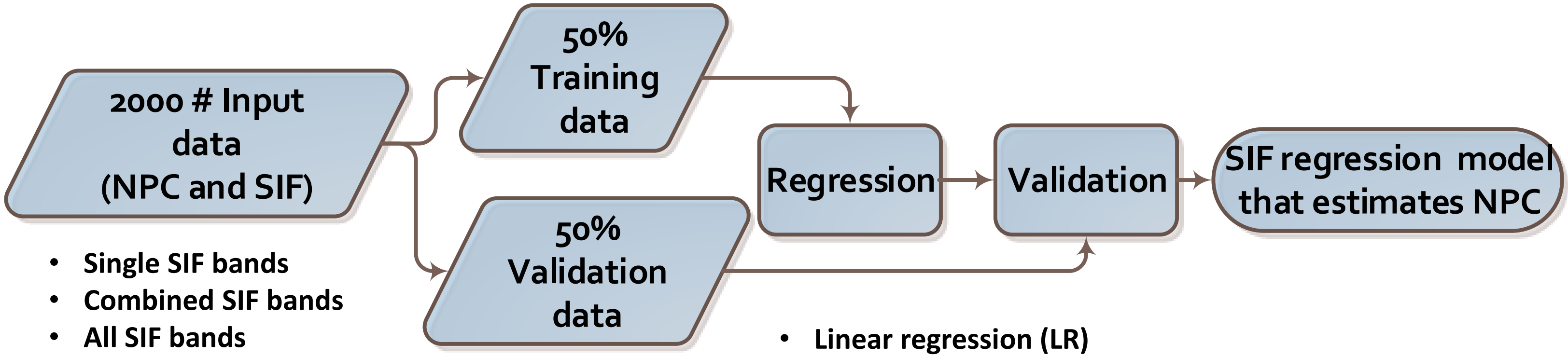
II: Exploiting the fluorescence signal towards "Net photosynthesis of the canopy" (NPC)

- **SCOPE modelling study on NPC retrieval strategies based on fluorescence data.** *(Reflectance data did not lead to any meaningful relationship)*

Objective:

- **To relate Fluorescence data (single bands, combined bands) to output NPC**

Regression problem with multiple SIF inputs and NPC as output. We have tested both linear and nonlinear regression algorithms



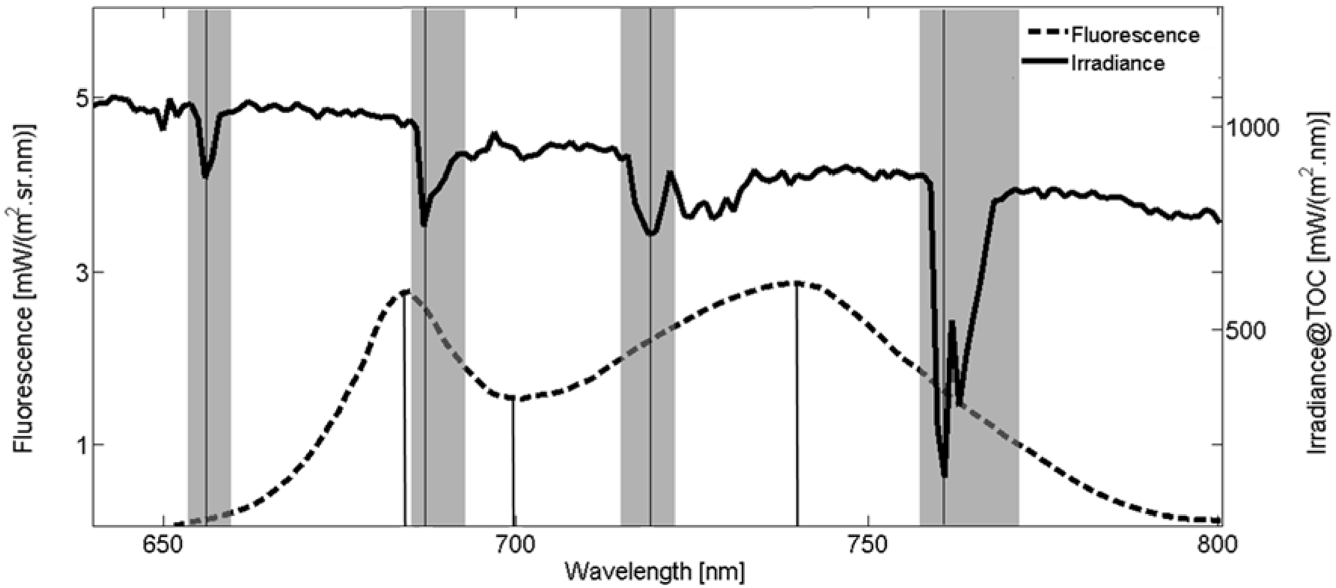
- Single SIF bands
- Combined SIF bands
- All SIF bands

- NPC

- Linear regression (LR)
- (nonlinear) Gaussian processes regression (GPR)

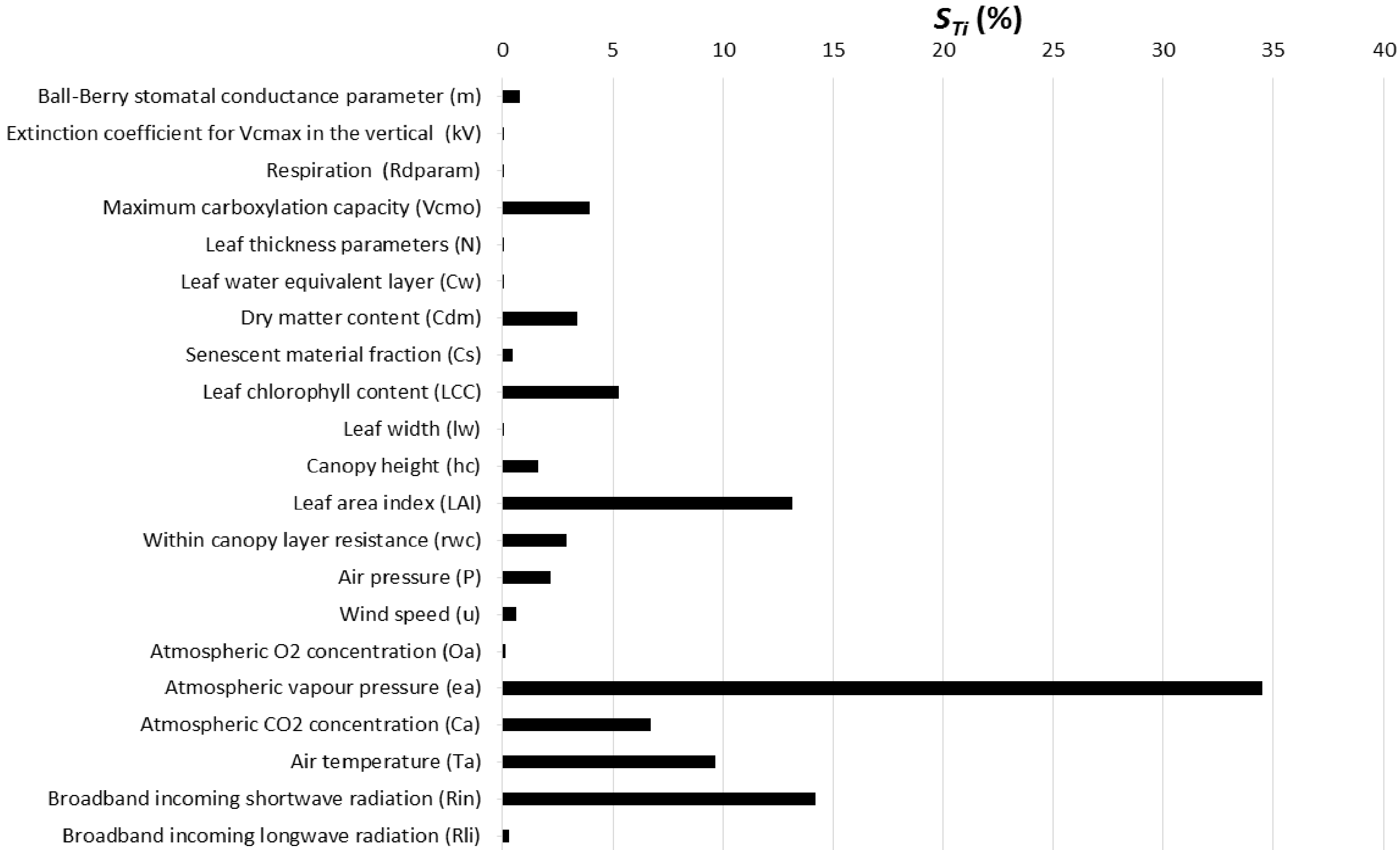
Sampling the broadband fluorescence signal

Important (absorption) wavelengths fluorescence retrieval:



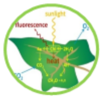
	Central Wavelength (nm)	Spectral range (nm) absorption lines
Hα absorption line	656	653-662
Red peak (attributed to SIF emission of PS II)	684	
O_2(-B) absorption line	687	683-692
Valley between red and NIR peaks	699	
Water vapor (Wv) absorption line	719	714-722
NIR peak (attributed to SIF emission of PS I and to a lesser extent PSII)	736	
O_2(-A) absorption line	761	757-771

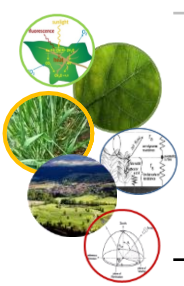
Driving SCOPE variables of F_{total} (integral of SIF 640 – 850 nm) as identified by GSA (S_{TI})
(without geometry, LAD).



12 driving variables explain 97.5 % of total variability (with interactions).

Retrieval strategies (#2000 sim. each)

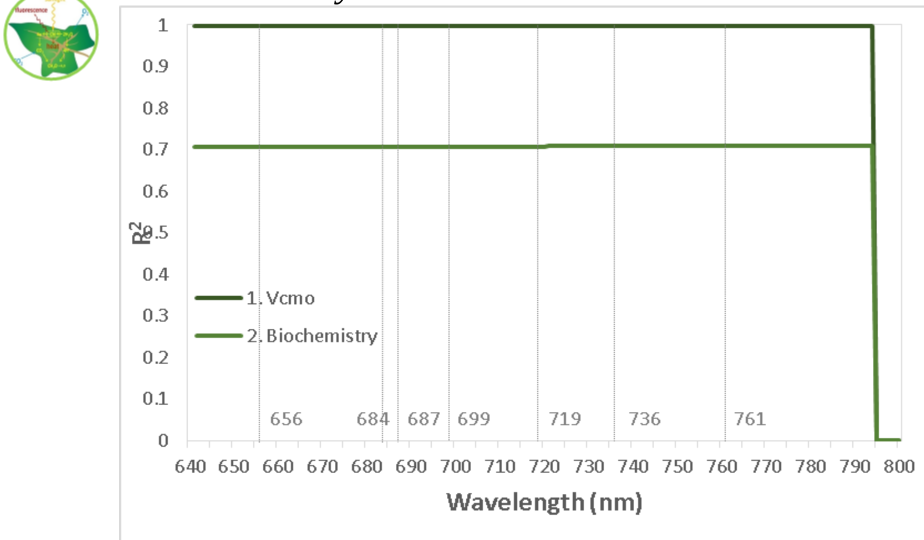


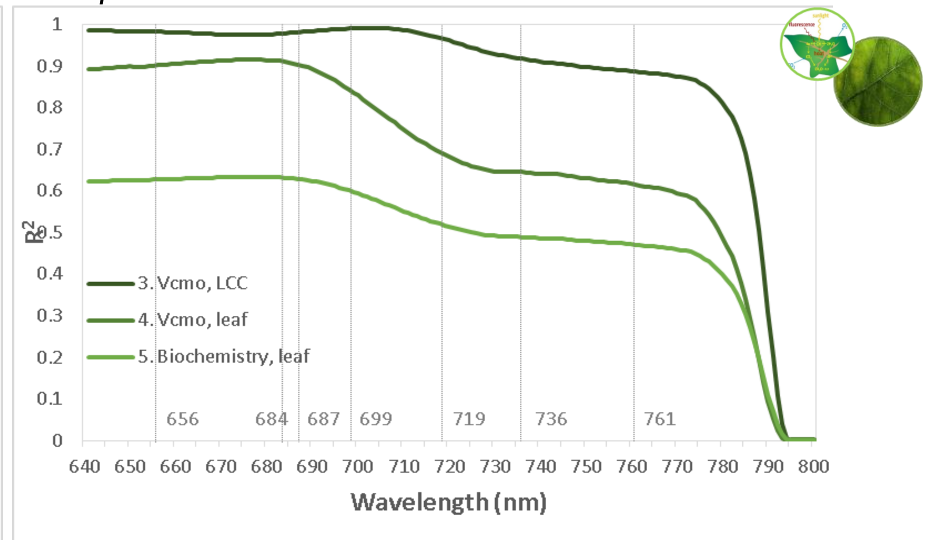
	Ranging variables	Justification
Biochemistry		
1	Vcmo	**Vcmo is the main biochemical driver of photosynthesis**. Hence, this is the theoretical baseline when SIF is not influenced by any other variable.
2	Biochemistry	**All biochemical variables** (Vcmo, m, Rdparam, kV). Represents the most heterogeneous situation at the biochemical scale.
Biochemistry, leaf		
3	Vcmo, LCC	**Driving biochemical and leaf variables**.
4	Vcmo, leaf	**Driving biochemical variable and all leaf variables** (N, Cw, Cdm, Cs, LCC).
5	Biochemistry, leaf	**All biochemical and leaf variables.** Represents the most heterogeneous situation at biochemical and leaf scales (Vcmo, m, Rdparam, kV, N, Cw, Cdm, Cs, LCC).
Biochemistry, leaf , canopy		
6	LCC, LAI	**Driving leaf and canopy variables.**
7	Vcmo, LAI	**Driving biochemical variable (Vcmo) with driving canopy variable (LAI)**
8	Vcmo, canopy	**Driving biochemical variable (Vcmo) with all varying canopy variables** (LAI, lw, hc).
9	Vcmo, N, Cw, Cdm, Cs, Cab, LAI, hw, hc (spherical LIDF)	**Driving biochemical variable (Vcmo) with all leaf and all canopy** (N, Cw, Cdm, Cs, Cab, LAI, lw, hc).
10	Biochemistry, leaf, canopy	**Al biochemical, leaf and canopy variables** (Vcmo, m, Rdparam, kV, N, Cw, Cdm, Cs, LCC, LAI, lw, hc). Represents the most heterogeneous situation at the canopy scale.
All biochemistry, leaf , canopy, geometry, micrometeorology		
11	**Key SCOPE variables driving SIF**	Vcmo, Cdm, LCC, LAI, hc, rwc, P, ea, Ca, Ta, Rin. **These variables and their interactions explain 97.5% of the variability in F_{total}.**
12	**All SCOPE variables**	All SCOPE variables (Vcmo, m, Rdparam, kV, N, Cw, Cdm, Cs, LCC, LAI, lw, hc, VZA, RAA, SZA, rwc, rb, P, u, Oa, ea, Ca, Ta, Rin, Rli). **Represents the most heterogeneous configuration.**

Results: R^2 validation SIF -NPC

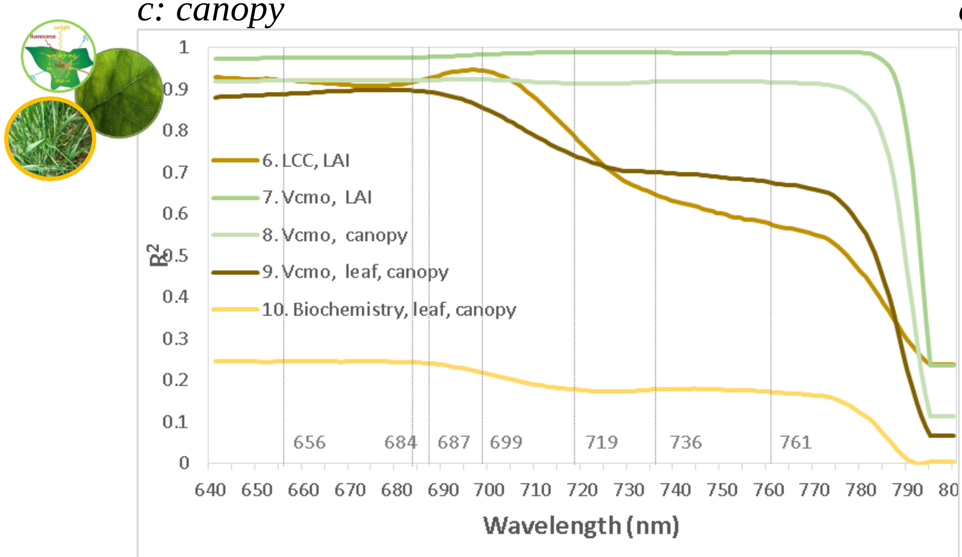
a: biochemistry



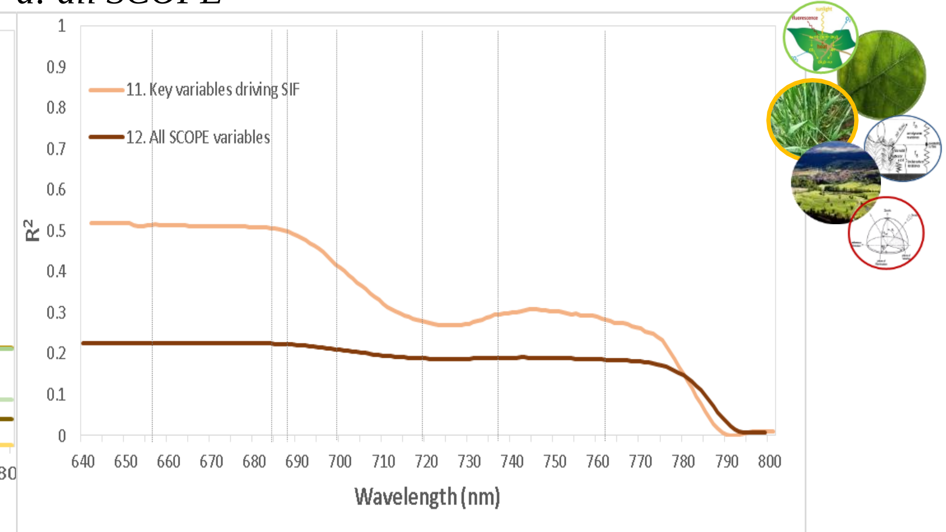
b: leaf

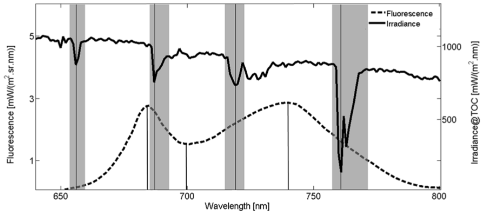


c: canopy

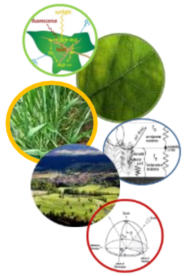


d: all SCOPE





NPC estimation by single bands



Most realistic situation: varying multiple variables at bi**ochemistry, leaf, canopy & micrometeorology** scale.

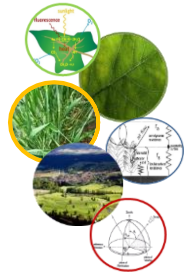
	R^2								
	656	**684**	**687**	**699**	**719**	**737**	**761**	**Best λ**	**R^2**
Vcmo, leaf, canopy	0.89	**0.90**	0.89	0.85	0.74	0.70	0.67	**678**	**0.90**
Biochemistry, leaf, canopy	**0.25**	0.24	0.24	0.22	0.18	0.18	0.17	**650**	**0.25**
Key SIF variables	**0.52**	0.50	0.50	0.41	0.28	0.30	0.28	**650**	**0.52**
All SCOPE variables	**0.23**	**0.23**	0.22	0.21	0.19	0.19	0.19	**650**	**0.23**

- **Rather poor results when relying on only one SIF wavelength in heterogeneous canopies.**

- **Most sensitive SIF bands related to NPC to be found <u>within first peak</u>.**
- **This because:**
  - **SIF_{Ned} reabsorbtion, thus, what leaves the canopy less affected by scattering.**
  - **SIF_{NIR} no reabsorption, more affected by leaf and canopy scattering effects.**

See also Van Wittenberghe et al., 2015; RSE

NPC estimation by multiple SIF bands



Combined wavelengths	Wavelengths (nm)
O2-B and O2-A	687, 761
Hα, O2-B, O2-A and water vapor (Wv)	656, 687, 719, 761
Two SIF emission peaks	684, 736
Peak ratio	684/736
Two SIF emission peaks and middle valley	684, 699, 736
F_{total}	Integrated SIF (from 640 to 850nm)
F_{all}	All individual SIF wavelengths (from 641 to 800)

Linear regression:

	O_2-B, O_2-A	Ha, O_2-B, Wv, O_2-A	Two peaks	Peak ratio	Two peaks and valley	F_{total}	F_{all}
Vcmo, leaf, canopy	0.90	**0.92**	0.90	0.43	0.91	0.72	**0.92**
Biochemistry, leaf, canopy	0.23	**0.27**	0.23	0.10	**0.27**	0.13	**0.28**
Key SIF variables	0.52	0.53	0.52	0.24	**0.54**	0.32	**0.54**
All SCOPE variables	0.22	0.22	0.22	0.14	**0.23**	0.19	0.22

(Nonlinear) Gaussian processes regression (GPR):

	O_2-B, O_2-A	Ha, O_2-B, Wv, O_2-A	Two peaks	Peak ratio	Two peaks and valley	F_{total}	F_{all}
Vcmo, leaf, canopy	0.92	**0.93**	0.92	0.56	0.92	0.73	**0.93**
Biochemistry, leaf, canopy	0.32	0.35	0.32	0.18	**0.36**	0.19	0.34
Key SIF variables	0.81	**0.82**	0.82	0.37	0.82	0.72	**0.82**
All SCOPE variables	0.30	**0.31**	0.30	0.14	0.30	0.24	**0.31**

- **Combining multiple SIF retrieval bands** lead to improved **predictive power** as compared so single bands.
- Moving away **from linear to nonlinear regression** further improved predictive power, particularly when considering all SCOPE key variables.
- When not having SIF retrieved at many bands, **using SIF retrievals at both O_2-B & O_2-A suffice**.

Conclusions:

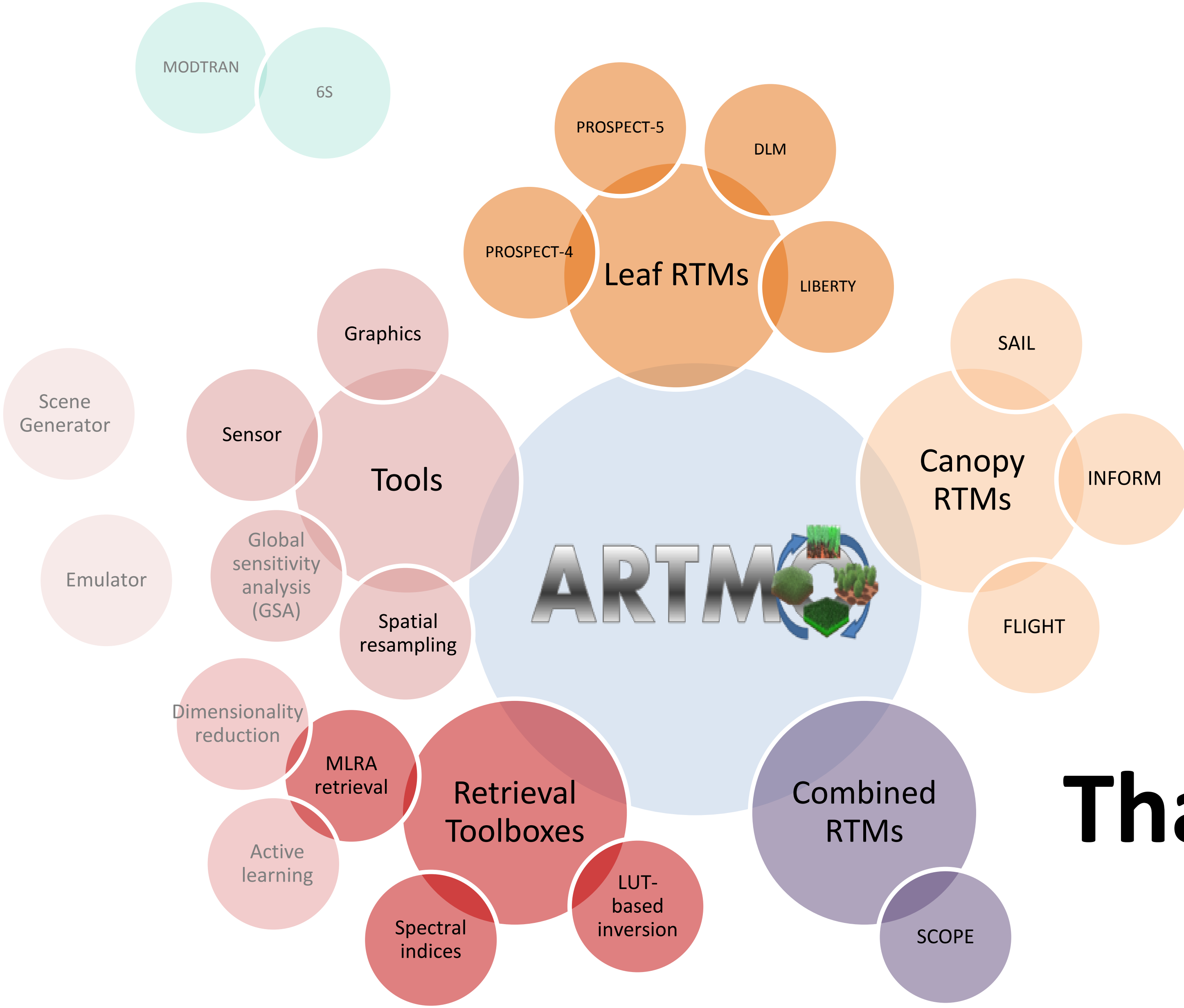
SCOPE v. 1.53 modeling studies were conducted to gain insight in fluorescence – photosynthesis relationships.

1. **Global Sensitivity Analysis (GSA):**

   - **V_{cmo} drives only for a relatively small portion the fluorescence signal. Key driving variables (LAI, Chl, Rin) need to be taken into account in order to realize unbiased interpretations of SIF.**

2. **Relating SIF to photosynthesis (NPC):**

   - **Most sensitive SIF bands to NPC** were located **around the first emission peak** for heterogeneous canopy configurations.
   - **Combining two SIF retrieval bands (e.g., O2-B and O2-A) led to stronger correlations than using only one SIF band.** Even stronger correlations were achieved using four main SIF retrieval bands (Hα, O2-B, water vapor, O2-A)
   - Using a **nonlinear regression** algorithm (GPR) can further increase predictive power.



Thanks

http://ipl.uv.es/artmo/