2012 FLEX/Sentinel-3 Tandem Mission Photosynthesis Study

EXECUTIVE SUMMARY

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Background

Chlorophyll fluorescence (CF) is a natural spectral emission resulting from the interaction of plant chlorophyll pigment with visible light (typically 400-700 nm). In photosynthesizing tissues, red and far-red light can be emitted from any chlorophyll-containing plant tissues which are exposed to light: primarily foliage, but also green stems, green exposed roots, floral structures, many fruits, and green seeds. This emission of chlorophyll fluorescence caused by sunlight is termed 'solar-induced' or 'sun-induced' fluorescence (SIF), and its measurement technique is deemed to be passive as no artificial excitation light is used to induce the fluorescence.

The capacity to observe SIF presents a totally novel option for space-based remote sensing: extracting information on the actual workings of the photosynthetic machinery of plant canopies. Because the production of chlorophyll fluorescence is related to the function of the two photosystems responsible for photosynthetic initiation in green plants, it provides a glimpse into the dynamics of the photosynthetic process itself, an insight not available from existing methodologies involving the usual vegetation reflectance indices.

Momentum is building within the scientific community to apply SIF to quantify terrestrial vegetation photosynthesis – including for the modelling of gross primary productivity (GPP). A second major application area is in detection of stress effects, especially before visual damage is apparent. Stress applications do not necessarily require quantification of photosynthetic rates or GPP, but instead may be able to utilize simple SIF indices.

Promising results in recent years from other investigators indicate that it is indeed possible to discriminate the subtle SIF signal from satellite platforms; however, existing satellite sensors are not optimized spatially or spectrally for SIF retrievals and applications. This presents a unique advantage for the FLuorescence EXplorer (FLEX), which is being designed specifically for the purpose of capture and usage of SIF from terrestrial vegetation. Key to that initiative is the development of methods to derive quantitative photosynthetic information from SIF.

Goals of the Photosynthesis Study

The Photosynthesis Study analysed the relationship between steady-state chlorophyll fluorescence and photosynthesis, and developed and tested a mechanistically-based model to derive photosynthesis from FLEX/Sentinel-3 Tandem Mission (FLEX/S3) measurements and auxiliary data. A secondary goal was to identify health & stress indicators from steady-state fluorescence features.

This dual focus allows full exploitation of the breadth of information potentially contained in the fluorescence signal from space.

Science tasks

The Photosynthesis Study was divided into four major tasks:

1. **Review of model availability and datasets: model/module assessment, comparison, and gap analysis.** A comprehensive review was conducted of available models linking photosynthesis and steady-state chlorophyll fluorescence. Sixty-five datasets were gathered into a database for model testing. Then based on performance results and suitability for the aims of the study, recommendations were made on the appropriate constitution of the consolidated model.
2. **Model implementation, validation, sensitivity analysis, and error quantification.** Software and documentation were produced for the model, which was then verified and validated for internal consistency and performance against field data. Sensitivity tests were performed to support model simplification, and error quantification was done for output variables versus uncertainties in input data.
3. **Algorithm development based on models.** Development of a Level-2 prototype algorithm was investigated to derive measures of photosynthesis from the FLEX/S3 tandem mission using this simplified approach.
4. **Fluorescence as an indicator of vegetation health and stress resilience.** A review was completed of SIF indicators for detection of water deficit, temperature extremes, and nitrogen insufficiency. Knowledge gaps were identified and prioritized, and a conceptual framework was formulated for SIF application in stress detection.

Model development

Because of the timeframe of the Study and the fact that previous studies have made progress in model development, the emphasis here was on utilizing existing models/modules, then integrating them into a consolidated program.

Evaluation of promising models/modules identified in the literature produced a shortlist of candidates which were tested for their capacity to link fluorescence and photosynthesis, and their suitability for the study’s goals.

Based on the findings of the model review and testing, the final consolidated model was designated to contain:

1. **for leaf biochemistry:** the MD12 model (developed by F. Magnani and colleagues) is an advanced model capturing fundamental processes in the leaf photosynthetic centres and containing routines for C3 and C4 vegetation, linking steady-state fluorescence and photosynthesis;
2. **for leaf radiative transfer:** the Fluspect optical model (developed by W. Verhoef) is a relatively simple model that operates efficiently and quickly due to its fast layer doubling algorithm;

3. **for canopy radiative transfer:** the SCOPE canopy model (developed by C. van der Tol and colleagues) links all modules in the chain and represents propagation of the fluorescence signals and fluxes to the top of the vegetation canopy.

The SCOPE model, first developed and published in 2009, was significantly updated here to its current version 1.53 – with new functionality, improved modularity, and up-to-date user documentation and manuals. Modules are usable individually or in combination, thus allowing for flexibility. (The model package also includes two leaf-level physiology modules that are empirically-calibrated and require fewer parameters than MD12.)

SCOPE v1.53 was automated in the PS Study to produce the Graphic User Interface A-SCOPE v1.53, which improves user-friendliness for aspects such as data input, storage, graphics and output management (Figure 1).

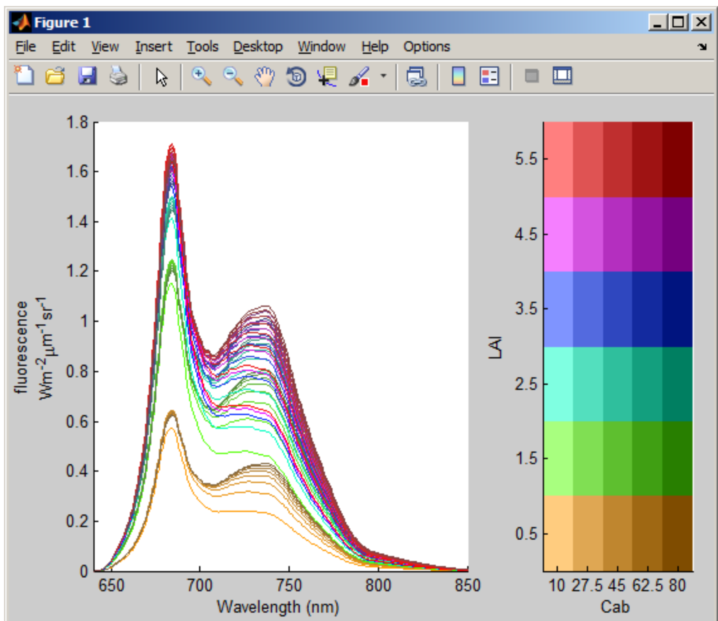

Figure 1. Example of Fluorescence graphic output from SCOPE/A-SCOPE, with color variations based on a broad range of two variables (Cab, LAI).

Model simplification and validation

SCOPE is a complex model with over 50 parameters, necessitating significant run times when all variables are in play. By identifying driving and non-driving parameters, the latter may be kept fixed (to default values) in most situations, thereby simplifying the model and increasing computational speed. Sensitivity analyses identified 10 to 12 core driving parameters for fluorescence and photosynthesis in the consolidated model (Table 1). Furthermore, if co-varying parameters are considered, the model can be streamlined even further. This does not mean that the full parameter matrix will not provide advantages in addressing diverse terrestrial vegetation canopies and conditions, hence, the full complement of variables is maintained at this time for greatest versatility.

Table 1. Major driving parameters of the SCOPE model for fluorescence and photosynthesis.

Driving parameters for fluorescence and photosynthesis	
• maximum carboxylation capacity	• leaf chlorophyll content
• Ball-Berry parameter ***m*** (stomatal conductance)	• dry matter content[1]
• **'Beta'** (fraction of photons partitioned to PSII)	• leaf area index
• rate of sustained non-photochemical quenching **kNPQs** (protection against high-light damage)	• incoming shortwave radiation
• fraction of functional reaction centres **qLs** (photodamage: a lower fraction=higher risk)	• air temperature
• **'stressfactor'**	• atmospheric vapour pressure (optional: C3 species only)

[1]Consistently important for fluorescence only.

The model was tested against field canopy data from a published study of winter wheat. In general, SCOPE was able to simulate canopy photosynthesis behaviour over the course of the day and with respect to the shape of the fluorescence emission. The model was able to simulate steady-state fluorescence especially in the O_2-A (far-red) band, but preliminary indications are that it may be overestimating fluorescence in the O_2-B (red) band. This will require further testing with additional datasets and fine-tuning of parameter settings and/or modules as appropriate.

Algorithms relating fluorescence and photosynthesis

Algorithm development based on the model was also investigated, including the possibility to deduce relatively simple relationships between SIF and GPP or net canopy photosynthesis (NPC). Model inversion work indicated that inclusion of fluorescence data resulted in substantive improvement in algorithm performance for the estimation of NPC. The two types of statistical algorithms – Gaussian processes regression (or GPR) and polynomial & rational functions fitting (or PRF) – gave highly accurate results for retrieval of canopy photosynthesis in the case of C3 plants, while with C4 plants excellent results were obtained using GPR (lower success with PRF). PRF using only simple optical data in a low number of channels was able to predict photosynthetic products (GPP, LUE, APARChl) for C3 plants in a non-stressed case with high performance; for C4 plants, only APARChl could be predicted with high accuracy. Both fluorescence bands were needed to predict GPP and LUE using PRF, meaning that the two bands do not carry the same information. Using GPR, although relationships were obtained using only the second emission peak F740, the most information apparently is contained within the first emission peak F685. An error threshold of 10% was already achievable with the F685 emission band in C3 species using GPR; including more bands, the whole fluorescence profile, and additional biophysical variables optimally yielded R^2 of 0.95 in C3 plants. In C4 plants, GPR required the full fluorescence profile to meet the error threshold. Neither reflectance data nor solely biophysical variables (Chl, LAI, *f*APAR) led to meaningful relationships with NPC. However, it is prudent to take chlorophyll content into account due to its effects on light absorption (which influences photosynthesis and fluorescence radiance positively) and reabsorption (which decreases fluorescence emission).

Although the models tested in this study were simple and used a limited number of variables, they proved their efficacy to predict photosynthetic products, at least in the absence of severe stress. Further investigations should be undertaken to test the robustness of the retrievals, preferentially with canopy SIF data such as that recently made available from the *HyPlant* airborne sensor, designed as an airborne prototype for FLORIS.

In the case of one-variable models, F760 surprisingly was found to be non-predictive for any products, regardless the plant type (C3, C4). This is in contrast with the previously reported high correlation between far-red fluorescence and GPP deduced from experimental data (Guanter *et al.* 2014; Berry *et al.* 2013; Frankenberg *et al.* 2011b; Rossini *et al.* 2010).

Stress detection

SIF was evaluated for use in detecting stress effects from water deficit, temperature extremes, and nitrogen deficiency. A random-effects meta-analysis identified clear benefits of the red and far-red fluorescence bands and the ratio of these bands for detection of stress-induced strain. Results of the meta-analysis were that:

- water deficit generally causes the red and far-red fluorescence at leaf and canopy levels to decrease;
- both types of temperature stresses cause the ratio of red to far-red fluorescence (stress to control ratio) to decrease;
- nitrogen deficit increases the red to far-red ratio.

Several novel fluorescence-based stress indices have been proposed here to assess stress intensity as well as stress quality in relation with water, temperature, and nitrogen stress. Further investigations and evaluations of these new stress indicators should be undertaken. These indicators are in addition to simple indices already known to be effective for identification of stress, most notably the ratio of red to far-red fluorescence (particularly expressed as a ratio of stressed:control values). The importance of normalizing SIF features was evident, which can be achieved through the use of control values as shown here, or, as others have shown, through the use of incident or absorbed PAR. Furthermore, with FLEX, the repeated measurements would create a change detection system whereby initial retrievals can serve as a baseline for comparison of subsequent retrievals. And finally, the photosynthesis model or its simplified formats – and the F-GPP algorithms developed in this study – provide even further choices for stress indices based on ratios of actual to potential photosynthesis.

Information gaps highlighted the need for better understanding of the effects of canopy structural complexity, environmental heterogeneity, stress interactions, and sources of error, among other factors. Sources of variability or error may be broadly categorized as arising from vegetation factors, environmental factors (including stresses), and instrumental or data processing factors. In remote sensing of SIF, clearly it is more practical to control instrumental or data processing methods than vegetation and environmental factors, necessitating the availability of adequate supporting and ground-truthing information to assist investigations.

To advance utilization of SIF, a conceptual framework has been formulated for application of remote SIF for stress detection (Figure 2), which also identified priorities for further study. Major elements of the framework include determination of goals and target applications; prioritization of vegetation sites; delineation of likely stresses and associated sources of variability/error; selection of SIF indicators; and definition of supporting measures needed for calibration, validation, data processing, and interpretation.

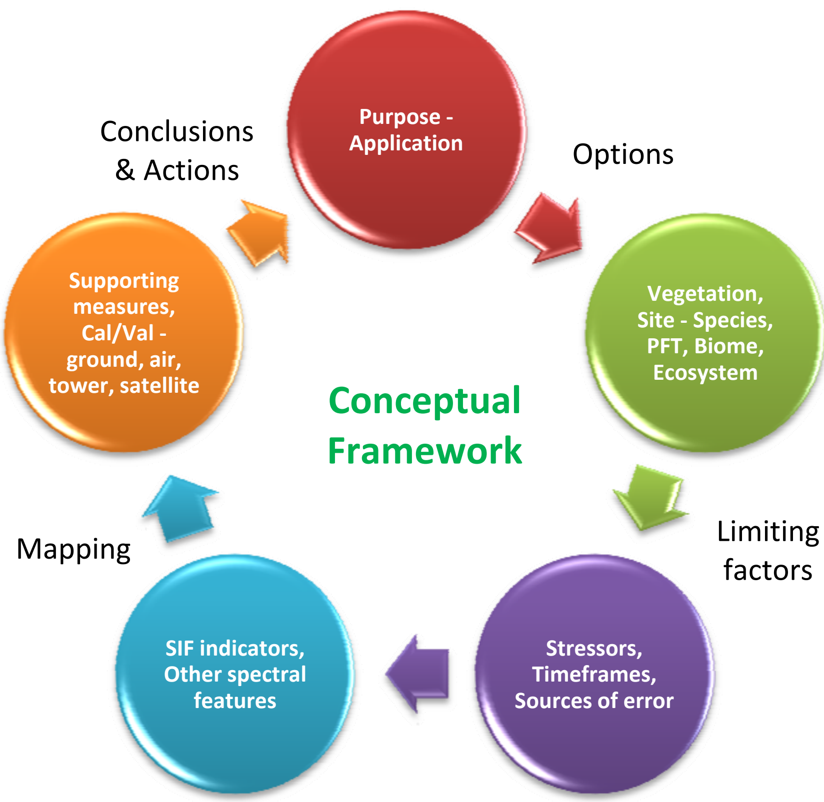

Figure 2. Conceptual framework for the use of remote SIF in stress detection.

Priorities for future study include consideration of the full range of potential applications, identification of the most suitable SIF indicators for different situations, understanding potential sources of variability and errors, establishment of ancillary technologies, and characterization and establishment of site networks for remote and ground-based assessments. Development of calibration and validation strategies and tools is a crucial subject that warrants concerted attention.

Significance for the FLEX mission

Outputs from the Photosynthesis Study that are of key relevance to the FLEX mission include:

1. **model advances** – the availability now of a powerful consolidated model for linking canopy SIF and photosynthesis, making it possible to derive photosynthesis from FLEX fluorescence retrievals (upon conversion to top-of-canopy signals);
2. **model GUI for users** – development of the new A-SCOPE Graphic User Interface, greatly facilitating usage of the photosynthesis model and opening the door to a potentially broad range of users for FLEX-derived products;
3. **calibration/validation tool** – availability of the SCOPE v1.53 model for calibration and validation activities during mission deployment;
4. **processing advancements** – demonstration of streamlining options for the photosynthesis model, thereby making more feasible the execution of large-volume analyses to be triggered from FLEX data;
5. **support of FLORIS spectral strategy** – substantiation in the model inversion work of the inherent value of both fluorescence peaks and the full fluorescence profile for estimating net photosynthesis of the canopy, thus conferring a singular advantage to the FLORIS sensor scheme to extract the complete emission profile;
6. **algorithms** – indications that simple regression models were able to predict photosynthetic products (NPC, GPP, LUE, APARChl) with high performance for C3 and C4 plants in a non-stressed case;
7. **stress applications** – development of novel stress indices, and confirmation of the benefits of having both red and far-red peaks for tracking strain induced by the stresses of water deficit, temperature extremes, and nitrogen insufficiency, which are all issues of contemporary concern in food production and management of significant vegetation systems worldwide;
8. **strategic approach** – depiction of a conceptual framework to support application of SIF to issues involving vegetation stresses and resource management.

Next steps

To build upon the findings of the Photosynthesis Study, the following developments are recommended:

- **advanced model parameterization** – advances in parameterization within the model of strategic physiological variables such light energy distribution between the photosystems, quantification of photoprotective quenching, and photodamage;
- **comprehensive model testing** – evaluation of model performance under a broader range of field situations, including stress scenarios;
- **algorithm testing** – evaluation of the robustness of simple regression models found here to relate SIF and photosynthetic products;

- **expanded stress detection** – consideration of a wider range of stresses – including multiple-stress situations – for which SIF might serve as an indicator, and identification of additional features from the full spectral emission profile that could be used;
- **stress indices testing & validation** – prototype stress indices have been suggested by the study activities which merit further testing and validation under various conditions and with a range of species and functional types;
- **calibration & validation** – development of a thorough strategy for calibration and validation of SIF from FLEX so that accurate interpretations may be drawn in the various application areas;
- **analysis & mitigation of errors** – elucidation of sources of variability and potential errors arising from biological and environmental factors which may constrain interpretations of SIF behaviour in response to stress, and presentation of strategies to mitigate errors and misinterpretation.

A comprehensive suite of recommendations has been drawn up for actions and studies which could span the timeframe leading up to and during FLEX deployment. These needs serve to underscore a significant reality: SIF from space is truly a fresh and emerging arena for understanding real-time photosynthetic behaviour of land vegetation – a possibility not envisaged before the prospect of the FLEX mission.

Even now, with intensifying efforts from researchers endeavouring to extract SIF data from non-optimized satellite platforms such as GOSAT, GOME-2, OCO-2, etc., it is evident that the FLEX mission would be unique and advantageously positioned to fully engage this extraordinary signal. FLEX and its sensor FLORIS would be the vanguard for this new way to view the actual functioning of terrestrial vegetation from space.

Acknowledgement

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