P & M Technologies
Innovations in Plant Science & Technology

FLEX/Sentinel-3 Tandem Mission

FLEX Bridge Study

EXECUTIVE SUMMARY

Final Report — January 2016

ESA ESTEC Contract No. 4000112341/14/NL/FF/gp

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Executive Summary

Background

The European Space Agency (ESA) has been investigating remote sensing methods for detection of chlorophyll fluorescence in terrestrial plants through its research activities over the past decade and more (e.g., Miller *et al.* 2005; Magnani *et al.* 2009; Mohammed *et al.* 2014; Moreno *et al.* 2014; Rascher *et al.* 2015). Current activities have focused on the Fluorescence Explorer (FLEX), one of two candidates included in Phase A/B1 assessments for ESA's Earth Explorer 8 mission (ESA 2015b). FLEX is oriented to bridging the land challenges identified in ESA's Living Planet Programme: Scientific Achievements and Future Challenges (ESA 2015a) through an advanced scientific Earth observation capacity that will support management of the world's vegetation resources (ESA 2015b).

As part of the FLEX Phase A/B1 activities, several initiatives were completed previously, including (i) the FLEX/Sentinel-3 Tandem Mission Photosynthesis (PS) Study, which developed a process-based model and simplified algorithms linking solar-induced fluorescence and photosynthesis, as well as fluorescence-based stress indicators (Mohammed *et al.* 2014); (ii) the Performance Analysis and Requirements Consolidation Study (PARCS), which developed approaches for retrieval of solar-induced chlorophyll fluorescence (SIF) from FLEX (Moreno *et al.* 2014); and (iii) the *HyFLEX* initiative, consisting of dedicated field campaigns executed with the airborne demonstrator *HyPlant*, to investigate fluorescence characteristics over a range of vegetation types and to explore the effects of stresses on SIF (Rascher *et al.* 2015). The current FLEX Bridge (FB) Study builds upon the foundation of those activities by focusing on optimisation of signal retrieval methodologies, extension of stress indicators, strengthening of the process-based modelling capabilities of the SCOPE model, and development of calibration/validation strategies for FLEX products.

Goals of the FLEX Bridge Study

The overall goals of the FLEX Bridge Study were to:

1. optimise approaches for SIF retrievals and applications in assessment of photosynthesis and stress status in terrestrial vegetation; and
2. develop a calibration/validation strategy for FLEX products.

Specific objectives were to:

- optimise the fluorescence retrieval algorithm developed under the PARCS activity;
- optimise the SCOPE photosynthesis model (v1.53) and related algorithms developed under the Photosynthesis Study;
- consolidate and develop retrievals for additional Level-2 data products;
- advance further applications based on Level-2 data products.

Science tasks

The FLEX Bridge Study was divided into four major science tasks:

1. **Solar induced fluorescence retrieval optimisation and analysis.** This task built upon the PARCS activities (Moreno *et al.* 2014) by: consolidating algorithms for atmospheric correction in FLEX configuration; optimising and improving algorithms for SIF retrieval; formalising fluorescence-derived indices; and developing biophysical products.

2. **Development of vegetation stress indicators and applications.** This activity advanced the range of applications and protocols for stress detection using SIF by: utilising datasets from campaigns with the airborne demonstrator *HyPlant* to extend stress-based applications of SIF; evaluating strategies to assess non-photochemical quenching (NPQ) using optical measurements; testing and reviewing stress indicators developed in the PS Study; and reviewing sources of variability and error in stress detection.

3. **Photosynthesis model optimisation, updates, and applications.** The SCOPE model version (1.53) that was developed in the PS Study was updated with new functionality, and foundations were laid for future developments by: considering effects of xanthophylls (known to contain additional information about stress); defining model parameters for specific plant functional types that can be linked to operational global dynamic vegetation models; further quantifying vegetation structural effects on the measured SIF signal; and investigating data assimilation techniques for a broader range of applications, including global ecology, climate- and carbon modelling.

4. **Development of a calibration/validation strategy.** The need for a comprehensive cal/val strategy was identified in the PS Study and at the 5th International Workshop on Remote Sensing of Vegetation Fluorescence (in 2014). This priority was addressed here by: determining validation error metrics and product accuracies; defining a cal/val strategy for basic fluorescence products; defining FLEX Level-2/3 products and their validation plan; and defining common protocols and state-of-the-art instruments to be used in estimation of fluorescence in the context of calibration/validation activities.

Results

Solar induced fluorescence retrieval optimisation and analysis

Capabilities were enhanced for the retrieval and analysis of sun-induced fluorescence from FLEX. These included provision of new simulation datasets, consolidation of algorithms for atmospheric correction of FLEX signals, improvements for SIF retrieval, formalisation of fluorescence-derived indices, and development of biophysical products.

In **data generation**, the existing FLEX/S3 spectral radiance databases were expanded with new simulations that allow for generation of either single pixels or synthetic composite imagery. Some of the new datasets were generated with the FLEX End-to-End Mission Performance Simulator (FLEX-E). The new databases afford versatility in simulating ideal or realistic scenarios and are valuable inputs for algorithm development.

The **atmospheric correction algorithm** was developed to a Level-2 processing chain, while also improving the coupling of atmospheric correction and fluorescence retrieval.

Fluorescence retrievals were improved for retrieval of the full SIF spectrum, and analyses conducted here demonstrated the feasibility of decoupling the Photosystem I and II (PSI and PSII) spectra from total canopy fluorescence.

Strategies were evaluated for better **estimates of absorbed photosynthetically active radiation (APAR)**, important for the calculation of yields. Further, insights were gained into potential causes of retrieval issues. **Normalisation strategies** of the SIF signal were evaluated for their capacity to minimise the impact of environmental conditions and vegetation structural parameters, and the importance of APAR and fAPAR for normalisation was substantiated.

Progress was made toward development of higher-level products for retrieval of **biophysical parameters** (or canopy state variables). For complex imagery, a retrieval strategy was developed to extract LAI estimates. A complementary approach for cases of relatively homogenous pixels showed that a simplified version of SCOPE was able to simultaneously retrieve surface reflectance, fluorescence, and most biophysical paramaters of the model.

Development of vegetation stress indicators and applications

Opportunities and protocols for stress detection were expanded and refined using published and new datasets, testing of indicator prototypes, and evaluation of strategies to assess non-photochemical quenching and minimise sources of variability and error.

SIF can be used to study a wide variety of **abiotic and biotic stresses** across many species. In addition to water stress, temperature stresses, and nitrogen deficit studied during the PS Study, the influence of air pollution, insecticides, senescence, biotic stress, combined stresses, heavy metals, herbicide, ozone, UV radiation, salt and micro- and macronutrients deficiency were evaluated. Stress indices introduced in the PS Study were tested, and the results reiterated the importance of having ancillary measures for interpretation of SIF and to distinguish among stresses. Application of SIF for stress detection requires a good understanding of vegetation ecophysiology, suitable sampling methods, techniques for merging of data from various domains, and sound mechanistic models. The spectral and spatial resolution of FLORIS and the complementarity of the tandem mission position FLEX advantageously for applications.

The value of the **photochemical reflectance index** (PRI) for interpretation of fluorescence is well known. Here, we have considered how best to incorporate PRI for canopy-level assessments and have proposed avenues by which PRI could be strengthened as a measure of non-photochemical quenching through compensating for the impacts of confounding factors, especially structural effects, illumination effects, and pigment pool sizes.

Finally, field datasets were utilised from stress experiments with the ***HyPlant*** airborne sensor which helped to quantitatively link vegetation stress and SIF. The far-red fluorescence was used here, for which the potential interplay of canopy characteristics with stress responses and fluorescence emission was indicated. An informative point was the apparent strong correlation of F_{760} to EVI (hence leaf area index, LAI), at least under heat stress. In the near future, as the extraction of the red fluorescence data from *HyPlant* campaigns is completed, this will more fully advance our understanding of stress responses in the field.

Photosynthesis model optimisation, updates, and applications

The SCOPE model and A-SCOPE graphic user interface were improved with new functionality for accommodating plant functional types, and SCOPE now has improved computation speed and greater accuracy of the fluorescence output. Further improvements will be facilitated with the creation here of a new leaf RT model that incorporates xanthophyll effects. Several types of applications were investigated.

Several modelling developments were relevant to applications of SIF for photosynthetic and stress evaluation. First, a new model, Fluspect_B_CX, was introduced to represent **xanthophyll pigment changes** related to NPQ and PRI. Second, a new model of **energy partitioning** between the two photosystems was proposed to provide preliminary estimation of PSI and PSII fluorescence radiance. Third, the possibility was investigated to estimate **sustained NPQ** from changes in leaf PRI, thereby strongly reducing model uncertainty.

Testing and evaluation of recent versions of the models were done. The **Fluspect model** provided realistic chlorophyll fluorescence simulations, with most of the fluorescence variability explicable from the PROSPECT parameters. However, the spectral distribution of the excitation light affected the shape of the chlorophyll fluorescence spectrum in a way that the Fluspect model could not fully reproduce. Ideally, measurements carried out under natural light conditions should be used to complete a full validation of the Fluspect model. The **SCOPE model** was compared to field data of far-red fluorescence from *HyPlant*. The model reproduced the magnitude and seasonal cycle of fluorescence. In unstressed conditions, the effects of canopy structure and leaf composition dominated fluorescence variations in the far-red band, with a smaller contribution of photosynthetic regulation due to photochemical and non-photochemical quenching.

To facilitate applications and user convenience, a **simple model** for red and far-red fluorescence and photosynthesis has been formulated based on SCOPE. The simple model runs approximately six orders of magnitude faster than the full SCOPE model. Also, an **Emulator toolbox**, developed as a complementary activity to the FB Study, is useful to evaluate various model emulators.

Data assimilation of fluorescence products will be key to applications. As a first attempt, data assimilation has been applied to a *HyPlant* scene, producing a map of canopy photosynthesis from the reflectance and retrieved fluorescence of *HyPlant*. Additional activity explored SIF datasets of coarse spatial resolution that could inform FLEX activities at the more detailed scale. Data assimilation using SIF to constrain the DVGM ORCHIDEE yielded promising results. Considering that canopy 3D geometry influences SIF values, there is merit to having ‘structure-corrected’ data for future use.

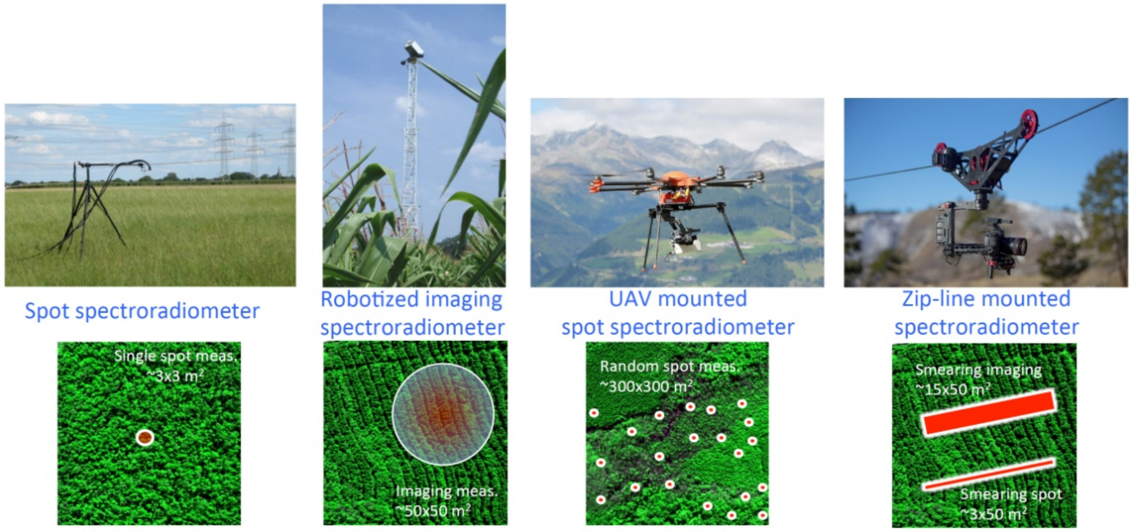
A further product was the '**Automated Scene Generator Module' (A-SGM)** for the generation of simulated scenes according to plant functional types. This module is available in a user-friendly GUI format in the ARTMO framework, and it can rapidly generate simulated scenes for any optical sensor specified within ARTMO. The A-SGM accommodates data from either a radiative transfer model (RTM) or an RTM emulator.

Development of a calibration/validation strategy

The FB Study has formulated a comprehensive cal/val strategy for FLEX mission products. The strategy covers methods to determine validation error metrics and product accuracies, cal/val for basic fluorescence products, validation of FLEX Level-2/3 products, and definition of common protocols and state-of-the-art instruments for use in the strategy.

A **"bottom-up" validation** strategy was proposed, with validation based on trusted top-of-canopy (TOC) SIF measurements over large relatively homogeneous sites from towers or masts, upscaled to moderate resolution via a combination of high resolution mapping with RT models.

The possibility exists to extend to several vegetation types (or even for inhomogeneous canopies of a single type) using *in-situ* imaging spectrometers and/or unmanned aerial vehicles (UAV)-based miniature spectrometers, along with RTMs and/or high-resolution mapping. Dedicated field campaigns with airborne FLEX simulators and extensive field measurements deployed at selected sites will provide high accuracy validation of upscaling processes, radiative transfer fluorescence models and TOC SIF measurements. Validation should extend globally over relevant biomes and latitudes, and continuously over seasonal changes, with data from the different validation sites compiled in a homogenised database. We have further proposed procedures for evaluation of instrument performances under natural illumination so as to identify the most suitable, cost-effective and precise instruments for deployment.



Spot spectroradiometer

Robotized imaging spectroradiometer

UAV mounted spot spectroradiometer

Zip-line mounted spectroradiometer

Instrumental setups to achieve field and landscape characterisation
using various sampling strategies

Significance for the FLEX mission

The FB Study supports the development of best practices for the retrieval, interpretation, and application of fluorescence measurements from space. These aspects are crucial in order to realise the full potential of space-based SIF technology in helping to meet the land challenges identified in ESA's Living Planet Programme (ESA 2015a). The completion of the FB Study also coincides with the conclusion of ESA's selection process for Earth Explorer 8 and the Agency's official announcement in mid-November 2015 that FLEX has been selected. Thus, the Study serves as a 'bridge' to future science activities.

Outputs of FLEX Bridge that are of key relevance to the FLEX/Sentinel-3 mission:

1. **fluorescence retrieval & quantification** – extension of FLEX/S3 spectral radiance databases to support algorithm development; improvement in atmospheric correction and development to a Level-2 processing chain; improvement in retrieval of the full SIF spectrum; decoupling of PSI and PSII spectra; normalisation strategies for estimation of APAR; progress in retrieval of biophysical parameters; definition of calibration/validation approaches.
2. **fluorescence interpretation** – strategies to incorporate PRI through compensating for confounding factors; evaluation of *HyPlant* campaign data on stress responses; strategies for quantifying and modelling NPQ and its components; formulation of a new leaf RT model incorporating xanthophylls; prototype model for energy partitioning between PSI and PSII; preliminary strategies to incorporate canopy 3D geometry effects; calibration/validation approaches.
3. **fluorescence applications** – identification of SIF indicators to study a wide variety of abiotic and biotic stresses; development of a prototype simplified model based on SCOPE; development of an Automated Scene Generator Module to incorporate plant functional types; creation of an emulator toolbox; testing of updated versions of SCOPE and Fluspect with simulated and field data.

Recommendations

To build upon the findings of this study, we offer several recommendations.

First, additional developments are needed on optimisation of **signal retrieval and analysis**. Algorithms for decoupling PSI/PSII contributions should be tested under realistic scenarios. Similarly, estimation of biophysical parameters should be studied in more detail under such scenarios. Further work is required on quantification and incorporation of canopy structural effects on the SIF signal and for the individual PAR terms (especially APAR), notably in complex vegetation canopies; and a strategy for normalisation of SIF in the red region to compensate for vegetation structure must be formulated, especially considering reabsorption of the red band fluorescence. In general, methodologies need to be tested with more 'real world' datasets.

Second, a concerted effort is required on **data assimilation** techniques amenable to a broad range of applications, including global ecology, climate- and carbon modelling. Preliminary activity here utilised GOME-2 data to inform the more detailed acquisitions that will be possible with FLEX, but future activity will need to focus on finer-resolution captures and on both red and far-red fluorescence, for which the *HyPlant* airborne sensor will be a valuable platform.

Third, the new and enhanced **models** developed here require fuller validation and testing with more datasets on a wider variety of vegetation types. The new leaf-level models of physiology or RT will need to be implemented into SCOPE once final testing and validation are completed. It should also be noted that a few very challenging areas of science were tackled here related to estimation of non-photochemical quenching. That story is not yet complete and further refinement or correction of these analytical models likely will be needed. Efforts should also continue on formulation and testing of simplified models or emulators for use at canopy level, and usage of the new emulator toolbox will expedite such investigation.

Fourth, pre-implementation of the **cal/val** strategy that was pioneered here needs to start soon so that the necessary infrastructure can be put in place. Developments on SIF proximal and remote sensing systems are needed to improve performances, accommodate heterogeneous landscapes, handle automatic sampling, and conduct automatic processing & archiving. Additionally, there would be benefits to establishing or engaging a common calibration facility and having portable cal/val standards. A helpful step will be to identify institutions, groups, and companies capable of such developments and manufacturing. To keep abreast of new developments, future activities will benefit from interaction with other initiatives (e.g., COST action OPTIMISE ES1309) involving diverse teams of scientists sharing a common interest in fluorescence spectroscopy under natural conditions.

Finally, a priority should be placed on advancement of SIF **applications** and supporting the **users** of FLEX. There is a need for studies on stress applications of SIF in a wide variety of vegetation systems, along with investigation into PSI/PSII behaviour and implications for SIF retrievals and quantification. The user network will need to be consolidated and supported with necessary expertise and other resources. A communications plan should be developed and implemented to keep the FLEX user community informed and ready to adopt new developments. This activity should occur contemporaneously with work on the cal/val pre-implementation, as these users will also be involved in refinement of site selection and methodologies for the different application areas.

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