2012 FLEX/S3 Tandem Mission Performance Analysis and Requirements Consolidation Study

EXECUTIVE SUMMARY

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Jose Moreno	University of Valencia (UVEG), Spain
Uwe Rascher	Forschungszentrum Jülich (FZJ), Germany
Yves Goulas	NRS – Laboratoire de Météorologie Dynamic (LMD), France
Roberto Colombo	University of Milan Bicocca (UNIMIB), Italy
Wouter Verhoef	University of Twente (UT-ITC), The Netherlands
Alexander Damm	University of Zurich (UZH), Switzerland
Luis Alonso	University of Valencia (UVEG), Spain
Sergio Cogliati	University of Milan Bicocca (UNIMIB), Italy
Fabrice Daumard	NRS – Laboratoire de Météorologie Dynamic (LMD), France
Juan Pablo Rivera	University of Valencia (UVEG), Spain
Neus Sabater	University of Valencia (UVEG), Spain
Anke Schickling	Forschungszentrum Jülich (FZJ), Germany
Carolina Tenjo	University of Valencia (UVEG), Spain
Joris Timmermans	University of Twente (UT-ITC), The Netherlands
Jochem Verreslt	University of Valencia (UVEG), Spain
Matthias Drusch	ESTEC, The Netherlands

<u>*Study Manager:*</u>
Prof. Jose Moreno
Laboratory for Earth Observation – IPL
Dept. Earth Physics and Thermodynamics
Faculty of Physics, University of Valencia
c/ Dr. Moliner, 50
46100, Burjassot, Valencia (Spain)
jose.moreno@uv.es

<u>*ESA/ESTEC Technical Manager:*</u>
Dr. Matthias Drusch
Land Surfaces Principal Scientist
Mission Science Division (EOP-SME)
European Space Agency, ESTEC
Earth Observation Programmes
Postbus 299
2200 AG, Noodwijk (The Netherlands)
Matthias.drusch@esa.int

Executive summary

Background

While most Earth Observation missions based on passive optical methods are intended to measure the light “reflected” by the surface, FLEX uses a completely innovative approach based on the measurement of the light “emitted” as fluorescence by terrestrial vegetation. Such fluorescence emission by vegetation has never been measured from space, which makes FLEX a true Explorer mission providing a type of information never available before.

The retrieval of vegetation fluorescence from measured spectral radiances at the top of the atmosphere requires a proper decoupling of the total measured signal into the different contributions that perturb the measurement: from the incoming solar irradiance at the top of the atmosphere to the illumination of the surface, then the surface reflection and the associated fluorescence emission, and finally the radiance travelling back through the atmosphere up to the satellite. In order to properly characterize all the effects on the fluorescence signal and to account for such effects in a retrieval scheme, spectral information from strong absorptions bands with high spectral resolution is required within specific spectral ranges, as well as other spectral information in a much larger spectral range (VNIR to SWIR) to characterize atmospheric effects, for cloud screening, to determine surface temperature and to help determining the vegetation status at the time of observation. Such requirements suggest the implementation of the FLEX mission concept as a single-instrument small satellite flying (FLORIS in FLEX) flying in tandem with Sentinel-3 (S3).

Goals of the PARCS Study

The FLEX/S3 Tandem Mission Performance Analysis and Requirements Consolidation Study (PARCS) was performed in the context of the Phase A/B1 activities carried out for the FLEX Earth Explorer 8 candidate mission. The main objective was to demonstrate the performance of FLEX in the context of observing fluorescence of the terrestrial vegetation from space, including both the retrieval concept and the adequacy of the FLEX/S3 tandem mission concept to perform the science associated with the objectives of the mission.

The objectives of the PARCS activity were:

- To assess and consolidate the mission observational requirements to retrieve vegetation fluorescence with the required accuracy to use fluorescence information into dynamical vegetation photosynthesis models, and the FLEX performances required to address the open issues in vegetation fluorescence.
- To establish the role of the different instruments included in Sentinel-3 and the FLEX payload, in conjunction with external data sources, to derive the final FLEX fluorescence products.
- To test the performances and evaluate feasibility of the evolving FLEX technical concept based on new iterations of the technical requirements and/or potential optimization of the payload, as a consequence of outputs from the industrial system concept studies, with the objective to provide the boundaries for optimization of the instrument concept.

Science tasks

PARCS was divided into four major tasks:

1. **Identification of open issues related to fluorescence retrieval in the context of the FLEX/S3 tandem concept**, and on the possible impact of these issues on the mission and instrument requirements. A comprehensive review was conducted of available fluorescence retrieval methods. Current knowledge on the impact of instrumental errors on the Fs retrieval accuracy was summarized and consolidated. Instrument requirements were prioritized and consolidated.
2. **Optimizing fluorescence retrieval methods with regards to the specific technical requirements and FLEX/FLORIS specifications.** Both theoretical and experimental reference datasets of simulated FLEX/S3 tandem observations were developed, using SCOPE 1.40 Beta and MODTRAN 5.2.1 as simulation tools. Using such simulated and experimental datasets, a detailed evaluation was performed including different possible retrieval strategies based on spectral fitting approaches. A full retrieval scheme including an atmospheric correction module and a new Fs retrieval module has been developed. Alternative retrieval approaches based on single-step model-inversion techniques have been also considered. The different investigated Fs retrieval approaches were extensively evaluated using the reference S3/FLORIS datasets. From this evaluation it appears that the SFM approach provides the most robust and accurate alternative with the advantage of retrieving the full Fs emission shape. This task ended with the definition of a validation plan for the retrieval method.
3. **Exploration of the FLEX/S3 tandem mission synergy concept.** The constraints imposed by the FLEX/S3 tandem solution, including the associated requirements, have been addressed. Potential temporal, radiometric and geometric synergy procedures have been reviewed. Solutions were proposed to achieve the required level of integration of information. Potential algorithms for the retrieval of biophysical information from S3 data were reviewed.
4. **Contribution to the development of the End-to-End Mission Performance Simulator (E2ES).** This task has been implemented by providing to the E2ES the so-called scientific modules of the simulator, so they comply with the architecture and interfaces of the full E2ES, which includes a Scene Generator Module (SGM) and a Level-2 Retrieval module (L2R).

Fluorescence retrieval method

Based on sensitivity studies performed and results from Task 1 of PARCS, and in the frame of previous studies related to FLEX, the spectral fitting method (SFM) proved to provide the best results and thus has been selected as baseline for Fs retrievals for FLEX. An assessment of possible strategies for Fs retrieval identified two main categories:

- Exploiting measured top-of-atmosphere (TOA) radiance and retrieving Fs, reflectance, and atmospheric properties in one step (one-step approach).
- Performing atmospheric correction and Fs retrieval sequentially (two-step approach).

Based on a theoretical database, three different fluorescence approaches have been developed and validated that follow two different strategies:

1. The **one-step Fs retrieval approach** is based on a consistent forward modelling, by means of radiative transfer models, of the sun-surface-sensor path and retrieves Fs directly from TOA data. This strategy provides the advantage of simultaneously retrieving atmospheric (e.g., AOD, CWV) and surface

variables (e.g., Fs, R, CAB, LAI). The applicability of the one-step approach is, however, limited due to the high number of variables involved in the inversion, which increases the inherent ill-posedness of the retrieval problem. Following this approach a new method has been developed based on the inversion of a canopy reflectance model coupled to an atmospheric RTM.

2. The **two-step Fs retrieval approach** applies sequentially an atmospheric correction followed by the retrieval of Fs on top-of-canopy radiance data (TOC) through SFM. This approach was commonly used in the past as a reduced number of variables is involved in the inversion scheme (only surface variables). Further, S3 data and products can be incorporated in this retrieval strategy to facilitate e.g., the atmospheric correction. Following this strategy there were two methods being tested: Polynomial SFM (SpecFit) that fits the full spectrum of fluorescence, and another method based on peak height in apparent reflectance.

While all three approaches allow retrieving Fs from TOA data by performing either the retrieval at TOA data or TOC data, the one-step approach requires perfect knowledge of the atmospheric status. In the two-step approach a full retrieval scheme including an atmospheric correction was developed, providing for the first time the possibility to realistically evaluate the retrieval as it will be the case for FLEX. The three investigated Fs retrieval approaches were extensively evaluated using the reference theoretical dataset. From this evaluation it appears that all three approaches provide good results, while the SFM approach provides the most robust and accurate alternative with the advantage of retrieving the full Fs emission shape.

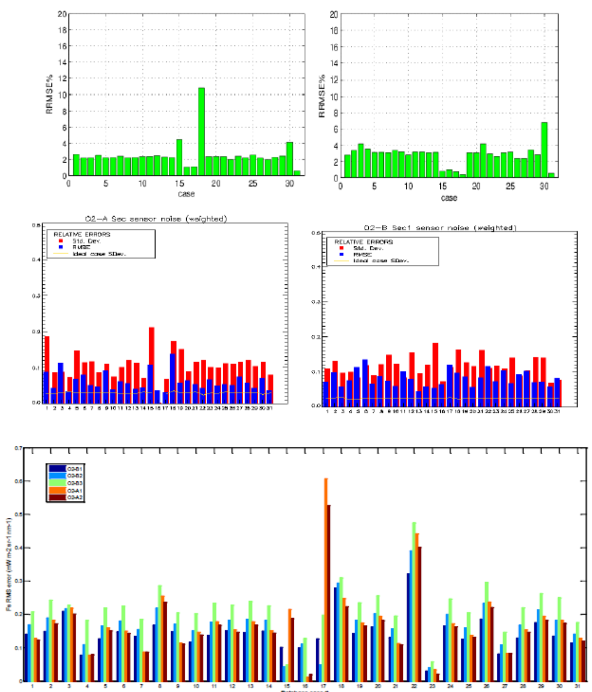

Figure 1. Summary of Fs retrieval accuracies considering the three investigated retrieval schemes. Top: Performance of the SFM method for the O_2-B band (left) and the O_2-A band (right); Middle: Performance of the two-step Fs retrieval approach O_2-B band (left) and the O_2-A band (right); Bottom: Performance of the one-step approach.

Given the results of the different methods tested, the selection for implementation on the retrieval module of the End-to-End Simulator was on the SpecFit SFM that allows retrieving the fluorescence's full spectrum.

However, whatever further developments and enhancements are achieved in the retrieval process, they could be considered for the final implementation of the retrieval module in FLEX processing chain.

Synergy concept

The benefit of having FLEX and S3 configured in tandem for improved retrievals of Fs and biophysical variables has been demonstrated. However, crucial hereby is that both datasets are merged with great accuracy, both in the radiometric and geometric domain, and thereby taking geometrical issues and the overpass time delay into account. To achieve this, geometric, temporal and radiometric synergy approaches have been proposed.

- The proposed geometry synergy builds further on co-registration approaches specifically developed for pushbroom sensors. This kind of approaches have also been implemented into other similar data processing schemes with platforms multi-sensors or missions using multi-platform data.
- Several parameters that change in the temporal domain have been analysed, finding that in the time span of the proposed FLEX-S3 tandem (6-15 s) only moving clouds might affect the results of synergistic products. The proposed temporal synergy is to account for cloud displacement and its related impacts. A S3-cloud mask that is enlarged with a buffer to account for this displacement would be a straightforward solution.
- Regarding radiometric synergy, several techniques have been presented in the scientific literature (e.g. histogram matching and image regression). However, these approaches have to be modified with spectral interpolation and extrapolation techniques to account for the non-overlapping spectral regions. When the E2ES is into place, proposed techniques can be evaluated.

E2E Simulator

The proposed Fs retrieval and FLEX/S3 synergy techniques can be evaluated within a controlled environment using the FLEX End-to-End Simulator (E2ES). The E2ES allows to assess the mission performance and to analyse the suitability of the developed Level-2 data processing algorithms. Within PARCS the so-called scientific modules have been developed, which includes a Scene Generator Module (SGM) and a Level-2 Retrieval module (L2R), so they comply with the architecture and interfaces of the full E2ES. The SGM simulates the stimuli to the instrument from bio-/geophysical and atmospheric parameters distributed over the observed area. The L2R module implements the processing algorithms for the retrieval of the geophysical parameters objective of the mission.

Significance for the FLEX mission

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

1. **Atmospheric correction module** – Development of FLORIS atmospheric correction procedure by making use of S3 OLCI and SLSTR data.
2. **Fluorescence retrieval module** - Development of a Fs retrieval processing chain that allows deriving Fs from FLORIS TOC radiance measurements with the required accuracy;
3. **Novel spectral fitting methods (SFM)** – Development and evaluation of SFMs led to a novel SpecFIt algorithm. SpecFIT offers the possibility to extract the full Fs emission spectrum from the FLORIS spectral radiance data;

4 **Reference dataset** – A theoretical dataset has been developed using SCOPE and MODTRAN models. This reference dataset has enabled quantitative evaluation of different retrieval strategies;

5 **Synergy strategies** – Identification of radiometric, geometric and temporal synergy strategies to support and fully exploit the FLEX/S3 tandem concept beyond the mere image co-registration;

6 **Scene Generator Module (SGM)** – Development of a SGM that enables the simulation of TOA radiance arriving to the FLORIS and OLCI/SLSTR sensors in exactly the way they observe the reflected/emitted light from the Earth surface. The complexity and realism of the generated scenes can range from toy examples to test basic performances to highly complex realistic scenes;

7 **Level-2 Retrieval module (L2R)** – Implementation of a module based on the developed algorithm that enables to retrieve the sun-induced fluorescence emission from the synergy between the S3 and FLORIS Level-1b products, as well as the associated biophysical products from FLEX.

Next steps

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

- Considering the intended **optimization of spectral fitting methods** for the Fs retrieval, it is recommended to quantitatively evaluate the sensitivity and performance of SFM methods in regard to the identified instrumental errors, including quantitative evaluation on the impact of subtle instrumental errors (i.e., detector non-linearity, stray light).
- Both the one-step and two-step approaches are promising and should be further investigated. It is recommended to systematically assess the impact of listed aspects **based on a common (experimental) validation data set** for all potential retrieval schemes.
- The results presented indicate that the Fs retrievals are indeed affected by effects of surface anisotropy. These effects deserve to be quantified in future studies.
- To strengthen the Fs retrieval method and to reinforce the identification of the sources of errors, it recommended to setup thorough **cal/val strategies** for these models by means of the E2ES.
- The **proposed radiometric, geometric and temporal co-registration methods** should be further elaborated within the E2ES environment.

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, even more so incorporating the data provided by Sentinel-3.

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