

Deriving Leaf Area Index Reference Maps Using Temporally Continuous *In Situ* Data: A Comparison of Upscaling Approaches

Luke A. Brown , Member, IEEE, Booker O. Ogutu , Fernando Camacho, Beatriz Fuster, and Jadunandan Dash 

Abstract—To further progress the validation of global leaf area index (LAI) products, temporally continuous reference data are a key requirement, as periodic field campaigns fail to adequately characterize temporal dynamics. Progress in cost-effective automated measurement techniques has been made in recent years, but appropriate upscaling methodologies are less mature. Recently, the use of multitemporal transfer functions has been proposed as a potential solution. Using data collected during an independent field campaign, we evaluated the performance of both vegetation index-based multitemporal transfer functions and a radiative transfer model (RTM)-based upscaling approach. Whether assessed using cross validation or data from the independent field campaign, the RTM-based approach provided the best performance ($r^2 \geq 0.88$, RMSE ≤ 0.41 , NRMSE $< 13\%$). For upscaling temporally continuous *in situ* data, the ability of RTM-based approaches to account for seasonal changes in sun-sensor geometry is a key advantage over vegetation index-based multitemporal transfer functions.

Index Terms—Digital hemispherical photography (DHP), INFORM, LAI, Sentinel-2, validation, vegetation indices.

I. INTRODUCTION

LEAF area index (LAI), defined as half the total leaf area per unit horizontal ground area [1], is a key parameter describing the structure of vegetation canopies and controlling processes including photosynthesis and respiration. Estimates of LAI are required in agricultural and forest monitoring, climate modeling, and numerical weather prediction, and are critical to understanding biosphere–atmosphere interactions [2]. To ensure satellite-derived LAI products are fit for purpose, validation using *in situ* measurements is required. Because field campaigns are time consuming and labour intensive, they are relatively infrequent, and for logistical reasons, are typically conducted during the peak of the growing season [3]. Their periodic nature

is a key factor limiting progress toward the third stage of the hierarchy proposed by the Land Product Validation (LPV) subgroup of the Committee on Earth Observation Satellites Working Group on Calibration and Validation. As such, the validation community has highlighted the need for temporally continuous LAI reference data [3], [4]. In response, a variety of automated *in situ* measurement techniques have been developed in recent years. These include systems based on digital hemispherical photography (DHP), digital cover photography, radiometric sensors, and terrestrial laser scanning [5]–[9].

Due to landscape heterogeneity, direct comparison of moderate spatial resolution (i.e., ≥ 300 m) LAI products and *in situ* measurements is impractical, necessitating upscaling approaches. Existing methods involve the use of an intermediate high spatial resolution image, which provides increased consistency with the spatial support of the *in situ* measurements [4], [10]. The radiometric information is related to the *in situ* measurements, enabling a high spatial resolution reference map covering multiple product pixels to be produced. The most widely applied upscaling protocols involve empirical transfer functions relating *in situ* measurements to, for example, vegetation indices, although radiative transfer model (RTM)-based retrievals can also be utilized [4], [10].

Although well-established, existing upscaling methods are designed for traditional field campaigns, in which replicate sampling of multiple (i.e., 20–100) elementary sampling units (ESUs) occurs. In this way, a robust transfer function can be derived using a single near-contemporaneous high spatial resolution image, describing the variation of LAI with spectral characteristics at the time of the campaign [4], [10]. In contrast, while automated *in situ* measurement techniques offer dense (i.e., \leq daily) temporal characterization of canopy dynamics, they are typically only available for a small number of locations (i.e., 1–5) within a site, preventing the derivation of a robust transfer function on any single date [5]–[9]. This is a key impediment to the use of temporally continuous *in situ* data for validating moderate spatial resolution LAI products, and there is a need to advance existing upscaling methodologies in this respect.

Recently, the use of multitemporal transfer functions has been proposed as a potential solution, in which *in situ* measurements and high spatial resolution images from multiple dates are used to derive a single relationship, which is then applied to all images [11], [12]. However, the method has not been explicitly evaluated

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Luke A. Brown, Booker O. Ogutu, and Jadunandan Dash are with the School of Geography and Environmental Science, University of Southampton, SO17 1BJ Southampton, U.K. (e-mail: l.a.brown@soton.ac.uk; b.o.ogutu@soton.ac.uk; j.dash@soton.ac.uk).

Fernando Camacho and Beatriz Fuster are with the Earth Observation Laboratory, 46980 Paterna, Spain (e-mail: fernando.camacho@eolab.es; beatriz.fuster@eolab.es).

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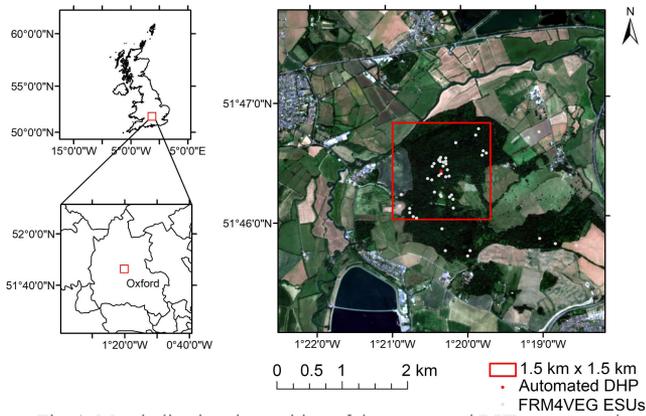


Fig. 1. Map indicating the position of the automated DHP system and independent *in situ* measurements from the FRM4VEG campaign. The background image is a multispectral instrument (MSI) true colour composite from July 6, 2018.

against independent reference data while direct comparison of multitemporal transfer functions to RTM-based approaches, which have the potential to provide more robust results by accounting for variations in sun-sensor geometry [13]–[15], have not been made in the case of upscaling temporally continuous *in situ* data. Using temporally continuous *in situ* data collected at a deciduous broadleaf forest site in Southern England, we compare both vegetation index-based multitemporal transfer functions and RTM-based methods for the generation of high spatial resolution LAI reference maps. We then evaluate the performance of each approach using data collected during an independent field campaign.

II. MATERIALS AND METHODS

A. Study Site and In Situ Data

The study was undertaken at Wytham Woods (51.7734°N, 1.3384°W), a deciduous broadleaf forest site in Oxfordshire, U.K. (see Fig. 1), featuring an automated DHP system that provides daily estimates of LAI [5]. As an example of ancient seminatural woodland, the main species are sycamore (*Acer pseudoplatanus*), ash (*Fraxinus excelsior*), and hazel (*Corylus avellana*) while the site is dominated by clay soils. Further details on the site, automated DHP system, and processing of automated DHP data are provided by Brown *et al.* [5], who demonstrate that the LAI estimates derived from the automated DHP system are in agreement with manual observations made under optimal illumination conditions over a surrounding 40 × 40 m forest plot. Automated DHP data were available on a daily basis from April 2018 to May 2019 ($n = 394$).

B. MSI Data Processing and Quality Control

In total, 28 Sentinel-2 MSI L2A bottom-of-atmosphere reflectance scenes were obtained over the study site during 2018. Data were obtained from the Copernicus Open Access Hub,¹ which, since March 2018, has systematically provided L2A

TABLE I
VEGETATION INDICES ADOPTED TO UPSCALE *IN SITU* ESTIMATES OF LAI, WHERE B8A, B7, B6, B5, B4, AND B3 ARE MSI BANDS CENTERED AT 865, 783, 740, 705, 665, AND 550 NM, RESPECTIVELY

	Index	Formula	Reference
Broadband indices	Normalised difference vegetation index (NDVI)	$\frac{B8A - B4}{B8A + B4}$	[17]
	Green normalised difference vegetation index (GNDVI)	$\frac{B8A - B3}{B8A + B3}$	[18]
	Soil adjusted vegetation index (SAVI)	$\frac{B8A - B4}{B8A + B4 + 0.5} (1 + 0.5)$	[19]
	Optimised soil adjusted vegetation index (OSAVI)	$\frac{B8A - B4}{B8A + B4 + 0.16}$	[20]
	Green chlorophyll index (C_{green})	$\frac{B7}{B3} - 1$	[21]
	Red-edge indices	Sentinel-2 terrestrial chlorophyll index (S2TCI)	$\frac{B6 - B5}{B5 - B4}$
Inverted red-edge chlorophyll index (IRECI)		$\frac{B7 - B4}{B5/B6}$	[22]
Sentinel-2 LAI index (SeLI)		$\frac{B8A - B5}{B8A + B5}$	[23]
Red-edge chlorophyll index ($C_{red-edge}$)		$\frac{B7}{B3} - 1$	[21]
Red-edge position (REP)		$705 + 35 \frac{(B4 - B7)/2 - B5}{B6 - B5}$	[24]
Modified chlorophyll absorption ratio index (MCARI)		$\frac{(B5 - B4) - 0.2(B5 - B3)}{B5 - B4}$	[25]

products generated from L1C MSI data over Europe using the Sen2Cor atmospheric correction algorithm [16]. Before further processing, each scene was resampled to a common spatial resolution of 20 m, using mean value downsampling for the 10 m bands. Pixels flagged as saturated/defective, dark, cloud/cloud shadow, water, thin cirrus, or snow were discarded from further analysis, as were unclassified pixels.

C. Upscaling In Situ LAI

To upscale *in situ* estimates of LAI using multitemporal transfer functions, relationships with 11 vegetation indices were established, using the daily maximum *in situ* LAI estimates corresponding to the acquisition dates of each available MSI scene. Two categories of vegetation indices were investigated: the first consisted of traditional broadband indices used to estimate LAI while the remaining indices were selected to investigate whether the incorporation of MSI's red-edge bands could provide additional information on LAI (see Table I). Data from all cloud-free acquisition dates ($n = 28$) were used to derive the transfer functions through ordinary least squares regression (see Table II). Once established, transfer functions were applied to each MSI scene to obtain a series of high spatial resolution reference maps.

To upscale *in situ* estimates of LAI using an RTM-based approach, a hybrid retrieval algorithm making use of leaf/canopy RTMs and machine learning techniques was applied. We adopted the Invertible Forest Reflectance Model (INFORM)-based retrieval algorithm presented by Brown *et al.* [26], as it was shown to provide improved retrieval accuracy over forest environments when compared to methods involving 1-D RTMs. The algorithm consists of an artificial neural network (ANN) trained with INFORM simulations designed to reflect the deciduous broadleaf forest site it was developed for. 50 000 simulations were carried out to establish the ANN training database

¹Online. [Available]: <https://scihub.copernicus.eu/>

TABLE II
CALIBRATION AND MULTITEMPORAL TRANSFER FUNCTIONS USED TO DERIVE
HIGH SPATIAL RESOLUTION LAI REFERENCE MAPS

Index/retrieval algorithm	Regression equation
NDVI	$y = 9.4139x - 5.2072$
GNDVI	$y = 9.3425x - 4.4651$
SAVI	$y = 9.1402x - 2.335$
OSAVI	$y = 10.8812x - 3.7503$
CI _{green}	$y = 0.1906x + 1.3887$
S2TCI	$y = 0.6166x + 0.5324$
IRECI	$y = 1.5165x + 0.9878$
SeLI	$y = 8.1768x - 2.327$
CI _{red-edge}	$y = 0.4835x + 1.0917$
REP	$y = 0.2139x - 151.8877$
MCARI	$y = 1.7049x + 1.8113$
INFORM	$y = 1.8181x - 4.3239$
INFORM _{broadband}	$y = 2.2461x - 6.174$

by randomly drawing from predefined distributions of model parameters (see Appendix). The inputs of the trained ANN were the bottom-of-atmosphere reflectance in eight MSI bands (B3, B4, B5, B6, B7, B8A, B11, and B12), in addition to the cosine of the associated viewing and illumination geometries. In addition to the standard algorithm, we also trained a further ANN using a subset of bands (B3, B4, B8A, B11, and B12) to assess whether a reduction in performance would occur if MSI's red-edge bands were not used as inputs (hereafter referred to as INFORM_{broadband}). For further information on the ANN training database and procedure, we refer the reader to [26]. Because the ANN training data were optimized for a different study site, some degree of bias in the INFORM-based LAI retrievals was expected. To address this issue, calibration functions were derived through ordinary least squares regression using the daily maximum LAI estimates from the automated DHP system. The calibration functions were subsequently applied to the INFORM- and INFORM_{broadband}-based LAI retrievals. As with the multitemporal transfer functions based on vegetation indices, the calibration functions (see Table II) were based on data from all cloud-free acquisition dates ($n = 28$).

D. Evaluation Using Cross Validation and Independent Data

To provide a first assessment of how the different upscaling methods might generalize to new observations, leave-one-out cross validation was carried out. Agreement was assessed in terms of the coefficient of determination (r^2), root-mean-square error (RMSE), normalized RMSE (NRMSE), bias, and precision. The NRMSE was calculated by dividing the RMSE by the mean of the reference values, whereas bias and precision were calculated as the mean and standard deviation of differences.

To evaluate the upscaling methods with independent data, we compared our results with those of an independent field campaign. For this purpose, we used *in situ* data collected at Wytham Woods between July 3rd and 6th, 2018 under the fiducial reference measurements for vegetation (FRM4VEG) project. Although the FRM4VEG field campaign also made use of DHP to estimate LAI, the dataset was not used in the derivation of calibration or multitemporal transfer functions. The campaign involved the characterization of 47 ESUs (see Fig. 1), 42 of which were sampled using DHP. Each ESU contained

13–15 sampling points, and was approximately 20×20 m in extent. DHP data were processed to estimate LAI in the same way as the automated DHP system [5]. LAI was derived from the estimates of plant area index (PAI) obtained using DHP by subtracting wood area index (WAI). Because a canopy walkway structure is present in the area surrounding the automated DHP system, the WAI value derived from leaf-off measurements at this location was not applicable to other areas of the study site, as the walkway structure itself could not be distinguished from woody material by the classification, leading to a higher WAI than would be experienced in areas without the walkway present. Instead, a previously published WAI value representative of similar deciduous broadleaf forest was adopted [35]. Five ESUs were not sampled using DHP, but were assigned an LAI of zero as they represented bare unvegetated soil. To assess the upscaling methods, the high spatial resolution reference maps derived from the MSI scene acquired during the FRM4VEG field campaign (July 6, 2018) were directly compared with the *in situ* estimates of LAI obtained during the campaign itself.

III. RESULTS

When evaluated through cross validation, the INFORM- and INFORM_{broadband}-based upscaling approaches provided the best performance, demonstrating the highest r^2 (0.91) and lowest RMSE/NRMSE values (0.34 and 12%), with points lying close to the 1:1 line [see Fig. 2(l) and (m)]. In comparison, the multitemporal transfer functions based on vegetation indices yielded reduced accuracy. The worst performance was observed for the MCARI-based transfer function, which demonstrated the lowest r^2 (0.18) and highest RMSE/NRMSE values (1.04 and 36%), with considerable scatter [see Fig. 2(k)]. Of the multitemporal transfer functions, the SAVI-based transfer function provided the best performance ($r^2 = 0.83$, RMSE = 0.47, NRMSE = 16%) [see Fig. 2(c)]. While all upscaling approaches demonstrated low overall bias (−0.01 to 0.02), the majority of vegetation index-based multitemporal transfer functions is subject to overestimation of lower LAI values [see Fig. 2(a)–(k)].

When evaluated against independent *in situ* measurements from the FRM4VEG field campaign, a similar pattern was observed, albeit with slightly reduced performance in all cases (see Fig. 3). Again, the best performance was achieved by the INFORM-based upscaling approach ($r^2 = 0.88$, RMSE = 0.41, NRMSE = 13%), whereas the multitemporal transfer functions based on vegetation indices were characterized by reduced accuracy. Of these, the NDVI-based transfer function demonstrated the best performance ($r^2 = 0.88$, RMSE = 0.48, NRMSE = 15%), whereas the REP-based transfer function provided the worst performance ($r^2 = 0.06$, RMSE = 2.59, NRMSE = 83%). All upscaling approaches overestimated LAI, though considerably reduced biases were observed in the case of the INFORM- and INFORM_{broadband}-based upscaling approaches and S2TCI-based transfer function (bias = 0.06 to 0.07) when compared to the other considered vegetation indices (bias ≥ 0.20). As in the results of cross validation, several of the vegetation index-based multitemporal transfer functions were subject to overestimation of lower LAI values (i.e., over bare soil), while this was not the case for the INFORM- or INFORM_{broadband}-based upscaling

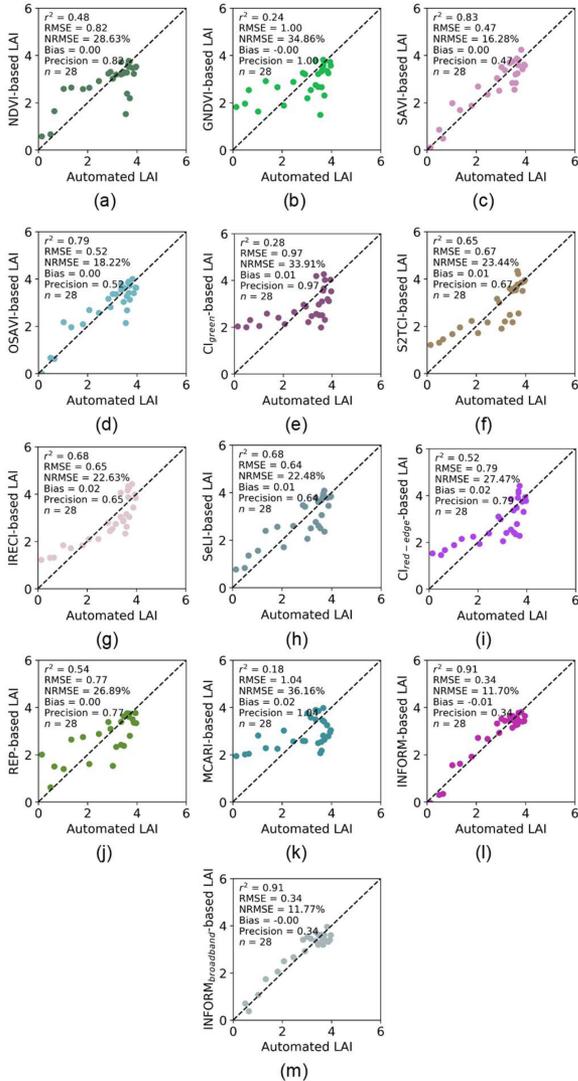


Fig. 2. (a)–(k) Comparison of multitemporal transfer function-based and (l)–(m) INFORM-based high spatial resolution reference maps of LAI with *in situ* measurements from the automated DHP system throughout 2018. The dashed line represents a 1:1 relationship.

approaches [see Fig. 3(l) and (m)]. Despite this, some vegetation index-based multitemporal transfer functions appeared to better capture variability at higher LAI values (though this could equally reflect uncertainty in the *in situ* measurements as opposed to increased capability of the indices).

In terms of their spatial characteristics, all upscaling approaches demonstrated reasonable consistency, resolving the major spatial structures over the 1.5×1.5 km area surrounding the automated DHP system during the FRM4VEG field campaign (see Fig. 4). The multitemporal transfer functions based on indices incorporating red-edge bands tended to demonstrate a greater degree of high frequency variation [see Fig. 4(f)–(k)], whereas these variations were less well resolved by most of the transfer functions based on broadband indices [see Fig. 4(a)–(e)]. The transfer functions based on the CI_{green} , IRECI, $CI_{\text{red-edge}}$, and MCARI substantially overestimated areas of low LAI, which were better captured by the other upscaling approaches (see Fig. 4).

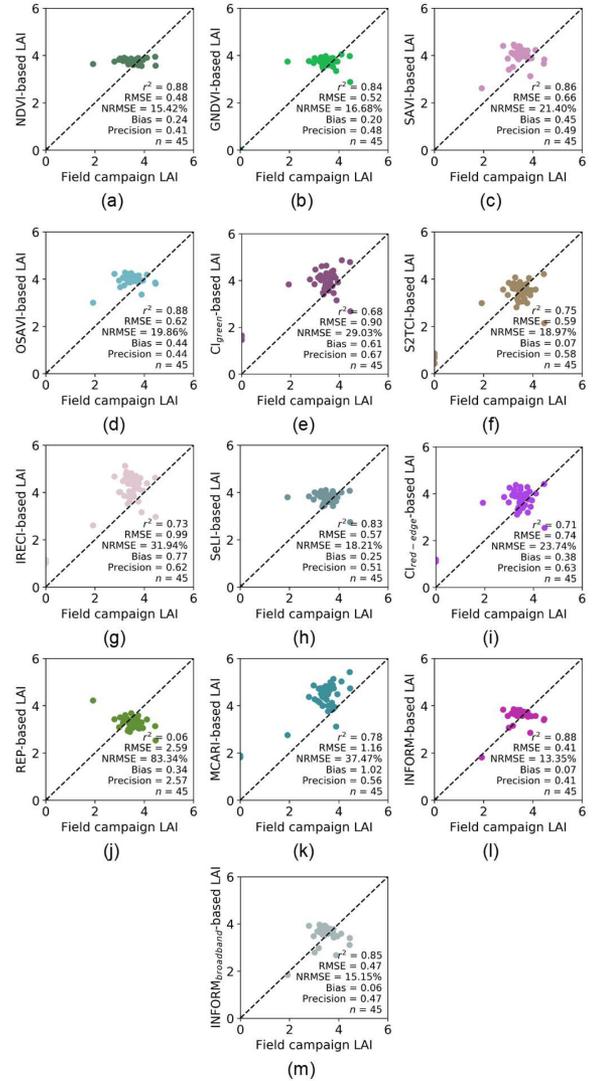


Fig. 3. (a)–(k) Comparison of multitemporal transfer function-based and (l)–(m) INFORM-based high-spatial resolution reference maps of LAI on July 6, 2018 with independent *in situ* measurements from the FRM4VEG field campaign (July 3–6, 2018). The dashed line represents a 1:1 relationship.

IV. DISCUSSION

When compared to the multitemporal transfer functions based on vegetation indices, the superior performance of the INFORM- and $INFORM_{\text{broadband}}$ -based upscaling approaches (both under cross validation and when evaluated against independent field data) reveals the advantages of RTM-based methods. Because viewing/illumination angles are an explicit input, the approach is better able to account for seasonal changes in sun-sensor geometry over the course of the year. In contrast, the vegetation index-based multitemporal transfer functions rely solely on the ability of the selected index to suppress bidirectional reflectance effects, despite the fact that no index is sensitive only to the desired biophysical variable [27]. This is one factor that can contribute to seasonal variations in the vegetation index–biophysical variable relationship, as observed in several previous studies [28]–[31], reducing its robustness.

While the RTM-based methods did demonstrate the best performance in our study, it is worth noting that reasonable

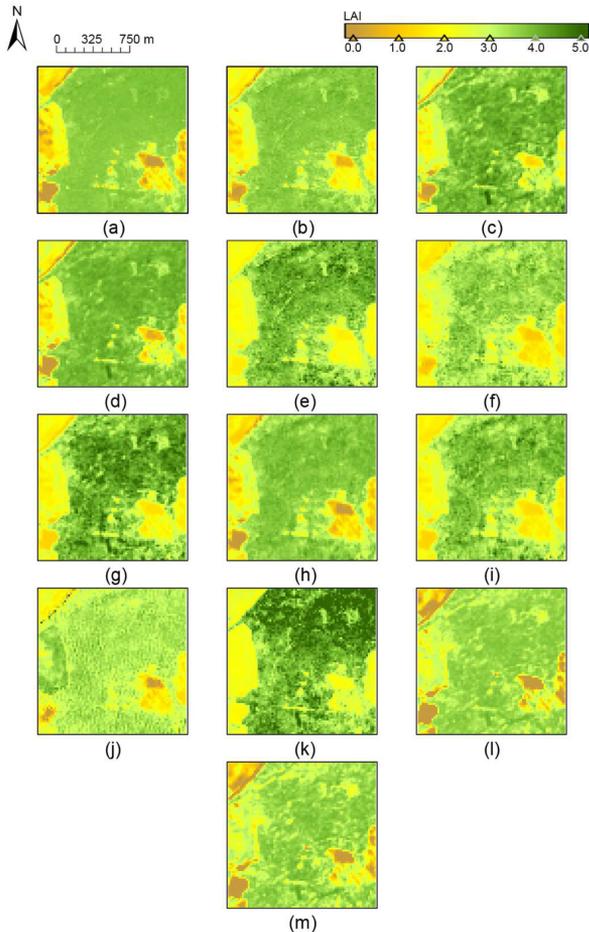


Fig. 4. (a) NDVI, (b) GNDVI, (c) SAVI, (d) OSAVI, (e) CI_{green} , (f) S2TCI, (g) IRECI, (h) SeLI, (i) $CI_{red-edge}$, (j) REP, (k) MCARI, and (l)–(m) INFORM-based high spatial resolution reference maps of LAI over a 1.5×1.5 km area surrounding the automated DHP system on July 6, 2018.

performance was also demonstrated by some of the vegetation index-based multitemporal transfer functions. Provided that a suitable range of vegetation indices is evaluated, and that careful calibration, assessment, and scrutiny of vegetation index-based multitemporal transfer functions is carried out (i.e., to verify that detrimental seasonal variations in the vegetation index–LAI relationship are not present), either approach could feasibly be used to derive time series of high spatial resolution LAI reference maps.

Amongst the investigated vegetation index-based multitemporal transfer functions, those that provided the best performance were based on traditional broadband indices (i.e., the NDVI and SAVI), reflecting their known association with LAI [32]. While comparable performance was demonstrated by some transfer functions based on red-edge indices (e.g., the SeLI), the incorporation of MSI’s red-edge bands did not universally improve performance. Similarly, the inclusion of MSI’s red-edge bands in the INFORM-based upscaling approach did not offer major gains in performance when compared to the $INFORM_{broadband}$ -based approach that excluded red-edge bands. Such results are not unexpected, since the red-edge region is most sensitive to biochemistry as opposed to canopy structure. Indeed, previous work has demonstrated that the incorporation

of information in the red-edge can increase sensitivity to variables related to pigmentation, including green LAI, leaf chlorophyll concentration (LCC), and canopy chlorophyll content (CCC) [22], [33]–[38]. In contrast, the automated DHP system adopted in our study does not discriminate between green and senescent leaves, making its measurements a purely structural quantity.

The fact that the majority of vegetation index-based multitemporal transfer functions overestimated lower LAI values is indicative of their sensitivity to the underlying soil background, which is another noncanopy factor known to perturb the vegetation index–biophysical variable relationship, particularly at low canopy densities [39], [40]. Indeed, those indices explicitly designed to minimize the influence of the soil background (i.e., the SAVI and OSAVI) were not subject to such overestimation. It is worth noting that other soil-resistant vegetation indices, such as the Enhanced Vegetation Index (EVI), were not analyzed in this study (the EVI was developed for the Moderate Resolution Imaging Spectroradiometer (MODIS) instrument, and its coefficients are not necessarily compatible with MSI data due to differences in band position and spectral response). Nevertheless, as an extension of the SAVI with additional terms to suppress atmospheric effects, the EVI is highly correlated to the SAVI [39], and would be expected to be similarly insensitive to the soil background. In the case of the RTM-based approach, reduced sensitivity to the soil background (and thus reduced bias at lower LAI values) is to be expected, since a variety of soil background reflectance spectra were explicitly incorporated in the INFORM simulations used to train the ANNs [26].

Despite the value of having independent *in situ* measurements with which to evaluate the considered upscaling approaches, it is important to recognize that the FRM4VEG dataset covered only the peak of the growing season, so performance could not be independently evaluated over the full range of LAI values experienced throughout the year (indeed, this a major drawback of one-off field campaigns). Additionally, the lack of leaf-off measurements meant a single WAI value had to be used to derive LAI over the FRM4VEG ESUs. Although this assumption may introduce some uncertainty into the absolute values of the performance statistics, its impact is the same for all investigated upscaling approaches, meaning their relative performances can still be reliably compared.

V. CONCLUSION

Whether assessed using cross validation or data from the independent field campaign, our results indicate that the RTM-based approach is most appropriate for upscaling temporally continuous *in situ* data. When compared to vegetation index-based multitemporal transfer functions, the ability of the RTM-based approach to account for seasonal changes in sun-sensor geometry is a key advantage. Future work should focus on more comprehensive evaluation of the RTM-based upscaling approach over a greater range of vegetation types and conditions. In this respect, independent field campaign datasets covering longer time periods (and ideally using alternative LAI measurement techniques over multiple growing seasons) will be required. Once suitably evaluated, the approaches demonstrated

in this study should prove useful for deriving time series of high spatial resolution LAI reference maps, enabling the validation of moderate spatial resolution (i.e., ≥ 300 m) LAI products using the emerging supply of temporally continuous *in situ* reference data.

APPENDIX

TABLE III

DISTRIBUTIONS FROM WHICH INFORM PARAMETERS USED TO ESTABLISH THE ANN TRAINING DATABASE WERE RANDOMLY DRAWN AFTER [26]

Parameter	Minimum	Maximum	Mean	Standard deviation	Reference
Structural parameter (N)	1.5	1.7	-	-	[41], [42]
Chlorophyll a + b ($\mu\text{g cm}^{-2}$)	10	60	50	20	[26]
Dry matter (g cm^{-2})	0.004	0.02	-	-	[41], [42]
Equivalent water thickness (g cm^{-2})	0.01	0.02	-	-	[41], [42]
Average leaf angle ($^{\circ}$)	55	55	-	-	[41], [42]
Single tree LAI	1.0	5.0	4.0	0.5	[26]
Understory LAI	0.5	0.5	-	-	[41], [42]
Stem density (ha^{-1})	72	536	256	106	[43]
Canopy height (m)	10	34	-	-	[44]
Crown diameter (m)	6	14	8	4	[43]
Solar zenith angle ($^{\circ}$)	29	64	-	-	[26]
Observer zenith angle ($^{\circ}$)	3	11	-	-	[26]
Relative azimuth angle ($^{\circ}$)	20	136	-	-	[26]
Soil brightness coefficient	0.5	0.5	-	-	[41]
Fraction of diffuse radiation	0.1	0.1	-	-	[41], [42], [45]

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Luke A. Brown (Member, IEEE) was born in Ascot, U.K., in 1993. He received the B.Sc. degree in geography and the M.Sc. degree in applied geographic information systems and remote sensing, in 2014 and 2015, respectively, from the University of Southampton, Southampton, U.K., where he is working toward the Ph.D. degree in remote sensing.

He is currently a Senior Research Assistant with the School of Geography and Environmental Science, University of Southampton, where he has previously worked as a Research Technician from 2017 to 2018.

His research interests are in the retrieval of vegetation biophysical and biochemical variables from optical remote sensing data, and in their validation using *in situ* measurement techniques.



Booker O. Ogutu received the B.Sc. degree in environmental science from Kenyatta University, Nairobi, Kenya, in 2001, the M.Phil. degree in geographic information systems and remote sensing from the University of Cambridge, Cambridge, U.K., in 2005, the joint M.Sc. degree in geoinformation science and earth observation for environmental modeling and management from Lund University, Lund, Sweden, the University of Warsaw, Warsaw, Poland, and the International Institute for Geo-Information Science and Earth Observation (ITC), University of Twente, Twente, The Netherlands, in 2008, and the Ph.D. degree in remote sensing from the University of Southampton, Southampton, U.K., in 2012.

From 2013 to 2015, he was a Lecturer in geographic information systems and remote sensing with the Department of Geography, University of Leicester, following a postdoctoral position from 2012 to 2013. He is currently a Lecturer in remote sensing with the School of Geography and Environmental Science, University of Southampton, where he has worked since 2015. His research interests include the exploitation and application of earth observation data to understand terrestrial ecosystem characteristics and dynamics.



Fernando Camacho received the Ph.D. degree in physics from the University of Valencia, Valencia, Spain, in 2004.

He is currently the Chief Executive Officer and Project Manager with the Earth Observation Laboratory, Paterna, Spain, which he founded in 2006 following a postdoctoral position at Medias-France. His research interests include the bidirectional reflectance distribution function, retrieval of biogeophysical variables from satellite optical data using empirical and physically-based methods, validation

of remote sensing products, and acquisition and upscaling of ground data in field campaigns for calibration and validation. He is currently the Chair of the Land Product Validation subgroup of the Committee on Earth Observation Satellites Working Group on Calibration and Validation.



Beatriz Fuster received the bachelor's degree in telecommunication technologies and services and the M.Sc. degree in telecommunication engineering from the Polytechnic University of Valencia, Spain, in 2015 and 2017, respectively.

From 2016 to 2019, she was a Research Engineer with the Earth Observation Laboratory, Paterna, Spain, where she worked in support of quality assurance of earth observation products for the Copernicus Global Land Service. Her research interests are in the training of neural networks and machine learning

procedures in order to develop algorithms to estimate biophysical products over croplands.



Jadunandan Dash received the M.Tech. degree in civil engineering from the Indian Institute of Technology, Kanpur, Kanpur, India, in 2002, and the Ph.D. degree in remote sensing from the University of Southampton, Southampton, U.K., in 2005.

He is currently a Professor in remote sensing with the School of Geography and Environmental Science, University of Southampton, where he has worked since 2006. He has a strong research background in pure and applied remote sensing, particularly in algorithm development, validation of vegetation bio-

physical products from earth observation data, and spatiotemporal analysis of earth observation data to understand the state of the world's ecosystems and the impacts of climate change.