Adapting a regularized canopy reflectance model (REGFLEC) for the retrieval challenges of dryland agricultural systems

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Keywords: LAI, leaf chlorophyll, REGFLEC, RapidEye, red-edge, aerosols, foliar dust, adjacency effects, precision agriculture

Abstract

A regularized canopy reflectance model (REGFLEC) is applied over a dryland irrigated agricultural system in Saudi Arabia for the purpose of retrieving leaf area index (LAI) and leaf chlorophyll content (Chl_i). To improve the robustness of the retrieved properties, REGFLEC was modified to 1) correct for aerosol and adjacency effects, 2) consider foliar dust effects on modeled canopy reflectances, 3) include spectral information in the red-edge wavelength region, and 4) exploit empirical LAI estimates in the model inversion. Using multi-spectral RapidEye imagery allowed Chl_i to be retrieved with a Mean Absolute Deviation (MAD) of $7.9 \mu\text{g cm}^{-2}$ (16%), based upon in-situ measurements conducted in fields of alfalfa, Rhodes grass and maize over the course of a growing season. LAI and Chl_i compensation effects on canopy reflectance were largely avoided by informing the inversion process with ancillary LAI inputs established empirically on the basis of a statistical machine learning technique. As a result, LAI was reproduced with good accuracy, with an overall MAD of $0.42 \text{ m}^2 \text{ m}^{-2}$ (12.5%). Results highlighted the considerable challenges associated with the translation of at-sensor radiance observations to surface bidirectional reflectances in dryland environments, where issues such as high aerosol loadings and large spatial gradients in surface reflectance from bright desert soils to dark vegetated fields are often present. Indeed, surface reflectances in the visible bands were reduced by up to 60% after correction for such adjacency effects. In addition, dust deposition on leaves required explicit modification of the reflectance sub-model to account for its influence. By implementing these model refinements, REGFLEC demonstrated its utility for within-field characterization of vegetation conditions over the challenging landscapes typical of dryland agricultural regions, offering a means through which improvements can be made in the management of these globally important systems.

1. Introduction

Dryland systems present a challenging environment for agricultural production, yet comprise 27% of total area under active cultivation globally (FAOSTAT, 2015; Wang et al., 2012). Rise in agricultural output and increasing demands on water supplies, coupled with variability in water quality and the

over-exploitation and depletion of aquifer systems (Rodell et al., 2009), severely impact the sustainability of dryland agriculture (Oki and Kanae, 2006). Remotely sensed information on within-field variability in crop growth and health offer an important mechanism to improve agricultural system management and optimize crop production.

Plant biochemical and biophysical quantities such as leaf chlorophyll content (Chl_l) and leaf area index (LAI), have significant utility in the characterization and monitoring of vegetation distribution, health and function and serve as valuable observational proxies for ecosystem functional behavior in both space and time domains (Houborg et al., 2015c; Musavi et al., 2015). For instance, Chl_l responds to changes in leaf nitrogen (Evans, 1989; Sage et al., 1987) and plant phenology (Croft et al., 2014; Houborg et al., 2011) and is recognized as a useful indicator of plant stress (Elarab et al., 2015; Zarco-Tejada et al., 2002), which is of particular interest in precision agriculture applications (Haboudane et al., 2002). Moreover, functional associations between Chl_l and photosynthetic efficiency have facilitated integration within physical land surface models as an observational constraint on coupled fluxes of water and carbon (Houborg et al., 2015c; Schull et al., 2015). Similarly, LAI is of use in models monitoring crop growth (Doraiswamy et al., 2004; Dorigo et al., 2007; Launay and Guerif, 2005) and land surface flux estimation (Kalma et al., 2008), in addition to being a useful metric for vegetation health (Anderson et al., 2015) and productivity (Gitelson et al., 2014).

Distributed information on within-field variability of non-optimal growing conditions is important in defining spatially explicit strategies for maximizing yield, as well as optimizing the application of water and fertilizer (Robert, 2002). However, the simultaneous requirements of very high spatial resolution ($<10m$) and time-critical acquisition have traditionally limited the utility of operational satellite systems for precision agriculture characterization (Moran et al., 1997). The advent of programmable commercial sensor systems has facilitated routine monitoring at 1–10 m resolution (Houborg et al., 2015a) and renewed opportunities in the context of precision agriculture. Examples such as the RapidEye (2008-) and WorldView (2009-) series of satellites provide multi-spectral sensor designs with pixel resolutions of between 2-5 m, potential revisit times of 1 to 5 days, and

enhancements to spectral monitoring with band(s) in the red-edge spectrum. The advantage of using the red-edge for agricultural applications has been observed in a number of investigations focusing on the estimation of leaf biochemistry (Clevers and Gitelson, 2013; Dash and Curran, 2007; Gitelson et al., 2003; Homolová et al., 2013) and vegetation density (Frampton et al., 2013; Viña et al., 2011). Developing retrieval techniques that exploit the enhanced information content of the red-edge is particularly pertinent in light of the recent launch of Sentinel-2, which will deliver multi-spectral data in critical regions of the spectrum (including two narrow bands in the red-edge) at resolutions down to 10 m and with a 5 – 10 day revisit capability. Exploiting these spectral advances however, is non-trivial.

Remotely sensed surface radiance fields represent a complex interaction of soil, leaf, canopy, and atmospheric influences that require careful treatment for translation into meaningful descriptors of vegetation properties. While the complexities of atmospheric absorption by gases and scattering by air molecules and aerosols can be modeled relatively accurately (Berk et al., 1999; Vermote et al., 1997), efficient removal of other atmospheric effects is challenged by uncertainties in the parameterization of atmospheric composition: especially aerosol optical thickness and size distribution (Hagolle et al., 2015). Uncertainties in the derived surface reflectance field can be particularly pronounced over dryland agricultural environments due to increased aerosol loadings and adjacency effects resulting from reflected background radiation scattered into the sensor field of view (Liang et al., 2001). Dust deposition on leaves adds an additional level of complexity in arid and semi-arid settings. The effect of foliar dust on reflectance spectra has received relatively little attention (Wu and Wang, 2015) and much remains unknown on this important element of dryland environments. In addition to spectral considerations, foliar dust has been shown to affect plant physiological response, with negative impacts on stomatal conductance, productivity and transpiration (Farmer, 1993; Hirano et al., 1995). Given an accurate representation of the surface reflectance field within discrete sensor bands, a canopy radiative transfer model (CRTM) can be used to invert reflectance spectra into relevant biophysical and biochemical vegetation characteristics (Darvishzadeh et al., 2008; Malenovský et al.,

2013; Rivera et al., 2013; Verrelst et al., 2014). However, a robust discrimination between soil, leaf, and canopy contributions is complicated by the ill-posedness of model inversion or compensation effects (Combal et al., 2002; Zurita-Milla et al., 2015), meaning that almost identical reflectance spectra can result from different parameter combinations. Introducing regularization strategies or constraints can improve the differentiation of component variables. These may be in the form of prior information (Dorigo et al., 2009; Houborg et al., 2007), additional spectral bands with enhanced sensitivity towards the target variable (Delegido et al., 2010), constraints based on spatial and temporal features in the satellite data (Atzberger, 2004; Houborg and Anderson, 2009) or via the integration of empirical data.

One approach developed to do explore these concepts is the regularized canopy reflectance model, REGFLEC (Houborg et al., 2015b). REGFLEC integrates leaf, canopy and atmospheric radiative transfer models, while maintaining a balance between sufficient physical realism and simplicity for application to remotely sensed reflectance fields across different vegetation types and landscapes. REGFLEC has previously been applied to multi-spectral sensors with standard bands in the green, red and near-infrared domains, including SPOT (Houborg and Boegh, 2008), Landsat (Houborg and Anderson, 2009; Houborg et al., 2007, 2015b, 2013), and aircraft (Houborg et al., 2009) sensors. A motivation of the current contribution is to extend REGFLEC to multi-spectral sensor systems with a band in the red-edge domain, in order to take advantage of the enhanced information content for Chl_l and LAI prediction (Clevers, 1999). Ancillary LAI, derived on the basis of an empirical statistical approach, is integrated as an additional constraint for improving the discrimination of Chl_l and LAI effects. Further, a module for considering foliar dust effects on canopy reflectance spectra is added to the REGFLEC framework.

The key objective of this study is to improve the robustness and utility of REGFLEC for application over dryland systems. Specifically, the research aims to 1) implement a correction for adjacency effects and evaluate the impact of these on the surface reflectance field and vegetation retrievals, 2) outline and evaluate a simple approach for considering foliar dust effects on modeled canopy spectra,

Fig. 1 Location of the Tawdeehiya commercial farm in Saudi Arabia with identification of intensive measurement zones (IMZ) during the three field campaigns in 2015. The image is a natural color representation of 5 m resolution RapidEye data collected on May 31 (DOY 151).

3) exploit the advantage of sensors with red-edge capability, and 4) exploit the combined benefits of physical and empirical retrievals to effectively constrain the inverse estimation of vegetation properties.

2. Material and methods

2.1 Study site

The Tawdeehiya Farm (24.174 °N, 48.015 °E) is located in the desert region of Al-Kharj, approximately 200 km southeast of the capital Riyadh, in Saudi Arabia (Fig. 1). This commercial property operates 47 fields with center-pivot irrigation systems (diameter ~ 800 m) installed on flat desert terrain approximately 380 m above sea level. Key crops under irrigation include alfalfa (22 fields), Rhodes grass (8 fields), maize (11 fields) and carrots (4 fields). The region is characterized by an extreme arid climate with hot summer months (average high of 43°C) and an average annual precipitation total of 95 mm that is concentrated during the months of December through April (PME, 2009; Kenaway and McCabe, 2015). The present study uses data collected across three intensive field campaigns in 2015 that took place between March 22 – March 25 (satellite overpass on March 28), April 12 – April 16 (satellite overpass on April 12), and May 31 – June 4 (satellite overpass on May 31), covering a range in plant development stages of the four crops. The daytime highs during the

Fig. 2 Time-series of aerosol optical thickness at 550 nm (τ_{550}) over Tawdeehiya and Solar Village retrieved from Terra MODIS and AERONET sun-photometer data at MODIS acquisition times. Gaps occasionally occur in the MODIS records due to the MODIS revisit capability (1 – 2 days) or lack of high quality retrievals. The shaded bars represent the timing and durations of the three field campaigns at Tawdeehiya. Time-series correlations (R^2) between the MODIS and AERONET datasets are indicated at the top.

three campaigns were 31°C, 40°C, and 46°C, respectively. Skies were cloud free throughout much of the period, but high frequencies of hazy conditions and occasional dust storms are evident in MODIS and nearby Aerosol Robotic Network (AERONET) records of aerosol optical thickness (τ) (Fig. 2). Atmospheric conditions were more turbid during the second campaign (April 12 – April 16) with regional τ at 550 nm (τ_{550}) occasionally above 1 and hazy field conditions associated with strong winds. Aerosol loadings were generally lower during the other two campaigns and winds were calmer, although day-to-day variations in τ could be significant.

2.2 In-situ measurements

During each of the campaigns, non-destructive sampling of biophysical properties was conducted within small (10 x 10 m) intensive measurement zones (IMZ) established in relatively homogeneous sections of the fields (Fig. 1). A total of 93 IMZs in fields of alfalfa (n=41), Rhodes grass (n=14),

maize (n=29), and carrots (n=9) were sampled over the duration of the three campaigns. Specific attention was given to LAI, defined as the one-sided green leaf area per unit horizontal ground area [$\text{m}^2 \text{ m}^{-2}$] and Chl_l , defined as the total chlorophyll *a* plus chlorophyll *b* content on a one-sided leaf area basis [$\mu\text{g cm}^{-2}$]. Within each IMZ, a grid of five plots was defined (i.e., a center plot and four plots positioned at the corners) and measurements at each plot were averaged to achieve a representative value for that specific IMZ. LAI was measured using a LAI-2200C plant canopy analyzer (LICOR, U.S.A.) using a 270° view cap to avoid interferences caused by the operator. At each plot, one above-canopy and four below-canopy readings were conducted and repeated once. For the row crops (maize and carrots), the four below-canopy readings were collected along diagonal transects between the rows to better approximate the ‘true’ (i.e., from destructive sampling) LAI (Houborg et al., 2013). Thus in each IMZ, the average of five LAI-2200C measurements (5 x 8 below canopy readings) was used.

Measurements were conducted throughout the day on clear days and corrected for light scattering (Kobayashi et al., 2013) to reduce uncertainties in LAI estimation for data taken in direct sun. The correction for light scattering was facilitated by instrument software (i.e. FV2200) using primary inputs of solar position (solar zenith and azimuth angles) and fraction of total incoming radiation (in the 230-490 nm waveband) that is in direct beam (f_{beam}). f_{beam} may be measured in the field by taking above canopy readings with a white diffuser cap for sunlit and shaded conditions followed by a shaded reading without a cap, as outlined in the LAI-2200C manual. f_{beam} can vary significantly over the course of the day and with changes in atmospheric turbidity, and not all of the LAI measurements could be associated with a near time-coincident scattering recording. In these cases, f_{beam} was calculated as a function of the sun zenith angle (θ_{sz}) and the atmospheric transmittance of direct sunlight in the blue band (T_{blue}) according to:

$$f_{\text{beam}} = T_{\text{blue}} \sqrt{\cos(\theta_{\text{sz}})} \quad \text{Eq. 1}$$

T_{blue} was derived from the aerosol optical thickness (τ) integrated over the blue waveband of the instrument (230 – 490 nm) based on representative day specific inputs of τ_{550} :

$$T_{blue} = \sum_{i=230}^{i=490} \exp(-\tau_i) / 260 \quad \text{Eq. 2}$$

where $\tau_i = \beta \cdot \lambda_i^{-\alpha}$ and $\beta = \tau_{550} / (550)^{-\alpha}$. Here β is Ångström's turbidity coefficient, λ is wavelength in microns and α is the Ångström exponent. τ_{550} was derived from a combination of MODIS and AERONET observations, whereas values of α were taken from AERONET observations at the Solar Village (see Section 2.4). The outlined approach considers variations in atmospheric turbidity during clear skies and facilitates scattering correction of measurements recorded with any LICOR plant canopy analyzer with inputs of solar position, τ_{550} , and α .

Chl_i was measured with a portable SPAD-502 meter (Konica Minolta, Inc., Osaka, Japan) in all IMZ except for carrot (leaves were too narrow). In maize, SPAD readings were taken at six locations on each leaf and averaged, with the procedure repeated for a total of four leaves (top-most) at each sampling plot. The resulting 5 x 4 measurements (i.e., 5 x 24 readings) were averaged over the IMZ. For alfalfa and Rhodes grass, five SPAD readings taken on random leaves were averaged and repeated five times on different leaves within each sampling plot to produce a single representative IMZ value based on a total of 5 x 5 measurements (i.e., 5 x 25 readings). The non-dimensional SPAD units (0 – 99) were converted to actual leaf chlorophyll content in units of $\mu\text{g cm}^{-2}$ using a calibration curve ($\text{Chl}_i = 87.889 \times \exp[0.0103 \times \text{SPAD}] - 92.911$, $R^2=0.93$, $\text{RMSD}=4.9 \mu\text{g cm}^{-2}$) derived on the basis of a spectrophotometrical analysis of multi-species agricultural leaf samples (Houborg and Anderson, 2009). Chl_i estimates from this calibration closely resembles ($R^2=0.99$, $\text{RMSD}=2.4 \mu\text{g cm}^{-2}$) estimates from the transformation equation ($\text{Chl}_i = [99\text{SPAD}]/[144-\text{SPAD}]$) derived based on a compilation of eight different calibration models (Cerovic et al., 2012), which suggests that using a single calibration curve irrespective of species type and SPAD sensor unit is robust.

2.3 RapidEye data

RapidEye (<http://www.blackbridge.com>) comprises a five-satellite constellation with identical multi-spectral sensors, providing imagery at a spatial resolution of 6.5 m at nadir in blue (440-510 nm),

Table 1 Inputs to 6SV during RapidEye satellite acquisitions over the Tawdeehiya farm in 2015. These include sun zenith (θ_{sz}), sun azimuth (θ_{saz}), sensor view zenith (θ_{vz}), and sensor azimuth (θ_{sataz}) angles, total columnar ozone (O_3), aerosol optical thickness at 550 nm (τ_{550}), and total precipitable water (TPW). H_r represent the source area (distance from target) for calculating the surface reflectance of the surrounding area in the adjacency correction (Eq. 3). Note that vertical profiles of humidity and ozone (from AIRS) were used in addition to the total columnar amounts. See Section 2.4 for further descriptions of data sources and retrieval techniques for the atmospheric parameters.

Dates	Doy	Time	τ_{550}	H_r [km]	TPW [g cm ⁻²]	O_3 [cm-atm]	θ_{sz} [°]	θ_{vz} [°]	θ_{saz} [°]	θ_{sataz} [°]
March 28	87	11:15	0.431	0.80	2.80	0.294	23.0	16.9	155	278
April 12	102	11:29	0.742	0.60	2.20	0.284	16.1	12.8	162	99
May 31	151	11:14	0.560	0.65	1.50	0.303	7.6	3.2	105	99

green (520-590 nm), red (630-685 nm), red-edge (690-730 nm) and near-infrared (760-850 nm) spectral bands. RapidEye level 3A products were provided as 25 by 25 km tiles radiometrically and geometrically corrected and aligned to a UTM map projection (with an orthorectified pixel size of 5 m) by incorporating ground control points and a digital elevation model. The standard locational accuracy is reported as 10 m root-mean-square-error or better (Blackbridge.com, 2015). A total of three scenes were acquired within 2–5 days of the in-situ data collections (Table 1) during cloud free conditions.

2.4 Atmospheric correction

At-sensor multi-spectral radiances were atmospherically corrected to bidirectional surface reflectances using the vector version of the Second Simulation of the Satellite Signal in the Solar Spectrum, 6SV (Kotchenova et al., 2006; Vermote et al., 1997), following the automated processing stream implemented in REGFLEC (Houborg et al., 2015b). Table 1 lists the various inputs required by 6SV. Information on Total Precipitable Water (TPW) and total columnar ozone (O_3) were acquired from the Terra MODIS water vapor product (MOD05) and the Aura Ozone Monitoring Instrument (OMI), respectively. Vertical profiles of temperature, humidity and ozone were taken from the Aqua AIRS standard product. Given the limited extent of the study region (Fig. 1) relative to the spatial resolution

of the atmospheric state data, a single parameter value or profile (average of available retrievals) was assumed to apply to the entire region.

The arid desert environment and high frequency of days with significant aerosol loadings (Fig. 1) warrant careful attention to the specification of τ_{550} . The closest AERONET (Holben et al., 1998) site (Solar Village; 24.91°N, 46.41°E) is located immediately west of Riyadh and approximately 200 km from the Tawdeehiya farm. While sun photometer measurements (level 1.5) of τ_{550} from the Solar Village are in good agreement ($R^2=0.80$, bias=-7.3%) with time- and space-coincident Terra MODIS Deep Blue algorithm (MOD04) retrievals (Levy et al., 2015), they are not directly useable over Tawdeehiya due to significant regional variations in τ_{550} , as reflected in the corresponding MODIS records from the two sites (Fig. 2). Site-specific AERONET measurements (τ_{550}^{aero}) and MODIS retrievals directly over the Solar Village ($\tau_{550}^{m_{sv}}$) and Tawdeehiya ($\tau_{550}^{m_{taw}}$) were combined to exploit the high accuracy of the in-situ observations and spatial information content of the satellite data for τ_{550} predictions over Tawdeehiya ($\tau_{550}^{c_{taw}}$). Specifically, the relative spatial difference between the MODIS retrievals (average value of a 3×3 pixel box centered over the sites) was used to adjust the AERONET measurement between the Solar Village and Tawdeehiya according to:

$$\tau_{550}^{c_{taw}} = \left(1 + \left[\tau_{550}^{m_{taw}} - \tau_{550}^{m_{sv}}\right] / \tau_{550}^{m_{sv}}\right) \cdot \tau_{550}^{aero} \quad \text{Eq. 3}$$

This approach resulted in values of $\tau_{550}^{c_{taw}}$ that were in good agreement with coincident MODIS retrievals over the farm, as evidenced by a largely unbiased relationship with an R^2 of 0.86 and differences generally less than $\pm(0.05+0.2\tau_{550})$ (Fig. S1a). The combined τ_{550} estimates ($\tau_{550}^{c_{taw}}$) are expected to more closely resemble actual turbidities, but the good inter-correlation (Fig. S1a) suggests that MODIS retrievals ($\tau_{550}^{m_{taw}}$) will provide a reasonable approximation in case inputs to Eq. 3 are missing. The measurements of τ_{550}^{aero} used in Eq. 3 were near time-coincident with the RapidEye acquisitions (Table 1).

The aerosol model parameterization represents another critical element in the atmospheric correction of satellite imagery (Hagolle et al., 2015). 6SV implements a number of standard aerosol models such

as rural, urban and desert, with predefined aerosol radiative characteristics. An alternative approach is to define the model on the basis of sun-photometer measurements of the aerosol size volume distribution and refractive index (Dubovik et al., 2006). The latter approach was adopted in this study, given the proximity of the Solar Village AERONET site to the Tawdeehiya farm. It is expected that doing this will better capture the regional characteristics of the size distribution and significant temporal variations caused by dust events (Fig. S1b).

Correction for adjacency effects are typically needed for high spatial resolution observations, particularly in landscapes with large contrasts in surface reflectance (Liang et al., 2001). The adjacency effect represents reflected radiation from surrounding pixels that are then scattered into the sensor field of view (Richter et al., 2006; Kaufman, 1985). Following Vermote et al. (1997), the correction for adjacency effects is directly related to the atmospheric turbidity and the reflectance contrasts between the target and surrounding area:

$$\rho_{s,adj}^{\lambda} = \rho_s^{\lambda} + \frac{t_{diffu}^{\lambda}}{t_{diru}^{\lambda}} (\rho_s^{\lambda} - \rho_{env}^{\lambda}) \quad \text{Eq. 4}$$

Here $\rho_{s,adj}^{\lambda}$ is the adjacency corrected surface reflectance for a given spectral band (λ), ρ_s^{λ} , t_{diffu}^{λ} and t_{diru}^{λ} are the atmospherically corrected surface reflectance, total diffuse upward transmission and total direct upward transmission respectively, all produced by 6SV for each acquisition and spectral band. The environmental surface reflectance contribution (ρ_{env}^{λ}) was estimated by applying a low pass filter to the initial image of ρ_s^{λ} . The relative kernel weights were assigned as a function of the distance of the contributing area from the target pixel as determined by the horizontal range (H_r) of the adjacency effect. Values between 0.5 – 1.5 km are typically used for H_r . A dependence on the atmospheric optical thickness was reported in (Kaufman and Joseph, 1982), with H_r values as low as 0.4 km during high atmospheric turbidities. A significantly larger adjacency range (i.e. > 5 km) is expected for very clear atmospheres where molecular scattering becomes dominant (Kaufman and Joseph, 1982). In this study, H_r was initially assigned a value of 1.5 km, and then iteratively optimized to avoid negative values in the adjacency corrected red band reflectances (Table 1).

2.5 LAI and Chl_l retrieval approach

REGFLEC was used for the retrieval of LAI and Chl_l. The model framework invokes a multi-step approach for regularizing (i.e. constraining) the inverse estimation of vegetation characteristics from satellite observed reflectance spectra, as described in detail in Houborg et al. (2015b). The introduction of additional information via regularization strategies is critically important, as the ill-posed nature of model inversion can otherwise result in non-unique solutions (Combal et al., 2002). Refinements in this study (REGFLEC Version 3.0) include consideration of adjacency effects (Section 2.4), the addition of a band in the red-edge region (Section 2.5.1), a correction scheme for considering the presence of foliar dust (Section 2.5.2), and ancillary LAI inputs empirically established on the basis of a statistical machine learning technique (Section 2.5.3). To briefly summarize, REGFLEC integrates atmospheric radiative transfer (6SV; Kotchenova et al., 2006; Vermote et al., 1997), canopy reflectance (4SAIL; Verhoef and Bach, 2007; Verhoef, 1984) and leaf optical (PROSPECT; Feret et al., 2008; Jacquemoud and Baret, 1990) models. The Scattering by Arbitrary Inclined Leaves model (4SAIL), calculates bidirectional canopy reflectance over relevant sensor-specific spectral bandwidths given inputs of observation geometry, LAI, mean leaf inclination angle (θ_l), two soil parameters (s_1 and s_2) (Houborg and Boegh, 2008; Price, 1990), canopy fraction of senescent leaf material (f_B), a hot spot parameter (s_L), the fraction of diffuse radiation, and leaf reflectance and transmittance. Leaf reflectance and transmittance spectra are simulated by PROSPECT with inputs of a leaf mesophyll structure parameter (N), Chl_l, equivalent water thickness (C_w), dry matter content (C_m), and leaf brown pigments (C_{bp}).

REGFLEC builds a suite of predictive (LAI and Chl_l) Vegetation Index (VI) relationships that consider spatio-temporal variations in the internal and external model parameters listed above. Careful attention to confounding factors in spectrum-trait relations is critical in order to improve the robustness and accuracy of retrieved properties and reduce the confusion between atmospheric, soil,

canopy and leaf contributions to the satellite observed reflectance field (Zurita-Milla et al., 2015). For this purpose, REGFLEC embeds a multi-step Look-Up-Table (LUT) based inversion scheme that 1) attempts to reduce obfuscating influences of the soil background signal on the vegetation retrievals by estimating representative ranges of s_1 and s_2 on the basis of bare or sparsely vegetated pixels and 2) retrieves optimal sets of land cover specific vegetation parameters based on spectral observations over intermediate to dense vegetation from multiple scenes available over a growing season. Optimal model parameter combinations (i.e., LAI, Chl_l , N , θ_l , f_B , D_f , C_m , s_1 , and s_2) are retrieved by minimizing the mean absolute error between modeled and observed spectral reflectances (i.e., green, red, red-edge, NIR) via a merit function:

$$\min \left(\frac{1}{n} \sum_{i=1}^n |\rho_{obs} - \rho_{pre}| + \overline{pen} \right) \quad \text{Eq. 5}$$

where p_{obs} and p_{pre} represent observed and model reflectances for the discrete wavebands of the remote sensor, n is the number of spectral observations, and pen is a penalty operator (Houborg et al., 2009). The process of matching modeled and measured LUT spectra is iterative (i.e., the merit function is evaluated for a wide range of parameter combinations), which facilitates effective use of spatial and temporal constraints and ancillary information (Houborg et al., 2015b). Finally, LAI and Chl_l are mapped over the modeling domain based on appropriate model-diagnosed VI relationships that reflect differences in the respective model parameters.

2.5.1 Integration of red-edge information

In previous applications (e.g., Houborg and Anderson, 2009; Houborg and Boegh, 2008), REGFLEC has been configured to use standard bands in the green (R_{gre}), red (R_{red}), and near-infrared (R_{nir}) for establishing high sensitivity VIs for mapping LAI (VI_{lai}) and Chl_l (VI_{chl}). In this study, REGFLEC was extended to include a band in the red-edge region in an effort to exploit the enhanced information content associated with this wavelength region (i.e. 690 – 740 nm) (Clevers and Gitelson, 2013;

Haboudane et al., 2002; Ramoelo et al., 2015). The MERIS Terrestrial Chlorophyll Index (MTCI) (Dash and Curran, 2004) has demonstrated greater linearity and improved sensitivity over the full range of Chl_l values (Dash and Curran, 2007) and was adopted as VI_{chl} using the spectral configuration of the RapidEye sensor (i.e. $MTCI = [R_{nir} - R_{redge}] / [R_{redge} - R_{red}]$). In this form, model simulated MTCI responds linearly to changes in Chl_l with a significantly enhanced sensitivity at the high range, in contrast to $R_{gre} - Chl_l$ relationships that start to saturate at intermediate values of Chl_l (Fig. S2). In addition, the index normalization reduces the effect of confounding factors, particularly at the lower Chl_l range. At the same time, red-edge reflectance is highly sensitive to variations in LAI and when combined with near-infrared reflectance in a simple ratio (R_{nir}/R_{redge}) constitutes a robust approach for the estimation of green LAI (Viña et al., 2011). An important feature of $R_{nir}/R_{redge} - LAI$ relationships is the improved predictability over dense vegetation relative to VIs based on red and near-infrared band reflectances, such as the NDVI and two-band Enhanced Vegetation Index (EVI2; Jiang et al., 2008) (Fig. S3), which are used in REGFLEC applications based on Landsat imagery (Houborg et al., 2015b). Given the enhanced canopy penetration ability and sensing depth of red-edge reflectance (Ciganda et al., 2012), the red-edge configuration (VI_{lai} and VI_{chl}) of REGFLEC is expected to provide estimates more representative of canopy layers from bottom to top. A full evaluation of the potential benefits of incorporating red-edge information is beyond the scope of this study but forms the central topic of a follow-up contribution.

2.5.2 Correction for foliar dust

The high frequency of dust events in the region warrants investigations into the effect of foliar dust on modeled canopy reflectance spectra. A simple correction was implemented into 4SAIL in an attempt to simulate the spatial and temporal impact of this phenomenon over the three field campaigns. Here, the reflective property of dust was assumed to mimic the local soil surface reflectance. When foliar dust is present, the spectral signature of dust will modulate the observed surface reflectance as a function of the density and characteristics of the vegetation and the fraction of foliar dust (D_f) on the

Fig. 3 Visualization of the simple correction for foliar dust implemented into 4SAIL. Modeled surface reflectances are modulated by changes in the fraction of foliar dust (D_f) as a function of the spectral signature of dust, which was assumed to approximate the local soil reflectance signal. Results are shown for a dense canopy with $LAI=4$, $\theta_{II}=57^\circ$, $Chl_I=50 \mu g cm^{-2}$, $C_m=50 g m^{-2}$, $N=1.75$, $s_1=0.4$, and $s_2=0$ assuming the observation geometry from DOY 102 (Table 1). The spectral responses of the green, red, red-edge and near-infrared RapidEye bands are shown on the secondary y-axis.

canopy. This was modeled by weighting the spectral signature of the bidirectional surface reflectance (R_s^λ) and soil surface reflectance (R_{soil}^λ) with D_f according to:

$$R_{s,dust}^\lambda = R_s^\lambda (1 - D_f) + R_{soil}^\lambda \cdot D_f \quad \text{Eq. 6}$$

where $R_{s,dust}^\lambda$ is the modeled surface reflectance with consideration of foliar dust and λ is the spectral wavelength. The impact of the correction is illustrated in Fig. 3 for a dense canopy with a given soil spectral signature ($s_2=0$, $s_1=0.4$). The contrast between green leaf and soil spectral signatures causes an increase in the visible domain and a decrease in the near-infrared domain, with an inflection point in the red-edge. In addition, the characteristic reflectance peak in the green domain

decreases with D_f and is largely indiscernible during significant dust amounts (ie. $D_f > 0.2$). This results from the typical increase in dust (i.e. soil) reflectance with wavelength (Fig. 3). These features are similar to results reported in Wu and Wang (2015) based on in-situ collected reflectance spectra over dust-affected areas in China.

D_f was added as a free variable in the REGFLEC inversion process to facilitate temporally varying foliar dust amounts on a crop-specific basis. The retrieval of crop-specific D_f was targeted towards the densest vegetation elements in order not to confuse the retrieval with changes in the soil background signal and to better approximate leaf level conditions. The LAI weighted average of these retrievals was then extrapolated to the entire vegetation type under examination.

2.5.3 Ancillary LAI constraint

The use of ancillary LAI within the REGFLEC inversion scheme has been shown previously to be an important regularization constraint for better discriminating LAI and Chl_l effects on observed reflectance spectra (Houborg et al., 2015b). The ancillary LAI maps serve to initialize the inversion process and better constrain the retrieval of land cover class-specific parameters (N , θ_l , C_m , D_f) and provide an informed basis for simultaneous retrieval of LAI and Chl_l (Houborg et al., 2015b).

In this study, the ancillary LAI data was derived from RapidEye spectral data based on an empirical multi-variate VI relationship established by Cubist (RuleQuest; www.rulequest.com). Cubist represents a data mining approach for identifying effective rule-based predictive models on the basis of a training dataset of observed target and explanatory variables. The training dataset consisted of the in-situ collected LAI (Section 2.2) from the three field campaigns, which were paired with a wide range of appropriate explanatory VIs extracted from the imagery within 2-5 days of the in-situ collections. These included the Simple Ratio (SR; Jordan, 1969), NDVI (Rouse et al., 1974), EVI2, Red-edge Simple Ratio (RSR), MTCI, Modified Triangular Vegetation Index (MTVI2; Haboudane, 2004), Transformed Chlorophyll Absorption Ratio Index (TCARI; Haboudane et al., 2002) and

Optimized Soil Adjusted Vegetation Index (OSAVI; Steven, 1998), in addition to the exponential and squared form of each VI. Single band reflectances were excluded from the list of attributes, as these are very sensitive to variations in confounding factors between acquisitions and lack generality compared to normalized VIs (Broge and Leblanc, 2001).

The Cubist software identifies the optimal combination of VIs based on the given training dataset, which are then used to map LAI over the full extent of the imagery. While the use of multiple rules may improve the agreement between the in-situ LAI and RapidEye spectral data, given the size of the training dataset (n=93) a single rule was enforced in order not to disrupt the spatial LAI value continuity (Houborg et al., 2016). The full training dataset was used to build the regression for generating the ancillary LAI inputs to REGFLEC. However, in order to test the predictive power on unseen data, the training database was separated into two groups, with the largest (70%) used for model training and the smaller (30%) used for independent model validation. Both groups contained LAI values distributed over the observed range from each of the acquisition days.

2.5.4 REGFLEC implementation

The specific canopy, leaf and soil parameter values and ranges used in the implementation of REGFLEC over the Tawdeehiya farm are listed in Table 2. f_B and C_{bp} were both assigned a value of zero, as leaf senescence was negligible over the course of the field campaigns. Leaf water content does not affect the spectrum observed by the RapidEye multi-spectral sensor so was arbitrarily fixed at 0.02 g cm^{-2} .

The separation of individual crop classes represents a critical element for constraining the estimation of the free model parameters (Houborg et al., 2015b). For this purpose, a land cover map was established by digitizing field pivot boundaries and assigning crop type based on visual inspections in the field. Knowledge of the actual cover types was used to assign representative estimates of the leaf

mesophyll structure (N). While the quantification of N is associated with uncertainty (Ceccato et al., 2001), it typically varies between 1–3 (Feret et al., 2011; Jacquemoud and Baret, 1990) and relates to

Table 2 Parameterizations of soil, leaf and canopy variables used in the present implementation of REGFLEC. The observation geometry for each overpass is provided in Table 1.

Parameters	Units	Symbol	Range
<i>Canopy</i>			
Leaf area index	$\text{m}^2 \text{m}^{-2}$	LAI	0 – 7
Mean leaf inclination angle	Deg	θ_l	15 – 80
Hot spot size	m m^{-1}	s_L	0.5/LAI
Fraction of senescent material	Unitless	f_B	0
Fraction of diffuse radiation	Unitless	skyl	$f(\tau_{550})$
Fraction of foliar dust	Unitless	D_f	0 – 0.3
<i>Soil</i>			
Weight of the 1 st Price function	Unitless	s_1	0.1 – 0.6
Weight of the 2 nd Price function	Unitless	s_2	-0.1 – 0.1
<i>Leaf</i>			
Leaf chlorophyll content	$\mu\text{g cm}^{-2}$	Chl_l	10 – 90
Leaf mesophyll structure	Unitless	N	1.0 ¹ , 2.5 ²
Leaf equivalent water thickness	g cm^{-2}	C_w	0.02
Dry matter content	g m^{-2}	C_m	25 – 100
Leaf brown pigment	Unitless	C_{bp}	0

¹Expert estimate used for maize and grass

²Expert estimate used for alfalfa and carrot

the compactness of the mesophyll, which can vary significantly dependent on vegetation type. Monocots (monocotyledons) such as maize have a compact structure, whereas dicots (dicotyledonous) such as alfalfa have more spongy leaves with air cavities (Verdebout et al., 1994). Accordingly, N for maize and Rhodes grass (monocots) were assigned a value of 1.0 whereas N=2.5 was used for alfalfa and carrot (dicots). Only limited variation (± 0.3) around these “expert” estimates were allowed in the inversion. The use of these prescribed N estimates serves to reduce the dimensionality of the ill-posed inversion process and compensating associations with θ_l (Houborg et al., 2015b; Zurita-Milla et al., 2015). A wide distribution space within realistic limits was assumed for the remaining free variables (Table 2). Of these, the soil parameters, Chl_l and LAI were allowed to vary on a per pixel basis, whereas optimized values of N, C_m , θ_l and D_f were derived for each crop class. While N and C_m are assumed to remain constant over the growing season, temporal adjustment of θ_l and D_f is achieved for each crop class by re-optimization against the observed reflectances on a scene-specific basis.

2.6 REGFLEC evaluations

The performance of REGFLEC was evaluated for three different configurations to investigate the impact of adjacency correction effects and foliar dust on vegetation retrievals and matching of modeled (REGFLEC) and observed (RapidEye) reflectance spectra. Two configurations assumed $D_f=0$, with inputs of atmospherically corrected reflectances both without (R_{noadj}) and with (R_{adj}) adjacency corrections applied. The final configuration ($R_{\text{adj_dust}}$) considered adjacency effects as well as foliar dust.

The vegetation retrievals were validated against in-situ measurement using standard statistics including the coefficient of determination (R^2), the Root-Mean-Square Difference (RMSD), the Mean Absolute Deviation (MAD), and the Mean Bias Deviation (MBD; positive when REGFLEC overestimates measurements). The relative RMSD, MAD, and MBD were calculated by dividing values with the mean of the in-situ measurements. Uncertainties in geolocation of the sampling units in combination with the geometric accuracy of the RapidEye data may introduce errors in the direct matching of measured and retrieved values. To correct for this, the pair of measured and retrieved value that provided the best agreement within a 3x3 search box centered on the sampling unit were retained. The search optimization was performed for LAI and Chl_l simultaneously to ensure that the same pixel location was used for both parameters.

The comparability between the modeled and observed surface reflectances was evaluated on a per-pivot basis for each of the REGFLEC run configurations. Surface reflectances were extracted from each crop pivot on the basis of digitized field boundaries and averaged to derive a set of pivot specific values. Note that the simulated spectra will differ for the three REGFLEC run configurations as a function of the optimized model parameter combinations (Section 2.5).

3. Results

The following section is divided into five sub-sections. Section 3.1 illustrates the effect of aerosol and adjacency effects on the atmospheric correction and is followed by the results of the empirically based ancillary LAI estimates (Section 3.2). REGFLEC evaluations are presented in the remaining sub-sections, first analyzing spatio-temporal features in LAI and Chl_l retrieved using red-edge and ancillary LAI data (Section 3.3), then evaluating retrievals based on three different REGFLEC configurations (Section 2.6) against in-situ measurements (Section 3.4), and finishing with an investigation into disparities between the satellite observed and modeled surface reflectance field as affected by adjacency effects and foliar dust (Section 3.5).

3.1 Atmospheric correction effects

Accurate observations of the surface reflectance field are critical for making reliable inferences of vegetation characteristics. In the case of remote observations, correction for atmospheric scattering and absorption effects constitutes a key element, which is primarily affected by ozone, water vapor and the amount and types of aerosol. Aerosol loadings were high ($\tau_{550} > 0.42$) during all three satellite acquisitions, with the haziness on day of year (DOY) 102 being particularly pronounced ($\tau_{550} = 0.74$). On this day, the aerosol size distribution recorded from the nearby AERONET site shows a single distribution peak at a particle radius of approximately $2 \mu\text{m}$, which diverges significantly from the more typical bi-modal distribution recorded during the two other acquisitions (Fig. S1b). Surface reflectances generated using the measured size distribution (DOY 102) as input to 6SV differ substantially from runs using a standard rural and desert (D’Almeida et al., 1991) aerosol model (Fig. S4). In fact, reflectances decrease by approximately 30% across all RapidEye spectral bands when replacing the standard rural model with the AERONET distribution on this particular day. On the two other overpasses, the rural model produces reflectance results more comparable to the AERONET-based results (Fig. S4).

Fig. 4 a) Effect of the adjacency correction (Eq. 5) on reflectances in the green, red, red-edge and near-infrared (NIR) band during the April 12th (DOY 102) overpass. The % reflectance difference is negative if the adjacency corrected reflectances are smaller than the uncorrected reflectances. b) The impact of the adjacency correction on magnitudes of the Normalized Difference Vegetation Index (NDVI) is included to demonstrate the relationship between the band-specific corrections and vegetation density.

The correction for adjacency effects induces further decreases in the surface reflectance field (Fig. 4a), particularly over vegetated pivots (Fig. 4b), while small increases may occur over the surrounding desert soil (Fig. 4a).

The correction is most pronounced in the visible bands, in part due to the increase in Rayleigh scattering intensity with decreasing wavelength, with up to a 60 % reduction in surface reflectances on DOY 102 (Fig. 4a). The adjacency corrections vary in space in response to the reflectance contrast between the target and environmental reflectance within the horizontal range of the adjacency effect (H_s). The bright desert soils surrounding the vegetated pivots represent a sharp reflectance contrast, particularly in the red domain due to radiation absorption by chlorophyll pigments (Fig. 3). In the near-infrared, bright desert and densely vegetated pixels (i.e., high values of NDVI) have more similar spectral signatures, which reduces the impact of radiation scattering from nearby pixels (Fig. 4a and b). The specification of H_s is clearly important and in this study was iteratively adjusted from an

Fig. 5 a) Agreement between the ancillary LAI, predicted on the basis of Eq. 7, and the in-situ measurements used to train the regression model. The error bars represent the standard deviation of the measurements within each IMZ. b) A single empirical regression model (Eq. 7) was used to generate the distributed ancillary LAI estimates for each RapidEye acquisition. This shows the results of a subset of the farm on April 12 (DOY 102).

initial value ($H_s=1.5$ km) to avoid negative values in the red spectral band. The resulting estimates show a dependence on τ_{550} , with the lowest value ($H_s=0.6$ km) retrieved during the highest atmospheric turbidity (Table 1). A similar tendency and range of H_s values were reported in Kaufman (1982).

3.2 Ancillary LAI

In this study, ancillary LAI information was used to constrain REGFLEC retrievals. The ancillary LAI maps (LAI_{anc}) (Fig. 5) were generated on the basis of a single empirical regression model of the form:

$$LAI_{anc} = -0.761 + 2.74 \cdot RSR - 0.285 \cdot (RSR)^2 \quad \text{Eq. 7}$$

Based on the available training data, Cubist identified the red-edge simple ratio (RSR) as the single most significant VI for LAI prediction, yielding an R^2 of 0.85, a MAD of 0.49 (14.4%), and an RMSD of 0.64 (18.6%) using the same dataset for training and validation (Fig. 5a). Interestingly, the use of

Fig. 6 Spatial and temporal features in REGFLEC predictions of (a) LAI and (b) ChlII over different crops. Non-labeled fields are all alfalfa.

in-situ LAI uncorrected for light scattering (Section 2.2) in the regression resulted in significantly reduced prediction accuracies ($\text{RMSD}=0.77$, $\text{RMSD}=23.2\%$, $R^2=0.79$), which highlights the importance of appropriate scattering corrections for LAI measurements conducted in direct sunlight with a LICOR plant canopy analyzer.

Independent validation using 70% ($n=65$) for training and 30% ($n=28$) for validation resulted in a similar regression ($\text{LAI}_{\text{anc}} = -0.864 + 2.88\text{RSR} - 0.3\text{RSR}^2$) characterized by a MAD of 0.51 (15.4%), an RMSD of 0.67 (20.1%), and an R^2 of 0.84. The Cubist-based selection of RSR as the optimal VI emphasizes the value of red-edge information for LAI prediction for different crops over a wide range of LAI values (0–6 in this study).

Table 3 Variations in model optimized (R_{adj_dust}) crop-specific parameters during the three acquisitions. Note that N and C_m were assumed to remain constant over the duration of the study period. The LAI and Chl_l values represent overall crop-specific averages $\pm$ one standard deviation.

Crops	87 - 151		Doy 87				Doy 102				Doy 151			
	C_m	N	LAI	Chl_l	θ_l	D_f	LAI	Chl_l	θ_l	D_f	LAI	Chl_l	θ_l	D_f
Alfalfa	46	2.5	1.9 $\pm$ 1.7	40 $\pm$ 12	54.5	0.01	1.6 $\pm$ 1.0	52 $\pm$ 12	64.2	0.17	2.7 $\pm$ 1.8	54 $\pm$ 9	53.7	0.02
Grass	36	1.0	1.7 $\pm$ 0.9	35 $\pm$ 6	30.3	0.11	2.1 $\pm$ 0.9	43 $\pm$ 7	51.1	0.24	2.8 $\pm$ 1.6	43 $\pm$ 6	27.3	0.05
Carrot	38	2.4	1.8 $\pm$ 1.2	40 $\pm$ 7	41.4	0.01	1.8 $\pm$ 1.0	45 $\pm$ 10	59.6	0.15	2.2 $\pm$ 1.4	34 $\pm$ 7	69.6	0.01
Maize	33	1.1	0.4 $\pm$ 0.4	16 $\pm$ 9	61.4*	0.03*	0.3 $\pm$ 0.2	38 $\pm$ 14	61.4*	0.03*	3.5 $\pm$ 1.5	46 $\pm$ 9	61.4	0.03

*Value from DOY 151 assumed due to the lack of vegetated ($NDVI > 0.7$) pixels for the retrieval

3.3 Spatio-temporal features in LAI and Chl_l retrievals

The spatial and temporal information content of the model-based retrievals of LAI and Chl_l are shown for a section of the Tawdeehiya farm in Fig. 6a and b, respectively. These retrievals were based on the REGFLEC configuration with consideration of both adjacency effects and foliar dust (R_{adj_dust}). The majority of the pivots (~800 m diameter) grow alfalfa, which tends to be characterized by significant within-field variations in vegetation density (i.e. LAI) during all stages of crop development (Fig. 6a). The center-pivot irrigation wheel trenches are clearly discernable and several field sections are characterized by patchy vegetation conditions, due in part to non-optimal growing conditions. The Chl_l retrievals on the other hand show relatively homogeneous intra-field distributions, except over very sparse vegetation cover ($LAI < 0.5$) where Chl_l retrieval is intrinsically uncertain (Houborg et al., 2015b) (Fig. 6b). While the spatial features in alfalfa Chl_l are more subtle, farm-wide statistics do indicate significant within-class variability, with standard deviations ranging from 9–12 $\mu g\ cm^{-2}$ (Table 3). Maize was in the emergence or early leaf development stage on DOY 87 and 102, entering the reproductive stage on DOY 151, with the farm-wide average of maize LAI increasing from ~0.3 to 3.5 (Table 3). The change in development stage and vegetation density increased Chl_l levels from 38 $\mu g\ cm^{-2}$ (DOY 102) to 46 $\mu g\ cm^{-2}$ (DOY 151). Fields of Rhodes grass and carrot are generally characterized by the lowest Chl_l values (Table 3), although Chl_l is comparatively low for all crops on DOY 87 (Fig. 6b). Across-field narrow sections of reduced LAI appear in the rightmost carrot field (Fig. 6a), which result from the installation of a wind-break style shield consisting of a row of maize plants.

Fig. 7 illustrates the degree of within field spatial detail achievable at the RapidEye spatial resolution for two Rhodes grass and one alfalfa field on DOY 151. Compared to the model derived LAI (Fig. 7a) Chl_l is more homogeneously distributed even over sections with significant changes in LAI. While strong correlations between LAI and Chl_l have previously been reported (Schull et al., 2015; Gitelson et al., 2014; Houborg et al., 2009), these were mainly associated with the onset of leaf senescence. The spatial disassociation recorded here occurs in fields with limited leaf yellowing and the field heterogeneity in LAI is mainly a reflection of within-field variations in ground elevation and soil conditions. Over the two grass fields, areas with relatively low soil reflectance (i.e. low values of s_l) (Fig. 9d) are generally characterized by the most vigorous vegetation development (high LAI) (Fig. 7a). These areas coincide with slightly lower ground elevations, resulting in wetter soils (and a corresponding slower rate of drying) and reduced loss of plant nutrients in response to natural hydraulic drainage, ensuring more optimal conditions for vegetation development. Large areas within the two grass fields have high soil reflectances. This is corroborated by relatively low (compared to field capacity) in-situ observations of volumetric soil moisture (17 – 21%) on DOY 154 (leftmost grass field) and sporadic activity of the grass center-pivot irrigation systems over the course of this campaign. The alfalfa field on the other hand was being actively irrigated throughout the campaign (~3 day watering cycle) as reflected by much lower soil reflectance values. The map of s_l records higher soil reflectances over the irrigation wheel trenches and towards the edges of the field, which is expected due to enhanced drying of the more exposed soil surfaces. LAI and Chl_l are adjusted for variations in soil background during the last step of the REGFLEC retrieval system (Houborg et al., 2015b). Proper consideration and accounting of this confounding influence is particularly pertinent in irrigated fields with heterogeneous patterns of wetting and drying. The realistic spatial distribution observed in LAI, Chl_l and s_l is an indication of the effectiveness of the soil background reflectance estimation and may serve as an independent and useful proxy for within-field variations in surface soil moisture conditions.

Fig. 7 Within-field variations in (a) REGFLEC LAI, (b) REGFLEC Chl, (c) empirical LAI, and (d) soil brightness (i.e. s_1) over Rhodes grass and alfalfa fields on May 31st (DOY 151).

Variations in soil background conditions are a likely cause for the significant discrepancies observed between the modeled (Fig. 7a) and ancillary (Fig. 7c) LAI maps. The empirically established ancillary LAI is based on a single regression equation (Eq. 7) and application over sections with widely different background conditions will inevitably add uncertainties to these estimates.

3.4 Validation of LAI and Chl_i retrievals

The value of the REGFLEC based LAI and Chl_i retrievals for dryland agricultural applications ultimately relies on the absolute retrieval accuracy and utility for reproducing observed gradients. Fig. 8 compares the REGFLEC model results against in-situ measurements collected over the course of the three field campaigns. When both foliar dust and adjacency effects (R_{adj_dust}) are considered in the retrieval, the overall predictive performance of the LAI retrievals is characterized by an R^2 of 0.89, an RMSD of 0.65 (19%), a MAD of 0.42 (12.5%), and an MBD of -0.37 (-10.8%) (Fig. 8a). On a crop-specific basis, lowest uncertainties are observed for alfalfa (RMSD=12.5%, MAD=7.5%) and maize (RMSD=20.8%, MAD=12.6%) (Table 4). The larger discrepancies associated with the grass and carrot retrievals are mainly attributed to a negative bias, as represented by an MBD of -18% and -26%, respectively (Table 4). At the Tawdeehiya farm, the carrots are planted in rows with a spacing of ~40 cm, whereas Rhodes grass in many places is heterogeneously distributed in clumps, with sections of bare soil interspersed between. This results in foliage clumping (i.e. divergence of the spatial organization of leaves in a canopy from the random leaf distribution characteristic of homogeneous canopies), which is not specifically considered in the turbid medium canopy reflectance model (4SAIL) used in REGFLEC. As a result, REGFLEC will predict an effective LAI that will be lower than the true LAI in clumped canopies (Houborg et al., 2015b). Similar limitations in the application of SAIL have been reported in canopies of maize planted in rows (Atzberger and Richter, 2012; Demarez et al., 2008). The relatively low MBD of -12% reported in the present study for maize may be attributed to the presence of significant understory vegetation in many of the fields. Even without correcting for the clumping issue, REGFLEC LAI retrievals represent an improvement over the empirically established LAI, in comparison with the independently validated dataset (Section 3.2).

For Chl_i the overall model performance (R_{adj_dust}) is described by an R^2 of 0.62, an RMSD of 10.9 $\mu\text{g cm}^{-2}$ (21.9%), a MAD of 7.9 $\mu\text{g cm}^{-2}$ (15.9%), and an MBD of -4.5 (-9.1%) (Fig. 8a). The model predictions are particularly encouraging for maize (Table 4), where almost all retrievals are within the

Fig. 8 Comparisons of REGFLEC retrieved LAI (left) and Chl_l (right) against in-situ observations. Results are shown for the (a) R_{adj_dust} , (b) R_{adj} , and (c) R_{noadj} REGFLEC run configurations (Section 2.6). The error bars represent the standard deviation of the measurements within each IMZ. Statistics of the overall retrieval accuracies are plotted on the plots. Crop-specific statistics are provided in Table 4.

589 standard deviations of the in-situ measurements over a wide range in Chl_l values (Fig. 8a).

Significantly larger deviations are reported for alfalfa. The most significant model underestimates occur on DOY 87, where the measured ($66 \mu\text{g cm}^{-2}$) and modeled ($49 \mu\text{g cm}^{-2}$) values diverge by 17

Table 4 Statistics of the crop-specific agreement between satellite-derived and in-situ measured LAI and Chl_l for each of the REGFLEC run configurations (Section 2.6).

Metric	Alfalfa			Grass			Maize			Carrot		
LAI [$\text{m}^2 \text{m}^{-2}$]	R_{noadj}	R_{adj}	$R_{\text{adj_dust}}$	R_{noadj}	R_{adj}	$R_{\text{adj_dust}}$	R_{noadj}	R_{adj}	$R_{\text{adj_dust}}$	R_{noadj}	R_{adj}	$R_{\text{adj_dust}}$
n	41	41	41	14	14	14	29	29	29	9	9	9
RMSD	2.13	0.67	0.43	2.42	1.61	0.97	1.44	0.56	0.54	2.24	1.28	1.02
RMSD [%]	57.3	17.9	11.4	63.3	42.1	25.3	55.2	21.6	20.8	59.6	34.4	27.4
MAD [%]	52.2	12.8	7.5	54.8	32.5	18.1	41.1	13.1	12.6	56.9	31.2	25.8
MBD [%]	-52.2	-9.4	-4.3	-54.8	-32.5	-17.9	-41.1	-13.0	-12.2	-56.9	-31.2	-25.8
Chl_l [$\mu\text{g cm}^{-2}$]												
n	41	41	41	14	14	14	29	29	29	-	-	-
RMSD	15.2	16.9	13.8	9.21	7.29	9.01	11.1	4.6	4.35	-	-	-
RMSD [%]	24.1	26.8	21.8	31.2	24.7	30.5	28.3	11.7	11.1	-	-	-
MAD [%]	19.4	22.3	17.2	27.9	21.5	26.2	19.9	7.4	7.6			
MBD [%]	-19.1	-22.2	-17.0	27.9	21.5	26.2	-8.8	-2.6	-2.3	-	-	-

$\mu\text{g cm}^{-2}$ on average. This could be related to uncertainties in the atmospheric correction or contamination from thin cirrus clouds in the imagery, which was a common occurrence during the first field campaign. The red-edge band is characterized by enhanced sensitivity to changes in Chl_l , but is also highly sensitive to LAI (Fig. S3). Their mutually compensating effect on canopy reflectance spectra (Lewis and Disney, 2007) can introduce uncertainties in the separation of Chl_l and LAI. This may provide a partial explanation for the overestimation of Chl_l and underestimation of LAI over Rhodes grass (Fig. 8a). In fact, a comparison of measured and estimated total canopy chlorophyll content (i.e. Chl_l multiplied by LAI) suggests only a small positive bias ($y=1.047x$, $R^2=0.86$). Several other factors can also affect estimation accuracies, including the calibration and predictive ability of PROSPECT (Feret et al., 2011, 2008; Houborg et al., 2015b), the confounding influence of partly polarized light scattered at the surface of leaves (Vanderbilt et al., 1985), model limitations over heterogeneous canopies, specifications of model parameters and ranges (Houborg et al., 2015b), and instrument measurement and calibration uncertainties (Section 2.2).

Over the arid sites examined here, the addition of the fraction of foliar dust in the model inversion constitutes a significant improvement over model results (R_{adj}) not corrected for foliar dust (Fig. 8b and Table 4). This is particularly evident for LAI, which sees the overall R^2 decreasing to 0.80 and the relative RMSD increasing to 27.1% when setting $D_f=0$ (Fig. 8b). The retrieved values of D_f are highest on DOY 102 (Table 3), where the addition of D_f as a free variable in the inversion causes a significant increase in the LAI estimation accuracy. Specifically, R^2 increases from 0.81 to 0.90, the RMSD decreases from 49% to 30%, and MBD decreases from -36% to -19% (not shown). Similarly for Chl_l , the R^2 , RMSD and MBD change from 0.73 to 0.80, 19% to 15%, and -7% to -2%, respectively. Since modeled foliar dust amounts are low on DOY 89 and 151 (Table 3), the impact of the foliar dust correction on the retrieval accuracies is minor on these days. This explains the statistics of the maize retrievals, which are largely unaffected by the correction, as these were predominantly from the DOY 151 overpass (Fig. 8b and Table 4).

If adjacency effects are not considered in the atmospheric correction (R_{noadj}), the LAI estimation accuracies deteriorate for all crops, with the RMSD ranging from 55% to 63% (Fig. 8c and Table 4). The effect on the Chl_l retrievals is mostly evident for maize, where retrievals fail (i.e., lower bound is reached) for low LAI (Fig. 8c and Table 4). The substantial difference between the adjacency corrected and uncorrected spectral surface reflectance field (Fig. 4) used as input to REGFLEC, is mostly compensated for by reductions in the model based LAI values. In most cases, the Chl_l retrievals remain reasonable (Fig. 8c). This is partly attributed to the empirical LAI constraint and the internal adjustment of the inversion parameters to optimize the agreement between the observed and modeled reflectance spectra (Houborg et al., 2015b).

3.5 Comparability between observed and modeled surface reflectances

Fig. 9 Comparisons between modeled and observed reflectances in the (a) green, (b) red, (c) red-edge, and (d) near-infrared band on a per-pivot basis over the duration of the three field campaigns. Results are shown for each of the REGFLEC run configurations (Section 2.6). Resulting relationships between ancillary and REGFLEC LAI are depicted in (e).

uncertainties in atmospheric correction and limitations in the physically-based representation and parameterization of canopy radiative transfer processes. These limitations can lead to disparities between the satellite observed and modeled surface reflectance field. The effect of the adjacency correction is clearly evident in comparisons between modeled and observed reflectances on a per-pivot basis (Fig. 9). The use of uncorrected reflectances in the REGFLEC inversion (R_{noadj}) results in significant discrepancies between modeled and observed pivot-averaged reflectances, with model underestimates in the green and red band up to 60 % (Fig. 9a and b). In the inversion process, the matching of modeled and observed reflectance spectra is informed by the ancillary LAI input. The significant bias (52% underestimation) between LAI_{anc} and $\text{LAI}_{\text{regflec}}$ (Fig. 9e) is a clear indication that the satellite observed reflectances used in the model inversion are not an accurate representation of the true top of canopy reflectance field. The agreement between LAI_{anc} and $\text{LAI}_{\text{regflec}}$ improves considerably when REGFLEC is inverted using surface reflectances with the adjacency correction applied (R_{adj}) (Fig. 9e). This results in a significant decrease in the relative reflectance differences across all wavebands (Fig. 9a-d). Improvements are particularly evident over intermediate to densely vegetated pivots (Fig. 9a-d).

Consideration of foliar dust ($R_{\text{adj_dust}}$) generally improves reflectance and LAI based compatibilities, especially on DOY 102 (Fig. 9). On this day, the model derived crop-specific fractions of foliar dust (D_f) vary between 0.15 and 0.24 (Table 3). The significant amount of modeled foliar dust is corroborated by dusty and windy conditions during and immediately preceding this image acquisition (Fig. 2 and Table 1). The two other RapidEye acquisitions occurred during periods with relatively lower aerosol loadings (Fig. 2) and less exposure to deposition of atmospheric dust, as also reflected in the records of D_f (Table 3).

For both configurations (R_{adj} and $R_{\text{adj_dust}}$), reflectance discrepancies are smallest in the red-edge band (Fig. 9c), as this is used in the VI based prediction of both LAI and Chl_l (Section 2.5.1). While the

optimal solution is based on minimizing the mean absolute error between modeled and observed reflectances across all 4 spectral bands (Eq. 5), the green band is not directly involved in the actual prediction of LAI or Chl_l. This in part explains the relatively large green reflectance deviations (Fig. 9a). In addition, the green band is located at a shorter wavelength and is therefore more sensitive to the quality of the atmospheric correction (Miura et al., 2008). This will affect the utility of this specific band in regions with significant aerosol loadings.

4. Discussion

4.1 Aerosol and adjacency effects

The challenging dryland environment explored here, with its relatively high and variable amounts of atmospheric dust particles, play a confounding role on the achievable accuracy of the atmospheric state data used as input into the 6SV atmospheric radiative transfer model. In an attempt to minimize uncertainties, τ_{550} was estimated by combining site-specific MODIS observations and nearby AERONET measurements, with aerosol radiative characteristics estimated from observations of aerosol optical properties and size distributions at the AERONET site. Clearly, the sparsely scattered network of AERONET sites represents a limitation of the adopted approach for application to any given satellite scene. Despite advances in the satellite-based estimation of τ_{550} over landscapes with bright surfaces (Bibi et al., 2015; Huang et al., 2015), the expected error envelope (around $\pm(0.05+0.20\tau_{550})$) imposes a constraint on the achievable surface reflectance accuracy level, particularly during periods of high aerosol loadings. Enhanced characterizations of site-specific aerosol properties from multi-sensor remote sensing observations based on physical modeling and advanced statistical optimization (Dubovik et al., 2014) is likely to prove particularly beneficial over such areas.

An accurate representation of the surface reflectance field is a fundamental prerequisite for robust parameter estimation through inversion of a canopy reflectance model. The implementation of a simple correction for adjacency effects was shown to be particularly important in the visible

wavelength domain due to typically large reflectance contrasts between target (e.g. vegetated) pixels and surrounding (e.g. bright desert) areas, in addition to high atmospheric turbidities, both of which are directly proportional to the magnitude of the adjacency correction. In fact, over densely vegetated pivots, green and red band reflectances were reduced by up to 60%. The adopted spectral corrections effectively reduced the negative bias in LAI estimation from 50% to 17%. Without corrections for adjacency effects, REGFLEC was unable to match the satellite observed reflectances and simultaneously achieve realistic LAI levels. Given the critical nature of atmospheric correction in these dryland environments, a key objective of ongoing work is to verify adopted atmospheric parameterizations using an in-situ validation dataset of surface reflectance spectra collected concurrently with the remote sensing acquisitions.

4.2 Foliar dust

The refinement of REGFLEC to simulate the effect of dust deposition on canopy spectral signatures further improved LAI and Chl_l retrieval accuracies and resulted in better matching of observed and modeled reflectance spectra. The reflectance modulation of foliar dust was tied to the spectral signature of the locally derived soil background signal, which resulted in reflectance increases in the visible and decreases in the near-infrared domain in proportion to the fraction of foliar dust (D_f). While this approach accounts for the impact of soil wetness on the spectral signature, it may be associated with significant uncertainty when the local soil texture conditions differ substantially from the source region of the depositing dust.

In the current implementation of REGFLEC, D_f was allowed to vary in time but was assumed uniform across the scene for each crop type. However, variations in foliar dust amounts may occur between pivots and within individual fields, depending on surface characteristics of the surrounding area and the cycle and efficiency of the center-pivot irrigation system in partial cleaning of the leaves for dust particles. While the REGFLEC modeling system can consider variations in D_f between individual pivots, it did not lead to improvements in the agreement between the satellite retrievals and in-situ

measurements (not shown). Also, the retrieval of D_f is best confined over the densest vegetation elements in order to avoid confusion of the foliar dust signal with changes in the soil background or other compensating factors such as foliage clumping and senescent leaf material (Houborg et al., 2009). In this study, the model performed best when using localized areas of high vegetation densities for the estimation of pixel-specific D_f values that were averaged to obtain a single crop-specific estimate. This approach is only meaningful over smaller regions where uniformity in dust conditions is a reasonable assumption.

Even though a simplified treatment of complex physical processes is a necessity in a remote sensing context, the correction for foliar dust in the spatial and temporal domain warrants further and more detailed investigations that should involve matching of model simulated spectra against spectral observations in plants with known amounts of dust deposition.

4.3 Red-edge information

The integration of regularization strategies or constraints is key to retrieving vegetation characteristics with sufficient accuracy from model inversion. The implementation of a new red-edge configuration in REGFLEC ensured robust retrievals over a wide range of both LAI and Chl_l for different crops, attributable to enhanced sensitivity at high ranges and reduced influence of atmospheric correction uncertainties relative to bands in the visible domain. The relatively high reflectance uncertainty reported for the green band may affect its usefulness for vegetation retrievals over dusty environments, although it potentially contains valuable information related to pigment content (Gitelson et al., 2005; Houborg et al., 2015b) and foliar dust (Wu and Wang, 2015). A full evaluation of the combined benefits of green and red-edge information within the REGFLFEC retrieval system is ongoing and will be the focus of a follow-up contribution.

The application to RapidEye data demonstrated significant utility in characterizing subtle within-field variations in LAI and Chl_l , which are valuable in the context of precision agriculture. The enhanced

definition of the red-edge offered by the newly launched Sentinel-2 (S-2) satellite could add further information for regularizing the ill-posed inverse problem (Laurent et al., 2014). However, the spatial detail achievable with S-2 (i.e., 20 m in the red-edge) may not always be sufficient for effective precision agricultural management, as within-field variations resulting from vegetation heterogeneity and non-optimal growing conditions often occur at much finer scales (Suárez et al., 2010). Advances made in unmanned aerial vehicles (UAV) sensor technology provide an enhanced capacity for timely sensing of vegetation health and condition at optimal resolutions and a unique platform for exploiting synergies in multispectral, hyperspectral and thermal sensing (Berni et al., 2009; Elarab et al., 2015; Zarco-Tejada et al., 2012) with reduced influence of atmospheric effects. Future research efforts should be directed towards developing extendable and well-constrained retrieval algorithms adapted to effectively exploit cross-sensor synergies and enhancement in spectral, spatial, and temporal remote sensor capabilities.

4.4 Combining benefits of physical and empirical retrievals

Consideration of spatial and temporal variations in confounding factors in the construction of the predictive model-based VI relationships remains a critical aspect in the mapping of both LAI and Chl_l . Variable irrigation scheduling and soil variability were evident in model derived estimates of the soil background signal, which significantly affected the within-field distribution of model estimated LAI. However, the same spatial features were not apparent in the ancillary LAI generated on the basis of a single empirically calibrated regression. While empirical regressions based on the red-edge simple ratio (RSR) have been shown to perform well in canopies (i.e., maize and soybean) with widely different leaf structures and canopy architectures (Vina et al., 2011), the RSR is strongly affected by variations in Chl_l (Fig. S3), which may not always be compensated by leaf structure tendencies (Gitelson et al., 2005). A physical framework has the capacity to re-parameterize the association between RSR and LAI in response to spatio-temporal variations in confounding contributions from the soil, canopy and atmosphere. In REGFLEC, the empirical LAI serves to improve the

discrimination of LAI and Chl_l effects by constraining the magnitudes of the modeled LAI estimates to realistic levels, while a physically realistic spatial distribution is ensured. Compared to empirical methods, physical approaches have the potential to be significantly more generic and transferable (Atzberger et al., 2015), but exploitation of the combined benefits, as shown here, may be needed to effectively constrain the inversion and achieve better-informed estimates in both space and time.

5. Conclusion

The utility of an integrated system of radiative transfer models (REGFLEC) for retrieving vegetation characteristics over a dryland irrigated agricultural system was examined on the basis of very high spatial resolution (i.e. 6.5 m) RapidEye imagery. Refinements to the REGFLEC framework were implemented to 1) correct for aerosol and adjacency effects, 2) consider foliar dust effects on modeled canopy reflectances, 3) extend application to high spatial resolution sensors with red-edge bands, and 4) exploit empirical LAI in the inversion. Evaluation against in-situ measurements conducted in fields of alfalfa, Rhodes grass, carrot, and maize over three separate field campaigns in the spring of 2015, demonstrated significant utility of the updated inversion system, with overall best-case LAI and Chl_l retrieval accuracies on the order of 12% and 16% (relative MAD), respectively.

However, the study highlighted a number of complexities associated with physically-based retrieval of LAI and Chl_l over dryland agricultural systems. The reflectance contrast between dark vegetated pivots and surrounding bright desert soils in combination with relatively high aerosol loadings, made corrections for adjacency effects critically important. The consideration of foliar dust improved the physical realism of the modeling framework for application over dryland systems following dust events. Additional regularization of the REGFLEC inversion framework, in the form of a band in the red-edge domain and empirically established ancillary LAI estimates, was instrumental in further improving retrieval accuracies.

The results advocate a needed investment in the development of well-constrained and physically realistic remote sensing retrieval techniques with the ability to robustly assess and discriminate within-field variability in plant biochemical and biophysical properties as mechanisms to improve production efficiencies and the sustainability of dryland agriculture.

6. Acknowledgements

Research reported in this publication was supported by the King Abdullah University of Science and Technology (KAUST). We greatly appreciate the logistical, equipment and scientific support offered to our team by Mr Jack King, Mr Alan King and employees of the Tawdeehiya Farm in Al Kharj, Saudi Arabia, without whom this research would not have been possible. We acknowledge the assistance with in-situ data collection from members of the Hydrology and Land Observation (HALO) team: in particular, Syed Haleem Shah, Bruno Aragon Solorio, Stephen D. Parkes, Samir K. Al-Mashharawi, Raghavendra B. Jana and Peter Z. Schulte. We thank PI Brent Holben for his effort in establishing and maintaining the Solar Village AERONET site.

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Fig. 1 Location of the Tawdeehiya commercial farm in Saudi Arabia with identification of intensive measurement zones (IMZ) during the three field campaigns in 2015. The image is a natural color representation of 5 m resolution RapidEye data collected on May 31 (DOY 151).

Fig. 2 Time-series of aerosol optical thickness at 550 nm (τ_{550}) over Tawdeehiya and Solar Village retrieved from Terra MODIS and AERONET sun-photometer data at MODIS acquisition times. Gaps occasionally occur in the MODIS records due to the MODIS revisit capability (1 – 2 days) or lack of high quality retrievals. The shaded bars represent the timing and durations of the three field campaigns at Tawdeehiya. Time-series correlations (R^2) between the MODIS and AERONET datasets are indicated at the top.

Fig. 3 Visualization of the simple correction for foliar dust implemented into 4SAIL. Modeled surface reflectances are modulated by changes in the fraction of foliar dust (D_f) as a function of the spectral signature of dust, which was assumed to approximate the local soil reflectance signal. Results are shown for a dense canopy with $LAI=4$, $\theta_{ll}=57^\circ$, $Chl_l=50 \mu g cm^{-2}$, $C_m=50 g m^{-2}$, $N=1.75$, $s_1=0.4$, and $s_2=0$ assuming the observation geometry from DOY 102 (Table 1). The spectral responses of the green, red, red-edge and near-infrared RapidEye bands are shown on the secondary y-axis.

Fig. 4 a) Effect of the adjacency correction (Eq. 4) on reflectances in the green, red, red-edge and near-infrared (NIR) band during the April 12th (DOY 102) overpass. The % reflectance difference is negative if the adjacency corrected reflectances are smaller than the uncorrected reflectances. b) The impact of the adjacency correction on magnitudes of the Normalized Difference Vegetation Index (NDVI) is included to demonstrate the relationship between the band-specific corrections and vegetation density.

Fig. 5 a) Agreement between the ancillary LAI, predicted on the basis of Eq. 7, and the in-situ measurements used to train the regression model. The error bars represent the standard deviation of the measurements within each IMZ. b) A single empirical regression model (Eq. 7) was used to generate the distributed ancillary LAI estimates for each RapidEye acquisition. This shows the results of a subset of the farm on April 12 (DOY 102).

Fig. 6 Spatial and temporal features in REGFLEC predictions of (a) LAI and (b) Chl_{ll} over a variety of different crops. Non-labeled fields are all alfalfa.

Fig. 7 Within-field variations in (a) REGFLEC LAI, (b) REGFLEC Chl_l , (c) empirical LAI, and (d) soil brightness (i.e. s_1) over Rhodes grass and alfalfa fields on May 31st (DOY 151).

Fig. 8 Comparisons of REGFLEC retrieved LAI (left) and Chl_l (right) against in-situ observations. Results are shown for the (a) R_{adj_dust} , (b) R_{adj} , and (c) R_{noadj} REGFLEC run configurations (Section 2.6). The error bars represent the standard deviation of the measurements within each IMZ. Statistics of the overall retrieval accuracies are plotted on the plots. Crop-specific statistics are provided in Table 4.

Fig. 9 Comparisons between modeled and observed reflectances in the (a) green, (b) red, (c) red-edge, and (d) near-infrared band on a per-pivot basis over the duration of the three field campaigns. Results are shown for each of the REGFLEC run configurations (Section 2.6). Resulting relationships between ancillary and REGFLEC LAI are depicted in (e).