Advanced radiometry measurements and Earth science applications with the Airborne Prism Experiment (APEX)

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ABSTRACT
We present the Airborne Prism Experiment (APEX), its calibration and subsequent radiometric measurements as well as Earth science applications derived from this data. APEX is a dispersive pushbroom imaging spectrometer covering the solar reflected wavelength range between 372 and 2540 nm with nominal 312 (max. 532) spectral bands. APEX is calibrated using a combination of laboratory, in-flight and vicarious calibration approaches. These are complemented by using a forward and inverse radiative transfer modeling approach, suitable to further validate APEX data. We establish traceability of APEX radiances to a primary calibration standard, including uncertainty analysis. We also discuss the instrument simulation process ranging from initial specifications to performance validation. In a second part, we present Earth science applications using APEX. They include geophysical and atmospheric considerations as well as reflectance anisotropy minimized Level 2 data. Further, we discuss retrieval of aerosol optical depth as well as vertical column density of NOx, a radiance data-based coupled canopy–atmosphere model, and finally measuring sun-induced chlorophyll fluorescence (Fs) and infer plant pigment content. The results report on all APEX specifications including validation. APEX radiances are traceable to a primary standard with <4% uncertainty and with an average SNR of >625 for all spectral bands. Radiance based vicarious calibration is traceable to a secondary standard with ≤6.5% uncertainty. Except for inferring plant pigment content, all applications are validated using in-situ measurement approaches and modeling. Even relatively broad APEX bands (FWHM of 6 nm at 760 nm) can assess Fs with modeling agreements as high as $R^2 = 0.87$ (relative RMSE = 27.76%). We conclude on the use of high resolution imaging spectrometers and suggest further development of imaging spectrometers supporting science grade spectroscopy measurements.

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1. Introduction

Imaging spectroscopy has emerged as an extremely efficient observational approach for mapping the Earth system (Schaepman et al., 2009a). The efficiency gain has its foundation in technical progress made on one hand, and on the improved understanding and modeling of the molecular scattering and absorption mechanisms, on the other. Imaging spectrometers—particularly airborne instruments—are frequently available nowadays, either targeting specific applications, or...
serving as 'general purpose' instruments, covering a wide range of applications (for a detailed review see Schaepman, 2009).

While the general procedure of constructing and operating airborne imaging spectrometers has reached a high level of maturity, requirements on specific instrument aspects might challenge any component of the full data acquisition chain, ranging from sensor modeling to calibration to product delivery. In particular, spectral fidelity (stability, Signal-to-Noise Ratio (SNR), etc.) was very early on identified as a key performance requirement for successful spectroscopy applications (Green et al., 1998).

Emerging satellite concepts utilizing principles of spectroscopy as their prime observational approach led to the idea to build a next generation airborne imaging spectrometer in Switzerland during the early 1990s. In fact, the idea emerged following a successful joint NASA/ESA Multisensor Airborne Campaign (MAC-Europe) in July 1991 in Europe (Itten, Meyer, Staenz, Kellenberger, & Schaepman, 1992). The funding source identified for such an endeavor was the European Space Agency’s PRODEX (PROgramme de Développement d’Expériences scientifiques) program, allowing small ESA member states to develop their own instruments. A joint Swiss–Belgian team proposed to build an airborne imaging spectrometer termed ‘Airborne Prism Experiment’ (APEX), under the scientific lead of Klaus Itten at the University of Zurich. He served as APEX principal investigator from 1995 to 2009 and Michael Schepman from 2009 onwards. A potential APEX system was for the first time presented to a wider audience in 1997 (Itten et al., 1997).

The scientific, industrial and operational consortium of APEX was subsequently established as follows. The science lead is with the University of Zurich, tasked to perform model simulations, establish system specifications and validate instrument performance, develop a science grade processing facility, and perform the project management. The institutional partner and co-investigator VITO is responsible for the operational implementation of the APEX processor, APEX operations and data distribution. The industrial consortium is composed of RUAG Aerospace, Switzerland (integration, mechanical and electrical subsystems, navigation and control), OIP Sensor Systems, Belgium (optical subsystem), and Netcetera AG, Switzerland (readout electronics, software). In addition, ESA as overall project responsible established two further contracts, one with Sofradir, France (short-wave infrared (SWIR) detector) and the German Aerospace Center (DLR), Germany (calibration home base). APEX went into operations in 2009 and acquires science grade spectroscopy data since 2010. APEX is on lease by ESA to the University of Zurich and VITO until 2015 and thereafter under ownership of the latter two institutions.

In this contribution, we discuss the evolution of the APEX instrument starting with simulating its key performance indicators, and definition of specifications, its optical, electronic and mechanical design. We then elaborate on the calibration procedure and finally demonstrate new Earth science applications allowing monitoring the Earth surface and atmosphere with unprecedented accuracy. We finally conclude by discussing emerging instrument capabilities and applications being of relevance for future, upcoming imaging spectrometers.

2. APEX advanced radiometry measurements

2.1. APEX specifications and performance modeling

The APEX system was specified to allow simulating spaceborne imaging spectrometers, supporting mission calibration and validation efforts. The following specifications are outlined as boundary conditions (Schaepman, De Vos, & Itten, 1998):

- Pushbroom imaging with $\leq 1000$ imaging pixels across track, covering a swath width of 2.5–5 km, depending on flight altitude,
- Spectral wavelength range covering 450–2500 nm,
- At least 200 programmable or 300 predefined spectral bands, adaptable to specific application requirements,
- Spectral sampling interval $< 15$ nm and a spectral sampling width of $<1.5$ the sampling interval, and
- Ability to provide calibrated data and products to geocoded and calibrated data.

Further on, the dispersive system of APEX had to be based on prisms, given a requirement from European Space Agency. The initial idea was do demonstrate that the ENVISAT/MERIS design can be used in APEX as a demonstrator for a full spectral coverage mission (400–2500 nm) as well as precursor mission of a planned imaging spectrometer in space (Menenti et al., 2002).

Using the above specifications, a performance modeling approach could be initiated. First, a forward model simulating 1D generic imaging spectrometers is implemented (Schaepman, Schläpfer, & Müller, 2002). Key science requirements from various applications are compiled as a list of 55 variables used to forward model the instrument performance. Application requirements are forward simulated using a reflectance model and then converted to at-sensor radiances using a radiance model and finally convolved using a sensor specific model. This leads to the possibility to model (still noise free and in 1D space) pixel-wise requirements for a given instrument. Subsequently, certain noise components are added (Schläpfer & Schaepman, 2002) as well as a spatial component allowing to assess spatial noise as well (Börner et al., 2001). These activities finally lead to a set of performance requirements for APEX which are used as engineering specifications (Schaepman, Schläpfer, & Itten, 2000) (Table 1, Section 4.1). However, not all specifications can be simulated using the above approach, such as stability requirements over time. These specifications are either taken over from existing publications (Green, 1998; Mroue, Green, & Chrien, 2000) or from engineering knowledge available through the support of ESA’s engineers.

2.2. APEX instrument description

APEX is composed of an optical system including two detector channels (Fig. 1), a mechanical subsystem, an electrical subsystem, and an in-flight calibration assembly. External to the core APEX imager is a control and storage unit (CSU), as well as a processing and archiving facility (PAF) and a calibration home base (CHB).

The optical system is a dual prism dispersion pushbroom spectrometer using a path-folding mirror followed by a ground imager with a slit in its image plane (Schaepman et al., 2003). The spectrometer consists of a collimator that directs the light transmitted by the slit towards the prisms, where a dichroic coating applied to the first prism separates the two spectrometer channels into a VNIR and SWIR channel (Visible/Near Infrared 372–1015 nm; Shortwave Infrared 904–2508 nm). The dispersed light is imaged on the detectors of these two channels. A commercial-off-the-shelf VNIR detector (CCD 55–30, E2V Technologies) and a custom made SWIR detector (Nowicki-Bringuijer & Chorier, 2009) are implemented. The SWIR focal plane array is a HgCdTe detecting module hybridized on a CMOS multiplexer. It has 1000 × 256 pixels with a 30 μm pitch. Integration time is variable, but limited by the detector frame rate (34.5 ms). Standard integration time is set to 29 ms [22 ... 34.5 ms], resulting in almost square pixels using the default aircraft (DO-228). Its spatial direction (1000 pixels) is parallel to the detector rows and its spectral direction (256 pixels) parallel to the detector columns, which is also the readout direction on the focal plane. The detector is implemented in a dewar with a sapphire window coated with anti-reflection material (transmission $>0.96$). A Stirling cycle cooler allows operating the SWIR detector with low dark current at 130 K detector temperature. The mount of the spectrometer is liquid cooled using a transfer line and cold finger (Ullrich et al., 2004). The 1000 across-track spatial pixels are recorded for both channels simultaneously. Both detectors are not fully illuminated in spectral direction, allowing non-illuminated lines to be used as dark current reference. The VNIR and SWIR detectors are externally
synchronized (uncertainty ± 0.5 ms) allowing us to acquire images simultaneously, even under varying integration time settings. Users receive a maximum of 334 (VNIR) + 198 (SWIR) = 532 spectral bands, which can be programmed to receive a maximum of 334 (VNIR) + 198 (SWIR) = 532 spectral bands, synchronized (uncertainty ±0.5 ms) allowing us to acquire images simultaneously.

Key to the mechanical subsystem is the optical compartment, including the optical base plate, on which all optical components are mounted. The optical base plate is isolated from the instrument housing and equipped with a separate, closed-loop cooling system. The temperature of the base plate is kept constant at 19 °C ± 1 °C, minimizing noise fluctuations and gradients as much as possible.

The electrical subsystem of APEX is composed of the frontend electronics, supporting frame rates of up to 43.3 Hz. Following an analog–digital conversion and multiplexing the two detector channels, data are processed in a Field Programmable Gate Array (FPGA) to stream 16 bit words in a serialized fashion through an optical high-speed link to the control and storage rack. Ancillary information is transmitted in parallel over a serial RS422 link to the control and storage rack. The APEX instrument is equipped with a separate, closed-loop cooling system. The temperature of the base plate is kept constant at 19 °C ± 1 °C, minimizing noise fluctuations and gradients as much as possible.

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filters used for instrument spectral stability monitoring. The filters are bandpass filters (Spectrogon) with transmission features at 700, 1000 and 2218 nm, and a Standard Reference Material (SRM) filter from the National Institute for Standards and Technology (NIST) with many distinct absorption features throughout the VNIR and SWIR spectral range. A fifth slot holds a neutral density glass filter (Schott NG4) and is used to avoid saturation in the VNIR channel at (very rare) expected maximum radiances levels (e.g., above snow). The sixth slot is left empty for standard Earth surface data acquisition. The APEX in-flight calibration capabilities are primarily used to assess spectral performance changes during in-flight and serve as comparison baseline between laboratory and in-flight conditions (D’Odorico, Alberti, & Schaepman, 2010). Simultaneous measurements of temperature and pressure ensure monitoring of environmental conditions in the lab, during in-flight calibration and data acquisition. This information is used for stability modeling and monitoring (Jehle, Hueni, Baumgartner, Lenhard & Schaepman, in press). IFC data analysis relies on the use of a feature-fitting algorithm comparing laboratory and in-flight shifts of particular filter absorption lines. In addition, the same method is used on atmospheric absorption lines during normal imaging, allowing monitoring the instrument’s spectral stability (D’Odorico, Guanter, Schaepman, & Schläpfer, 2011). Remaining spectral and radiometric variations are mostly due to changing pressure/humidity/temperature affecting the prisms refraction properties, and can be estimated using ancillary data recorded by the APEX instrument (Jehle et al., in press).

2.3. Control and storage unit

The control and storage unit (CSU) hosts instrumentation to operate APEX (Fig. 2). This includes the Inertial Navigation System (INS) with dGPS data processing capabilities (Applanix POS/AV 410 IMU/GPS). APEX optical and positional data are linked using GPS based timestamps.
during processing by forming a smoothed, best-estimate trajectory for each acquired imaging frame. Further components are the flight management system with interfaces to the operator and pilot (TRACK'AIR XTrack), the APEX computer with its storage unit (Solid State Disks) and the power supply units. While largely everything in the CSU is available as commercial-off-the-shelf, only a custom-made PCI card is needed to be developed in order to connect the optical link from the instrument to the host system. Data originating from the PCI card use a multi-threaded shared memory architecture to ensure sufficient data throughput to the solid-state-memory disks. All of the CSU is driven by a tiered software approach. Low-level interfaces control disk read/write operations, while a middle tier level handles all logging and alerting. High-level software controls and enables configuring the system, its status and displays a waterfall image in real-time on screen for the operator. Finally, the power distribution unit connects the aircraft power supply with all APEX instruments requiring power.

2.4. Calibration and validation approach

APEX calibration and validation invokes a full set of integrated activities with the aim to producing high quality, reproducible radiometric measurements for each pixel–spectral band combination (Fox et al., 2003; Nieke et al., 2004). Unique to the APEX overall calibration approach is the use of a combination of laboratory, in-flight, and vicarious calibration activities (Schläpfer et al., 2000) based on methods using combined in-flight, scene-based and atmospheric approaches (Brazile et al., 2006; D’Odorico et al., 2011). Vicarious calibration is methodologically based on Kneubühler, Schaepman, Thome, and Schläpfer (2003), while in situ measurements (spectral radiance and reflectance using field spectrometers) are performed on standard targets (artificial sportgrounds, concrete) (Jehle et al., 2010), covering a limited range of radiances measured at sensor (Hueni et al., 2009a). The initial design foresees to assimilate calibration measurements into a coherent set of radiance measurements (Kaiser et al., 2004). This results in the development of both, a calibration and validation approach and software supporting in-situ measurements of field spectroradiometer measurements (Bojinski, Schaepman, Schläpfer, & Itten, 2002; Hueni et al., 2009a; Schaeppman & Dangel, 2000) as well as handling calibration data (Hueni, Malthus, Kneubuehler, & Schaepman, 2011; Hueni et al., 2009a; Hueni, Lenhard, Baumgartner and Schaepman, 2013).

The laboratory calibration approach is based on a calibration home base (CHB, located at the German Aerospace Center (DLR)), which is
particularly designed to calibrate APEX and other airborne imaging spectrometers with similar properties, as well as the spectrometers used for on-ground reference measurements (Gege et al., 2009). This has been demonstrated with a number of airborne and field spectrometers calibrated in the CHB (Lenhard, Baumgartner, & Schwarzmaier, 2014 (in revision)). This traceable calibration approach facilitates the intercomparison of calibration data, and close cooperation with the German national metrology institute PTB (Physikalisch-Technische Bundesanstalt) assures state-of-the-art accuracy and traceability. By providing light sources with fully characterized properties (Taubert et al., 2013), the CHB allows to determine the functional relationship between at-sensor radiances and the signal measured by APEX (Nieke et al., 2008). The measurements can be classified in three categories: a) radiometric, allowing to convert raw sensor signals to physical units of radiance traceable to the système international (SI) (Taubert et al., 2013); b) spectral, allowing to assign center wavelength and spectral resolution for each detector element; and c) geometric, allowing to determine the view angles and angular resolution of each detector element. The latter two include the characterization of the optical distortions typical for pushbroom sensors known as smile and keystone. In addition, the CHB supports a multitude of auxiliary measurements required to fully characterize an imaging spectrometer such as detector linearity, sensitivity to linearly polarized light, radiometric noise or pixel response non-uniformity.

Finally, vicarious calibration efforts are performed in every flight season using selected reference targets on ground while the APEX instrument is acquiring data. The approach used follows guidelines as developed for other imaging spectrometer vicarious calibration (Kneubühler et al., 2003; Milton et al., 2009).

2.5. Processing and archiving facility

APEX data processing and archiving is split into the development of a science grade APEX processor, designed to produce calibrated radiances in a coherent observation geometry (i.e., Level 1), and an operational grade APEX processor and archiving facility, facilitating reproducible data processing and distribution (Hueni et al., 2009a). All processing beyond Level 1 (e.g., orthorectification, atmospheric compensation, and higher level products) are discussed in the application development section.

The science grade APEX processor is designed to process large quantities of imaging spectrometer data, including calibration and housekeeping data (Schaepman, Schläpfer, BIZE, & BOJINSKI, 2002). Its design is based on an iterative prototyping approach and from beginning on includes considerations to build look-up tables for atmospheric compensation (BRAZILE et al., 2004), as well as optimized processing speed requirements (BRAZILE, RICHTER, SCHLÄPFER, SCHAEPMAN, & ITTEN, 2008; BRAZILE et al., 2005).

The science grade APEX processor is developed to integrate calibration data with actual measurements, allowing to reconstruct each geometrical position and each radiance of any given detector element (Fig. 4). Processing data from raw to Level 1 is a two-stage process. Raw data generated by the APEX CSU computer are first segregated into imaging, in-flight calibration and dark current data blocks basing on a finite-state machine (FSM) fed with sensor parameters. Level 1 data processing is frame based, applying a sequence of algorithms comprising true dark current correction based on a shutter mechanism in front of the ground imager, de-smearing of the VNIR channel, compensations of radiometric effects due to spectral shifts (Hueni et al., 2014), radiometric calibration by applying gains and offsets, bad pixel replacement by spatial interpolation and optional spectral/spatial resampling to register the data within the nominal geometric and spectral coordinate space, thereby compensating for spectral and spatial misregistration. All calibration data is contained in the Calibration Parameters Cube’ (cf. Fig. 4) and available upon request. The raw to Level 1 processor as well as the APEX Calibration Information System are continuously improved to refine the sensor model (Huenni, Sterckx, & Jehle, 2013) and data calibration. (See Fig. 3.)

3. APEX Earth science applications

3.1. Introduction

Increasingly, imaging spectrometer data are delivered as calibrated radiance data (Level 1) as well as science products (Levels 2 & 3). Reasons to deliver a multitude of processing levels are based on modeling requirements using radiance based approaches (LAURENT, VERHOEF, CLEVERS, & SCHAEPMAN, 2011a; LAURENT, VERHOEF, CLEVERS, & SCHAEPMAN, 2011b; LAURENT et al., 2010), or applications of narrow- and broadband indices at surface reflectance or radiance levels (VERRELST, SCHAEPMAN, KÖTZ, & KNEUBÜHLER, 2008). Imaging spectrometer data are used for many purposes nowadays and comprehensive overviews are found in the scientific literature (cf., BEN-DOR et al., 2009; DOZIER, GREEN, NOLIN, & PAINTER, 2009; GAO, MONTES, DAVIS, & GOETZ, 2009; JACQUEMONT et al., 2009; KOKALY, ASNER, OLLINGER, MARTIN, & WESSMAN, 2009; MILTON et al., 2009; PLAZA et al., 2009; SCHAEPMAN et al., 2009b; USTIN et al., 2009). We concentrate here on describing a few key applications, which are either unique to APEX or significantly advance the use of APEX-like data. APEX data itself are available as a general purpose APEX data set, which can be downloaded (http://www.apex-esa.org) (Hueni et al., 2012). On the same site, APEX quick-looks are also listed. Many of those datasets can be obtained free of charge for scientific use by contacting the responsible person.

Although representative at regional scale, advanced APEX products have also implications for environmental research at larger scales. Process models, for example dynamic global vegetation models (LGPGUESS (Smith et al., 2001)), are unique tools to quantify the impact of environmental change on ecosystem functioning. Their reliability is however limited due to static parameterization or model assumptions (Friedlingstein et al., 2006). APEX like EO-data at local and regional scale face increasing attention to improve models (Plummer, 2000; Poulter et al., 2011). Long term environmental monitoring programs are usually based on modeling approaches and continuous satellite data series (Scholes et al., 2009). Providing continuous series of satellite data is non-trivial, especially in case of instrument replacement or sensor degradation, and can only be guaranteed by applying data harmonization strategies (Teillet et al., 1997). APEX data are suited to simulate data and products of current and future space missions (e.g., Sentinel-2; D’ODORICO, CONSANO, DAMM, & SCHAEPMAN, 2013). Such simulations provide the base to define technical specifications of incoming instruments or for identifying data harmonization needs and strategies (Steven et al., 2003). The traceability of EO data quality is of outstanding importance if data are intended to be assimilated in process models (Fox et al., 2003). The rigorous implementation of physical based algorithms for the APEX product retrieval (e.g., Bayesian optimization algorithm in combination with coupled atmosphere–canopy models; Laurent et al., 2011), and the comprehensive data quality assessment of APEX (i.e., calibration in CHB, IFC monitoring) enables to trace uncertainties throughout the entire processing chain. Products following the above reasoning are discussed in the following section.

3.2. Operational and science grade processing

APEX operational grade data processing is performed within the Central Data Processing Centre (CDPC) at VITO. First, spectral misregistration is performed using a spectrum-matching technique (GAO, MONTES, & DAVIS, 2004). Geometric processing is performed using direct georeferencing, including the use of standard or user-provided Digital Elevation Models (DEM). Subsequently, a smile-aware atmospheric correction is performed to retrieve hemispherical–conical reflectance factors (HCRF) in combination with MODTRAN5. Finally coordinate
Fig. 3. Laboratory calibration of APEX. Top: APEX mounted on integrating sphere for radiance calibration. Bottom: APEX mounted on optical bench for spectral/geometric calibration. Photo: M. Jehle, Calibration Home Base at DLR, Oberpfaffenhofen (GER)

Fig. 4. High level processing scheme of the APEX processor. DIC = Dichroic Filter Correction (Hueni, Schlaepfer, Jehle, & Schaepman, 2014; Hueni, Wooliams, & Schaepman, 2014), NG4 = Neutral density glass filter (Schott NG4), L1 = Level 1 Processor, BIL = Band Interleaved by Line format, Pol. = Polarization, VNIR = Visible/Near Infrared, SWIR = Shortwave Infrared.
projection is performed using the General Cartographic Transformation Package (GCTP) (USGS, 1998). For all reprojections, a seven parameter Helmert transformation is used. In a final step, HCRF data are resampled to the central wavelengths as calibrated in the CHB for the actual acquisition (Biesemans et al., 2007).

APEX science grade data processing is corrected to minimize the impact of atmospheric and topographic effects (Richter & Schläpfer, 2002; Schläpfer & Richter, 2002). The subsequent automated atmospheric compensation process accounts for irradiance properties in complex terrain, atmospheric scattering and absorbers, as well as instrument smile effects (Richter, Schläpfer, & Muller, 2011). This combined geo-atmospheric processing is used for all situations, where users wish to obtain uniform geo-locatable bottom of atmosphere reflectance values. In addition, APEX data can be normalized to contain nadir-viewing geometries by applying a Li-Ross BRDF correction based on a continuous land cover classification (Weyermann, Damm, Kneubuhler, & Schaepman, 2014). Using a spectral unmixing based approach, land cover types with substantial BRDFs are extracted from the APEX scene and expressed as linear combinations of three kernels (isotropic, geometric (Li-kernel), volumetric (Ross-kernel)). This approach allows seamless mosaicking of several APEX flight lines, while minimizing angular effects dominating flight patterns that are chosen to comply with minimal operational constraints and not optimized for minimal directional illumination influences (Laurent, Schaepman, Verhoef, Weyermann, & Chavez, 2014).

While operational APEX data processing is available to everyone browsing data in the CDPC archive of VITO, science grade data processing is highly experimental and only applied on request. However, the APEX PAF is upgraded to include always latest developments of the science grade processing.

3.3. AOD and critical surface albedo

If able to directly retrieve aerosol optical depth (AOD) from APEX data, it is possible to improve the atmospheric compensation procedure by generating a priori probability distribution functions. We suggest a forward model approach, identifying a SNR of ≥ 100 at 550 nm being sufficient for AOD retrieval on surfaces with 10% reflectance or less (Seidel, Schläpfer, Nieke, & Itten, 2008). However, even if reflectance spectroscopy data are combined with dedicated aerosol remote sensing instruments measuring at multiple angles including polarization sensitivity (Diner et al., 2013), aerosol optical and especially microphysical property retrieval remain challenging. Computationally extensive algorithms limit the AOD retrieval to far real-time data processing. We suggest a simple model for atmospheric radiative transfer (SMART), critically balancing computational speed and retrieval accuracy to the benefit of AOD retrievals (Seidel, Kokhanovsky, & Schaepman, 2010) as well as simulations of Hemispherical–Conical Reflectance Factors (HCRF, following (Schaepman-Strub, Schaepman, Painter, Dangel, & Martonchik, 2006)) for space- and airborne sensors. SMART is used in a fast optimization scheme for the retrieval of AOD using APEX data (Seidel, Kokhanovsky, & Schaepman, 2012) avoiding the critical surface albedo regions (Seidel & Popp, 2012) to maximize the AOD retrieval sensitivity on radiance data at sensor level.

3.4. NO2 vertical column densities

Atmospheric trace gas retrievals using Earth looking airborne imaging spectrometers are of increasing interest and with increased instrument performance and spectral resolution become more feasible (Marion, Michel, & Faye, 2004; Thorpe, Frankenber, & Roberts, 2014). Nitrogen dioxide (NO2) is a reactive trace gas in the troposphere, which acts as an ozone and aerosol precursor and can negatively affect human health and ecosystem functions. Anthropogenic emissions are a major source of atmospheric NO2 and NO2 thresholds are still regularly exceeded in many European countries. We take advantage of the APEX band binning/unbinning capability (Dell’Endice et al., 2009) to derive vertical column densities (VCD) of NO2 from APEX. A two-step approach (Popp et al., 2012) based on differential optical absorption spectroscopy (DOAS) is applied to unbinned APEX measurements whose higher spectral sampling enables good coverage of the narrow absorption lines of atmospheric gases. First, the number of NO2 molecules along the average photon path through the atmosphere to the sensor (slant column densities (SCD)) are computed by fitting absorption cross sections of NO2 and other interfering gases (i.e., H2O, O3–O2, or O2) in the 470–510 nm spectral region to the differential optical depth calculated from image-based reference spectra. Second, the resulting NO2-SCD is normalized to NO2-VCD with a so-called air mass factor (AMF). The AMF is computed by radiative transfer calculations including forward model parameters such as surface reflectance retrieved from the APEX data, a digital elevation model, a-priori model NO2 profiles, and an aerosol extinction profile (Popp et al., 2012). The resulting two-dimensional NO2-VCD maps now allow the quantification of the spatio-temporal highly variable NO2 field as well as the detection of major NO2 sources at an unparalleled local scale and synoptic view.

3.5. Coupled canopy–atmosphere modeling

Imaging spectrometers are used to map dedicated absorption features present in Earth surface materials or in the atmosphere. This requires that spectral bands should be positioned at (or sufficiently close to) the absorption features. Spectral instabilities will lead to detection of unrelated phenomena and even render retrieval algorithms (such as vegetation indices) instrument specific and/or dependent. In addition, data are usually converted to surface reflectance. For this conversion to be successful, we must assume certain parameters at the interface between canopy and atmosphere (i.e., topography, surface anisotropy, adjacency effects, location of top-of-canopy). We therefore suggest the use of a coupled canopy–atmosphere RT model combined with a Bayesian optimization algorithm for vegetation (Laurent, Verhoef, Damm, Schaepman, & Clevers, 2013). This approach does not invoke atmospheric compensation before applying the inverse model and is largely independent of the number of bands used (limitations are related to larger uncertainties when using fewer bands). Using the hybrid canopy RT model Soil–Leaf–Canopy (SLC) (Verhoef & Bach, 2007) and the atmosphere RT model MODTRAN (Berk et al., 2004), the canopy–atmosphere coupling is based on the 4-stream theory (Laurent et al., 2011b), making full use of the directional information contained in the four canopy reflectance components as modeled by SLC. Variable estimation is then performed using Bayesian optimization of the coupled model (Tarantola, 2005).

3.6. Sun-induced chlorophyll fluorescence (Fs) retrieval

From the early APEX instrument development phase on, the pushbroom design allowed only one given wavelength to be chosen for the adjustment between dispersing elements and detector(s). Once this wavelength is chosen, all the others are defined by geometric constraints. This wavelength was set to be the 760 nm O2–A absorption line in the VNIR detector since it has the advantage of being useful for in-flight calibration purposes. With the advent of having this line well calibrated, it became evident that APEX can be used for the retrieval of sun-induced chlorophyll fluorescence (Fs) (Damm et al., 2011). In the near infrared, emitted Fs contributes to about 2–5% to the reflected radiance flux of a vegetation canopy (R). Both fluxes have to be decoupled to quantify the Fs emission signal. For medium resolution instruments, the Fraunhofer Line Depth (FLD) approach introduced by Plaszczyk (1975) serves as de-facto standard for Fs retrieval using medium resolution instruments (Meroni et al., 2009). The Fs retrieval algorithm implemented for APEX data follows the approach proposed by Guanter et al. (2010) and is based on a constrained FLD approach exploiting the broader O2–A absorption feature. Reference surfaces with known Fs
emission (e.g., bare soil) are used to constrain the Fs retrieval (Damm et al., 2014; Guanter et al., 2010).

3.7. Pigment retrieval

Retrieval of plant pigments and pigment systems has seen substantial progress paralleled with increased performance of imaging spectrometers (Kokaly et al., 2009; Ustin et al., 2009). Pigments are not only relevant to determine leaf functioning (Carvalho, Takaki, & Azevedo, 2011), but are used as proxies for light use efficiency in models of net primary productivity (Coops, Hilker, Hall, Nichol, & Drolet, 2010) or assessing functional traits (Homolova, Malenovsky, Clevers, Garcia-Santos, & Schaepman, 2013). However, high accurate retrieval of functional traits is highly dependent on narrow and stable bands in a spectrometer system. Finally, as photoacclimation and time kinetics (Hallik, Niinemets, & Kull, 2012) become more feasible to be measured, accurate pigment estimates will steadily gain in importance. We use index based approaches for combined retrieval of chlorophyll, carotenoids and anthocyanins from APEX data (Gitelson, Keydan, & Merzlyak, 2006). The original band positions are adapted to match specific APEX bands, which are smaller in bandwidth than the sensor used for the original development of the retrievals.

4. Results

4.1. APEX advanced radiometry measurements

Following acceptance testing in 2009, APEX was transferred to the University of Zurich and VITO in spring 2010 for regular operations. Since summer 2010, APEX is producing science grade spectrometry measurements and has acquired >3 Terabytes of data corresponding to >3 Mio. scan-lines (approx. 30,000 km²) and several factors more in calibration and product data until the end of 2013. APEX has received airworthiness certification for two of DLR's research aircraft (Dornier DO-228-101 (D-CODE), Dornier DO-228-212 (D-CFFU)) with VITO and the University of Zurich providing instrument operators for data flights. In parallel, updates to the instrument, CHB, and PAF have been made to further improve the instruments measurements. We present the following table (Table 1) summarizing the initial specifications used to design the instrument and list validated performances for all specifications as well as other relevant instrument parameters including associated references following upgrades and calibration efforts.

APEX radiometric performance is validated using a four-fold approach. Following calibration in the CHB, APEX is calibrated traceable to a primary calibration standard with less than 4% uncertainty (Fig. 5A). Second, APEX is calibrated using radiance based vicarious calibration approaches with in-situ measurements performed using a field spectroradiometer (ASD FieldSpec Pro FR) and a sunphotometer (CIMEL) (Fig. 5B). Uncertainties are in the range of ≤6.5%, but lower spectral resolution of the field spectroradiometer as compared to APEX are limiting the calibration effort. Also with a spatial resolution of 1–2 m, identifying homogeneous areas on ground is very challenging. At this spatial scale, sports fields, concrete or other artificial targets are usually not homogeneous enough to serve as calibration surfaces. Therefore, validation efforts are also put in place using spatially distributed data and inverse (Fig. 5C) as well as forward (Fig. 5D) modeling approaches. The latter two still show deviations from the APEX measurements, largely due to simplified model approaches.

In-flight calibration information is used in combination with atmospheric measurements allowing to monitor (D’Odorico et al., 2011) and model instrument stability (Jehle et al, in press) and can therefore not be used in addition as independent calibration source.

4.2. APEX Earth science applications development

APEX Earth science applications span a wide range of products. While calibrated radiances are a standard product for many science grade instruments, we have developed individual and joint approaches for atmospheric correction and allowing minimizing the impact of surface anisotropy effects. These products are of high operational use,

**Fig. 5.** Comparison of four APEX validation approaches. A) traceable, calibrated laboratory measurements (Hueni, Schlaepfer, Jehle, & Schaepman, 2014; Hueni, Wooliams, & Schaepman, 2014); B) radiance based vicarious calibration effort using in-situ spectroradiometric measurements (Damm, pers. comm.; C) radiance level based comparison from Bayesian optimization (Laurent et al., 2013); and D) forward simulated at-sensor-radiances using 3D modeling (Schneider et al., 2014 (in revision)).
since increasingly well corrected surface reflectance data are required for more operational or stakeholder-oriented user communities. However, a complete physically based surface anisotropy correction remains challenging. Instruments like APEX are limited in angular data acquisition as well as by having a relatively small FOV. Additional efforts are needed to constrain the BRDF correction, likely with the support of a priori information.

We report on a second class of Earth science applications, namely retrieving information from the atmosphere (VCD of NO2 as well as AOD), and deriving the concept of critical surface albedo, allowing to decouple atmospheric and land surface based products, further increasing the retrieval quality of the atmospheric products. Columnar retrievals of NO2 using airborne instruments cannot be compared with in-situ point measuring networks. However, current existing in situ measurements can be complemented by columnar NO2 information, allowing policy validation with a higher level of process understanding in the coupled surface–atmosphere system (Popp et al., 2012). Finally AOD retrievals are optimized using simplified approaches, carefully balancing retrieval accuracy and computational requirements. The AOD information can be later used as prior information in an atmospheric compensation procedure in an iterative fashion.

Many of the current retrieval schemes used in spectroscopy rely on retrieving surface reflectance and subsequently infer biochemical or biophysical information. We demonstrate with APEX a new retrieval scheme by coupling a canopy–atmosphere model and invert the coupled model. This allows us to avoid two separate steps of atmospheric correction and invoking an inverse canopy model in a second step. The coupled model approach clearly shows advantages by minimizing interfacing complexity between these two models at the cost of increased inversion complexity. The particular model combination (SLC and MODTRAN) shows excellent performance in vegetation corresponding closest turbid media scattering, which is the physical foundation of the SLC model. Validation of this process is performed using a radiance based vicarious calibration procedure, ensuring consistency when comparing in-situ and airborne measurements (see Fig. 4B).

We finally apply simultaneous fluorescence line depth (FLD) and pigment retrieval approaches to APEX data (Fig. 6). Vegetation fluorescence (Fs) is derived using the constrained 3FLD approach (Damm et al., 2014). Because of a very low Fs signal, residual along-track striping is still visible in the APEX data. Fs values range between 0 ... 10 mW m⁻² nm⁻¹ sr⁻¹. Simultaneous field validation using a field spectroradiometer (ASD FieldSpec FR Pro) is carried out. We use a spectral deconvolution approach to minimize Fs retrieval differences between APEX and the field spectroradiometer measurements (Zhao, Jia, & Li, 2010). In situ data were collected using a stratified random sampling approach while measuring reflected and emitted radiances at each calibration point (n = 16), resulting in a good agreement between airborne and in situ Fs (R² = 0.87, relative RMSE = 27.76%). Spatial distribution of Fs, such as measured with APEX, can serve as proxy for instantaneous plant photosynthesis. Pigments are derived in relative units and visual validation suggests feasibility of the method. Measurements of pigments in leaves are well understood (Gitelson, Chivkunova, & Merzlyak, 2009), however their validation using leaf pigment concentrations is ongoing, and leaf models including separate representation of these pigments and plant structure are sparse (Townsend, Serbin, Kruger, & Gamon, 2013) and not applied in an inverse fashion to remotely sensed data as of yet. Relative pigment abundances will support improved plant functioning and estimates of light use efficiency. Also they represent an important functional trait per se.

5. Conclusions and outlook

We report on the latest status of APEX with focus on advanced radiometry measurements and Earth science applications. APEX has undergone a complete development cycle, ranging from modeling system specifications to analyzing APEX data in a coherent fashion. Following the start of the operational activities of APEX in 2010, small improvements were made to the hardware (more reliable electronics boards, update of storage capacity, etc.), and major improvements to sensor modeling, refinement of the PAF and development of science grade retrieval algorithms. APEX has very high compliance with its initial specifications (though not in all parts), and currently allows operational data acquisition of traceable radiometric measurements and production of Earth science applications.

The APEX instrument has demonstrated to deliver traceable spectroradiometric measurements. The PAF processes data using the latest calibration information, individually optimized for each single scene. This results in scene-specific band positions. While this is no threat to individually analyzing scenes, most of the commercially available software does not support convolution techniques ‘on-the-fly’, putting a de-convolution/convolution effort on those users using multiple scenes for their analysis. Controversial discussions are ongoing, if

![Fig. 6. Left: Fs retrieval following Damm et al. (2014) in absolute units [0–10 mW m⁻² nm⁻¹ sr⁻¹, black–white]. Right: Pigment content retrieval following Gitelson et al. (2006) in relative units [0–100%]. Pigment abundances are red: carotenoids, green: chlorophyll-a and blue: anthocyanin (APEX data June 16, 2012; 10:48 UTC; Oensingen, Fluxnet site 314; 47.2863°N, 7.7343°E, Switzerland). For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)](image-url)
APEX band settings should be resampled to a ‘common band set’, or leaving the original measurements unaltered. Currently, the latter is the case.

APEX was designed using a robust approach to sensor modeling. Even though the instrument model was updated on a regular basis, a key challenge remains to develop a sensor independent model, allowing for forward and inverse modeling approaches. Currently, the APEX PAF contains substantial APEX specific correction algorithms, being inherent to the functioning and performance of this specific instrument (Hueni et al., 2009). A more generic and generally applicable instrument and application model would serve all of the hyperspectral community much better, allowing for instrument and product cross-comparison in a much more coherent fashion.

While APEX, with its very high spectral resolution, is capable of simulating existing and future missions at very high accuracy, it can also be used to ensure consistency of indices-based approaches. Many of the existing narrow- and (and broad-) band indices are developed using a specific instrument. High spectral resolution instruments can easily be convolved to fit original band settings, but can in addition be used as a model intermediate to ensure continuity and uncertainty estimates of different instruments (D’Odorico et al., 2013) in combination with in situ measurements. Availability of spatial and temporal discontinuous data of high spectral resolution is of key importance to fulfilling this goal.


