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Considerations on Water Vapor and Surface Reflectance Retrievals for a Spaceborne Imaging Spectrometer

Rudolf Richter and Daniel Schläpfer

Abstract—The retrievals of atmospheric water vapor column and surface reflectance from air- or spaceborne hyperspectral imagery require accurate spectroradiometric calibration and a radiative transfer (RT) code. Since RT codes are too time consuming to be run on a per-pixel basis, a common technique employs the offline compilation of an atmospheric database and its subsequent use for the atmospheric correction of the image cube. The challenge is to design the size of the database as small as possible for a requested retrieval accuracy. We present a methodology to compile the database for a specified retrieval accuracy in water vapor and surface reflectance for a given set of input surface reflectance spectra and a chosen RT algorithm. The method is applied as a case study conducted for the planned German imaging spectrometer EnMAP. Some tradeoff considerations are also discussed. For the specified range of columnar water vapor (0.5–4.5 cm), results demonstrate that five water vapor grid points in the database are sufficient to achieve the requested relative root-mean-square retrieval accuracies of 2% and 3% in water vapor and surface reflectance, respectively. It should be pointed out that this is not intended as a general claim of retrieval accuracy achievable under typical remote sensing conditions, but these figures apply only to the theoretical conditions of the calculation, i.e., assuming the same conditions for forward simulation and retrieval. Nevertheless, these figures are indispensable for the design of a database, which is an important step for the atmospheric correction of imaging spectrometer data and the sole topic of this paper.

Index Terms—Atmospheric effects, EnMAP, imaging spectrometer, surface reflectance, water vapor.

I. INTRODUCTION

The history of imaging spectrometers acquiring data in the solar-reflective region (0.4–2.5 µm) goes back to 1984 [1], [2]. In 1989, AVIRIS was the first operational instrument covering the 0.4–2.5-µm electromagnetic spectrum with more than 200 contiguous narrow spectral bands [3]. After atmospheric correction, i.e., using the retrieved surface reflectance spectra, its data enabled a large range of applications in geology, agriculture, forestry, ecology, etc. In the 1990s, progress was also achieved in algorithms for the scene-based automatic retrieval of atmospheric parameters from hyperspectral imagery, i.e., aerosol type, optical thickness [4], and atmospheric water vapor [5], [6]. Additionally, the accuracy of radiative transfer (RT) codes was improved [7]–[9].

In the 1990s, software packages for the atmospheric correction of multispectral and hyperspectral imagery became publicly available (e.g., ATCOR [10], ATREM [11], ISDAS [12], FLAASH [13], ACORN [14], and HATCH [15]). As the number of air- and spaceborne hyperspectral instruments increased, the idea of a general-purpose fine spectral resolution (“narrow band model”) database of atmospheric lookup tables (LUTs) became attractive. If once compiled, it could be used for any hyperspectral instrument (e.g., Hyperion [16], AVIRIS [17], and CHRIS/Proba [18]) by resampling the database with the channel spectral filter curves, which is much faster than running an RT code for an additional sensor to be supported [19]. However, since the database has to cover a large range of atmospheric parameters (different aerosol types, visibilities, and water vapor columns), geometric conditions (different sensor altitudes for airborne instruments, view or tilt angles, and ground elevations), and solar geometries, the size of the database is huge. The fine spectral resolution ATCOR database in 2002 for airborne sensors was about 2 GB; it is about 5 GB in 2007. The database size for satellite sensors is a factor of eight smaller, because a common altitude above the Earth’s atmosphere can be taken.

Another approach was implemented in FLAASH. Here, the MODTRAN code [9] is run for the specified view and solar geometry pertaining to a scene, several surface reflectance values, and a range of atmospheric parameters (water vapor and visibility). Results are stored in LUTs, which are then used for the surface reflectance retrieval. Both approaches have advantages and drawbacks. The advantage of the first approach is that no RT runs are necessary when the database has been compiled; the drawback is that interpolations in the parameter space have to be performed, and updates to the RT algorithm cannot be included without regenerating the database. The advantage of the second approach is that no interpolations for the view/solar geometry are required, and interpolation errors for the remaining parameters (e.g., water vapor column and visibility) will be smaller, because more grid points per parameter interval can be afforded. The drawback is the need to run the RT code, although results can be stored for later use.

This contribution investigates the first approach. The background is the approved German EnMAP mission, a spaceborne imaging spectrometer covering the 0.42–2.45-µm electromagnetic spectrum with approximately 200 bands, a spectral resolution of 10 nm in the land mode, and a spatial resolution of

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30 m [20]. In the water mode, which is not treated here, some
channels have a 5-nm bandwidth but with the same spatial reso-
lution. The instrument is scheduled for launch in 2012. A deci-
sion was made to use the general-purpose atmospheric-database
approach for EnMAP. Since the locations of the channel-center
positions have not yet been finalized, the following work was
conducted for an instrument with a 10-nm channel spacing
with the first and last channel centers at 0.4 and 2.45 μm,
respectively, employing Gaussian channel filter curves with
FWHM = 10 nm (full width at half maximum). The objective
of this paper is to design a method of compiling a high spectral
resolution database with specified retrieval accuracies of water
vapor and surface reflectance and a minimum database size.
This database shall support instruments with FWHM ≥ 10 nm,
requiring a sampling distance of about 1 nm.

If the specific atmosphere used in a forward RT simulation
is one of the atmospheres of the retrieval database, then the
retrieval will essentially produce an exact match of the water
vapor column and surface reflectance. Additional errors occur
when interpolated or extrapolated atmospheric conditions are
used in the retrieval. The objective of this paper is to insure
that these additional errors are small, i.e., relative rms retrieval
errors do not exceed 2% and 3% for water vapor and surface
reflectance, respectively.

II. METHODOLOGY TO OBTAIN AN
ACCURACY-TAILORED DATABASE

A short description of the basic RT equation is needed before
we begin the discussion of the method. Under clear-sky condi-
tions and assuming an isotropic (Lambertian) reflectance law,
the at-sensor spectral radiance for a small target of reflectance
ρ is in a large background of reflectance ρb, ρ is described by [21]

\[ L(ρ, ρ_b) = L_p + \frac{τ_{dr} E_g(0)ρ}{1 - s ρ_b} + \frac{τ_{df} E_g(0)ρ_b}{1 - s ρ_b} \]  

(1)

where \( L \), \( L_p \), \( E_g(0) \), \( τ_{dr} \), \( τ_{df} \), and \( s \) are the total at-sensor
radiance, path radiance, global solar flux (direct plus diffuse)
on the ground for a surface reflectance of zero, direct and diffuse
ground-to-sensor transmittance, and the spherical albedo of the
atmosphere, respectively. All quantities depend on wavelength,
but the wavelength index is omitted for brevity. If \( ρ_b = ρ_b = ρ \),
(1) can be simplified to contain only two terms on the right-
hand side (path radiance and reflected radiance) by introducing
the total transmittance \( τ = τ_{dr} + τ_{df} \). When solving for the
surface reflectance of image data, (1) is solved iteratively.

The first step neglects the neighborhood effect and obtains
\( ρ_1(x, y) \); the second step employs a moving low-pass filter
of twice the adjacency range (typically, 1 km for satellite
sensors) to get \( ρ_2(x, y) \); and the third step calculates the final
surface reflectance with the removed adjacency influence as
\( ρ_3(x, y) = ρ_1(x, y) + (τ_{df}/τ_{dr})(ρ_1(x, y) - ρ_2(x, y)) \) (see [10]
for details). For flat-terrain applications, it would be sufficient
to store the global flux \( E_g(0) \), but in mountainous terrain, the
direct \( E_{dr} \) and diffuse flux \( E_{df} \) terms are required (\( E_g = E_{dr} + E_{df} \)) [19], [22]. Therefore, the atmospheric database will store
the set of six quantities \( Q = (L_p, τ_{dr}, τ_{df}, E_{dr}, E_{df}, s) \) after
each run of an RT code. In principle, the calculations can be
conducted with any RT code that has a sufficient accuracy and
spectral resolution. We use the well-known MODTRAN4 code
[9] to calculate LUTs for these functions and store them in the
database.

The quantities \( Q \) are computed for a discrete set of at-
mospheric parameters. In terms of MODTRAN, these input
parameters are as follows: atmospheric model (e.g., midlatitude
summer and tropical), aerosol type (e.g., rural and urban),
visibility, water vapor column, observation geometry (sensor
altitude, view angle, and ground elevation), and solar geometry
(zenith and azimuth angle).

For the accuracy estimate analysis of this paper, RT calcula-
tions have to be performed for two parameter sets: one with a
narrow spacing of grid points to be used as a reference for the
retrieval accuracy (index “ref”) and a second one with a wider
spacing for the finally recommended database (index “db”).

The retrievals will be performed with the quantities from the coarse
spacing \( Q_{db} \) evaluated at the grid points of the narrow reference
spacing. For this purpose, suitable interpolation/extrapolation
has to be provided. For the columnar water vapor parameter
\( W \), an appropriate function type is [23]

\[ g(W, λ) = \exp \left( a(λ) + b(λ) W^{1/2} \right) \]  

(2)

where \( λ \) is the wavelength, and \( a(λ) \) and \( b(λ) \) are coefficients
obtained by a least squares fit using the coarse grid. Thus,
for all six quantities in \( Q_{db} \), separate wavelength-dependent fit
coefficients have to be computed.

The surface reflectance retrieval evaluates the reference
at-sensor or top-of-atmosphere (TOA) spectral radiance cube
\( L_{ref} \) using the interpolated quantities \( Q_{db} \) and solves (1) for
the surface reflectance \( ρ \) for each spectral band employing
\( ρ = ρ_1 = ρ_2 \), because the simulated \( L_{ref} \) is calculated for iso-
lated large homogeneous pixels. This can be written as a short
symbolic equation

\[ ρ(λ) = f^{-1} (L_{ref}(λ) + n(λ), Q_{db}(λ)) \]  

(3)

where \( ρ(λ) \) is the retrieved surface reflectance and \( n(λ) \)
is an optional channel-dependent noise term which may include
different noise sources (instrument and shot noise [24]). A
comparison with the known input \( ρ(λ) \) allows the calculation
of the retrieval error. All scenario variables other than water
vapor column are being set to nominal values, as described in
Section II-A. As the retrieval accuracy generally depends on the
spectral behavior of the surface, typical surface types encoun-
tered in earth remote sensing have to be included, e.g., soil,
sand, fresh and dry vegetation, and spectrally flat reflectances.
Then, a relative (percent) root-mean-square (rms) error can be
evaluated for the retrieved water vapor map as a function of
\( W_k (k = 1, \ldots, n_{ref} = \text{number of forward simulations with}
the narrow reference grid, see Section II-A)

\[ \Delta W_k = 100 \left( \frac{1}{m} \sum_{j=1}^{m} \left( \frac{W_k - W_{k,j}}{W_k} \right)^2 \right) \]  

(4)

where \( W_k \) represents the known input values, the asterisk
denotes the corresponding retrieved values, and the summation

...
is performed over all $m$ input surfaces employed in the forward simulation (see Sections II-A and III).

Similarly, the relative rms reflectance-retrieval error can be evaluated as

$$
\Delta \rho(\lambda, W_k) = 100 \sqrt{\frac{1}{m} \sum_{j=1}^{m} \left( \frac{\rho_j(\lambda) - \rho^*_{j,k}(\lambda, W_k)}{\rho_j(\lambda)} \right)^2} \quad (5)
$$

A. Details of Methodology

First, a short overview on the methodology is given, explaining the principle for one parameter (water vapor column). Then, the general multiparameter description is outlined.

The method creates a 2-D image (map of Fig. 1) for a discrete reference grid of water vapor columns, and for each surface of the input set of surface types and each reference water vapor grid point, the TOA radiance cube (3-D image) is calculated. The initial database has a much lower number of water vapor grid points than the reference grid. Then, the reference radiance cube is inverted using the atmospheric database, requiring appropriate interpolation at the reference water vapor grid points. The water vapor and the surface reflectance cube are retrieved, and relative rms errors with respect to the known input values (water vapor and reflectance) can be calculated. If the specified retrieval accuracy is not met, another water vapor grid point is added to the database, and the iteration continues until the specifications are met or the maximum number of iterations is reached.

Detailed Description: The first step is the definition of the spectral coverage and bandwidth of the hyperspectral sensor to be studied. Then, the interval $I_{p_j}$ for each parameter $p_j$ ($j = 1, \ldots, n$) of the database has to be specified, together with a set of input reflectance spectra $\rho_i(\lambda)$ ($i = 1, \ldots, m$). For each interval, a discrete set of database grid points $p^{db}_{j,k}$ ($k = 1, \ldots, n^{db}_{j}$) is employed to compute the LUTs and provide interpolated values with appropriate functions, e.g., (2). A second much finer spaced reference grid $p^{ref}_{j,k}$ ($k = 1, \ldots, n^{ref}_{j}$) with $n^{ref}_{j} > n^{db}_{j}$ is also specified, which serves as the accuracy check for the interpolated values of the coarse grid.

Then, the at-sensor radiance cube $L(\lambda, p^{ref}_{j,k}; \rho_i(\lambda))$ for this instrument is calculated for a certain parameter (e.g., $p^{ref}_{j} = W =$ water vapor column) using the narrow reference grid points. The last step is the $p^{ref}_{j}$ and surface reflectance retrieval with the coarse parameter grid points of the database and the calculation of the corresponding retrieval errors with respect to the reference grid.

Fig. 1 shows a schematic sketch of the generated synthetic maps with $p^{ref}_{j}$ = water vapor $W(x, y)$ and $L(x, y, \lambda)$. The rows of the $W$ map are repeated $m$ times corresponding to the selected $m$ reflectance spectra $\rho_i(\lambda)$. The $m$ rows of the $L$ map also correspond to the $m$ surface reflectance types.

Fig. 2 shows a flowchart of the proposed methodology. For simplicity, the iteration of database grid points is only shown for one parameter $p_j$, and the index $j$ is omitted in Fig. 2. The procedure starts with a small number $n^{db}$ of $p^{db}_{j}$ grid points, which is usually three or four. The number of points is iteratively increased until the required retrieval accuracy is met or the maximum number of iterations $(n^{max})$ is reached. An equidistant or user-specified spacing in the range of the $I^{db}_{p_j}$ interval is supported.

Example with parameter water vapor column $W$: interval $I_{W}^{db} = (0.4, 4.5)$ cm, initial coarse set of database grid points $p^{db}_{j,k} = W^{db}_{k} = (0.4, 1.0, 2.0, 2.9)$ cm with interpolation functions of (2). Retrieval errors are evaluated at the exact locations of the reference grid $W^{ref}_{k} = (0.5, 1.0, 1.5, \ldots, 4.5)$ cm (a detailed discussion of results of a case study is presented in the next section).

Theoretically, a complete accuracy study should include all parameters of the database, i.e., it consists of the flowchart of Fig. 2 enhanced by a third loop for all parameters. This is a tremendous task, because all $L(x, y, \lambda, p^{ref}_{j})$ image cubes with the narrow reference grids have to be calculated, and the corresponding retrievals have to be performed. As an example, with eight parameters and ten grid points for each parameter interval, the total number of combinations for the narrow reference grid is $10^8$. Therefore, a more practical approach is to fix all parameters but one at typical values (e.g., visibility 23 km, solar zenith angle = 40°, ground at sea level, etc.) and investigate the accuracy requirements for only one parameter.
The next section illustrates this approach with a case study on the water vapor parameter. The complete all-parameter accuracy investigation is also not recommended, because there are other tradeoff considerations discussed in Section IV.

The final compilation of the fine spectral resolution database can be conducted when the parameter grid spacing for the most demanding instrument has been determined.

III. Application of the Methodology: Case Study

This section applies the proposed method to a nadir-view spaceborne imaging spectrometer covering the 0.4–2.45-µm electromagnetic spectrum with 206 channels at a 30-nm spatial resolution and 1024 pixels per line. As mentioned in the Introduction, these specifications closely match the characteristics of the EnMAP spectrometer. The channel filter curves are Gaussian with a bandwidth of FWHM = 10 nm, and the sampling distance of the center wavelengths is also 10 nm. We consider the case of an "ideal" sensor, i.e., the channel noise term \( n(\lambda) = 0 \) in (3). The sensor shall retrieve the columnar water vapor and surface reflectance in the interval (0.5, 4.5 cm) with an average relative rms accuracy better than 2% and 3%, respectively, in the spectral regions influenced by atmospheric water vapor absorption: 0.9–1, 1.1–1.2, and 2–2.45 µm. The very strong absorption regions 1.35–1.45 and 1.8–1.95 µm are not considered, because the ground-reflected signal reaching the sensor is close to zero (see Fig. 3).

Several water vapor retrieval techniques have been published: the narrow/wide band ratio (N/W) [25], continuum interpolated band ratio (CIBR) [23, 26], atmospheric precorrected differential absorption technique (APDA) [6], and curve-fitting methods [27]–[29]. The robust and fast APDA method proved to perform better than N/W and CIBR, particularly in the low-to-medium reflectance interval (0.1, 0.3), and it is often used for operational processing (e.g., [30]). Curve-fitting techniques may achieve higher accuracy than APDA but are time-consuming, and some are not yet operational [28], [29].

The simulation scenario fixes the following parameters at typical remote sensing conditions: a midlatitude summer atmosphere, rural aerosol, visibility of 23 km, ground at sea level, and solar zenith angle = 40°. We employ the APDA algorithm for the water vapor retrieval using measurement bands at 940 and 1130 nm and two reference bands in the adjacent atmospheric windows at 880/1000 and 1070/1240 nm, respectively. The separate 940/1130-nm water vapor calculations are averaged to obtain the final water vapor column. To keep the scope of the results within limits, we assume the following situation: the initial database (db) water vapor grid points are fixed at 0.4, 1.0, 2.0, and 2.9 cm. Failure to meet accuracy requirements will add a grid point near the failure point. In our scenario, the next grid point to be added according to Fig. 2 is selected at 4.0 cm. The reference points use an equidistant 0.5-cm grid.

Since the performance of the APDA algorithm deteriorates for very low reflectance surfaces (water and shadow areas) [6], we select the following input surface types with \( \rho \geq 0.1 \) (in the 0.85–1.25-µm region): surfaces with a spectrally flat reflectance at \( \rho = 0.10, 0.15, 0.30, 0.50, \) fresh vegetation, bright soil, dry vegetation, dark soil, and sand, which are labeled one to nine, respectively (see Fig. 4). Although this case study depends somewhat on the chosen input surface materials, similar results are obtained with larger sets of input spectra of the same surface types as long as low reflectance materials (\( \rho < 0.1 \), for \( 0.85 < \lambda < 1.25 \) µm) are avoided. Section IV includes a discussion of the influence of selecting different surface reflectance sets.

The first objective is the study of the influence of the interpolation functions \( g(W, \lambda) \) of (2) on the accuracy of the water vapor and surface reflectance retrievals with a small clearly arranged set of input spectra, which still yields typical representative results. Retrieval errors also depend on other factors, e.g., a shift in channel locations, coregistration between different channels, type of spectral interpolation between absorption and window channels, haze particles, subpixel clouds, etc. (these are not considered here; a discussion of these effects is presented in [23] and [31]).

After the specification of the coarse parameter grid of the database, the RT quantities \( Q^\text{db} \) have to be interpolated over the complete range of \( W \) from 0.4–4.5 cm using (2). Fig. 5(a) shows normalized functions \( E_{dir} = E_{dir} \tau \), i.e., the direct solar flux at the ground times the ground-sensor transmittance, for several channels. It is obvious that channels in weak absorption regions (910 nm) display an almost linear decrease with \( W \), while the stronger absorption regions show a pronounced nonlinear behavior due to saturated water vapor absorption.
Fig. 5. Normalized fluxes at (a) different wavelengths and (b) comparison of fit results for the subinterval $W = 2 – 4.5$ cm with the 2.45-µm channel.

Fig. 5(b) shows results of different curve fits with (2) in the 2.0- to 4.5-cm subinterval for the channel at 2450 nm. Although the SNR of all current sensors is very low near 2450 nm, we have included the 2450-nm channel to investigate the “worst case.”

Fig. 5 shows the following:

1) fit with the initial four water vapor grid points of the (0.4, 2.9)-cm interval;
2) fit with five grid points of the (0.4, 4.0)-cm interval;
3) fit with three grid points using the (2.0, 4.0) subinterval.

The triangle symbol in Fig. 5(b) marks the exact calculations with the 0.5-cm reference grid. It can be seen that a suitable subinterval fitting provides more accurate results. This fact will also be demonstrated later for the water vapor and reflectance retrievals, but the situation can be best explained with the behavior of the RT functions. It also illustrates that an accuracy improvement can be achieved when the RT quantities $Q_{db}$ are evaluated using the appropriate water vapor subinterval.

Fig. 6(a) shows the rms errors for the retrieval of the water vapor column. The triangle indicates the case of using the initial four database grid points (0.4, 2.9)-cm interval; the square symbol indicates the case with the added 4.0-cm grid point, and the diamond symbol indicates the latter case but with the fit functions of (2) for the quantities $Q_{db}$ calculated for the appropriate subinterval with the nearest three grid points (“optimized” subinterval fit). Overall, the optimized subinterval fit provides the lowest error levels, although the other cases may sometimes yield a smaller error by chance.

Although the presented curves depend on the chosen type of fit function (2), an increase in accuracy with the optimized subinterval approach is a general feature and can also be obtained with other types of fit functions. Fig. 6(b) shows a comparison of the reflectance-retrieval results for the channels 910 and 940 nm and two of the same conditions from earlier, specifically, four $W$ grid points in the (0.4, 2.9)-cm interval versus five grid points in the (0.4, 4.0)-cm interval with optimized subinterval fits. For both channels, the retrieval accuracy is distinctly improved for higher water vapor columns ($W \geq 3.5$ cm), and it is nearly the same for $W \leq 3$ cm. The errors for the 940-nm channel are generally higher than for the 910-nm channel, because the latter channel is less influenced by atmospheric water vapor.

Fig. 7 shows the reflectance-retrieval errors of four selected channels in weak and strong atmospheric-absorption regions as a function of water vapor column. For all bands, the average rms error is below 3%, although the 3% limit is occasionally exceeded. Obviously, a band with weak absorption (910 nm) is less sensitive to water vapor retrieval errors.

Fig. 8 shows the results of the reflectance retrieval for surface 5 (fresh vegetation, see Fig. 4). Fig. 8(a) is based on the five $W$ grid points to calculate the fit functions of (2) for the quantities $Q_{db}$ over the complete water vapor interval (0.4–4.5 cm). Fig. 8(b) calculates the fit functions for the appropriate optimized subinterval with the nearest three grid points. Each plot contains retrieval results for three water vapor cases: $W = 4.0$, 4.5, and 5.0 cm. Although the case $W = 5.0$ cm is not considered in our previous rms error budgets, it is still included.
Here to obtain an impression of the trend. Due to the better performance of the subinterval fits, results in Fig. 8(b) are clearly superior to those in Fig. 8(a) where pronounced artifacts occur near 0.940 and 1.14 µm; the strongest are related to the W = 5.0 cm case. Small artifacts at these wavelengths can also be observed in Fig. 8(a). They are caused by small water vapor retrieval errors and spectral resampling effects in regions with strong spectral gradients of surface reflectance, atmospheric transmittance, and the solar fluxes [32], [33]. Reflectance values in the 1.4- and 1.8-µm region were not retrieved but were provided with a nonlinear spline interpolation.

Note: The following results are always based on the case with five water vapor grid points and the optimized subinterval fits.

IV. TRADEOFF CONSIDERATIONS

The calculations of the previous section were based on a typical remote sensing scenario with a midlatitude summer atmosphere, rural aerosol, and visibility of 23 km. The coarse parameter grid of the database and the reference TOA radiance cubes were both computed with the same scenario. In this section, we investigate the sensitivity of the retrieval and restrict the discussion to four cases.

1) The reference TOA radiance cube is calculated for a visibility of 23 km and the vertical temperature/humidity profile of MODTRAN’s midlatitude summer atmosphere for W < 4.0 cm but with the temperature/humidity profile of the tropical atmosphere for W ≥ 4.0 cm (labeled MIX23). The retrieval is still performed with the temperature/humidity profile of the midlatitude summer atmosphere (labeled MS23). The mixed mode of height profiles (MS for W < 4.0 cm and tropical for W ≥ 4.0 cm) is chosen to investigate the influence of a moderate error in the moisture-height profile. The MS23/MS23 (input/retrieval) configuration is included for comparison.

2) Same as 1) but using MODTRAN’s U.S. standard atmosphere during the retrieval scaled to the same water vapor column grid W = (0.4, 1.0, 2.0, 2.9, 4.0) cm, labeled US23. When the relative humidity per height layer exceeds 100% and the requested column W is not attained, the humidity of higher altitude layers is iteratively increased until the requested W is achieved. Since the U.S. standard atmosphere has much lower temperatures than the midlatitude summer or tropical atmosphere, a very large influence on the water vapor retrieval accuracy is expected, because the retrieval accuracy depends not only on the total column W but also on its height distribution.

3) The influence of the set of input surface reflectance spectra on the relative rms error of the retrieved water vapor column.

4) The number of water vapor grid points in the database is increased to eight, i.e., the same number as the reference grid. The complete set is (0.4, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0) cm, i.e., a 0.5-cm spacing except for the first subinterval. Input is the MS23 atmosphere; the retrieval will also be performed with MS23 to investigate the most favorable situation concerning potential reduction of errors due to a narrower grid. Again, the interpolation will be performed with the appropriate subinterval fit using the nearest three grid points for each water vapor value. This case serves as a check on how much the interpolation errors can be reduced if a relatively large set of grid points is employed.

Case 1: Fig. 9(a) shows the rms water vapor retrieval errors for case 1). The influence of the MIX23/MS23 (input/retrieval) configuration is about 0.5% in ∆W, and accidentally, the retrieval error is less than for the MS23/MS23 configuration for W = 3–4 cm. Different values are already obtained starting at W = 3 cm because of the use of the optimized three-grid
subintervals, i.e., for $W = 3$ cm, the employed grid points are $W = 2.0, 2.9,$ and 4.0 cm.

Fig. 9(b) shows the relative rms surface reflectance-retrieval errors for four selected channels and the MIX23/MS23 configuration. The highest error is usually found at the 2450-nm channel, but average errors are below the requested 3% in all cases, although the 2450-nm channel distinctly exceeds this limit for $W \geq 3.5$ cm. All calculations are intentionally performed for a noise-free instrument to ascertain the theoretical performance limits and to design the database for a general use, i.e., independent of the noise characteristics of instruments. Since the noise level of current-technology imaging spectrometers typically increases in the region 2.4–2.5 $\mu$m (compared to 2.1–2.35 $\mu$m), these results indicate that larger reflectance-retrieval errors have to be expected in reality.

Fig. 10 shows the results of the MIX23/MS23 and MS23/MS23 configurations for the flat spectrum $\rho = 0.1$ of surface one of Fig. 4. A flat spectrum is selected for demonstration, as any deviation from the constant value is most easily seen. The zoomed 2–2.45-$\mu$m region is chosen, because retrieval errors are often higher than in the 940- or 1140-nm region [compare Fig. 9(b)]. Fig. 10(a) shows results for the MS23/MS23 (input/retrieval) case to be compared with the MIX23/MS23 case in Fig. 10(b). The black and gray curves represent the retrievals for $W = 4$ cm and $W = 4.5$ cm, respectively. The case $W = 5$ cm is included for a trend overview but was not considered for the previous error budgets, because the requirements are restricted to the water vapor column interval (0.5, 4.5 cm).

Accidentally, the retrieval results for $W = 5.0$ cm are slightly better than for $W = 4.5$ cm for MS23/MS23. Thus, the least squares fit of the set of $Q^{\text{db}}$ functions [see (2)] provides a closer match at $W = 5.0$ cm than at $W = 4.5$ cm in this case. For the MIX23/MS23 situation [Fig. 10(b)], the retrieved surface reflectance is underestimated for $\lambda \geq 2.3$ $\mu$m, while the MS23/MS23 case usually overestimates the retrieved reflectance.

Case 2: Fig. 11 shows the results of the water vapor retrieval for the MIX23/US23 case and the MIX23/MS23 for comparison. For moderate water vapor columns ($W \leq 2$ cm), there is not a large difference between both cases. However, for $W > 2$ cm, retrieval errors distinctly increase for the MIX23/US23 case, because the lower atmospheric layers of the U.S. standard atmosphere are saturated in humidity, and moisture is shifted into higher atmospheric layers. The maximum error reaches 38%, but the plot is scaled in the 0%–12% range for a better comparison with the MIX23/MS23 configuration. This is probably a pessimistic error budget; in most practical cases, the error will be much lower. Nevertheless, the comparison illustrates the importance of using reasonable temperature/moisture profiles, i.e., for winter conditions, the retrieval with the midlatitude summer atmosphere will not be appropriate.

Case 3: The influence of the selected input set of surface reflectance spectra was investigated for several sets that are relevant to environmental applications because of the EnMAP background. For the land mode of EnMAP, this means that emphasis is put on surface covers, such as fresh and dry
vegetation, different soils, sand, urban spectra such as asphalt, etc. Although the field of mineral exploration will also be an interesting topic with EnMAP, this paper intentionally excludes sets of the different mineral groups (carbonate, sulfate, Al–OH bearing, Mg–OH bearing, etc.) and is restricted to the types aforementioned. The results for five different sets of input reflectance spectra can be summarized as follows: In most cases, the relative rms water vapor retrieval errors agree within ±0.5% with the results presented in Section III; occasionally, deviations up to ±1.0% occur, which are caused by a stronger nonlinear surface reflectance behavior in the sensible spectral regions (940/1130 nm). Averaged over the whole water vapor column interval (0.5, 4.5 cm), relative rms errors stay below 2% for all sets.

**Case 4):** Fig. 12 shows the results for the water vapor retrieval using eight grid points. The former case of five grid points from Fig. 6(a) is included for comparison. With eight grid points, the relative rms error decreases, on the average by about 0.33%; however, this is a modest accuracy improvement compared with the case of five grid points. The residual errors are caused by the nonlinear reflectance behavior of surfaces in the 940/1130-nm region (APDA algorithm errors) and interpolation errors due to (2).

**V. Conclusion**

In this paper, a method for the design of an atmospheric database for the correction of general imaging spectrometer data was presented. The objective is the compilation of a database that enables water vapor and surface reflectance retrievals at a specified accuracy level while keeping the database size as small as possible. During a case study, some critical parameters and tradeoff considerations were discussed.

An improved reflectance-retrieval accuracy can be achieved if the least squares fit of the RT functions is not performed over the general broad water vapor interval (e.g., 0.4–4.5 cm) but for the smaller subinterval corresponding to the actual pixel-dependent water vapor value.

With five water vapor grid points for the interval (0.4–4.5 cm), the average relative rms water vapor and surface reflectance-retrieval errors are less than 2% and 3%, respectively, for the investigated spectrometer with a 10-nm bandwidth. A slightly better accuracy can be achieved with more grid points, at the cost of increasing the size of an already huge database. However, as demonstrated, the potential improvements are limited, because the achievable accuracy not only depends on the number of grid points but also on other parameters, e.g., nonlinear surface reflectance behavior and spectral interpolation between window and absorption channels in the water vapor algorithm.

The accuracy of the surface reflectance retrieval depends on the atmospheric absorption depth, and the general trend is that a higher absorption depth lowers the accuracy. If the vertical atmospheric-moisture profile of the retrieval deviates moderately from the actual profile of the scene, a small rms water vapor retrieval error of about 0.5%–1% can be expected; much larger errors occur for large discrepancies in actual and retrieved moisture distributions.

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**References**


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