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Averaging kernels for DOAS total-column satellite retrievals

H. J. Eskes and K. F. Boersma

Royal Netherlands Meteorological Institute, De Bilt, The Netherlands

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Correspondence to: H. J. Eskes (eskes@knmi.nl)

Abstract

The Differential Optical Absorption Spectroscopy (DOAS) method is used extensively to retrieve total column amounts of trace gases based on UV-visible measurements of satellite spectrometers, such as ERS-2 GOME. In practice the sensitivity of the instrument to the tracer density is strongly height dependent, especially in the troposphere. The resulting tracer profile dependence may introduce large systematic errors in the retrieved columns that are difficult to quantify without proper additional information, as provided by the averaging kernel (AK). In this paper we generalise the AK concept to total column retrievals, and derive an explicit expression for the DOAS AK. It is shown that the additional AK information corrects for the *a priori* dependence of the retrieval. The availability of averaging kernel information as part of the total column retrieval product is essential for the interpretation of the observations, and for applications like chemical data assimilation and detailed satellite validation studies.

1. Introduction

The Global Ozone Monitoring Experiment (GOME) spectrometer on ESA ERS-2 (Burrows et al., 1999) has demonstrated the unique ability to observe trace gases in the troposphere, including the boundary layer. GOME observes several key species of tropospheric chemistry, such as O_3 (Von Bargen and Thomas, 1999; Valks et al., 2002), NO_2 (Leue et al., 2001; Richter and Burrows, 2002), HCHO (Chance et al., 2000), BrO (Hegels et al., 1998; Wagner and Platt, 1998; Richter et al., 1998; Van Roozendael et al., 1999) and SO_2 (Eisinger and Burrows, 1998). Column amounts of these tracers have been retrieved using the DOAS technique (Platt, 1994). These data sets contain important information on aspects like fossil fuel burning emissions, natural hydrocarbon emission, biomass burning, NO_x produced by lightning, and volcano emissions.

The derivation of quantitative tropospheric column amounts for these species is complicated and remains a major challenge. The retrieval depends strongly on aspects like

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clouds, the assumed profile shape, surface albedo, the presence of a stratospheric background and aerosols. All these aspects can give rise to large errors in the retrieved vertical column for individual measurements.

The DOAS total column retrieval is implicitly dependent on an *a priori* tracer profile. The radiative transfer calculation in DOAS accounts for the sensitivity of the measurement to tracer concentrations at all altitudes. These sensitivities are implicitly weighted with the assumed tracer profile to produce the retrieved column. The averaging kernel (AK) is proportional to this measurement sensitivity profile, and provides the relation between the retrieved quantities and the true tracer profile. The kernel therefore provides important information needed for a quantitative analysis of the satellite data (Rodgers, 2000; Rodgers and Connor, 2003).

The averaging kernel concept is by now well established in the retrieval of profiles of atmospheric quantities like temperature and tracers like ozone from satellite measurements. Retrieval groups are increasingly including the kernel information in the profile data products disseminated to users. This is in contrast to the retrieval of total column data such as the DOAS products mentioned above, or for instance Total Ozone Mapping Spectrometer (TOMS) total ozone. It is well known for all these retrievals that the sensitivity of the satellite instrument is (strongly) height dependent (e.g. Hudson et al., 1995; Martin et al., 2002; Lamarque et al., 2002, and the references given above). This profile dependence implies that kernel information is needed to make optimal use of the retrieved tracer columns. However, AKs have not been defined in the literature on DOAS, and they are not included in DOAS total column data products.

Recently an improved approach has been introduced (Palmer et al., 2001; Martin et al., 2001) to address the profile dependence of the retrieval. This consists of a direct coupling of the retrieval with a chemistry-transport model, in which the *a priori* profile used in the air-mass factor calculation is replaced by a more realistic model-derived time and space dependent profile. In fact, the results described in these papers can also be obtained when averaging kernels are used in the model/satellite intercomparisons and vertical column reconstructions. The latter approach has the practical

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advantage that there is no need to join the retrieval code and the chemistry-transport model.

The paper consists of three topics. First, the DOAS approach will be discussed based on the general retrieval formalism developed by Rodgers. In this alternative approach to DOAS averaging kernels arise naturally. Second, an explicit expression of the DOAS AK is derived in terms of the familiar DOAS air-mass factors. Third, in Sect. 4 the application of the AK will be discussed.

2. Retrieval and averaging kernels

There is an important difference between *in situ* and remote sensing (e.g. satellite) observations. The former can normally be interpreted as true point measurements, while retrieved satellite quantities *always* represent a weighted average over all parts of the atmosphere that contribute to the signal observed by the satellite instrument. The averaging kernel matrix defines the relation between the retrieved quantities and the true atmospheric state. In the derivation below we will closely follow the discussion in the book of Rodgers (Rodgers, 2000), but concentrating on column observations of atmospheric trace gases.

An observation vector $\mathbf{y}$, e.g. a spectrum of reflectivities in the UV-visible, can be related to the true distribution of the trace gas $\mathbf{x}$ by a forward model $\mathbf{F}$,

$$\mathbf{y} = \mathbf{F}(\mathbf{x}, \hat{\mathbf{b}}) + \mathbf{\Delta F} + \frac{\partial \mathbf{F}}{\partial \mathbf{b}}(\mathbf{b} - \hat{\mathbf{b}}) + \epsilon. \quad (1)$$

The forward model accounts for the radiative transfer in the atmosphere, and instrument effects. The vector of parameters $\mathbf{b}$ is a subset of all quantities – apart from the trace gas under consideration – that influence the measurement, and $\hat{\mathbf{b}}$ is the best estimate of these forward model parameters. Examples of $\mathbf{b}$ are the satellite observation geometry (solar zenith angle, viewing angle), properties of clouds, surface properties, the presence of other tracers and aerosols, Ring effect, spectral line strengths

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and instrument aspects. The right-hand side includes three sources of errors: ϵ is the measurement noise, $\mathbf{\Delta F}$ is the (often systematic) error in the forward model, and $\partial\mathbf{F}/\partial\mathbf{b}(\mathbf{b}-\hat{\mathbf{b}})$ describes the errors resulting from uncertainties in the model parameters $\mathbf{b}$.

For (weakly) non-linear forward models (moderately optically thin absorbers), Eq. (1) can be expanded around an *a priori* trace gas distribution $\mathbf{x}_a$ when $\mathbf{x} \approx \mathbf{x}_a$,

$$\mathbf{y} = \mathbf{F}(\mathbf{x}_a, \hat{\mathbf{b}}) + \mathbf{K}_x(\mathbf{x} - \mathbf{x}_a) + \text{error terms}. \quad (2)$$

The term $\mathbf{K}_x = \partial\mathbf{F}/\partial\mathbf{x}$ is the weighting function or Jacobian matrix, evaluated at $\mathbf{x} = \mathbf{x}_a$

A retrieval method $\mathbf{R}$ computes a vector (or scalar) of estimated trace gas quantities $\hat{\mathbf{x}}$ based on the measured values $\mathbf{y}$, the *a priori* information and forward model parameters,

$$\hat{\mathbf{x}} = \mathbf{R}(\mathbf{y}, \mathbf{x}_a, \hat{\mathbf{b}}) \quad (3)$$

Note that the number of elements of the retrieved state $\hat{\mathbf{x}}$ may differ from that of the $\mathbf{x}$. A matrix equation is obtained when this expression is linearised around the *a priori* state $\mathbf{y}_a = \mathbf{F}(\mathbf{x}_a, \hat{\mathbf{b}})$,

$$\hat{\mathbf{x}} = \mathbf{R}[\mathbf{F}(\mathbf{x}_a, \hat{\mathbf{b}}), \mathbf{x}_a, \hat{\mathbf{b}}] + \mathbf{G}_y[\mathbf{K}_x(\mathbf{x} - \mathbf{x}_a) + \text{error terms}]. \quad (4)$$

Here we have used Eq. (2), and $\mathbf{G}_y = \partial\mathbf{R}/\partial\mathbf{y}$. Subtract the *a priori* $\hat{\mathbf{x}}_a$ on both sides ($\mathbf{A} = \mathbf{G}_y\mathbf{K}_x$),

$$\hat{\mathbf{x}} - \hat{\mathbf{x}}_a = \mathbf{A}(\mathbf{x} - \mathbf{x}_a) + \mathbf{G}_y[\mathbf{\Delta F} + \partial\mathbf{F}/\partial\mathbf{b}(\mathbf{b} - \hat{\mathbf{b}}) + \epsilon] + \mathbf{R}[\mathbf{F}(\mathbf{x}_a, \hat{\mathbf{b}}), \mathbf{x}_a, \hat{\mathbf{b}}] - \hat{\mathbf{x}}_a. \quad (5)$$

$\hat{\mathbf{x}}_a$ is related to $\mathbf{x}_a$ by, for instance, a summation over subsets of vertical layers (see remarks below). For total column retrievals, the *a priori* column $\hat{x}_a = \sum_l x_{a,l}$, where $x_{a,l}$ is the *a priori* sub-column in layer l.

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Remarks:

1. The first term on the right in Eq. (5) describes the relation between the retrieved quantities and the true distribution of the tracer through the matrix **A**, called the averaging kernel. For column retrievals the AK is a vector. In the framework of data assimilation the AK is part of the observation operator: a recipe to calculate a forecast of the retrieved observations based on the model state.

2. The other terms describe sources of error related to the forward model and knowledge of the model parameters. The second term on the right describes errors related to the forward model. The last term on the right describes how well the retrieval is able to reproduce the *a priori*. Normally the retrieval method is constructed in such a way that this is the case, and this last term = 0. Note that this is not automatically guaranteed for the DOAS retrieval (e.g. for $\mathbf{x}_a = 0$).

3. A discussion of the error sources can be based on Eq. (5), but is beyond the scope of this note (Boersma et al., 2002).

4. Equation (5) is a generalisation of the discussion by Rodgers (2000). In our derivation the trace gas state vector $\mathbf{x}$ and the vector of retrieved quantities $\hat{\mathbf{x}}$ may be of different dimension. In his book, Rodgers discusses profile retrieval problems with the forward model and retrieval method both defined for the same set of vertical levels, and $\hat{\mathbf{x}}_a = \mathbf{x}_a$. In practice it will often be natural to choose different sets of vertical layers for the forward model and the retrieval method (this general extension is discussed in Rodgers and Connor, 2003). The total column retrieval is an extreme example of this. A forward model often requires a large number of vertical layers to achieve a good accuracy. In the retrieval the number

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of levels may reflect the degrees of freedom of signal. One example of this are the ozone profiles provided on "Umkehr" layers in the case of the Solar Backscatter UltraViolet (SBUV) satellite instruments.

3. DOAS total column retrieval

In the DOAS approach it is assumed that the reflectivity spectrum can be well approximated by the following equation (Platt, 1994; Burrows et al., 1999),

$$\ln R(\lambda) \sim \sum_t \sigma_t(\lambda)\mathcal{S}_t + \text{polynomial}. \quad (6)$$

The sum over t is over all tracers that influence the measurement in a predefined spectral window, and may also contain a correction for the Ring effect (inelastic Raman scattering). The remaining spectrum is assumed to be smooth and is approximated by a low-order polynomial of the wavelength λ. Based on this approximation, DOAS becomes a two step retrieval approach. The first step is a fit of the differential spectral features with the absorption cross section of the tracer σ_λ to be retrieved. This results in a slant column $\mathcal{S}$: the effective total column of the tracer along the mean path the light has followed through the atmosphere. Next, an air-mass factor $\mathcal{M}$ is computed that relates the slant column to the vertical column amount $\mathcal{V} = \mathcal{S}/\mathcal{M}$, expressed in Dobson units (ozone) or in molecules cm^{-2}. The slant column fit does not depend directly on *a priori* information. $\mathcal{M}$ accounts for the atmospheric aspects, and is calculated with a radiative transfer model, based on an *a priori* profile $\mathbf{x}_a$.

For weak absorbers (such as NO_2) the forward model can be linearised around $\mathbf{x}_a = 0$.

$$\mathbf{y} = \mathbf{F}(0, \hat{\mathbf{b}}) + \mathbf{K}_x\mathbf{x} + \text{error terms}, \quad (7)$$

where $\mathbf{x}$ is an array of tracer partial columns in the layers defined by the forward model. $\mathbf{F}(0, \hat{\mathbf{b}})$ and $\mathbf{K}_x$ no longer depend on $\mathbf{x}$. They do, however, strongly depend on the forward model parameters $\hat{\mathbf{b}}$. The term $\mathbf{F}(0, \hat{\mathbf{b}})$ is dominated by scattering terms (Rayleigh,

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surface) and absorption by other gases like ozone. The term $\mathbf{K}_x$ describes the differential spectral structure, roughly proportional to the absorption cross-section of the trace gas. It specifies the height-dependence of the sensitivity of the spectrum to changes in the tracer concentration.

Similarly, the retrieval method R can be linearised around $\mathbf{F}(0, \hat{\mathbf{b}})$. Note that the retrieval still depends on the *a priori* tracer profile shape because of the profile dependence of the air-mass factor. We can write $\mathbf{x}_a = \lim_{\epsilon \to 0} \epsilon \mathbf{x}_a^0$, where $\mathbf{x}_a^0$ represents a non-zero *a priori* profile that is used in the calculation of $\mathcal{M}$,

$$\mathcal{V} = \hat{x} = R[\mathbf{F}(0, \hat{\mathbf{b}}), \mathbf{x}_a^0, \hat{\mathbf{b}}] + \mathbf{G}_y \mathbf{K}_x \mathbf{x} + \text{error terms}. \quad (8)$$

With the definition of the averaging kernel, and because $R[\mathbf{F}(0, \hat{\mathbf{b}}), \mathbf{x}_a^0, \hat{\mathbf{b}}] \approx 0$,

$$\mathcal{V} = \mathbf{A}\mathbf{x} + \text{error terms}. \quad (9)$$

In terms of the two DOAS steps,

$$\mathcal{V} = R(\mathbf{y}, \hat{\mathbf{b}}, \mathbf{x}_a^0) = \mathcal{S}/\mathcal{M}(\mathbf{x}_a^0, \tilde{\mathbf{b}}),$$
$$\mathbf{G}_y = \partial R/\partial \mathbf{y} = 1/\mathcal{M}(\mathbf{x}_a^0, \tilde{\mathbf{b}})\ \partial \mathcal{S}/\partial \mathbf{y}. \quad (10)$$

Here $\tilde{\mathbf{b}}$ is the subset of the parameters $\hat{\mathbf{b}}$ that describe atmospheric aspects. In a similar way the forward model may be approximated,

$$\mathbf{y} = \mathbf{F}(\mathbf{x}, \hat{\mathbf{b}}) \approx \mathbf{Y}[S(\mathbf{x}, \tilde{\mathbf{b}}), \hat{\mathbf{b}}], \mathbf{K}_x = \partial \mathbf{Y}/\partial S\ \partial S/\partial \mathbf{x}. \quad (11)$$

The operator $S(\mathbf{x}, \tilde{\mathbf{b}})$ in Eq. (11) (to be distinguished from the retrieved $\mathcal{S}$) computes a slant column based on the tracer profile, and $\mathbf{Y}$ computes a spectrum based on S.

The two-step approximation assumes that the dependence of the spectrum on the tracer distribution can be described by a single quantity, namely the slant column. One important exception to this is the temperature-dependence of the cross section. This introduces an indirect profile dependence. Equation (11) assumes that this dependence is small and can be neglected (or that an efficient *a posteriori* correction can be applied).

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Assume that the DOAS fit of the retrieval method accurately reproduces the slant column in the forward model, or $\partial S/\partial \mathbf{y}\ \partial \mathbf{Y}/\partial S \approx 1$. In this case the averaging kernel can be expressed in terms of the air-mass factor. For optically thin tracers the slant column is linear with respect to the tracer amount, $S = \sum_l \mathcal{M}_l x_l$, and is a sum of the contributions of each of the layers,

$$\frac{\partial S}{\partial x_l} = \mathcal{M}_l = \mathcal{M}(\epsilon \mathbf{e}_l, \tilde{\mathbf{b}}). \tag{12}$$

Here $\mathcal{M}_l$ is the air-mass factor for layer l. The right side shows that this is computed in the same way as the total air-mass factor, but for an optically thin amount ϵ of tracer confined to layer l only (the unit vector $\mathbf{e}_l$ is = 1 for index l, and = 0 elsewhere).

The elements of the averaging kernel vector A_l are the ratio of the air-mass factor of layer l and the total air-mass factor computed from the *a priori* profile,

$$A_l = \frac{\mathcal{M}(\epsilon \mathbf{e}_l, \tilde{\mathbf{b}})}{\mathcal{M}(\mathbf{x}_a^0, \tilde{\mathbf{b}})}. \tag{13}$$

The air-mass factor of layer l can be identified as the Jacobian of the forward model $\partial S/\partial \mathbf{x}$. This term determines the height dependence of the averaging kernel and is independent of the tracer distribution. For stronger absorbers the forward model will become non-linear and the Jacobian will depend on $\mathbf{x}$. In this case the appropriate starting point is Eq. (5) which describes the retrieval in terms of departures from the *a priori* $\mathbf{x}_a$.

Figure 1 shows examples of the AK computed for the NO_2 retrieval. The actual shape of the kernel changes from one ground pixel to the next, depending in particular on the presence of clouds, aerosols and on the surface albedo of the scene. For this illustration a simplified *a priori* profile $\mathbf{x}_a^0$ is used which peaks in the middle/upper stratosphere, where the air-mass factor approaches the simple geometrical expression $A = 1/\cos(\theta^{sza}) + 1/\cos(\theta^{v})$. The solar zenith angle θ^{sza} is 45 degree and the viewing angle θ^{v} is zero (nadir view) in the examples. The air-mass factor is calculated at 437 nm.

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For curve c we have approximated the cloud top of an optically thick cloud by a Lambertian reflector. This description of clouds is crude, but it is consistent with assumptions that are often used in cloud retrieval algorithms (e.g. the Fresco algorithm, Koelemeijer et al., 2001) that are used in the DOAS retrieval. These cloud algorithms will retrieve an effective, light path derived, cloud top, which can be expected to be somewhat lower than the actual cloud top.

The figure demonstrates the large range of sensitivities between 200 hPa and 1000 hPa, and the low sensitivity in the lower troposphere for cloud free pixels with a dark surface. Because of the large variability of the short-lived NO_2 compound in the (lower) troposphere, and because of the presence of NO_2 in the stratosphere, NO_2 profile shapes show a similar large variability. Generally there is a large difference between the sensitivities of the retrieval in the stratosphere as compared to the lower troposphere. For instance, curve (a) in the figure shows roughly a factor 3 difference of the air-mass factor between boundary layer and stratospheric NO_2. Since the retrieved vertical column is directly proportional to the air-mass factor, this profile variability implies a large profile dependence of the vertical column retrieved. As a result, errors of the order of 100% can be expected in the retrieved total column for individual pixels for simplified *a priori* profile assumptions.

4. Use of averaging kernel information

There is one important aspect related to averaging kernels as discussed above. As mentioned, the retrieved total column $\mathcal{V}$ depends on the *a priori* profile shape. In contrast, a comparison of the DOAS retrieved $\mathcal{V}$ with profile information $\mathbf{x}$ from models or other measurements, based on the averaging kernels (Eq. 9), is *independent of the a priori profile* for optically thin absorbers. The air-mass factor in the retrieval of the vertical column, Eq. (10) cancels against the air-mass factor in the denominator of Eq. (13). The averaging kernel describes the sensitivity of the measured spectra to changes in tracer concentrations at a given altitude (given $\hat{\mathbf{b}}$ is known accurately). It contains the

information needed to understand the relation between the retrieved vertical column and the DOAS slant column.

One should be careful to identify the DOAS retrieved $\mathcal{V}$ as the total vertical tracer column. When most of the tracer is in the stratosphere (e.g. total ozone), or if the profile variation is small, the retrieval is only weakly *a priori* dependent and $\mathcal{V}$ will be an accurate estimate of the vertical column. In general, $\mathcal{V}$ is related to the true tracer profile by $\mathbf{A}$ and $\mathbf{x}_a$, and the additional AK information is crucial:

1. *Data assimilation.* A successful assimilation of satellite measurements requires accurate observation operators. The relation $\hat{\mathbf{x}} - \hat{\mathbf{x}}_a = \mathbf{A}(\mathbf{x} - \mathbf{x}_a)$ describes how the model state $\mathbf{x}$ (e.g. a model NO_2 profile) should be related to the retrieved quantities $\hat{\mathbf{x}}$ (the retrieved DOAS NO_2 column).

2. *Comparisons with model simulations.* The averaging kernels allow for a direct comparison between model results and the observations. When the averaging kernels are used, this comparison is no longer complicated by systematic biases caused by unrealistic *a priori* assumptions (as was shown above). Effectively the GOME slant column is then directly compared with a modelled slant column.

3. *Interpretation of the retrieved columns.* The averaging kernels describe the sensitivity of the satellite observations to the trace gas profile. This is valuable additional information to understand the measurements. An example is an area with large boundary layer concentrations related to local emissions: despite the large vertical column, the satellite retrieval may show small values of $\mathcal{V}$ at such locations. This may be related to a small sensitivity near the surface in combination with unrealistic *a priori* profile information.

4. *Detailed validation of the satellite retrievals.* If additional profile information is available from independent (ground-based) measurements, the averaging kernel relates this local profile to collocated satellite column observations (Rodgers and Connor, 2003).

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The derivatives of the forward model with respect to the state or the retrieval parameters (the Jacobians) play a central role in all retrievals. Because of this, most modern radiative transfer codes contain efficient subroutines to compute these Jacobians. For operational use these Jacobians can for instance be stored in look-up tables. The extra effort of providing the averaging kernel information will therefore often be small. For DOAS the averaging kernel is the ratio of two air-mass factors, Eq. (13), and can be computed with the existing DOAS software.

5. Conclusions

The averaging kernel provides a direct interpretation of the satellite retrieval to users. In particular, the AK quantifies the contribution of the stratosphere, troposphere and boundary layer to the observation, depending on aspects like clouds, surface albedo, viewing and solar zenith angle. It also provides an interpretation of the value of the air-mass factor. The use of the AK together with the retrieved column removes the (often large) dependence on *a priori* assumptions about the profile shape.

The AK provides an alternative and more direct way of implementing the combined retrieval/modelling approach described by (Palmer et al., 2001; Martin et al., 2001): the AK is proportional to the height-dependent sensitivity of the satellite observation to changes in the tracer concentration, which is the central information needed in this approach. However, the retrieval and modelling of atmospheric chemistry and transport can now be performed independently, which is a practical advantage. The retrieval depends on a detailed knowledge of the instrument aspects, (time-dependent) calibration procedure and knowledge of the radiative transfer, and therefore instrument teams in general have the best information to perform the retrievals.

With this paper we hope to stimulate retrieval groups to routinely include averaging kernel information in the data products of GOME and new satellite instruments like SCIAMACHY on Envisat and OMI on EOS-Aura. The above discussion is more general than the application to DOAS only. Averaging kernel information (related to the

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Jacobians) can be provided for alternative column retrieval approaches such as, for instance, the TOMS total ozone algorithm. The additional kernel information is important for remote sensing retrievals in general, and in particular for tropospheric trace gas retrievals.

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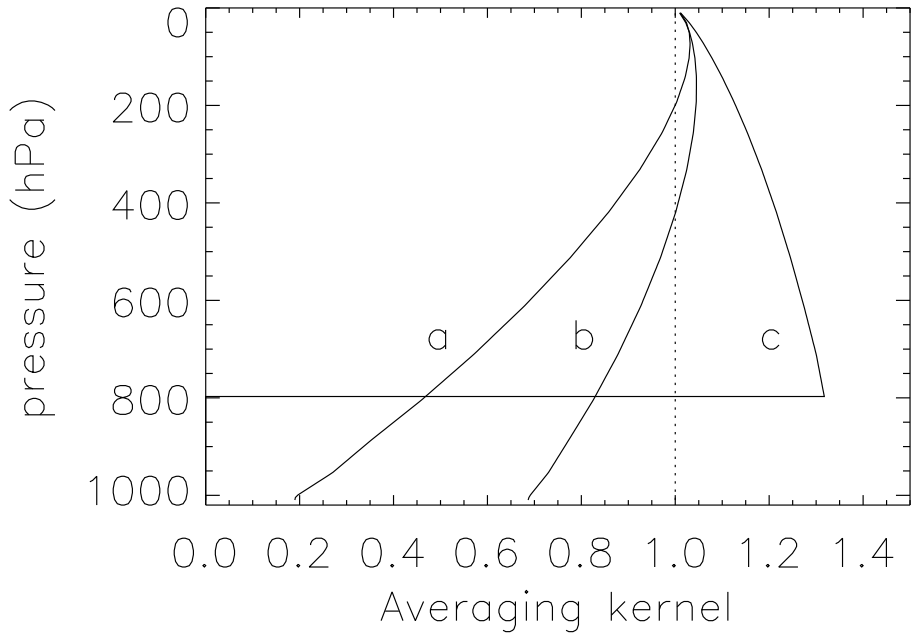

Fig. 1. Example of DOAS averaging kernels: **(a)** clear pixel with a surface albedo of 0.02; **(b)** clear pixel with a surface albedo of 0.15; **(c)** pixel with an optically thick cloud and cloud top at 800 hPa.

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