Meteorol. Z. (Contrib. Atm. Sci.), PrePub DOI 10.1127/metz/2020/0985

DACH 2019

The contribution and weighting functions of radiative transfer – theory and application to the retrieval of upper-tropospheric humidity

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(Manuscript received June 25, 2019; in revised form December 11, 2019; accepted January 7, 2020)

Abstract

Several interesting problems in remote sensing can be traced back to the question of the origin along the line of sight of the registered photons. In this paper we revive old concepts that directly follow from the equation of radiative transfer, namely the contribution and weighting functions. We give them, however, a new mathematical form by transforming them into a pair of probability density functions which have the advantage that they can be used in a more flexible manner. We derive these functions, demonstrate a simple relation between them and show how they can be used in principle. Then we proceed with simple applications to a case of upper-tropospheric humidity (UTH) retrieval. In particular, we show how the mean emission pressure level and mean emission temperature change with increasing UTH. We show that the mean emission pressure increases with increasing humidity and remains almost unchanged for UTH values greater than 50 %. The mean emission temperature is decreasing exponentially as UTH increases. The sensitivities of the mean emission pressure to various quantities, e.g. the temperature lapse rate, or retrieval situations, e.g. whether UTH or UTH with respect to ice is considered or which of two different versions of a receiver is used, is generally small compared to the $2\sigma_p$-width of the layer. The relation of the contribution and weighting functions to Jacobians is discussed as well. We note that the dependence of the mean emission pressure level and other statistical quantities can be formulated using the radiances or brightness temperatures directly. The new method thus offers additional possibilities for interpretation of data from passive remote sensing, and examples are given. In addition of deriving the desired product (for instance, UTH) one can derive and map the mean emission location, its width, and other physical properties like mean temperature of the emission layer. The necessary probability density functions are contained in the solution of the radiative transfer equation and can thus be obtained from runs of the corresponding models. We recommend that radiative transfer models be equipped with facilities to compute and output the contribution and weighting functions.

Keywords: statistical methods, upper-tropospheric humidity, satellite data, contribution function

1 Introduction

Satellite radiance measurements are often expressed as brightness temperatures. The brightness temperature is a measure of the intensity of radiation travelling upward from the top of the atmosphere to the satellite. It is expressed in units of temperature as it relates to the physical temperature at which the atmospheric constituents radiate photons to space. This relation is, however, a vague one and has, to our knowledge, never been characterised. All retrievals that are based on a brightness temperature face the situation that the brightness temperature is *somehow* related to the physical temperature of the emitting layer, but since this layer has a certain depth along the line of sight, it has a temperature distribution (or profile) rather than a distinct temperature.

The point of origin of the registered photons (that is, from where they are emitted or scattered into the line of sight) lies at the core of such considerations. Not only the temperature, but also the pressure and further properties of the emitting layer may be of interest in a retrieval problem. The solution of the radiative transfer equation offers methods to answer such questions, but it seems that these methods have rarely been exploited in the past (examples are POC et al., 1980; FISCHER et al., 1981; SCHMETZ et al., 1995). These tools are two probability density functions (pdfs) that can be derived from the solution of the radiative transfer equation. These two pdfs are called contribution function following STERANKA et al. (1973); POC et al. (1980) and weighting function following for instance FISCHER et al. (1981); HARRIES (1997). The contribution function describes the probability that a recorded photon originates from a certain location along the line of sight while the weighting function decomposes the measured radiance (intensity) into contributions from the Planck function along the line of sight. These concepts will be presented in the next section.

The equation of radiative transfer that we start from is completely general for non-polarised radiation, and

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DOI 10.1127/metz/2020/0985
Gebrüder Borntraeger Science Publishers, Stuttgart, www.borntraeger-cramer.com

this generality applies as well to the method that we develop. It can be used for radiation in the terrestrial atmosphere, in ocean water, in clouds, in the interstellar medium and so on. An extension to polarised radiation is probably straightforward. It is not necessary to make assumptions on the radiative properties of the medium, e.g. whether it is in local thermodynamic equilibrium or not. The method is valid for any wavelength of the radiation. The method is based on fundamental radiative transfer and shares this fundamentality.

As an application ground for the theory we will use the retrieval of upper-tropospheric humidity (UTH). The motivation for this choice is that an analytic expression for the contribution function is available as explained below. Just as brightness temperature relates *somehow* to the temperature in the emitting layers of the atmosphere, UTH relates *somehow* to the relative humidity in the emitting layers. Local humidity values are obtained from in-situ measurements in the upper troposphere which are performed from balloons and aircraft (e.g. Sherwood et al., 2010). Non-local humidity averages over broad layers can be retrieved from satellite radiance measurements at infrared and microwave frequencies (e.g. Soden and Bretherton, 1993; Schmetz et al., 2002; Brogniez and Pierrehumbert, 2006; Buehler et al., 2008; Shi and Bates, 2011; Schröder et al., 2014). To develop methods for retrieving UTH from radiance measurements, it is common practice to run forward radiative transfer calculations using a large variety of profiles of temperature and relative humidity. These calculations form the basis for a regression of UTH on brightness temperature. The resulting radiance for each calculation, translated into brightness temperature, must be related to a certain weighted mean over the profile of relative humidity, which is intended to represent a large part of the profile with a single value, that is, UTH. There are several possibilities for the weighting along the profile (see, e.g. Schmetz and Turpeinen, 1988; Jackson and Bates, 2001; Brogniez et al., 2004; Brogniez et al., 2015; Schröder et al., 2014), and the one that produces the smallest scatter in the regression is used. These types of weighting make often use of Jacobians, that is, expressions of the sensitivity of the radiance to changes of the relative humidity or temperature at certain locations along the line of sight. The relation of such Jacobians to the contribution and weighting functions is therefore discussed below. An alternative method for UTH retrieval that directly uses the contribution function mentioned above has recently been devised by the authors (Gierens and Eleftheratos, 2019) following the retrieval method originally developed by Soden and Bretherton (1993) and Stephens et al. (1996). All methods serve the same purpose; to define a weighted average of relative humidity in the upper troposphere.

As mentioned, the theory underlying the contribution and weighting functions is described in the next section. Applications of the theory are presented for the UTH case in section 3, followed by a discussion of how Jacobians are related to contribution and weighting functions. The paper ends with a short summary and conclusions section.

2 Theory

The intensity of radiation (radiance) at a certain point in space, $I(s_0)$, is the amount of energy $\mathrm{d}E$ transported by photons coming from a certain direction within a very narrow cone of solid angle $\mathrm{d}\omega$ to an infinitesimal disk around this point with projected area $\mathrm{d}\sigma$ (projection with respect to the ray direction) within a short time interval $\mathrm{d}t$. If necessary, a certain wavelength band, $\mathrm{d}\lambda$ may be singled out in the consideration and then we speak of specific intensity, $I_\lambda(s_0)$. A filter response function, $\Psi(\lambda)$, can easily be included in the developments, letting $I(s_0) = \int \Psi(\lambda)\, I_\lambda(s_0)\,\mathrm{d}\lambda$. The following considerations are valid in all these cases. The mentioned photons originate somewhere in the cone either by true emission (that is, an atom or molecule lowers its quantum state and the energy difference is radiated away as a photon) or by scattering from another direction into the direction of the cone. The intensity changes along the cone's direction, measured for instance with a coordinate s, by emission and by extinction (including true absorption and scattering), are described by a very basic form of the equation of radiative transfer:

$$\frac{\mathrm{d}\,I(s)}{\mathrm{d}\,s} = \eta(s) - I(s)\chi(s), \qquad (2.1)$$

with the coefficients of emission, $\eta(s)$, and extinction, $\chi(s)$. The formal solution of this differential equation is

$$I(s_0) = \int_{-\infty}^{s_0} \eta(s)\, \exp\left[-\int_{s}^{s_0} \chi(s')\,\mathrm{d}s'\right] \mathrm{d}s, \qquad (2.2)$$

which states that the intensity at s_0 is composed of the energy carried by the photons emitted from all locations in front of s_0 that have not been absorbed or scattered into another direction on the way towards s_0. The long expression under the integral will be abbreviated as $\Phi(s)$ in the following such that the formal solution of the equation of transfer is simply

$$I(s_0) = \int_{-\infty}^{s_0} \Phi(s)\,\mathrm{d}s. \qquad (2.3)$$

So far this is standard textbook knowledge. In the present paper we will use $\Phi(s)$ in its normalised form, that is

$$\varphi(s|s_0) := \frac{\Phi(s)}{I(s_0)} = \frac{\Phi(s)}{\int_{-\infty}^{s_0} \Phi(s')\,\mathrm{d}s'}. \qquad (2.4)$$

The notation $\varphi(s|s_0)$ is borrowed from probability theory. The quantities after the "|" are given parameters; here it is a certain point in space; later we will have another parameter as well. We note that $\varphi(s|s_0)$ is a probability density function which we call "contribution function" following Steranka et al. (1973); Poc et al. (1980); Fischer et al. (1981). $\varphi(s|s_0)\,\mathrm{d}s$ is the probability that a photon which arrives at s_0 originated (by true emission or scattering) in the immediate vicinity ($\mathrm{d}s$) of the point s along the considered direction. Thus, the contribution function describes how the energy that arrives at point s_0 is composed from contributions of all positions in front of that point. This solves an important problem in passive remote sensing where one likes to know from which locations in the atmosphere the photons emerge that reach a satellite instrument. If an expression for $\varphi(s|s_0)$ is known, such problems and related ones can be treated. Poc et al. (1980) and Fischer et al. (1981) studied the origin of registered photons directly using $\Phi(s)$ or $\Phi(s)/\max(\Phi)$, but we deem the approach using the normalised form $\varphi(s|s_0)$ offers more potential for further analyses, since with this approach we can employ the methods of probability theory.

As $\varphi(s|s_0)$ is a probability density function, moments of any order k are defined, if the corresponding integrals exist:

$$\mu_k(s_0) = \int_{-\infty}^{s_0} s^k\,\varphi(s|s_0)\,\mathrm{d}s. \tag{2.5}$$

The moments depend on the given parameters and their variation with these parameters is of interest as well. The first moment, $\overline{s}(s_0) := \mu_1(s_0)$, is the mean location along the considered direction from which the registered photons emerge, and the second moment is related to the corresponding standard deviation: $\sigma_s(s_0) := (\mu_2 - \mu_1^2)^{1/2}$. Higher-order moments of the pdfs, related to skewness (3rd moment) and kurtosis (4th moment), can be also computed with Eq. (2.5).

It is possible as well to compute more general characteristics, for instance the mean temperature at which the photons are emitted. Let $T(s)$ be the temperature profile along the direction s. Then

$$\overline{T}(s_0) := \int_{-\infty}^{s_0} T(s)\,\varphi(s|s_0)\,\mathrm{d}s \tag{2.6}$$

is the mean temperature of the layers from which the detected photons emerge. Note that $\overline{T}$ only equals $T(\overline{s})$ if T is a linear function of s. Generally, the numerical values of $\overline{T}(s_0)$, $T(\overline{s})$, and the measured brightness temperature, should be similar. This is the main motivation to use brightness temperature in remote sensing applications.

The formal solution of the equation of radiative transfer, Eq. 2.2, offers further possibilities for weighing certain properties of the medium along the line of sight. The ratio η/χ, known as the source function, equals under the condition of local thermodynamic equilibrium the Planck function, $B[T(s)]$. This will be assumed here for convenience, although the following argumentation is valid in the more general case as well. The exponential function in Eq. 2.2 is the transmission between s and s_0, $\mathcal{T}(s, s_0)$ such that we can rewrite it as

$$I(s_0) = \int_{-\infty}^{s_0} B[T(s)]\,\mathcal{T}(s,s_0)\,\chi(s)\,\mathrm{d}s. \tag{2.7}$$

Now, the product

$$\mathcal{T}(s,s_0)\,\chi(s) = \frac{\mathrm{d}\mathcal{T}(s,s_0)}{\mathrm{d}s} \tag{2.8}$$

has been called by various authors (e.g. Fischer et al., 1981; Harries, 1997; Gierens and Eleftheratos, 2016) the weighting function or weighting kernel, $W(s)$. The weighting function is embedded in the contribution function giving weight to each individual contributing layer, depending, *inter alia*, on the vertical humidity profile, the temperature profile and the viewing angle. Fischer et al. (1981) note that in order to associate the phenomena in water vapour images with an atmospheric layer, the weighting function is not appropriate and that the product of the weighting function and the Planck function, called the contribution function, must be analysed. The relation between this weighting function and the radiation integrand $\Phi(s)$ is thus:

$$W(s) = \Phi(s)/B[T(s)]. \tag{2.9}$$

We normalise the weighting function to get another probability density function

$$w(s|s_0) = \frac{\Phi(s)/B[T(s)]}{\int_{-\infty}^{s_0} \frac{\Phi(s)}{B[T(s)]}\,\mathrm{d}s} \tag{2.10}$$

and compute with it a mean value of the Planck function, viz.

$$\int_{-\infty}^{s_0} B[T(s)]\,w(s|s_0)\,\mathrm{d}s = \frac{\int_{-\infty}^{s_0}\Phi(s)\,\mathrm{d}s}{\int_{-\infty}^{s_0}\frac{\Phi(s)}{B[T(s)]}\,\mathrm{d}s} = \left[\int_{-\infty}^{s_0}\frac{1}{B[T(s)]}\,\varphi(s|s_0)\,\mathrm{d}s\right]^{-1} = \overline{\left(\frac{1}{B}\right)}^{-1}. \tag{2.11}$$

This mean is the harmonic mean of the Planck function with respect to φ. Thus, the following relations hold:

$$\int B(s)\,\varphi(s)\,\mathrm{d}s = \overline{B} \quad \text{(arithmetic mean)} \tag{2.12}$$

$$\int B(s)\,w(s)\,\mathrm{d}s = \overline{\left(\frac{1}{B}\right)}^{-1} \quad \text{(harmonic mean)}. \tag{2.13}$$

This is a simple relation that we can express in the form: The arithmetic mean of the Planck function along the line of sight $B(s)$ with respect to the weighting function $w(s|s_0)$ equals the harmonic mean of the same quantity with respect to the contribution function $\varphi(s|s_0)$. As the harmonic mean is never larger than the arithmetic mean, we have finally

$$\int B(s)\,w(s|s_0)\,\mathrm{d}s \le \int B(s)\,\varphi(s|s_0)\,\mathrm{d}s. \tag{2.14}$$

For any arbitrary quantity $Q(s)$ the relation is more complex:

$$\int Q(s)\, w(s|s_0)\, \mathrm{d}s = \overline{\left(\frac{Q}{B}\right)} \cdot \overline{\left(\frac{1}{B}\right)}^{-1}, \qquad (2.15)$$

that is, the arithmetic mean of Q with respect to $w(s|s_0)$ equals the product of the arithmetic mean of Q/B times the harmonic mean of the Planck function, both with respect to $\varphi(s|s_0)$.

3 Application to the retrieval of upper-tropospheric humidity

3.1 Mean emission pressure level

The radiation-based quantity upper-tropospheric humidity (UTH) is a measure of the radiance resulting from emitting and absorbing water molecules in a deep layer in the upper troposphere and lowermost stratosphere. It is expressed as a relative humidity, and its retrieval is constructed in a way that UTH is a *measure of central tendency* for the respective profile of relative humidity. While relative humidity is a local quantity, UTH is non-local. As it is based on radiances measured by satellite instruments (infrared or microwave), it is characteristic of a relatively thick layer, not of a point in space as relative humidity itself is. The location of this layer is not fixed, it has no clear upper and lower boundaries and these characteristics depend on the UTH itself. The layer is located higher in the atmosphere when UTH is large and vice versa (e.g. Fischer et al., 1981, their Figure 6), but the amount of this shift and the sensitivity of the layer altitude to changes in UTH has not been documented extensively in the published literature. Using the contribution function from above allows to get a clearer picture of these issues, if an expression for φ is known. This is the case for the new UTH-retrieval method by Gierens and Eleftheratos (2019) that is applicable to channel 12 radiances from the High-resolution Infrared Sounder (HIRS) on the series of polar-orbiting National Oceanic and Atmospheric Administration (NOAA) satellites as well as on the European Metop series of satellites. HIRS channel 12 comes in two versions, one with a central wavelength of 6.7 µm (HIRS/2) and one with a central wavelength of 6.5 µm (HIRS/3 and HIRS/4). The retrieval method distinguishes between these two versions.

The formal solution of the radiative transfer equation in the mentioned UTH retrieval is

$$\begin{aligned} I &= B_0 C_\lambda \beta \qquad (3.1)\\ &\times \int_{-\infty}^{\infty} \exp\left\{-A_\lambda \sqrt{U}\left[1 + \operatorname{erf}\left(\sqrt{\kappa}\beta x - \sqrt{\kappa}/2\right)\right]^{1/2}\right\}\\ &\times \exp[C_\lambda(\beta x - \beta^2 x^2)]\,(1 - 2\beta x)\,\mathrm{d}x\\ &= \int_{-\infty}^{\infty} \Phi(x|U)\,\mathrm{d}x. \end{aligned}$$

Here, B_0 is the value of the Planck function at 6.7 µm and 6.5 µm at 240 K. All constants are explained in Gierens and Eleftheratos (2019). For the convenience of the reader, a short list of values, units and meanings is given in the Appendix. U is the value of the upper-tropospheric humidity and is considered a parameter in the following. The coordinate along the ray is the logarithm of pressure, $x = \ln(p/p_0)$, such that the HIRS instrument is at $x = -\infty$ and the value of x *increases* downward into the atmosphere. The parameter that gives the location of the sensor is suppressed in the following (that is, the fact that $x = -\infty$ at the sensor is not explicitly written down), but the parameter U is given explicitly, because it is the variation of the probabilistic quantities with U forming the focus of the current investigation. The shape of the radiance integrand $\Phi(x)$ for various values of U can be seen in Fig. 3b of Gierens and Eleftheratos (2019).

The contribution function $\varphi(x|U)$ is

$$\varphi(x|U) = \Phi(x|U) \Big/ \int \Phi(x|U)\,\mathrm{d}x. \qquad (3.2)$$

With this contribution function we are able to compute the first moments of the distribution of x, the location of emission. But moments of x cannot easily be interpreted; it would be better to compute the moments of the corresponding pressure levels. Here we have two possibilities: as $x = \ln(p/p_0)$ we can either employ the substitution rule for probability density functions to compute a contribution function that refers to the pressure coordinate, $\psi(p|U) = \varphi[\ln(p/p_0)|U]\,(\mathrm{d}x/\mathrm{d}p)$ and with that function we can estimate the mean emission altitude using the following equation:

$$\overline{p} = \int p\,\psi(p|U)\,\mathrm{d}p. \qquad (3.3)$$

The alternative is to compute a mean pressure level as $\overline{p} = p_0 \int e^x \varphi(x|U)\,\mathrm{d}x$. We use the first alternative since in this form the computation of higher moments is clearer.

Figure 1 shows $\overline{p}$ as a function of U, that is, how the mean pressure level from which the channel 12 photons emerge changes with upper-tropospheric humidity according to Eq. (3.3). The $\pm\sigma_p(U)$ curves are given as well. The necessary integrals have been computed numerically (Romberg integration). The calculations have been performed for both versions of the HIRS receiver. Based on Fig. 1 we can notice the following results:

- The moister the upper troposphere the higher the mean emission level. However, the curves are rather flat already for moderate values of U, that is, the mean height of emission is rather insensitive to U if U exceeds about 0.5 (or 50 % in relative humidity units). For these cases the mean emission level is between 383 and 336 hPa for HIRS/2 and between 329 and 290 hPa for the HIRS/3 and HIRS/4 receivers.

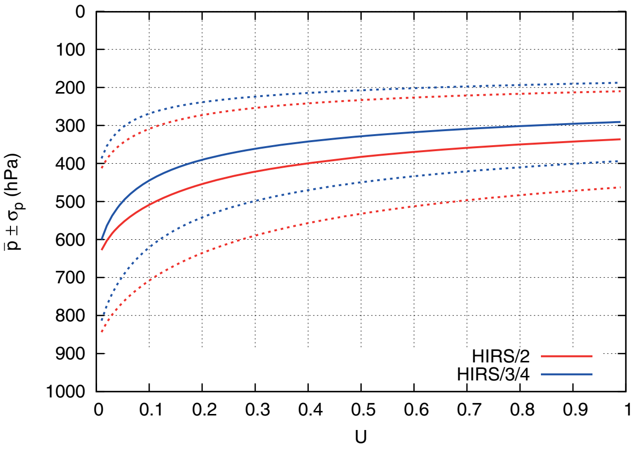

Figure 1: Mean emission pressure levels (solid) and their standard deviations (dashed) for HIRS/2 (6.7 µm) and HIRS/3/4 (6.5 µm) water vapour channels, as a function of upper tropospheric humidity. The mean height of emission has little dependence on U for $U > 50\%$.

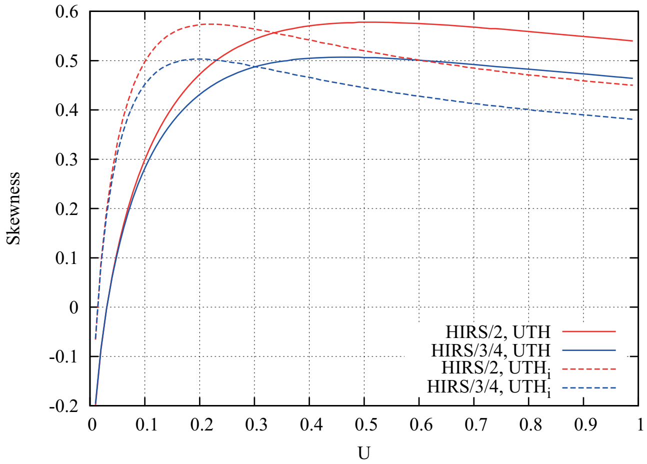

Figure 2: Skewness of the distribution functions of emission pressure levels for UTH and UTH$_i$ and for HIRS/2 (6.7 µm) and HIRS/3/4 (6.5 µm) water vapour channels, as a function of upper tropospheric humidity. Except for very dry situations the distributions have a tail to higher pressures (positive skewness).

- In the tropics almost all photons originate from the troposphere, because the tropical tropopause is at about 150 hPa, which is about 50 hPa lower than the mean emission level minus one standard deviation at $U = 1$. In the midlatitudes, however, the signal can have contributions from the lowermost stratosphere.
- The emission layer for HIRS/3/4 is located higher than that for HIRS/2, as expected, since the atmosphere is more opaque at the channel 12 central wavelength of HIRS/3/4 (6.5 µm) than at the corresponding wavelength of HIRS/2 (6.7 µm).
- The emission layer depth, measured as plus/minus one standard deviation, is quite large; it is larger for HIRS/2 than for HIRS/3/4.
- The standard deviations of the distributions get smaller with increasing U.
- In very dry situations (e.g. less than 5 %) some photons can reach the satellite directly from levels below 700 hPa, but more so with HIRS/2 than with HIRS/3/4.

Figure 2 displays in a similar way the skewness of the distributions of emission pressures. With the exception of the driest situations ($U < 0.03$) all distributions have positive skewness, that is, a tail to higher pressure, which means that the distribution of the emission pressure levels is not symmetric around the mean emission pressure but skews towards lower altitudes.

3.2 Mean temperature

Next we show the mean emission temperature as a function of U for both version of HIRS, see Fig. 3. We note that the retrieval method for UTH assumes a certain temperature profile (Eq. 4 in Gierens and Eleftheratos, 2019), that can be written again in pressure coordinates as $T(p) = T_0(p/p_0)^\beta$ with the normalised lapse rate constant $\beta = 0.22$ and with $T_0 = 240$ K and $p_0 = 388$ hPa.

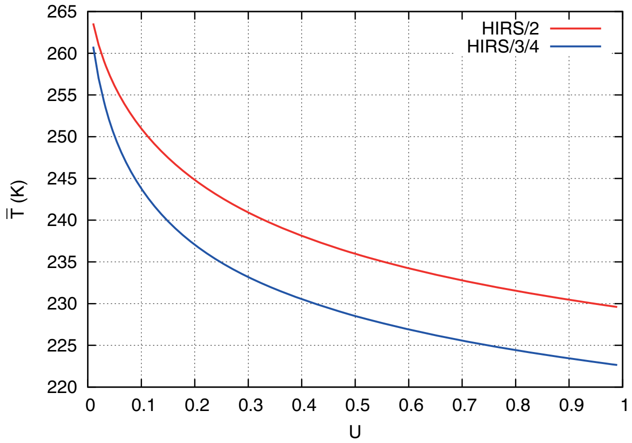

Figure 3: Mean emission temperatures for HIRS/2 (6.7 µm) and HIRS/3/4 (6.5 µm) water vapour channels, as a function of upper tropospheric humidity. The mean temperature of emission decreases with increasing U. Differences between HIRS/2 and HIRS3/4 curves are the order of 7 K.

The mean emission temperature is then

$$\overline{T} = T_0 \int (p/p_0)^\beta \, \psi(p|U) \, \mathrm{d}p, \qquad (3.4)$$

that is, it is proportional to the moment of order β of the contribution function in pressure coordinates. Figure 3 shows how the mean emission temperatures for both HIRS versions decrease with increasing UTH according to Eq. (3.4). As expected, the mean emission temperature is about 7 K higher for HIRS/2 than for HIRS/3/4. The curves are quite steep in dry situations, but they get flatter with increasing UTH. The temperature $T_0 = 240$ K, which is assumed as the pivot for several approximations in the retrieval methods for UTH, both the original by Soden and Bretherton (1993) and the second-order one by Gierens and Eleftheratos (2019), is the mean emission temperature at a quite

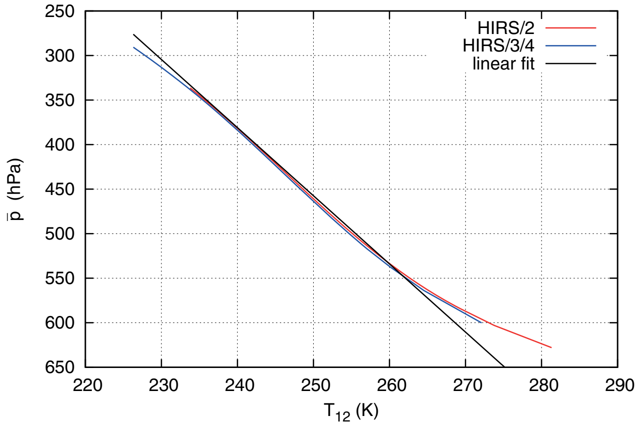

Figure 4: The mean emission pressure as a function of the channel 12 brightness temperature for HIRS/2 (6.7 µm) and HIRS/3/4 (6.5 µm) water vapour channels. The black line is a simple linear fit.

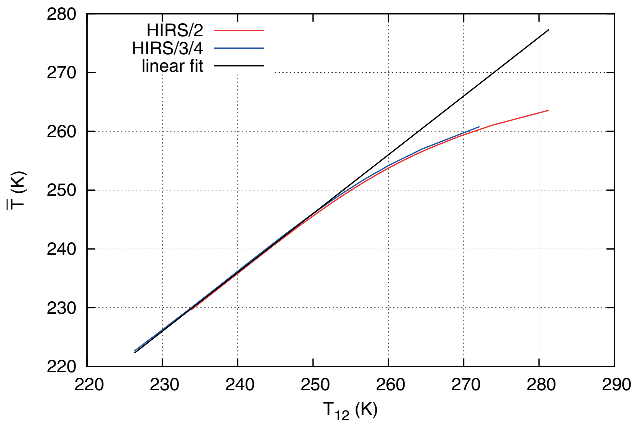

Figure 5: The mean emission temperature as a function of the channel 12 brightness temperature for HIRS/2 (6.7 µm) and HIRS/3/4 (6.5 µm) water vapour channels. The black line is a simple linear fit. The mean emission temperature is very nearly 4 K lower than the brightness temperature in the regime $T_{12} < 255$ K.

dry situation of about $U = 0.15$ for HIRS/3 and HIRS/4. For the older HIRS/2 this mean temperature is achieved at a higher UTH, about $U = 0.33$.

The upper-tropospheric humidity is a bijective function of the brightness temperature in HIRS channel 12, T_{12}. Expressions of this functional dependence are given in Gierens and Eleftheratos (2019). It is thus possible to relate the mean emission pressures and temperatures directly to measured brightness temperatures. A detour via UTH is not necessary. Figures 4 and 5 display these relations. Evidently both relations are quasi-linear over a wide range of brightness temperatures and they are almost equal for both versions of the HIRS detector. This might suggest that the variation of the mean altitude and temperature of the peak emission layer with respect to the T_{12} measured by the satellite, does not depend on which version of the HIRS instrument is used. However, please note that if HIRS/2 and HIRS/3/4 would sense the same situation, the resulting brightness temperaures would differ by (absolutely) 4 to 12 K (Gierens et al., 2018) and thus the resulting mean emission pressures and temperatures would differ as well. There are distinct deviations from linearity at the high end of the brightness temperature range (i.e. when the atmosphere is quite dry), but on the low end the deviations are small for the mean emission pressure or nearly absent for the mean emission temperature. It is noteworthy that the mean emission temperature in this regime is constantly about 4 K lower than the measured respective brightness temperature. This is a result of the retrieval formulation where a monotonically decreasing temperature profile with decreasing pressure is assumed. Whenever an actual temperature profile is available, the mean emission temperature should be computed directly from Eq. (2.6).

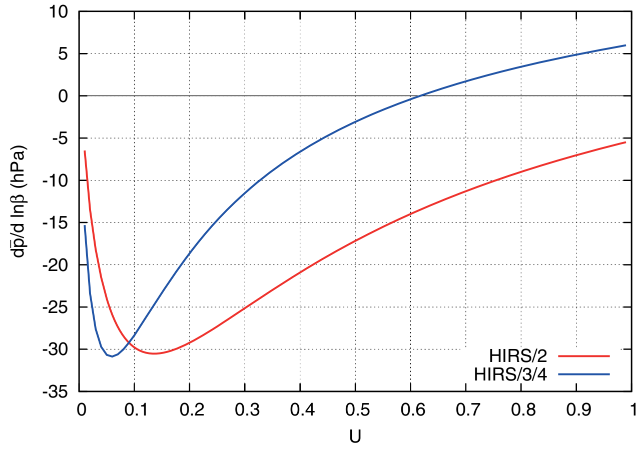

Figure 6: The derivative of mean emission pressure to relative change of the lapse rate parameter β at its standard value $\beta = 0.22$ for HIRS/2 (6.7 µm) and HIRS/3/4 (6.5 µm) water vapour channels, as a function of upper tropospheric humidity. A ten-percent change of β from its standard value thus implies an absolute pressure change of less than about 3 hPa.

3.3 Influence of atmospheric stability

The non-dimensional lapse rate parameter β has the constant value 0.22 in the standard retrieval, but actually it varies with geographical latitude (Jackson and Bates, 2001). The effect of varying β has been corrected for using the brightness temperature in HIRS channel 4 (Stephens et al., 1996) or channel 6 (Jackson and Bates, 2001). This means for the current investigation that for instance the mean emission pressure level would vary with varying β. The derivative $d\overline{p}/d\ln\beta$, taken at $\beta = 0.22$, has been numerically computed for both HIRS versions and the result is shown in Fig. 6. For HIRS/2 the derivative is negative for the whole range of UTH, while it is positive for HIRS/3/4 when U exceeds 0.6. The static stability of the troposphere increases with decreasing β and vice versa. This means that the mean emission pressures are mostly higher in a more stable than in a more neutral troposphere. The effect is however quite weak. In summary, we find small impact in

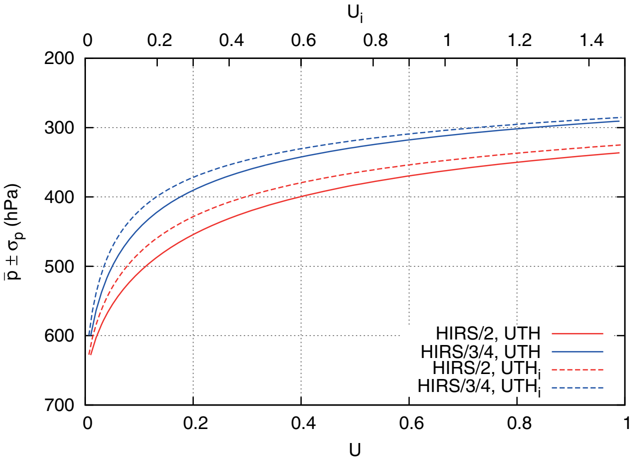

Figure 7: Mean emission pressure levels for the retrieval of UTH (solid lines, bottom axis) and UTH$_i$ (dashed lines, top axis) for HIRS/2 (red) and HIRS/3/4 (blue).

the calculations of the mean emission altitude by changing the lapse rate parameter. A change in the lapse rate parameter by 10 % from its standard value is associated with an absolute change of less than about 3 hPa in the mean emission altitude. This is much less than the $\pm\sigma_p$-width of the emission layer and it is about one hundred times smaller than the value of the mean emission altitude itself.

3.4 Application to upper-tropospheric humidity with respect to ice

The retrieval method by Gierens and Eleftheratos (2019) has also been derived for upper-tropospheric humidity with respect to ice (UTHi). The derivation implies slight differences in the assumed atmospheric structure relative to the UTH retrieval. It should be noted that the ratio between the values of UTHi and UTH at upper-tropospheric temperatures is typically about 1.5. Taking this into account, the mean emission pressure levels differ by about 30 to 40 hPa in dry cases and the difference reduces to 10 to 20 hPa towards moister situations, see Fig. 7. These differences are small compared to the standard deviations of the distribution of emission pressure levels.

3.5 Application to profiles of relative humidity

Gierens and Eleftheratos (2016) considered the problem of how UTH might change in consequence of global warming when, as often assumed, regional and global means of relative humidity stay constant. As UTH can be interpreted as a weighted mean of the relative humidity profile in the upper troposphere, $r(z)$, UTH may change without a change of $r(z)$ when the weights change. Gierens and Eleftheratos (2016) assumed a generic weighting function, such that UTH = $\int K(z,\bar{z},H)\, r(z)\, \mathrm{d}z$. The weighting function has two free parameters, namely a water vapour scale height, H, and the pressure altitude (or any other vertical coordinate)

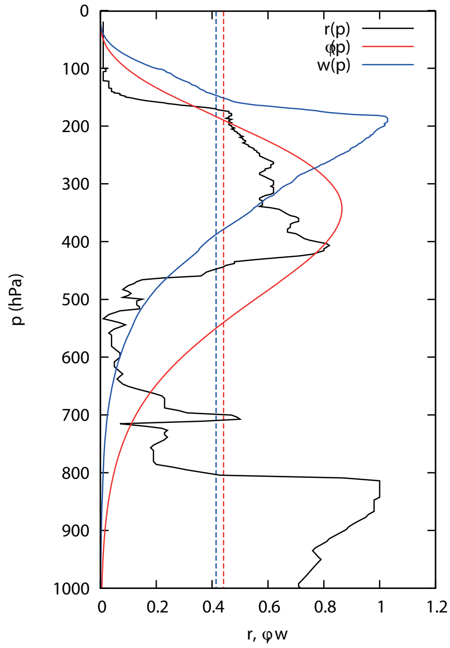

Figure 8: Example profiles of relative humidity, r (black), the contribution function φ (thick red), the weighting function, w (thick blue), and the two UTH values (dotted vertical lines) resulting from application of the fixpoint equations.

where the optical depth reaches unity, $\bar{z}$. We computed theoretically but also documented with real data, how a warming would affect these parameters and concluded from that how UTH would change. In order to avoid thousands of radiative transfer calculations, we ignored that $\bar{z}$ actually depends on $r(z)$. This is evidently a shortcoming of Gierens and Eleftheratos (2016). With the new version of the weighting and contribution functions, $w(z|U)$ and $\varphi(z|U)$ there is more flexibility; in fact, the weighting and contribution functions adjust themselves to the actual $r(z)$ if we use the following fixpoint equations:

$$U_\varphi = \int r(z)\, \varphi(z|U_\varphi)\, \mathrm{d}z \tag{3.5}$$

$$U_w = \int r(z)\, w(z|U_w)\, \mathrm{d}z \tag{3.6}$$

which can be solved iteratively; generally a few (say 5) iterations suffice. Figure 8 shows an example, using a real profile of relative humidity from the meteorological observatory Lindenberg (February 1st, 2000, 18 Z, cf. Spichtinger et al., 2003), the two functions $\varphi(z|U_\varphi)$ and $w(z|U_w)$ as well as the resulting values U_φ and U_w which differ little, by about 2 %. Note that $w(z|U_w)$ has been computed with the actual temperature profile for the Planck function. Using the academic linear profile that is assumed for the derivation of the UTH retrieval leads to too much weight in the dry stratosphere and thus to unrealistic results.

We have then two versions of UTH which will generally differ. This is no problem since as we stated in Gierens and Eleftheratos (2019) there is no unique value of UTH. They are just two different measures of central tendency for the distribution of relative humidity along the line of sight.

4 The relation to Jacobians

The sensitivity of the registered radiance to changes in the underlying atmospheric profiles is labelled Jacobian in the retrieval community, a name that has its origin in the numerical discretisation of the atmosphere into distinct layers. In principle, the so-called Jacobians are discrete versions of functional derivatives. In the present section we derive the relation between Jacobians and the contribution and weighting functions. To that end we consider the sensitivity of the radiance to changes in the profile of an arbitrary quantity, $Q(s)$. Q can be anything that affects the radiance, e.g. mixing ratios of water vapour and other species, temperature, electron density in an astrophysical setting, and so on. s is used for a general coordinate along the line of sight.

Let us write the solution of the RT equation again

$$I = \int \Phi(s, Q(s))\,\mathrm{d}s, \tag{4.1}$$

where we make the dependence of the integrand on the Q-profile explicit. Now assume that a very small change $\delta Q(s)$ occurs in a very small range around an arbitrary location s^* on the line of sight, $[s^*, s^* + \delta s]$, with $\delta Q(s) = 0$ outside this range. This leads to a new radiance

$$I' = \int \Phi[s, Q(s) + \delta Q(s)]\,\mathrm{d}s. \tag{4.2}$$

If the change is really small it is possible to make a first order approximation of Φ, namely

$$\Phi[s, Q(s) + \delta Q(s)] \approx \Phi(s, Q(s)) + \left(\frac{\partial \Phi}{\partial Q}\right)_{s^*} \delta Q(s). \tag{4.3}$$

The difference of the two radiances is then

$$I' - I = \int_{s^*}^{s^*+\delta s} \left(\frac{\partial \Phi}{\partial Q}\right)_{s^*} \delta Q(s)\,\mathrm{d}s. \tag{4.4}$$

Now, taking the limits $\delta Q \to 0$ and $\delta s \to 0$ gives the general Jacobian as

$$\mathfrak{J}_Q\, I(s^*) := \lim_{\delta s\to 0}\, \lim_{\delta Q\to 0} \frac{I' - I}{\delta s\, \delta Q} = \left(\frac{\partial \Phi}{\partial Q}\right)_{s^*}, \tag{4.5}$$

where we assume that in the limits both $\delta Q(s)$ and the derivative of Φ with respect to Q can be considered constant. The Jacobian is thus the partial derivative of Φ to the quantity in question at an arbitrary location along the line of sight (and thus it is itself a function of s). Obviously, we can divide both sides of this equation by the measured radiance which yields a *relative sensitivity* with respect to changes of Q:

$$\mathfrak{j}_Q\, I(s^*) := \lim_{\delta s\to 0}\, \lim_{\delta Q\to 0} \frac{I' - I}{I\, \delta s\, \delta Q} = \left(\frac{\partial \varphi}{\partial Q}\right)_{s^*}, \tag{4.6}$$

and here we have the desired relation between the contribution function φ and the Jacobian.

Now we consider the case that Q is the relative humidity, $r(s)$. The Planck function does not depend on the relative humidity. Thus we have

$$I' - I = \int B(s)\,[W[s, r(s) + \delta r(s)] - W(s, r(s))]\,\mathrm{d}s. \tag{4.7}$$

Again we assume that $\delta r(s)$ vanishes outside a very small range $[s^*, s^* + \delta s]$. The function W is approximated to first order, we take the limits as above, and the result is

$$\mathfrak{J}_r\, I(s^*) := \lim_{\delta s\to 0}\, \lim_{\delta r\to 0} \frac{I' - I}{\delta s\, \delta r} = B(s^*) \left(\frac{\partial W}{\partial r}\right)_{s^*}. \tag{4.8}$$

Using $W(s, r(s)) = \mathcal{T}(s, r(s))\chi(s, r(s))$ we have further

$$\left(\frac{\partial W}{\partial r}\right)_{s^*} = \left(\frac{\partial \mathcal{T}}{\partial r}\right)_{s^*} \chi(s^*, r(s^*)) + \mathcal{T}(s^*, r(s)) \left(\frac{\partial \chi}{\partial r}\right)_{s^*}. \tag{4.9}$$

In this expression the first term on the left vanishes since

$$\left(\frac{\partial \mathcal{T}}{\partial r}\right)_{s^*} = 0. \tag{4.10}$$

This can be formally derived, but it is easily understood from the physics involved. $\mathcal{T}(s^*, .)$ is the transmission probability at s^*, that is, the probability that photons emitted at s^* reach the receiver. It can only be changed if the absorber distribution is changed *between* s^* and the receiver, not with a change directly *at or before* s^*. With this consideration the result simplifies to

$$\left(\frac{\partial W}{\partial r}\right)_{s^*} = \mathcal{T}(s^*, r(s)) \left(\frac{\partial \chi}{\partial r}\right)_{s^*} \tag{4.11}$$

and eventually

$$\mathfrak{J}_r\, I(s^*) = B(s^*)\,\mathcal{T}(s^*, r(s)) \left(\frac{\partial \chi}{\partial r}\right)_{s^*}. \tag{4.12}$$

It is seen that the Jacobian with respect to changes of the relative humidity profile is ultimately given by the local derivative of the extinction coefficient with respect to the local relative humidity, with a preceding factor $B(s^*)\mathcal{T}(s^*)$. Contributions to extinction from other gases, aerosols, etc. affect the result only indirectly via the transmission function, not via the extinction coefficient. The presence of the transmission function in the final expression explains that the "local relative humidity" Jacobian (Brogniez et al., 2004) peaks in the upper troposphere (at around the level where the optical depth reaches unity) even for humidity profiles that have low RH in the upper troposphere. There cannot be much sensitivity far below the level where the optical depth is unity.

5 Summary and conclusions

The formal solution of the equation of radiative transfer contains implicit information on the locations from where the photons registered at a certain location (e.g. a receiver on a satellite) originated by either true emission or scattering into the line of sight. Earlier studies (Poc et al., 1980; Fischer et al., 1981) confined themselves in using the radiance integrands $(\Phi(s), W(s))$, their mode values and the widths at half maximum to obtain such information. However, the integrands can mathematically be cast in the form of probability density functions by appropriate normalisation and this results in what we prefer to call contribution and weighting functions $(\varphi(s|s_0), w(s|s_0))$. In particular the contribution function $\varphi(s|s_0)$ allows to compute the mean location from where the photons originate, the corresponding standard deviation, mean temperatures and mean Planck- (or more generally, source-) functions that characterise the emission regions. We have given application examples for a case where the contribution function is explicitly known, but it is certainly possible to obtain it from numerical solutions of the radiative transfer equation as well.

A more familiar function that can be obtained from the formal solution of the equation of radiative transfer is the so-called weighting function, which is the derivative of the transmission function along the line of sight. It turns out that there is a quite simple relation between mean values obtained either using the contribution function or the weighting function. The arithmetic mean of the Planck function with respect to the weighting function equals the harmonic mean of that function with respect to the contribution function. For other arbitrary functions the corresponding relation is more complex, but still relatively simple.

We applied the analysis of the contribution function to the recently developed retrieval method for upper-tropospheric humidity (UTH) for channel 12 radiances measured by the series of HIRS instruments on NOAA and Metop polar-orbiting satellites. It turned out that the mean emission pressure decreases (that is, the altitude increases) with increasing upper-tropospheric humidity (as expected), but the variation is not very large when UTH exceeds about 50 %. The depth of the emitting layer (measured as $\pm\sigma_p$ distance) is much larger than the variation of the mean pressure with UTH.

Jacobians are used to express the sensitivity of the measured radiance or brightness temperature to changes in the underlying profiles of any quantity (in particular temperature and relative humidity) along the line of sight. In this paper we show that a general Jacobian is simply the derivative of the radiance integrand $\Phi(s, Q(s))$ to the quantity $Q(s)$ at arbitrary locations. Introducing a relative Jacobian, which gives the relative sensitivity of the radiance to a change in a profile, we show that this equals the corresponding derivative of the contribution function φ. The Jacobian for changes in the relative humidity profile is the product of

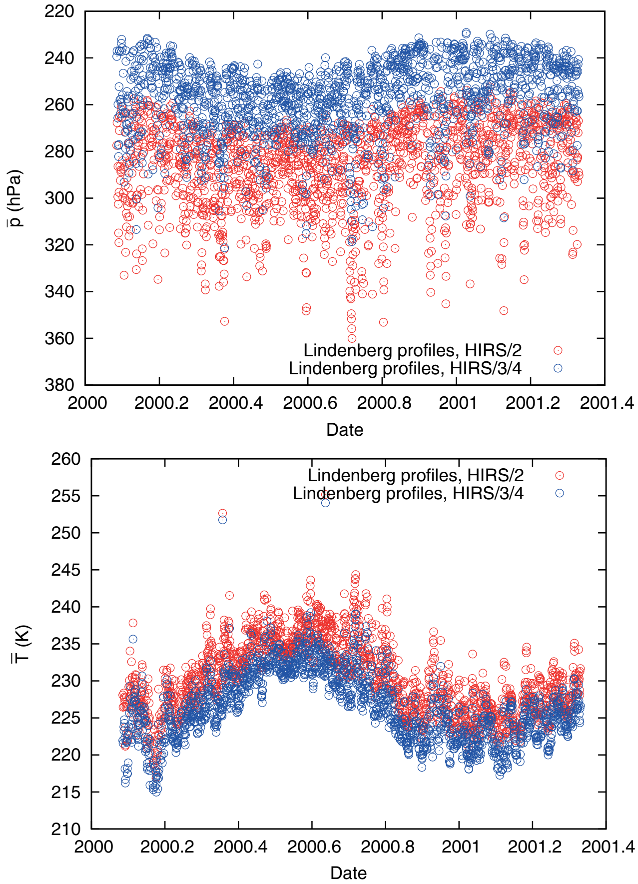

Figure 9: Mean emission pressure levels (top panel) and temperatures (bottom panel) computed from brightness temperatures for HIRS/2 on NOAA 14 (red) and HIRS/3 on NOAA 15 (blue) that have been computed using a set of radiosonde profiles obtained at Lindenberg, Germany, with a radiative transfer code. The x-axis is the date of the respective radiosonde launch.

the Planck function with the transmission function and the derivative of the extinction coefficient to the relative humidity at an arbitrary location along the line of sight.

Finally, we note that use of the contribution function offers new possibilities to interprete satellite data. Figures 4 and 5 show that brightness temperature measurements can be used to infer $\overline{p}$ and $\overline{T}$, the mean emission pressures and temperatures. As an example for such an application we took the HIRS/2 (on NOAA 14) and HIRS/3 (on NOAA 15) channel 12 brightness temperatures that have been computed (Gierens et al., 2018) for a large data set of radiosonde profiles obtained from the meteorological observatory Lindenberg (Spichtinger et al., 2003). Figure 9 shows the mean emission pressure levels and temperatures for both sensors and for each launch. The daily and even sub-daily variability of $\overline{p}$ is quite large which reflects the corresponding large variability of relative humidity. The mean emission temperatures show additionally the typical seasonal variation, i.e. low temperature in winter and higher temperature in summer. Instead of producing maps of UTH from HIRS radiances it is possible to produce maps of the corresponding $\overline{p}$ and $\overline{T}$. These have the same information content but allow different points of view on the data. Furthermore, $\overline{p}$ corresponds roughly to the level where the optical depth, τ, in channel 12 reaches unity, at least for all situations where UTH exceeds 5 (HIRS/3/4) to 15 % (HIRS/2). For larger UTH, we get that $\overline{\tau} \approx 1.05$ (not shown). Thus another interpretation arises, namely that of the level where the optical depth reaches unity value. These new possibilities can be exploited in future analyses of HIRS data, but they can be exploited for other data as well once the contribution function is either given or obtainable numerically.

Acknowledgments

K. Gierens thanks his son Jakob for the idea that certain moments in the theory are simply arithmetic and harmonic means. The authors thank Dennis Piontek and Luca Bugliaro for critically reading the manuscript before submission. We are grateful for the comments of two reviewers which helped to improve the paper.

Appendix

Here we provide the values and meanings of the constants in the expression on the right hand side of Eq. (3.1). Values that are given as pairs, like (x_1, x_2), are the versions for HIRS/2 (x_1) and HIRS/3/4 (x_2), respectively.

$B_0 = (10.4224, 11.0738)\,\mathrm{W\,m^{-2}\,sr^{-1}}$: Planck function at $T_0 = 240\,\mathrm{K}$.

$C_\lambda = (8.95, 9.22)\,\mathrm{W\,m^{-2}\,sr^{-1}}$: radiation constant $(2hc^2/\lambda^3)$ with the Planck constant h, speed of light c and wavelength λ.

$\beta = 0.22$: dimensionless lapse rate $(d\ln T/d\ln p)$.

$A_\lambda = (46.98, 72.37)$ for UTH and

$A_\lambda = (53.87, 82.99)$ for UTHi.

$\kappa = 23.1$ for UTH and $\kappa = 25.7$ for UTHi: parameter for the approximation of the water vapour saturation pressure.

For details please consult Gierens and Eleftheratos (2019).

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