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ABSTRACT

To retrieve vertical profiles of temperature and moisture from infrared spectral measurements, surface emissivity must be accounted for in the physical solution of the inverse problem. A radiative model that includes the emission and reflection on the lower atmospheric boundary is introduced. An algorithm is developed for the solution of the vertical temperature–humidity profile and the estimation of an effective surface emissivity and temperature within the sounding area. Results using spectral measurements from the Geostationary Operational Environmental Satellite (GOES)-8 sounder are presented. It is found that accounting for the surface emissivity in the solution of the inverse problem has a positive impact on the meteorological profiles.

1. Introduction

An objective of meteorological remote sensing is to assess the temperature–humidity distribution of the ‘‘surface + atmosphere’’ system. Quantitative estimation of these parameters is based upon the numerical solution of the radiative transfer equation (RTE) wherein contributions to the measured radiances from the observed system are modeled. The model must account for emissions from both the earth’s surface and the atmosphere. How well this accounting is done plays a critical role in the accuracy of the solution because the inverse problem is ill posed. The primary goals of this work are 1) to estimate the influence of the spatial–temporal variability of the surface emissivity on the satellite infrared measurements and 2) to demonstrate the importance of accounting for surface emissivity variations in meteorological remote sensing when using infrared (IR) spectral measurements. There are many papers that present laboratory and field measurements of the optical properties of different material and surfaces; they demonstrate the physical complexity of the radiance reflection phenomena and the difficulty of modeling them (see Nerry et al. 1991). In satellite remote sensing the infrared radiometer measures the outgoing thermal radiance of the surface + atmosphere system within the sensor field of view (FOV). The spatial size of the Geostationary Operational Environmental Satellite (GOES) sounder FOV is about 10 km × 10 km. For such spatial scales, we can estimate surface emissivity only when sensing spatially homogeneous surfaces like the sea surface. For other non-homogeneous surfaces, we observe a spatially averaged reflection from a spatial mix of materials and surfaces.

In Plokhenko and Menzel (2000), we estimated the influence of surface emissivity on retrievals of atmospheric temperature–moisture profiles by using infrared measurements from the Moderate Resolution Imaging Spectroradiometer airborne simulator (MAS; King et al. 1996). In that paper, an effective surface emissivity was directly estimated within the solution of the inverse problem. It was shown that the derived effective surface emissivity varies significantly with each MAS 50-m FOV over nonhomogeneous land scenes, and accounting for this emissivity in the solution of the radiative transfer equation positively affects the atmospheric part of the solution. In this paper we describe the algorithm and its application to the measurements from the GOES sounder.
As stated in Plokhenko and Menzel (2000), the major reasons to include a parameter describing the surface reflection into the solution of the inverse problem are the following.

• Emissivity variations cause measurable changes in infrared radiances.
• Measurements from meteorological satellite instruments demonstrate a relative accuracy of approximately 0.2 K. To realize the potential information content of this measurement, an appropriate radiative transfer model accounting for surface emissivity must be used.
• Modeling errors, reinforced by the instability of the inverse problem, can drastically reduce the accuracy of the temperature and moisture profile retrievals.
• The first-guess temperature and moisture spatial fields (from numerical weather prediction models) used to initialize the profile retrievals from the measured radiance fields are already very accurate. Thus, the measurement model must be of high quality so that its errors do not amplify the measurement errors.
• The varieties of surface cover, with different surface optical properties and extremely high spatial and temporal variations, restrict using a priori estimates of the surface effects. Therefore, the direct evaluation of emissivity is a more effective approach for modeling.

This work is aimed at improving the inversion algorithms for GOES data processing that do not explicitly account for the spatial variability of the surface emissivity; many use a graybody emissivity of 0.98 for sea surfaces and 0.96 for land surfaces (Hayden 1988). The effective emissivities in our GOES processing are derived for very large areas (the window channel measurements are averaged over 3 × 3 fields of view corresponding to areas of 900–2500 km², depending on viewing angle). Interpretation of these effective emissivities estimated for large nonuniform surface areas (available only under cloud-free atmospheres) is challenging. They do not compare with finescale tabulations of spectral surface emissivities, nor did we expect them to. However, we will show that they do have the general spectral, spatial, and temporal properties one expects.

This paper is organized as follows. In section 2, we present a short description of the measurement model, inverse problem, and solution algorithm. In section 3, we describe and analyze the GOES sounder infrared spectral measurements. Conclusions are offered in section 4. Appendix A presents some of the details in the solution algorithm, and appendix B contains an analysis of the estimates of the atmospheric temperature–moisture profiles.

2. Measurement model, description of the problem, and the estimation algorithm

The physical model for the GOES measurements and the mathematical basis for the algorithms developed for retrieving temperature and moisture profiles, accounting for the surface emissivity, are described in this section.

The RTE that describes the satellite measurement of the outgoing thermal radiance for the cloud-free, non-scattering, azimuthally homogeneous atmosphere can be written as

\[
\bar{J}(\theta) = \frac{\varepsilon(\theta)B(T_s)\tau_i(\theta) + \int_{\tau_{i}^{0}(\theta)} \tau_{i}^{+}(p, \theta) B[T(p)] \, d\tau_{i}^{+}(p, \theta) \, d\tau_{i}^{0}(\theta)}{\tau_{i}^{0}(\theta) \tau_{i}^{+}(\theta) + 1} + r(\theta)\tau_{i}^{+}(\theta) \int_{\tau_{i}^{0}(\theta)}^{1} B[T(p)] \, d\tau_{i}^{+}(p, \theta^{*}) + \xi, \tag{1}
\]

where \(\bar{J}(\theta)\) is the measured radiance at the angle of incidence \(\theta\); \(\varepsilon(\theta)\) and \(r(\theta)\) are the effective hemispheric directional emissivity and reflectivity, respectively (Nicodemus 1965); \(B(\cdot)\) is the Planck function; \(T_s\) is the surface temperature; \(T(p)\) is the temperature at pressure \(p\); \(\tau_{i}^{+}(p, \theta)\) is the transmittance of the upwelling radiance from pressure \(p\) to the top of the atmosphere in a given spectral interval at zenith angle \(\theta\); \(\tau_{i}^{+}(p, \theta^{*})\) is the transmittance of the downwelling radiance from pressure \(p\) to the surface at zenith angle \(\theta^{*}\); \(\tau_{i}^{0}(\theta)\) designates the value of any parameter on the surface level; \(\theta^{*}\) is the effective angle of incidence of downwelling radiance; and \(\xi\) is the measurement error.

Solar radiance is disregarded in Eq. (1); hence, it should be considered as a nighttime version of the RTE. Term I describes the upwelling radiation, and term II describes the downwelling radiance reflected by the surface upward to the sensor. The transmittance is a known function of the atmospheric temperature–moisture profile.

The effective emissivity \(\varepsilon\) of the scene observed in the radiometer FOV is given by

\[
\varepsilon(\theta) = \frac{\int_{0}^{1} \varepsilon(\theta, \beta) [B(\beta)\Psi(\beta)] d\beta}{B(T_s)}
\]

\[
T_s = \int_{0}^{1} T_s(\beta)\Psi(\beta) \, d\beta, \tag{2}
\]

where \(\varepsilon(\theta, \beta)\) is the hemispherical directional emissivity of surface type \(\beta\), which occupies a fraction \(\Psi(\beta)\) within the FOV and has temperature \(T_s(\beta)\), and \(T_s\) is the average surface temperature within the FOV.

The effective angle of incidence \(\theta^{*}\) of the downwelling radiance \(J^{+}(\theta^{*})\) is understood as
Here, \( \rho(\theta, \vartheta, \beta) \) is a bidirectional reflectance function of surface \( \beta \) described by a surface shape distribution function \( \Phi(\theta, \beta) \) (Beckmann and Spizzichino 1963; Nicodemus 1965; Hapke 1993). The product \( \Phi(\theta, \beta)\Psi(\beta) \) describes the composite structure of the surface within the FOV. The effective angle \( \vartheta^* \) is a function of wavelength.

Conservation of radiance energy in isothermal conditions in Eq. (1) implies a relation analogous to Kirchhoff’s law:

\[
r(\theta) = 1 - \varepsilon(\theta). \tag{4}
\]

In Eq. (1), the surface optical effects are described by both \( \varepsilon(\theta) \) and \( \vartheta^* \). However \( \varepsilon(\theta) \) dominates because the functional derivative of the radiance with respect to the effective angle of incidence will be approximately two orders of magnitude less than the corresponding derivative with respect to the effective emissivity.

To bound the inverse problem in Eq. (1), a priori information that characterizes the effective emissivity \( \varepsilon(\theta) \) is required. In Eq. (1), the geometrical characteristics of \( \varepsilon(\theta) \) are implicitly defined by the angle \( \vartheta^* \). We assume \( \vartheta^* = \theta \), which corresponds to the traditional “specular reflection.” Furthermore, we partition the spectrum into intervals within which the surface is considered to be a “graybody.” Thus, the unknown parameters in Eq. (1) are the spectral profile of effective emissivity \( \varepsilon(\theta) \), surface temperature \( T_s \), temperature profile \( T(p) \), and moisture profile \( Q(p) \).

The inverse solution of Eq. (1) is ill posed. To solve Fredholm’s equation of the first kind numerically, it must be regularized. The initial problem must be approximated by a well-posed problem whose solution is unique, stable, and corresponds in some sense to the solution of the initial problem (Tikhonov and Arsenin 1977). We construct a well-posed problem with a solution using the minimum-variance estimator (Rao 1965) with respect to atmospheric moisture–temperature profiles. The surface emissivity is a control parameter within known bounds (0.72–0.98). The corresponding minimization problem is solved using the Gauss–Newton iterative scheme. See appendix A for details.

3. Analysis of GOES sounder data and interpretation of algorithm applications

Description of the GOES-8 sounder can be found in Menzel et al. (1998) and the GOES I–M Data Book (Space Systems-Loral 1996). GOES-8 sounder spectral channels, measurement characteristics, and their intended purposes are briefly summarized in Table 1, where \( \sigma(\xi) \) designates the standard deviation of the instrument noise (converted into a temperature value for a scene temperature typical to each spectral channel). Significant variations of \( \sigma(\xi) \) from one spectral channel to another are evident. The parameter \( \sigma(\hat{\xi}) \) represents the noise remaining after spatial filtering (see, Plokhenko and Menzel 2000) is used to improve the signal-to-noise ratio (SNR).

Infrared sounder measurements, and the GOES sounder, as well, have demonstrated the following properties:

1) land surface reflection is substantially larger in shortwave (SW) bands (channels 13–18) than in longwave (LW) bands (channels 1–8),

2) radiation absorption by cloud ice particles is substantially larger in LW than in SW bands, and

3) SW bands are less affected by variations of atmospheric moisture than are LW bands, including “atmospheric windows” sensitive to the atmospheric moisture.

Examples of the temperature weighting functions and moisture sensitivities are shown in Fig. 1. We find that the vertical distributions of the contributions to measurements in pairs of LW and SW spectral bands are
nearly the same; channels 3 and 15 (in Fig. 1a), 5 and 14 (in Fig. 1a), and 6 and 16 (in Fig. 1b) have very similar weighting functions. We use these similarities in the different spectral measurements to assist with filtering noise and detecting clouds (Plokhenko and Menzel 2001; Plokhenko et al. 2003). Spatial smoothing is used to improve the SNR of the GOES measurements relative to the background first
A spectral measurement represents a specific atmospheric layer (sometimes in combination with the surface; see Fig. 1) and has the corresponding spatial properties. Atmospheric temperature fields are smooth. In particular, spectral bands sensitive to upper-tropospheric and stratospheric layers exhibit large spatial uniformity. Therefore, variations on small spatial scales (shortwave spatial variations) in the measurements mostly describe surface variations or noise. The spatial smoothing is accomplished by a moving average within a square box; the size of the box is adjusted with spectral band.

Spatial averaging and cloud identification are combined in a joint algorithm. The preparation of the data for sounding analysis starts with spatial smoothing, followed by cloud detection, followed by averaging the clear-sky (cloud free) subsamples. Cloud detection tests for spatial smoothness (second differential should be large) and spectral smoothness [differences between LW and SW band channels (14, 5), (15, 6), (16, 8) should be large]. Details regarding the spatial smoothing and characteristics of resulting spectral fields are given in Plokhenko and Menzel (2001) and Plokhenko et al. (2003). The procedure provides a uniform accuracy of estimates in all spectral channels [see the parameter $\sigma(\xi)$ in Table 1] and is especially effective in the upper-tropospheric and stratospheric channels (1, 2, 3, 4, and 15).

To stabilize the solution of Eq. (1) and to reduce its physical uncertainty, we use a priori information about the modeled surface + atmosphere system. To initialize the data analysis, we use a forecast of temperature–moisture profiles (first guess) from the Eta Model (Black 1994; Rogers et al. 1996). The retrieval solutions will be successful if they improve upon the accuracy of the first-guess profiles with respect to radiosonde observations (raobs). Because the first guess is already very good, we face the problem that model uncertainties are comparable to the amplitude of signal variations. That effect is demonstrated in Fig. 2; the spectral distribution of calculated radiance (brightness temperature) variations is shown as a function of variations in atmospheric temperature, atmospheric moisture, and surface emissivity (with surface temperature fixed). We plot the brightness temperature response in the GOES sounder spectral bands when the temperature and moisture profiles change by as much as the Eta Model differences with respect to raobs, and we plot the brightness temperature response in the GOES sounder spectral bands when the surface emissivity increases from 0.96 to 0.98.

In Fig. 2 we find that

1) the Eta Model temperature first guess is very accurate (variation in the midtropospheric temperatures is less than 0.5 K),
2) the SW bands respond to the vertical variation of the atmospheric temperature profile and the surface emissivity [the latter affects the measurements in channels 13 and 16 and will affect the temperature profile estimate in the lower troposphere (see Fig. 1)],
3) the LW bands respond to variation in the lower atmosphere (see Fig. 1; the measurement model for channels 5–8 must include variations of the atmospheric temperature–moisture profiles and the surface emissivity), and
4) contributions from the GOES sounder measurements toward improving upon the first guess will be in the upper-tropospheric and lower-stratospheric temperature profile (from channels 14 and 15 in the SW band and channels 1–4 in the LW band) and in the upper-troposphere moisture profile (from channels 10–12 in the 6.5–7.5-μm water vapor absorption band).

Figure 2 also demonstrates that the emissivity in the
measurement model must be properly addressed if the first guess in the lower troposphere is to be improved.

GOES sounder data for 1 June 2000 at 1000 UTC were processed and analyzed. Figure 3 presents the measurements in the SW (4 μm; Fig. 3a) and the brightness temperature difference of the SW minus the LW (11 μm) window bands (ΔT = Tsw − Tw) (in kelvins; Fig. 3b). The East Coast appears to be clear, showing a cooler land surface and warmer sea surface on Fig. 3a. Dark areas indicate cloud cover. The strong similarity in spatial distributions of measurements in the SW and LW (11 μm) window bands was evident (LW window is not shown). Differences in spectral signatures from different surface and cloud cover show up readily (differences between −5 and 5 K are shown). Dark red areas (positive differences of up to 20 K) correspond to upper-tropospheric ice clouds, and dark blue areas correspond to low-tropospheric clouds. Figure 3b shows that measurements over the land surface are noticeably cooler (∼2 K) in the SW window than in the LW window. Over the water the situation is reversed; the SW window is more “clear,” and hence warmer, than the LW window, which is contaminated by water vapor absorption. The East Coast of North America (for similar atmospheric conditions) is very evident, with the larger decrease of the SW emissivity (reflection increasing) going from water to land than for LW. In accordance with Eq. (1), the surface emissivity reduction decreases the contribution of the warm surface into the outgoing radiance and increases the contribution of the cooler atmosphere. The water surface is characterized by significantly larger emissivity values with a small spectral variation. Figure 4 shows laboratory reflection measurements of surface constituents relatively frequently observed by satellite.
(soil, sand, granite, and asphalt; ASTER 2000). It helps to explain the spatial–spectral variability of the land measurements seen in Fig. 3b; the land surface contains elements for which emissivities in the SW band are noticeably less than emissivities in the LW band.

We now proceed to solve Eq. (1) for the GOES sounder measurements. In accordance with the algorithm (Appendix A), we use a two-parameter emissivity model, 
\[ \varepsilon = (\varepsilon_{SW}, \varepsilon_{LW}), \]
where \( \varepsilon_{SW} \) describes the surface emissivity for channels 13–18 (3.8–4.6 \( \mu \)m) and \( \varepsilon_{LW} \) for channels 4–8 (11.0–13.7 \( \mu \)m). For channels 10–12 (water vapor absorption band 6.5–7.5 \( \mu \)m), the surface influence is less than 0.1% of signal variation. This emissivity spectrum partition is based upon direct emissivity measurements (see Fig. 4). The solution is constrained so that \( \varepsilon \approx 0.98 \).

Figure 5 presents SW and LW emissivity estimates that correspond to solutions using the GOES data in Figs. 3a and 3b (dark blue areas with values of \( \varepsilon \times 1000 < 800 \) signify missing data). The SW emissivity is noticeably less than that of the LW, the correlation of SW and LW emissivity components is 0.9, and the SW and LW emissivity estimates exhibit a strong spatial variability. The emissivity fields are spatially consistent; random variations of emissivity estimates from pixel to pixel are not observed. The local maxima of the emissivities (left center of Fig. 5) indicate the location of Mississippi River. The local emissivity minima at boundaries of "clear–cloudy" areas (bluish shadows around missing data areas) indicate problems with the a priori emissivity information (an a priori emissivity estimate is required for estimating outgoing thermal radiation used for cloud detection).

Temporally averaged SW and LW emissivity maps at grid spacing of 0.1° latitude and 0.1° longitude for 25 cases at 1000 UTC 12 May–12 June 2000 are shown in Fig. 6 (dark blue areas with values of \( \varepsilon \times 1000 < 800 \) signify missing data). We see the spectral–spatial variability and the spatial consistency of the emissivity estimates. The monthly average of the emissivity varies within the whole map; the average SW emissivity is \( \sim 0.86 \) and average LW emissivity is \( \sim 0.92 \). The range of the emissivity variation is larger in the SW (\( \sim 0.80–0.98 \)) than in the LW (\( \sim 0.86–0.98 \)). The spatial consistency of the emissivity estimate is apparent, as is the obvious relationship between ecosystem and emissivity. Local SW emissivity maxima indicate river or lake locations (Rio Grande River, Mississippi River, Lake Okeechobee, the Great Lakes) and nearby agricultural areas (vegetation contributions increase the surface emissivity). Local SW emissivity minima are evident in the vicinity of the Appalachian Mountains (the lower vegetation cover and the higher rock cover reduce the SW emissivity in accordance with Fig. 4). The LW emissivity does not show a corresponding reduction (as predicted by Fig. 4); the LW spatial pattern is different from that of the SW. These emissivity characteristics
over land show a good relationship with the land surface physical characteristics. The temporal consistency of the emissivity estimates of Fig. 6 is demonstrated in Figs. 7a and 7b; showing the standard deviation of the emissivity estimates. There are only a few locations at which the standard deviation of the emissivity estimate exceeds 0.045, implying that the emissivity estimates are stable for this time period. Note that the standard deviation of the emissivity estimate includes contributions of the spatial averaging and the temporal variability of the emissivity; thus, we can assume that the emissivity estimate error is actually less than the standard deviation value. Over the land surface in the image, the average standard deviation is approximately 0.023 for the SW and approximately 0.017 for the LW.

In an attempt to find the influence of the emissivity estimate on the atmospheric parameter estimates, we calculate the standard deviation of the spatial differential of the Laplace operator of spatial fields of atmospheric temperature estimate and the average absolute difference of radiosonde minus satellite temperature profiles. The statistics of the spatial differential of the retrieved atmospheric temperature field describes the spatial "roughness" of the estimated field. The differentiation affects the physical signal and the retrieval error of the atmospheric temperature field in different ways; it weakens the large-scale physical signals and amplifies the small-scale retrieval errors. The spatial roughness of the atmospheric temperature estimate is a function of the measurement and model errors, reinforced by the instability of the inverse problem. The variance of the spatial roughness of an atmospheric parameter estimate is an indication of the measurement and model accuracy; a smaller variance indicates more accurate measurements and models. The emissivity and thermal properties of land surfaces have a strong spatial variability; that is, they are described by changes on small scales. In correspondence, the model errors, associated with the emissivity estimate error, are also found on small spatial scales. In the same way, a more accurate emissivity estimate produces a more spatially smooth atmospheric temperature esti-
Fig. 6. Average (a) SW and (b) LW emissivity (scaled by 1000) on a 0.1° lat by 0.1° lon grid for 25 cases at 1000 UTC 12 May–12 Jun 2000.

mate in the model. The appropriate criteria for atmospheric temperature spatial smoothness are dictated by the continuity equation that contains a velocity divergence term. The spatial variations in the estimate of the atmospheric temperature field \( T(x, y, p) \) generate variations in the thermal wind field \( u_x \) and \( u_y \) terms. The spatial variations in the estimate of the atmospheric temperature field \( T(x, y, p) \) generate variations in the thermal wind field \( u_x \) and \( u_y \) terms. The initial thermal fields \( T(x, y, p) \) correspond to the initial velocity fields and satisfy the continuity equation; \( \delta^2 T \) should be small, where \( \delta T(x, y, p) = T(x, y, p) - T(x, y, p) \), so as to comply with the continuity equation under given initial velocity fields.

The spatial smoothness criteria can be used for a relative evaluation of different surface reflection models. We use a radiative transfer model with the optically “black” surface as a reference point in evaluating the efficiency of the model with reflection. The results of experiments for the radiative transfer models with and without reflection are presented in Fig. 8, showing the standard deviation of the second spatial differential \( \delta^2 T / \delta x^2 (\delta x)^2 + \delta^2 T / \delta y^2 (\delta y)^2 \) and the average absolute difference of the temperature from the raobs and satellite estimates. It follows from Fig. 8a that the surface emissivity estimate noticeably reduces the spatial variability of the estimated temperature fields in the lower troposphere in comparison with the spatial variability of the solution without surface reflection. The solution with reflection is smoother and, hence, more in concert with the continuity equation. The significance of the roughness reduction is emphasized by the smoothness of the first-guess fields. The estimates of accuracy in Fig. 8b show that the solution with reflection is more in agreement with raobs, especially in the atmospheric layers at 700–850 and 950–1000 hPa.
4. Conclusions

Analysis of nighttime measurements from the GOES-8 sounder shows that surface emissivity significantly affects the GOES infrared measurements. An assumption of fixed emissivity is not effective for retrieving temperature and moisture profiles, especially over land where the surface emissivity has strong spatial variability. Temporally averaged land surface emissivity for shortwave and longwave spectral bands of the GOES sounder was estimated for May–June 2000. The results show strong spatial variability and temporal consistency. The spatial distribution of the surface emissivity estimates is coherent with the ecosystem characteristics. Direct evaluation of surface emissivity in the inverse solution of the radiative transfer equation produces atmospheric temperature profile solutions that have better agreement with radiosonde observations and corresponding horizontal temperature fields that are smoother and more in concert with the continuity equation.

The derived emissivity estimates are affected by low spectral–spatial resolution, missing spectral channels, and cloud identification errors. They are found to be slightly low. In particular:

1) The results presented are derived from the spectral measurements spatially averaged over 900–2500 km² (depending on viewing angle); the elements with low emissivities within the scene reduce the average emissivity value (especially in the SW).

2) The satellite viewing angle is large (on average 45°), and emissivity is a nonlinear decreasing function of viewing angle (especially in the SW).

3) Orographic effects magnify the emissivity angular effects.
4) Undetected cloud contamination is driving the effective emissivity estimate down. 

Comparison with a standard emissivity chart is difficult. However, the surface emissivity estimates do have the general spectral, spatial, and temporal properties one expects.

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APPENDIX A

Details of the Solution Algorithm

We construct a well-posed problem with a solution that uses the minimum-variance estimator (Rao 1965): estimates of the desired parameters \( x \) and \( \varepsilon \) must satisfy the following conditions:

1) \( x \) is a random value (vector) that has statistical characteristics so that the average \( \bar{x} = 0 \) and the covariance matrix \( \overline{xx^T} = R \), where the overbar denotes the mathematical expectation and \( X = \bar{x} + x \), where \( \bar{x} \) designates the first guess;

2) \( \xi \) is a random value (vector) that has statistical characteristics so that the average \( \bar{\xi} = 0 \) and the covariance matrix \( \overline{\xi \xi^T} = S_{\xi} \), and \( \xi \) is uncorrelated with \( x \) so that \( \overline{\xi x^T} = 0 \); and

3) \( \varepsilon \) is a control parameter in a known spectral interval of interest, \( \varepsilon \) designates some first guess, and \( \varepsilon = \bar{\varepsilon} + \delta \varepsilon \) where we need \( \bar{\varepsilon} \) to introduce a priori information about the spectral profile of emissivity.

Then a linearized model of measurement with respect to the variation of the unknown parameters \( (\delta \varepsilon, x) \) can be written as

\[
\begin{align*}
\mathbf{f}(\varepsilon, \delta \varepsilon, x) &= \mathbf{J} - \mathbf{J}(x) - (1 - \varepsilon)\mathbf{J}(\bar{x}) \\
&= -\delta \varepsilon \cdot \mathbf{J} + A(\varepsilon)x + \xi,
\end{align*}
\]
where \( f(\pi, \delta \pi, x) \) designates the measurement variation vector and \( A(\pi) = A[J(\pi)] \) is a matrix of the algebraic system approximating Eq. (1). The matrix \( A(\pi) \) can be represented in the form

\[
A(\pi) = A[J(\pi)] = A[J_0 + (1 - \pi)J_s]
\]

\[
= A + (1 - \pi)G,
\] (A2)

where \( A = A[J_0] \) designates the linear approximation of the emissive integral term

\[
J_s = B(T_s)\tau_i^s(\theta) + \int_{\tau_i^s(\theta)}^{1} B(T(p)) \, d\tau^s(p, \theta),
\] (A3)

and \( G = A[J_s] \) designates the linear approximation of the reflective integral term

\[
J_r = -B(T_r)\tau_i^r(\theta)
\]

\[
+ \tau_i^r(\theta) \int_{\tau_i^s(\theta)}^{1} B(T(p)) \, d\tau^s(p, \theta).
\] (A4)

For estimating \( \delta \pi \) (scalar), we use the least squares solution min\(\pi\) \( f(\pi, \delta \pi, x)D(\pi)^{-1}f(\pi, \delta \pi, x) \):

\[
\delta \pi = - \beta(\pi)J^T_s D(\pi)^{-1}f(\pi, \delta \pi, x)
\]

\[
\hat{\pi} = \pi + \delta \pi,
\] (A5)

where

\[
\beta(\pi) = 1/[J_s^T D(\pi)^{-1}J_s],
\]

\[
D(\pi) = A(\pi)R A(\pi)^T + S,
\] (A6)

and superscripts \( T \) and \( -1 \) are transposition and inversion operators, respectively. The error of the estimate (A5) is

\[
\xi(\hat{\pi}, x) = - \beta(\pi) J_s D(\pi)^{-1} [A(\pi) x + \xi]
\]

\[
\xi(\hat{\pi}, x)^T = \beta(\pi).
\] (A7)

Equation (A5) smooths the influence of \((x, \xi)\), with the statistical weight in the signal defined by the matrix \( D(\pi) \). Under fixed estimate \( \hat{\pi} \), the estimate \( \hat{x} \) has the following form:

\[
\hat{x}(\hat{\pi}) = RA(\hat{\pi})^T D(\hat{\pi})^{-1} f(\hat{\pi}, \delta \pi, x)\big|_{\delta \pi = 0}
\]

\[
f(\hat{\pi}, \delta \pi, x)\big|_{\delta \pi = 0} = \tilde{J} - J_0[\tilde{X}] - (1 - \hat{\pi})J_s[\tilde{X}]
\]

\[
= A(\hat{\pi}) x + \xi.
\] (A8)

We split the solution of Eq. (1) into components because the functional derivative of radiance with respect to emissivity is much larger than the other derivatives. Considering substitutions \( \hat{\pi} \Rightarrow \pi, \hat{x} \Rightarrow x \) in (A5), we solve (A5)-(A8) iteratively. For the scalar parameter \( \delta \pi \), the iteration is defined by the following relations:

\[
J[e^{(n)}, T_s^{(n)}, X^{(n)}]
\]

\[
= J_s[T_s^{(n)}, X^{(n)}] + [1 - e^{(n)}]J_s[T_s^{(n)}, X^{(n)}]
\]

\[
f^{(n)} = \tilde{J} - J[e^{(n)}, T_s^{(n)}, X^{(n)}]
\]

\[
\beta^{(n)} = 1/[J_s[T_s^{(n)}, X^{(n)}]^T D[e^{(n)}]^{-1} J_s[T_s^{(n)}, X^{(n)}]]
\]

\[
e^{(n+1)} = e^{(n)} - \beta^{(n)} J_s[T_s^{(n)}, X^{(n)}]^T D[e^{(n)}]^{-1} f^{(n)}
\]

\[
f_s^{(n)} = \tilde{J} - J[e^{(n)}], T_s^{(n)}, X^{(n)}]
\]

\[
T_s^{(n+1)} = T_s^{(n)} + \beta^{(n)} D[e^{(n)}]^{-1} f_s^{(n)}
\]

\[
f_s^{(n)} = \tilde{J} - J[e^{(n)}, T_s^{(n)}, X^{(n)}]
\]

\[n := n + 1\]

\[
\text{if}[f_s^{(n+1)}]_s - f_s^{(n+1)} > \text{trace}(S D[e^{(n+1)}])^{-1},
\]

(A9)

with the initial values \( e^{(1)} = \pi, T_s^{(1)} = \tilde{T}_s, \) and \( X^{(1)} = \tilde{X} \). In (A9) we separate the surface parameter estimates ( emissivity, temperature) from the atmospheric parameter estimates (temperature–moisture profiles) to achieve stability in the solution (see appendix B). The matrix \( A_{(\pi)}(e) \) designates \( \partial J[e, T_s, X]/\partial T_s \), and the matrices \( A_{(\pi)}(e) \) and \( D_{(\pi)}(e) \) correspond to the matrices \( A(e) \) and \( D(e) \), respectively, with matrix elements corresponding to the surface parameters modified [i.e., \( A_{(\pi)}(e) \) and \( D_{(\pi)}(e) \) describe only atmospheric temperature–moisture contributions]. The first-guess emissivity \( \pi \) comes from an a priori information or can be constructed using (A5) in the form

\[
\pi = 1 - \frac{1}{[J_s(\tilde{X})^T S^{-1} J_s(\tilde{X})]} J_s(\tilde{X})^T S^{-1} [\tilde{J} - J_s(\tilde{X})].
\] (A10)

For the vector parameter \( \delta \pi \), the iteration (A9) must be modified with respect to the estimate \( \delta \pi \):

\[
\delta \pi = -[\Delta_s^T D(e)^{-1} \Delta_s]^{-1} \Delta_s D(e)^{-1} [\tilde{J} - J(e, T_s, X)]
\]

\[
\Delta_s \equiv \frac{\partial J}{\partial (\delta \pi)},
\] (A11)

and (A7) is transformed to

\[
\xi(\pi, x) = -[\Delta_s^T D(e)^{-1} \Delta_s]^{-1} \Delta_s D(e)^{-1} [A(\pi) x + \xi]
\]

\[
S_s = \xi(\pi, x)^T \xi(\pi, x) = [\Delta_s^T D(e)^{-1} \Delta_s]^{-1}.
\] (A12)

APPENDIX B

Analysis of Estimates of the Atmospheric Temperature–Moisture Profiles

We consider a sensitivity of the estimate \( \hat{x}(\hat{\pi}) \) from (A8) to the uncertainty \( \xi(\pi, x) \) of the estimate \( \hat{\pi}, \hat{\pi} = \pi + \xi(\pi, x) \). The estimate (A8) is the solution approximation, depending on the parameter \( \hat{\pi}, \) and its accuracy is defined by the expansion
\[ x(\varepsilon) - \hat{x}(\varepsilon) = \frac{\partial \hat{x}(\varepsilon)}{\partial \varepsilon} \xi(\varepsilon, x) + \frac{1}{2} \frac{\partial^2 \hat{x}(\varepsilon)}{\partial \varepsilon^2} \xi(\varepsilon, x)^2 + \cdots \]  
(B1)

Let us examine the terms \( \frac{\partial \hat{x}(\varepsilon)}{\partial \varepsilon} \xi(\varepsilon, x) \) and \( \frac{\partial^2 \hat{x}(\varepsilon)}{\partial \varepsilon^2} \xi(\varepsilon, x)^2 \). Using the measurement model (A1),

\[ f(\varepsilon, \hat{\varepsilon}, x) = J_1(\tilde{x} + x) + (1 - \varepsilon)J_1(\tilde{x} + x) + \xi - J_2(\tilde{x}) - (1 - \varepsilon)J_2(\tilde{x}), \]  
(B2)

and the solution estimate (A8),

\[ \hat{x}(\varepsilon) = RA(\varepsilon)^T \hat{D}(\varepsilon)^{-1} f(\varepsilon, \hat{\varepsilon}, x) = L(\varepsilon) f(\varepsilon, \hat{\varepsilon}, x), \]  
(B3)

the corresponding derivatives are defined as

\[ \frac{\partial \hat{x}(\varepsilon)}{\partial \varepsilon} = \frac{\partial L(\varepsilon)}{\partial \varepsilon} f(\varepsilon, x) + L(\varepsilon) J_1, \]
\[ \frac{\partial^2 \hat{x}(\varepsilon)}{\partial \varepsilon^2} = \frac{\partial^2 L(\varepsilon)}{\partial \varepsilon^2} f(\varepsilon, x) + 2 \frac{\partial L(\varepsilon)}{\partial \varepsilon} J_1. \]  
(B4)

For the emissivity error amplitude \( \sqrt{\xi(\varepsilon, x)^2} \approx 0.03 \) we can discard the quadratic term in (B1), if the amplitudes of the derivatives are close \( \frac{\partial \hat{x}(\varepsilon)/\partial \varepsilon = \partial^2 \hat{x}(\varepsilon)/\partial \varepsilon^2} \). The major factor affecting the amplitudes of the derivatives is the inverse matrix \( \hat{D}(\varepsilon)^{-1} \); a norm of \( \hat{D}(\varepsilon)^{-1} \) is \( ||\hat{D}(\varepsilon)^{-1}|| \approx 25 \) (K=1) for the regularized matrix \( \hat{D}(\varepsilon) = A(\varepsilon)RA(\varepsilon)^T + S \). The properties of the derivatives of \( \hat{D}(\varepsilon)^{-1} \) define the accuracy of estimate (A8) and the linearity of approximation (B1), which describes the estimate stability with respect to the emissivity variations.

We consider \( \frac{\partial \hat{D}(\varepsilon)^{-1}}{\partial \varepsilon} \) and \( \frac{\partial^2 \hat{D}(\varepsilon)^{-1}}{\partial \varepsilon^2} \) for \( \varepsilon = 1 \): \( \varepsilon = 1 - \delta \). For the linear approximation:

\[ \hat{D}(\varepsilon) = D[\delta \cdot D^{-1}(RA^T + ARG^T)], \]  
(B5)

where \( D = D(\varepsilon = 1) \) and \( A(\varepsilon) = A + (1 - \varepsilon)G \) from (A2); then

\[ \hat{D}(\varepsilon)^{-1} = D^{-1} - \delta \cdot D^{-1}GRA^T + ARG^TD^{-1}. \]  
(B6)

Further, we suggest the approximation \( D^{-1}(ARA^T) \approx E_1 \) for the signal-to-noise ratio \( ARA^T \gg S \), where \( E_1 \) is the identity matrix in the space of measurements. Then, \( \frac{\partial \hat{D}(\varepsilon)^{-1}}{\partial \varepsilon} = \hat{D}(\varepsilon)^{-1}(GRA^T + ARG^TD^{-1}) \), \( \frac{\partial^2 \hat{D}(\varepsilon)^{-1}}{\partial \varepsilon^2} \) and, retaining linear terms,

\[ \left. \frac{\partial \hat{D}(\varepsilon)^{-1}}{\partial \varepsilon} \right|_{\varepsilon=1-\delta} = D^{-1}(ARG^T + GRA^T)D^{-1} \]
\[ + 2 \delta \cdot D^{-1}(GRA^T - (GRA^T + ARG^T) \times D^{-1}(ARG^T + GRA^T)D^{-1}. \]  
(B7)

From the above, it follows that

\[ \left. \frac{\partial^2 \hat{D}(\varepsilon)^{-1}}{\partial \varepsilon^2} \right|_{\varepsilon=1-\delta} = -2D^{-1}[GRA^T - (GRA^T + ARG^T) \times D^{-1}(ARG^T + GRA^T)D^{-1}, \]  
(B9)

Let us consider the physical properties of the terms \( Ax \) and \( Gx \). They describe variations in the downwelling and upwelling radiances. It should be noted that the downwelling and upwelling signals share a common scale because the same atmospheric layer generates both. Term \( Gx \) describes the thermal contrast between the surface radiance and reflected downwelling radiance. We suggest that the variations in surface temperature, atmospheric temperature profile, and atmospheric moisture profile contribute to the measurement variation independently. From the RTE and our suppositions about the properties of the solution, the following representation can be used:

\[ A = A_T - A_H + A_S, \]
\[ G = \tilde{\lambda}(A_T + A_H) - A_S, \]  
(B10)

where \( A_T, A_H, \) and \( A_S \) are matrices that describe contributions of atmospheric temperature and moisture and surface temperature, correspondingly. The matrix \( \tilde{\lambda} \) is a diagonal: \( \lambda_{ij} = [\tau_i(\rho_j)^2]/[\tau_i(\rho_j)^2] \leq 1 \), where \( \tau_i(\rho_j) \) is the transmittance for the effective atmospheric layer \( \rho \) in the spectral channel \( i \), in the sense of the RTE. It follows from the approximation \( \tau_i(\rho) \approx [\tau_i(\rho_i)/[\tau_i(\rho_j)] \in Eq. (1). The matrix \( A_T \) is defined by \( A_{ij} = \tau_i(\rho_j) \delta_{ij} \), where \( \delta_{ij} = 1 \) when \( i = j \) and 0 otherwise and \( N \) is the index of the surface level (\( p_j = p_N \)) in a finite-difference approximation of the RTE. It is assumed that the RTE (in terms of variations) was normalized by \( \partial T/\partial T \), the derivative of the Planck function with respect to the temperature. The matrices \( A_T, A_H, \) and \( A_S \) are positive (all elements are positive).

The different sign of the operator \( A_H \) in the expressions for \( A \) and \( G \) corresponds to the upwelling radiance reduction and the downwelling radiance increase, respectively, by the water vapor absorption under the standard atmospheric temperature vertical stratification (\( \partial T/\partial z > 0 \)).

Let us suppose that the surface temperature, atmospheric temperature profile, and atmospheric moisture profile are not correlated and that the corresponding signal variations are not correlated. Then, \( A_TRA^T_{HH} = A_HRA^T_{HH} = 0 \), and \( A_TRA^T_{TT} = A_HRA^T_{TT} = 0 \), where \( \sigma_T \) and \( \tau_T \) are the surface temperature variance and \( \tau_T \) is the vector of transmittances at the surface. Using these terms we obtain the approximation

\[ \left. \frac{\partial \hat{D}(\varepsilon)^{-1}}{\partial \varepsilon} \right|_{\varepsilon=1} = -D^{-1}[\lambda(\rho_j - A_TRA^T_{HH})(\rho_i \delta_{ij} - A_HRA^T_{HH} \tilde{\lambda} + \tilde{\lambda}(A_TRA^T_{HH} - A_HRA^T_{HH}) + A_HRA^T_{HH}D^{-1}. \]  
(B11)

The derivative \( \partial \hat{D}(\varepsilon)^{-1}/\partial \varepsilon \) defines the amplitude of variations of atmospheric parameter estimates with respect
to the emissivity variation. That variation should be as small as possible to reduce the effect of the emissivity estimate error on the atmospheric parameter estimate. It follows from (B11) that the surface temperature term has the amplitude of $D(e)^{-1}$. Because $\|D(e)^{-1}\| \sim 25 (K^{-2})$ and $\sigma_{RT} \sim 10 (K^2)$, the surface temperature variation is one of the primary parameters that affect the atmospheric part of the solution. From the condition $\max \| (E - \lambda \tau_{i} \tau_{j}^{T}) \|$ it follows that the measurements in spectral channels with $\tau_{i} = 0.7$ (for corresponding atmospheric parameters) will propagate that kind of instability to the atmospheric solution. To reduce the instability of the atmospheric solution with respect to the uncertainty of the surface temperature estimate, we separate the atmospheric estimate from the surface temperature estimate in the sense that the atmospheric parameters are estimated under given surface temperature. In practical terms, it means that we construct the solution estimate in three consecutive stages: emissivity $\Rightarrow$ surface temperature $\Rightarrow$ atmospheric temperature–moisture profiles. In the third stage, the surface temperature parameter is treated as a control parameter in the solution in addition to the surface emissivity parameter. In formal terms, it means that the term $A_{4}$ is removed from the matrices $A$, $G$, and $D(e)$. Corresponding matrices were designated in (A9) as $A(e) \Rightarrow A_{4}(e)$ and $D(e) \Rightarrow D_{4}(e)$. For that solution we have

$$
\frac{\partial D_{4}(e)^{-1}}{\partial e} \bigg|_{e=1} = -D_{4}^{-1} \{\hat{\lambda} (A_{4}R_{A}^{T} - A_{4}R_{A}^{T}) + \hat{\lambda} (A_{4}R_{A}^{T} - A_{4}R_{A}^{T})\} D_{4}^{-1},
$$

(B12)

where $(D_{4}^{-1} = D_{4}(e = 1)^{-1}$. For the measurement interpretation, when the first guess of the atmospheric temperature profile is very accurate, $\|A_{4}R_{A}\| \sim 0.25 (K^{-2})$ and the measurement quality is high—$\|S\| \sim 0.04 (K^{-2})$—the moisture factor can change the sign of $\partial D_{4}(e)^{-1}/\partial e$ and the solution properties. It follows from the above that $\partial D_{4}(e)^{-1}/\partial e \leq 0$ for the atmospheric conditions defined by $A_{4}R_{A}^{T} \geq A_{4}R_{A}^{T}$; that is, the atmospheric moisture contribution into the measurement variance exceeds the atmospheric temperature contribution. It implies that the solution’s numerical properties are case sensitive; that is, the emissivity effect on the solution stability depends on meteorological characteristics of the atmosphere. These properties obviously vary also within the spectrum with the variation of the water vapor absorption (see Fig. 2).

At the 4-$\mu m$ window band, the atmosphere is clear with respect to the water vapor absorption; that is, $A_{4}R_{A}^{T} = 0$ and correspondingly $0 < \partial D_{4}(e)^{-1}/\partial e \leq 2D_{4}^{-1}$. It follows that the solution instability at the 4-$\mu m$ band reaches a maximum for the optically black surfaces.

At the 11–13-$\mu m$ window band, the water vapor contribution $A_{4}R_{A}^{T}$ can vary substantially with time (increasing in the daytime and decreasing in the night), season (increasing at the warm humid summer and decreasing at the cold dry winter), and geographical location of the soundings. For the wet atmosphere with $A_{4}R_{A}^{T} \gg A_{4}R_{A}^{T}$, we have $-2D_{4}^{-1} < \partial D_{4}(e)^{-1}/\partial e \leq 0$. Then, the derivative varies within the range

$$
-2D_{4}^{-1} \leq \frac{\partial D_{4}(e)^{-1}}{\partial e} \bigg|_{e=1} \leq 2D_{4}^{-1}.
$$

(B13)

Repeating the corresponding analysis of $\partial \ln D_{4}(e)^{-1}/\partial e$ from (B9), using (B10) for cases $A_{4}R_{A}^{T} \ll A_{4}R_{A}^{T}$, $A_{4}R_{A}^{T} \approx A_{4}R_{A}^{T}$, and $A_{4}R_{A}^{T} \gg A_{4}R_{A}^{T}$, we obtain the relation

$$
-2D_{4}^{-1} \leq \frac{\partial D_{4}(e)^{-1}}{\partial e} \bigg|_{e=1} \leq 6D_{4}^{-1}.
$$

(B14)

The relations (B13) and (B14) show that the quadratic term in (B1) is small for the amplitude $\sqrt{\zeta(e, \chi)^{2}} = 0.03$ of the emissivity error.

REFERENCES


