

1 **Long-term accuracy assessment of land surface temperatures derived from**
2 **the Advanced Along-Track Scanning Radiometer**

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10
11 **ABSTRACT**

12 The accuracy of land surface temperatures (LSTs) derived from the Advanced Along-Track
13 Scanning Radiometer (AATSR) was assessed in a test site in Valencia, Spain from 2002-
14 2008. AATSR LSTs were directly compared with concurrent ground measurements over
15 homogeneous, full-vegetated rice fields in the conventional temperature-based (T-based)
16 method. We also applied the new radiance-based (R-based) method over bare soil and water
17 surfaces, where ground LST measurements were not available. In the R-based method,
18 ground LSTs are simulated from AATSR brightness temperatures in the 11 μm band and
19 radiative transfer simulations using surface emissivity data and atmospheric water vapor and
20 temperature profiles. The accuracy of the R-based ground LSTs depends on how well the
21 profiles used in simulations represent the actual atmosphere at the time of AATSR
22 observations. This can be checked with the difference $\delta(T_{11}-T_{12})$ between the actual AATSR
23 and the profile-based simulated difference in the 11 and 12 μm brightness temperatures (T_{11}
24 and T_{12} , respectively). We found that for $-0.6 \text{ K} < \delta(T_{11}-T_{12}) < 0.6 \text{ K}$, the R-based LSTs were
25 accurate within $\pm 1.0 \text{ K}$ and can be used for LST validation. For the data analyzed here, the

26 AATSR operational algorithm overestimated the ground LST by 2 to 5 K, showing that the
27 auxiliary data utilized within the retrieval scheme (biome classification and fractional
28 vegetation cover maps at $0.5^{\circ}\times 0.5^{\circ}$ resolution) should be improved and provided at the same
29 spatial resolution as the AATSR data (1 km^2). When the AATSR algorithm was optimized
30 with biome and fractional vegetation cover selected according to the nature of each surface,
31 LST errors showed negligible average biases and $\text{rmse}=\pm 0.5\text{ K}$ for full vegetation and water,
32 and $\pm 1.1\text{ K}$ for bare soil. Furthermore, we checked an alternative algorithm explicitly
33 dependent on emissivity, which provided accurate LSTs for all the surfaces studied, with
34 small biases, rmse from ± 0.4 to $\pm 0.6\text{ K}$ and most LST errors within $\pm 1.0\text{ K}$. The algorithm
35 requires monthly emissivity maps at 1 km^2 , which can be derived from classification and
36 fractional vegetation cover estimated from optical AATSR data. The results of this paper
37 show the high LST accuracy achievable with AATSR data in ideal conditions. While it is
38 necessary to establish and maintain highly homogeneous T-based validation sites, the R-based
39 method provides an alternative for the semi-operational, long-term evaluation of LST
40 products at global scale, since it is applicable over surfaces with varied LST and atmospheric
41 regimes where ground LST measurements are not feasible.

42 1. INTRODUCTION

43 Land Surface Temperature (LST) is a key parameter in meteorological, climatological and
44 hydrological studies since it results from the physical interactions in the surface-atmosphere
45 system, including the energy and water fluxes (Anderson et al., 1997; Sánchez et al., 2008).
46 LST is sensitive to local atmospheric conditions, land cover type, soil moisture and vegetation
47 water stress. Therefore it can be used to monitor desertification, deforestation and climate
48 change (Allen et al., 1994; Lambin and Ehrlich, 1997). Thermal infrared (TIR) remote
49 sensing is probably the most suitable technique to obtain LST measurements at regional and
50 global scales. Currently, there are a number of LST products derived from TIR remote
51 sensing observations at different spatial scales and temporal periodicities. Examples are the
52 products generated from the Moderate Resolution Imaging Spectroradiometer (MODIS)
53 (Wan, 2008), the Atmospheric Infrared Sounder (AIRS) (Susskind et al., 2003), the Advanced
54 Spaceborne Thermal Emission and Reflection radiometer (ASTER) (Gillespie et al., 1998)
55 and the Meteosat Second Generation (MSG) Spinning Enhanced Visible and Infrared Imager
56 (SEVIRI) (PUM_LST, 2008).

57

58 The Advanced Along-Track Scanning Radiometer (AATSR) (Llewellyn-Jones et al., 2001)
59 onboard the European Space Agency (ESA) satellite Envisat provides an operational LST
60 product at 1 km² resolution, which is currently included in the Level 2 AATSR data
61 (ATS_NR_2P). The operational LST algorithm is also applied to predecessors ATSR-1 and
62 ATSR-2, then providing LSTs back to 1991. The AATSR has two on-board calibration
63 targets, low-noise detectors and mechanical coolers that provide high radiometric accuracy
64 and stability to the TIR data (better than 0.05 K for the 11 and 12 μm bands). Therefore
65 instrumental error in AATSR LST estimation will be very small. The conical scanning
66 mechanism of AATSR gives a dual-view of the Earth's surface, first in the forward view at

67 zenith angles about 55°, and 150 s later in the nadir view at zenith angles from 0° to 21.7°. The
68 nominal spatial resolution of AATSR is 1 km × 1 km in the nadir view and 1.5 km × 2 km in
69 the forward view, with a swath width of about 500 km. Equator crossing time is 10:00 a.m.
70 local time (descending node) and revisit time is about 3 days.

71

72 The operational AATSR LST product is based on the split-window technique using the 11
73 and 12 μm bands at nadir view (Prata, 2002a). Different sets of split-window coefficients are
74 used for 14 land cover classes or biomes predefined in a static classification map, and tuned
75 with monthly fractional vegetation cover maps based on climatology. Both classification and
76 fractional vegetation cover maps are implemented in the operational algorithm at spatial
77 resolution of 0.5°×0.5° in longitude and latitude. The generation of LST products involves the
78 correction of the satellite-observed radiances for atmospheric absorption and emission
79 (mainly due to water vapor) and non-unity of land surface emissivity. This is a challenging
80 problem because of the water vapor and surface emissivity variability. It is therefore
81 necessary to assess the accuracy and precision of the products to provide LST users with data
82 quality information. Long-term validation is required to identify possible deficiencies and
83 subsequently introduce improvements in the algorithms.

84

85 Since the launch of Envisat in 2002, the AATSR LST product has been validated with
86 concurrent ground LST measurements performed over homogeneous surfaces such as rice
87 fields with full vegetation cover in Valencia, Spain and inland waters in Lake Tahoe, USA
88 (Coll et al., 2005, 2006, and 2009a). For both sites, results showed that the product
89 overestimated the in situ LSTs by 3 to 4 K. The large LST errors were attributed to the spatial
90 resolution of the classification and fractional vegetation cover maps (0.5°), which is too coarse
91 to resolve the land surface heterogeneity at the AATSR 1 km² scale. Noyes et al. (2007a)

92 observed both positive and negative biases, with AATSR being typically warmer (colder) in
93 the summer (winter), which was attributed to the algorithm's sensitivity to atmospheric water
94 vapor, temperature and LST. In order to address the above problems, Noyes et al. (2007b)
95 proposed several modifications in the current operational algorithm.

96

97 The objective of this paper is to show the long-term accuracy assessment of AATSR derived
98 LSTs at the Valencia test site in the period 2002-2008. We checked not only the operational
99 LST product but also the impact of using more appropriate values for the auxiliary parameters
100 over the test site, and the performance of an alternative split-window algorithm with explicit
101 emissivity dependence applicable to AATSR (Galve et al., 2008). The overall aim of such
102 validations is to stress the need for modifications in the current AATSR LST processor.

103

104 Two types of validation methods were used in the present study. First, we show conventional
105 temperature-based (T-based) validation, where concurrent ground LST measurements were
106 directly compared with AATSR retrievals over homogeneous rice crops with full vegetation
107 cover, much in the same way as in Coll et al. (2005, 2006 and 2009a). Due to the dissimilarity
108 in the spatial scale between ground instruments and satellite measurements, only highly
109 homogeneous surfaces are suitable for T-based validation, which reduces the number of
110 biomes and climatic conditions available for a meaningful LST assessment. Therefore, we
111 propose the new radiance-based (R-based) method (Wan and Li, 2008) that has been used for
112 MODIS LST validation (Wan, 2008; Coll et al 2009b) and does not require ground LST
113 measurements. Instead, ground LSTs are calculated from satellite brightness temperatures
114 through radiative transfer simulations using surface emissivity data, and atmospheric
115 temperature and water vapor profiles. Since homogeneous sites in 10-13 μm emissivity are
116 more frequent than homogeneous sites in LST, the R-based method can be potentially applied

117 to a larger number of sites with different LST and atmospheric regimes. The R-based method
118 is not a validation method in strict sense, because it does not rely on independently measured
119 LSTs. However, it can be an alternative or complement to the T-based method when ground
120 LST measurements are not feasible.

121
122 The paper follows with a brief description of the operational AATSR LST algorithm and the
123 alternative explicit emissivity-dependent algorithm. In section 3, the T-based validation
124 results for full vegetation cover are presented and discussed. Section 4 shows the principles
125 and sensitivity analysis of the R-based method, and the validation results for two different
126 biomes (bare soil and lake). Finally, the main conclusions of the paper are presented in
127 section 5.

128

129 **2. LST RETRIEVAL FROM AATSR**

130 LST can be retrieved from AATSR brightness temperatures in the 11 and 12 μm bands, nadir
131 view using the split-window technique. The AATSR forward view is not used due to
132 difficulties in accounting for angular effects on temperature and emissivity, the different field
133 of view and the non-simultaneity of the two views, which may have an important impact over
134 heterogeneous land surfaces (Prata, 2002a; Coll et al., 2006). The application of split-window
135 algorithms requires that the characteristics of the surface must be well known. It can be done
136 through explicit dependence on surface emissivity data at the two bands considered (Becker
137 and Li, 1990; Wan and Dozier, 1996; Coll and Caselles, 1997). Another possibility is to
138 derive specific sets of algorithm coefficients for different land cover biomes weighted by
139 fractional vegetation cover (Kerr et al., 1992). The operational AATSR LST algorithm (Prata,
140 2002a) adopted the latter approach. Therefore it does not depend explicitly on emissivity, but
141 accounts implicitly for surface emissivity effects through biome-dependent coefficients and

142 fractional vegetation cover. The operational algorithm is described next and an alternative
143 algorithm with explicit emissivity dependence is presented in section 2.2.

144

145 *2.1. Operational AATSR LST algorithm*

146 The algorithm expresses the LST (T) as a nearly-linear combination of the brightness
147 temperatures in the 11 and 12 μm bands, T_{11} and T_{12} , with coefficients determined by
148 regression over simulated brightness temperatures and depending on the biome (i), the
149 fractional vegetation cover (f), the precipitable water (W) and the satellite zenith viewing
150 angle (θ):

$$151 \quad T = a_{f,i,W} + b_{f,i}(T_{11}-T_{12})^n + (b_{f,i} + c_{f,i})T_{12} \quad (1)$$

$$152 \quad a_{f,i,W} = 0.4[\sec(\theta)-1]W + f a_{v,i} + (1-f) a_{s,i}$$

$$153 \quad b_{f,i} = f b_{v,i} + (1-f) b_{s,i}$$

$$154 \quad c_{f,i} = f c_{v,i} + (1-f) c_{s,i}$$

$$155 \quad n = 1/\cos(\theta/5)$$

156 Coefficients a , b , and c of Eq. (1) were determined for 13 land biomes defined in Dorman and
157 Sellers (1989) plus a lake class ($i=1$ to 14), and are shown in Table 1 (Prata, 2002b). For each
158 land cover biome, two separate sets of coefficients are specified for the fully vegetated surface
159 (subscript v) and for the bare surface (subscript s), which are weighted by the fractional
160 vegetation cover f . For some biomes ($i=4, 7, 9, 10, 12, 13$, and 14), coefficients are identical
161 for the vegetated and bare surface, which makes the algorithm insensitive to f . For the lake
162 class, different coefficients are given for day and night. In Eq. (1), all temperatures are in $^{\circ}\text{C}$.

163

164 Since the algorithm only uses the nadir view ($\theta < 21.7^{\circ}$), the impact of W on the LST
165 calculated from Eq. (1) is rather small, e.g., a LST difference < 0.03 K for a W variation of 1

166 cm. For the same reason, coefficient n is close to unity and the algorithm is nearly linear on
167 $T_{11}-T_{12}$. Given that $1 < n < 1.0029$, the difference with the LST derived using $n=1$ in Eq. (1) is
168 between 0 and 0.03 K for $T_{11}-T_{12}=3$ K. Similarly, the impact of θ in the algorithm, both
169 through coefficients $a_{f,i,w}$ and n , is small. Taking $\theta=0^\circ$ instead of the correct angle yields
170 differences in the calculated LST less than 0.06 K for $W=3$ cm.

171

172 The ancillary data necessary for the application of the algorithm (i , f and W) are tabulated at
173 spatial resolution of $0.5^\circ \times 0.5^\circ$ in longitude/latitude. Land biomes are determined from global
174 classification and are static. The fractional vegetation cover has monthly variability, and is
175 obtained from Dorman and Sellers (1989) and an estimate of the “greenness” derived from
176 global normalized difference vegetation index from the International Satellite Land-Surface
177 Climatology Project (ISLSCP). Precipitable water data are taken from the NASA Water
178 Vapor Project (NVAP) global climatology at monthly intervals. The target accuracy of the
179 LST product is ± 1.0 K at nighttime and ± 2.5 K at daytime. For more details on the algorithm
180 and the operational implementation see Prata (2002a).

181

182 As pointed out in previous validation studies (Coll et al., 2005, 2006, and 2009a), the 0.5°
183 resolution of the ancillary data is too coarse to account for the natural heterogeneity of LST at
184 the AATSR scale. Noyes et al. (2007b) and Coll et al. (2009a) also noted the high sensitivity
185 of the LST retrievals to the fractional vegetation cover. Noyes et al. (2007b) proposed to
186 increase the resolution of the biome and f maps to $1-3 \text{ km}^2$, to use the GLOBCOVER biome
187 map derived from Envisat/Medium Resolution Imaging Spectrometer (MERIS), and to
188 increase the accuracy of the fractional cover by introducing an observational component, e.g.,
189 estimating f by using vegetation indices derived from the AATSR optical bands.

190

191 2.2. *Explicit emissivity-dependent LST algorithm*

192 As an alternative, the split-window method can be applied with algorithms explicitly
193 dependent on the surface emissivity at the 11 and 12 μm AATSR bands, namely the mean
194 emissivity ($\epsilon=(\epsilon_{11}+\epsilon_{12})/2$) and the band emissivity difference ($\Delta\epsilon=\epsilon_{11}-\epsilon_{12}$), which are the
195 physical magnitudes accounting for the effect of land surface biome and fractional vegetation
196 cover on TIR measurements. This is the approach adopted by the generalized split-window
197 algorithm (Wan and Dozier, 1996) used to generate the MODIS LST products MOD11_L2
198 (Terra) and MYD11_L2 (Aqua) (Wan, 2008), and by the MSG-SEVIRI LST product
199 (PUM_LST, 2008). This approach is feasible since the emissivity values of natural surfaces at
200 10-13 μm show relatively small variability at global scale. According to Pinheiro et al.
201 (2004), ϵ and $\Delta\epsilon$ range from 0.968 to 0.990 and from -0.014 to 0.009, respectively, for the
202 Advanced Very High Resolution Radiometer (AVHRR) bands 4 and 5, which are comparable
203 to the AATSR bands. Similarly, Snyder et al. (1998) found ϵ varying from 0.969 to 0.990 and
204 $\Delta\epsilon$ from -0.006 to 0.011 for the MODIS split-window bands 31 and 32. However, the
205 sensitivity of LST to these small emissivity changes can be large (typically ± 0.8 K for
206 uncertainty of ± 0.010 in both ϵ_{11} and ϵ_{12} ; Galve et al., 2008).

207

208 The explicit emissivity-dependent split-window algorithm proposed here is based on the
209 model of Coll and Caselles (1997) particularized for AATSR as described in Galve et al.
210 (2008). It can be written as

$$\begin{aligned} 211 \quad T = T_{11} + 0.02 + 0.782(T_{11}-T_{12}) + 0.302(T_{11}-T_{12})^2 + \\ 212 \quad + (1-\epsilon)[53+1.13(W/\cos\theta)-1.023(W/\cos\theta)^2] - \Delta\epsilon[79-11.06(W/\cos\theta)] \end{aligned} \quad (2)$$

213 The algorithm coefficients were obtained from radiative transfer simulations of AATSR
214 brightness temperatures using a database of 382 continental, cloud-free radiosonde profiles

215 with global coverage and precipitable water up to 6 cm (Galve et al., 2008). The quadratic
216 dependence on $T_{11}-T_{12}$ accounts for the increase of the atmospheric attenuation for large
217 amounts of atmospheric water vapor. The algorithm depends explicitly on precipitable water
218 in the emissivity terms only; however, the impact of W in LST is small (typically less than 0.1
219 K for a variation of 0.5 cm in W). Eq. (2) does not take into account directional temperature
220 and emissivity effects, which are expected to be small in the nadir view of AATSR ($\theta < 21.7^\circ$).
221 In Eq. (2), temperatures can be either in K or $^\circ\text{C}$.

222

223 Since emissivity only appears explicitly in the last two terms of the right-hand side of Eq. (2),
224 it seems that atmospheric and emissivity effects are separated in the LST retrieval. However,
225 it should be noted that emissivity effects are also implicit in the “non-emissivity” or
226 “atmospheric” part of Eq. (2) through the brightness temperature T_{11} and the temperature
227 difference $T_{11}-T_{12}$, which are determined by both the atmosphere and the surface emissivity.
228 For surfaces where $\Delta\varepsilon$ is positive (negative), $T_{11}-T_{12}$ is larger (smaller) than it would be for
229 the same atmosphere over a black-body. Therefore, when $T_{11}-T_{12}$ is multiplied by
230 “atmospheric” coefficients in Eq. (2), there is an over or under-correction of atmospheric
231 effects depending on the sign of $\Delta\varepsilon$. The over or under-correction induced by emissivity is
232 compensated by the corresponding emissivity term in Eq. (2). Similarly, emissivity effects on
233 T_{11} are also accounted for by the emissivity terms. Note that the theoretical definitions of the
234 “emissivity” coefficients contain the “atmospheric” coefficients (see Eq. 5 and 6 of Coll and
235 Caselles, 1997)

236

237 The critical issue for the application of the algorithm is the need of accurate emissivity maps
238 as ancillary data. For the present study, emissivity maps were derived using the vegetation
239 cover method (Valor and Caselles, 1996), which is based on a physical surface model and

240 estimations of fractional vegetation cover through spectral indices. In this method, the
241 emissivity in band k is estimated through the relationship:

$$242 \quad \epsilon_k = \epsilon_{kv} f + \epsilon_{kg} (1-f) + 4 \langle d\epsilon_k \rangle f (1-f) \quad (3)$$

243 where ϵ_{kv} and ϵ_{kg} are the vegetation and ground emissivity, respectively, $\langle d\epsilon_k \rangle$ is the
244 maximum cavity term, and f is the fractional vegetation cover. The cavity term accounts for
245 the effect of radiance internal reflections between the different components of a structured and
246 rough surface (Caselles and Sobrino, 1989).

247

248 Since ϵ_{kv} , ϵ_{kg} and $\langle d\epsilon_k \rangle$ depend on the surface type, they were obtained by combining the
249 Advanced Spaceborne Thermal Emission and Reflection Radiometer (ASTER) Spectral
250 Library (Baldrige et al. 2009) and the GLOBCOVER (GLC) global classification (Bicheron
251 et al., 2008). The ASTER Spectral Library is the most extensive published dataset of TIR
252 reflectance spectra including both natural (soils, rocks, vegetation, minerals) and manmade
253 (asphalt, tar, concrete, brick, tile) materials. The GLC biome map provides the global
254 classification with best spatial resolution (300 m) to date, which is one of the key factors to
255 improve classification accuracy (Herold et al., 2008; Heiskanen, 2008). It is generated from
256 MERIS data (with reasonably good spectral resolution) using an unsupervised classification
257 regional expert-tuned procedure similar to the predecessor GLC2000 classification
258 (Bartholomé and Belward 2005), and is compatible with the standardized legend of the United
259 Nations Food and Agriculture Organization Land Cover Classification System (LCCS). It
260 should be noted that the approach used here for modeling surface emissivity based on land
261 surface classes and fractional vegetation cover is similar to that used by the operational
262 AATSR LST algorithm to define the coefficients of Eq. (1).

263

264 Surface type maps were derived from GLC data. Each GLC surface type was assigned an
265 emissivity class depending on the soil and vegetation type contained and the surface structure
266 (see Table 2), and then the vegetation and ground emissivities for each class were estimated
267 from the ASTER Spectral Library data. Using this procedure, the initial 22 classes (and
268 associated subclasses) were reduced to only 10 classes, taking into account the components
269 included in each class and the similarity between surface structures (Table 2).

270

271 Table 3 gives the corresponding ϵ_{kv} , ϵ_{kg} and $\langle d\epsilon_k \rangle$ values for Eq. (3), or alternatively effective
272 emissivity values, for each class. For the case of vegetated surfaces, classes were grouped
273 attending to structure (low grasses/crops, shrubs/trees lower than 5 m, shrubs/trees higher than
274 5 m), background (soil or water depending on flooding conditions), and vegetation type
275 (green grasses, evergreen or deciduous shrubs/trees). In each case, the emissivity values for
276 vegetation and ground (or water) were calculated using the emissivity spectra of the samples
277 given in the ASTER Spectral Library. The spectra were first convolved with the AATSR
278 spectral response curves for the 11 and 12 μm bands to get the band emissivity values. These
279 values were then averaged for the selected samples. In the case of soils, all samples available
280 in the library (52) were used, which showed low variability in these bands (standard deviation
281 smaller than ± 0.005). There are only four vegetation samples. The green grass sample was
282 used for classes 1 and 3, the average between conifer and deciduous samples for classes 2 and
283 4, the conifer sample for class 6, and the deciduous sample for class 5. Rocks were excluded
284 since they should not be usual in these surface types.

285

286 For vegetated surfaces with a significant structure (emissivity classes 2, 4, 5 and 6) the
287 maximum cavity term was determined with a simulation procedure. According to Caselles
288 and Sobrino (1989), the cavity term for nadir observation is given by $d\epsilon_k = (1 - \epsilon_{kg})\epsilon_{kv}F(1-f)$,

289 where F is a shape factor that depends on the height and separation between the surface
 290 elements, and considers the energy transmission between them. The cavity term was
 291 simplified and parameterized in terms of fractional vegetation cover only and a maximum
 292 cavity term ($\langle d\epsilon_k \rangle$ in Eq. 3) that represents the maximum value for a given surface geometry
 293 with f ranging from 0 to 1 (Valor and Caselles, 1996). The cavity term was calculated for
 294 different geometric structures, using the vegetation and ground/water emissivities obtained
 295 above, and for fractional vegetation cover ranging from 0 to 1. The maximum value for each
 296 case was selected. Then, the average of the maximum values was calculated for each class,
 297 resulting in the $\langle d\epsilon_k \rangle$ values given in Table 3.

298

299 In the case of non-vegetated surfaces, such as bare rock, water, or snow and ice, average
 300 values were calculated from the samples provided by the ASTER Spectral Library (389 rock
 301 samples, 2 water samples and 4 snow and ice samples), and a unique effective value for each
 302 AATSR band was calculated. Certainly, rock emissivities show high standard deviations, and
 303 probably it would be necessary to distinguish them using additional rock maps. Finally,
 304 effective emissivity values were calculated for urban areas using the spectra for manmade
 305 materials (tiles, asphalt, concrete, etc.) and considering regular city structures.

306

307 Fractional vegetation cover required in Eq. (3) was calculated from normalized difference
 308 vegetation index (NDVI) and reflectance values in AATSR red (0.66 μm) and near infrared
 309 (0.87 μm) bands using the following relationship (Valor and Caselles, 1996):

$$310 \quad f = \frac{\left(1 - \frac{\text{NDVI}}{\text{NDVI}_s}\right)}{\left(1 - \frac{\text{NDVI}}{\text{NDVI}_s}\right) - K \left(1 - \frac{\text{NDVI}}{\text{NDVI}_v}\right)} \quad (4)$$

311 where NDVI is the pixel vegetation index, $NDVI_s$ and $NDVI_v$ are the index values for bare
312 soil and full vegetation, and factor K is

$$313 \quad K = \frac{\rho_{2v} - \rho_{1v}}{\rho_{2s} - \rho_{1s}} \quad (5)$$

314 where ρ_{1v} and ρ_{2v} are respectively the red and near infrared reflectance values over full
315 vegetation, and ρ_{2s} and ρ_{1s} are the corresponding reflectances over bare soil. All these
316 coefficients can be extracted from the AATSR scene itself. As an example, Figure 1 shows
317 mean emissivity ($\varepsilon=(\varepsilon_{11}+\varepsilon_{12})/2$) and band emissivity difference ($\Delta\varepsilon=\varepsilon_{11}-\varepsilon_{12}$) maps derived for
318 the Eastern part of Spain using two AATSR scenes acquired on March and July, 2007. In
319 order to minimize the impact of cloud cover, the procedure can be repeated for several dates
320 along the year to produce monthly emissivity composites at regional or global scales.

321

322 **3. T-BASED VALIDATION**

323 The T-based method for satellite LST validation is the direct comparison with ground
324 measurements performed at a field site concurrently with the satellite overpass. Thus, it
325 provides an independent evaluation of the radiometric quality of the satellite instrument
326 together with the ability of the LST retrieval algorithm to correct for atmospheric and
327 emissivity effects. However, it is necessary that the LST observed by the ground instruments
328 at several points over the test site is truly representative of the average LST over the
329 instantaneous field of view of the satellite sensor, for which the site must be thermally
330 homogeneous from the point scale to several kilometers. Since most of the Earth's surface is
331 heterogeneous at these spatial scales, high-quality ground validation data are limited to few
332 biomes such as lakes, silt playas, grasslands and agricultural fields collected during dedicated
333 campaigns (Wan et al., 2002 and 2004; Coll et al., 2005). An exception is the Lake Tahoe

334 automated validation site (Hook et al., 2007), where lake surface temperatures are
335 continuously measured since 1999.

336

337 A homogeneous site for LST validation was established in a large ($>30 \text{ km}^2$), flat area of rice
338 fields close to Valencia, Spain since 2002. In July and August, rice crops are well irrigated
339 and attain nearly full vegetation cover (see Figure 2). It makes the site highly homogeneous in
340 terms of both surface temperature and emissivity and eases the radiometric measurement of
341 LST. Ground data from the Valencia test site have been used in previous studies (Coll et al.,
342 2005, 2006, 2007 and 2009a). The daytime thermal homogeneity of the site was assessed with
343 AATSR and MODIS data at $1 \times 1 \text{ km}^2$, and with ASTER TIR data at $90 \times 90 \text{ m}^2$. Results
344 showed typical variability (standard deviation) ranging from 0.2 to 0.5 K depending on the
345 spatial resolution.

346

347 Several TIR radiometers were distributed over a 1 km^2 grid to measure the ground LST and its
348 variability concurrent to AATSR daytime overpasses (10:20-10:40 UTC). The instruments
349 were two CIMEL CE 312-1 radiometers with four bands (8.0-13.3 μm , 11.5-12.4 μm , 10.2-
350 11.3 μm , and 8.3-9.3 μm) (Brogniez et al., 2003), one CIMEL CE 312-2 radiometer with six
351 bands (8.0-13.3 μm , 8.3-8.6 μm , 8.5-8.9 μm , 9.0-9.3 μm , 10.2-11.0 μm , and 10.9-11.7 μm),
352 and two Everest model 112.2L thermometers (8-13 μm) (www.everestinterscience.com). The
353 instruments were calibrated against a reference blackbody before and after each field
354 measurement day and intercompared in the field. The ground LSTs were calculated by
355 averaging the ground temperatures measured by the available radiometers within three
356 minutes centered on the satellite overpass time. The standard deviation of the ground
357 temperatures was calculated as a measure of the spatial and temporal variability of LST

358 (typically ≤ 0.5 K). More details on the ground LST measurements can be found in Coll et al.
359 (2005 and 2006).

360

361 Radiometric temperatures were corrected for emissivity effects, including the reflection of the
362 sky irradiance. Surface emissivity was measured in the field using the box method (Rubio et
363 al., 2003) for the four channels of the CE 312-1 radiometers. The CE 312-1 channels at 10.2-
364 11.3 and 11.5-12.4 μm are similar to the AATSR bands at 11 and 12 μm , respectively. A total
365 of 30 emissivity measurements were taken at different spots on the test site for each channel.
366 More details on the field emissivity measurements are given in Coll et al. (2007). We
367 obtained uniform and high emissivity values ($\epsilon=0.985\pm 0.005$) with small spectral variation in
368 the 8-13 μm range, as expected for full vegetation cover.

369

370 Together with the average ground LST, we estimated the total uncertainty including the
371 radiometer calibration error, the emissivity correction error (~ 0.2 K for measured emissivity
372 uncertainty of 0.005), and the LST variability. A total of 28 cloud-free, daytime concurrences
373 of ground and AATSR data were collected in July and August, 2002-2007. Table 4 lists the
374 ground LST (T_g) and uncertainty for each case. The center of the 1 km^2 grid was at
375 $0^\circ 17' 50'' \text{W}$, $39^\circ 14' 27'' \text{N}$ in 2002-2003; $0^\circ 17' 43'' \text{W}$, $39^\circ 15' 01'' \text{N}$ in 2004; and $0^\circ 18' 28'' \text{W}$,
376 $39^\circ 15' 54'' \text{N}$ in 2005-2007. For each case, we extracted the concurrent AATSR brightness
377 temperatures in the 11 and 12 μm bands, nadir view from L1b scenes (ATS_TOA_1P,
378 georeferenced, top of atmosphere data). We used arrays of 3×3 pixels centered on the
379 measurement site, for which the average value was calculated (see Table 4). The standard
380 deviation of T_{11} and T_{12} for the 3×3 pixels was typically 0.1 K.

381

382 For each validation case, Table 4 shows the AATSR-derived LST (T_{AATSR}) as obtained from:

383

384 (i) The operational LST product in the AATSR Level 2 data. It is the result of applying Eq.
385 (1) with the operational classification and fractional vegetation cover maps. The Valencia test
386 site is classified as biome $i=6$ (broadleaf trees with ground cover) and the assigned f value is
387 0.40-0.47 in July-August. The data in Table 4 are the average for 3×3 pixels centered on the
388 site.

389

390 (ii) The optimized AATSR algorithm, in which we assigned biome $i=8$ (broadleaf shrubs with
391 ground cover) and $f=1$ (full vegetation cover) in Eq. (1) for application to the brightness
392 temperatures in Table 4. This selection of i and f yields the best agreement of LSTs derived
393 from Eq. (1) with the ground data (Coll et al., 2009a).

394

395 (iii) The explicit emissivity-dependent algorithm (Eq. 2) applied to the brightness
396 temperatures using the emissivity values obtained from Eq. (3) ($\epsilon=0.986$ and $\Delta\epsilon=-0.005$ at the
397 site, with $f=0.91$, emissivity class 1, and GLC class 11) and the mean precipitable water for
398 July and August (2.5 and 2.7 cm, respectively) as obtained from the National Centers for
399 Environmental Prediction (NCEP) global tropospheric analyses product (Kalnay et al., 1996).

400

401 Figure 3 shows the comparison between T_{AATSR} and T_{g} , and Figure 4 plots the LST error
402 $\delta T = T_{\text{AATSR}} - T_{\text{g}}$ as a function of time for the three options of LST retrieval. The operational
403 LST product clearly overestimated the ground LST by 2 to 5 K depending on the validation
404 case. For the 28 cases, the average value of δT or bias was 3.6 K with standard deviation of
405 0.7 K. However, the optimized AATSR algorithm and Eq. (2) agreed very well with each
406 other and with the ground LSTs, δT values ranging between -1.0 and +1.0 K for most of the
407 cases. In Figure 3, the correlation coefficient (R) between T_{AATSR} and T_{g} is 0.88 for the

408 optimized algorithm and 0.90 for Eq. (2). For the optimized algorithm the average bias was
409 0.2 K and the standard deviation was 0.5 K, yielding $rmse=\pm 0.5$ K, while for Eq. (2) the bias
410 was 0.4 K, and the standard deviation was 0.5 K ($rmse=\pm 0.6$ K). Although the validation
411 cases are few, covering one surface type with limited atmospheric and LST variability, the
412 results show the good accuracy achievable with AATSR data. On the other hand, Figure 4
413 suggests that the positive bias in AATSR LSTs is slightly increasing in the 2006 and 2007
414 campaigns. This effect may be due to the small number of validation cases available for the
415 last two years, and it will be investigated in forthcoming field campaigns.

416

417 The large overestimation given by the operational LST product is due to incorrect
418 classification and fractional vegetation cover assigned to the test site. Using the same biome
419 ($i=6$) but setting $f=1$ in Eq. (1), the AATSR algorithm would yield better agreement with the
420 ground data (δT between 0.4 and 2.4 K, average bias of 1.4 K). As an alternative to the
421 AATSR classification, Noyes et al. (2007b) considered high-resolution (1 km) global biome
422 classification maps such as those from the University of Maryland (UMD) (Hansen et al.,
423 2000) and the International Geosphere-Biosphere Project (IGBP) (Loveland et al., 1998). The
424 Valencia site is classified as cropland in both cases, which corresponds to AATSR biome 12
425 (broadleaf-deciduous trees with winter wheat). Using $i=12$ and $f=1$ in Eq. (1), the AATSR-
426 derived LSTs overestimated the ground LSTs by a range from 1.2 to 3.3 K for the 28
427 validation cases, with average bias of 2.3 K.

428

429 Excluding the optimized algorithm mentioned above ($i=8$, $f=1$), the best agreement with the
430 ground LST was obtained for vegetation biomes 2 (broadleaf deciduous trees), 3 (broadleaf
431 and needleleaf trees) and 5 (needleleaf-deciduous trees) using $f=1$, resulting in biases of -0.3,
432 -0.4 and 0.5 K, respectively. Other vegetation biomes (e.g., 1, 4, 9, 10 and 12 in Table 1)

433 yielded large positive biases (2.3-2.5 K) even with $f=1$. In terms of surface emissivity, all the
434 above fully-vegetated biomes should be quite similar, with ϵ and $\Delta\epsilon$ values close to those used
435 for the Valencia site and thus the retrieved LSTs should be similar. However, they produce
436 rather different LST estimates showing the high sensitivity of the AATSR LST algorithm to
437 the biome assignment. Noyes et al. (2007b) also noted a high sensitivity of the algorithm to
438 the fractional vegetation cover. For comparison, an uncertainty of ± 0.005 in both ϵ_{11} and ϵ_{12}
439 results in an LST uncertainty of ± 0.5 K in the explicit emissivity-dependent algorithm (Eq. 2).

440

441 **4. R-BASED VALIDATION**

442 The R-based method (Wan and Li, 2008) does not require ground LST measurements and
443 thus provides an alternative for satellite LST validation over a wide range of biomes and LST
444 and atmospheric regimes. The ground temperatures are calculated from radiative transfer
445 simulations using at-sensor brightness temperatures in the 11 μm band, near concurrent
446 atmospheric temperature and water vapor profiles and surface emissivity measurements. As
447 mentioned above, emissivity in AATSR bands at 11 and 12 μm is high and exhibits small
448 variations for most land cover biomes, so the R-based method could be applied, with care,
449 globally. In this study, radiative transfer simulations were performed using the MODTRAN 4
450 code (Berk et al., 1999). In the next section, the R-based method is described. In section 4.2,
451 the feasibility of the method is assessed through a comparison with ground LST
452 measurements and a sensitivity analysis is performed. R-based validation results for two new
453 biomes (bare soil and lake) are presented in section 4.3.

454

455 *4.1. Description of the R-based method*

456 The R-based method is physically based on the radiative transfer equation. For a surface at
 457 temperature T and with spectral emissivity ϵ_λ , the at sensor spectral radiance measured in
 458 band k at zenith viewing angle θ (L_k^{sen}) can be written as

$$459 \quad L_k^{\text{sen}} = \int_0^\infty f_k(\lambda) \left\{ [\epsilon_\lambda B_\lambda(T) + (1-\epsilon_\lambda) \frac{F_\lambda^\downarrow}{\pi}] \tau_\lambda(\theta) + L_\lambda^\uparrow(\theta) \right\} d\lambda \quad (6)$$

460 where $f_k(\lambda)$ is the normalized spectral response function of band k ($\int_0^\infty f_k(\lambda) d\lambda = 1$), B_λ is the
 461 Planck function for blackbody spectral radiance, τ_λ is the atmospheric transmittance, L_λ^\uparrow is
 462 the atmospheric radiance emitted towards the sensor, and F_λ^\downarrow is the downwelling sky
 463 irradiance (Lambertian reflection assumed). The brightness temperature, T_k , corresponding to
 464 the at-sensor radiance is defined as $L_k^{\text{sen}} = B_k(T_k)$, B_k being the band-averaged Planck function,

$$465 \quad B_k(T^*) = \int_0^\infty f_k(\lambda) B_\lambda(T^*) d\lambda \quad (7)$$

466 where T^* is a generic temperature. Using Eq. (7), look-up tables for T^* - $B_k(T^*)$ conversion
 467 can be generated for a given band at small temperature steps in order to calculate T_k from
 468 L_k^{sen} . Equation (6) is the basis of the so-called forward simulation, in which the at-sensor
 469 radiances or brightness temperatures are simulated from surface temperature and emissivity
 470 data, and atmospheric parameters (τ_λ , L_λ^\uparrow , and F_λ^\downarrow) calculated with MODTRAN 4 from
 471 temperature and water vapor profiles. Similarly, Eq. (6) can also be used for inverse
 472 simulation, that is, the calculation of surface temperature (T) from satellite T_k or L_k^{sen} . In this
 473 case, the right-hand side of Eq. (6) can be calculated iteratively for different T values until it
 474 agrees with the prescribed L_k^{sen} value.

475

476 The R-based method requires accurate temperature and water vapor profiles representing the
 477 actual atmospheric conditions at the time of the satellite observation. The accuracy of the

478 atmospheric profiles can be assessed with the test suggested by Wan and Li (2008), which
479 involves the calculation of $\delta(T_{11}-T_{12})=(T_{11}-T_{12})_{obs}-(T_{11}-T_{12})_{sim}$, that is, the difference between
480 the $T_{11}-T_{12}$ value observed by AATSR and the $T_{11}-T_{12}$ value simulated from the atmospheric
481 profiles and the surface emissivity data. The test relies on the fact that the atmospheric effect
482 is larger at 12 μm , owing to the water vapor continuum absorption. Then $T_{11}-T_{12}$ is usually
483 positive and increases with the atmospheric water vapor. When the atmospheric profile used
484 for the R-based LST calculation is over (under) correcting the atmospheric effect, then $\delta(T_{11}-$
485 $T_{12})<0$ (>0) since the calculated, profile based $T_{11}-T_{12}$ value is larger (smaller) than the actual
486 AATSR value. Therefore, $\delta(T_{11}-T_{12})$ should be close to zero when the atmospheric profiles
487 used in simulations represent the real atmospheric conditions and the effect of the surface
488 emissivity uncertainties is small. The R-based method can be summarized as follows:

489

490 a) Calculation of the R-based in situ LST (T_{R-b}) from the 11 μm band at-sensor radiance using
491 atmospheric profiles and surface emissivity data (inverse simulation). The 11 μm band is used
492 because it is less affected by variations in atmospheric water vapor and temperature. The LST
493 error (δT) is the difference between the product LST and T_{R-b} .

494

495 b) Calculation of brightness temperatures in bands at 11 and 12 μm using T_{R-b} as ground LST,
496 atmospheric profiles and surface emissivity data (direct simulation). The difference $\delta(T_{11}-T_{12})$
497 between the actual and the simulated $T_{11}-T_{12}$ value is obtained. Note that the brightness
498 temperature T_{11} simulated here is equal to the measured T_{11} used in step a). Thus, $\delta(T_{11}-T_{12})$
499 is equal to the difference between the simulated and the measured brightness temperature T_{12} .
500 Since the 12 μm band is not used in the T_{R-b} calculation, it provides an independent
501 assessment of the atmospheric profiles.

502

503 A good knowledge of the spectral emissivity of the site is necessary for the application of the
504 method. It should be applied over long time periods at each site to analyze the relationship
505 between δT and $\delta(T_{11}-T_{12})$ and select the cases with $\delta(T_{11}-T_{12})$ values around zero for which
506 the error introduced by the atmospheric profiles is small.

507

508 *4.2. Feasibility and sensitivity analysis of the R-based method*

509 In order to show the feasibility of the R-based method, we compared the ground LSTs derived
510 from radiative transfer simulations with concurrent, ground-measured LSTs. Two ground LST
511 datasets were used. (1) The Valencia data shown in Table 4 corresponding to full vegetation
512 cover, with LSTs ranging from 25 to 31 °C and W ranging from 2 to 4 cm. (2) A set of 99
513 ground measurements of lake surface temperature from Lake Tahoe, USA (Hook et al., 2007)
514 concurrent to AATSR overpasses in 2002 and 2003, both daytime and nighttime, which have
515 been used previously in Coll et al. (2009a). Cloud-free conditions were ensured by means of a
516 statistical cloud masking algorithm (any scenes with a mean <4.4 °C and/or a standard
517 deviation >0.44 K were excluded). For the Lake Tahoe data, surface temperature ranges from
518 7 to 22 °C, and W from 0.2 to 2 cm. Therefore, the two datasets cover a wide range of LST
519 and atmospheric conditions. Moreover, the two sites are homogeneous in terms of emissivity
520 with well-known emissivity values based on ground measurements ($\epsilon_{11}=0.985$ and $\epsilon_{12}=0.980$
521 for the rice fields) or spectral libraries ($\epsilon_{11}=0.991$ and $\epsilon_{12}=0.985$ for water; Baldrige et al.,
522 2009), which facilitates the application of the R-based method.

523

524 For the Valencia site, we used three types of atmospheric profiles. Radiosonde balloons were
525 launched at the test site near-concurrently with AATSR overpasses for 5 cases (cases 16, 19,
526 21, 23, and 27 in Table 4). Since local radiosondes measurements are seldom and limited to
527 dedicated campaigns, we also used the NCEP global tropospheric analyses product (Kalnay et

528 al., 1996), which provides global atmospheric data at $1^\circ \times 1^\circ$ grids at 00:00, 06:00, 12:00 and
529 18:00 UTC. For each case in Table 4, the NCEP profiles for the four grids closest to the site
530 and the two times closest to the overpass were linearly interpolated to obtain the NCEP
531 profile at the site and the overpass time. Finally, we also used atmospheric profiles derived
532 from the Aqua/AIRS instrument (Susskind et al., 2003) with spatial resolution of 45 km and
533 overpass time at the site between 12:30 and 13:30 UTC. AIRS profiles were available for 16
534 cases in Table 4 (10-12, 14, 16-23, and 25-28). For the Lake Tahoe dataset, we only used
535 spatially and temporally interpolated NCEP atmospheric profiles for the 99 validation cases.

536

537 The profiles were entered in MODTRAN 4 to calculate the atmospheric transmittance and
538 emitted upwelling and downwelling radiances. Using Eq. (6), we calculated the ground LST
539 (T_{R-b}) from the corresponding brightness temperature T_{11} , and the difference $\delta(T_{11}-T_{12})$ for
540 each case. Figure 5 plots the difference between the ground-measured LSTs and the R-based
541 LSTs ($\delta T = T_g - T_{R-b}$) against $\delta(T_{11}-T_{12})$ for all the sites and atmospheric profiles considered (49
542 cases in Valencia and 99 in Lake Tahoe). For all datasets, a close relationship ($R=0.91$) is
543 observed between δT and $\delta(T_{11}-T_{12})$, with large positive (negative) values of δT
544 corresponding to large positive (negative) values of $\delta(T_{11}-T_{12})$, and small LST errors
545 associated with a narrow range of $\delta(T_{11}-T_{12})$ values in the vicinity of zero. The correlation is
546 slightly higher for the Lake Tahoe dataset alone because the uncertainties in the ground LST
547 measurements and the water emissivity are smaller than in Valencia, as well as the
548 precipitable water.

549

550 For most of the cases with local radiosondes, the δT and $\delta(T_{11}-T_{12})$ values were relatively
551 small, showing that the atmospheric profiles were accurate. The NCEP profiles provided
552 large, negative values of δT and $\delta(T_{11}-T_{12})$ in some cases, meaning that the simulations

553 overestimated the atmospheric effect. For other cases, however, the NCEP profiles yielded
554 accurate results with δT and $\delta(T_{11}-T_{12})$ close to zero. Most of the cases with AIRS profiles
555 resulted in large, positive δT and $\delta(T_{11}-T_{12})$ values. The bad performance of AIRS profiles
556 may be due to the temporal gap between Envisat and Aqua (2-3 h.), and the coarse spatial
557 resolution of AIRS data (45 km). The data in Figure 5 correspond to a wide set of LST and
558 atmospheric regimes and cover wide ranges of δT and $\delta(T_{11}-T_{12})$. The linear regression for all
559 data yields $\delta T = 1.78 \times \delta(T_{11}-T_{12}) + 0.02$. From it, we can obtain $-0.6 \text{ K} < \delta(T_{11}-T_{12}) < 0.6 \text{ K}$ as the
560 condition for which the error in the calculated R-based LST is within $\pm 1.0 \text{ K}$.

561

562 The data in Figure 5 are affected by uncertainties in both the ground LSTs and the radiative
563 transfer calculations involved in the R-based method. A sensitivity analysis was performed to
564 assess the accuracy of the simulated T_{R-b} and $T_{11}-T_{12}$ values using the radiosonde profile of
565 case 16 as a representative case ($W=2.5 \text{ cm}$). The effect of atmospheric uncertainties was
566 simulated in two ways. First, the water vapor mixing ratio was increased by 10% at each
567 profile level. Second, the air temperature was increased by 1 K at each level. These changes
568 represent small temporal and spatial atmospheric variations or typical radiosonde errors.
569 Table 5 shows the effect of the atmospheric variations on T_{R-b} (inverse simulation), T_{11} , T_{12}
570 (forward simulation) and the difference $T_{11}-T_{12}$. Atmospheric effects on T_{11} and T_{12} have the
571 same sign, so they cancel in part in $T_{11}-T_{12}$. The uncertainty in the MODTRAN 4 code was
572 assumed as the root square sum (rss) of the errors due to the water vapor and air temperature
573 changes.

574

575 We assumed an uncertainty of 0.005 in ϵ_{11} and ϵ_{12} , which is justified for vegetated surfaces
576 and is a typical uncertainty in field emissivity measurements (Rubio et al., 2003). However,
577 larger uncertainties may be expected for bare surfaces. For the present case, the resulting

578 uncertainty in the simulated temperatures is shown in Table 5. Emissivity uncertainties are
579 regarded as random and may have opposite signs in the two bands. For this reason, the
580 emissivity uncertainty in the simulated T_{11} - T_{12} is obtained as the rss of the errors in T_{11} and
581 T_{12} . Finally, the total uncertainty in the simulated temperatures is estimated as the rss of the
582 above atmospheric, MODTRAN 4 and emissivity errors, resulting in ± 0.7 K for T_{R-b} and ± 0.4
583 K for the simulated T_{11} - T_{12} .

584

585 NCEP and AIRS profiles may be less accurate than assumed in the previous uncertainty
586 analysis, thus the errors in the calculated T_{R-b} and T_{11} - T_{12} may be larger. To assess the
587 accuracy of the NCEP and AIRS profiles, we compared the five cases of the Valencia dataset
588 with local radiosondes with the same cases with NCEP and AIRS profiles. If we assume that
589 the local radiosondes represent accurately the atmospheric state, then the difference between
590 T_{R-b} calculated from radiosonde and NCEP/AIRS profiles is the LST error due to the incorrect
591 profile. Similarly, the difference between the radiosonde T_{11} - T_{12} and the corresponding
592 NCEP/AIRS value is the $\delta(T_{11}$ - $T_{12})$ difference due to the incorrect profile. Figures 6a and 6b
593 show the difference δT between radiosonde and NCEP/AIRS T_{R-b} values against the
594 precipitable water difference W_{rad} - $W_{NCEP/AIRS}$ and $\delta(T_{11}$ - $T_{12})$, respectively. δT shows a good
595 correlation ($R=0.82$) with the water vapor differences, with NCEP/AIRS overestimating
596 (underestimating) radiosonde T_{R-b} when NCEP/AIRS water vapor overestimated
597 (underestimated) radiosonde water vapor. Furthermore, the correlation between δT and $\delta(T_{11}$ -
598 $T_{12})$ is excellent ($R=0.94$) and shows a similar behavior as in Figure 5. The correlation in
599 Figure 6b is higher than in Figure 6a because the difference in the R-based LSTs depends not
600 only on the precipitable water difference but also on the difference in temperature profiles and
601 viewing angle, and all these effects are also largely reflected in $\delta(T_{11}$ - $T_{12})$.

602

603 The results of this section show that large errors in R-based LSTs are due to inappropriate
604 atmospheric profiles, and that the $\delta(T_{11}-T_{12})$ test may be used to select the profiles that
605 reasonably represent the actual atmosphere for the AATSR observation. Cases meeting the
606 condition $-0.6 \text{ K} < \delta(T_{11}-T_{12}) < 0.6 \text{ K}$ correspond to errors within $\pm 1.0 \text{ K}$ in the calculated in situ
607 LST, which is appropriate for LST validation. This condition was derived using ground
608 measured LSTs covering a wide range of conditions (Figure 5), and is compatible with the
609 preceding uncertainty analysis and the $\delta T - \delta(T_{11}-T_{12})$ relationship shown in Figure 6b.

610

611 *4.3. Application of the R-based method*

612 The R-based method was applied to two different biomes in the Valencia test site for a total of
613 47 cloud-free, daytime and nighttime AATSR scenes from March to early May in 2003-2008.
614 Cloud-free conditions were assessed by means of visual inspection and threshold tests using
615 $LST - T_{11}$, $T_{11} - T_{12}$, and the standard deviation of T_{11} . On these dates, rice fields are fallow and
616 the soil is left dry before the start of the growing season in mid May. Therefore the site
617 appears as a wide area of uniform, dry bare soil. As for the summer full-cover conditions, we
618 assessed the uniformity of the site with satellite data at different resolutions (AATSR and
619 MODIS at 1 km, ASTER and Landsat at $\sim 100 \text{ m}$) and field surveys. We tried to use the bare
620 soil for T-based validation, but preliminary tests showed that the ground-scale thermal
621 heterogeneity of the site was higher than for the full-vegetation case, and thus the ground
622 LSTs may not be accurate enough for AATSR LST validation. For this reason, we applied the
623 R-based method to the bare soil site using concurrent NCEP atmospheric profiles (local
624 radiosondes were not available), and laboratory emissivity measurements. Different samples
625 were taken from the site for mineralogy analysis, resulting in homogeneous composition of
626 14% sand, 35% clay, 4.5% organic matter and 44% carbonate (Mira et al., 2007). According
627 to the measurements (30 per channel), the soil emissivity was quite uniform with values

628 $\epsilon_{11}=0.957$ and $\epsilon_{12}=0.954$ (uncertainty of ± 0.005) for dry conditions (Mira et al., 2007).
629 Additionally, we applied the R-based method over the nearby Albufera Lake (about 7 km in
630 diameter, a few kilometers north of the rice fields site, see Fig. 2b) using the same AATSR
631 scenes and NCEP profiles, and taking $\epsilon_{11}=0.991$ and $\epsilon_{12}=0.985$ for water.

632

633 The AATSR viewing angle (θ) and brightness temperatures (T_{11} and T_{12}) for the bare soil and
634 lake cases are shown in Tables 6 and 7, respectively. These data are the average values for
635 3×3 pixels centered on the validation sites. In both Tables, we also show the AATSR-derived
636 LSTs (T_{AATSR}) using the three algorithms as in section 3: (i) the operational algorithm, which
637 assigns biome $i=6$ and $f=0.35-0.40$ in March-May for both sites; (ii) the optimized AATSR
638 algorithm selecting biome $i=11$ (bare soil) for the bare soil cases and $i=14$ -d/n (lake day/night)
639 for the lake cases; and (iii) the explicit emissivity-dependent algorithm (Eq. 2) using the
640 emissivity values derived from Eq. (3) ($\epsilon=0.974$ and $\Delta\epsilon=-0.007$ with $f=0.06$ for bare soil,
641 $\epsilon=0.988$ and $\Delta\epsilon=0.006$ for water) and the NCEP mean precipitable water for March-May (1.2-
642 1.9 cm). T_{AATSR} values from options (i) and (ii) are quite similar for the bare soil site (Table
643 6), with differences of a few tenths of K. For the lake site (Table 7), options (ii) and (iii) agree
644 very well with each other and differ by 1-4 K from option (i).

645

646 Table 8 shows the calculated R-based LST ($T_{\text{R-b}}$) and the difference $\delta(T_{11}-T_{12})$ for each bare
647 soil and lake validation case from Tables 6 and 7. The precipitable water obtained from the
648 NCEP profiles (W_{NCEP}) is also shown. When comparing each case, the differences between
649 $\delta(T_{11}-T_{12})$ values for bare soil and lake are relatively small (root mean square difference of
650 0.2 K), being compatible with the uncertainty due to small emissivity errors (most likely
651 affecting the soil). Nearly all the validation cases met the condition $-0.6 \text{ K} < \delta(T_{11}-T_{12}) < 0.6 \text{ K}$
652 derived in section 4.2. The outliers are marked with * in Table 8. This means that, for most

653 cases, the NCEP profiles provided a sufficiently accurate description of the atmosphere over
654 the site at the time of AATSR observations, and the R-based LSTs can be used for AATSR
655 LST validation. Figure 7 shows the AATSR LST error ($\delta T = T_{\text{AATSR}} - T_{\text{R-b}}$) against $\delta(T_{11} - T_{12})$
656 for the three algorithm options and the two sites. For all algorithms and sites, Figure 7 points
657 out a high correlation between δT and $\delta(T_{11} - T_{12})$, especially for algorithm (iii) in both sites,
658 and algorithm (ii) in the lake site. The relationship between δT and $\delta(T_{11} - T_{12})$ is similar as in
659 Figure 5, which gives confidence in the R-based results.

660

661 Considering only the δT values for the cases meeting the above $\delta(T_{11} - T_{12})$ condition, we
662 computed the average bias, standard deviation and rmse for each algorithm and site, which are
663 given in Table 9 together with the range of δT . Algorithm (iii) yielded the smallest LST errors
664 for both sites (rmse= ± 0.4 K), with δT values within ± 1.0 K for all cases. The optimized
665 algorithm (ii) resulted in small errors for the lake site (rmse= ± 0.5 K), in good agreement with
666 the T-based validation in Lake Tahoe shown in Coll et al. (2009a). For the bare soil site, LST
667 errors were still acceptable (rmse= ± 1.1 K) and generally met the target accuracy of the
668 AATSR algorithm (± 1.0 K at nighttime and ± 2.5 K at daytime). Again, the largest LST errors
669 were provided by the operational algorithm (i) for the lake cases because of the
670 misclassification of the site. However, results were better for bare soil (rmse= ± 1.3 K), with
671 similar LST errors as the optimized algorithm.

672

673 We did not find any significant long-term temporal variability in the R-based LST errors for
674 the data used in this section (2003-2008). Comparing the daytime and nighttime results, the
675 operational algorithm showed lower biases at nighttime, with rmse close to ± 1 K for both bare
676 soil and water. For the optimized algorithm over bare soil, the bias changed from 0.9 K at

677 daytime to -0.9 K at nighttime. For Eq. (2), no significant differences were found between
678 daytime and nighttime at both sites.

679

680 We observed a high dependence of the LST errors of the operational and the optimized
681 algorithm on the actual AATSR brightness temperature difference $T_{11}-T_{12}$, a magnitude that
682 plays a key role in the split-window algorithms (see Eqs. 1 and 2). $T_{11}-T_{12}$ is a function of
683 atmospheric precipitable water, but also depends on the temperature profile, LST, surface
684 emissivity and observation angle. Figure 8 plots the LST errors against $T_{11}-T_{12}$ for the three
685 algorithms over bare soil. It appears that AATSR LSTs based on Eq. (1) overestimate
686 (underestimate) the R-based LSTs for large (small) values of $T_{11}-T_{12}$, which suggests that
687 coefficients $b_{f,i}$ in Eq. (1) may be overestimated. For the algorithm of Eq. (2), the LST error
688 dependence on $T_{11}-T_{12}$ was much smaller. A few validation cases (32, 34, 38, 40 and 41, all
689 corresponding to nighttime in March) showed small values of $T_{11}-T_{12}$ (-0.05 to 0.13 K over
690 water, see Table 7) and T_{11} values close to the ground LST, which suggests that they may be
691 affected by near surface atmospheric temperature inversions (Platt and Prata, 1993).
692 According to the NCEP profiles, air temperatures at 100-135 m were 9 to 13 K warmer than
693 T_{11} in these cases. In these possible inversion conditions, Eq. (2) resulted still in reasonable
694 LST errors (biases of -0.5 K over water and -0.7 K over bare soil).

695

696 **5. CONCLUSIONS**

697 AATSR-derived LSTs were validated over the Valencia test site during the period 2002-2008.
698 Validation included the conventional T-based method over full-vegetated rice fields, and the
699 new R-based method (Wan and Li, 2008) over bare soil and lake. T-based validation provides
700 a direct assessment of the AATSR and algorithm performance since it relies on independently
701 measured ground LSTs. However, validation sites must be large enough, highly homogeneous

702 in surface temperature from ground to satellite scales, and equipped with accurate ground
703 radiometers for multiple spatial and temporal sampling in an area of at least 1 km². While it is
704 necessary to establish and maintain high-quality validation sites, the T-based method is not
705 suitable for the global validation of satellite LST products because of the large heterogeneity
706 of land surfaces.

707

708 The R-based method provides an alternative for the semi-operational, long-term validation
709 and diagnostics of the AATSR LST product at global scale. It could be applied over surfaces
710 with varied LST and atmospheric regimes where ground LST measurements are not feasible
711 (forests, partially vegetated surfaces, semi-arid areas, deserts, remote regions, etc.). Accurate
712 measurements of surface emissivities are necessary. The R-based method requires
713 atmospheric profiles representing adequately the atmospheric state at the time of the AATSR
714 observation. This can be checked with the $\delta(T_{11}-T_{12})$ test, which must be applied for each
715 atmospheric profile at each site in long periods of time to select a range of $\delta(T_{11}-T_{12})$ values
716 around zero for which the R-based ground LSTs are sufficiently accurate. In this paper, we
717 used spatially and temporally interpolated NCEP profiles for R-based validation over the
718 Valencia and Lake Tahoe sites. Local radiosonde measurements and AIRS profiles were also
719 used at the Valencia site. Another possibility for R-based validation is to select suitable
720 validation areas around permanent radio sounding stations with launching times close to
721 AATSR overpasses.

722

723 Results of this paper stress the need for modifications on the operational AATSR LST
724 algorithm. The most obvious conclusion is that the ancillary data (classification and fractional
725 vegetation cover maps) must be provided at the same spatial resolution as the AATSR data (1
726 km²). Otherwise, LST errors from 2 to 5 K can be obtained. When the AATSR algorithm (Eq.

727 1) was optimized with i and f values selected for each validation site according to their nature,
728 LST errors were within the target accuracy of the LST product, with negligible biases and
729 $rmse=\pm 0.5$ K for full-vegetated and lake surfaces, and ± 1.1 K for bare soil. For the vegetated
730 surface, we found that the algorithm is very sensitive to the assigned biome since the various
731 vegetation biomes of Table 1 (with $f=1$) resulted in rather different biases (AATSR minus
732 ground) ranging from -0.4 to 2.5 K. Furthermore, LST errors from Eq. (1) showed certain
733 dependence on the brightness temperature difference $T_{11}-T_{12}$.

734

735 The explicit emissivity-dependent algorithm (Eq. 2) provided accurate LSTs for all the
736 biomes studied, with small biases, $rmse$ from ± 0.4 to 0.6 K and LST errors within ± 1.0 K for
737 most validation cases. This shows the high accuracy achievable with AATSR data in ideal
738 conditions. The ancillary data required for Eq. (2) (ϵ and $\Delta\epsilon$ maps at 1 km² resolution) can be
739 derived from classification maps and monthly fractional vegetation cover estimated from
740 visible and near infrared AATSR data. It is the approach adopted by other satellite LST
741 products such as MODIS and SEVIRI (Wan and Dozier, 1996; PUM_LST, 2008). The land
742 cover biomes studied here (vegetation, water and bare soil) likely span the emissivity range of
743 natural surfaces. However, these results only apply to the geographical area used in the study
744 and the accuracy of the AATSR LST retrievals may be different in other regions and under
745 different conditions. More validation datasets are necessary especially over deserts where
746 emissivity may have a larger variability in response to differences in soil composition, texture
747 and moisture content.

748

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904

905 **TABLES**

906 **Table 1.** Coefficients for the operational AATSR LST algorithm (Eq. 1) for the different
 907 biomes (from Prata, 2002b).

908

| Biome | <i>i</i> | a_{vi} | a_{si} | b_{vi} | b_{si} | c_{vi} | c_{si} |
|---|-----------------|----------------------------|----------------------------|----------------------------|----------------------------|----------------------------|----------------------------|
| Broadleaf evergreen trees | 1 | 0.6907 | 6.0951 | 3.8129 | 4.5637 | -2.8456 | -3.3617 |
| Broadleaf deciduous trees | 2 | -0.5393 | 4.6301 | 3.6472 | 4.3652 | -2.7218 | -3.2155 |
| Broadleaf and needleleaf trees | 3 | -0.6885 | 4.8786 | 3.6472 | 4.3652 | -2.7218 | -3.2155 |
| Needleleaf-evergreen trees | 4 | 1.0801 | 1.0801 | 3.2972 | 3.2972 | -2.2909 | -2.2909 |
| Needleleaf-deciduous trees | 5 | 0.7804 | 1.491 | 3.2721 | 3.8117 | -2.3374 | -2.7233 |
| Broadleaf trees with groundcover | 6 | 0.9089 | 0.0348 | 3.3511 | 3.9038 | -2.389 | -2.7891 |
| Groundcover | 7 | 0.7994 | 0.7994 | 3.5088 | 3.5088 | -2.5065 | -2.5065 |
| Broadleaf shrubs with groundcover | 8 | 1.5662 | 0.7833 | 3.1384 | 3.656 | -2.2419 | -2.6121 |
| Broadleaf shrubs with bare soil | 9 | 0.8965 | 0.8965 | 3.4867 | 3.4867 | -2.4908 | -2.4908 |
| Dwarf trees, shrubs with groundcover | 10 | 1.0817 | 1.0817 | 3.3039 | 3.3039 | -2.2955 | -2.2955 |
| Bare soil | 11 | 0.7075 | 0.7041 | 3.7832 | 3.7832 | -2.7868 | -2.7868 |
| Broadleaf-deciduous trees with winter wheat | 12 | 0.881 | 0.881 | 3.4106 | 3.4106 | -2.4133 | -2.4133 |
| Perennial land ice | 13 | 1.0801 | 1.0801 | 3.2972 | 3.2972 | -2.2909 | -2.2909 |
| Lake-day | 14-d | -0.0005 | -0.0005 | 2.4225 | 2.4225 | -1.4344 | -1.4344 |
| Lake-night | 14-n | -0.3658 | -0.3658 | 2.3823 | 2.3823 | -1.3556 | -1.3556 |

909

910

911 **Table 2.** Emissivity classes by surface type and their correspondence with the biomes defined
 912 by the GLOBCOVER (GLC) dataset.

| Emissivity class | GLC Class | Description |
|--|--|--|
| 1. Flooded vegetation, crops and grasslands | 11 | Post-flooding or irrigated croplands (or aquatic) |
| | 13 | Post-flooding or irrigated herbaceous crops |
| | 180 | Closed to open (>15%) grassland or woody vegetation on regularly flooded or waterlogged soil - Fresh, brackish or saline water |
| | 185 | Closed to open (>15%) grassland on regularly flooded or waterlogged soil - Fresh or brackish water |
| 2. Flooded forest and shrublands | 170 | Closed (>40%) broadleaved forest or shrubland permanently flooded - Saline or brackish water |
| 3. Croplands and grasslands | 14 | Rainfed croplands |
| | 15 | Rainfed herbaceous crops |
| | 20 | Mosaic cropland (50-70%) / vegetation (grassland/shrubland/forest) (20-50%) |
| | 21 | Mosaic cropland (50-70%) / grassland or shrubland (20-50%) |
| | 120 | Mosaic grassland (50-70%) / forest or shrubland (20-50%) |
| | 140 | Closed to open (>15%) herbaceous vegetation (grassland, savannas or lichens/mosses) |
| | 141 | Closed (>40%) grassland |
| | 150 | Sparse (<15%) vegetation |
| 4. Shrublands | 151 | Sparse (<15%) grassland |
| | 16 | Rainfed shrub or tree crops (cash crops, vineyards, olive tree, orchards...) |
| | 30 | Mosaic vegetation (grassland/shrubland/forest) (50-70%) / cropland (20-50%) |
| | 130 | Closed to open (>15%) (broadleaved or needleleaved, evergreen or deciduous) shrubland (<5m) |
| | 131 | Closed to open (>15%) broadleaved or needleleaved evergreen shrubland (<5m) |
| | 134 | Closed to open (>15%) broadleaved deciduous shrubland (<5m) |
| 5. Broadleaved/needleleaved deciduous forest | 152 | Sparse (<15%) shrubland |
| | 40 | Closed to open (>15%) broadleaved evergreen or semi-deciduous forest (>5m) |
| | 50 | Closed (>40%) broadleaved deciduous forest (>5m) |
| | 60 | Open (15-40%) broadleaved deciduous forest/woodland (>5m) |
| | 90 | Open (15-40%) needleleaved deciduous or evergreen forest (>5m) |
| 6. Broadleaved/needleleaved evergreen forest | 91 | Open (15-40%) needleleaved deciduous forest (>5m) |
| | 32 | Mosaic forest (50-70%) / cropland (20-50%) |
| | 70 | Closed (>40%) needleleaved evergreen forest (>5m) |
| | 92 | Open (15-40%) needleleaved evergreen forest (>5m) |
| | 100 | Closed to open (>15%) mixed broadleaved and needleleaved forest (>5m) |
| | 101 | Closed (>40%) mixed broadleaved and needleleaved forest (>5m) |
| 110 | Mosaic forest or shrubland (50-70%) / grassland (20-50%) | |
| 7. Urban area | 190 | Artificial surfaces and associated areas (Urban areas >50%) |
| 8. Bare rock | 200 | Bare areas |
| | 201 | Consolidated bare areas (hardpans, gravels, bare rock, stones, boulders) |
| | 202 | Non-consolidated bare areas (sandy desert) |
| | 203 | Salt hardpans |
| 9. Water | 210 | Water bodies |
| 10. Snow and ice | 220 | Permanent snow and ice |

913

914 **Table 3.** Coefficients for the vegetation cover method emissivity (Eq. 3) for AATSR bands at
 915 11 and 12 μm based on the classes shown in Table 2.

916

| Emissivity class | 11 μm | | | 12 μm | | |
|--|--|---------------------------|-----------------------------|--|---------------------------|-----------------------------|
| | ϵ_v | ϵ_g | $\langle d\epsilon \rangle$ | ϵ_v | ϵ_g | $\langle d\epsilon \rangle$ |
| 1. Flooded vegetation, crops and grasslands | 0.983 \pm 0.005 | 0.970 \pm 0.005 (soil) | 0 | 0.989 \pm 0.005 | 0.977 \pm 0.004 (soil) | 0 |
| | | 0.991 \pm 0.001 (water) | 0 | | 0.985 \pm 0.001 (water) | 0 |
| 2. Flooded forest and shrublands | 0.981 \pm 0.008 | 0.970 \pm 0.005 (soil) | 0.014 \pm 0.004 (soil) | 0.982 \pm 0.009 | 0.977 \pm 0.004 (soil) | 0.010 \pm 0.003 (soil) |
| | | 0.991 \pm 0.001 (water) | 0.004 \pm 0.001 (water) | | 0.985 \pm 0.001 (water) | 0.007 \pm 0.002 (water) |
| 3. Croplands and grasslands | 0.983 \pm 0.005 | 0.970 \pm 0.005 | 0 | 0.989 \pm 0.005 | 0.977 \pm 0.004 | 0 |
| 4. Shrublands | 0.981 \pm 0.008 | 0.970 \pm 0.005 | 0.014 \pm 0.004 | 0.982 \pm 0.009 | 0.977 \pm 0.004 | 0.010 \pm 0.003 |
| 5. Broadleaved/needleleaved deciduous forest | 0.973 \pm 0.005 | 0.970 \pm 0.005 | 0.019 \pm 0.006 | 0.973 \pm 0.005 | 0.977 \pm 0.004 | 0.015 \pm 0.004 |
| 6. Broadleaved/needleleaved evergreen forest | 0.989 \pm 0.005 | 0.970 \pm 0.005 | 0.019 \pm 0.005 | 0.991 \pm 0.005 | 0.977 \pm 0.004 | 0.015 \pm 0.004 |
| | Effective emissivity, 11 μm | | | Effective emissivity, 12 μm | | |
| 7. Urban area | 0.969 \pm 0.006 | | | 0.976 \pm 0.004 | | |
| 8. Bare rock | 0.93 \pm 0.05 | | | 0.95 \pm 0.05 | | |
| 9. Water | 0.991 \pm 0.001 | | | 0.985 \pm 0.001 | | |
| 10. Snow and ice | 0.990 \pm 0.004 | | | 0.971 \pm 0.014 | | |

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922 **Table 4.** Ground-measured LSTs (T_g) and uncertainties (σ) over full-vegetated rice fields in
923 the Valencia test site, and concurrent AATSR brightness temperatures in the 11 and 12 μm
924 bands, nadir view. θ is the satellite zenith viewing angle. The AATSR-derived LSTs (T_{AATSR})
925 using different options (see text) are shown in the last three columns.

926

| case | date (d/m/y) | $T_g \pm \sigma$ (°C) | θ (°) | T_{11} (°C) | T_{12} (°C) | operational T_{AATSR} (°C) | optimized T_{AATSR} (°C) | Eq. (2) T_{AATSR} (°C) |
|------|--------------|-----------------------|--------------|---------------|---------------|--|--------------------------------------|------------------------------------|
| 1 | 10/07/02 | 28.6±0.6 | 3.7 | 25.04 | 22.99 | 32.1 | 28.6 | 28.8 |
| 2 | 13/07/02 | 27.6±0.9 | 13.8 | 22.28 | 19.26 | 31.8 | 28.3 | 28.3 |
| 3 | 26/07/02 | 27.9±0.6 | 1.11 | 23.39 | 20.68 | 32.0 | 28.6 | 28.6 |
| 4 | 08/08/02 | 26.5±0.7 | 16.2 | 20.29 | 17.31 | 29.4 | 26.5 | 26.2 |
| 5 | 14/08/02 | 28.5±0.5 | 3.9 | 23.69 | 21.52 | 30.8 | 27.7 | 27.7 |
| 6 | 17/08/02 | 29.1±0.6 | 13.91 | 22.81 | 19.84 | 32.0 | 28.7 | 28.7 |
| 7 | 05/09/02 | 28.0±0.8 | 19.06 | 24.10 | 22.03 | 31.2 | 27.9 | 27.9 |
| 8 | 08/07/03 | 28.3±0.7 | 11.13 | 25.30 | 23.03 | 33.1 | 29.4 | 29.5 |
| 9 | 11/07/03 | 29.1±0.7 | 1.20 | 27.03 | 25.50 | 33.0 | 29.2 | 29.9 |
| 10 | 14/07/03 | 28.6±0.6 | 8.66 | 24.73 | 22.39 | 32.7 | 29.0 | 29.1 |
| 11 | 24/07/03 | 28.8±0.6 | 16.25 | 24.68 | 22.36 | 32.5 | 28.9 | 29.0 |
| 12 | 30/07/03 | 28.9±0.6 | 3.74 | 23.44 | 20.63 | 32.5 | 28.9 | 28.9 |
| 13 | 12/08/03 | 31.3±0.6 | 11.13 | 28.10 | 26.51 | 33.9 | 30.3 | 31.0 |
| 14 | 28/06/04 | 29.2±0.6 | 8.66 | 26.41 | 24.36 | 34.0 | 29.8 | 30.2 |
| 15 | 08/07/04 | 25.7±0.6 | 16.33 | 23.15 | 21.60 | 28.8 | 25.8 | 26.0 |
| 16 | 14/07/04 | 27.2±0.7 | 3.74 | 22.45 | 19.78 | 31.1 | 27.7 | 27.6 |
| 17 | 27/07/04 | 27.7±0.4 | 11.05 | 25.02 | 23.35 | 31.2 | 27.8 | 28.1 |
| 18 | 30/07/04 | 27.8±0.4 | 1.19 | 23.37 | 20.58 | 32.1 | 28.8 | 28.8 |
| 19 | 12/08/04 | 28.4±0.6 | 16.25 | 25.50 | 23.98 | 31.0 | 27.9 | 28.3 |
| 20 | 12//07/05 | 27.0±0.6 | 11.13 | 24.64 | 23.04 | 30.6 | 27.1 | 27.6 |
| 21 | 21/07/05 | 28.5±0.6 | 18.97 | 25.40 | 23.63 | 31.8 | 28.4 | 28.6 |
| 22 | 28/07/05 | 28.8±0.5 | 16.33 | 24.75 | 22.67 | 32.0 | 28.5 | 28.6 |
| 23 | 06/08/05 | 28.0±0.5 | 13.66 | 25.35 | 23.68 | 31.0 | 28.1 | 28.4 |
| 24 | 03/07/06 | 29.5±0.6 | 8.7 | 27.50 | 25.90 | 33.6 | 29.8 | 30.4 |
| 25 | 22/07/06 | 29.5±0.5 | 13.7 | 26.39 | 24.44 | 33.3 | 29.6 | 30.0 |
| 26 | 04/07/07 | 27.8±0.9 | 3.7 | 23.40 | 20.63 | 32.3 | 28.8 | 28.8 |
| 27 | 20/07/07 | 27.8±0.4 | 1.3 | 24.03 | 21.65 | 32.0 | 28.4 | 28.5 |
| 28 | 26/07/07 | 27.5±0.4 | 19.1 | 24.70 | 22.90 | 31.2 | 27.8 | 28.0 |

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929 **Table 5.** Uncertainty (in K) of the simulated temperatures in the R-based method (T_{R-b} , T_{11} ,
930 T_{12} , and $T_{11}-T_{12}$) for different sources of uncertainty (see text).

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| | T_{R-b} | T_{11} | T_{12} | $T_{11}-T_{12}$ |
|--------------------------------------|-----------|----------|----------|-----------------|
| W (10%) | 0.33 | 0.26 | 0.39 | 0.13 |
| T_{air} (1 K) | 0.28 | 0.21 | 0.33 | 0.12 |
| MODTRAN 4 | 0.43 | 0.33 | 0.51 | 0.18 |
| ϵ (0.005) | 0.35 | 0.28 | 0.22 | 0.36 |
| Total (rss) | 0.71 | 0.55 | 0.76 | 0.43 |

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934 **Table 6.** R-based validation cases over bare soil in the Valencia test site. The AATSR-derived
 935 LSTs (T_{AATSR}) using different options (see text) are shown in the last three columns.

| case | Date (d/m/y) | Time (UTC) | θ (°) | T_{11} (°C) | T_{12} (°C) | operational T_{AATSR} (°C) | optimized T_{AATSR} (°C) | Eq. (2) T_{AATSR} (°C) |
|------|--------------|------------|--------------|---------------|---------------|-------------------------------------|-----------------------------------|---------------------------------|
| 1 | 09/03/2003 | 10:25 | 7.0 | 11.49 | 10.46 | 15.2 | 15.0 | 14.5 |
| 2 | 12/03/2003 | 10:31 | 4.1 | 12.76 | 12.06 | 15.7 | 15.4 | 15.3 |
| 3 | 25/03/2003 | 10:22 | 12.5 | 11.45 | 9.98 | 16.4 | 16.2 | 15.1 |
| 4 | 10/04/2003 | 10:19 | 18.0 | 13.18 | 11.91 | 17.7 | 17.4 | 16.5 |
| 5 | 02/05/2003 | 10:28 | 1.3 | 15.25 | 13.71 | 20.6 | 20.2 | 18.9 |
| 6 | 21/05/2003 | 10:31 | 4.1 | 17.41 | 15.61 | 23.5 | 23.1 | 21.6 |
| 7 | 12/03/2004 | 10:28 | 1.4 | 11.18 | 10.05 | 15.2 | 15.0 | 14.3 |
| 8 | 03/04/2004 | 10:37 | 15.2 | 12.33 | 11.04 | 16.8 | 16.6 | 15.7 |
| 9 | 13/04/2004 | 10:22 | 12.4 | 12.63 | 11.39 | 17.0 | 16.8 | 15.9 |
| 10 | 06/05/2005 | 10:28 | 1.4 | 16.99 | 15.91 | 21.2 | 20.6 | 19.9 |
| 11 | 25/05/2005 | 10:31 | 4.1 | 19.16 | 17.72 | 24.4 | 23.8 | 22.7 |
| 12 | 14/03/2006 | 10:22 | 12.5 | 11.89 | 10.93 | 15.5 | 15.2 | 14.8 |
| 13 | 30/03/2006 | 10:19 | 18.2 | 13.45 | 12.13 | 18.1 | 17.8 | 16.9 |
| 14 | 18/04/2006 | 10:22 | 12.5 | 14.56 | 12.85 | 20.3 | 20.0 | 18.6 |
| 15 | 21/04/2006 | 10:28 | 1.5 | 14.64 | 12.95 | 20.3 | 20.0 | 18.6 |
| 16 | 26/05/2006 | 10:28 | 1.5 | 17.36 | 15.61 | 23.3 | 22.9 | 21.4 |
| 17 | 29/05/2006 | 10:34 | 9.6 | 19.01 | 17.51 | 24.4 | 23.8 | 22.6 |
| 18 | 05/03/2007 | 10:34 | 9.6 | 12.68 | 11.71 | 16.3 | 16.1 | 15.6 |
| 19 | 15/03/2007 | 10:19 | 18.0 | 12.16 | 10.98 | 16.4 | 16.1 | 15.4 |
| 20 | 18/03/2007 | 10:25 | 6.9 | 13.08 | 12.02 | 17.0 | 16.7 | 16.1 |
| 21 | 03/04/2007 | 10:22 | 12.6 | 11.97 | 10.44 | 17.1 | 16.9 | 15.7 |
| 22 | 08/05/2007 | 10:22 | 12.5 | 16.88 | 15.58 | 21.7 | 21.2 | 20.2 |
| 23 | 14/05/2007 | 10:34 | 9.6 | 17.14 | 15.81 | 22.0 | 21.5 | 20.5 |
| 24 | 30/05/2007 | 10:31 | 4.1 | 17.85 | 16.29 | 23.4 | 22.8 | 21.6 |
| 25 | 02/03/2008 | 10:25 | 7.0 | 13.28 | 12.28 | 17.0 | 16.7 | 16.2 |
| 26 | 05/03/2008 | 10:31 | 4.1 | 12.34 | 11.42 | 15.8 | 15.6 | 15.2 |
| 27 | 18/03/2008 | 10:22 | 12.5 | 12.74 | 11.66 | 16.7 | 16.4 | 15.8 |
| 28 | 21/03/2008 | 10:28 | 1.4 | 11.55 | 9.84 | 17.1 | 17.0 | 15.6 |
| 29 | 03/04/2008 | 10:19 | 18.0 | 13.92 | 12.80 | 18.1 | 17.7 | 17.0 |
| 30 | 25/04/2008 | 10:28 | 1.5 | 12.65 | 11.30 | 17.3 | 17.1 | 16.1 |
| 31 | 09/03/2003 | 21:40 | 16.7 | 8.94 | 8.70 | 10.5 | 10.3 | 11.0 |
| 32 | 19/03/2003 | 21:26 | 10.9 | 4.77 | 4.73 | 5.5 | 5.6 | 6.7 |
| 33 | 25/03/2003 | 21:37 | 11.1 | 1.65 | 0.82 | 4.3 | 4.7 | 4.4 |
| 34 | 03/03/2004 | 21:26 | 11.0 | 4.84 | 4.68 | 5.9 | 6.0 | 6.8 |
| 35 | 22/03/2004 | 21:29 | 5.4 | 6.67 | 6.19 | 8.7 | 8.7 | 9.0 |
| 36 | 13/04/2004 | 21:38 | 11.1 | 7.45 | 7.18 | 9.0 | 8.9 | 9.5 |
| 37 | 15/05/2004 | 21:32 | 0.1 | 12.54 | 11.49 | 16.4 | 16.1 | 15.5 |
| 38 | 07/03/2005 | 21:29 | 5.5 | 0.71 | 0.70 | 1.1 | 1.4 | 2.6 |
| 39 | 26/03/2005 | 21:32 | 0.1 | 11.90 | 11.44 | 14.2 | 13.8 | 14.2 |
| 40 | 12/03/2007 | 21:29 | 5.5 | 5.26 | 5.02 | 6.6 | 6.6 | 7.3 |
| 41 | 15/03/2007 | 21:35 | 5.5 | 6.53 | 6.42 | 7.6 | 7.5 | 8.5 |
| 42 | 16/04/2007 | 21:29 | 5.4 | 10.12 | 9.33 | 13.2 | 13.0 | 12.7 |
| 43 | 19/04/2007 | 21:35 | 5.6 | 11.42 | 10.64 | 14.5 | 14.3 | 14.0 |
| 44 | 08/05/2007 | 21:37 | 11.1 | 15.63 | 14.92 | 18.8 | 18.3 | 18.1 |
| 45 | 02/03/2008 | 21:40 | 16.6 | 11.46 | 11.37 | 12.7 | 12.4 | 13.4 |
| 46 | 18/03/2008 | 21:37 | 11.1 | 10.91 | 10.17 | 13.9 | 13.6 | 13.5 |
| 47 | 31/03/2008 | 21:29 | 5.5 | 11.09 | 10.65 | 13.3 | 13.0 | 13.3 |

937 **Table 7.** R-based validation cases over Albufera Lake in the Valencia test site. The AATSR-
 938 derived LSTs (T_{AATSR}) using different options (see text) are shown in the last three columns.

| case | Date (d/m/y) | Time (UTC) | θ (°) | T_{11} (°C) | T_{12} (°C) | operational T_{AATSR} (°C) | optimized T_{AATSR} (°C) | Eq. (2) T_{AATSR} (°C) |
|------|--------------|------------|--------------|---------------|---------------|-------------------------------------|-----------------------------------|---------------------------------|
| 1 | 09/03/2003 | 10:25 | 7.5 | 11.91 | 10.91 | 15.6 | 13.2 | 13.3 |
| 2 | 12/03/2003 | 10:31 | 3.5 | 13.01 | 12.32 | 15.9 | 13.8 | 14.0 |
| 3 | 25/03/2003 | 10:22 | 13.0 | 12.04 | 10.62 | 16.9 | 13.9 | 14.0 |
| 4 | 10/04/2003 | 10:19 | 18.5 | 13.75 | 12.48 | 18.3 | 15.4 | 15.5 |
| 5 | 02/05/2003 | 10:28 | 1.9 | 16.05 | 14.55 | 21.3 | 18.0 | 18.2 |
| 6 | 21/05/2003 | 10:31 | 3.5 | 17.85 | 15.95 | 24.3 | 20.4 | 20.7 |
| 7 | 12/03/2004 | 10:28 | 1.9 | 9.45 | 7.67 | 15.1 | 11.9 | 12.1 |
| 8 | 03/04/2004 | 10:37 | 14.6 | 11.95 | 10.69 | 16.3 | 13.6 | 13.7 |
| 9 | 13/04/2004 | 10:22 | 12.9 | 12.50 | 11.22 | 17.0 | 14.2 | 14.3 |
| 10 | 06/05/2005 | 10:28 | 1.9 | 17.45 | 16.35 | 21.7 | 18.8 | 19.0 |
| 11 | 25/05/2005 | 10:31 | 3.5 | 18.82 | 17.44 | 23.9 | 20.6 | 20.8 |
| 12 | 14/03/2006 | 10:22 | 13.0 | 11.91 | 10.96 | 15.5 | 13.1 | 13.2 |
| 13 | 30/03/2006 | 10:19 | 18.7 | 13.64 | 12.29 | 18.4 | 15.5 | 15.5 |
| 14 | 18/04/2006 | 10:22 | 13.0 | 14.81 | 13.16 | 20.4 | 17.0 | 17.2 |
| 15 | 21/04/2006 | 10:28 | 2.0 | 14.83 | 13.02 | 20.8 | 17.2 | 17.5 |
| 16 | 26/05/2006 | 10:28 | 2.0 | 17.15 | 15.36 | 23.2 | 19.5 | 19.8 |
| 17 | 29/05/2006 | 10:34 | 9.0 | 19.09 | 17.52 | 24.7 | 21.1 | 21.4 |
| 18 | 05/03/2007 | 10:34 | 9.1 | 12.91 | 11.94 | 16.6 | 14.2 | 14.2 |
| 19 | 15/03/2007 | 10:19 | 18.6 | 12.33 | 11.14 | 16.6 | 13.9 | 14.0 |
| 20 | 18/03/2007 | 10:25 | 7.5 | 12.92 | 11.91 | 16.7 | 14.2 | 14.3 |
| 21 | 03/04/2007 | 10:22 | 13.1 | 12.04 | 10.51 | 17.1 | 14.1 | 14.2 |
| 22 | 08/05/2007 | 10:22 | 13.0 | 16.76 | 15.49 | 21.5 | 18.4 | 18.5 |
| 23 | 14/05/2007 | 10:34 | 9.0 | 16.54 | 15.36 | 21.0 | 18.0 | 18.2 |
| 24 | 30/05/2007 | 10:31 | 3.5 | 17.99 | 16.33 | 23.8 | 20.2 | 20.4 |
| 25 | 02/03/2008 | 10:25 | 7.5 | 13.49 | 12.53 | 17.2 | 14.7 | 14.8 |
| 26 | 05/03/2008 | 10:31 | 3.5 | 12.19 | 11.21 | 15.8 | 13.5 | 13.5 |
| 27 | 18/03/2008 | 10:22 | 13.1 | 12.89 | 11.82 | 16.8 | 14.3 | 14.4 |
| 28 | 21/03/2008 | 10:28 | 2.0 | 11.05 | 9.28 | 16.7 | 13.5 | 13.7 |
| 29 | 03/04/2008 | 10:19 | 18.6 | 14.32 | 13.23 | 18.4 | 15.7 | 15.8 |
| 30 | 25/04/2008 | 10:28 | 2.0 | 11.32 | 9.91 | 16.1 | 13.2 | 13.3 |
| 31 | 09/03/2003 | 21:40 | 16.5 | 8.11 | 7.94 | 9.4 | 8.2 | 8.5 |
| 32 | 19/03/2003 | 21:26 | 11.2 | 4.36 | 4.41 | 4.8 | 4.0 | 4.6 |
| 33 | 25/03/2003 | 21:37 | 10.9 | 6.44 | 5.81 | 8.8 | 7.1 | 7.3 |
| 34 | 03/03/2004 | 21:26 | 11.2 | 3.68 | 3.65 | 4.3 | 3.5 | 4.0 |
| 35 | 22/03/2004 | 21:29 | 5.7 | 5.78 | 5.37 | 7.6 | 6.1 | 6.4 |
| 36 | 13/04/2004 | 21:38 | 10.9 | 7.56 | 7.26 | 9.2 | 7.8 | 8.1 |
| 37 | 15/05/2004 | 21:32 | 0.1 | 11.33 | 10.53 | 14.5 | 12.4 | 12.5 |
| 38 | 07/03/2005 | 21:29 | 5.7 | 0.04 | 0.04 | 0.4 | -0.3 | 0.3 |
| 39 | 26/03/2005 | 21:32 | 0.2 | 11.59 | 11.12 | 13.9 | 12.2 | 12.3 |
| 40 | 12/03/2007 | 21:29 | 5.7 | 4.56 | 4.43 | 5.5 | 4.5 | 5.0 |
| 41 | 15/03/2007 | 21:35 | 5.3 | 5.73 | 5.68 | 6.6 | 5.6 | 6.1 |
| 42 | 16/04/2007 | 21:29 | 5.7 | 9.57 | 8.87 | 12.3 | 10.4 | 10.6 |
| 43 | 19/04/2007 | 21:35 | 5.4 | 11.59 | 10.81 | 14.7 | 12.6 | 12.7 |
| 44 | 08/05/2007 | 21:37 | 10.9 | 14.39 | 13.84 | 17.0 | 15.2 | 15.2 |
| 45 | 02/03/2008 | 21:40 | 16.4 | 11.03 | 10.87 | 12.5 | 11.2 | 11.4 |
| 46 | 18/03/2008 | 21:37 | 10.9 | 10.27 | 9.57 | 13.1 | 11.1 | 11.3 |
| 47 | 31/03/2008 | 21:29 | 5.7 | 9.96 | 9.63 | 11.8 | 10.3 | 10.5 |

940 **Table 8.** Calculated R-based LST (T_{R-b}) and difference $\delta(T_{11}-T_{12})$ for each validation case in
 941 Table 6 (bare soil) and Table 7 (lake). W_{NCEP} is the precipitable water from NCEP profiles.
 942 Cases not meeting $-0.6 \text{ K} < \delta(T_{11}-T_{12}) < 0.6 \text{ K}$ are marked with *.

| case | W_{NCEP} (cm) | bare soil | | lake | |
|------|-----------------|----------------|-----------------------------|----------------|-----------------------------|
| | | T_{R-b} (°C) | $\delta(T_{11}-T_{12})$ (K) | T_{R-b} (°C) | $\delta(T_{11}-T_{12})$ (K) |
| 1 | 0.98 | 14.4 | 0.47 | 13.1 | 0.13 |
| 2 | 0.84 | 15.5 | 0.29 | 13.9 | 0.09 |
| 3 | 1.23 | 14.7 | 0.54 | 13.6 | 0.24 |
| 4 | 1.46 | 16.8 | 0.13 | 15.7 | -0.19 |
| 5 | 2.53 | 18.4 | 0.29 | 18.1 | -0.13 |
| 6 | 1.83 | 21.1 | 0.37 | 19.9 | 0.26 |
| 7 | 1.68 | 13.8 | 0.40 | 10.1 | 1.05* |
| 8 | 1.15 | 15.6 | 0.29 | 13.3 | 0.16 |
| 9 | 0.81 | 15.9 | 0.32 | 13.9 | 0.22 |
| 10 | 1.16 | 20.2 | 0.18 | 18.9 | -0.05 |
| 11 | 1.54 | 22.8 | 0.11 | 20.6 | -0.14 |
| 12 | 1.09 | 14.8 | 0.26 | 13.2 | 0.10 |
| 13 | 2.71 | 17.5 | -0.44 | 16.3 | -0.67* |
| 14 | 1.77 | 18.5 | 0.29 | 17.1 | -0.09 |
| 15 | 2.11 | 18.2 | 0.31 | 17.0 | 0.17 |
| 16 | 2.20 | 21.4 | 0.15 | 19.5 | -0.02 |
| 17 | 3.34 | 23.3 | -0.49 | 22.2 | -0.67* |
| 18 | 1.30 | 15.9 | 0.12 | 14.5 | -0.13 |
| 19 | 1.13 | 15.4 | 0.16 | 13.8 | 0.03 |
| 20 | 1.28 | 16.4 | 0.10 | 14.4 | -0.13 |
| 21 | 1.33 | 15.5 | 0.32 | 13.9 | 0.17 |
| 22 | 1.57 | 20.1 | 0.30 | 18.2 | 0.06 |
| 23 | 1.37 | 20.6 | 0.23 | 18.1 | -0.09 |
| 24 | 2.22 | 21.3 | 0.39 | 20.0 | 0.22 |
| 25 | 1.62 | 16.0 | 0.40 | 14.8 | 0.04 |
| 26 | 0.55 | 15.7 | -0.15 | 13.5 | -0.19 |
| 27 | 1.02 | 15.8 | 0.21 | 14.2 | 0.01 |
| 28 | 1.45 | 15.1 | 0.48 | 12.7 | 0.38 |
| 29 | 1.48 | 16.8 | 0.36 | 15.6 | 0.12 |
| 30 | 1.69 | 15.0 | 0.91* | 11.9 | 0.93* |
| 31 | 0.85 | 11.6 | -0.20 | 8.9 | -0.39 |
| 32 | 0.81 | 7.3 | -0.32 | 5.1 | -0.54 |
| 33 | 1.53 | 3.2 | 0.91* | 7.3 | -0.07 |
| 34 | 0.53 | 7.5 | -0.29 | 4.4 | -0.47 |
| 35 | 0.89 | 9.6 | -0.19 | 6.8 | -0.36 |
| 36 | 0.93 | 10.2 | -0.24 | 8.5 | -0.41 |
| 37 | 1.60 | 15.9 | 0.01 | 12.8 | -0.32 |
| 38 | 0.38 | 3.3 | -0.40 | 0.8 | -0.48 |
| 39 | 1.68 | 15.3 | -0.63* | 13.3 | -0.81* |
| 40 | 1.24 | 7.9 | -0.26 | 5.4 | -0.49 |
| 41 | 0.87 | 9.1 | -0.31 | 6.5 | -0.48 |
| 42 | 1.80 | 13.1 | -0.05 | 10.9 | -0.38 |
| 43 | 2.42 | 14.3 | -0.29 | 13.1 | -0.55 |
| 44 | 1.80 | 18.2 | 0.06 | 15.2 | -0.17 |
| 45 | 1.59 | 13.5 | -0.08 | 11.5 | -0.18 |
| 46 | 1.15 | 13.9 | -0.08 | 11.4 | -0.26 |
| 47 | 1.06 | 14.3 | -0.53 | 11.2 | -0.73* |

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944 **Table 9.** Statistics of the R-based validation ($\delta T = T_{\text{AATSR}} - T_{\text{R-b}}$) for the AATSR-derived LSTs
 945 using the three options (see text) over the bare soil and lake sites.

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| LST algorithm | operational | | optimized | | Eq. (2) | | |
|---------------------------------------|-------------|-----------|-----------|-----------|---------|-----------|------|
| | site | bare soil | lake | bare soil | lake | bare soil | lake |
| bias (K) | | 0.6 | 2.2 | 0.3 | -0.2 | -0.2 | 0.0 |
| std. dev. (K) | | 1.2 | 1.3 | 1.1 | 0.4 | 0.4 | 0.4 |
| rmse (K) | | 1.3 | 2.5 | 1.1 | 0.5 | 0.4 | 0.4 |
| min. δT (K) | | -2.2 | -0.4 | -1.9 | -1.1 | -0.8 | -0.5 |
| max. δT (K) | | 2.4 | 4.4 | 2.0 | 0.7 | 0.6 | 0.9 |

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949 **FIGURE CAPTIONS**

950 **Figure 1.** Mean emissivity ($\epsilon=(\epsilon_{11}+\epsilon_{12})/2$) and emissivity difference ($\Delta\epsilon=\epsilon_{11}-\epsilon_{12}$) in AATSR

951 bands at 11 and 12 μm derived from Eq. (3) over East Spain on March and July, 2007.

952 Clouds and water are masked in white.

953 **Figure 2.** (a) Photograph showing part of the Valencia test site in July. (b) RGB composite of

954 ASTER bands 2 (0.66 μm), 3 (0.81 μm) and 1 (0.56 μm) showing the Valencia rice

955 field area and environs on August 3, 2004. (c) RGB composite of AATSR bands at

956 0.87, 0.66 and 0.55 μm over Valencia on July 11, 2003.

957 **Figure 3.** AATSR-derived LST (T_{AATSR}) against ground-measured LST (T_{g}) for the three

958 LST retrieval options. The dashed line is the 1:1 line.

959 **Figure 4.** Difference between AATSR-derived and ground-measured LST ($T_{\text{AATSR}}-T_{\text{g}}$) as a

960 function of time.

961 **Figure 5.** Difference between ground-measured and R-based LSTs against $\delta(T_{11}-T_{12})$ for the

962 datasets and atmospheric profiles indicated. The linear regression for all data is shown.

963 **Figure 6.** Difference between R-based LSTs obtained from local radiosonde and NCEP/AIRS

964 profiles against a) precipitable water difference, and b) difference in $T_{11}-T_{12}$ simulated

965 from local radiosonde and NCEP/AIRS profiles.

966 **Figure 7.** AATSR-derived LST minus R-based LST calculated with NCEP profiles against

967 $\delta(T_{11}-T_{12})$ in the bare soil and lake sites for a) the operational algorithm, b) the

968 optimized algorithm, and c) the explicit emissivity-dependent algorithm.

969 **Figure 8.** AATSR-derived LST minus R-based LST calculated with NCEP profiles against

970 the actual AATSR brightness temperature difference $T_{11}-T_{12}$ in the bare soil site for the

971 operational, the optimized and the explicit emissivity-dependent algorithm (Eq. 2). The

972 solid lines are the linear regressions for each algorithm.

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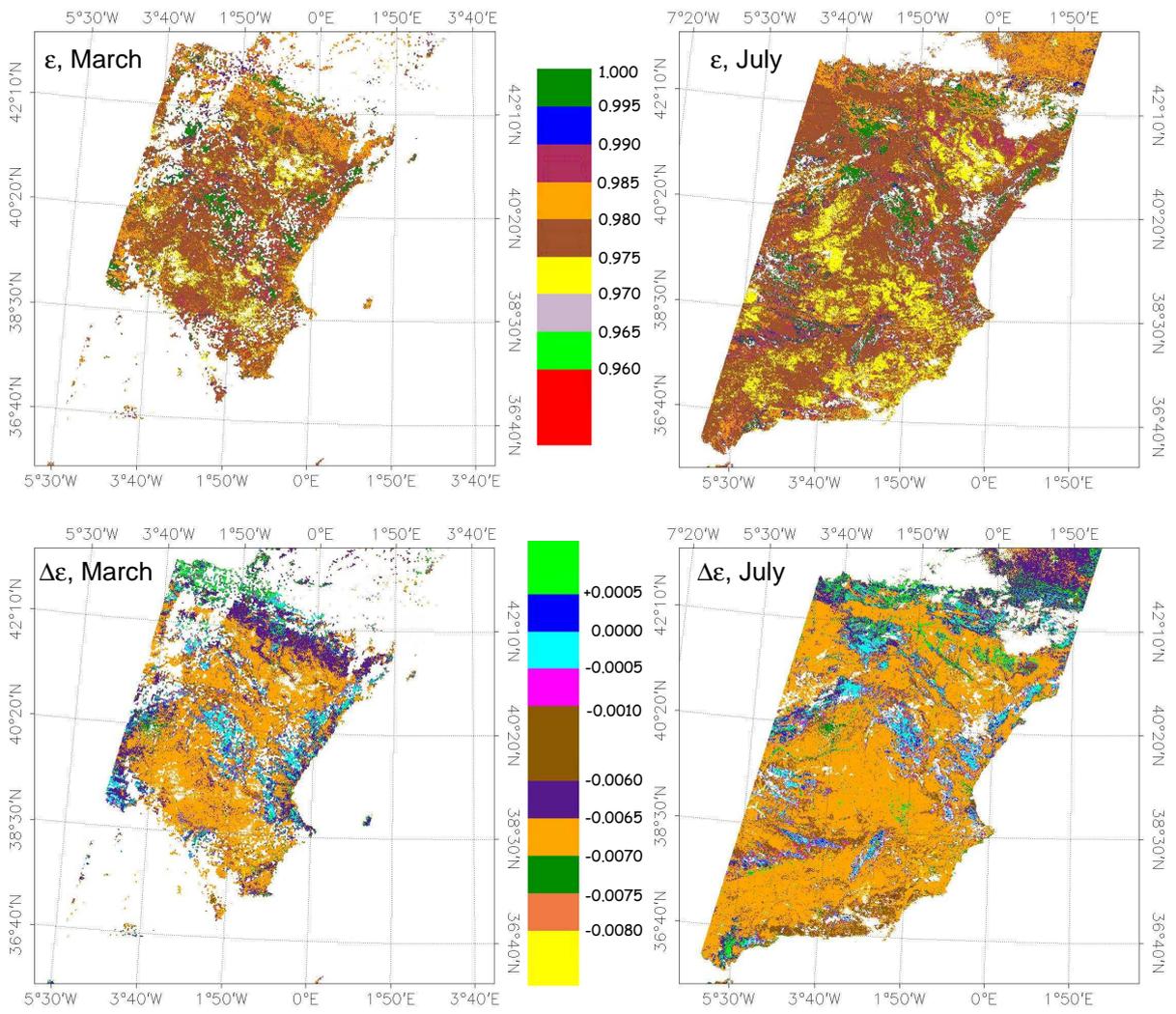


Figure 1

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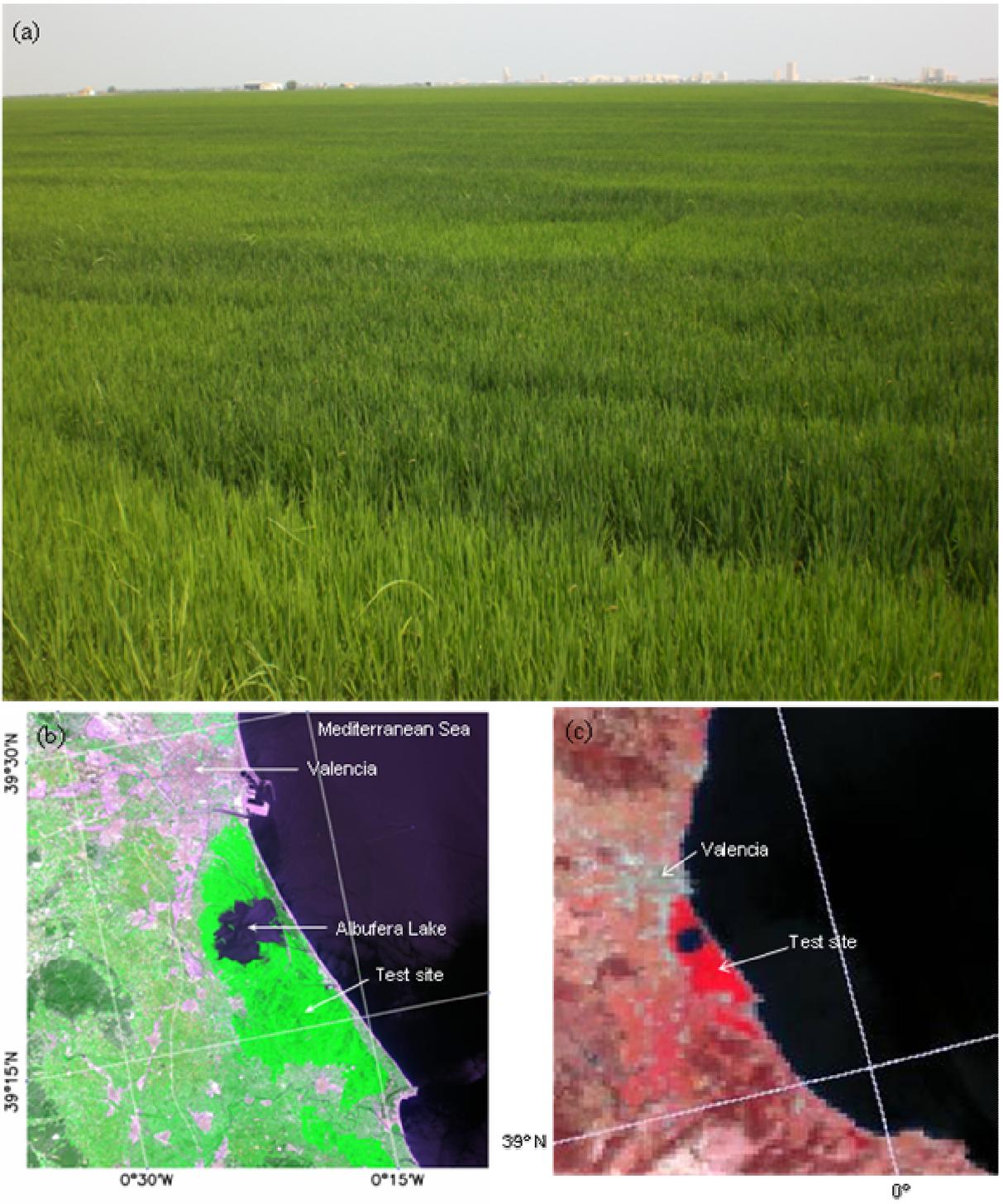


Figure 2

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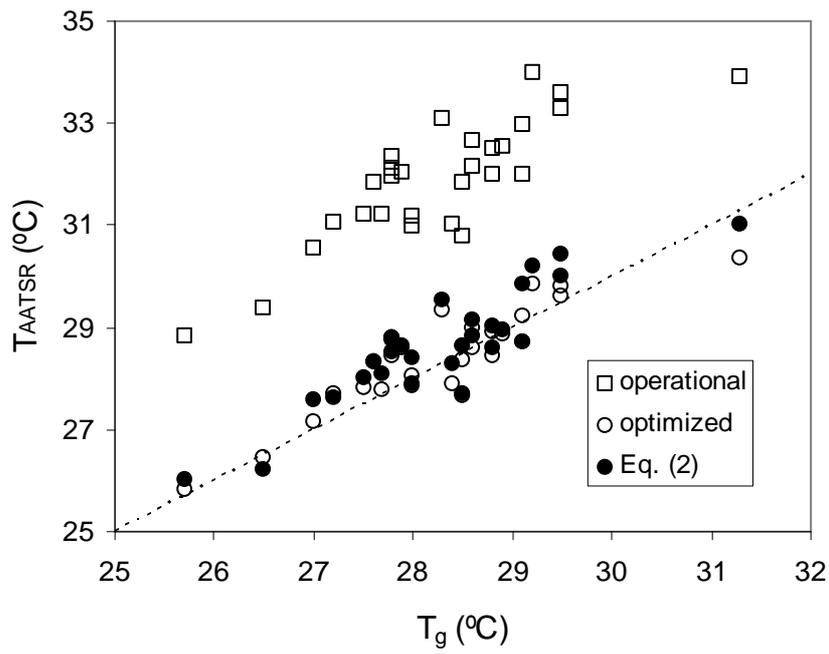


Figure 3

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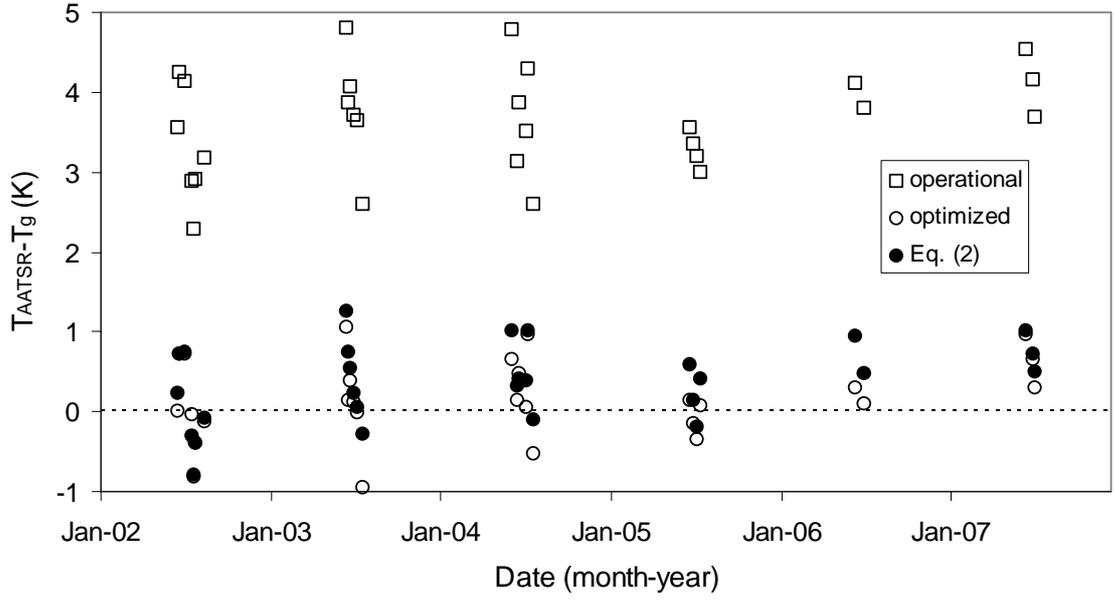


Figure 4

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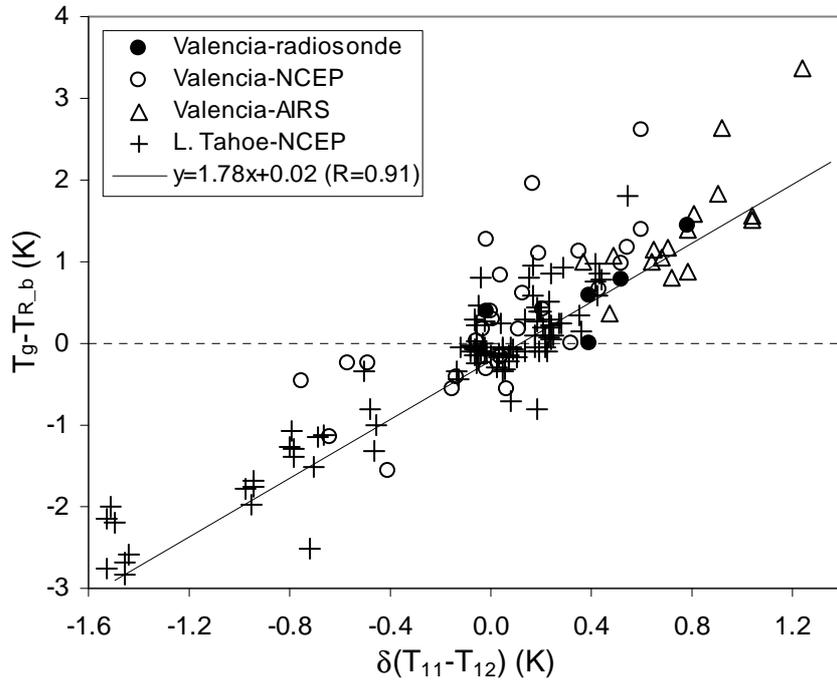


Figure 5

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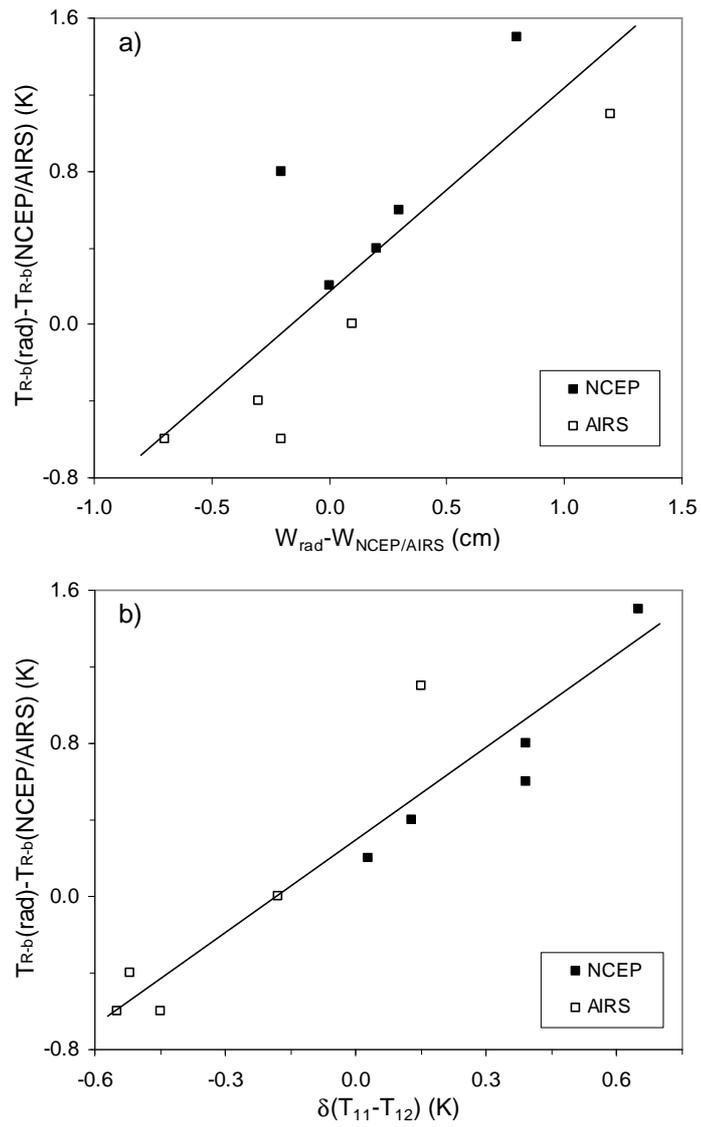


Figure 6

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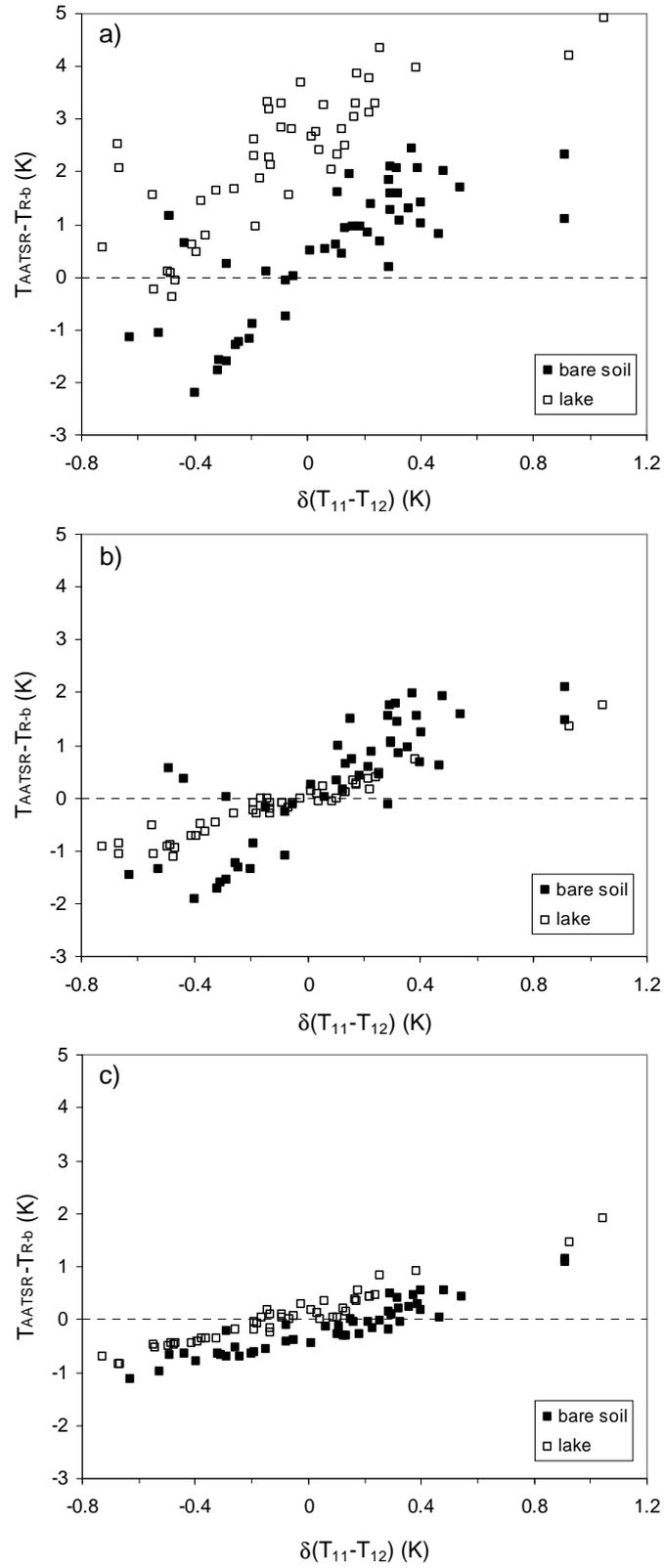


Figure 7

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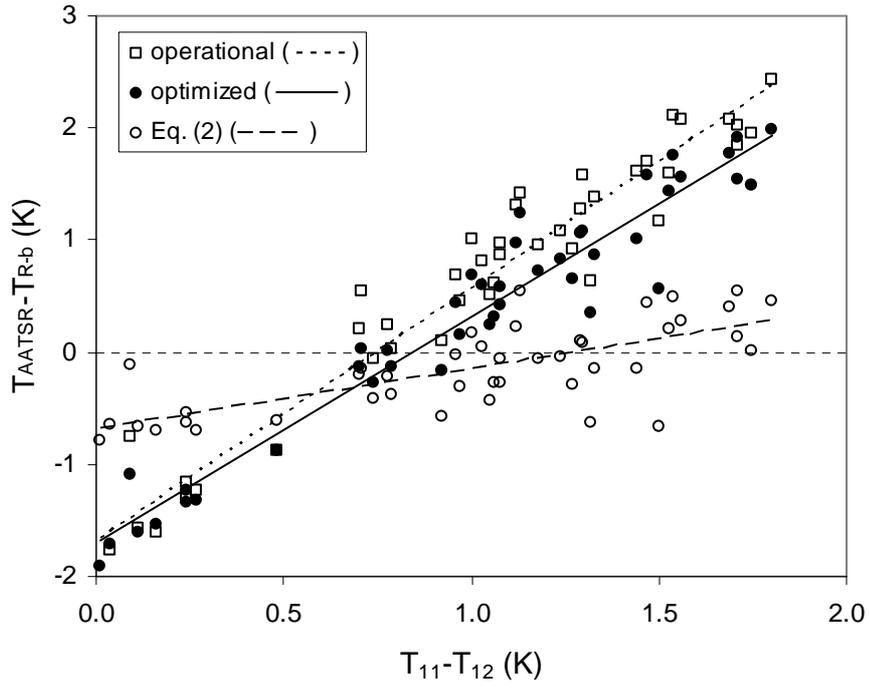


Figure 8