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## A physical method for downscaling land surface temperatures using surface energy balance theory

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22 **Abstract**

23 Fine-resolution land surface temperature (LST) derived from thermal infrared remote sensing  
24 images is a good indicator of surface water status and plays an essential role in the exchange of  
25 energy and water between land and atmosphere. A physical surface energy balance (SEB)-based  
26 LST downscaling method (DTsEB) is developed to downscale coarse remotely sensed thermal  
27 infrared LST products with fine-resolution visible and near-infrared data. The DTsEB method is  
28 advantageous for its ability to mechanically interrelate surface variables contributing to the spatial  
29 variation of LST, to quantitatively weigh the contributions of each related variable within a  
30 physical framework, and to efficaciously avoid the subjective selection of scaling factors and the  
31 establishment of statistical regression relationships. The applicability of the DTsEB method was  
32 tested by downscaling 12 scenes of 990 m Moderate Resolution Imaging Spectroradiometer  
33 (MODIS) and aggregated Advanced Spaceborne Thermal Emission and Reflection Radiometer  
34 (ASTER) LST products to 90 m resolution at six overpass times between 2005 and 2015 over three  
35 9.9 km by 9.9 km cropland (mixed by grass, tree, and built-up land) study areas. Three typical LST  
36 downscaling methods, namely the widely applied TsHARP, the later developed least median  
37 square regression downscaling (LMS) and the geographically weighted regression (GWR), were  
38 introduced for intercomparison. The results showed that the DTsEB method could more effectively  
39 reconstruct the subpixel spatial variations in LST within the coarse-resolution pixels and achieve  
40 a better downscaling accuracy than the TsHARP, LMS and GWR methods. The DTsEB method  
41 yielded, on average, root mean square errors (RMSEs) of 2.01 K and 1.42 K when applied to the  
42 MODIS datasets and aggregated ASTER datasets, respectively, which were lower than those  
43 obtained with the TsHARP method, with average RMSEs of 2.41 K and 1.71 K, the LMS method,  
44 with average RMSEs of 2.35 K and 1.63 K, and the GWR method, with average RMSEs of 2.38  
45 K and 1.64 K, respectively. The contributions of the related surface variables to the subpixel spatial  
46 variation in the LST varied both spatially and temporally and were different from each other. In  
47 summary, the DTsEB method was demonstrated to outperform the TsHARP, LMS, and GWR  
48 methods and could be used as a good alternative for downscaling LST products from coarse to fine  
49 resolution with high robustness and accuracy.

50 **Keywords:** Land surface temperature; Thermal infrared remote sensing; Surface energy balance;  
51 Downscaling; DTsEB

## 52 **1. Introduction**

53 As a key parameter in the characterization of energy and water exchange between land and  
54 atmosphere [Li *et al.*, 2013; Duan & Li, 2016; Anderson *et al.*, 2008], land surface temperature  
55 (LST) has been widely applied in a variety of disciplines and related studies on evapotranspiration  
56 estimation [Tang *et al.*, 2010; Tang & Li, 2017a], urban heat island monitoring [Weng *et al.*, 2004;  
57 Quan *et al.*, 2014], forest fire detection [Eckmann *et al.*, 2008] and biogeochemical process  
58 modeling [Zhan *et al.*, 2016]. Satellite-based thermal infrared (TIR) data are directly linked to  
59 LSTs through the radiative transfer equation and are recognized as the most reliable source for  
60 deriving regional LSTs in a globally consistent and economically feasible manner. However,  
61 because of technical constraints, satellite-derived LST datasets always reflect a tradeoff between  
62 temporal and spatial resolutions [Bindhu *et al.*, 2013; Liu *et al.*, 2020]. Even within the same  
63 satellite, thermal sensors have much lower spatial resolution than visible and near-infrared (VNIR)  
64 sensors due to the relatively lower levels of thermal radiation that are emitted by land surface. The  
65 relatively low spatial resolution of satellite-derived TIR LSTs often leads to a thermal mixture  
66 effect (i.e., blending of multiple thermal elements within a single coarse spatial resolution pixel)  
67 [Yang *et al.*, 2011; Zhan *et al.*, 2013] and provides a weak representation of the heterogeneity of  
68 the land surface water status and energy exchange. Therefore, techniques to enhance the spatial  
69 resolution of satellite-derived LST datasets are highly desirable [Atkinson, 2013; Hutengs &  
70 Vohland, 2016].

71 Over the past decades, a large number of LST downscaling (also called *LST sharpening* or  
72 *LST disaggregating*) methods have been proposed to transform coarse-resolution LSTs to fine  
73 resolution with thermal radiances at the two resolutions invariantly maintained [Kustas *et al.*, 2003;  
74 Zhan *et al.*, 2012, 2013]. Most of these LST downscaling methods assume that the relationships  
75 between surface parameters (e.g., independent variables) and LSTs (e.g., dependent variable) are  
76 scale invariant, and they first construct a mathematical relationship at coarse resolution and  
77 subsequently apply the relationship to surface parameters at fine resolution to obtain fine-  
78 resolution LSTs. The surface parameters used in LST downscaling have been collectively referred  
79 to as scaling factors in some studies (also called *kernels* or *modulation factors* in some other  
80 studies); they represent indicators that connect the LSTs and should be achieved at both coarse and  
81 fine resolutions [Zhan *et al.*, 2011, 2013; Liu & Moore, 1998; Stathopoulou & Cartalis, 2009;  
82 Chen *et al.*, 2014]. Based on the fact that the regional LST variability is most affected by vegetation

83 coverage, vegetation indices (VIs) are the most widely used scaling factors in LST downscaling  
84 algorithms. Since the pioneering LST downscaling methods developed by *Kustas et al. [2003]* and  
85 *Agam et al. [2007]* (named *DisTrad* and *TsHARP*) were proposed, successful tests and applications  
86 of various VIs, such as the normalized difference vegetation index (NDVI) or its derivatives –  
87 fractional vegetation cover ( $f_c$ ), soil-adjusted vegetation index (SAVI) [*Yang et al., 2011*],  
88 enhanced vegetation index (EVI) [*Zakšek & Oštir, 2012*], and green ratio vegetation index (GRVI)  
89 [*Bonafoni, 2016*] – over different land cover types (especially agricultural areas) have been  
90 reported in the LST downscaling literature [*Jeganathan et al., 2011; Essa et al., 2012; Bisquert et*  
91 *al., 2016a; Bisquert et al., 2016b; Olivera-Guerra et al., 2017*]. However, because the LST is  
92 influenced by multiple factors, the relationships between VIs and LSTs display great limitations  
93 for heterogeneous underlying surfaces [*Inamdar & French, 2009; Nichol, 2009; Stathopoulou &*  
94 *Cartalis, 2009; Zakšek & Oštir, 2012*]. To compensate for the deficiency of using only simple  
95 vegetation parameters in LST downscaling, spectral indices representing different types of land  
96 surfaces, such as the normalized difference water index (NDWI), the normalized difference built-  
97 up index (NDBI), the enhanced built-up and bareness index (EBBI), the bare soil index (BI), and  
98 the temperature vegetation dryness index (TVDI), have also been introduced [*Yang et al., 2011;*  
99 *Zakšek & Oštir, 2012; Merlin et al., 2012; Bonafoni, 2016; Li et al., 2019; Agathangelidis &*  
100 *Cartalis, 2019; Liu et al., 2020*]. In addition, to modulate the land surface energy distribution,  
101 topographic variables, namely, digital elevation models (DEMs) and slope angle, surface  
102 emissivity and broadband albedo, were also suggested to be good scaling factors [*Duan & Li, 2016;*  
103 *Li et al., 2019; Agathangelidis and Cartalis, 2019; Inamdar & French, 2009; Nichol, 2009;*  
104 *Stathopoulou & Cartalis, 2009; Zakšek & Oštir, 2012; Merlin et al., 2010, 2012; Dominguez et*  
105 *al., 2011*]. However, although many studies have reported that the accuracy of LST downscaling  
106 results increases with the introduction of new or multiple scaling factors, the selection of scaling  
107 factors (usually without explicit physical implications) remains mostly subjective, uncertain, and  
108 application-specific.

109 For the relationships between scaling factors and LSTs, statistical regression has been widely  
110 used in LST downscaling. Both simple linear or quadratic regression relationships and multivariate  
111 nonlinear regression relationships between single/multiple scaling factors (e.g., NDVI, DEM,  
112 broadband albedo, and surface emissivity) and LSTs were explored in early years [*Kustas et al.,*  
113 *2003; Agam et al., 2007; Dominguez et al, 2011; Yang et al., 2011; Merlin et al., 2010, Merlin et*

114 *al.*, 2012; Bonafoni, 2016; Bisquert *et al.*, 2016a]. In recent years, more advanced regression  
115 methods, including tree-based regression techniques (such as the gradient boosting machine),  
116 kernel-based regression techniques (such as the support vector machine), artificial neural networks,  
117 and random forest techniques, which have great advantages in establishing stable relationships  
118 between multiple scaling factors and LST, have attracted extensive attention [Yang *et al.*, 2010;  
119 Ghosh *et al.*, 2014; Hutengs and Vohland, 2016; Li *et al.*, 2019; Wu and Li, 2019; Agathangelidis  
120 and Cartalis, 2019]. Although great success has been reported for LST downscaling, the lack of a  
121 clear physical mechanism in these empirical regression relationship-based methods has resulted in  
122 difficulties in understanding the interactions of various scaling factors with LSTs and has further  
123 hindered the extension of LST downscaling methods to other study areas. Moreover, the selection  
124 of different scaling factors and the establishment of corresponding empirical relationship between  
125 scaling factors and LST in these different statistics-based methods can even result in different  
126 LSTs for the same pixel under different relationship expression formulas and/or different sizes of  
127 areas of interest (such as the different LST downscaling results for Changping area in the  
128 researches of Yang *et al.* [2011] and Wu & Li [2019]). To date, compared to the statistics-based  
129 LST downscaling methods, (semi)physical methods for achieving LST downscaling have seldom  
130 been proposed [Bechtel *et al.*, 2012]. While tests have been developed to enhance the thermal  
131 details, the apparently unreasonable assumptions of invariable emitted energy (with surface  
132 emissivity as the sole factor influencing temperature variation) among the subpixels [Nichol, 2009]  
133 or isothermal pixels [Liu & Pu, 2008; Liu & Zhu, 2012] have greatly hindered the wide application  
134 of these (semi)physical methods. The dual band method proposed by Dozier [Dozier, 1981] to  
135 estimate the percentage of thermally anomalous coverage and its temperature also faces technical  
136 limitations because of the requirements of a priori knowledge (such as the predefined specific end  
137 members) [Zakšek & Oštir, 2012; Bechtel *et al.*, 2012]. In fact, in the energy and water exchange  
138 between land and atmosphere, the spatial variation of LST is more physically and fundamentally  
139 linked to the surface energy budget (i.e., the surface net radiation, soil heat flux, sensible heat flux  
140 and latent heat flux) than the land surface vegetation information or land cover details [Zhan *et al.*,  
141 2013]. From this point of view, the surface energy balance is very likely to provide a robust and  
142 physical LST downscaling framework to take into account all parameters that drive the spatial  
143 variation of LSTs [Zhan *et al.*, 2013; Merlin *et al.*, 2010].

144 The objective of this study is to develop a physical surface energy balance (SEB)-based LST  
145 downscaling method (DTsEB) to avoid a subjective selection of scaling factors and the  
146 establishment of statistical regression relationships. To this end, the theoretical relationship  
147 between scaling factors and LSTs is at first deduced from the SEB equation and Penman-Monteith  
148 equation. Subsequently, the DTsEB method is developed by calculating the total differential of the  
149 LST, and then, the fine-resolution LSTs can be obtained by converting the differences between the  
150 LSTs at fine and coarse resolutions into differences between the VNIR/SWIR scaling factors at  
151 the two resolutions. Finally, this new approach is tested on both 990 m resolution Moderate  
152 Resolution Imaging Spectroradiometer (MODIS) LST and aggregated 990 m resolution Advanced  
153 Spaceborne Thermal Emission and Reflection Radiometer (ASTER) LST data at six overpass  
154 times between 2005 and 2015 over three 9.9 km by 9.9 km cropland (mixed by grass, tree, and  
155 built-up land) study areas. As a reference, three typical LST downscaling methods, namely the  
156 well-known and most widely applied TsHARP method, the later developed least median square  
157 regression downscaling (LMS) method, and the geographically weighted regression (GWR)  
158 method, are intercompared with the DTsEB method. Section 2 describes the study areas, the  
159 remotely sensed MODIS and ASTER data, and the auxiliary ground-based meteorological data  
160 involved in this study. Section 3 presents the methodology of how LST downscaling is performed  
161 with the DTsEB method. Section 4 provides the LST downscaling results and discusses the  
162 uncertainty, superiority, and weakness of the DTsEB method. Finally, a summary and conclusions  
163 are presented in Section 5.

## 164 **2. Study Area and Data**

### 165 **2.1. Study area**

166 Three study areas (Figure 1) with spatial dimensions of 9.9 km by 9.9 km and characterized  
167 by different climates and soil types were selected to evaluate the adaptability and accuracy of the  
168 DTsEB method.

169 Study area A, which surrounds the Yucheng site (36.8291 °N/116.5703 °E, indicated by  
170 the solid black triangle in Figure 1), is located in the southwestern part of Yucheng County,  
171 Shandong Province, North China. This area is characterized by a subhumid monsoon climate with  
172 a mean annual temperature and precipitation of 13.1 °C and 528 mm, respectively. The soil type  
173 is classified as sandy loam and the land cover types primarily consist of croplands, bare soil and

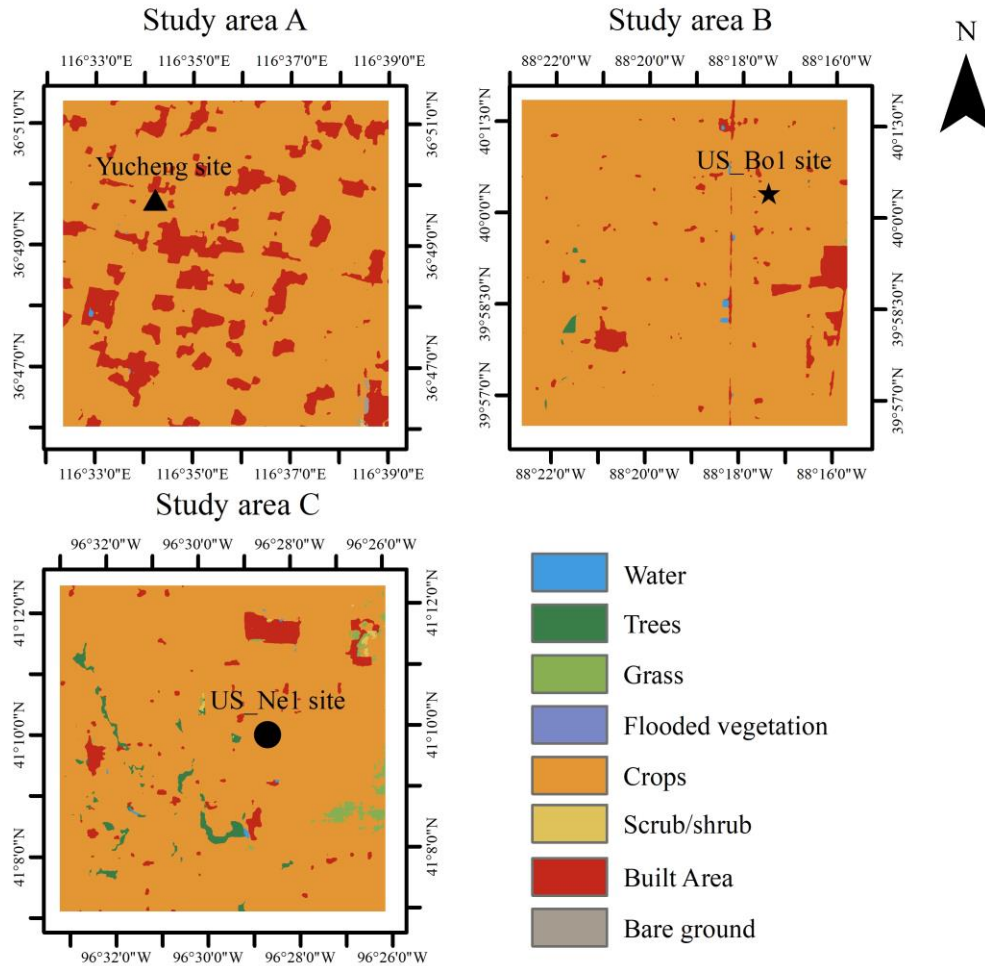
174 built-up lands (including roads and buildings). Winter wheat (seeded in mid-October and harvested  
175 in mid-June) and summer corn (seeded in late June and harvested in early October) are rotated in  
176 this study area. More details of regarding the characteristics of this area can be found in the work  
177 by *Tang & Li [2017b]*.

178 Study area B, which surrounds the US\_Bo1 site (40.0062 °N/88.2904 °W, marked by the  
179 solid black star in Figure 1), is located in the midwestern part of the United States near Champaign,  
180 Illinois. Study area B has a deep silty clay loam soil type and is characterized by a humid  
181 continental climate with a mean annual temperature of 11 °C and mean annual precipitation of 991  
182 mm. The land cover types mainly include crops, trees, and built-up lands. Corn and soybeans are  
183 rotated annually in this study area. The detailed information on study area B was provided by  
184 *Meyers & Hollinger [2004]*.

185 Study area C, which surrounds the US\_Ne1 site (41.1651 °N/96.4766 °W, indicated by the  
186 solid black circle in Figure 1), is located at the University of Nebraska Agricultural Research and  
187 Development Center near Mead, Nebraska, United States. Study area C has a humid continental  
188 climate with a mean annual temperature of 10 °C and mean annual precipitation of 790 mm. The  
189 soil type is classified as deep silty clay loam and the land cover/land use types of this study area  
190 are mainly crops, built-up areas, trees, and grass. Maize and soybeans are seeded under no-till and  
191 are harvested in early November and October, respectively. The detailed information of study area  
192 C was provided by *Verma et al. [2005]*.

193 Surface four-component radiation (downwelling and upwelling shortwave and longwave  
194 radiation) and meteorological variables, including precipitation, wind speed, relative humidity, air  
195 temperature, and atmospheric pressure were regularly measured at half-hourly intervals at the three  
196 ground-based sites. The auxiliary meteorological data required for evaluating the LST  
197 downscaling methods were obtained from the three sites over the three study areas (Yucheng site  
198 in study area A, US\_Bo1 site in study area B and US\_Ne1 site in study area C).





199  
 200 **Figure 1.** Site geolocations (Yucheng site in study area A, US\_Bo1 site in study area B and US\_Ne1 site in  
 201 study area C) and land use/land cover (LULC) types of the three study areas (retrieved from ESA Sentinel-2  
 202 imagery at 10 m resolution), including water, trees, grass, flooded vegetation, crops, built-up area, and bare  
 203 ground.

204 **2.2 Data**

205 The data used in this study include remotely sensed MODIS and ASTER datasets onboard  
 206 the same satellite platform and ground-based meteorological datasets. In each study area, datasets  
 207 from two different dates were used to test the LST downscaling algorithm.

208 **2.2.1 MODIS datasets**

209 MODIS data collected from the MODIS/Terra platform, including the MODIS/Terra Land  
 210 Surface Temperature/Emissivity Daily L3 Global 1 km SIN Grid product (MOD11A1, Collection  
 211 6) and MODIS/Terra Surface Reflectance Daily L2G Global 1 km and 500 m SIN Grid product  
 212 (MOD09GA, Collection 6), were used as the original coarse-resolution data in this study. These

213 data were downloaded from the National Aeronautics and Space Administration's (NASA's)  
214 Level-1 and Atmosphere Archive and Distribution System (LAADS) Distributed Active Archive  
215 Center (DAAC) (<https://ladsweb.modaps.eosdis.nasa.gov/search/>). The two MODIS products  
216 were acquired on April 24, 2006, and October 3, 2010, for study area A, on April 15, 2005 and  
217 July 29, 2005, for study area B, and on September 2, 2014, and August 20, 2015, for study area C  
218 in HDF-EOS format and were reprojected into UTM WGS 1984 50 N, UTM WGS 1984 16 N,  
219 and UTM WGS 1984 14 N, respectively, with a resampling interval of 990 m by using the MODIS  
220 Reprojection Tool (MRT).

221 Coarse-resolution parameters, such as the normalized difference vegetation index (NDVI)  
222 and fractional vegetation cover ( $f_c$ ) (used to calculate the soil heat flux), broadband albedo and  
223 surface emissivity (used to calculate the surface net radiation), and surface resistance and  
224 aerodynamic resistance (used to solve the Penman-Monteith equation) at 990 m can be obtained  
225 with the MOD11A1 and MOD09GA products. For example, the NDVI is calculated using the  
226 reflectance values in the red and near-infrared bands; the surface broadband albedo,  $r$ , is estimated  
227 using the method of *Liang [2001]* (the method of *Mokhtari et al. [2013]* is applied for ASTER  
228 data after April 2008 due to the malfunction of the shortwave infrared detectors), and the surface  
229 emissivity,  $\epsilon_s$ , is calculated using the algorithm proposed by *Qin et al. [2004]* (see the Appendix  
230 D).

### 231 **2.2.2 ASTER datasets**

232 Concurrent remote sensing data from the ASTER sensor onboard the Terra satellite, including  
233 the ASTER L2 Surface Kinetic Temperature product (AST\_08) and ASTER L2 Surface  
234 Reflectance Visible and Near Infrared (VNIR) and Shortwave Infrared (SWIR) product (AST\_07),  
235 were used as the fine-resolution data in this study. These data were collected from NASA's  
236 Earthdata Search web application (<https://search.earthdata.nasa.gov/search/>).

237 The ASTER surface reflectance products (AST\_07), with a pixel size of 15 m in the VNIR  
238 region and 30 m in the SWIR region were spatially aggregated to 90 m to match the original spatial  
239 resolution of ASTER LST (AST\_08) in this study. The surface parameters, including NDVI,  $f_c$ ,  $r$ ,  
240  $\epsilon_s$ , surface resistance, and aerodynamic resistance at 90 m resolution can be calculated with the  
241 AST\_07 data (see the Appendix D).

### 242 **2.2.3 Ground-based meteorological data**

243 Half-hourly surface meteorological variables from the three ground sites (e.g., the Yucheng  
 244 site in study area A, the US-Bo1 site in study area B and the US\_Ne1 site in study area C),  
 245 including downward solar radiation, wind speed, relative humidity, air temperature and vapor  
 246 pressure, were collected at the Terra satellite overpass times as the auxiliary data in this study.  
 247 Given the limited spatial dimensions of the study areas, the spatial variation of near-surface  
 248 meteorological data was low and might contribute less to the downscaled LST than the subpixel  
 249 heterogeneity of surface parameters. The meteorological data from the ground sites were thus  
 250 regarded as spatially representative over the entire study area.

## 251 2.2.4 Digital elevation data

252 The digital elevation data (DEM) was used as the auxiliary data in the GWR method. 30 m  
 253 DEM data of the three study areas (N36E116 for study area A, N39W089 and N40W089 for study  
 254 area B, and N41W097 for study area C) collected from the ASTGTM product (Version 3,  
 255 <https://search.earthdata.nasa.gov/search/>) were spatially aggregated to 90 m and 990 m to match  
 256 the fine and coarse resolution ASTER and MODIS datasets, respectively.

## 257 3. Methodology

### 258 3.1 DTsEB method

259 LST is a direct indicator in the exchange of long-wave radiation and turbulent heat fluxes at  
 260 the land–atmosphere interface and can effectively characterize the physical processes of surface  
 261 energy and water balance at local to global scales [Li *et al.*, 2013]. Considering the physical  
 262 interconnections between LSTs and land surface energy, we propose the DTsEB method (the flow  
 263 chart is shown in Figure 2) by introducing the surface energy balance equation and Penman-  
 264 Monteith equation, as follows:

$$265 \quad R_n = G + H + LE \quad (1)$$

$$266 \quad LE = \frac{\Delta(R_n - G) + \rho C_p VPD / r_a}{\Delta + \gamma(1 + r_s / r_a)} \quad (2)$$

267 where  $R_n$  is the surface net radiation,  $\text{W/m}^2$ ;  $G$  is the soil heat flux,  $\text{W/m}^2$ ;  $H$  is the sensible heat  
 268 flux,  $\text{W/m}^2$ ;  $LE$  is the latent heat flux,  $\text{W/m}^2$ ;  $\Delta$  is the slope of the saturated vapor pressure versus  
 269 air temperature curve,  $\text{kPa/}^\circ\text{C}$ ;  $\rho$  is the air density,  $\text{kg/m}^3$ ;  $C_p$  is the specific heat of air,  $\text{J}/(\text{kg }^\circ\text{C})$ ;

270  $VPD$  is the vapor pressure deficit of air, kPa;  $r_a$  is the aerodynamic resistance, s/m;  $r_s$  is the surface  
 271 resistance, s/m; and  $\gamma$  is the psychrometric constant, kPa/ °C.

272 The sensible heat flux ( $H$ ) can be approximated by combining the difference between LST  
 273 and air temperature ( $T_a$ ) with the aerodynamic resistance ( $r_a$ ), as follows:

$$274 \quad H = \rho C_p \frac{LST - T_a}{r_a} \quad (3)$$

275 The soil heat flux ( $G$ ) is often expressed as a fraction of the surface net radiation ( $R_n$ ) from  
 276 the remote sensing perspective and it is estimated following the work of *Su [2002]* in this study,  
 277 as follows:

$$278 \quad G = R_n \left[ \Gamma_c + (1 - f_c)(\Gamma_s - \Gamma_c) \right] \quad (4)$$

279 where  $f_c$  is the fractional vegetation cover, and  $\Gamma_c$  and  $\Gamma_s$  are the fractions of  $G$  to  $R_n$  for fully  
 280 covered vegetation and dry bare soil, respectively.

281 By combining and rearranging equations (1), (2), (3) and (4), we can mathematically express  
 282 the LST with the following equations:

$$283 \quad LST = \frac{r_a \left[ 1 - \Gamma_s + (\Gamma_s - \Gamma_c) f_c \right] R_n}{\rho C_p} \frac{\gamma (1 + r_s / r_a)}{\Delta + \gamma (1 + r_s / r_a)} - \frac{VPD}{\Delta + \gamma (1 + r_s / r_a)} + T_a \quad (5)$$

284 with

$$285 \quad R_n = (1 - r) R_g + \varepsilon_s \varepsilon_a \sigma T_a^4 - \varepsilon_s \sigma LST^4 \quad (6)$$

$$286 \quad f_c = \left( \frac{NDVI - NDVI_{min}}{NDVI_{max} - NDVI_{min}} \right)^2 \quad (7)$$

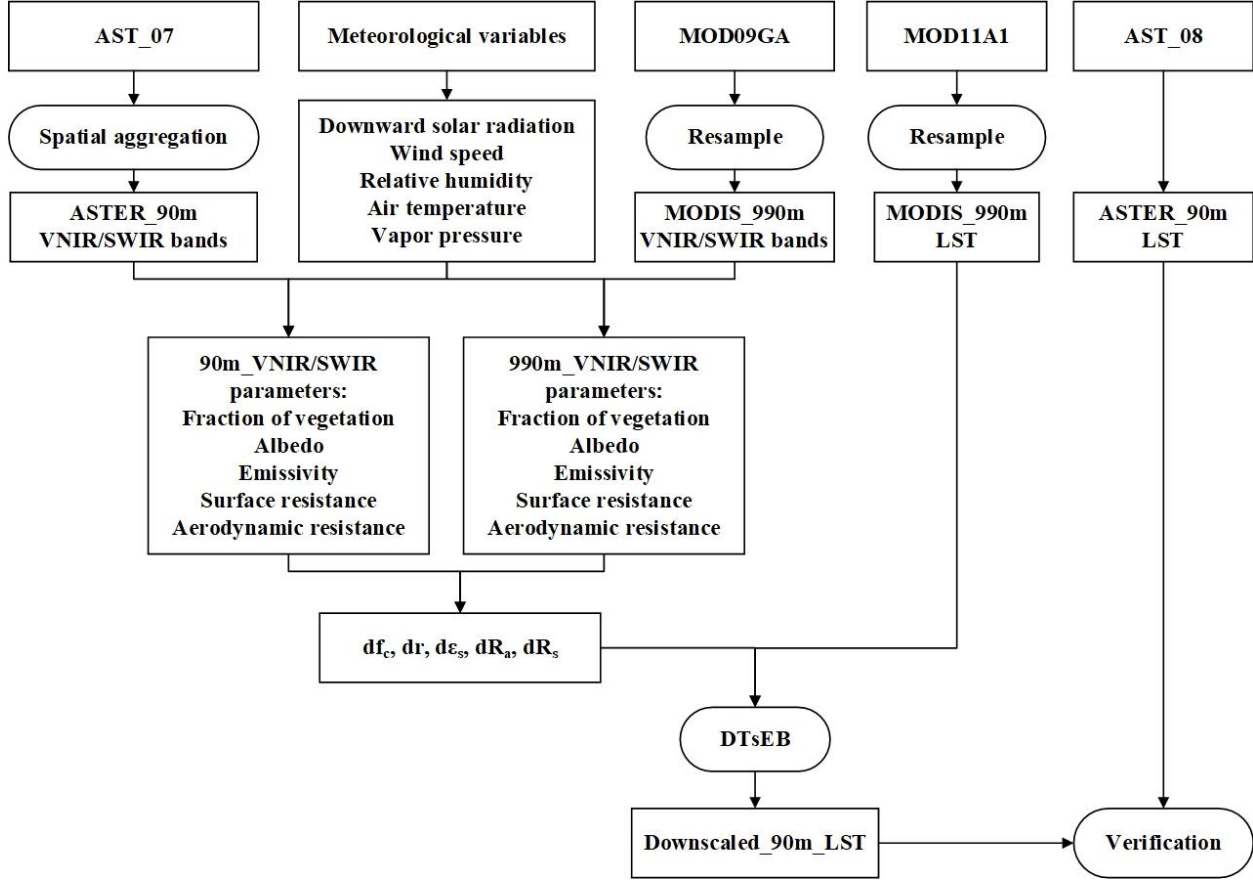
$$287 \quad r_a = \frac{\left[ \ln \left( \frac{Z_u - d}{Z_{om}} \right) - \Psi_m \right] \left[ \ln \left( \frac{Z_t - d}{Z_{oh}} \right) - \Psi_h \right]}{k^2 u} \quad (8)$$

$$288 \quad r_s = \frac{1}{C_L m(T_{min}) m(VPD) LAI} \quad (9)$$

289 where  $R_g$  is the global solar radiation,  $\text{W/m}^2$ ;  $r$  is the surface albedo;  $\varepsilon_s$  is the surface emissivity;  $\varepsilon_a$   
 290 is the atmospheric emissivity;  $\sigma$  is the Stefan-Boltzmann constant; and  $NDVI_{min}$  and  $NDVI_{max}$  are  
 291 the minimum NDVI corresponding to bare soil and the maximum NDVI corresponding to fully  
 292 vegetated surfaces, respectively;  $Z_u$  and  $Z_t$  are the heights at which the wind speed and air  
 293 temperature are observed, respectively, m;  $k$  is the von Karman constant;  $u$  is the wind speed, m/s;  
 294  $d$  is the zero plane displacement height, m;  $z_{om}$  is the surface momentum roughness height, m;  $z_{oh}$   
 295 is the roughness height for surface heat transfer, m;  $\Psi_m$  and  $\Psi_h$  are the stability correction functions  
 296 for momentum and heat transfer, respectively [Paulson, 1970];  $LAI$  is the leaf area index;  $C_L$  is the  
 297 mean potential stomatal conductance per unit leaf area;  $m(T_{min})$  is a multiplier that limits the  
 298 potential stomatal conductance by the minimum air temperature; and  $m(VPD)$  is a multiplier used  
 299 to reduce the potential stomatal conductance when the VPD is sufficient to reduce the canopy  
 300 conductance [Mu et al., 2007, 2011]. In Eq. (5), all the surface environmental and ecophysiological  
 301 parameters including the fractional vegetation cover, surface emissivity, broadband albedo,  
 302 aerodynamic resistance, surface resistance, and surface net radiation that are involved in the  
 303 surface energy budget and drive the spatial variation of the LSTs are mechanically interrelated.

304 In this work,  $\Gamma_c = 0.05$  and  $\Gamma_s = 0.4$  are assumed in the soil heat flux calculations [Daughtry  
 305 et al., 1990; Li & Lyons, 1999; Tang et al., 2010];  $z_{oh} = 0.1z_{om}$  where  $z_{om}$  is 0.125 times the  
 306 vegetation height,  $h$  ( $z_{om} = 0.125h$ ), and in this study, following the work of Tang et al. [2013] and  
 307 Teixeira et al. [2009],  $h$  is estimated as a function of the surface albedo and NDVI. A summary of  
 308 how these intermediate variables/parameters are estimated is provided in the Appendix D.

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**Figure 2.** Flow chart of LST downscaling based on the DTsEB algorithm

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Given the negligible spatial variations in the atmospheric parameters over the subpixels within a coarse pixel, the difference between fine-resolution LST and coarse-resolution LST primarily comes from the heterogeneity of the surface parameters (e.g., albedo, emissivity, fractional vegetation cover, resistance) within the coarse pixel and can be obtained by calculating the total differential of Eq. (5), as follows:

317

$$dLST = \frac{\partial LST}{\partial R_n} dR_n + \frac{\partial LST}{\partial f_c} df_c + \frac{\partial LST}{\partial r_a} dr_a + \frac{\partial LST}{\partial r_s} dr_s \quad (10)$$

318 with

319

$$dR_n = -R_g dr + (\epsilon_a \sigma T_a^4 - \sigma LST_{CR}^4) d\epsilon_s - 4\epsilon_s \sigma LST_{CR}^3 dLST \quad (11)$$

320

We combine equation (11) into equation (10), as follows:

$$dLST = \frac{\frac{\partial LST}{\partial R_n} \left[ -R_s dr + (\varepsilon_a \sigma T_a^4 - \sigma LST_{CR}^4) d\varepsilon_s \right] + \frac{\partial LST}{\partial f_c} df_c + \frac{\partial LST}{\partial r_a} dr_a + \frac{\partial LST}{\partial r_s} dr_s}{1 + \frac{\partial LST}{\partial R_n} 4\varepsilon_s \sigma LST_{CR}^3} \quad (12)$$

in which,

$$\frac{\partial LST}{\partial R_n} = \frac{r_a \left[ 1 - \Gamma_s + (\Gamma_s - \Gamma_c) f_c \right]}{\rho C_p} \frac{\gamma (1 + r_s/r_a)}{\Delta + \gamma (1 + r_s/r_a)} \quad (13)$$

$$\frac{\partial LST}{\partial f_c} = \frac{r_a (\Gamma_s - \Gamma_c) R_n}{\rho C_p} \frac{\gamma (1 + r_s/r_a)}{\Delta + \gamma (1 + r_s/r_a)} \quad (14)$$

$$\frac{\partial LST}{\partial r_a} = \frac{\left[ 1 - \Gamma_s + (\Gamma_s - \Gamma_c) f_c \right] R_n}{\rho C_p} \frac{\gamma \Delta + \gamma^2 (1 + r_s/r_a)^2}{\left[ \Delta + \gamma (1 + r_s/r_a) \right]^2} - \frac{\gamma VPD r_s / r_a^2}{\left[ \Delta + \gamma (1 + r_s/r_a) \right]^2} \quad (15)$$

$$\frac{\partial LST}{\partial r_s} = \frac{\left[ 1 - \Gamma_s + (\Gamma_s - \Gamma_c) f_c \right] R_n}{\rho C_p} \frac{\gamma \Delta}{\left[ \Delta + \gamma (1 + r_s/r_a) \right]^2} + \frac{\gamma VPD / r_a}{\left[ \Delta + \gamma (1 + r_s/r_a) \right]^2} \quad (16)$$

where the  $\frac{\partial LST}{\partial R_n}$ ,  $\frac{\partial LST}{\partial f_c}$ ,  $\frac{\partial LST}{\partial r_a}$  and  $\frac{\partial LST}{\partial r_s}$  can be calculated with the coarse resolution VNIR/SWIR and ground-based meteorological data, the  $dR_n$ ,  $df_c$ ,  $dr_a$ ,  $dr_s$ ,  $dr$ , and  $d\varepsilon_s$  are the variations of  $R_n$ ,  $f_c$ ,  $r_a$ ,  $r_s$ ,  $r$ , and  $\varepsilon_s$  between fine and coarse resolutions, respectively, and the  $\frac{\partial LST}{\partial R_n} dR_n$ ,  $\frac{\partial LST}{\partial f_c} df_c$ ,  $\frac{\partial LST}{\partial r_a} dr_a$ , and  $\frac{\partial LST}{\partial r_s} dr_s$  represent the contribution of surface net radiation, the contribution of fraction of the vegetation, the contribution of aerodynamic resistance, and the contribution of surface resistance to  $dLST$ , respectively. The subscript CR stands for the variable at coarse resolution.

Overall, combining the surface energy balance equation and Penman-Monteith equation, we can express the differences between LSTs at fine and coarse resolutions as a function of the differences between the surface parameters (i.e.,  $\frac{\partial LST}{\partial R_n} dR_n$ ,  $\frac{\partial LST}{\partial f_c} df_c$ ,  $\frac{\partial LST}{\partial r_a} dr_a$  and  $\frac{\partial LST}{\partial r_s} dr_s$ , which can be obtained with VNIR/SWIR data) at the two resolutions. The final downscaled fine-resolution LST ( $LST_{FR}$ ) can be expressed as the sum of the coarse-resolution LST ( $LST_{CR}$ ) and the LST difference, as follows:

339 
$$LST_{FR} = LST_{CR} + dLST \quad (17)$$

340 **3.2 Model application**

341 To better understand error propagation in LST downscaling and how the reference LST truth  
342 affects the model performance, the proposed physical-based DTsEB method is evaluated for two  
343 different cases. As a reference, the downscaling results from the widely applied TsHARP method  
344 [Agam *et al.*, 2007; Kustas *et al.*, 2003], the LMS method [Mukherjee *et al.*, 2014; Bisquert *et al.*,  
345 2016], and the GWR method [Duan *et al.*, 2016] (see the Appendix A, B, and C for a description  
346 of these three methods) are also intercompared.

347 Case 1: downscaling of the 990 m MODIS LST product to 90 m and validation against the  
348 concurrent 90 m ASTER LST product. In this case, six scenes of original coarse-resolution  
349 MODIS LST data (990 m) for different growing dates of crops over three study areas were first  
350 downscaled to 90 m. Then, the fine-resolution ASTER LST products at 90 m (AST\_08) were used  
351 as the reference LST data to validate the downscaled results. Because both the MODIS and ASTER  
352 sensors are onboard the same satellite platform (Terra), errors caused by altitude and time  
353 differences between different satellites can be eliminated.

354 Case 2: downscaling of 990 m aggregated ASTER LST data to 90 m and validation against  
355 the 90 m ASTER LST product that was used for aggregation. In this case, the original 90 m ASTER  
356 datasets were first spatially aggregated to a resolution of 990 m by assuming the conservation of  
357 surface emitted energy for AST\_08 LST products and by the arithmetic mean for the AST\_07  
358 reflectance products. The LST downscaling methods were then performed on these aggregated  
359 datasets. The aggregated 990 m LSTs were used here with an implicit assumption that the coarse-  
360 resolution LSTs are highly consistent with the reference fine-resolution LSTs. The uncertainties  
361 introduced by the differences between the coarse-resolution LSTs and reference fine-resolution  
362 LSTs can therefore be excluded to some extent.

363 During model application, essential quality control procedures were conducted to remove  
364 pixels (~ 0.3%) characterized by low vegetation cover (NDVI < 0.1) with extremely high  $r_a$  and  $r_s$   
365 (> 1,000 s/m) values at 90 m resolution, to reduce the abnormalities in the downscaled LSTs in the  
366 DTsEB method. Note that fine-resolution data in this study were from 90 m ASTER NVIR and  
367 SWIR reflectance products. More generally, for a targeted coarse-resolution LST to be downscaled



368 in practical applications, concurrent (or adjacent) reflectance measurements with the sensor  
 369 onboard the same (or other) satellite platform can be used as the fine-resolution data.

### 370 3.3 Statistical Analyses

371 Once the LST downscaling results are obtained, they were compared with the 90 m reference  
 372 fine-resolution ASTER LST. The following statistical metrics, namely the root mean square error  
 373 (RMSE), mean absolute error (MAE), mean bias (BIAS), normalized root mean square error  
 374 (NRMSE), and correlation coefficient (R), were calculated to measure the model performance, as  
 375 shown in Equations (18) - (22):

$$376 \quad RMSE = \sqrt{\frac{\sum_{i=1}^n (LST_{dsl,i} - LST_{ref,i})^2}{n}} \quad (18)$$

$$377 \quad MAE = \frac{\sum_{i=1}^n |LST_{dsl,i} - LST_{ref,i}|}{n} \quad (19)$$

$$378 \quad BIAS = \frac{\sum_{i=1}^n (LST_{dsl,i} - LST_{ref,i})}{n} \quad (20)$$

$$379 \quad NRMSE = \frac{RMSE}{SD} \quad (21)$$

$$380 \quad R = \frac{\sum_{i=1}^n (LST_{dsl,i} - \overline{LST_{dsl,i}})(LST_{ref,i} - \overline{LST_{ref,i}})}{\sqrt{\sum_{i=1}^n (LST_{dsl,i} - \overline{LST_{dsl,i}})^2} \sqrt{\sum_{i=1}^n (LST_{ref,i} - \overline{LST_{ref,i}})^2}} \quad (22)$$

381 where,  $LST_{dsl}$  is the downscaled LST,  $LST_{ref}$  is the reference LST,  $\overline{LST_{dsl}}$  and  $\overline{LST_{ref}}$  are the  
 382 average values of  $LST_{dsl}$  and  $LST_{ref}$ , respectively, SD is the standard deviation of reference LST.

## 383 4. Results and Discussion

### 384 4.1 Application to MODIS datasets

385 Before using the ASTER LST data to evaluate the downscaling results of the coarse-  
 386 resolution MODIS LST data, the original 990 m MODIS LST data, the aggregated 990 m ASTER

387 LST data and the reference 90 m ASTER LST data from study areas A, B and C were compared,  
388 as shown in Table 1 and Figure 3. A deviation was found between the ASTER LST products  
389 (AST08) and the MODIS LST products (MOD11A1) because the former were generated from the  
390 Temperature/Emissivity Separation (TES) algorithm while the latter were generated from the  
391 generalized spilt-window (GSW) algorithm. From a visual comparison, clear spatial pattern  
392 differences between the MODIS LST (Figure 3a) and ASTER LST (Figure 3b) data were observed.  
393 The spatial distribution of the MODIS LSTs was smooth, whereas the ASTER LSTs could more  
394 effectively reflect sharp variations and spatial heterogeneity over the three study areas. In addition,  
395 compared with the ASTER LSTs, the MODIS LSTs were lower overall (approximately 2 K lower  
396 on average, see Table 1), especially in the high value range of LSTs. For example, the differences  
397 between the highest ASTER and MODIS LSTs on April 24, 2006 for study area A, on July 29,  
398 2005 for study area B and on August 20, 2015 for study area C were as great as ~10 K, ~14 K and  
399 ~12 K, respectively, while in the low value range of LSTs, the MODIS LSTs were observed to be  
400 somewhat higher than the ASTER LSTs (Figure 3 and Table 1). These differences imply that the  
401 MODIS LSTs had a narrower value distribution than the ASTER LSTs, and this narrower value  
402 distribution was much remarkable than that of aggregated ASTER LSTs.

403 **Table 1.** The minimum, maximum, and mean of the coarse-resolution MODIS LSTs and the aggregated ASTER  
404 LSTs for model applications and the reference fine-resolution ASTER LSTs for validation.

| Study Area & Date |                      | MODIS LST   |             |             | Aggregated ASTER LST |             |             | ASTER LST   |             |             |
|-------------------|----------------------|-------------|-------------|-------------|----------------------|-------------|-------------|-------------|-------------|-------------|
|                   |                      | at 990 m    |             |             | at 990 m             |             |             | at 90 m     |             |             |
|                   |                      | Min.<br>(K) | Max.<br>(K) | Mean<br>(K) | Min.<br>(K)          | Max.<br>(K) | Mean<br>(K) | Min.<br>(K) | Max.<br>(K) | Mean<br>(K) |
| A                 | April 24, 2006       | 294.36      | 297.80      | 295.94      | 295.85               | 303.43      | 298.30      | 294.30      | 307.34      | 298.25      |
| A                 | October 3, 2010      | 297.64      | 300.16      | 298.73      | 298.63               | 302.06      | 300.00      | 295.20      | 306.16      | 299.97      |
| B                 | April 15, 2005       | 298.10      | 303.74      | 301.28      | 299.60               | 307.19      | 303.89      | 293.78      | 310.47      | 303.86      |
| B                 | July 29, 2005        | 299.56      | 304.18      | 300.79      | 300.36               | 309.91      | 302.32      | 298.70      | 318.20      | 302.35      |
| C                 | September 2,<br>2014 | 298.0       | 301.48      | 299.19      | 298.66               | 304.60      | 300.84      | 296.50      | 312.90      | 300.83      |
| C                 | August 20, 2015      | 298.64      | 302.04      | 299.64      | 300.72               | 305.93      | 302.42      | 296.50      | 314.30      | 302.41      |

405 Figures 3 and 4 show the spatial patterns of the LSTs downscaled from MODIS products  
406 using the DTsEB, TsHARP, LMS and GWR methods and scatter plots of the comparisons between  
407 the downscaled LSTs and ASTER LSTs, respectively. In general, the spatial distributions of the  
408 downscaling results based on the DTsEB (Figure 3c), TsHARP (Figure 3d), LMS (Figure 3(e))  
409 and GWR (Figure 3(f)) were basically consistent with the spatial distribution of the ASTER LSTs  
410 (Figure 3b). All the four LST downscaling methods were able to enhance the spatial details of the  
411 original coarse pixels to some extent. However, in reference to the ASTER LSTs, the DTsEB  
412 method could more successfully reconstruct the subpixel spatial variations within a coarse MODIS  
413 LST pixel and, in particular, display the texture features better than the TsHARP, LMS, and GWR  
414 methods for all three study areas. For example, from circled region 1 in study area A on April 24,  
415 2006 and circled region 3 in study area C on September 2, 2014, the high-value subpixels within  
416 the low-value coarse-resolution pixels were better reproduced in the DTsEB downscaled LSTs,  
417 whereas smooth subpixel variation was represented in the TsHARP, LMS, and GWR downscaled  
418 LSTs. For the generally high LST values in study area B on April 15, 2005 (see circled region 2  
419 in Figure 3), the spatial details of the low LST subpixels that were mixed with high-value pixels  
420 could also be better displayed by the DTsEB method. In summary, the DTsEB method  
421 outperformed the TsHARP, LMS, and GWR methods in all the study areas, i.e., A, B and C.  
422 Especially for high value ranges of LSTs, the DTsEB method better reproduced the spatial details  
423 of ASTER LSTs (but possibly with some scatters over study areas B and C, as shown in Figure 4)  
424 whereas the TsHARP, LMS, and GWR methods significantly underestimated the reference LSTs.  
425 In addition, the LST downscaling results of study areas A and C were better than those of study  
426 area B regardless of which method was used. Overall, for the six scenes of LST downscaling, the  
427 DTsEB method, with a lower root mean square error (RMSE) of 1.46~3.02 K, mean absolute error  
428 (MAE) of 1.20~2.53 K, mean bias of -2.06~-0.23 K, normalized RMSE (by standard deviation of  
429 90 m reference ASTER data) of 0.70~1.29 and correlation coefficient of 0.38~0.79, achieved a  
430 higher accuracy than the TsHARP, LMS, and GWR methods. By contrast, the TsHARP method,  
431 with RMSE values of 1.57~3.21 K, MAE values of 1.31~2.71 K, mean bias values of -2.43~-1.19  
432 K, normalized RMSE values of 0.90~1.39 and correlation coefficient values of 0.46~0.76,  
433 performed slightly worse than the LMS method, and the GWR method. With an intermediate  
434 performance, the LMS method had RMSE values of 1.56~3.38 K, MAE values of 1.30~2.88 K,  
435 mean bias values of -2.59~-1.04 K, normalized RMSE values of 0.89~1.44 and correlation

436 coefficient of values 0.39~0.77 and the GWR method had RMSE values of 1.57~3.25 K, MAE  
437 values of 1.30~2.74 K, mean bias values of -2.41~-1.15 K, normalized RMSE values of 0.90~1.33  
438 and correlation coefficient of values 0.40~0.83 (Table 2 and 4). In other words, the RMSE  
439 decreased by 0.11~0.70 K (~17% on average), 0.04~0.50 K (~14% on average), and 0.08~0.58 K  
440 (~16% on average) and the MAE decreased by 0.11~0.71 K (~16% on average), 0.09~0.51 K (~14%  
441 on average) and 0.10~0.67 K (~15%) when the DTsEB method was applied for LST downscaling  
442 instead of the TsHARP method, the LMS method, and the GWR method, respectively.

443 As mentioned in the Methodology section, the sum of the surface net radiation ( $R_n$ ), fractional  
444 vegetation cover ( $f_c$ ), aerodynamic resistance ( $r_a$ ), and surface resistance ( $r_s$ ) contributions  
445 constitutes the final  $dLST$  (the difference in LST between 990 m and 90 m resolutions) in the  
446 DTsEB method. Figure 5 displays the spatial distribution of the contributions of the above four  
447 surface parameters in study areas A, B and C. From a visual comparison, the contributions of each  
448 of the four parameters varied both spatially and temporally and were different from each other.  
449 Compared with those of the other three parameters, the spatial variation of the contribution of  $r_s$   
450 (Figure 5(d)) was more similar to that of  $dLST$  (Figure 5e). The contribution of  $r_s$  ( $1.26 \pm 1.39$  K  
451 on average) had the greatest impact on the final  $dLST$  results, especially for the high-value ranges  
452 of  $dLST$ , whereas the lowest impacts and narrower variation ranges were found for the  
453 contributions of  $R_n$  ( $0.33 \pm 0.21$  K on average, Figure 5a). In addition, the contributions of  $f_c$   
454 (Figure 5b) were negatively correlated with  $dLST$ , while the contributions of  $r_s$  were positively  
455 correlated with  $dLST$ , which means that in the process of LST downscaling from a coarse  
456 resolution to a fine resolution, an increase in  $f_c$  or decrease in  $r_s$  could lead to a decrease in LST  
457 and vice versa. However, no simple correlation relationship was found between the contribution  
458 of  $R_n$  or  $r_a$  and  $dLST$ .

459 **Table 2.** Statistical metrics of the validation of the downscaled 90 m LST by the DTsEB, TsHARP, LMS, and GWR methods from the 6 scenes of 990 m  
 460 MODIS LST over three study areas with the corresponding 90 m ASTER LST. RMSE is the root mean square error, MAE is the mean absolute error, and  
 461 NRMSE is the RMSE normalized by the standard deviation (SD) of the reference 90 m ASTER LST.

| Study area & Date |               | Methods  |         |          |       |          |         |          |       |          |         |          |       |          |         |          |       |
|-------------------|---------------|----------|---------|----------|-------|----------|---------|----------|-------|----------|---------|----------|-------|----------|---------|----------|-------|
|                   |               | DTsEB    |         |          |       | TsHARP   |         |          |       | LMS      |         |          |       | GWR      |         |          |       |
|                   |               | RMSE (K) | MAE (K) | BIAS (K) | NRMSE | RMSE (K) | MAE (K) | BIAS (K) | NRMSE | RMSE (K) | MAE (K) | BIAS (K) | NRMSE | RMSE (K) | MAE (K) | BIAS (K) | NRMSE |
| A                 | Apr. 24, 2006 | 1.84     | 1.37    | -0.89    | 0.70  | 2.37     | 1.72    | -1.51    | 0.90  | 2.34     | 1.71    | -1.51    | 0.89  | 2.36     | 1.69    | -1.56    | 0.90  |
| A                 | Oct. 3, 2010  | 1.46     | 1.20    | -1.04    | 1.22  | 1.57     | 1.31    | -1.24    | 1.31  | 1.56     | 1.30    | -1.22    | 1.30  | 1.57     | 1.30    | -1.23    | 1.32  |
| B                 | Apr. 15, 2005 | 3.02     | 2.53    | -2.06    | 1.29  | 3.21     | 2.71    | -2.43    | 1.37  | 3.38     | 2.88    | -2.59    | 1.44  | 3.25     | 2.74    | -2.41    | 1.38  |
| B                 | Jul. 29, 2005 | 2.03     | 1.26    | -0.74    | 0.79  | 2.46     | 1.54    | -1.38    | 0.96  | 2.32     | 1.46    | -1.27    | 0.91  | 2.44     | 1.53    | -1.39    | 0.95  |
| C                 | Sept. 2, 2014 | 1.92     | 1.33    | -0.23    | 0.91  | 2.10     | 1.52    | -1.19    | 1.00  | 1.96     | 1.42    | -1.04    | 0.93  | 2.00     | 1.45    | -1.15    | 0.95  |
| C                 | Aug. 20, 2015 | 2.06     | 1.54    | -1.05    | 1.04  | 2.76     | 2.25    | -2.22    | 1.39  | 2.52     | 2.05    | -2.00    | 1.27  | 2.64     | 2.22    | -2.20    | 1.33  |
| Overall           |               | 2.01     | 1.54    | -1.00    | 0.99  | 2.41     | 1.84    | -1.66    | 1.16  | 2.35     | 1.80    | -1.61    | 1.12  | 2.38     | 1.82    | -1.66    | 1.14  |

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**Table 3.** Same as Table 2, but for the 990 m aggregated ASTER data.

| Study area & Date |               | Methods  |         |          |       |          |         |          |       |          |         |          |       |          |         |          |       |
|-------------------|---------------|----------|---------|----------|-------|----------|---------|----------|-------|----------|---------|----------|-------|----------|---------|----------|-------|
|                   |               | DTsEB    |         |          |       | TsHARP   |         |          |       | LMS      |         |          |       | GWR      |         |          |       |
|                   |               | RMSE (K) | MAE (K) | BIAS (K) | NRMSE | RMSE (K) | MAE (K) | BIAS (K) | NRMSE | RMSE (K) | MAE (K) | BIAS (K) | NRMSE | RMSE (K) | MAE (K) | BIAS (K) | NRMSE |
| A                 | Apr. 24, 2006 | 1.54     | 1.25    | 0.30     | 0.59  | 1.74     | 1.35    | -0.06    | 0.66  | 1.69     | 1.28    | 0.05     | 0.65  | 1.76     | 1.34    | 0.05     | 0.67  |
| A                 | Oct. 3, 2010  | 0.95     | 0.72    | 0.12     | 0.79  | 1.17     | 0.90    | 0.41     | 0.98  | 1.10     | 0.86    | 0.03     | 0.92  | 1.12     | 0.87    | 0.03     | 0.94  |
| B                 | Apr. 15, 2005 | 1.85     | 1.45    | 0.14     | 0.79  | 2.32     | 1.73    | -0.03    | 0.99  | 2.03     | 1.58    | 0.03     | 0.86  | 2.36     | 1.79    | 0.02     | 1.00  |
| B                 | Jul. 29, 2005 | 1.46     | 0.99    | 0.06     | 0.57  | 1.97     | 1.35    | -0.24    | 0.77  | 2.12     | 1.30    | -0.03    | 0.83  | 1.67     | 1.11    | -0.08    | 0.65  |
| C                 | Sept. 2, 2014 | 1.45     | 1.03    | 0.25     | 0.69  | 1.53     | 1.13    | -0.09    | 0.73  | 1.52     | 1.10    | 0.01     | 0.72  | 1.59     | 1.16    | -0.01    | 0.75  |
| C                 | Aug. 20, 2015 | 1.29     | 0.92    | 0.24     | 0.65  | 1.51     | 1.11    | -0.08    | 0.76  | 1.31     | 0.89    | 0.01     | 0.66  | 1.32     | 0.90    | 0.01     | 0.66  |
| Overall           |               | 1.42     | 1.06    | 0.19     | 0.68  | 1.71     | 1.26    | -0.02    | 0.82  | 1.63     | 1.17    | 0.03     | 0.77  | 1.64     | 1.20    | 0.003    | 0.78  |

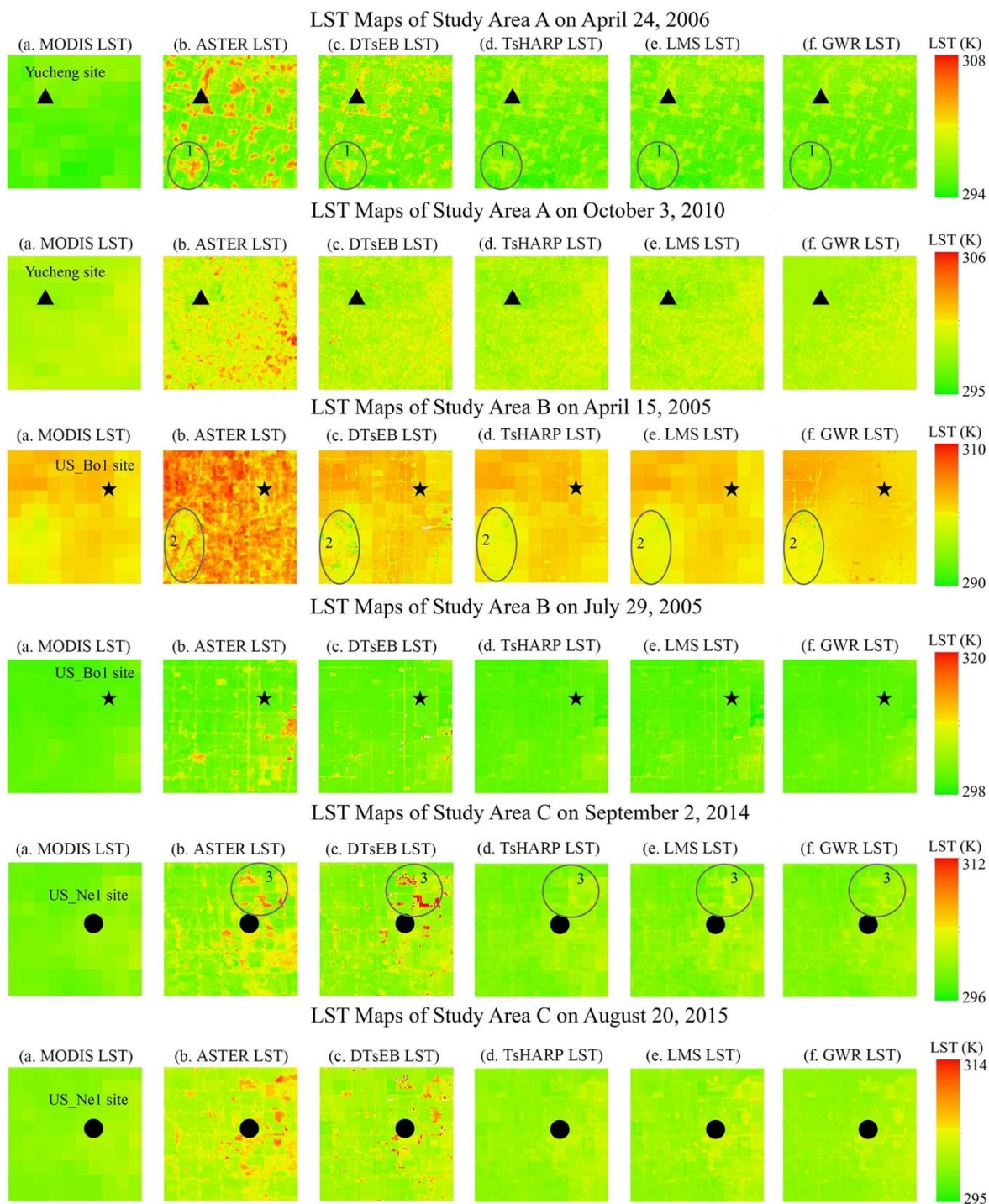
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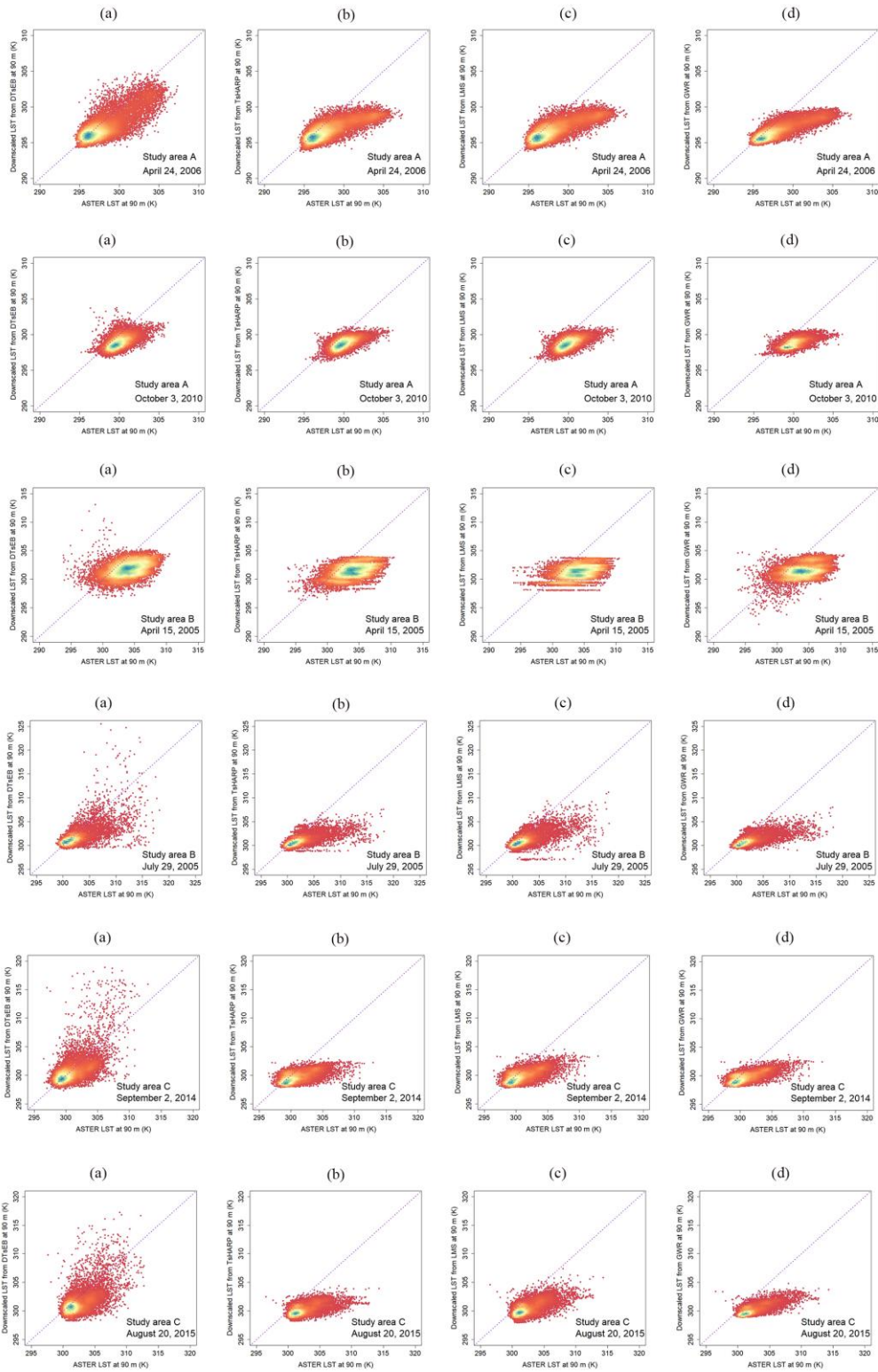
466 **Table 4.** The correlation coefficient (R) between 90 m downscaled LST by the DTsEB, TsHARP, LMS, and GWR methods and the reference 90 m ASTER  
 467 LST over the three study areas.

| Study area & Date |               | Methods      |                         |              |                         |              |                         |           |                         |
|-------------------|---------------|--------------|-------------------------|--------------|-------------------------|--------------|-------------------------|-----------|-------------------------|
|                   |               | DTsEB        |                         | TsHARP       |                         | LMS          |                         | GWR       |                         |
|                   |               | MODIS<br>LST | Aggregated<br>ASTER LST | MODIS<br>LST | Aggregated<br>ASTER LST | MODIS<br>LST | Aggregated<br>ASTER LST | MODIS LST | Aggregated<br>ASTER LST |
| A                 | Apr. 24, 2006 | 0.79         | 0.83                    | 0.76         | 0.84                    | 0.77         | 0.85                    | 0.83      | 0.85                    |
| A                 | Oct. 3, 2010  | 0.55         | 0.63                    | 0.59         | 0.61                    | 0.58         | 0.61                    | 0.58      | 0.57                    |
| B                 | Apr. 15, 2005 | 0.38         | 0.63                    | 0.46         | 0.56                    | 0.39         | 0.60                    | 0.40      | 0.47                    |
| B                 | Jul. 29, 2005 | 0.66         | 0.82                    | 0.66         | 0.80                    | 0.67         | 0.80                    | 0.69      | 0.80                    |
| C                 | Sept. 2, 2014 | 0.61         | 0.75                    | 0.59         | 0.76                    | 0.63         | 0.76                    | 0.68      | 0.74                    |
| C                 | Aug. 20, 2015 | 0.59         | 0.78                    | 0.58         | 0.72                    | 0.64         | 0.80                    | 0.73      | 0.79                    |
| Overall           |               | 0.60         | 0.74                    | 0.61         | 0.72                    | 0.61         | 0.74                    | 0.65      | 0.70                    |

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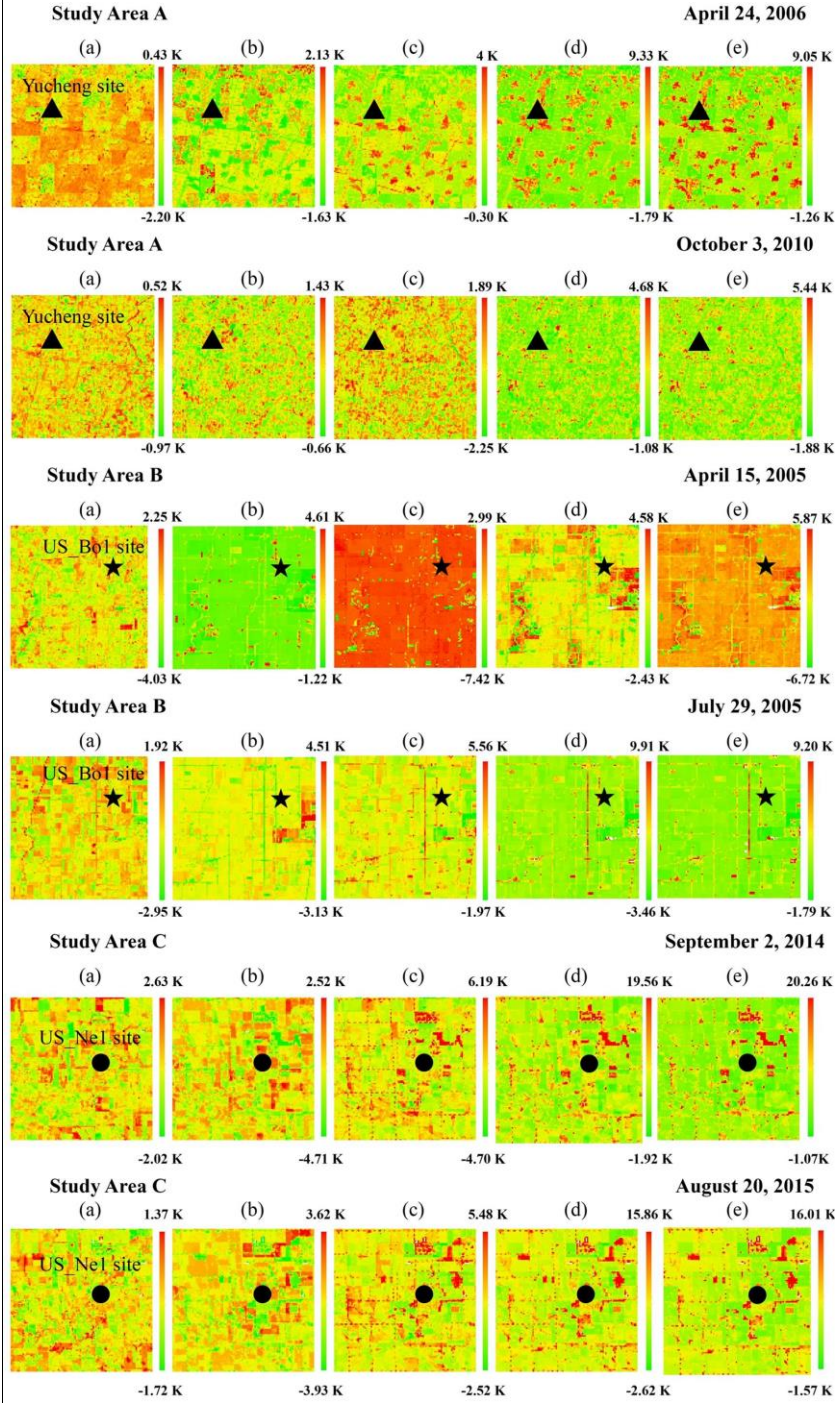


469  
 470 **Figure 3.** Spatial distribution of the (a) 990 m MODIS LST, (b) 90 m ASTER LST, (c) 90 m LST downsampled  
 471 by the DTsEB method, (d) 90 m LST downsampled by the TsHARP method, (e) 90 m LST downsampled by the  
 472 LMS method, and (f) 90 m LST downsampled by the GWR method for study areas A, B and C. Circles 1, 2 and 3  
 473 (in study area A on April 24, 2006, in study area B on April 15, 2005, and in study area C on September 2, 2014,  
 474 respectively) are typical areas highlighted for comparison.



475  
 476 **Figure 4.** Comparisons of the 90 m LST downscaled from 990 m MODIS products using the (a) DTsEB (left  
 477 panel), (b) TsHARP, (c) LMS, and (d) GWR methods with the ASTER LST for the three study areas.





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**Figure 5.** Spatial distribution of the contributions of the four surface parameters to the final  $dLST$  results in study areas A, B and C by using the MODIS datasets: (a) contribution of the surface net radiation,  $\frac{\partial LST}{\partial R_n} dR_n$ ; (b) contribution of fraction of the vegetation,  $\frac{\partial LST}{\partial f_c} df_c$ ; (c) contribution of the aerodynamic resistance,  $\frac{\partial LST}{\partial r_a} dr_a$ ; (d) contribution of the surface resistance,  $\frac{\partial LST}{\partial r_s} dr_s$ ; and (e) the estimated  $dLST$ .

## 483 4.2 Application to aggregated ASTER datasets

484 Similar to the application to the MODIS datasets, the DTsEB, TsHARP, LMS, and GWR  
485 methods were also applied to downscale the 990 m resolution aggregated ASTER LSTs to 90 m  
486 resolution. Overall, the aggregated ASTER LSTs (Figure 6a) were higher than the MODIS LSTs  
487 (Figure 3a) in all the study areas, i.e., A, B and C. Especially in the high-value LST ranges, the  
488 aggregated coarse-resolution ASTER LSTs presented a much broader value distribution. The  
489 maximum value of the aggregated ASTER LSTs (Table 1) was approximately 4 K higher than that  
490 of the MODIS LSTs on average. Furthermore, from a visual comparison, the pixel-to-pixel LST  
491 variations were also observed to be larger in the aggregated coarse-resolution LSTs than in the  
492 MODIS LSTs. Compared with the reference ASTER LSTs without aggregation, the aggregated  
493 ASTER LSTs roughly exhibited the expected similar spatial distributions in all the study areas,  
494 i.e., A, B and C. The differences between the mean aggregated ASTER LSTs and the mean fine-  
495 resolution ASTER LSTs over the three study areas were less than 0.1 K. The notable differences  
496 between the coarse-resolution LSTs and fine-resolution reference LSTs were largely reduced with  
497 the use of aggregation datasets.

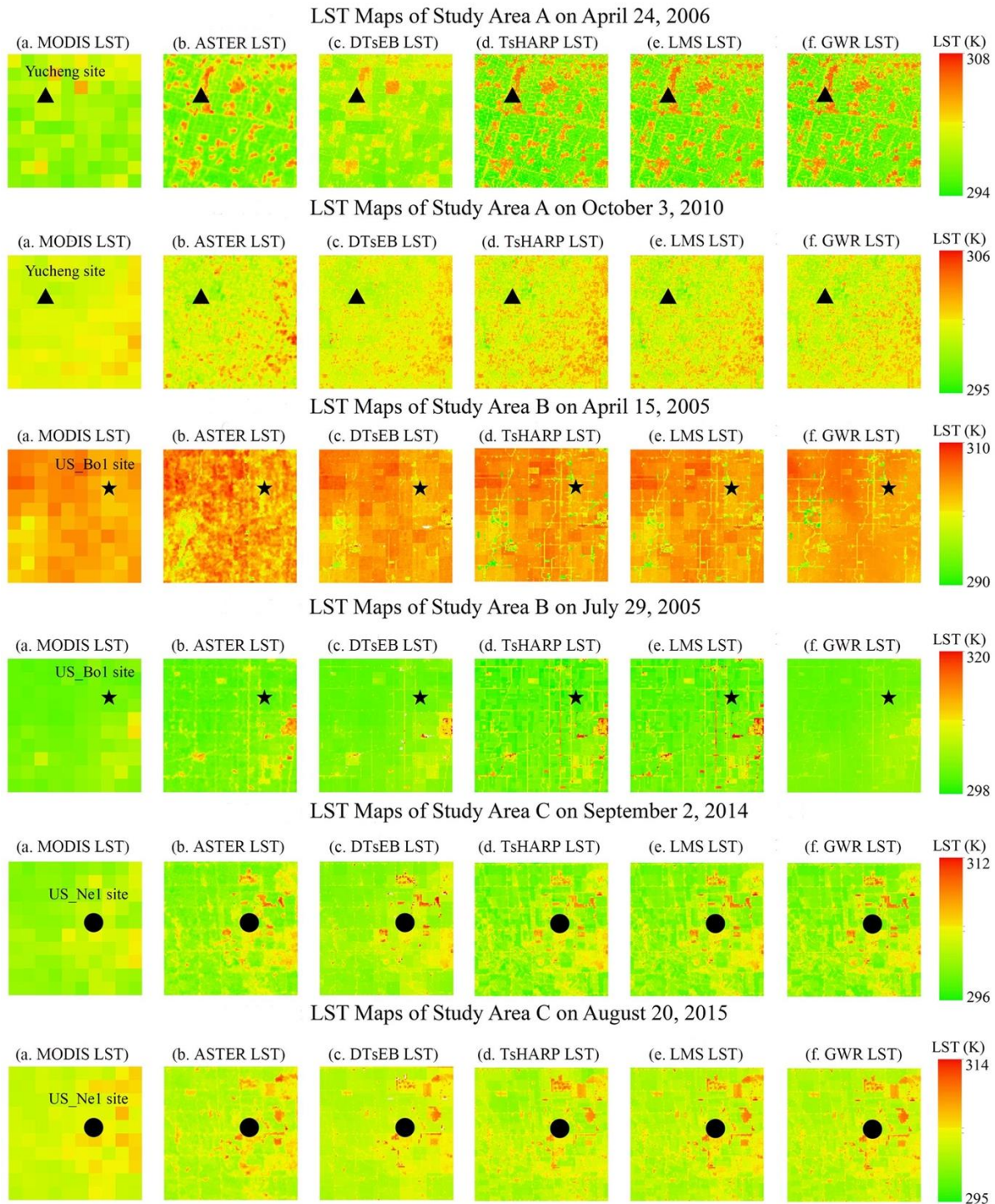
498 The spatial patterns of the 90 m LSTs downscaled from the aggregation datasets using the  
499 DTsEB, TsHARP, LMS, and GWR methods over the three study areas are displayed in Figure 6  
500 and a scatterplot of the comparison between the downscaled LSTs and the reference fine-resolution  
501 ASTER LSTs is presented in Figure 7. Overall, although an overestimation of low LST extremes  
502 and an underestimation of high LST extremes were present, the DTsEB, TsHARP, LMS, and  
503 GWR methods could all effectively reconstruct subpixel spatial variations within coarse-resolution  
504 pixels. The spatial distribution and texture characteristics of the three downscaled LST results were  
505 similar and basically consistent with those of the 90 m reference ASTER LSTs. The accuracy of  
506 LST downscaling results obtained by the DTsEB method was higher than that obtained by the  
507 TsHARP, LMS, and GWR methods, while the LMS method slightly outperformed the TsHARP  
508 and GWR method. The RMSE decreased by 0.08~0.51 K (~17% on average) from 1.17~2.32 K  
509 for the TsHARP method, by 0.02~0.66 K (~13% on average) from 1.10~2.12 K for the LMS  
510 method, and by 0.03~0.51 K (~13% on average) from 1.12~2.36 K for the GWR method, to  
511 0.95~1.85 K for the DTsEB method (Table 3). As expected, the normalized RMSE of 0.57~0.79  
512 for the DTsEB method was lower than that for the TsHARP method (0.66~0.99), the LMS method  
513 (0.65~0.92) and the GWR method (0.65~1.00). Except for the results on August 20, 2015, over

514 study area C, where the MAE of the LMS method and GWR method was negligibly lower (0.03  
515 K and 0.02 K, respectively) than that of the DTsEB method, the MAE decreased by 0.10~0.36 K  
516 (16% on average) from 0.90~1.73 K for the TsHARP method, by 0.03~0.31 K (9% on average)  
517 from 0.86~1.58 K for the LMS method, and by 0.09~0.34 K (12% on average) for the GWR  
518 method, to 0.72~1.45 K for the DTsEB method. The correlation coefficient (Table 4), which varied  
519 between 0.63 and 0.83, for the DTsEB method was comparable to that for the TsHARP method  
520 (between 0.56 and 0.84), the LMS method (between 0.60 and 0.85), and the GWR method  
521 (between 0.47 and 0.85), while the bias for the DTsEB method was slightly higher than that for  
522 the latter three methods. Furthermore, for all the DTsEB, TsHARP, LMS, and GWR methods,  
523 better LST downscaling results were obtained in study areas A and C. The RMSE values obtained  
524 in the evaluation of the 90 m LSTs downscaled by the DTsEB method on October 3, 2010 in study  
525 area A, for example, were lower than 1 K. However, in the LST downscaling results on April 15,  
526 2005 in study area B, a larger bias was observed in the low-value ranges of LSTs for the TsHARP,  
527 LMS, and GWR methods (Figure 7).

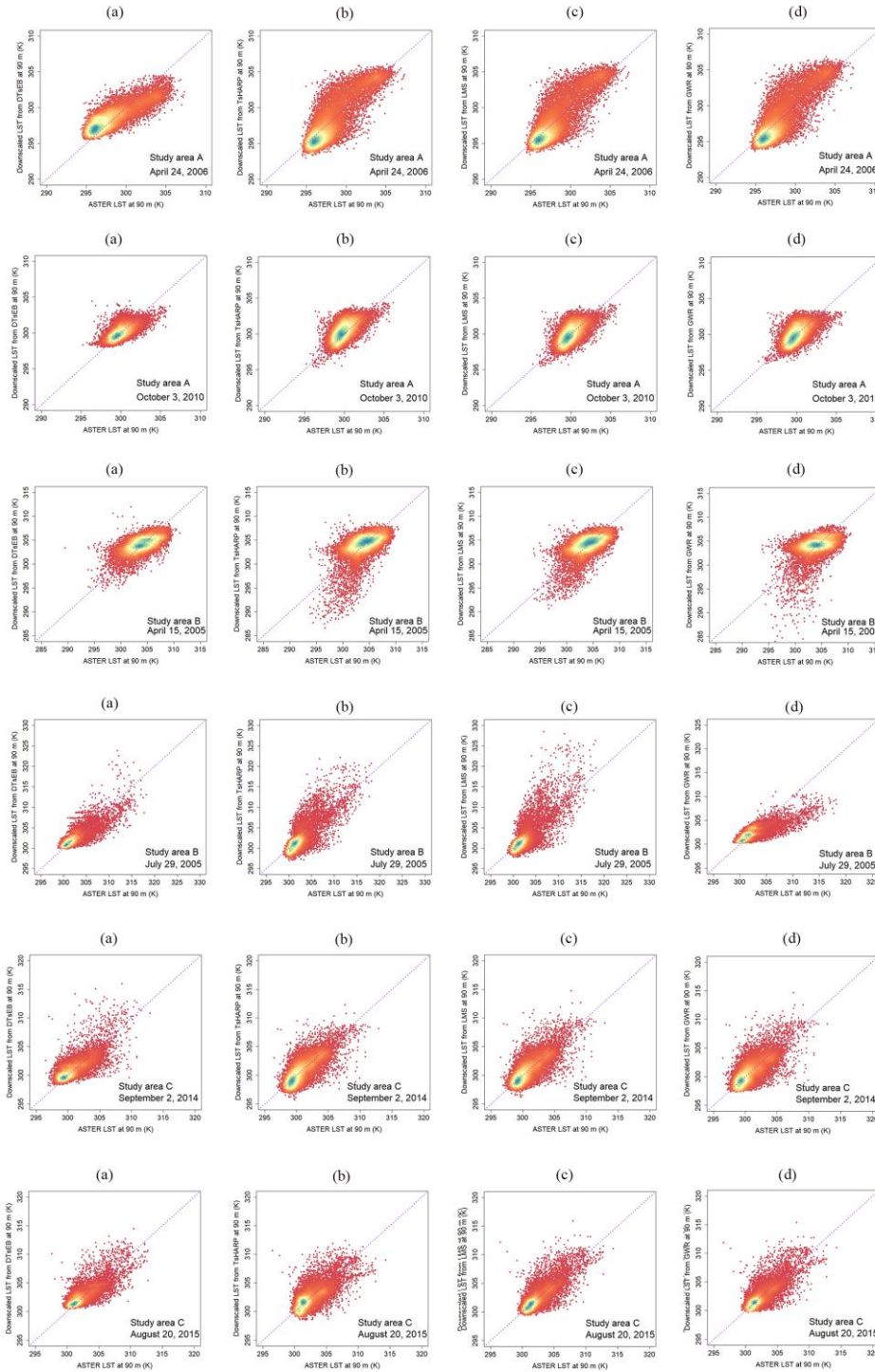
528 Compared with the application to MODIS datasets, the use of aggregated ASTER LST  
529 datasets for the DTsEB, TsHARP, LMS, and GWR methods all resulted in improved accuracy of  
530 the downscaled results for study areas A, B and C. When using the aggregated ASTER datasets  
531 instead of the MODIS datasets, the mean RMSE (MAE) values of the DTsEB, TsHARP, LMS,  
532 and GWR downscaled results decreased by 0.59 K (0.48 K), 0.70 K (0.58 K), 0.72 K (0.63 K), and  
533 0.74 K (0.62 K), respectively. For study area B on April 15, 2005, the RMSE and MAE values  
534 obtained by using the DTsEB decreased by 39% and 43%, respectively, while the TsHARP yielded  
535 a 28% decrease in RMSE and a 36% decrease in MAE, the LMS produced a 40% decrease in  
536 RMSE and a 45% decrease in MAE, and the GWR yielded a 27% decrease in RMSE and a 35%  
537 decrease in MAE compared to the application to the MODIS LSTs. Furthermore, the obvious  
538 underestimation in the high-value ranges of LSTs by using the MODIS datasets was effectively  
539 improved in the application to the aggregated ASTER LST datasets (see the scatter plot  
540 distribution in Figures 4 and 7).

541 Figure 8 displays the spatial patterns of the contributions of the four scaling factors (e.g.,  $R_n$ ,  
542  $f_c$ ,  $r_a$ , and  $r_s$ ) to the final  $dLST$  when the DTsEB method was applied to the aggregated ASTER  
543 LST downscaling. Similar to the findings of the application to the MODIS datasets, the results  
544 showed that the contributions of the four parameters were different from each other and varied

545 both spatially and temporally in the application to the aggregated ASTER LSTs; the contributions  
546 of all four scaling factors varied from negative to positive. The contribution of  $r_s$  was most affected  
547 by environmental variables and had a broader value distribution than the other three scaling factors  
548 whereas the contribution of  $R_n$  had the narrowest value distribution. For example, in study area A  
549 on April 24, 2006 and October 3, 2010, the contribution of  $R_n$  to the final  $dLST$  was less than  $\pm 1$   
550 K while in study area B on July 29, 2005 and in study area C on September 2, 2015, the greatest  
551 contributions of  $r_s$  to the final  $dLST$  were larger than 18 K and 14 K, respectively. Furthermore,  
552 the contributions of  $r_s$  (Figure 8c) were positively correlated with the  $dLST$  (Figure 8e) and had  
553 the greatest impact on the final  $dLST$  results ( $0.72 \pm 0.84$  K on average), which was similar to the  
554 findings in the application to the MODIS LSTs. Meanwhile, the contributions of  $f_c$  (Figure 8b)  
555 were negatively correlated with  $dLST$ , which is consistent with the negative correlation  
556 relationship between surface vegetation and LSTs. The lowest impact on the final  $dLST$  was found  
557 in the contributions of  $R_n$  ( $0.19 \pm 0.18$  K on average, Figure 8a). Compared with the application to  
558 the MODIS datasets, the spatial distribution of the contributions of the four scaling factors was  
559 smoother, and the contributions of  $r_a$  and  $r_s$  to the final  $dLST$  in high-value ranges were larger.



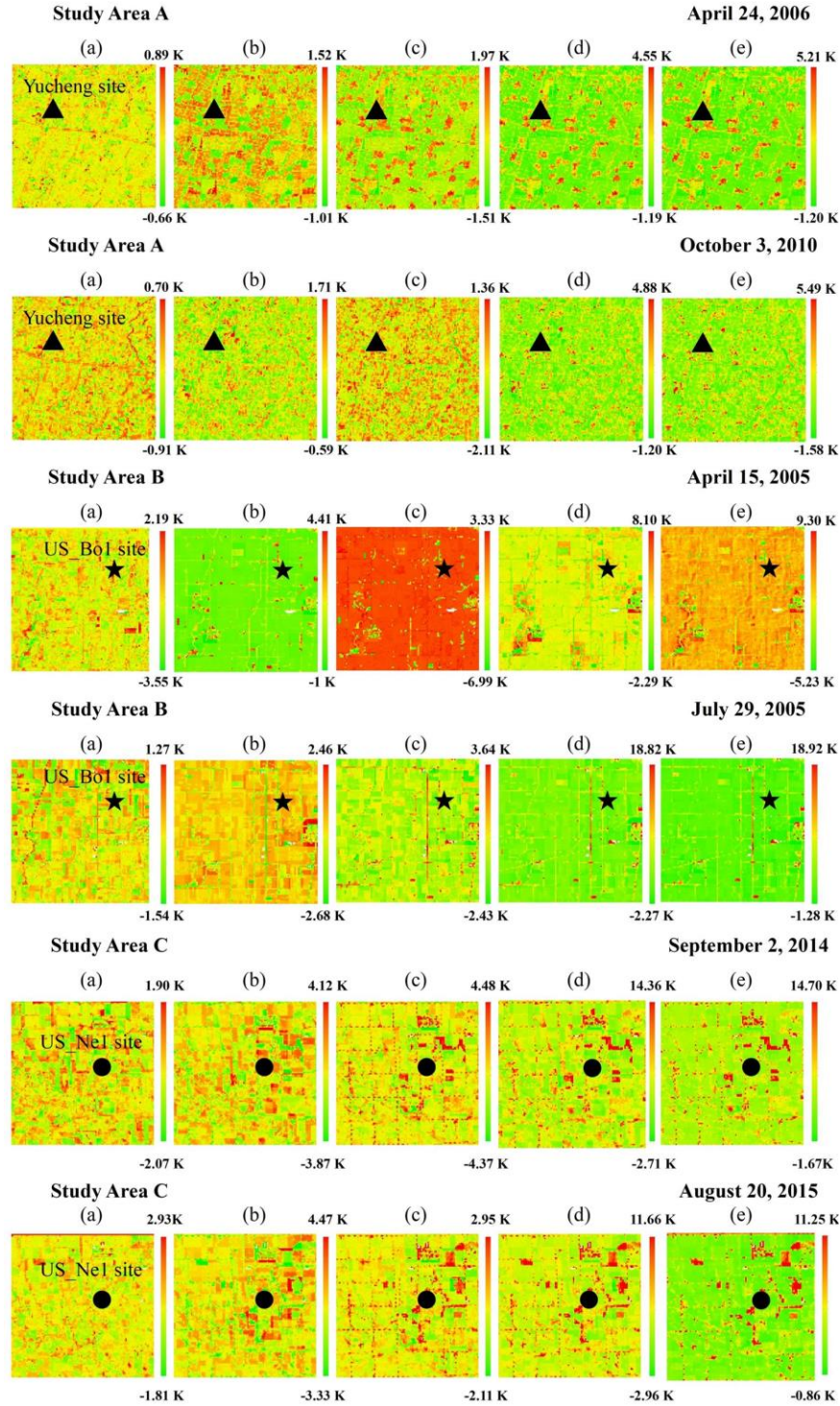
560  
561 **Figure 6.** Spatial distributions of the (a) 990 m aggregated ASTER LSTs, (b) 90 m reference ASTER LSTs, (c)  
562 90 m LSTs downscaled by the DTsEB method, (d) 90 m LSTs downscaled by the TsHARP method, (e) 90 m  
563 LSTs downscaled by the LMS method, and (f) 90 m LSTs downscaled by the GWR method for study areas A,  
564 B and C.  
565



566

567 **Figure 7.** Comparisons of the 90 m LSTs downscaled from the 990 m aggregated ASTER LSTs using the DTsEB

568 (a), TsHARP (b), LMS (c), and GWR (d) methods with ASTER LSTs for the three study areas.



569

570 **Figure 8.** Spatial distribution of the contributions of four surface parameters to the final  $dLST$  results in study  
 571 areas A, B, and C determined by using the aggregated ASTER datasets: (a) contribution of the surface net  
 572 radiation,  $\frac{\partial LST}{\partial R_n} dR_n$ ; (b) contribution of the fraction of vegetation,  $\frac{\partial LST}{\partial f_c} df_c$ ; (c) contribution of the aerodynamic  
 573 resistance,  $\frac{\partial LST}{\partial r_a} dr_a$ ; (d) contribution of the surface resistance,  $\frac{\partial LST}{\partial r_s} dr_s$ ; and (e) the estimated  $dLST$ .

### 574 4.3 Discussion

575 The improvements in LST downscaling methods made in recent years mainly include the  
576 following two aspects: 1) selecting more appropriate scaling factors and 2) establishing more  
577 accurate relationships between LSTs and scaling factors. Regrettably, many of the scaling factors  
578 chosen in previous works simply remedied the regressed negative correlation relationships  
579 between NDVI and LSTs [Merlin *et al.*, 2010; Yang *et al.*, 2011; Bonafoni, 2016; Duan & Li,  
580 2016], which is somewhat arbitrary and site-specific. Furthermore, most of the established  
581 relationships between LSTs and scaling factors were from statistical regressions [Agam *et al.*, 2007;  
582 Bindhu *et al.*, 2013], which limited the applicability and robustness of the LST downscaling  
583 algorithm and even resulted in different LSTs for the same pixel under different regression  
584 equations and sizes of areas of interest. Instead of selecting the scaling factors subjectively and  
585 using statistical regression relationships with no explicit physical mechanism, the DTsEB method  
586 proposed in this paper improves the downscaling of coarse-resolution LSTs by proposing  
587 analytical equations. These equations make use of surface energy balance constraints to provide a  
588 physically intuitive mechanism for combining the thermal infrared spectrum data (coarse  
589 resolution) with the VNIR and SWIR spectrum data (fine resolution).

590 The performance improvements in the DTsEB method against the TsHARP, LMS, and GWR  
591 methods varied among different scenes and different underlying surface conditions. The DTsEB  
592 downscaled results were better than the TsHARP, LMS, and GWR results, especially in high LST  
593 ranges. The underestimations of TsHARP, LMS, and GWR over high LST value pixels (see the  
594 scatter plots in Figures 4 and 7) indicate the limitations in the extension of regression equations  
595 constructed with narrower NDVI ranges at coarse resolution to applications at wider NDVI ranges  
596 at fine resolution. Taking the concurrent 90 m ASTER LST product as the reference LST, the  
597 TsHARP method yielded average RMSE (MAE) values of 2.41 K (1.84 K) and 1.71 K (1.26 K)  
598 in the downscaling of the 990 m MODIS LSTs and the aggregated ASTER LSTs to 90 m,  
599 respectively. By contrast, for the LMS method the average RMSE (MAE) values were 2.35 K  
600 (1.80 K) and 1.63 K (1.17 K), respectively, and for the GWR method the average RMSE (MAE)  
601 values were 2.38 K (1.82 K) and 1.64 K (1.20 K), respectively. These LST downscaling accuracies  
602 of the TsHARP, LMS, and GWR methods are comparable to those achieved in previous studies.  
603 For example, Hutengs & Vohland [2016] applied TsHARP to downscale 960 m aggregated ETM+  
604 LST to 240 m resolution and obtained an average RMSE of 1.48 K (referenced to 240 m ETM+



605 LST data). In the downscaling of 990 m MODIS LSTs to 90 m resolution, the TsHARP method  
606 achieved RMSEs of 3.62 K and 2.16 K (referenced to 90 m ASTER LST data) for two different  
607 study areas in *Wu & Li's* work [2019]. The LMS method in *Mukherjee et al.'s* [2014] work  
608 produced an average RMSE of 1.43 K in the downscaling of 1000 m MODIS LSTs to 250 m  
609 (referenced to 250 m TM LST data) and in *Bisquert et al.'s* [2016] work generated average RMSE  
610 values of 1.80 K and 2.10 K in downscaling 960 m MODIS LSTs and aggregated ETM+ LSTs to  
611 60 m (referenced to 60 m ETM+ LST data), respectively. *Duan & Li* [2016] introduced the GWR  
612 to downscale the 990 m MODIS LST to 90 m (referenced to 90 m ASTER LST data), and obtained  
613 an average RMSE (MAE) of 3.1 K (2.3 K). Compared to the TsHARP, LMS, and GWR, the  
614 DTsEB method in this study improved LST downscaling, with average RMSEs (MAEs) of 2.01  
615 K (1.54 K) and 1.42 K (1.06 K) in the application to the 990 m MODIS datasets and aggregated  
616 ASTER datasets, respectively, indicating the effectiveness of this new proposed method. The  
617 average RMSE decrease achieved by using the DTsEB (17% and 17% compared to the TsHARP,  
618 14% and 13% compared to the LMS, and 16% and 13% compared to the GWR in application to  
619 the MODIS datasets and aggregated ASTER datasets, respectively) in the LST downscaling  
620 compared favorably to those achieved by the Extended-RFD method (13% to 26% relative to the  
621 TsHARP) in *Hutengs & Vohland* [2016] and the regression tree-based method (averages of 20%  
622 and 25% relative to the TsHARP for an irrigated agricultural site and heterogeneous naturally  
623 vegetated area, respectively) in *Gao et al.* [2012]. Furthermore, compared to the downscaling  
624 methods suggested by *Merlin et al.* [2010], *Chen et al.* [2014] and *Duan & Li* [2016], the DTsEB  
625 method is also observed to produce similar or better LST accuracy in downscaling kilometer-  
626 resolution LSTs to fine resolution. In the work of *Merlin et al.* [2010], broadband albedo was  
627 introduced into the TsHARP method to distinguish photosynthetically and nonphotosynthetically  
628 active vegetation and finally achieved average RMSEs of 3.81 K and 2.78 K in downscaling 1 km  
629 resolution MODIS LSTs and aggregated ASTER LSTs to 100 m resolution, respectively. *Chen et*  
630 *al.* [2014] combined the TsHARP method with thin-plate spline interpolation to downscale 1-km-  
631 resolution MODIS LSTs to 250 m resolution and obtained an RMSE of 2.38 K. *Duan & Li* [2016]  
632 introduced geographically weighted regression to the TsHARP method and obtained an average  
633 RMSE of 2.7 K in downscaling 990 m resolution MODIS LSTs to 90 m resolution.

634 The improved LST downscaling results obtained in the application to aggregated ASTER  
635 datasets compared to the application to MODIS datasets for the DTsEB, TsHARP, LMS, and GWR

636 methods mainly resulted from the smaller differences between the coarse-resolution aggregated  
637 ASTER LSTs and fine-resolution reference ASTER LSTs than between the coarse-resolution  
638 MODIS LSTs and fine-resolution reference ASTER LSTs, which is consistent with the previous  
639 findings that differences between coarse and reference fine resolution LSTs could directly affect  
640 evaluations of downscaling results [Agam *et al.*, 2007; Merlin *et al.*, 2010]. Yang *et al.* [2011]  
641 also found that downscaled LSTs often have a relatively high accuracy by using resampling and  
642 aggregation methods. Different from the intercalibration of the coarse- and fine-resolution LSTs  
643 and surface parameters (such as NDVI) that were obtained from different sensors in the works of  
644 Bindhu *et al.* [2013], the datasets from the MODIS and ASTER sensors onboard the same satellite  
645 platform, which avoided errors caused by different satellite altitudes and overpass times, were used  
646 directly without extra processing in this study. In this aspect, reasonably enhancing the spatial  
647 details of original coarse-resolution MODIS LSTs (Real data) is crucial to LST downscaling  
648 methods. Given the relatively large differences between the LSTs from these two sensors, the  
649 better performance of the DTsEB method compared with the TsHAPR, LMS, and GWR methods,  
650 especially in the high-value ranges of LSTs, highlights the high robustness, generality, and  
651 accuracy of DTsEB. Nevertheless, both the coarse-resolution remotely sensed LST products and  
652 the reference fine-resolution LST products have an intrinsic bias, which is difficult to exclude in  
653 LST downscaling.

654 Another advantage of the DTsEB method is its ability to properly quantify the contributions  
655 of each scaling factor (e.g., surface net radiation, fraction of vegetation, aerodynamic resistance  
656 and surface resistance) within a physical framework. Although the values of these scaling factors  
657 are likely to vary with the spatial resolution of the VNIR/SWIR images, the physical relationship  
658 remains inviable, whereas the regression-based TsHARP, LMS, and GWR methods and others  
659 only attribute the subpixel spatial variations of LST to one or more vegetation indices and  
660 topographic variables (e.g., NDVI, NDWI, NDBI, EBBI, BI, TVDI, and DEM, see Introduction  
661 Section), and their regression relationships are different from one another. The test results in this  
662 study revealed that the surface resistance and aerodynamic resistance were, overall, the largest and  
663 second largest factors, respectively, which contributed to the subpixel spatial variations of coarse-  
664 resolution land surface temperature for the whole spatial domain in the three study areas. An  
665 exception, for which the largest contribution was from the aerodynamic resistance in the  
666 downscaling of MODIS surface temperatures, occurred and was possibly due to the intrinsic

667 difference in the surface temperature and reflectance measurements between the MODIS and  
668 ASTER sensors. Different from the DTsEB method, the regression-based downscaling techniques  
669 (e.g., TsHARP, LMS, GWR and other methods) were flawed in their attribution of the  
670 contributions and different attribution results could be obtained from these techniques with  
671 different independent variables (e.g., scaling factors), which clearly does not make sense.

672 Downscaled LSTs are often accompanied by the notorious “boxy effect” [Agam *et al.*, 2007,  
673 2008; Duan & Li, 2016; Bindhu *et al.*, 2013], which results from the addition of the constant  
674 residuals obtained at coarse resolutions. This addition is necessary and can help improve LST  
675 downscaling when there are LST differences at coarse resolution between the values calculated by  
676 the constructed relationship with the scaling factors and the values extracted from the remotely  
677 sensed image to be downscaled. The boxy effects become more pronounced when the residual  
678 errors are larger and disappear if LST downscaling is performed without adding the constant  
679 residual or the constructed relationship can perfectly (no residual error) represent the remotely  
680 sensed LSTs at coarse resolution. Compared to the TsHARP, LMS and GWR methods, the DTsEB  
681 method makes use of the dLST that represents the differences between LSTs at fine and coarse  
682 resolutions and is expressed as a function of the differences between surface parameters (e.g.,  $dR_n$ ,  
683  $df_c$ ,  $dr_a$ , and  $dr_s$ ). The addition of residual field is actually not applied in the DTsEB method.  
684 Therefore, the DTsEB method can more effectively reduce the “boxy effect” and thus improve  
685 LST downscaling compared to the TsHARP, LMS, and GWR methods because of the higher  
686 accuracy of the physical LST equation relative to the regression equation.

687 In brief, the TsHARP, LMS, GWR and other regression-based methods are simple in model  
688 structure, do not require auxiliary near-surface data as input but are deficient in their poor  
689 spatiotemporal extensibility and in quantifying the contributions of influencing factors (namely,  
690 attribution analysis). In contrast, the DTsEB method, developed by theoretical derivations of  
691 surface energy balance and Penman-Monteith equation under the assumption of negligible spatial  
692 variations in atmospheric parameters over the subpixels within a coarse pixel, has the advantages  
693 of a solid physical foundation, the capability to separate the contributions of the influencing factors,  
694 and LST downscaling results with a high accuracy. The main limitation of the DTsEB method lies  
695 in the requirements for near-surface meteorological data (e.g., incoming solar radiation, air  
696 temperature, VPD, and wind speed), which may introduce a certain degree of uncertainty in LST  
697 downscaling, especially when the DTsEB method is applied regionally or globally, because pixel-

698 by-pixel meteorological data (e.g., sourced from reanalysis data) should be introduced to consider  
699 the spatial variation in near-surface meteorology under such conditions. This data requirement  
700 does not add much computational cost. For instance, in-situ meteorological data, such as the  
701 FLUXNET and AMERIFLUX datasets, can be used in small-scale study areas (e.g. the study areas  
702 (Figure 1) with spatial dimensions of 9.9 km by 9.9 km). As for regional or global study areas,  
703 interpolated meteorological data and reanalysis data (such as ERA5 datasets) can be used.  
704 Moreover, the uncertainty of the parameterization in the DTsEB algorithm also introduces biases  
705 in LST downscaling to some extent. For example, the scatters in the downscaling of high LSTs  
706 (primarily over built-up lands) in this study likely resulted from the uncertainty in the  
707 determination of roughness height (influencing aerodynamic resistance) and soil heat flux by  
708 following the general parameterizations over vegetated surfaces (e.g., cropland, grassland,  
709 forestland), indicating that improved parameterization of the DTsEB method for these two  
710 parameters is required over built-up lands (beyond the scope of this study). In particular, we did  
711 not distinguish the parameterization of surface resistance between crop and built-up lands but  
712 applied the same equation as shown in Appendix D to parameterize surface resistance for all land  
713 cover types, primarily because the focus of our study was not on the parameterization but on the  
714 development of DTsEB downscaling method. Parameterizing surface resistance differently are  
715 strongly recommended over cropland, built-up land and other land cover types. In addition, due to  
716 the complexities of LST downscaling that come from the uncertainty/error of coarse-resolution  
717 and fine-resolution LSTs and VNIR/SWIR reflectance products, downscaling algorithm,  
718 parameterization, and inputs, none of the three methods could obtain a normalized RMSE  $< 0.5$  in  
719 this study, although these methods have reported RMSE values of similar magnitude to those from  
720 previous studies. In short, despite the great progress made in the past for LST downscaling, there  
721 remains a long way to go.

## 722 **5. Summary and Conclusions**

723 A physical LST downscaling method, DTsEB, has been developed to downscale coarse-  
724 resolution LST data to a fine resolution. By theoretical derivations of the surface energy balance  
725 equation and Penman-Monteith equation, analytical equations for combining thermal infrared data  
726 with visible and near-infrared data have been constructed in the newly proposed LST downscaling  
727 method. The differences in surface net radiation, fractional vegetation cover, aerodynamic  
728 resistance and surface resistance between coarse and fine resolutions are first calculated, and fine-

729 resolution LSTs can then be obtained by converting the differences between the LSTs at the two  
730 resolutions to the differences between these surface parameters. The surface energy balance  
731 constraint in the DTsEB method provides a robust and physical connection between the scaling  
732 factors and LSTs and thus avoids the subjective selection of scaling factors and the use of statistical  
733 regression relationships.

734 Because of the comprehensive consideration of various surface parameters related to LSTs,  
735 the DTsEB method can effectively reconstruct subpixel spatial variations within coarse-resolution  
736 pixels and achieve better downscaling accuracy than the widely adopted TsHARP, LMS, and  
737 GWR methods, when tested on 990 m MODIS and aggregated LST products collected between  
738 2005 and 2015 over three 9.9 km by 9.9 km cropland (mixed by grass, tree, and built-up land)  
739 study areas. The average RMSE (MAE) values in DTsEB decreased by 17% (16%) relative to the  
740 TsHARP method, 14% (14%) relative to the LMS method, and 16% (15%) relative to the GWR  
741 method for application to 6 scenes of MODIS datasets and by 17% (16%) relative to the TsHARP  
742 method, 13% (9%) relative to the LMS method, and 13% (12%) relative to the GWR method for  
743 application to 6 scenes of aggregated ASTER datasets.

744 In summary, the DTsEB method has great potential in LST downscaling over various land  
745 cover types and satellite sensor data as long as the parameters are properly estimated, because 1)  
746 the solid physical foundation makes it robust and highly accurate and 2) the physical association  
747 between scaling factors and the LSTs can quantitatively separate the specific contributions of  
748 different scaling factors to the LST downscaling results. In the context that most existing LST  
749 downscaling methods are based on statistical regression, the physical DTsEB method proposed in  
750 this study is instructive and worthwhile. When other high-resolution satellite sensor (e.g. Landsat  
751 TM, ETM+, OLI) LST data are used to test the applicability of this new method, one may only  
752 perform a simulation of downscaling coarse-resolution aggregated LST to high-resolution LST (as  
753 in case 2 shown in Section 3.2) because no coarse-resolution satellite sensor LST concurrent with  
754 the high-resolution satellite sensor LST is available. To allow more general conclusions to be made,  
755 further work is recommended to evaluate the DTsEB method and the regression-based LST  
756 downscaling methods in more regions of the world that are characterized by a wider range of  
757 climates and land cover conditions.

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## 770 Appendix

### 771 A. TsHARP method

772 For a comparative analysis of the LST downscaling performance of the DTsEB method, the  
773 widely used vegetation-based regression method, TsHARP (more specifically, the TsHARP  
774 version, named TsHARPFcS, which was recommended by Agam *et al.* [2007]), was applied in this  
775 study. The TsHARP method, a refinement of the disaggregation procedure for radiometric surface  
776 temperatures (DisTrad, proposed by Kustas *et al.* [2003]), assumes that the relationship between  
777 LSTs and NDVI-based transformed variables is scale invariant. A linear regression between LSTs  
778 and the NDVI-based transformed variable is first performed at coarse resolution, as follows:

$$779 \quad f(NDVI_{CR}) = a_0 - a_1(1 - NDVI_{CR})^{0.625} \quad (A1)$$

780 where the subscript CR represents the coarse resolution.

781 Subsequently, the divergence ( $\Delta LST$ ) between the regressed LSTs and the source LSTs,  
782 which comes from the spatial variability in LSTs that is driven by factors other than the vegetation  
783 cover fraction at coarse resolution, can be calculated, as follows:

$$784 \quad \Delta LST = LST_{CR} - f(NDVI_{CR}) \quad (A2)$$

785 This residual field is finally applied to derive the downscaled fine-resolution LSTs  
 786 ( $LST_{TsHARP}$ ), as follows:

$$\begin{aligned}
 787 \quad LST_{TsHARP} &= f(NDVI_{FR}) + \Delta LST \\
 &= a_0 - a_1(1 - NDVI_{FR})^{0.625} + \Delta LST
 \end{aligned}
 \tag{A3}$$

788 where the subscript FR represents the fine resolution.

### 789 B. LMS method

790 According to the work of Mukherjee *et al.* [2014], least median square regression  
 791 downscaling (LMS), which is less sensitive to outliers than the ordinary least square regression  
 792 algorithm (used in TsHARP method), could achieve a better accuracy in LST downscaling.

793 In the ordinary least square regression, the regression parameters slope and intercept are  
 794 estimated by minimizing the sum of square residuals, as follows:

$$795 \quad MinSSR = \sum_{i=1}^n (LST_i - f(NDVI_i))^2 \tag{B1}$$

796 In the LMS, the parameter slope and intercept are calculated to yield the least median of the  
 797 square residuals, as follows:

$$798 \quad MinMedSR = Median \left\{ (LST_1 - f(NDVI_1)), (LST_2 - f(NDVI_2)), \dots, (LST_n - f(NDVI_n)), \right\} \tag{B2}$$

799 The least median square regression between LST and NDVI is first performed at coarse  
 800 resolution, and the divergence ( $\Delta LST$ ) between the regressed LSTs and the source LSTs can be  
 801 subsequently calculated. Finally, this residual field  $\Delta LST$  is added at fine resolution to obtain the  
 802 fine-resolution LST.

### 803 C. GWR method

804 Compared with traditional regression method, geographically weighted regression (GWR)  
 805 can fully consider the geographic similarity relationship between the dependent variables and the  
 806 independent variables. According to the work of Duan *et al.* [2016], a nonstationary relationship  
 807 at coarse-resolution is first established, which can be expressed as:

$$LST_i^{CR} = a_0^{CR}(\mu_i, \nu_i) + a_1^{CR}(\mu_i, \nu_i)NDVI_i^{CR} + a_2^{CR}(\mu_i, \nu_i)DEM_i^{CR} + \Delta_i^{CR} \quad (C1)$$

where the superscript *CR* represents the coarse resolution, the  $\alpha_0^{CR}(\mu_i, \nu_i)$ ,  $\alpha_1^{CR}(\mu_i, \nu_i)$ , and  $\alpha_2^{CR}(\mu_i, \nu_i)$  are the regression coefficients, and the  $\Delta_i^{CR}$  is the residual at coarse resolution.

Subsequently, the coarse-resolution regression coefficients  $\alpha_0^{CR}(\mu_i, \nu_i)$ ,  $\alpha_1^{CR}(\mu_i, \nu_i)$  and  $\alpha_2^{CR}(\mu_i, \nu_i)$  and the residual  $\Delta_i^{CR}$  are interpolated to fine resolution by using the ordinary kriging interpolation technique (according to the work of Duan *et al.* [2016]).

Finally, the fine resolution downscaled LST can be obtained by using the fine resolution NDVI and DEM, as follows:

$$LST_i^{FR} = a_0^{FR}(\mu_i, \nu_i) + a_1^{FR}(\mu_i, \nu_i)NDVI_i^{FR} + a_2^{FR}(\mu_i, \nu_i)DEM_i^{FR} + \Delta_i^{FR} \quad (C2)$$

where the superscript *FR* represents the fine resolution, the  $\alpha_0^{FR}(\mu_i, \nu_i)$ ,  $\alpha_1^{FR}(\mu_i, \nu_i)$ ,  $\alpha_2^{FR}(\mu_i, \nu_i)$ , and  $\Delta_i^{FR}$  are the regression coefficients and residual, respectively, which can be obtained with the ordinary kriging interpolation technique.

## D. Parameterization of DTsEB

Table D1. Methods for estimating the intermediate variables/parameters in DTsEB

| Parameters           | Calculation formula  | Description   | References                                       |
|----------------------|--|---|--|
|                      | for MODIS:<br>$albedo = 0.160b_1 + 0.291b_2 + 0.243b_3 + 0.116b_4 + 0.112b_5 + 0.081b_7 - 0.015$   |   |  |
|                      | for ASTER:<br>before April 2008,<br>$albedo = 0.484b_1 + 0.335b_3 - 0.324b_5 + 0.551b_6 + 0.305b_8 - 0.367b_9 - 0.0015$<br>after April 2008,<br>$albedo = 0.697b_1 + 0.298b_3 + 0.008$ | <i>r</i> is the broadband albedo,<br><i>b<sub>i</sub></i> is the short-wave band spectral reflectances.   | Liang, 2003;<br>Mokhtari et al., 2013            |
| <i>G</i>             | $G = R_n [\Gamma_c + (1 - f_c)(\Gamma_s - \Gamma_c)]$  | <i>G</i> is the soil heat flux,<br>$\Gamma_c = 0.05$ ; $\Gamma_s = 0.4$ .   | Su, 2002   |
| <i>f<sub>c</sub></i> | $f_c = \left( \frac{NDVI - NDVI_{min}}{NDVI_{max} - NDVI_{min}} \right)^2$   | $NDVI_{min} = 0.2$ ; $NDVI_{max} = 0.86$ ;<br>$NDVI > NDVI_{max}$ , $f_c = 1$ ;<br>$NDVI < NDVI_{min}$ , $f_c = 0$ .  | Prihodko & Goward,<br>1997; Tang et al.,<br>2010 |
| <i>r<sub>a</sub></i> | $r_a = \frac{\left[ \ln \left( \frac{Z_u - d}{Z_{om}} \right) - \Psi_m \right] \left[ \ln \left( \frac{Z_r - d}{Z_{oh}} \right) - \Psi_h \right]}{k^2 u}$                              | <i>r<sub>a</sub></i> is the aerodynamic resistance,<br>$\Psi_m$ and $\Psi_h$ are the stability correction functions for momentum and heat transfer, respectively. | Paulson, 1970;<br>Li et al., 2009                |



|              |   |  |                                      |
|--------------|---|--|--------------------------------------|
| $Z_{om}$     | $Z_{om} = \exp(aNDVI / albedo + b)$   | $Z_{om}$ is the roughness length for momentum transfer   | Tang et al., 2013;                   |
| $VegHeight$  | $VegHeight = Z_{om} / 0.123$  | $a = 0.26$ ; $b = -2.21$   | Teixeira et al., 2009                |
| $d$          | $d = \frac{2}{3} VegHeight$   | $d$ is the zero-plane displacement height  | Allen et al., 2007                   |
| $Z_{oh}$     | $Z_{oh} = 0.1Z_{om}$  | $Z_{oh}$ is the roughness length, governing the transfer of heat and vapour  | Allen et al., 2007                   |
| $r_s$        | $r_s = \frac{G_{s1} + G_{s2} + G_{cu}}{G_{s2} \times (G_{s1} + G_{cu}) \times LAI}$ | $r_s$ is the surface resistance,<br>$G_{s1}$ , $G_{s2}$ and $G_{cu}$ is the stomatal conductance, leaf boundary-layer conductance, and leaf cuticular conductance, respectively.   | Mu et al., 2007;<br>Mu et al., 2011; |
|              | $G_{s1} = C_L \times m(T_{min}) \times m(VPD) \times r_{corr}$                      | $C_L$ is the mean potential stomatal conductance per unit leaf area, assumed to 0.007 for cropland   |                                      |
| $\epsilon_s$ | $\epsilon_s = \epsilon_v f_c R_v + \epsilon_s (1 - f_c) R_s + d\epsilon$            | $\epsilon_s$ is the surface emissivity,<br>$\epsilon_v=0.986$ and $\epsilon_s=0.972$ are the emissivities of bare soil and vegetation, respectively; $R_v$ and $R_s$ are the temperature ratio for vegetation and bare soil, respectively. | Qin et al., 2004                     |
|              | $R_v = 0.0585 f_c + 0.9332$   |  |                                      |
|              | $R_s = 0.1068 f_c + 0.9902$   |  |                                      |
| $\epsilon_a$ | $\epsilon_a = 1.08(-\ln \tau_{sw})^{0.265}$   | $\epsilon_a$ is the atmospheric emissivity,<br>$\tau_{sw}$ is the atmospheric transmissivity for short wave radiation  | Bastiaanssen, 1995                   |

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