

# A Coupled Ground Heat Flux-Surface Energy Balance Model of Evaporation Using Thermal Remote Sensing Observations

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29 **Abstract**

30 One of the major undetermined problems in evaporation (ET) retrieval using thermal infrared  
31 remote sensing is the lack of a physically based ground heat flux (G) model and its integration  
32 within the surface energy balance (SEB) equation. Here, we present a novel approach based on  
33 coupling a thermal inertia (TI)-based mechanistic G model with an analytical surface energy  
34 balance model, Surface Temperature Initiated Closure (STIC, version STIC1.2). The coupled  
35 model is named STIC-TI. The model is driven by noon-night (1:30 pm and am) land surface  
36 temperature, surface albedo, and vegetation index from MODIS Aqua in conjunction with a clear-  
37 sky net radiation sub-model and ancillary meteorological information. SEB flux estimates from  
38 STIC-TI were evaluated with respect to the *in-situ* fluxes from eddy covariance measurements in  
39 diverse ecosystems of contrasting aridity in both northern and southern hemispheres. Sensitivity  
40 analysis revealed substantial sensitivity of STIC-TI-derived fluxes due to the land surface  
41 temperature uncertainty. An evaluation of noontime G ( $G_i$ ) estimates showed 12 – 21% error across  
42 six flux tower sites and a comparison between STIC-TI versus empirical G models also revealed  
43 the substantially better performance of the former. While the instantaneous noontime net radiation  
44 ( $R_{Ni}$ ) and latent heat flux ( $LE_i$ ) were overestimated (15% and 25%), sensible heat flux ( $H_i$ ) was  
45 underestimated (22%). Overestimation (underestimation) of  $LE_i$  ( $H_i$ ) was associated with the  
46 overestimation of net available energy ( $R_{Ni} - G_i$ ) and use of unclosed SEB flux measurements in  
47  $LE_i$  ( $H_i$ ) validation. The mean percent deviations in  $G_i$  and  $H_i$  estimates were found to be strongly  
48 correlated with satellite day-night view angle difference in parabolic and linear pattern, and a  
49 relatively weak correlation was found between day-night view angle difference versus  $LE_i$   
50 deviation. Findings from this parameter-sparse coupled G-ET model can make a valuable  
51 contribution to mapping and monitoring the spatiotemporal variability of ecosystem water stress  
52 and evaporation using noon-night thermal infrared observations from future Earth Observation  
53 satellite missions such as TRISHNA, LSTM, and SBG.

54 **Keywords:** Thermal remote sensing, water stress, evaporation, ground heat flux, thermal inertia,  
55 surface energy balance, STIC, terrestrial ecosystem

## 56 **1 Introduction**

57 One of the outstanding challenges in evaporation (ET) estimation through surface energy balance  
58 (SEB) model concerns an accurate characterization of ground heat flux in the open canopy  
59 architecture with mixed vegetation such as savanna or in ecosystems with low mean fractional  
60 vegetation cover, prevailing water stress, and strong seasonality in soil moisture. Ground heat flux  
61 (G) is an intrinsic component of SEB (Sauer and Horton, 2005), affecting the net available energy  
62 for ET (the equivalent water depth of latent heat flux, LE) and sensible heat flux (H). It represents  
63 an energy flow path that couples surface with the atmosphere and has important implications for  
64 the underlying thermal regime (Sauer and Horton, 2005). Depending on the vegetation fraction  
65 and water stress, the magnitude of instantaneous G varies greatly across different ecosystems. In  
66 the humid ecosystems with predominantly dense canopies and high mean fractional vegetation  
67 cover, G contributes to a small proportion in the surface energy balance. Dense canopy cover leads  
68 to less transmission of radiative fluxes through multiple layers of canopies, which results in low  
69 warming of the soil floor. Due to persistently high soil water content, humid ecosystems generally  
70 show low diurnal and seasonal variability in G. In contrast, the magnitude of G is substantially  
71 large in arid and semi-arid ecosystems with sparse and open canopy and soil moisture deficits. Due  
72 to prevailing feedback between the physics of ground heat flux, land-atmosphere interactions and  
73 vegetation ecophysiology, evaporation modelling in the complex ecosystems remains a  
74 challenging task (Wang et al., 2013; Kiptala et al., 2013). This paper addresses the challenge of  
75 simultaneous estimation of G and ET by combining thermal remote sensing observations with a  
76 mechanistic G model and a SEB model.

77 SEB models mainly emphasize on estimating sensible heat flux (H) by resolving the aerodynamic  
78 conductance ( $g_A$ ) and computes LE as a residual SEB component as follows:

$$LE = R_N - G - H \quad (1)$$

79  $R_N$  is the net radiation. The proportion of  $R_N$  that is partitioned into G depends upon soil properties  
80 like its albedo, soil moisture, soil thermal properties such as thermal conductivity and heat  
81 capacity, which vary with mineral, organic and soil water fractions. SEB models use land surface  
82 temperature (LST or  $T_S$ ) as an important lower boundary condition for estimating H and LE. Due  
83 to the extraordinarily high sensitivity of  $T_S$  to evaporative cooling and soil water content variations,

84 thermal infrared (TIR) remote sensing is extensively used in large scale evaporation diagnostics  
85 (Kustas and Anderson, 2009; Mallick et al., 2014, 2015a, 2018a; Cammalleri and Vogt, 2015;  
86 Anderson et al., 2012). Evaporation estimation through SEB models commonly employ empirical  
87 sub-models of  $G$  in a stand-alone mode. Despite the utility of mechanistic  $G$  models is  
88 demonstrated in different studies (Verhoef, 2004; Murray and Verhoef, 2007; Verhoef et al.,  
89 2012), no TIR-based evaporation study attempted to couple a mechanistic  $G$  model with a SEB  
90 model.

91 The SEB models for ET estimation driven by remote sensing observations generally use linear and  
92 non-linear relationships for estimating  $G$  and such methods generally employ  $R_N$ ,  $T_S$ , albedo ( $\alpha_R$ ),  
93 and NDVI (e.g., Bastiaanssen et al., 1998; Friedl, 2002; Santanello and Friedl, 2003). While the  
94 inclusion of  $T_S$  and albedo serves as a proxy for soil moisture and surface characteristics effects in  
95  $G$ , inclusion of NDVI provides a scaling of  $G - R_N$  ratio for different fractional vegetation cover.  
96 Unfortunately, the empirical approaches do not include any information of soil temperature or  
97 daily temperature amplitude. These empirical models also lack the universal consensus. Setting  $G$   
98 as a fraction of  $R_N$  does not solve the energy balance equation and disregards the role of thermal  
99 inertia of the land surface (Mallick et al., 2015b). This could introduce substantial uncertainty in  
100 LE estimation because  $G$  effectively couples the surface energy balance with energy transfer  
101 processes in the soil thermal regime. It provides physical feedback to LE through the effects of  
102 soil moisture, temperature, and conductivity (thermal and hydraulic) (Sauer and Horton, 2005).  
103 Such feedbacks are most critical in the arid and semi-arid ecosystems where LE is significantly  
104 constrained by the soil moisture dry-down. The limits imposed on LE by the water stress  
105 consequently result in greater partitioning of the net available energy (i.e.,  $R_N - G$ ) into  $H$  and  $G$   
106 (Castelli et al., 1999).

107 When LE is reduced due to soil moisture dry-down, both  $G$  and  $T_S$  tend to show rapid intra-  
108 seasonal rise. Therefore, the surface energy balance equation could be linked with mechanistic  $G$   
109 model,  $T_S$  harmonics (Verhoef, 2004), and soil moisture availability. Realizing the importance of  
110 direct estimates of  $G$  in LE and invigorated by the advent of TIR remote sensing, Verhoef et al.  
111 (2012) demonstrated the potential of a TI-based mechanistic model (Murray and Verhoef, 2007)  
112 (MV2007 hereafter) for spatiotemporal  $G$  estimates in semi-arid ecosystems of Africa. Some  
113 studies also emphasized the importance of using noontime and nighttime  $T_S$  and  $R_N$  for estimating

114 G (Mallick et al., 2015b; Bennet et al., 2008; Tsuang, 2005). The method of MV2007 has so far  
115 been tested in a stand-alone mode, and no remote sensing method has so far been attempted to  
116 combine such a mechanistic G model (e.g., MV2007-TI model) with a SEB model for coupled  
117 energy-water flux estimation and validation.

118 By integrating  $T_s$  into a combined structure of the Penman-Monteith (PM) and Shuttleworth-  
119 Wallace (SW) model, an analytical SEB model was proposed by Mallick et al. (2014, 2015a,  
120 2016). The model, Surface Temperature Initiated Closure (STIC), is based on finding analytical  
121 solution for aerodynamic and canopy-surface conductance ( $g_A$  and  $g_S$ ) where the expressions of  
122 the conductances were constrained by an aggregated water stress factor. Through physically  
123 linking water stress ( $T_s$  derived) with  $g_A$  and  $g_S$ , STIC established direct feedback between  $T_s$ , H  
124 and LE, and simultaneously overcame the need of empirical parameterization for estimating the  
125 conductances (Mallick et al., 2016, 2018a). Different versions of STIC have been extensively  
126 validated in different ecological transects (Tropical rainforest to woody savanna) and aridity  
127 gradients (humid to arid) (Trebs et al., 2021; Bai et al., 2021; Mallick et al., 2015a; 2016; 2018a,  
128 b; Bhattarai et al., 2018, 2019). Based on the conclusions of Verhoef et al. (2012), Mallick et al.  
129 (2014; 2015a,b; 2016; 2018a,b, 2022), Bhattarai et al. (2018, 2019), and Bai et al. (2021), there is  
130 a need to address some of the challenges in SEB modeling, which are, (i) accurate estimation of G  
131 and ET in sparse vegetation, (ii) testing the utility of coupling a TI-based G model with an  
132 analytical SEB model for accurately estimating G and ET, and (iii) detailed evaluation of a coupled  
133 G-SEB model at the ecosystem scale. Realizing the significance of mechanistic G model  
134 (MV2007), the advantage of the analytical STIC model, and to mitigate some of the overarching  
135 gaps in SEB modeling in sparsely vegetated open canopy systems, this study presents the first-  
136 ever coupled implementation of MV2007 G with the most recent version of STIC (STIC1.2). We  
137 name this new coupled model as STIC-TI and it requires noon-night  $T_s$  and associated remotely  
138 sensed land surface variables as inputs. We performed subsequent evaluation of STIC-TI in nine  
139 terrestrial ecosystems in arid, semi-arid and sub-humid climate in India, the United States of  
140 America (USA) (northern hemisphere) and Australia (southern hemisphere) at the eddy covariance  
141 flux tower sites. The current study addresses the following research questions and objectives:

142 (i) What is the performance of STIC-TI G estimates when compared with conventionally used  
143 empirical G models in ecosystems having low mean fractional vegetation cover ( $f_c$ ) ( $\leq 0.5$ ) and  
144 having larger soil exposure to radiation for example in Savanna?

145 (ii) How do the estimates from STIC-TI LE and H fluxes compare with LE and H observations in  
146 diverse terrestrial ecosystems that represent a varied range of  $f_c$  (0.25 – 0.5) covering cropland,  
147 savanna, mulga vegetation (woodlands and open-forests dominated by the mulga tree [*Acacia*  
148 *aneura*]) spread across arid, semi-arid, sub-humid, humid climates over a vast range of rainfall  
149 (250 to 1730 mm), temperature (-4 to 46°C) and soil regimes?

150 (iii) What is the seasonal variability of G and evaporative fraction from STIC-TI model in a wide  
151 range of ecosystems having contrasting aridity and vegetation cover?

152 It is important to mention that assessing the performance of STIC-TI LE and H with respect to  
153 other SEB models is not within the scope of the present study. The prime focus of the current study  
154 is to assess the sensitivity of STIC-TI, temporal variability of the retrieved SEB fluxes, and cross-  
155 site validation of the individual SEB components.

156 A list of variables, their symbols and corresponding units are given in Table A1 in Appendix A.

## 157 **2 Study area and datasets**

### 158 **2.1 Study site characteristics**

159 The present study was conducted using data from nine flux tower sites (four sites in India; three  
160 sites in Australia; two sites in USA) equipped with Eddy Covariance (EC) measurement systems.

161 The distribution of the flux tower sites considered for the present study are shown in Fig.1 below.

162 The sites cover a wide range of climate, vegetation types, low fractional vegetation cover ( $f_c$ ) of  
163 around 0.5 and have contrasting aridity (Table 1). In India, a network of EC towers was set up

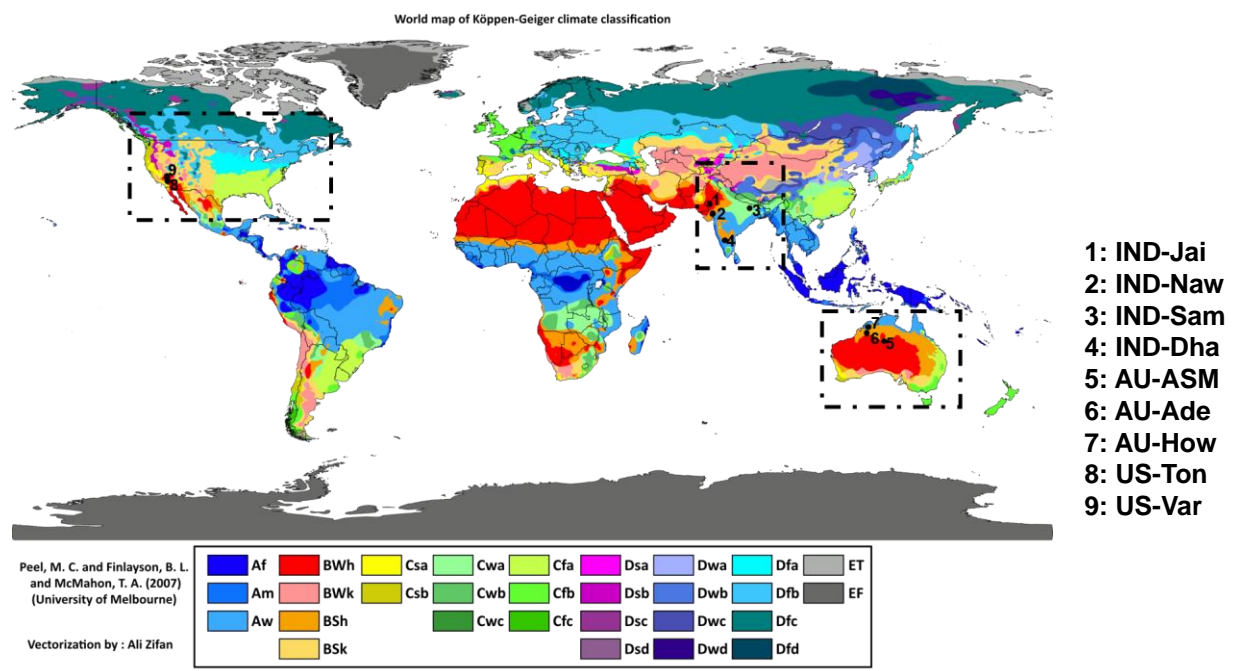
164 under Indo-UK INCOMPASS (INteraction of Convective Organization and Monsoon  
165 Precipitation, Atmosphere, Surface and Sea) Program (Turner et al., 2019) at Jaisalmer (IND-Jai)

166 in Rajasthan state, Nawagam (IND-Naw) in Gujarat state, Samastipur (IND-Sam) in Bihar state  
167 and under Newton-Bhaba programme (Morisson et al., 2019 a,b) at Dharwad (IND-Dha) in

168 Karnataka state. The flux footprint for EC towers in India varied from 500 m – 1 km (Bhat et al.,  
169 2019). In the present study, about 90% of the fluxes came from an area within 500 m to 1 km from

170 the EC tower. Therefore, the relative contribution of vegetated land surface area to the fluxes is  
 171 close to 90% (Schmid, 2002; Vesala et al., 2008). The remaining percentage of fluxes originated  
 172 from an area beyond the flux footprint. The mean annual  $f_c$  was found to vary from 0.25 to 0.52  
 173 with standard deviation (SD) ranging from 0.1 to 0.16.

174 The IND-Jai site represents arid western zone over desert plains of natural grassland ecosystem.  
 175 The region receives very low rainfall (100 – 300 mm) during monsoon and experiences a wide  
 176 range in air temperature, high solar radiation, wind speed and high evaporative demand (Raja et  
 177 al., 2015). The IND-Naw site represents semi-arid agroecosystem in the middle Gujarat  
 178 agroclimatic zone of north-west India and has a pre-dominant rice-wheat cropping system. The  
 179 IND-Sam site has sub-humid climate of north-west alluvial plain zone in the Indo-Gangetic Plain  
 180 (IGP) situated in the eastern India and this site also follows rice-wheat crop rotation. IND-Dha  
 181 represents humid sub-tropical climate of transition zone in the southern India and this site  
 182 comprises of crops.



**Figure 1:** Locations of the flux tower sites in India, Australia and USA overlaid on climate type map. (Image Source: By Peel, M. C., Finlayson, B. L., and McMahon, T. A. (University of Melbourne) enhanced, modified, and vectorized by Ali Zifan; Hydrology and Earth System Sciences: "Updated world map of the Köppen-Geiger climate classification". Legend explanation, CC BY-SA 4.0, <https://commons.wikimedia.org/w/index.php?curid=47086879>)

183 In USA, two EC tower sites were located at Tonzi Ranch (US-Ton) and Vaira Ranch (US-Var), in  
184 the lower foothills of the Sierra Nevada Mountains. Both the EC stations are part of the  
185 AMERIFLUX Management Project (<https://ameriflux.lbl.gov/>). US-Ton is classified as an oak  
186 savanna woodland. While the overstorey is dominated by blue oak trees (40% of total vegetation)  
187 with intermittent grey pine trees (3 trees per hectare), the understory species include a variety of  
188 grasses and herbs. The mean annual rainfall at this site is 559 mm. US-Var is a grassland dominated  
189 site and the growing season is confined to the wet season only, typically from October to early  
190 May. The mean annual rainfall at this site is 559 mm. The mean annual  $f_c$  was found to vary from  
191 0.18 to 0.26 and SD of the order of 0.06 to 0.07.

192 In Australia, three EC tower sites were located at Howard Springs (AU-How), Alice Springs Mulga  
193 (AU-ASM), Adelaide river (AU-Ade) in the Northern Territory as part of the OzFlux network  
194 (Beringer et al., 2016) and the Terrestrial Ecosystem Research Network (TERN), which is  
195 supported by the National Collaborative Infrastructure Strategy (NCRIS)  
196 (<http://www.ozflux.org.au/monitoringsites/index.html>). The AU-How is situated in the Black  
197 Jungle Conservation Reserve representing an open woodland savanna and the mean annual rainfall  
198 is 1750 mm. The AU-ASM is located on Pine Hill cattle station near Alice Springs. The woodland  
199 is characterized by mulga canopy and mean annual rainfall is 306 mm. AU-Ade represents savanna  
200 with a mean annual rainfall of 1730 mm. The mean annual  $f_c$  varied from 0.21 to 0.48 having SD  
201 range of 0.08 - 0.17. A description of Australian flux sites is given in Beringer et al. (2016).  
202 Average heights of vegetation are 1.15 m at IND-Naw, 1 m at IND-Jai, 1.23 m at IND-Sam, 1.5  
203 m at IND-Dha, 6.5 m at AU-ASM, 15m at AU-How, 7 m at AU-Ade, 10 m at US-Ton, and  $\leq 0.5$   
204 m at US-Var.

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214 **Table 1:** An overview of the EC flux tower site characteristics in the present study

Hemisphere	Sites	Latitude (°N), Longitude (°E)	Climate & Vegetation	Mean $f_c$ (SD)	Soil texture	T <sub>A</sub> range (°C)	Mean Annual P (mm)	Observation period
Northern	Jaisalmer (IND-Jai)	26.99, 71.34	Arid grassland	0.25(±0.1)	Loamy fine sand to coarse sand	8 – 40	250	2017 – 2018
	Nawagam (IND-Naw)	22.80, 72.57	Semi-arid cropland	0.41(±0.13)	Sandy loam	9 – 39	700	2017 – 2018
	Samastipur (IND-Sam)	26.00, 85.67	Humid subtropical cropland	0.52(±0.16)	Sandy loam to loam	10 – 39	1000	2017 – 2018
	Dharwad (IND-Dha)	15.50, 74.99	Tropical Savanna	0.36(±0.11)	Shallow to medium black clay and red sandy loam soils	12 – 40	650	2016 – 2018
	Tonzi ranch (US-Ton)	38.43, -120.96	Woody Savanna	0.18(±0.06)	Red sandy clay loam	0 – 40	559	2011 – 2019
	Vaira ranch (US-Var)	38.41, -120.95	Arid grassland	0.26(±0.07)	Rocky silt loam	0 – 40	559	2011 – 2019
Southern	Alice Springs Mulga (AU-ASM)	-22.28, 133.24	Semi-arid mulga	0.21(±0.09)	Loamy sand	(-4) – 40	305	2011 – 2014
	Howard Springs (AU-How)	-12.49, 131.15	Tropical savanna	0.48(±0.17)	Red kandasol	19 – 34	1700	2011 – 2014
	Adelaide River (AU-Ade)	-13.07, 131.11	Savanna	0.42(±0.08)	Yellow hydrosol, shallow, loamy sand with coarse gravel	16 – 37	1730	2007 – 2009

215 T<sub>A</sub>: Air temperature during the observation period; P: rainfall (mm) measured using rain gauge at flux tower site during the study  
 216 period. IND is for India, AU is for Australia, and US is for the United States; SD is standard deviation of annual mean  $f_c$  which is  
 217 computed from NDVI as mentioned in section 3.1.

## 218 2.2 Datasets

### 219 2.2.1 Micrometeorological data at flux tower sites

220 Standardized, controlled, and harmonized surface energy balance (SEB) flux and meteorological  
221 data from nine EC towers were used in the present analysis. In Australia, H and LE were measured  
222 through the EC systems and  $R_N$  were measured through net radiometers at varying heights of 15  
223 m (AU-Ade), 23 m (AU-How), and 11.6 m (AU-ASM), respectively. In India, the EC  
224 measurement height was maintained approximately at 8 m above the surface, except at IND-Dha  
225 where it was installed at a height of 4.2 m. In USA, the SEB measurements were carried out at  
226 tower heights of 23 m at US-Ton and 2 m US-Var. A summary of the instrumentation is given in  
227 Table A2 of Appendix A. All the flux tower sites were equipped with a range of meteorological  
228 instrumentation which measured diurnal air temperature ( $T_A$ ) and relative humidity ( $R_H$ ), four  
229 components of the net radiation ( $R_N$ , consisting of down- and up-welling shortwave and long-wave  
230 radiation ( $SW\downarrow$ ,  $SW\uparrow$ ,  $LW\uparrow$  and  $LW\downarrow$ , respectively)) above the vegetated canopy. In addition, the  
231 diurnal soil heat flux ( $G$ ) and soil temperature ( $T_{ST}$ ) were measured at all the three Australian sites  
232 and two US sites. In India, the diurnal soil heat flux was measured only at IND-Dha.

233 For the Indian sites, the raw EC measurements of the turbulent wind vectors ( $u$ ,  $v$  and  $w$ , for  
234 horizontal, meridional and vertical, respectively), sonic temperature ( $T$ ), and  $CO_2$  and water vapor  
235 mass density were recorded at a sampling rate of 20 Hz. Raw EC data were post-processed to  
236 obtain level-3 quality controlled and harmonized surface fluxes at 30-minute flux averaging  
237 intervals using EddyPRO® Flux Calculation Software (LI-COR Biosciences, Lincoln, Nebraska,  
238 USA) using the data handling protocol described by Bhat et al. (2019). The EC data from the  
239 OzFlux sites was averaged over 30 minutes recorded by the logger and processed through levels  
240 using the PyFluxPro standard software processing scripts as mentioned in Isaac et al. (2017). The  
241 Level 3 (L3) used in this paper was produced using PyFluxPro (Isaac et al., 2017) employing the  
242 Dynamic INtegrated Gap filling and partitioning for Ozflux (DINGO) system as described in  
243 Donohue et al. (2014) and Beringer et al. (2016). The quality checked EC data at 30 minute  
244 intervals for two AMERIFLUX sites US-Ton and US-Var was acquired from  
245 <https://doi.org/10.17190/AMF/1245971> & <https://doi.org/10.17190/AMF/1245984>, respectively.

246 **2.2.2 Remote sensing data**

247 Optical and thermal remote sensing observations available from Moderate Resolution Imaging  
 248 Spectroradiometer (MODIS) (Didan et al., 2015) on-board Aqua platform were used in the present  
 249 study (Table 2) for estimating G and associated SEB fluxes. These include eight-day land surface  
 250 temperature (LST or  $T_S$ ) at 1:30 pm and 1:30 am, and surface emissivity ( $\epsilon_s$ ) (MYD11A2), daily  
 251 surface albedo ( $\alpha_R$ ) (MCD43A3), 16-day NDVI (MYD13A2). The overpass times of MODIS  
 252 Aqua are at 1:30 pm and 1:30 am. The 8-day average values of clear-sky  $T_S$  available from  
 253 MYD11A2 data were used (Source: <https://vip.arizona.edu/documents/viplab/MYD11A2.pdf>) for  
 254 all nine flux tower sites. Since MYD21A2 LST product is known to provide better accuracy (1 –  
 255 1.5 K) (Hulley et al, 2016) as compared to MYD11A2 LST over semi-arid and arid ecosystems,  
 256 the former was also used in STIC-TI to compare LE and H estimates (see Table 5 in section 4.4)  
 257 with the estimates of MYD11A2 LST over the arid and semi-arid sites (IND-Jai, IND-Naw, US-  
 258 Ton). The noon-night pair of thermal remote sensing observations from Aqua are close to the time  
 259 of occurrences of maximum and minimum soil surface temperature (see Figure 2) and are therefore  
 260 ideal for soil heat flux modeling using thermal inertia. The MODIS Terra overpass times are at 11  
 261 am and 11 pm and are far from the time of occurrences of minimum-maximum soil temperatures.  
 262 Therefore, MODIS Aqua acquisition times were used in the present study.

263 **Table 2:** A summary of MODIS Aqua optical and thermal remote sensing products used in the  
 264 present study

Data type	Product ID (version)	Variables used	Spatial resolution (m)	Temporal resolution	Purpose	Inputs to equation numbers
LST and emissivity	MYD11A2 (V006) MYD21A2	$T_S$ (1:30 pm and am) and $\epsilon_s$	923	8-day	For estimating $R_{Ni}$ , $G_i$ , $LE_i$ , $H_i$	(5), (13), (C6), (C7), (B8)
Surface albedo	MCD43A3 (V006)	$\alpha_R$	462	8-day composite from daily	For estimating $R_{Ni}$ , $G_i$	(5), (B3)

Vegetation index	MYD13Q1 (V006)	NDVI	250	16-day	For estimating $G_i$	(4)
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## 265 **3 Methodology**

### 266 **3.1 Coupled soil heat flux-SEB model**

267 In this paper, we modified a thermal inertia (TI) based soil heat flux (G) model using noon-night  
268 thermal remote sensing observations and thereafter coupled the TI-based G with STIC1.2. A clear-  
269 sky net radiation ( $R_N$ ) model was also introduced into this coupled model and  $R_N$  estimation  
270 algorithm is described in Appendix B. The estimation of G through modifying MV2007-TI  
271 approach and its coupling with STIC1.2 is the most novel component of the modeling scheme, and  
272 it is therefore described in the main body of the paper (section 3.1.1). Such a coupling enabled the  
273 implementation of a mechanistic G model along with an analytical SEB model using optical-  
274 thermal remote sensing data. The coupled model is hereafter referred as STIC-TI.

#### 275 **3.1.1 MV2007 soil heat flux model based on Thermal Inertia (TI)**

276 The functional form for estimating instantaneous G ( $G_i$ , hereafter) (eq. 2 below) is based on the  
277 harmonic analysis of soil surface temperature and is described in detail by Murray and Verhoef  
278 (2007) and Maltese et al. (2013).

$$G_i = \Gamma \left[ (1 - 0.5f_C) \left( \sum_{n=1}^k A \sqrt{n} \omega \sin \left( n\omega t + \phi'_n + \frac{\pi}{4} - \frac{\pi \Delta t}{12} \right) \right) \right] = \Gamma J_s \quad (2)$$

279  $G_i$  is the soil heat flux at the surface at a particular instance ( $\text{Wm}^{-2}$ ),  $\Gamma$  is the soil thermal inertia ( $\text{J}$   
280  $\text{m}^{-2} \text{K}^{-1} \text{s}^{-0.5}$ ),  $k$  is the total number of harmonics used,  $A$  is the amplitude ( $^{\circ}\text{C}$ ) of the  $n^{\text{th}}$  soil  
281 surface temperature ( $T_{\text{ST}}$ ) harmonic,  $\omega$  is the angular frequency ( $\text{rads}^{-1}$ ),  $t$  is the time (s),  $\phi'_n$  is the  
282 phase shift of the  $n^{\text{th}}$  soil surface temperature harmonic (rad),  $J_s$  is the summation of harmonic  
283 terms of soil surface temperature (K), and  $\Delta t$ (s) is time offset between the canopy composite  
284 temperature and the below-canopy soil surface temperature. Here, we represent  $G_i$  and  $A$  as  
285 ecosystem-scale ( $\leq 1\text{km}$ ) soil heat flux and surface soil temperature amplitude (averaged from soil  
286 surface to 10 cm depth), respectively and assume it to be valid for different vegetated landscape.

287 Since we have considered a single pair (noon-night corresponding to 1:30 pm and 1:30 am) of  
 288 MODIS aqua LST data in the present study, the phase shift ( $\phi'_n$ ) is taken as zero and number of  
 289 harmonics is taken as one ( $k=1$ ) for estimating  $G_i$ . Thus equation (2) is modified as follows:

$$G_i = \Gamma \left[ (1 - 0.5f_c) \left( A\sqrt{\omega} \sin \left( \omega t + \frac{\pi}{4} - \frac{\pi \Delta t}{12} \right) \right) \right] = \Gamma J_S \quad (3)$$

290 With the two boundary values (i.e.,  $\Delta t = 1.5$  h for  $f_c = 1$  and  $\Delta t = 0$  for  $f_c = 0$ ,  $f_c$  being the vegetation  
 291 fraction), a linear approach is proposed here to describe the time offset  $\Delta t$  as a function of  $f_c$   
 292 (Maltese et al., 2013). For a given day,  $f_c$  was derived by normalizing NDVI with the upper-lower  
 293 limits of annual NDVI cycle.

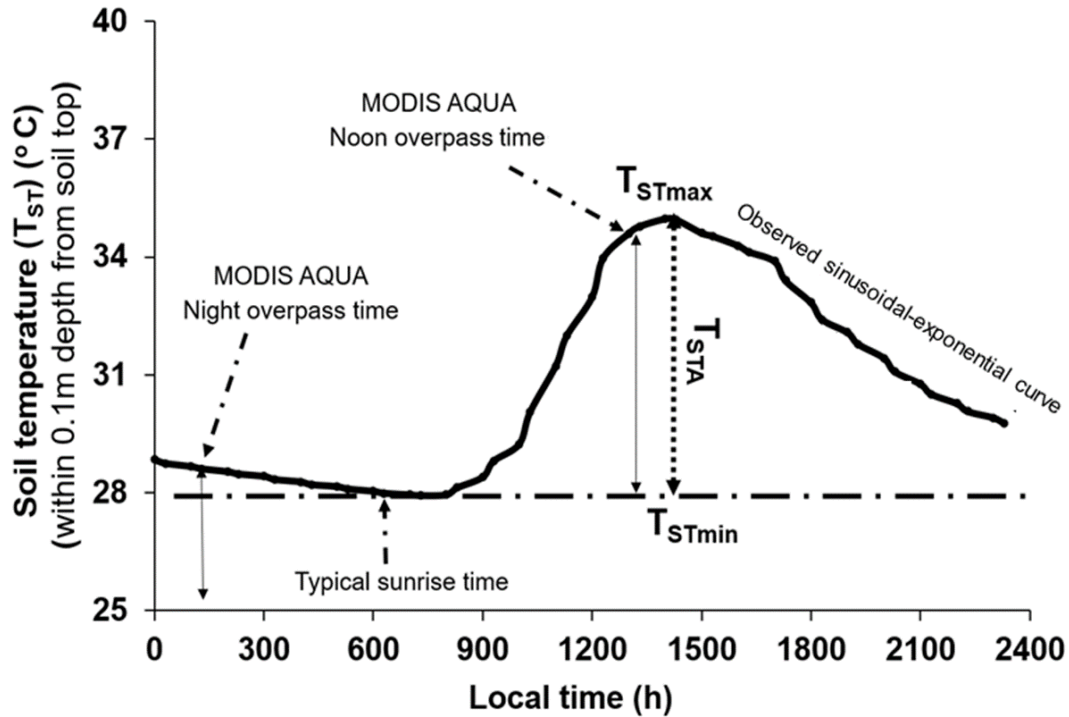
$$\Delta t = 1.5 f_c \quad (4)$$

### 294 ***3.1.1.1 Scaling function for estimating ecosystem-scale surface soil temperature amplitude (A)***

295 Estimating ecosystem-scale  $A$  involves two steps, (a) computing point-scale soil surface  
 296 temperature amplitude (from surface to 0.1m depth) ( $T_{STA}$ , hereafter) from the available  
 297 measurements of soil surface temperature, and (b) linking  $T_{STA}$  with remote sensing variables to  
 298 develop scaling functions for  $A$ . Point-scale soil temperature measured at different depths within  
 299 top 10 cm soil layer at AU-ASM, US-Ton, US-Var was averaged and considered as representative  
 300 surface soil temperature (0 – 10 cm). For Ind-Dha and AU-Ade, single-depth (10 cm) soil  
 301 temperature measurement was used. Studies also showed that LST carries some signal beneath the  
 302 skin of the surface (Johnston et al., 2022).

303 Several studies suggested theoretical sinusoidal trajectory of soil surface and sub-surface  
 304 temperatures (Gao et al., 2010), where the amplitude is maximum at the surface, and it gradually  
 305 decreases with depth to become 37% of surface amplitude until the damping depth (Hillel, 1982).  
 306 However, at deeper depths, soil temperatures remain constant with time and do not show many  
 307 fluctuations as compared to surface or near-surface soil temperatures. This invariant soil  
 308 temperature is called deep soil temperature (Mihailovic et al., 1999). However, the diurnal surface  
 309 soil temperature measurements (within top 0.1 m depth) across different flux tower sites showed  
 310 a sinusoidal-exponential behavior, i.e., sinusoidal pattern from sunrise until the afternoon and  
 311 exponential pattern from afternoon through sunset to the next sunrise. An illustrative example of

312 the theoretical and observed trajectories of surface soil temperature is shown in Fig. 2. This diurnal  
 313 surface soil temperature variation has a single harmonic component (Gao et al., 2010). For  
 314 computing  $T_{STA}$ , theoretical half-curve of sinusoidal pattern is assumed and was derived from  
 315 measurements as exemplified in Fig 2.



**Figure 2.** An illustrative example of typical diurnal variation of observed soil temperature ( $T_{ST}$ ) (from surface to 0.1m depth) at OzFlux sites and timings of MODIS AQUA observations. Here,  $T_{STmax}$  and  $T_{STmin}$  are maximum and minimum point-scale observed soil surface temperatures

316  
 317 It is evident from Fig. 2 that  $T_{STmin}$  represents minimum surface soil temperature occurring 1-1.5h  
 318 after sunrise and  $T_{STmax}$  occurs during 12.30 – 15.00h local time. The *in-situ* measured  $T_{ST}$  on  
 319 completely clear-sky days at OzFlux sites were used to extract  $T_{STmax}$  and  $T_{STmin}$  and  $T_{STA}$  was  
 320 derived as  $(T_{STmax} - T_{STmin})$  from the theoretical half-curve of sinusoidal pattern.

321  $T_{STA}$  is generally influenced by several land surface characteristics such as surface temperature  
 322 and surface albedo of soil-canopy complex, surface heat capacities, fractional canopy cover and  
 323 thermal conductivity (White, 2013).  $T_s$  and  $\alpha_R$  are the major thermal and reflective land surface  
 324 properties that have strong synergy with surface soil temperature dynamics. Hence, we have used  
 325 bivariate regression analysis to develop a scaling function for estimating ecosystem-scale  $T_{STA}$  (top  
 326 to 0.1m depth). The bivariate regression is based on the difference of noon (d) and night (n)  $T_s$

327 data and  $\alpha_R$  (Duan et al., 2013, Li Tian et al., 2014) from MODIS Aqua. The scaling function given  
 328 in eq. (5) estimates ecosystem-scale  $T_{STA}$  (symbolized as ‘A’ in equation 5) from surface to 0.1 m  
 329 soil depth:

$$A = B_1(T_{Sd} - T_{Sn}) + B_2(\alpha_R) + B_3 \quad (5)$$

330 Here, B1, B2, B3 are coefficients of regression model;  $T_{Sd}$  and  $T_{Sn}$  are noon and nighttime LST,  
 331 respectively. The results of this regression analysis are elaborated in section 4.1.

### 332 *3.1.1.2 Estimating $\Gamma$*

333  $\Gamma$  is the key variable for estimating  $G_i$  using eq. (2). MV2007 adopted the concept of normalized  
 334 thermal conductivity (Johansen, 1975) and developed a physical method to estimate  $\Gamma$  as follows:

$$\Gamma = e^{[\gamma'(1 - S_r^{\gamma' - \delta})]}(\tau_* - \tau_0) + \tau_0 \quad (6)$$

335 where  $\tau_*$  and  $\tau_0$  are the thermal inertia for saturated and air-dry soil ( $J m^{-2} K^{-1} s^{-0.5}$ );  $\tau_0 = D_1\theta^* + D_2$ ;  
 336  $\tau_* = D_3(\theta^*)^{-1.29}$ ;  $\gamma'$  (–) is a parameter depending on the soil texture (Murray and Verhoef, 2007;  
 337 Minasny, 2007; Anderson et al., 2007);  $S_r$  ( $m^3 m^{-3}$ ) is relative saturation and is equal to  $(\theta/\theta^*)$ ;  $\delta$   
 338 (unitless) is the shape parameter which is dependent on the soil texture.  $\theta^*$  ( $m^3 m^{-3}$ ) is the soil  
 339 porosity (equal to the saturated soil moisture content when soil moisture suction is zero),  $\theta$  ( $cm^3$   
 340  $cm^{-3}$ ) is the volumetric soil moisture and  $D_1, D_2, D_3$  are coefficients which were derived from a  
 341 large number of experimental data. The reported global values of  $D_1, D_2,$  and  $D_3$  were taken as -  
 342 1062.4, 1010.8, 788.2, respectively (Maltese et al., 2013). The value for  $\theta^*$  and shape parameter  
 343 for soil textures across study sites were specified according to Van Genuchten et al. (1980). The  
 344 details are mentioned in Table E1 of Appendix E.

345 In the present study, the relative soil moisture saturation,  $S_r(\theta/\theta^*)$  is represented in terms of an  
 346 aggregated moisture availability (M) of canopy-soil complex through a linear function (eq. 12). In  
 347 case of zero canopy cover, M represents the soil moisture availability from surface to 0.1 m depth.  
 348 In sparse and open canopy, rates of moisture availability from soil to root and root to canopy were  
 349 assumed same.

350 Theoretically, M is expressed as available soil moisture fraction between field capacity ( $\theta_{fc}$ ) and  
 351 permanent wilting ( $\theta_{wp}$ ) point as given in eq. (7) below.

$$M = \frac{\theta - \theta_{wp}}{\theta_{fc} - \theta_{wp}} \quad (7)$$

352 Where,  $\theta_{fc}$  ( $m^3 m^{-3}$ ) is the volumetric soil moisture at the field capacity (at a suction of 330 hPa)  
 353 and  $\theta_{wp}$  ( $m^3 m^{-3}$ ) is the volumetric soil moisture at the permanent wilting point (at suction of 15000  
 354 hPa) (Singh, 2007). Since  $\theta_{fc}$ ,  $\theta_*$ ,  $\theta_{wp}$  are characteristic volumetric soil moisture contents  
 355 corresponding to specific suctions and depends on the soil texture, dividing the numerator and  
 356 denominator in eq. (7) by  $\theta_*$  gives the following expression:

$$M = \frac{\frac{\theta}{\theta_*} - \frac{\theta_{wp}}{\theta_*}}{\frac{\theta_{fc}}{\theta_*} - \frac{\theta_{wp}}{\theta_*}} \quad (8)$$

357 Due to their dependence on soil texture, the ratios ( $\theta_{fc}/\theta_*$ ) and ( $\theta_{wp}/\theta_*$ ) are treated as constants.  
 358 These are represented as C and C' in the later equations (eq. 9, 10, and 11). The constants, C and  
 359 C' vary from 0.3 to 0.8 and from 0.1 to 0.4 (Murray and Verhoef, 2007; Minasny et al., 2011;  
 360 Anderson et al., 2007), respectively over different soil textures.

$$M = \frac{\frac{\theta}{\theta_*} - C'}{C - C'} \quad (9)$$

$$M(C - C') = \left(\frac{\theta}{\theta_*}\right) - C' \quad (10)$$

361 By replacing  $S_r$  in eq. (6) as  $\theta/\theta_*$  and by rearranging eq. (10), the following linear function is  
 362 obtained.

$$S_r = \frac{\theta}{\theta_*} = M(C - C') + C' = M' \quad (11)$$

363 Thus, the modified equation to calculate  $\Gamma$  is given by eq. (12) as follows:



$$\Gamma = e^{\left[ \gamma' \left( 1 - M^{\gamma'(\gamma' - \delta)} \right) \right]} (\tau_* - \tau_0) + \tau_0 \quad (12)$$

364 By substituting the values obtained from eq. (4), (5) and (12) into eq. (3), we obtained the  
 365 instantaneous ecosystem-scale  $G_i$  corresponding to MODIS Aqua noontime overpass. The intrinsic  
 366 link between  $G_i$  estimates through MV2007-TI and SEB scheme in STIC1.2 is made through  $M$ ,  
 367 where the computation of  $M$  follows the procedure as described in Mallick et al. (2016, 2018a, b)  
 368 and Bhattarai et al. (2018). (description in Appendix C).

### 369 **3.1.1.3 Estimating $M$**

370 In STIC1.2, an aggregated moisture availability ( $M$ ) of canopy-soil complex is expressed as the  
 371 ratio of the ‘vapor pressure difference’ between the aerodynamic roughness height of the canopy  
 372 (i.e., source/sink height) and air to the ‘vapor pressure deficit’ between aerodynamic roughness  
 373 height to the atmosphere:

$$M = \frac{(e_0 - e_A)}{(e_0^* - e_A)} = \frac{(e_0 - e_A)}{\kappa(e_S^* - e_A)} = \frac{s_1(T_{0D} - T_D)}{\kappa s_2(T_S - T_D)} \quad (13)$$

374 Where  $e_0$  and  $e_0^*$  are the actual and saturation vapor pressure at the source/sink height;  $e_A$  is the  
 375 atmospheric vapor pressure;  $e_S^*$  is the saturation vapor pressure at the surface;  $T_{0D}$  is dew point  
 376 temperature at the source/sink height;  $T_S$  is the LST;  $T_D$  is the air dew point temperature;  $s_1$  and  $s_2$   
 377 are the psychrometric slopes of the saturation vapor pressure and temperature between  $(T_{0D} - T_D)$   
 378 versus  $(e_0 - e_A)$  and  $(T_S - T_D)$  versus  $(e_S^* - e_A)$  relationship; and  $\kappa$  is the ratio between  $(e_0^* - e_A)$   
 379 and  $(e_S^* - e_A)$ . To solve the eq. (13), estimation of  $T_{0D}$  is necessary. An initial estimate of  $T_{0D}$  [ $T_{0D}$   
 380 =  $[(e_S^* - e_A) - s_3 T_S + s_1 T_D] / (s_1 - s_3)$ ] and  $M$  were obtained following Venturini et al. (2008) where  
 381  $s_1$  and  $s_3$  were approximated in  $T_D$  and  $T_S$ , respectively. However, eq. (13) cannot be directly  
 382 solved because there are two unknowns in one equation. However, since  $T_{0D}$  also depends on LE  
 383 (Mallick et al., 2016, 2018a), an iterative updation of  $T_{0D}$  (and  $M$ ) was carried out by expressing  
 384  $T_{0D}$  as a function of LE [ $T_{0D} = T_D + (\gamma LE / \rho c_p g_A s_1)$ ] which is described in detail by Mallick et al.  
 385 (2016, 2018a) and Bhattarai et al. (2018). In the numerical iteration,  $s_1$  was not updated to avoid  
 386 numerical instability and it was expressed as a function of  $T_D$ .

387 **3.1.2 STIC-TI: Coupling modified MV2007-TI and STIC 1.2**

388 The initiation of the coupling between MV2007-TI and STIC1.2 was executed through linking  $G_i$   
389 estimates from the modified MV2007-TI with  $M$  estimates from STIC1.2. Having the initial  
390 estimates of  $M$  (through eq. 13), an initial estimation of  $G_i$  was made from eq. (2) where  $S_r$  in eq.  
391 11 was replaced with the initial estimates of  $M'$ . From the initial estimates of  $G_i$  (eq. 2) and  $R_{Ni}$   
392 (equations in Appendix B), initial estimates of  $LE_i$  and  $H_i$  were obtained through the Penman-  
393 Monteith Energy Balance (PMEB) equation. Analytical expressions of the conductances for  
394 estimating  $H$  and  $LE$  through the PMEB equation were obtained by solving the state equations as  
395 described in the Appendix. The process was then iterated by updating  $T_{0D}$  [ $T_{0D} = T_D +$   
396  $(\gamma LE / \rho c_p g_{AS1})$ ] and  $M$  in every time step (as mentioned in Mallick et al., 2016, 2018a), and re-  
397 estimating  $G_i$  (using eq. 3), net available energy ( $R_{Ni} - G_i$ ), conductances,  $LE_i$  and  $H_i$ , until stable  
398 estimates of  $LE_i$  were obtained. The conceptual block diagram and algorithm flow of STIC-TI is  
399 shown in Fig. 3a and Fig 3b, respectively.

400

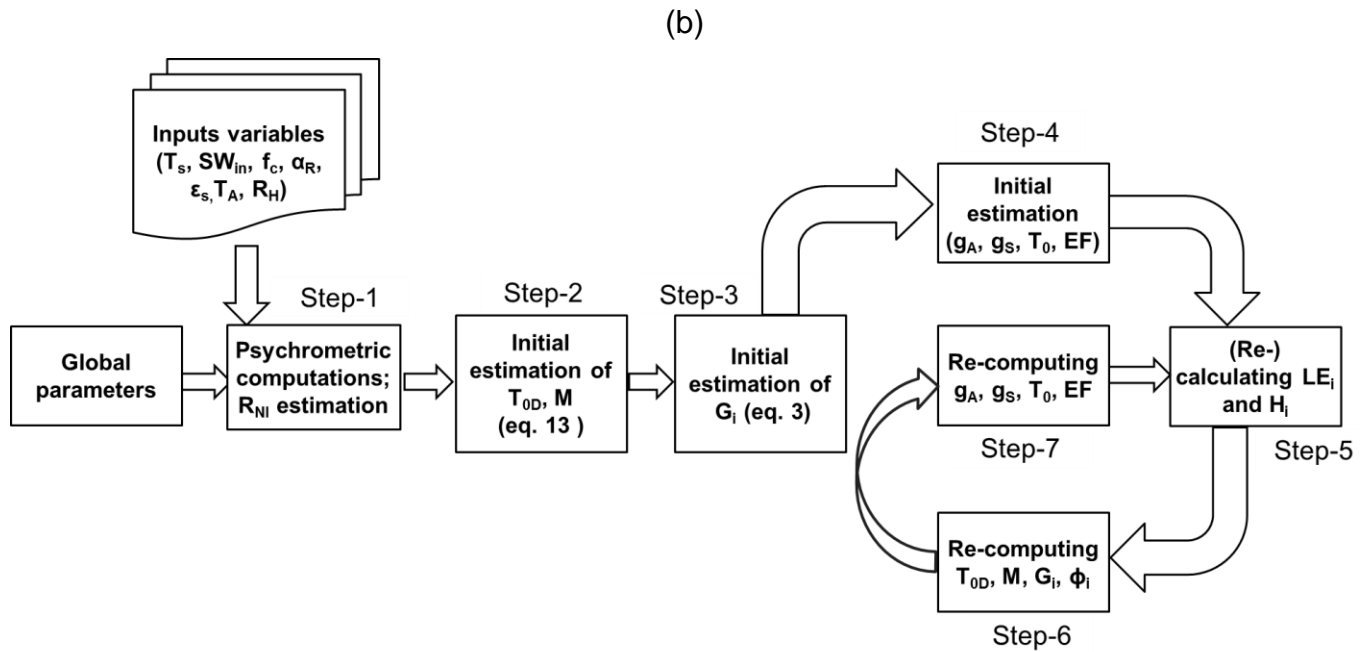
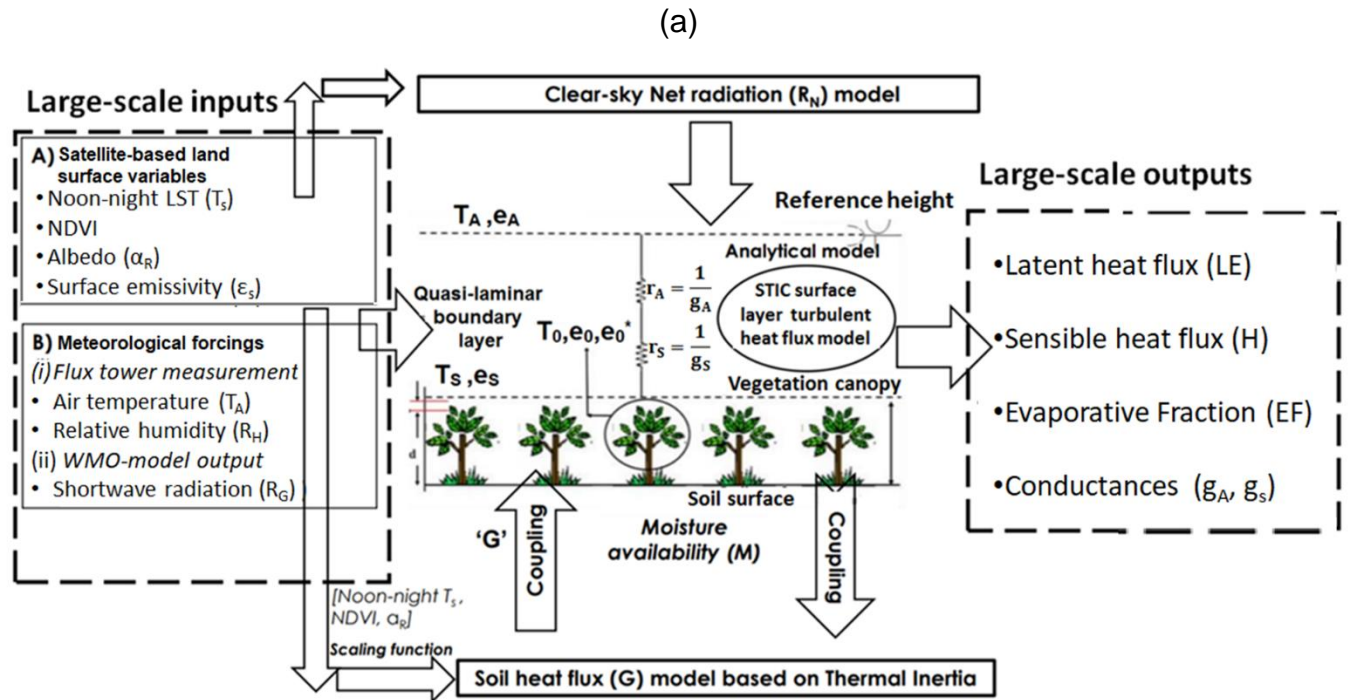
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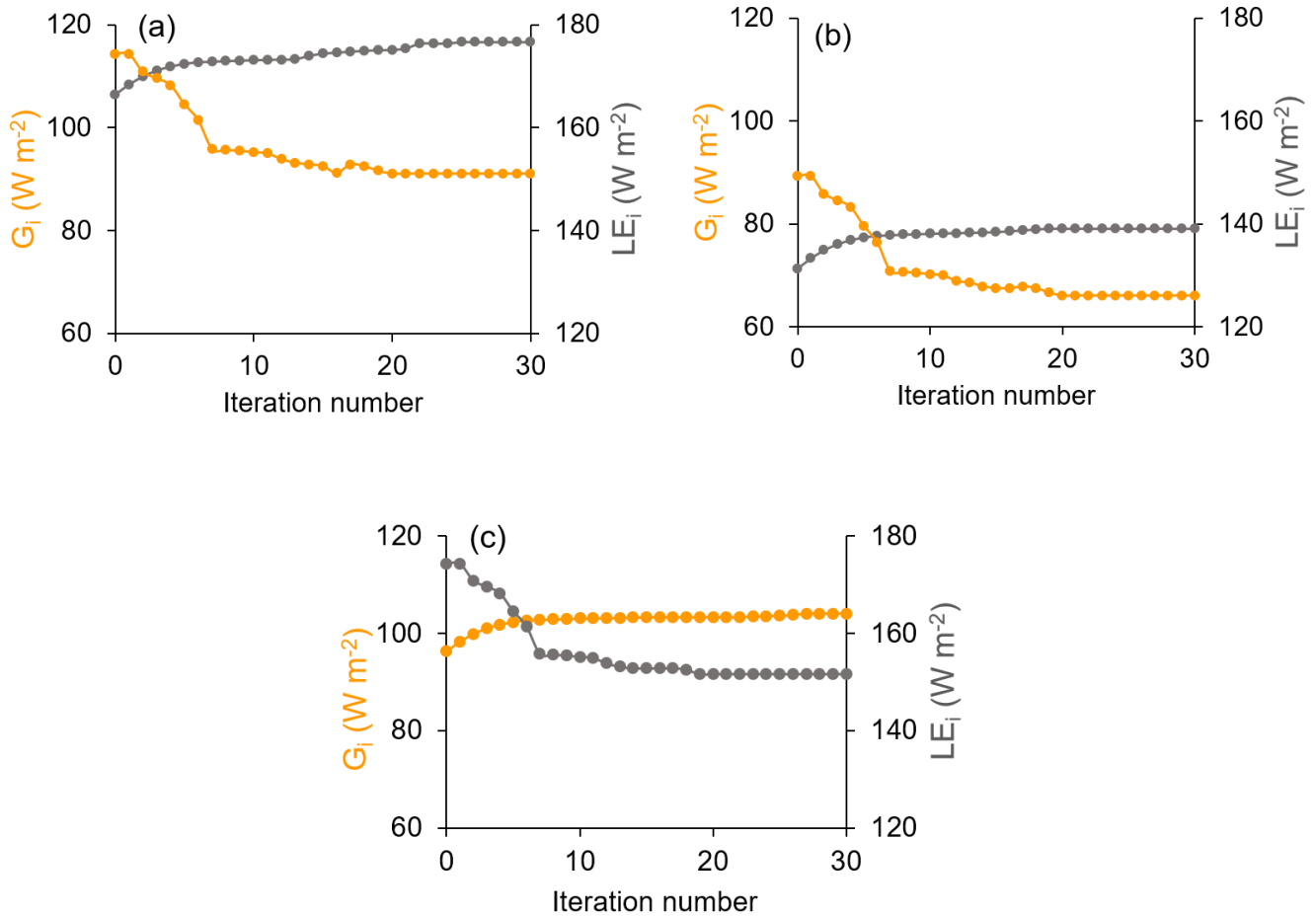
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**Figure 3:** (a) Conceptual diagram of STIC-TI model showing different input variables and model outputs, (b) Algorithmic flow for estimating G and associated SEB fluxes through STIC-TI.

406 Examples of iterative stabilization of  $G_i$  and  $LE_i$  for Indian, Australian and US ecosystems of India  
 407 are shown in Fig. 4. The iterative stabilization of  $G_i$  and  $LE_i$  was obtained between 8-25 iterations  
 408 for all sites.



**Figure 4:** Illustrative examples of iterative stabilization of STIC-TI  $G_i$  (yellow marker line) and  $LE_i$  (grey marker line) in (a) IND-Jai, (b) AU-ASM, (c) US-Ton

409  
 410 The noteworthy features of STIC-TI are: (1) estimating  $G$  by modifying the mechanistic MV2007-  
 411 TI model using noon and midnight  $T_s$  information from thermal remote sensing observations  
 412 available through polar orbiting satellite platform (e.g. MODIS Aqua), (2) coupling the  
 413 mechanistic MV2007-TI  $G$  model with STIC1.2 to simultaneously estimate surface moisture  
 414 availability ( $M$ ),  $G$ , and SEB fluxes, (3) introducing water stress information in  $G$  (through  $M$ ) to  
 415 better constrain the aerodynamic and canopy-surface conductances as well as the SEB fluxes, and

416 (4) derivation of amplitude of ecosystem-scale surface soil temperature (from top soil to 0.1 m soil  
417 depth).

### 418 **3.1.3 Generation of remote sensing inputs**

419 Two of the key variables in SEB modeling are  $T_s$  and  $\epsilon_s$ . These two variables were retrieved at  
420 923m spatial resolution from MODIS Aqua noon-night TIR observations (MYD11A2) in bands  
421 11.03  $\mu\text{m}$  and 12.02  $\mu\text{m}$  using a generalized split-window algorithm (Wan et al., 2015). For  
422 optimal retrieval, tractable sub-ranges of atmospheric column water vapor and lower boundary air  
423 surface temperature were used. Land surface emissivity was estimated from land cover types and  
424 anisotropy factors. The MYD21A2 LST product was generated using Temperature-Emissivity  
425 Separation (TES) algorithm (Hulley et al, 2016) and improved water vapor scaling method to  
426 remove the atmospheric effects. Albedo was estimated from MODIS (MCD43A2 Version 6.0)  
427 Bidirectional Reflectance Distribution Function and Albedo (BRDF/Albedo) daily dataset (Schaaf  
428 et al., 2002)) at 462 m spatial resolution. Actual albedo is a value which is interpolated between  
429 white-sky and black-sky albedo as a function of fractional diffuse skylight (which is a function of  
430 aerosol optical depth). NDVI was obtained from level 3 MODIS vegetation indices product  
431 (MYD13Q1, version 6.1), which are generated every 16-day at 250 meter (m) spatial resolution.  
432 All the input remote sensing variables mentioned in table 2 were resampled to spatial resolution  
433 of MYD11A2 product (923 m).

### 434 **3.2 Sensitivity and statistical analysis**

435 The accuracy of STIC-TI heavily depends on the accuracy of  $T_s$ , NDVI, and  $\alpha_R$  due to the dual  
436 role of  $T_s$  in estimating  $M$  and  $G_i$ , the role of NDVI in  $G_i$ , and the combined role of  $T_s$  and  $\alpha_R$  in  
437 estimating  $R_{Ni}$ . Therefore, one-dimensional sensitivity analysis was conducted to assess the  
438 impacts of uncertainty in  $T_s$ , NDVI and  $\alpha_R$  on  $G_i$ ,  $H_i$  and  $LE_i$ . The sensitivity was assessed by  
439 varying noon-time  $T_s$  by  $\pm 0.5$  K,  $\pm 1.0$  K and  $\pm 1.5$  K (keeping nighttime  $T_s$  constant so that  
440 amplitude can vary automatically); varying NDVI by  $\pm 0.05$ ;  $\pm 0.10$ ,  $\pm 0.15$ ; and varying albedo by  
441  $\pm 0.02$ ,  $\pm 0.05$ ,  $\pm 0.10$ , respectively. SEB fluxes were computed by using  $T_s$ , NDVI, and  $\alpha_R$  for three  
442 different periods of the year in all the eight ecosystems. Sensitivity analyses were conducted by  
443 increasing and decreasing systematically  $T_s$ , NDVI,  $\alpha_R$  from its central value while keeping the  
444 other variables and parameters constant. This procedure was selected because the fluxes and

445 intermediate outputs of the STIC-TI model reflect an integrated effect due to uncertainty in  $T_s$ . In  
 446 the first run, SEB fluxes were computed using *in-situ*  $T_s$  measurements obtained from the flux  
 447 tower outgoing longwave radiation measurements. Then  $T_s$  was increased and decreased at  
 448 constant interval and a new set of fluxes were estimated. In the similar way,  $\alpha_R$  and NDVI were  
 449 increased and decreased at constant intervals and new set of fluxes were computed. The sensitivity  
 450 of STIC-TI was assessed by the equation 14.

$$\text{Sensitivity} = \frac{E_{i0} - E_{iM}}{O_i} * 100 \quad (14)$$

451  $E_{i0}$  is the estimated (original) model output and  $E_{iM}$  is the estimated (modified) output obtained by  
 452 changing the variable whose sensitivity is to be tested.  $O_i$  is actual measurements. Apart from the  
 453 sensitivity analysis, the following set of statistical metrics were used to assess model performances.

$$R^2 = \left( \frac{\sum_{i=1}^n (E_i - \bar{E}) (O_i - \bar{O})}{\sqrt{\sum_{i=1}^n (E_i - \bar{E})^2} \sqrt{\sum_{i=1}^n (O_i - \bar{O})^2}} \right)^2 \quad (15)$$

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^n (E_i - O_i)^2}{n}} \quad (16)$$

$$\text{BIAS} = \frac{\sum_{i=1}^n (E_i - O_i)}{n} \quad (17)$$

$$\text{MAPD} = \frac{100}{n} \sum_{i=1}^n \left| \frac{E_i - O_i}{O_i} \right| \quad (18)$$

$$\text{KGE} = 1 - \sqrt{(r - 1)^2 + \left( \frac{\sigma_E}{\sigma_o} - 1 \right)^2 + \left( \frac{\bar{E}}{\bar{O}} - 1 \right)^2} \quad (19)$$

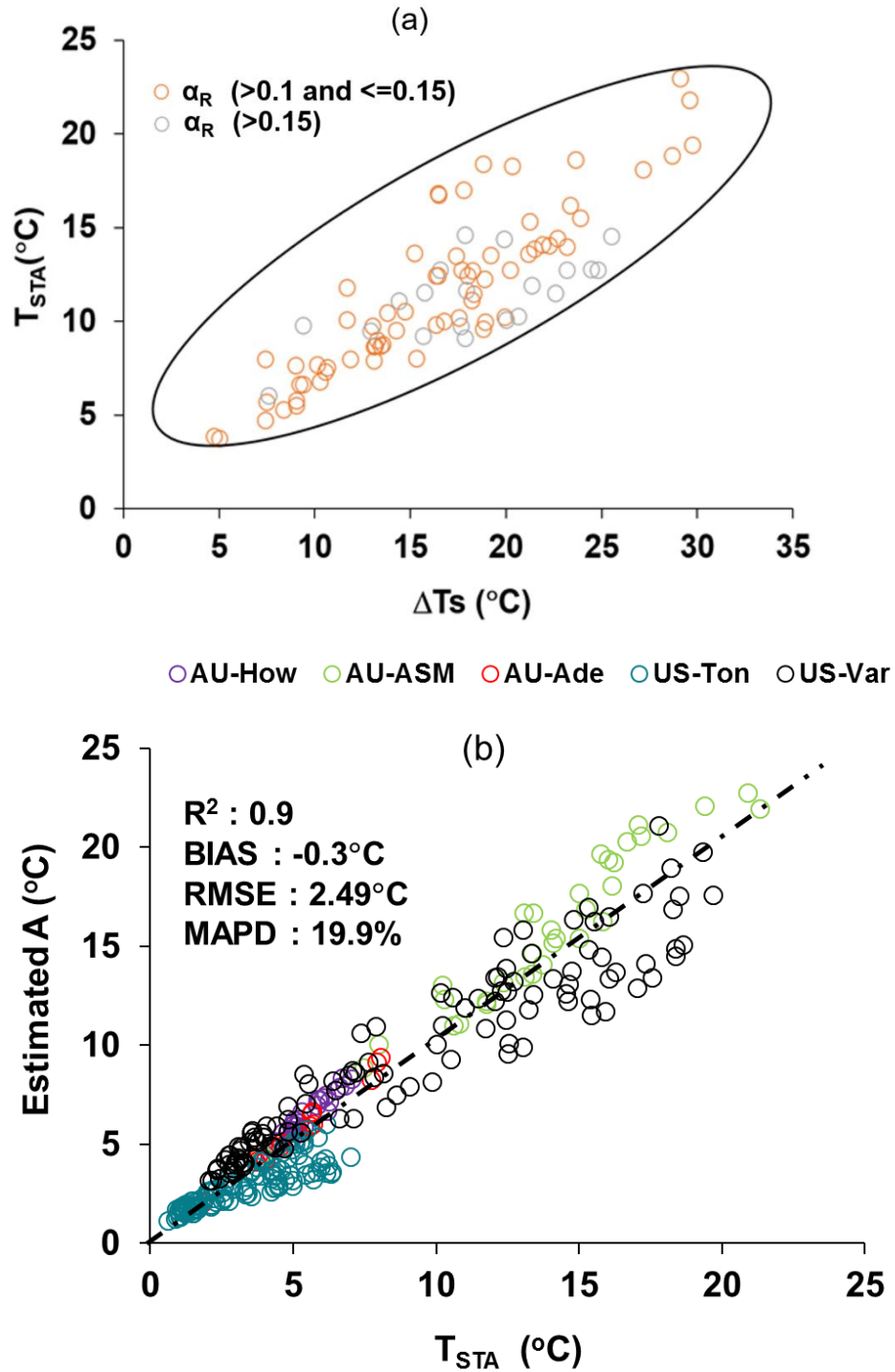
454 Where  $R^2$  is the coefficient of determination, RMSE is root-mean-square error, BIAS is the mean  
 455 bias, MAPD is the mean absolute percent deviation, KGE is Kling-Gupta efficiency,  $n$  is the total  
 456 number of data pairs, the bar indicates mean value of the measured variable and model estimates  
 457 of the same variable.  $E_i$  and  $O_i$  are the model estimated and measured SEB fluxes,  $r$  is the Pearson's  
 458 correlation coefficient and  $\bar{O}$  is the average of measured values and  $\bar{E}$  is the average of estimated

459 values and  $\sigma_o$  is standard deviation of observation values and  $\sigma_E$  is the standard deviation of  
460 estimated values. The KGE has been widely used for calibration and evaluation hydrological  
461 models in recent years and it combines the three components of Nash-Sutcliffe efficiency (NSE)  
462 of model errors (i.e., correlation, bias, ratio of variances or coefficients of variation) in a more  
463 balanced way. But it has not been widely used for analyzing the ET model performances.  $KGE = 1$   
464 indicates perfect agreement between modeled estimates and observations. The performance of a  
465 model is considered ‘poor’ for KGE between 0 and 0.5 and models with negative KGE values is  
466 considered ‘not satisfactory’.

## 467 **4 Results**

### 468 **4.1 Ecosystem- scale surface soil temperature amplitude (A)**

469 The scaling functions developed to estimate ecosystem-scale (1km) surface soil temperature  
470 amplitude (A) from point-scale  $T_{STA}$  were used to estimate  $G_i$ . However, before the development  
471 of the scaling functions, analysis was carried out to investigate the relationship of soil temperature  
472 amplitude between the two different spatial scales. The scatterplot (Fig. 5a) of noon-night LST  
473 difference ( $\Delta T_s$ ) versus  $T_{STA}$  for different albedo classes showed a linear increase in  $\Delta T_s$  with  
474 increasing  $T_{STA}$ . However, some divergence of data points within the cluster were also noticed  
475 which could be associated with different albedo ( $\alpha_R$ ) levels. Bivariate linear function was fitted  
476 between  $T_{STA}$  as predictand (Y) versus  $\Delta T_s$  ( $T_{sd} - T_{sn}$ ) and  $\alpha_R$  as predictors (X1 and X2,  
477 respectively). The function was found to be  $Y = 0.59X1 - 51.3X2 + 8.66$  by combining the data  
478 of nine ecosystems ( $r = 0.86$ ). The coefficients in the above expressions correspond to B1 (0.59),  
479 B2 (51.3), B3 (8.66) of eq. 5 in section 3.1.1.1. The estimated amplitude from this ecosystem-scale  
480 predictors and scaling functions was treated as ecosystem-scale surface soil temperature amplitude  
481 (A).



**Figure 5.** (a) Two-dimensional scatterplots between ( $\Delta T_s$ ) versus  $T_{STA}$  at different  $\alpha_R$  levels over different ecosystems. Here  $T_{STA}$  in y-axis is the observed soil temperature amplitude that is used to develop the scaling function and delta  $\Delta T_s$  is noon-night LST difference of MODIS AQUA; (b) Validation of ecosystem-scale estimates of A from the above functions over different sites.



482 Validation of ecosystem-scale estimates of A from the above functions over different sites is  
483 shown in Fig. 5b with respect to  $T_{STA}$  for the independent datasets. The estimated A was found to  
484 have MAPD of 19.9%, negative bias, and  $R^2 = 0.90$  over different ecosystems. The temporal  
485 variation of estimated A and  $T_{STA}$  is shown in Fig D1 in Appendix D. Further analysis was carried  
486 out to investigate the bias in A at three fractional vegetation cover ( $f_c$ ) classes ( $f_c < 0.3$ ;  $0.3 \leq f_c$   
487  $\leq 0.5$ ;  $f_c > 0.5$ ) representing bare soil (class 1), 30 – 50% canopy cover (class 2) and more than 50%  
488 canopy cover (class 3), respectively. While negative bias was noted for class 1 and class 3 ( $-0.54^\circ\text{C}$   
489 and  $-0.83^\circ\text{C}$ ), the bias was positive ( $0.49^\circ\text{C}$ ) in the intermediate  $f_c$  which represents sparse and  
490 patchy canopy cover. The signals of surface albedo, emissivity and temperatures of soil surface  
491 and canopy are relatively pure in class 1 and class 3 as compared to class 2, where the surface  
492 signal carries more heterogeneity. Given  $T_{STA}$  is computed from the in-situ measurements, it is  
493 likely to carry more heterogeneity in class 2 as compared to the other two classes. The land surface  
494 emissivity in MYD11A2 was estimated from land cover types and anisotropy factor, which have  
495 differential impacts on  $T_{ST}$  and  $T_S$  leading to such opposite bias in class 2 as compared to class 1  
496 and class 3.

## 497 **4.2 Sensitivity analysis of STIC-TI $G_i$ , $LE_i$ and $H_i$ to land surface variables**

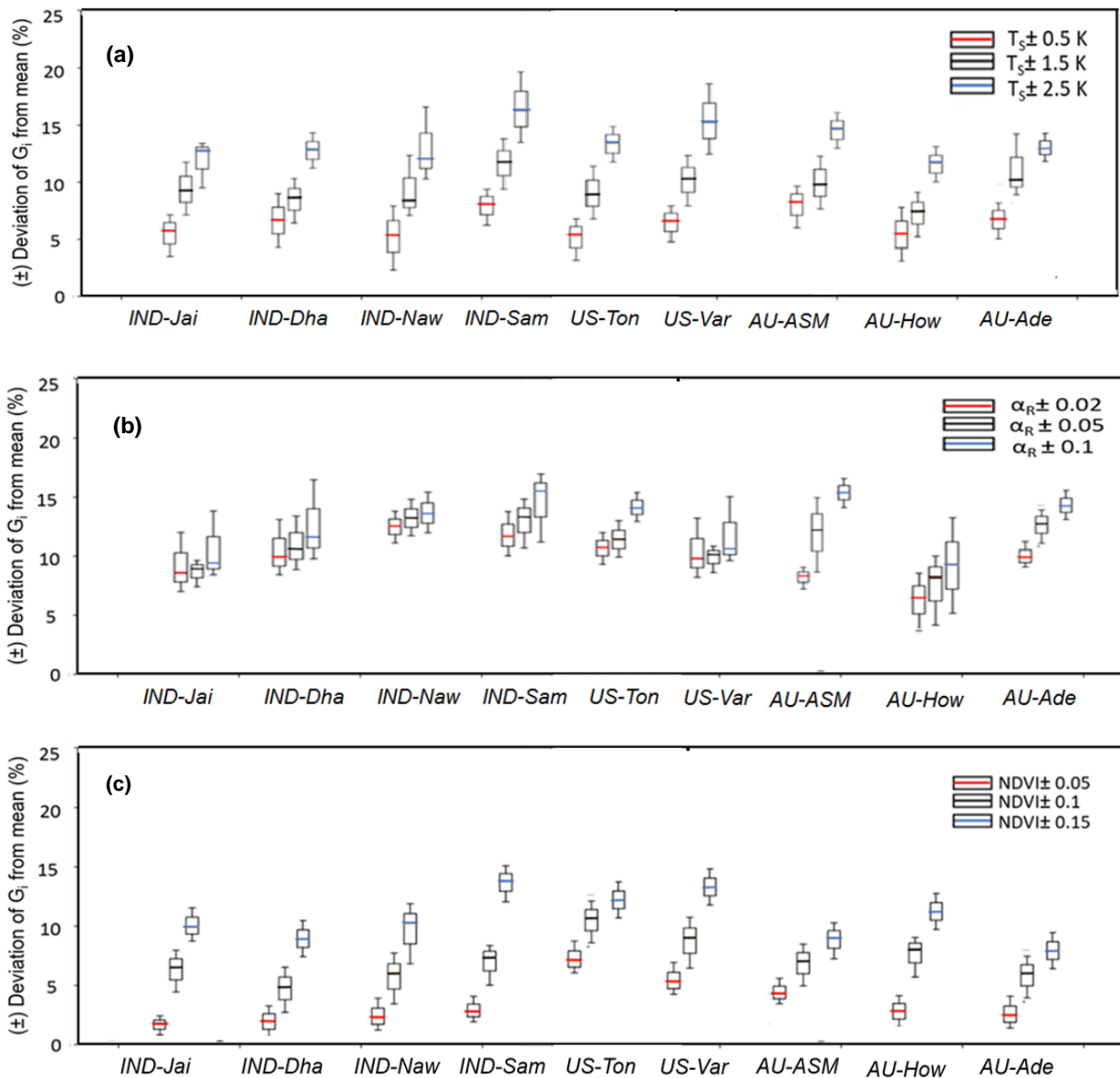
### 498 **4.2.1 Sensitivity of $G_i$ to land surface variables**

499 The average sensitivity of  $G_i$  to three land surface variables ( $T_S$ , NDVI,  $\alpha_R$ ) by combining the  
500 estimates of wet and dry periods is shown in Fig. 6.  $G_i$  was found to be substantially sensitive to  
501  $T_S$  with error magnitude ranging from 2 – 18% due to  $T_S$  uncertainties of  $\pm 0.5 - 2.5$  K (Fig. 6a),  
502 with greater sensitivity to  $T_S$  during the summer season. The median sensitivity of  $G_i$  due to  $\pm 5 -$   
503 10% uncertainty in  $\alpha_R$  varied from 5 to 12% in all the ecosystems (Fig. 6b). The uncertainties in  
504 NDVI revealed 2 to 15% error in  $G_i$  estimates (Fig. 6c), and no significant difference in the mean  
505 sensitivity due to NDVI uncertainties was noted between the ecosystems. The sensitivity of  $G_i$   
506 decreased with increasing values of NDVI.

### 507 **4.2.2 Sensitivity of $LE_i$ and $H_i$ to land surface variables**

508 Both  $LE_i$  and  $H_i$  were sensitive to  $T_S$  to the order of 2 – 29% ( $LE_i$ ) and 5 – 35% ( $H_i$ ) for  $T_S$   
509 uncertainty of  $\pm 0.5 - 2.5$  K from its mean values (Table 3). Interestingly,  $LE_i$  was more sensitive  
510 to  $T_S$  uncertainties as compared to  $H_i$  in the rainfed ecosystems. The highest mean sensitivity of

511  $LE_i$  to  $T_S$  was found in arid (IND-Jai: 2 – 28%), semi-arid (AU-ASM: 5 – 21%), tropical savanna  
 512 (IND-Dha: 3 – 26%), savanna (US-Ton: 4-29%) and arid (US-Var: 3-26%) ecosystems. The mean  
 513 sensitivity of  $H_i$  to  $T_S$  was maximum in sub-humid (IND-Sam: 2 – 32%), semi-arid (IND-Naw: 2  
 514 – 28%), savanna (AU-Ade: 8 – 17%) (Table 3). A greater sensitivity of the SEB fluxes due to  $\alpha_R$   
 515 uncertainties was found than due to NDVI. The median sensitivity of  $LE_i$  and  $H_i$  due to 10%  
 516 uncertainty from mean  $\alpha_R$  varied within 2 – 16% in all the ecosystems (Table 3). By contrast,  
 517 errors in the two SEB fluxes were substantially low (2 – 13%) due to  $\pm 0.05 – 0.15$  uncertainty  
 518 from mean NDVI (Table 3).



**Figure 6:** Sensitivity of STIC-TI  $G_i$  due to uncertainties in  $T_s$  (a),  $\alpha_R$  (b), and NDVI (c) for eight flux tower sites in India and Australia. The uncertainties were introduced by taking the mean values of these variables during three different periods (summer, rainy and winter) of a year. Mean uncertainties of the three periods are presented in the figure.

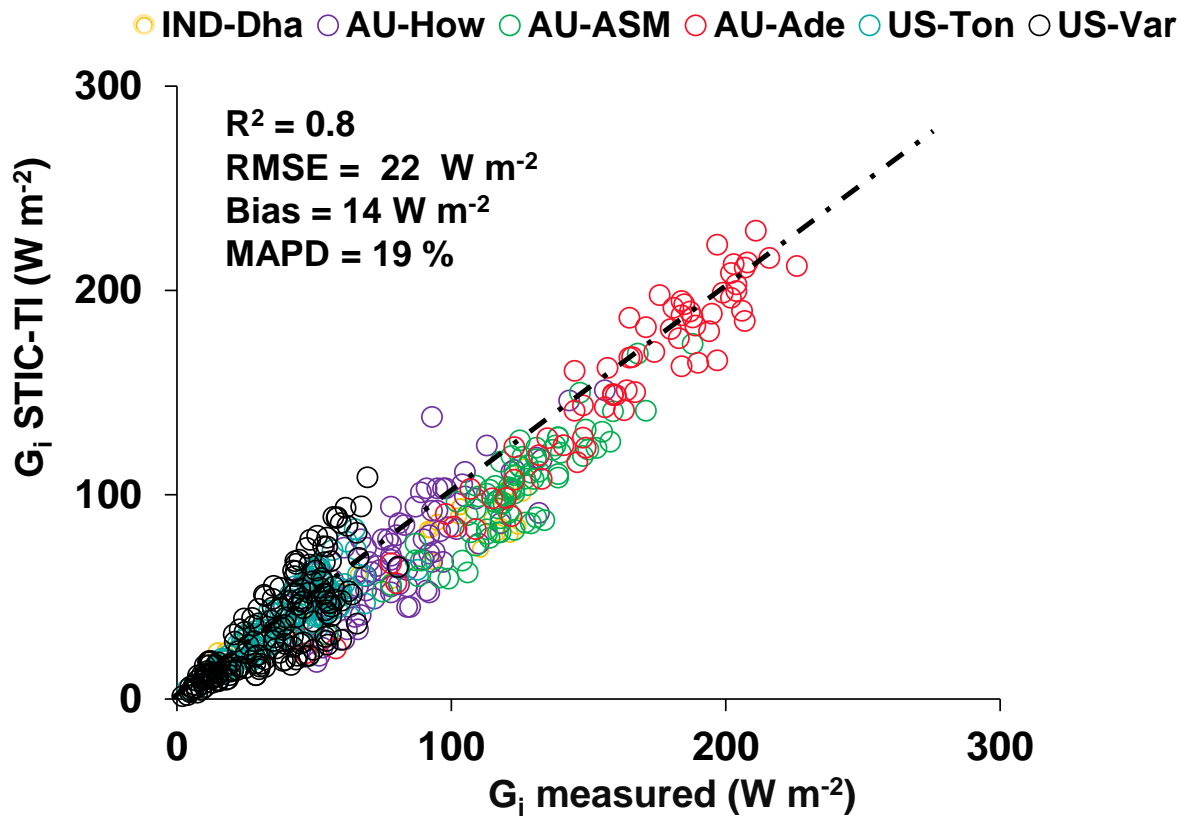
519 **Table 3:** Sensitivity (in percent) of  $LE_i$  and  $H_i$  due to  $T_s$ , NDVI, and  $\alpha_R$  uncertainties

Study sites	Sensitivity of $LE_i$ and $H_i$ to $T_s$ , NDVI and $\alpha_R$ (percent change)					
	$T_s$ uncertainty ( $\pm 0.5 - 2.5 K$ )		$\alpha_R$ uncertainty ( $\pm 5 - 10\%$ )		NDVI uncertainty ( $\pm 0.05 - 0.15$ )	
	$LE_i$	$H_i$	$LE_i$	$H_i$	$LE_i$	$H_i$
IND-Jai	2-28	1-6	3-14	2-13	2-8	2-6
IND-Dha	3-26	2-8	2-12	3-12	3-10	3-9
IND-Naw	1-20	2-28	2-10	3-10	2-7	2-6
IND-Sam	1-16	5-32	4-13	6-11	2-5	2-7
US-Ton	4-29	4-12	3-12	4-12	3-8	5-7
US-Var	3-26	6-14	4-11	2-10	4-10	2-8
AU-ASM	5-21	2-10	3-12	2-13	2-10	2-11
AU-How	8-13	2-15	2-11	4-16	3-12	3-13
AU-Ade	2-17	8-17	3-12	2-10	3-10	3-9

520 **4.3 Comparative evaluation of STIC-TI and contemporary  $G_i$  models**

521 The performances of STIC-TI and existing  $G_i$  models were evaluated and compared with respect  
522 to *in-situ*  $G_i$  measurements. The existing models reported by Moran et al. (1989), Bastiaanssen et  
523 al. (1998), Su (2002), and Boegh et al. (2004) have been considered for comparing with TI-based  
524 model. These four existing models are referred here as MOR89, BAS98, SU02 and BO04,  
525 respectively. While the models MOR89, SU02 and BO04 are based on linear regression between  
526  $G$  versus NDVI, BAS98 is based on multivariate regression of  $G$  with NDVI, LST and  $\alpha_R$ . The  
527 performance of the STIC-TI was substantially better as compared to MOR89, SU02 and BO04  
528 with respect to MAPD (19%), RMSE ( $22 \text{ Wm}^{-2}$ ) and coefficient of determination ( $R^2 = 0.8$ ) when  
529 compared with *in-situ* measurements over one Indian, three Australian and two US flux tower sites

530 (Table 4) and comparable with BAS98  $G_i$  model. The validation plot of retrieved noontime  $G_i$   
 531 from STIC-TI is shown in Fig. 7.



**Figure 7:** Validation of noontime (1:30 pm)  $G_i$  estimates with respect to in-situ measurements in different ecosystems. The regression between the two sources of  $G_i$  is  $G_i(\text{STIC-TI}) = 0.90G_i(\text{tower}) - 0.10$ .

532 **Table 4:** A comparison of error statistics of  $G_i$  estimates from STIC-TI and existing  $G_i$  models  
 533 over different ecosystems

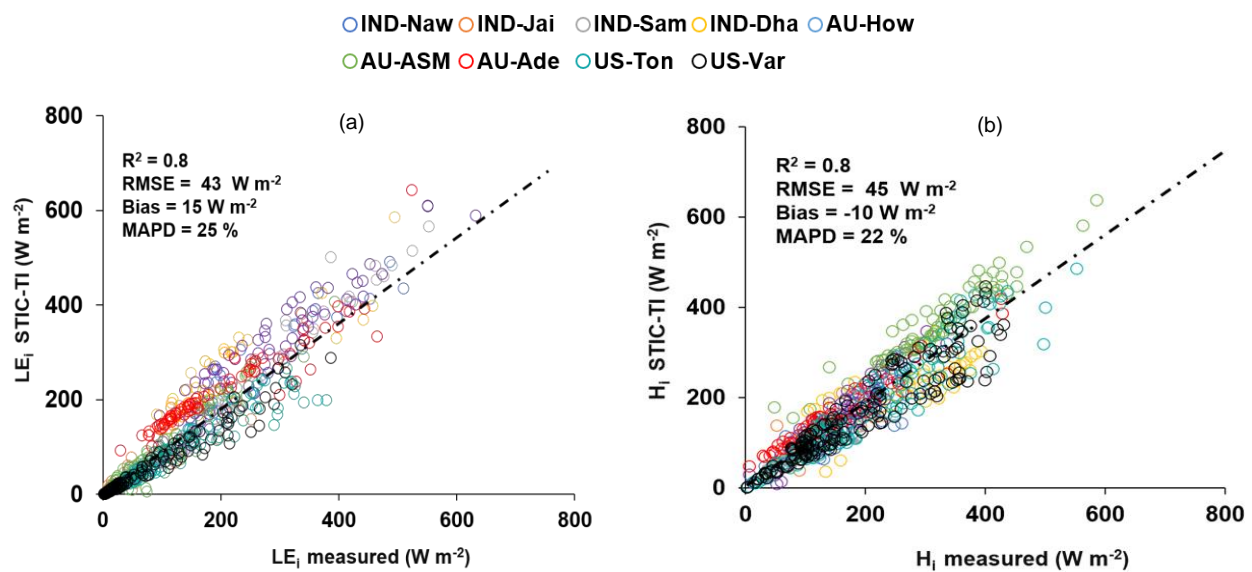
<b>G models</b>	<b>R<sup>2</sup></b>	<b>RMSE (W m<sup>-2</sup>)</b>	<b>MAPD (%)</b>	<b>KGE</b>
STIC-TI	0.80	22	19	0.74
MOR89	0.70	31	29	0.46
BAS98	0.80	20	18	0.61
SU02	0.80	30	26	0.54
BO04	0.70	35	29	0.48

534 The RMSE varied from 9 to 20  $\text{W m}^{-2}$  with MAPD ranging from 12 to 21% across individual flux  
 535 tower sites. High magnitude of  $G_i$  was predicted in the arid and semi-arid systems (120 – 240  $\text{W}$

536  $\text{m}^{-2}$ ) as compared to the humid systems ( $20 - 90 \text{ W m}^{-2}$ ), which was in close correspondence with  
 537 the observations. The model also captured the range of  $G_i$  that are generally found in different  
 538 biomes ( $20 - 140 \text{ W m}^{-2}$  for grasslands,  $20 - 90 \text{ W m}^{-2}$  for cropland) (Purdy et al., 2016). Due to  
 539 the paucity of  $G_i$  measurements, direct validation of  $G_i$  was only possible for 32 days (concurrent  
 540 to MODIS overpass) at the IND-Dha site. Overall, STIC-TI tends to provide reasonable  $G$   
 541 estimates for the terrestrial ecosystems having soil temperature amplitude above  $5^\circ\text{C}$ .

#### 542 4.4 Evaluation of STIC-TI $LE_i$ , $H_i$ , and EF

543 The modeled versus measured  $LE_i$  and  $H_i$  showed good agreement in all the nine ecosystems with  
 544 RMSE in  $LE_i$  and  $H_i$  estimates using MYD11 LST product to the order of  $29 - 62 \text{ W m}^{-2}$  and  $26 -$   
 545  $61 \text{ W m}^{-2}$ , MAPD of  $9 - 31\%$  and  $20 - 36\%$ , BIAS of  $-29$  to  $38 \text{ W m}^{-2}$  and  $-44$  to  $32 \text{ W m}^{-2}$  (Fig.  
 546 8a, b; Table 5) and high  $R^2$  of 0.8.



**Figure 8:** (a) Validation of STIC-TI  $LE_i$  estimates with respect to *in-situ* measurements in different ecosystems; (b) Validation of STIC-TI  $H_i$  estimates with respect to *in-situ* measurements in different ecosystems.

547

548 **Table 5:** Error statistics of STIC-TI  $LE_i$  and  $H_i$  estimates with respect to EC measurements in  
 549 different ecosystems of India, US, and Australia using MYD11A2 LST product for all nine sites  
 550 and using MYD21A2 LST product for three semi-arid and arid sites. The statistics obtained by  
 551 using MYD21A2LST are shown in the parentheses.

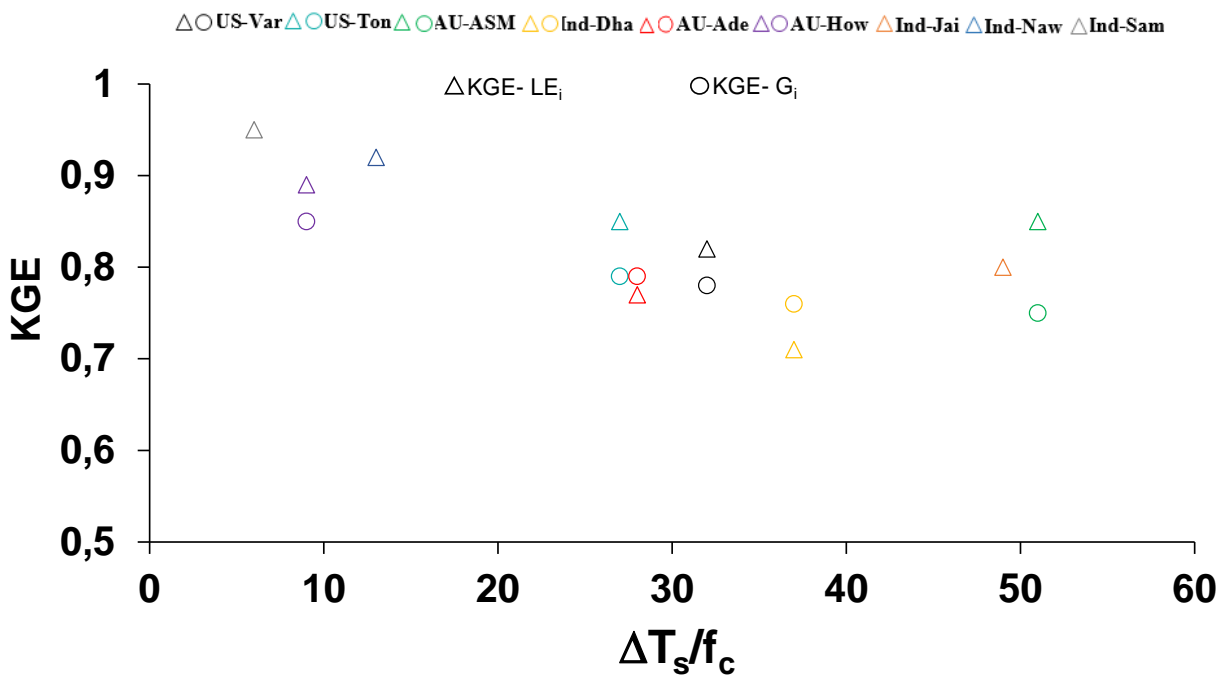
552

Sites	STIC-TI ( $LE_i$ and $H_i$ )									
	$R^2$		BIAS ( $W\ m^{-2}$ )		RMSE ( $W\ m^{-2}$ )		MAPD (%)		KGE	
	$LE_i$	$H_i$	$LE_i$	$H_i$	$LE_i$	$H_i$	$LE_i$	$H_i$	$LE_i$	$H_i$
IND-Jai	0.90 (0.91)	0.90 (0.92)	-21 (-16)	12 (9)	57 (45)	27 (21)	31 (24)	22 (19)	0.80 (0.82)	0.76 (0.79)
IND-Naw	0.90 (0.92)	0.80 (0.85)	19 (12)	-26 (-16)	44 (37)	51 (46)	17 (16)	28 (25)	0.92 (0.92)	0.71 (0.73)
IND-Dha	0.90	0.90	38	-44	43	35	27	25	0.71	0.64
IND-Sam	0.90	0.80	12	-10	32	61	9	27	0.95	0.70
US-Ton	0.90 (0.91)	0.90 (0.92)	-29 (-18)	-32 (-21)	53 (45)	34 (27)	25 (22)	17 (15)	0.85 (0.87)	0.91 (0.93)
US-Var	0.90	0.80	-19	-28	49	39	27	20	0.82	0.89
AU-ASM	0.90 (0.93)	0.90 (0.91)	-3 (6)	22 (16)	46 (37)	26 (18)	29 (24)	20 (17)	0.94 (0.95)	0.83 (0.85)
AU-How	0.90	0.90	16	-25	42	27	17	21	0.89	0.85
AU-Ade	0.90	0.90	21	15	29	53	28	36	0.77	0.80

553

554 Arid ecosystems in India (IND-Jai), US (Ton and Var) and semi-arid ecosystem in Australia (AU-  
555 ASM) revealed relatively high MAPD (31%, 25%, 27%, and 28%) (Table 5). In general, STIC-TI  
556 was able to produce the dominant convective heat fluxes with respect to the EC measurements as  
557 evident through low RMSE for  $H_i$  and high RMSE for  $LE_i$  in the IND-Jai, US-Ton, US-Var, and  
558 AU-Ade where  $LE_i$  is inherently low except few rainy days. A uniform distribution of data points  
559 around 1:1 validation line (Fig. 8a) indicated overall low BIAS in  $LE_i$  estimates. However,  
560 modeled  $H_i$  was consistently lower than the observations (negative BIAS) in the tropical savanna  
561 (IND-Dha and AU-How) and semi-arid (IND-Naw) ecosystems [(-44) – (-25)  $W\ m^{-2}$  and -26  $W$   
562  $m^{-2}$ ] while a consistent positive BIAS was observed in the AU-ASM (semi-arid) and AU-Ade  
563 (savanna), US-Var (arid) (Fig. 8b; Table 5). This consequently led to overall low negative BIAS  
564 (-10  $W\ m^{-2}$ ), relatively low  $R^2$  in  $H_i$  ( $R^2 = 0.8$ ) as compared to the errors in  $LE_i$  (BIAS = 15  $W\ m^{-2}$ ,  
565  $R^2 = 0.9$ ). The regression between the modeled and tower measurements of  $LE_i$  is  $LE_i(STIC-TI)$   
566  $= 0.98LE_i(tower) - 0.266$ . The regression between the modeled and tower measurements of  $H_i$  is  
567  $H_i(STIC-TI) = 0.93H_i(tower) + 4.90$ . The KGE statistics varied in the range of 0.71 – 0.95 for  $LE_i$   
568 and in the range of 0.64 – 0.91 for  $H_i$ , respectively across all nine flux tower sites, thus revealed  
569 reasonably high efficiency of the model to capture the magnitude and variability of SEB fluxes.

570 The impact of MODIS Aqua day-night view angle difference ( $\delta VZA$ ) on STIC-TI fluxes was  
 571 further investigated. Estimated errors in terms of mean percent deviation in  $LE_i$ ,  $H_i$  and  $G_i$  with  
 572 respect to measurements for each  $10^\circ$  bin over 16 angular bins within  $\pm 80^\circ$  were analysed in  
 573 response to mean  $\delta VZA$  of each angular bin.  $G_i$  errors (X) were found to be significantly correlated  
 574 with  $\delta VZA$  (Y) in a parabolic ( $Y = 0.0027X^2 - 0.0025X + 1.4919$ ;  $r = 0.73$ ) pattern (Refer  
 575 Appendix F, Figure F1(a)). Errors in  $G_i$  to the order of -5 to 10%, 10-15% and >15% were largely  
 576 found to be within  $\pm 30^\circ$ ,  $\pm 45^\circ$ , and  $>45^\circ$  to  $-80^\circ$   $\delta VZA$ , respectively. The errors in  $H_i$  were found  
 577 to have strong linear ( $Y = -0.1452X + 1.1146$ ,  $r = 0.77$ ) dependence on  $\delta VZA$  (Refer Appendix F,  
 578 Figure F1(b)). However, a weak dependence of  $LE_i$  errors ( $Y = -0.0878X + 2.0314$ ,  $r = 0.5$ ) on  
 579  $\delta VZA$  (Refer Appendix F, Figure F1(c)) was found, as majority of the errors were within  $\pm 10\%$   
 580 that corresponded to  $\pm 60^\circ$   $\delta VZA$ . The nature of relations and degree of dependency of model flux  
 581 errors on  $\delta VZA$  in this study would be helpful to minimize the error budget in surface energy  
 582 balance fluxes from future thermal infrared missions having day-night observations.



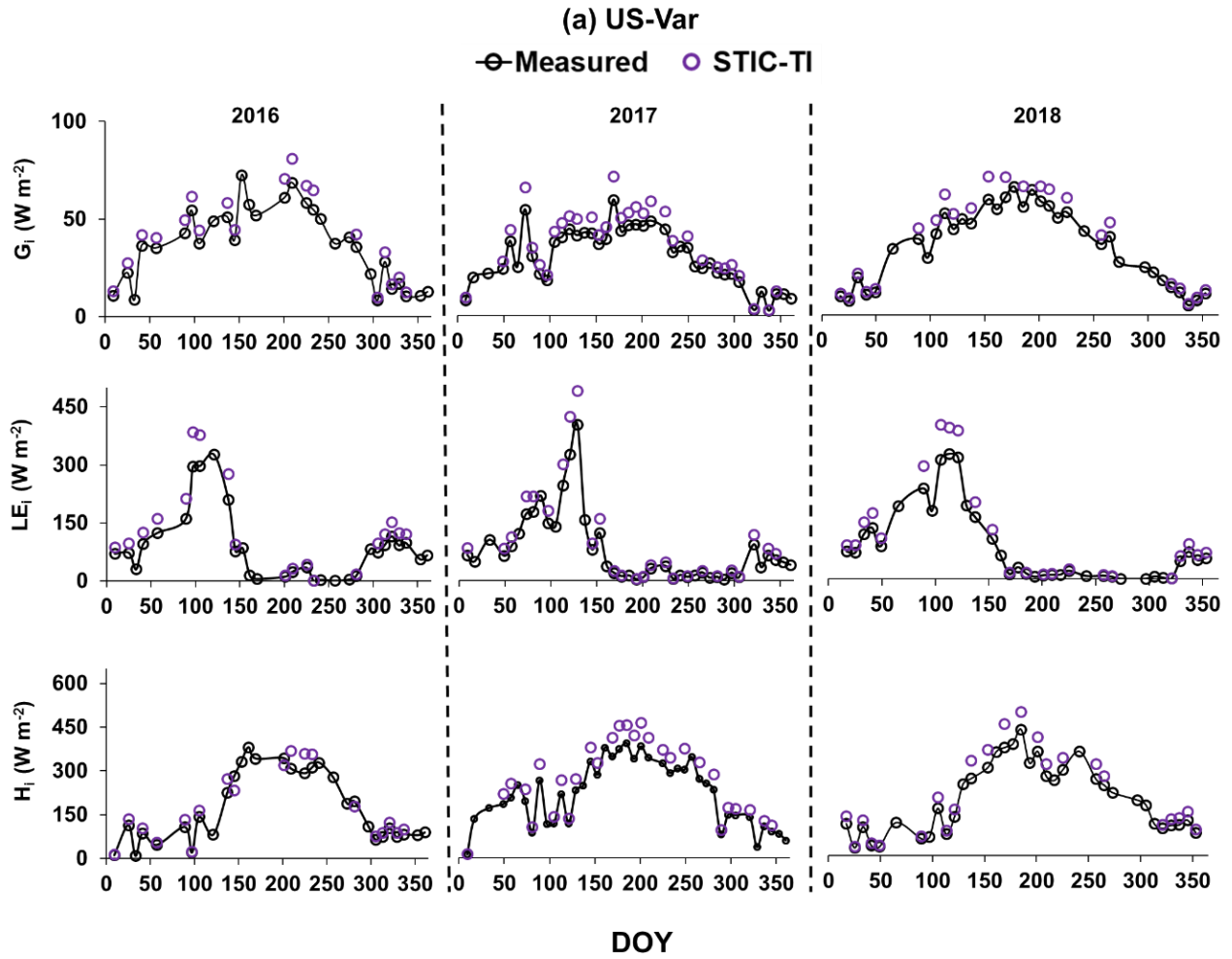
**Figure 9:** Relationship between KGE of STIC-TI ( $G_i$  and  $LE_i$ ) with  $\Delta T_s/f_c$  in different terrestrial ecosystems.

583 Further investigation was made on whether KGE for STIC-TI  $G_i$  and  $LE_i$  follow any systematic  
 584 pattern and the ratio  $\Delta T_s$  and  $f_c$  was used as proxy for surface heterogeneity and dryness. The plot

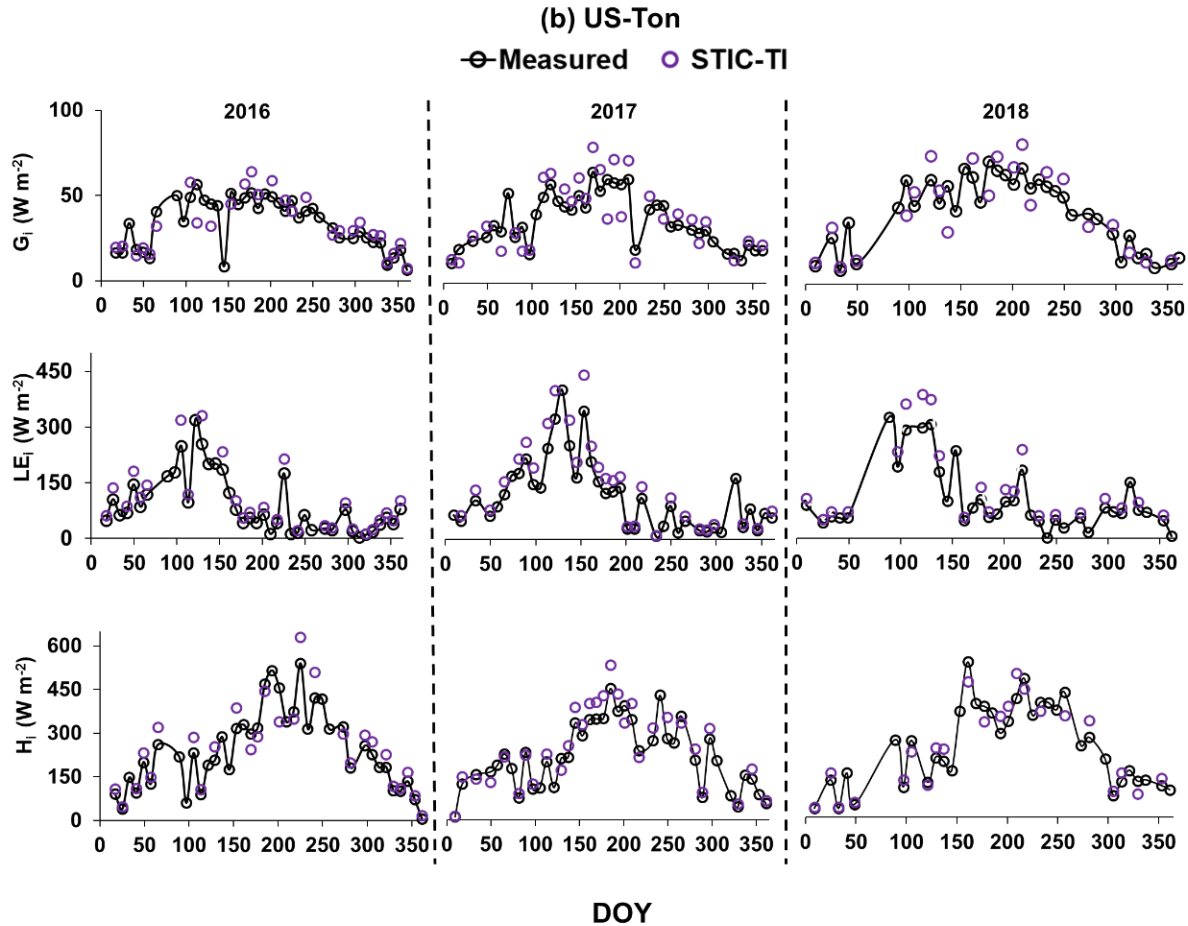
585 of KGE of  $G_i$  and  $LE_i$  with this ratio is shown in Fig. 9. KGE- $G_i$  was found to show a systematic  
586 decrease with increase in  $\Delta T_s-f_c$  ratio up to 40, after which it remained unchanged with increase  
587 in the ratio. Although KGE of  $LE_i$  also decreased (20% reduction) with increase in  $\Delta T_s-f_c$  ratio,  
588 KGE- $LE_i$  was found to increase beyond  $\Delta T_s-f_c$  40. This revealed that the model efficiency  
589 remained high ( $>0.8$ ) within certain dryness limits ( $\Delta T_s-f_c$  ratio  $<20$  and  $>50$ ) and the efficiency  
590 reduced moderately (within  $0.7 - 0.8$ ) for intermediate dryness. Interestingly, the use of  
591 MYD21A2 LST in STIC-TI showed improvements (see the parentheses in different columns in  
592 Table 5) in  $LE_i$  and  $H_i$  error statistics as compared to using MYD11A2 LST in terms of higher  $R^2$   
593 and KGE, and lower RMSE in  $LE_i$  (3-8% less) and  $H_i$  (2-3% less) for semi-arid and arid sites such  
594 as IND-Jai, IND-Naw and US-Ton.

595 An independent evaluation of multi-temporal heat fluxes over two US flux sites for the years 2016-  
596 2018 is shown in Fig. 10 and Fig 11. STIC-TI  $G_i$  estimates with MYD11A2 LST product showed  
597 close match with *in-situ* measurements with respect to intra and inter-annual variability in  $G_i$   
598 followed by  $LE_i$  and  $H_i$ . This further demonstrates the merit of the coupled model for reproducing  
599 ecosystem-scale  $G_i$  estimates especially for shorter and open canopies.





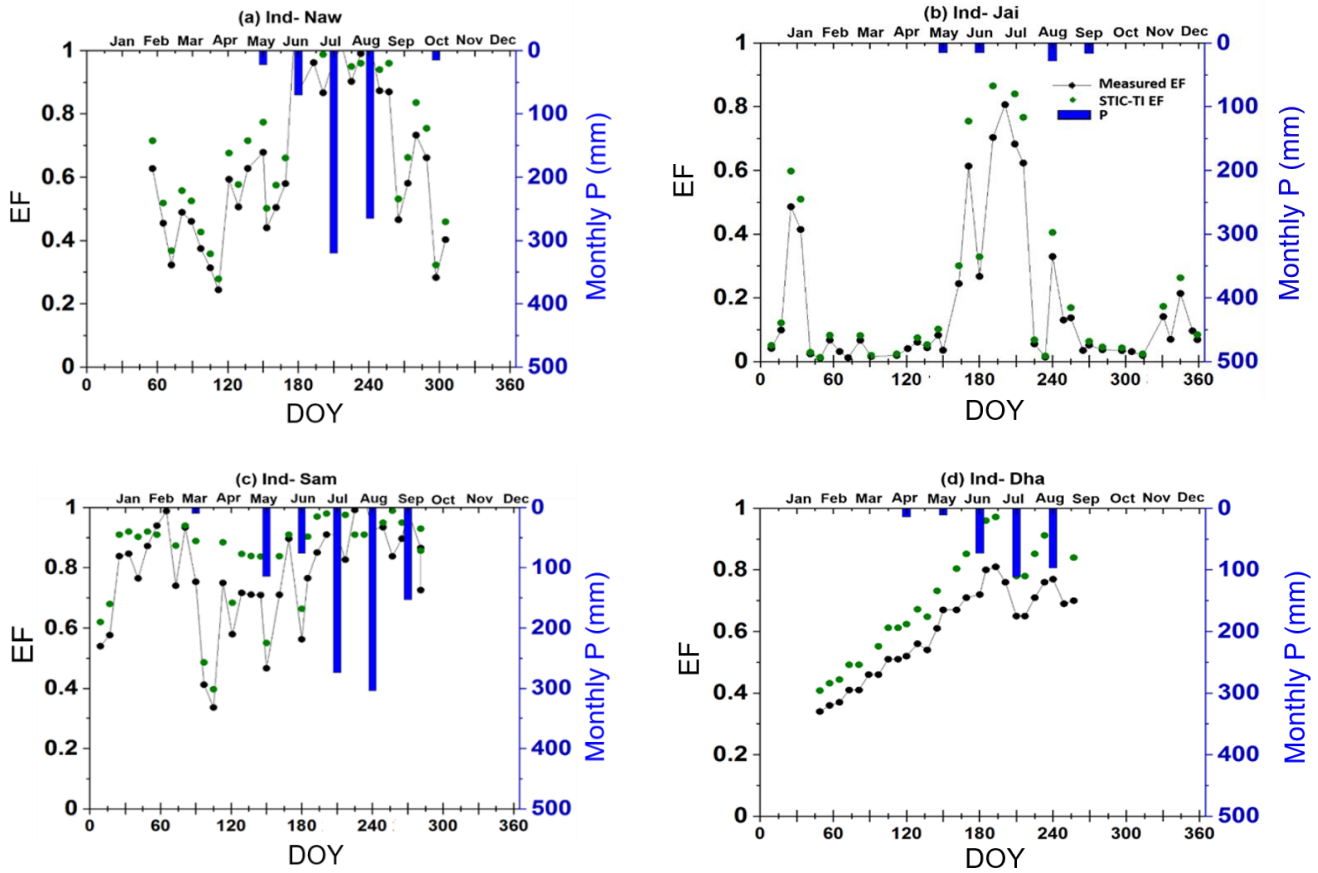
**Figure 10:** Illustrative examples of temporal evolution of STIC-TI derived fluxes using MYD11A2 LST product versus observed SEB fluxes for three consecutive years from 2016 to 2018 in a grassland ecosystem in United States (e.g., US-Var).



**Figure 11:** Illustrative examples of temporal evolution of STIC-TI derived fluxes using MYD11A2 LST product versus observed SEB fluxes for three consecutive years from 2016 to 2018 in a woody savanna ecosystem in the United States (e.g., US-Ton).

600 The temporal behavior of STIC-TI and observed evaporative fraction (EF) (ratio of LE and  $R_N -$   
 601 G) (Fig. 12) along with observed monthly rainfall (P) distinctly captured the substantial temporal  
 602 variability in EF during the dry-to-wet transition in the Indian study sites, which also corresponded  
 603 to low (high)  $\theta$  and P. In IND-Naw and IND-Sam, a marked rise ( $>0.4$ ) in STIC-TI EF was noted  
 604 during day-of-the-year (DOY) 25 to 75 where wheat is grown under assured irrigation. The impact  
 605 of irrigation is thus captured by the substantial increase in EF in the absence of P. In contrast, the  
 606 rainfed grassland system (IND-Jai) showed peak EF ( $\sim 0.8$ ), which corresponded to south-west  
 607 monsoon rainfall during June to September and a progressive decline in EF during the dry down  
 608 period in October to April corresponding to post south-west monsoon phase. Some intermittent  
 609 spikes in EF were also noted during dry-down phase in both STIC-TI and observations. The  
 610 intermittent EF spikes during the soil moisture dry down phase could be due to enhanced LE

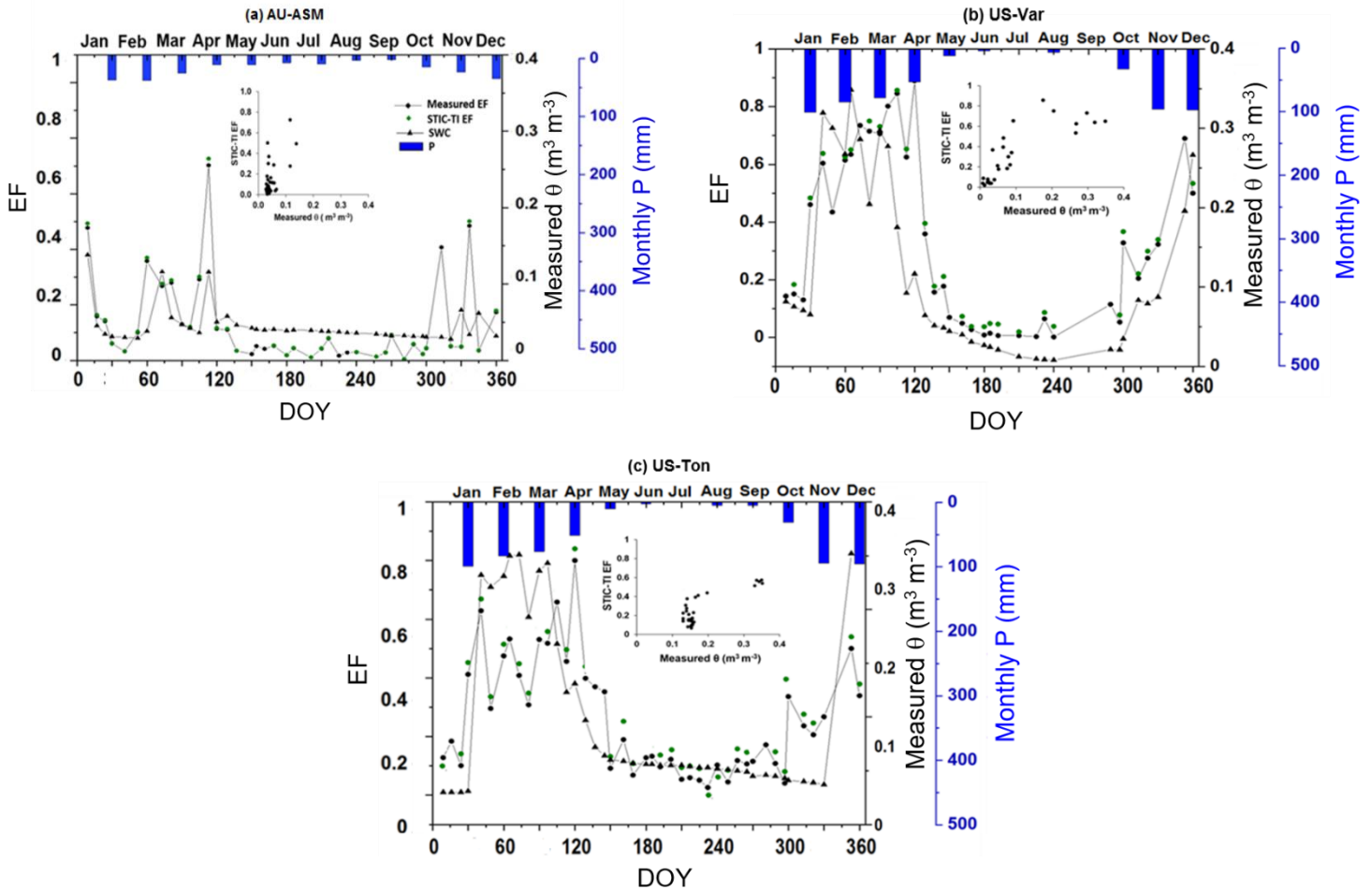
611 through moisture advection from the surrounding vegetation causing an enhancement of  
 612 evaporation than expected. This is known as the ‘clothesline effect’ which frequently occurs in  
 613 semi-arid and arid ecosystems. In addition to IND-Jai, the response of both modeled and measured  
 614 EF to wet and dry spells was also noted during south-west monsoon period at all other flux tower  
 615 sites of India.



**Figure 12:** Illustrative examples of temporal variation of STIC-TI derived EF using MYD11A2 LST product with respect to measured EF and P in (a) IND-Naw, (b) IND-Jai, (c) IND-Sam, and (d) IND-Dha

616 The temporal behavior of EF from STIC-TI using MYD11A2 LST product and EC measurements  
 617 along with measured  $\theta$  and P at the OzFlux and AmeriFlux sites also revealed (Fig. 13) close  
 618 correspondence of STIC-TI with EC observations. Low EF (0.05 – 0.40) during the dry season  
 619 around DOY 100 – 250 and high EF (>0.4) during the wet season (DOY 1 – 120 and 300 to 360)  
 620 in AU-ASM, US-Ton and US-Var was observed. The analysis showed that STIC-TI EF can  
 621 capture the annual variability of observed EF and its responses across different ecosystems during  
 622 wet and dry seasons. The plots of STIC-TI EF versus measured  $\theta$  (in the inset of Fig. 13) revealed

623 triangular scatter close to right-angled triangle with positive slope of hypotenuse in three  
 624 ecosystems AU-ASM, US-Var and US-Ton. This showed that in the water-controlled ecosystems,  
 625 where distinct wet-dry seasons exist, the positive EF- $\theta$  relationship is an outcome of the soil  
 626 moisture controls on transpiration during the dry season.



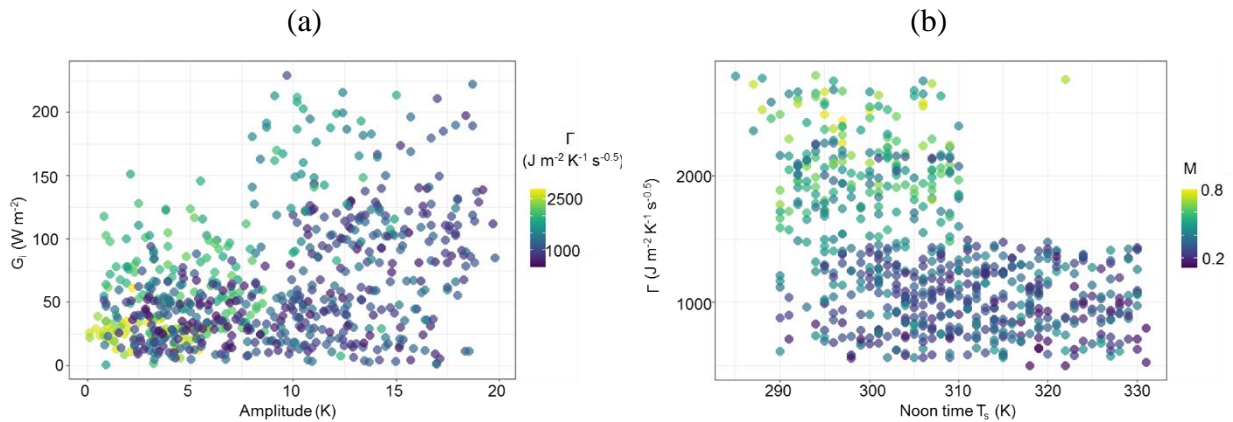
**Figure 13:** Comparison of temporal variation of STIC-TI derived EF using MYD11A2 LST with respect to measured EF,  $\theta$  and Pin (a) AU-ASM, (b) US-Var, (c) US-Ton. The scatterplots in the inset shows the relationship between STIC-TI EF with respect to measured  $\theta$ .

## 627 5 Discussion

### 628 5.1 Interaction of flux and internal SEB metrics

629 From section 4.1 we found relatively reduced sensitivity of  $G_i$  to  $T_s$  uncertainties. In any given  
 630 condition, if an over(under) estimation of  $M$  due to noontime  $T_s$  uncertainties (through eq. 13)  
 631 leads to an over(under) estimation of  $\Gamma$ , the effects of such over(under) estimation of  $\Gamma$ (due to

632 noontime  $T_s$  uncertainties) tend to be compensated by under(over) estimation of amplitude  $A$  (in  
 633 eq. 5), ultimately leading to a reduction of the sensitivity of  $G_i$  to  $T_s$ . While the scatter between  $G$   
 634 versus  $A$  for a wide range of  $\Gamma$  (Fig. 14a) revealed large scatter with increasing amplitude under  
 635 the dry conditions (low  $\Gamma$ ), the scatter between  $\Gamma$  versus  $T_s$  for different  $M$  (Fig. 14b) revealed  
 636 exponential reduction of  $\Gamma$  with increasing  $T_s$  and dryness, and almost no significant change in  $\Gamma$   
 637 with increasing  $T_s$  at a constantly high dryness ( $M < 0.25$ ). Thus, the confounding effects of  $\Gamma$ ,  $A$ ,  
 638 and  $M$  through eq. 3, 5, 12 and 13 led to a reduction of sensitivity of  $G$  to  $T_s$ , as exemplified in  
 639 Fig. 14.



**Figure 14:** Response plots among parameters of TI-based  $G_i$  model, such as (a)  $G_i$  versus Amplitude ( $A$ ) for varying  $\Gamma$ , and (b) Noon-time  $T_s$  versus  $\Gamma$  with varying  $M$ .

640  
 641 Concerning  $LE_i$  and  $H_i$ , dual uncertainties could be propagated in both the fluxes through  
 642 daytime  $T_s$  (through  $M$  and  $G_i$ ), leading to high sensitivity of these two SEB fluxes due to  $T_s$   
 643 perturbations. The relatively high sensitivity of  $LE_i$  to  $T_s$  (as compared to  $H_i$ ) in the non-  
 644 irrigated ecosystems could be due to partial compensation of  $g_A/g_s$  in both numerator and  
 645 denominator of the PMEB equation for  $H$  (eq. C7 of Appendix C). A recent study (Fig.10 in  
 646 Mallick et al., 2018a) showed high sensitivity of  $g_s$  due to  $T_s$  (1% change in  $T_s$  led to 5.2–7.5%  
 647 change in  $g_s$ ) as compared to  $g_A$  sensitivity to  $T_s$  (1% change in  $T_s$  led to 1.6–2% change in  $g_A$ ),  
 648 suggesting that errors in  $g_s$  due to  $T_s$  uncertainty tend to be larger than errors in  $g_A$ . Partial  
 649 cancellation of the conductance errors in the numerator of eq. (C7 of Appendix C) might have  
 650 resulted in compensation of  $H_i$  errors in the water-limited ecosystems. In this environment, the  
 651 variability of  $LE_i$  is mainly dominated by  $g_A/g_s$ , which makes  $LE_i$  highly sensitive due to  $T_s$   
 652 uncertainties. Combined uncertainty due to  $g_A/g_s$  in the denominator and  $g_A$  in the numerator

653 of eq. (C6 of Appendix C) resulted into greater sensitivity in  $LE_i$  to  $T_s$  in the arid and tropical  
654 savannah ecosystems (Mallick et al., 2015, 2018a; Winter & Eltahir, 2010). The very low  
655 sensitivity of  $LE_i$  and  $H_i$  due to uncertainties in NDVI is because NDVI was not used in the  
656 conductance parameterizations and effects due to NDVI in STIC-TI was only propagated  
657 through  $G_i$ . The sensitivity of  $LE_i$  and  $H_i$  to albedo was mainly due to the dependence of net  
658 radiation ( $R_{Ni}$ ) on albedo, and any resultant uncertainty in  $R_{Ni}$  (due to albedo) tends to be  
659 reflected in the sensitivity of  $LE_i$  and  $H_i$  to albedo.

## 660 **5.2 Possible sources of errors in SEB flux evaluation**

661 In STIC-TI, underestimation and overestimation errors in  $G_i$  in different ecosystems (Fig. 7) could  
662 originate due to the errors in MYD11A2 LST product. A host of studies previously reported that  
663 the standard deviations of errors in retrieved emissivity in bands 31 and 32 are 0.009, and the  
664 maximum error in retrieved  $T_s$  of MOD11A1 LST falls within 2-3 K, which is mainly due to the  
665 errors in surface emissivity correction (Duan et al., 2017; Wan, 2014; Lei et al., 2018). In the  
666 present analysis, we found an overestimation error of MODIS  $T_s$  in the range of 0.5 – 1.5 K when  
667 compared with *in-situ* infrared temperature measurements at the tropical savanna site. As  
668 mentioned in section 3.1, a positive (negative) bias in  $T_s$  would tend to an overestimation  
669 (underestimation) of amplitude (A) in eq. (5); underestimation (overestimation) of M in eq. (13),  
670 and consequent underestimation (overestimation) of  $\Gamma$  (eq. 12) and  $G_i$ , respectively. Furthermore,  
671 the standard deviation of NDVI surrounding the tower sites varied from 0.01 – 0.05 when  
672 compared to the ground measurements, which could be another source of error in the STIC-TI  
673 model. In addition, NDVI saturates at  $LAI > 3$ . However, STIC-TI provides direct estimates of  
674 ecosystem G and is independent of  $R_N$ .

675 Despite the comparable accuracy of current G estimates with the G model of Bastiaanssen et al  
676 (1998), the foundation of STIC-TI lies in the use of soil moisture characteristics with varying soil  
677 textural types which are known to influence the soil heat conductance and thereby G. Thus, the  
678 control of soil moisture on evaporation is explicitly included in STIC-TI as opposed to the semi-  
679 empirical G function of Bastiaanssen et al (1998). The higher accuracies of TI-based thermal  
680 diffusion model as compared to  $R_N$ -based empirical G models were also reported by Purdy et al.  
681 (2016) at daily or longer time scales in cropland, grassland. All these G model estimates many a

682 times differ from in situ measurements because of the no accounting of leaf litter presence or layer  
683 on soil floor in the remote sensing-based G-model.

684 The overestimation (underestimation) of  $LE_i(H_i)$  is also due to the effects of spatial resolution of  
685 different input variables on these two SEB fluxes and conducted statistical evaluation with respect  
686 to the measured SEB fluxes. Eswar et al. (2017) demonstrated the need for spatial disaggregation  
687 models for monitoring  $LE_i$  at field scale using contextual models by disaggregation of evaporative  
688 fraction ( $\Lambda$ ) and downwelling shortwave radiation ratio ( $R_G$ ). Using different disaggregation  
689 models, they estimated  $LE_i$  at 250m spatial resolution and reported RMSE of  $30 - 32 \text{ W m}^{-2}$  as  
690 compared to  $LE_i$  obtained at 1000m spatial resolution with RMSE of  $40 - 70 \text{ Wm}^{-2}$  over different  
691 sites in India. Anderson et al. (2007) reviewed different validation experiments conducted in  
692 diverse agricultural landscapes (Anderson et al., 2004, 2005; Norman et al., 2003) and reported  
693 RMSE in  $LE_i$  in the range of  $35 - 40 \text{ W m}^{-2}$  (15%) at  $30 - 120 \text{ m}$  disaggregated spatial resolution.  
694 Current analysis also brought out the need for noon-night thermal imaging with spatial resolution  
695 finer than 1000m to adequately capture the magnitude and variability of  $LE_i$  in the terrestrial  
696 ecosystems especially agroecosystems where average field sizes are less ( $< 0.5 \text{ ha}$ ) and fragmented  
697 such as in India and other sub-continent.

698 As seen in Fig. 8a and Table 5, there is a gross overestimation of  $LE_i$  with respect to the tower  
699 observations when MYD11A2 LST was used. The consistent positive BIAS in STIC-TI  $LE_i$  in  
700 five out of nine sites is presumably due to the overestimation of  $R_{Ni}$  (Figure B1 of Appendix B)  
701 and underestimation of  $G_i$ . Figure 7 shows overestimation of  $G_i$  for three OzFlux sites and US sites  
702 and underestimation of  $G_i$  for Indian site with  $G_i(\text{STIC-TI}) = 0.90 G_i(\text{tower}) - 0.10$  and  
703 overestimation of  $R_{Ni}$  at the ecosystem-scale, with  $R_{Ni}(\text{STIC-TI}) = 0.78R_{Ni}(\text{tower}) + 58.92$   
704 (Appendix-B2). This means a systematic overestimation of net available energy ( $R_{Ni} - G_i$ ) will be  
705 obvious in cases where STIC-TI shows underestimation of  $G_i$ . Since available energy is an  
706 important component for estimating LE through the PMEB equation, an overestimation of net  
707 available energy leads to an overestimation of LE by STIC-TI. Sensible heat flux will be  
708 consequently underestimated due to the complementary nature of the PMEB equation. It may be  
709 also noted that the use of MYD21A2 LST led to relatively better accuracy in  $LE_i$  (3-8%) and  $H_i$   
710 (2-3%) as compared to using MYD11A2 LST in semi-arid and arid ecosystems. The higher  
711 retrieval accuracy of MYD21A2 LST using TES (Temperature-Emissivity Separation) algorithm

712 over MYD11A2 LST that uses split-window algorithm (Wan et al, 2015) is the main reason for  
713 obtaining higher accuracy in  $LE_i$  and  $H_i$  estimates.

714 The standard deviations of MODIS Aqua day-night overpass time over study sites were found to  
715 be within 30-45 minutes (Sharifnezhadazizi et al, 2019) and the expected deviation in LST from  
716 the mean local time would be around  $\pm 0.75K$  (Sharifnezhadazizi et al, 2019). Sensitivity analysis  
717 showed that resultant uncertainties in STIC-TI heat flux estimates would be of the order of  $\pm 5-7\%$   
718 due to this LST uncertainty.

### 719 **5.3 Effects of SEB closure**

720 Given there is a widespread lack of SEB closure ( $H + LE \neq R_N - G$ ) or residual energy balance,  
721 knowledge of the impact of different vegetation types and climatic variables on SEB ‘non-closure’  
722 is essential. A recent study by Dare-Idowu et al. (2021) covering 8 growing seasons and 3 crops  
723 (maize, wheat, and rapeseed) in two sites of south-western France showed that the systematic effect  
724 of each site on SEB closure was stronger than the influence of crop type and stage. Same study  
725 revealed a greater percentage of SEB closure under unstable atmospheric conditions and in the  
726 prevailing wind directions, and sensible heat advection accounted for more than half of the  
727 imbalance at both the sites.

728 In our study, using unclosed SEB observations for Indian sites in the absence of *in-situ*  $G_i$   
729 observations also added to the consistent positive BIAS in the statistical evaluation of  $LE_i$ . A  
730 ubiquitous lack of energy balance closure to the order of 10 – 20% worldwide at most of the EC  
731 sites is reported in different literatures (Stoy et al., 2013; Wilson et al., 2002), which implies a  
732 systematic underestimation (overestimation) of  $LE_i$  (EC tower) (and/or  $H_i$ (EC tower)).  
733 Accommodating an average 15% imbalance in  $LE_i$  (EC tower) would tend to diminish the positive  
734 BIAS in STIC-TI. Therefore, the pooled gain (0.98) and positive BIAS between the STIC-TI and  
735 tower  $LE_i$  is determined by the overestimation of  $(R_{Ni} - G_i)$ , combined with the underestimation  
736 of measured  $LE_i$  from the EC towers. An underestimation of  $H_i$  (negative BIAS) is associated with  
737 two reasons; (a) ignoring the two-sided aerodynamic conductance of the leaves (Jarvis and  
738 McNaughton, 1986; Monteith and Unsworth, 2013; Schymanski et al., 2017), which could lead to  
739 substantial underestimation of  $H_i$ , and (b) due to the complementary nature of the PMEB equation,  
740 if  $LE_i$  is overestimated,  $H_i$  will be underestimated. In addition, frequent micro-advection fluxes  
741 alter measured in situ H and LE fluxes. But these advection conditions are not explicitly accounted



742 in the current STIC-TI model. At the EC tower sites, the fraction of residual energy balance to  $R_N$   
743 can be quantified with respect to vegetation/crop growth characteristics or biophysical properties.  
744 However, where G observations are lacking such as in many Indian EC tower sites, the TI-based  
745 G model can be used to fill up the missing G observations to quantify residual energy balance and  
746 to correct the SEB non-closure.

## 747 **6 Summary and conclusions**

748 This study addressed one of the long-term uncertainties in thermal remote sensing of evaporation  
749 modeling in open canopy heterogeneous ecosystems, which is associated with empirical methods  
750 of estimating ground heat flux. We demonstrated for the first-time physical integration and  
751 coupling of a mechanistic ground heat flux model with an analytical evaporation model (Surface  
752 Temperature Initiated Closure, STIC) within the surface energy balance equation. The model is  
753 called STIC-TI, which uses satellite-based land surface temperature from MODIS Aqua and  
754 associated biophysical variables, and it has minimal independence on *in-situ* measurements. The  
755 estimation of evaporation through STIC-TI does not require any empirical function for inferring  
756 the biophysical conductances. STIC-TI is independent of uncertain parameterizations of surface  
757 roughness and atmospheric stability and does not also involve any look-up table for biome or plant  
758 functional attributes. By linking noon-night land surface temperature with harmonics equation of  
759 thermal inertia and soil moisture availability, STIC-TI derived the ground heat flux, and  
760 subsequently coupled it with evaporation. Independent validation of STIC-TI with respect to eddy  
761 covariance flux measurements from nine terrestrial ecosystems in arid, semi-arid and sub-humid  
762 climate in India, USA and Australia led us to the following conclusions:

- 763 (i) While the MODIS Aqua day-night view angle difference showed strong impact on ground  
764 heat flux and sensible heat flux estimate deviations of STIC-TI (with respect to  
765 measurements), relatively weak dependence of latent heat flux errors on the day-night view  
766 angle difference was noted.
- 767 (ii) The most notable advantages of STIC-TI are firstly, it provides direct estimates of ground heat  
768 flux while simultaneously integrates the effects of soil water stress on ground heat flux and  
769 evaporation through the inclusion noon-night land surface temperature information. Secondly,

770 the ecosystem-scale surface soil temperature amplitude used in the ground heat flux model  
771 can advance our understanding on associated terrestrial ecosystem processes.

772 The requirement of few input variables in STIC-TI generates promise for surface-atmosphere  
773 exchange studies using readily available data from the current generation remote sensing satellites  
774 (e.g., MODIS, VIIRS) that have noon-night land surface temperature observations. STIC-TI can  
775 also be potentially used for distributed ET mapping from future high spatial resolution (~ 50 – 60  
776 m) TIR missions having noon-night observations with high revisit such as the Indo-French  
777 mission, TRISHNA (Thermal infrared Imaging Satellite for High-resolution Natural Resource  
778 Assessment) (Lagouarde et al., 2018, 2019), ESA's LSTM (Land Surface Temperature  
779 Monitoring), and NASA SBG (Surface Biology and Geology), respectively.

#### 780 **Author contributions**

781 KM and BKB conceptualized the idea; DD conducted STIC-TI model coding, simulations; BKB  
782 and DD conducted the data analysis in consultation with KM; DD and BKB wrote the first version  
783 of the manuscript with KM writing the introduction, discussions, and conclusions; BKB and KM  
784 conducted all the analysis and writing during revision; all authors contributed to discussions,  
785 editing and corrections; BKB and KM jointly finalized the manuscript.

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## 800 **Data and code availability**

801 Harmonized time series datasets over the study grids are available in  
802 <https://doi.org/10.5281/zenodo.5806501>. The model code is available to the first author upon  
803 reasonable request.

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1102 **Appendix A**1103 **Table A1: A list of symbols, their descriptions and units used in the present study**

<b>Attributes</b>	<b>Symbol</b>	<b>Description</b>
Temperature	$T_A$	Air temperature ( $^{\circ}\text{C}$ )
	$T_{\text{Max}}$	Maximum air temperature ( $^{\circ}\text{C}$ )
	$T_{\text{Min}}$	Minimum air temperature ( $^{\circ}\text{C}$ )
	$T_D$	Air dew-point temperature ( $^{\circ}\text{C}$ )
	$T_{\text{STA}}$	point-scale soil temperature amplitude
	$\Delta T_s$	noon-night LST difference ( $^{\circ}\text{C}$ )
	$T_{\text{ST}}$	Soil temperature ( $^{\circ}\text{C}$ )
	$T_s$	Land surface temperature (LST) ( $^{\circ}\text{C}$ )
Humidity, vapor pressures	$R_H$	Relative humidity (%)
	$e_A$	Atmospheric vapor pressure at the level of $T_A$ measurement (hPa)
	$e_A^*$	Saturation vapor pressure at the level of $T_A$ measurement (hPa)
	$e_s^*$	Saturation vapor pressure at surface (hPa)
	$D_A$	Atmospheric vapor pressure deficit at the level of $T_A$ measurement (hPa)
Radiation	$R_G$	Downwelling shortwave radiation (or global radiation) ( $\text{W m}^{-2}$ )
	$R_R$	Upwelling or reflected shortwave radiation ( $\text{W m}^{-2}$ )
	$R_{L\downarrow}$	Downwelling longwave radiation ( $\text{W m}^{-2}$ )
	$R_{L\uparrow}$	Upwelling longwave radiation ( $\text{W m}^{-2}$ )
	$\tau_{\text{sw}}$	Atmospheric transmissivity for shortwave radiation (unitless)
	$\alpha_R$	Broadband shortwave surface albedo (unitless)
SEB components	$LE_i$	Latent heat flux ( $\text{W m}^{-2}$ ); subscript 'i' signifies 'instantaneous'
	$H_i$	Sensible heat flux ( $\text{W m}^{-2}$ ); subscript 'i' signifies 'instantaneous'
	$G_i$	Ground heat flux ( $\text{W m}^{-2}$ ); subscript 'i' signifies 'instantaneous'
	$R_{N_i}$	Net radiation ( $\text{W m}^{-2}$ ); subscript 'i' signifies 'instantaneous'
	$\phi$	Net available energy ( $\text{W m}^{-2}$ ); i.e., $R_N - G$
	$A$	Ecosystem-scale surface soil temperature amplitude ( $^{\circ}\text{C}$ )

MV2007 model	$T_{sd}$	Daytime $T_s$ ( $^{\circ}\text{C}$ )
	$T_{sn}$	Nighttime $T_s$ ( $^{\circ}\text{C}$ )
	$\omega$	Angular frequency ( $\text{rad s}^{-1}$ )
	$\phi'_n$	Phase shift of the $n^{\text{th}}$ soil surface temperature harmonic (rad)
	$\Delta$	Shape parameter (unitless)
	$S_r$	Relative soil moisture saturation ( $\text{m}^3 \text{m}^{-3}$ )
	$f_s$	Sand fraction (unitless)
	$\theta_{fc}$	Soil water content at field capacity ( $\text{m}^3 \text{m}^{-3}$ )
	$\theta_{wp}$	Soil water content at permanent wilting point ( $\text{m}^3 \text{m}^{-3}$ )
	$\theta^*$	Soil porosity ( $\text{cm}^3 \text{cm}^{-3}$ )
	$J_s$	Summation of harmonic terms of soil surface temperature (K)
	$\Upsilon'$	Soil textural parameter (unitless)
	$\Gamma$	Soil thermal inertia ( $\text{J K}^{-1} \text{m}^{-2} \text{s}^{-0.5}$ )
	$\tau_0$	Thermal inertia of air-dry soil ( $\text{J K}^{-1} \text{m}^{-2} \text{s}^{-0.5}$ )
	$\tau^*$	Thermal inertia of saturated soil ( $\text{J K}^{-1} \text{m}^{-2} \text{s}^{-0.5}$ )
	$t'$	Time of satellite overpass (seconds)
	$\Delta t$	Time offset between the canopy composite temperature and the below-canopy soil surface temperature (seconds)
	$\kappa$	Total number of harmonics used (unitless)
	$f_c$	Vegetation fraction (unitless)
	$\theta$	Volumetric soil moisture ( $\text{cm cm}^{-3}$ )
Clear-sky $R_{Ni}$ model	$R_{ns}$	Net shortwave radiation ( $\text{W m}^{-2}$ )
	$R_{nl}$	Net long wave radiation ( $\text{W m}^{-2}$ )
	$G_{sc}$	Solar constant ( $1367 \text{ W m}^{-2}$ )
	$\beta_e$	Sun elevation angle ( $^{\circ}$ ).
	$\varepsilon_s$	Infrared surface emissivity (unitless)
	$\varepsilon_a$	Atmospheric emissivity (unitless)
	$E$	Eccentricity correction factor due to variation in Sun-Earth distance (unitless)
	$M$	Aggregated moisture availability (0-1)

STIC-TI model	$g_A$	Aerodynamic conductance ( $m s^{-1}$ )
	$g_s$	Canopy-surface conductance ( $m s^{-1}$ )
	$T_0$	Aerodynamic temperature (or source/sink height temperature) ( $^{\circ}C$ )
	$T_{0D}$	Dewpoint temperature at the source/sink height ( $^{\circ}C$ )
	$\Lambda$	Evaporative fraction (unit less)
	$e_0$	Vapor pressure at the source/sink height (hPa)
	$e_0^*$	Saturation vapor pressure at the source/sink height (hPa)
	$D_0$	Vapor pressure deficit at source/sink height (hPa)
	$s_1$	Psychrometric slope of vapor pressure and temperature between ( $T_{0D} - T_D$ ) versus ( $e_0 - e_A$ ) ( $h Pa K^{-1}$ )
	$s_2$	Psychrometric slope of vapor pressure and temperature between ( $T_s - T_D$ ) versus ( $e_s^* - e_A$ ) ( $h Pa K^{-1}$ )
	$s_3$	Psychrometric slope of vapor pressure and temperature between ( $T_{0D} - T_D$ ) versus ( $e_s^* - e_A$ ).
	$\kappa$	Ratio between ( $e_0^* - e_A$ ) and ( $e_s^* - e_A$ ) (unitless)
Ancillary meteorological variables	$U$	Wind speed at 8 m height ( $m s^{-1}$ )
	$u^*$	Friction velocity ( $m s^{-1}$ )
Constants	$P$	Precipitation ( $mm d^{-1}$ )
	$\gamma$	Psychrometric constant ( $h Pa k^{-1}$ )
	$c_p$	Specific heat capacity of air at constant pressure ( $MJ kg^{-1} K^{-1}$ )
	$\rho$	Density of air ( $Kg m^{-3}$ )
	$\sigma$	Stefan–Boltzmann constant ( $5.67 \times 10^{-8} Wm^{-2}K^{-4}$ )
Sensor view geometry	VZA	MODIS Aqua sensor view angle ( $^{\circ}$ )
	$\delta VZA$	Difference in MODIS Aqua day-night sensor view angle ( $^{\circ}$ )

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1106 **Table A2:** Summary of instruments used, height or depth and period of measurements, measured  
 1107 variables at nine EC flux tower sites

Type of primary instruments used for in situ data recording at flux tower sites	Measurement height/ depth (m)	Measured variables
Net radiometer	<ul style="list-style-type: none"> <li>• 3m (IND-Naw, IND-Jai, IND-Sam)</li> <li>• 15m (AU-Ade)</li> <li>• 12.2m (AU-ASM)</li> <li>• 23m (AU-How) 2m (US-Ton, US-Var)</li> </ul>	Four radiation flux components: shortwave incoming ( $R_G$ ) and outgoing ( $R_R$ ); longwave incoming ( $R_{L\downarrow}$ ) and outgoing ( $R_{L\uparrow}$ )
EC assembly with IRGA (Infrared Gas Analyzer), three-dimensional sonic anemometer, TC probe	<ul style="list-style-type: none"> <li>• 8m (IND-Naw; IND-Jai; IND-Sam)</li> <li>• 4.5m (IND-Dha)</li> <li>• 15m (AU-Ade)</li> <li>• 11.6m (AU-ASM)</li> <li>• 23m (AU-How)</li> <li>• 2m (US-Ton, US-Var)</li> </ul>	High response wind vectors ( $u$ , $v$ and $w$ ), sonic temperature, and $CO_2$ - water vapor mass at 10/20 Hz frequency
Humidity and temperature probe	<ul style="list-style-type: none"> <li>• 8m (IND-Naw, IND-Jai, IND-Sam)</li> <li>• 4.5m (IND-Dha)</li> <li>• 15m (AU-Ade), 11.6m (AU-ASM)</li> <li>• 23m (AU-How), 70m (AU-How)</li> <li>• 2m (US-Ton, US-Var)</li> </ul>	$T_A$ and $R_H$
Soil temperature probe	<ul style="list-style-type: none"> <li>• -0.1m (IND-Dha)</li> <li>• -0.15m (AU-Ade)</li> <li>• (-0.02, -0.06m) (AU-ASM)</li> <li>• -0.08m (AU-How)</li> <li>• -0.02m, -0.04m, -0.08m, and -0.16m (US-Ton, US-Var)</li> </ul>	$T_{ST}$
Soil heat flux plates	<ul style="list-style-type: none"> <li>• Ground, 0.1 m (IND-Dha)</li> <li>• Ground, -0.15 m (AU-Ade)</li> <li>• Ground, -0.08 m (AU-ASM)</li> <li>• Ground, -0.15 m (AU-How)</li> <li>• -0.01m (US-Ton, US-Var)</li> </ul>	Soil heat flux ( $G$ )

1108 **Appendix B**

1109 **B1: Clear-sky instantaneous net radiation ( $R_{Ni}$ ) model**

1110 Net radiation ( $R_N$ ) is defined as the difference between the incoming and outgoing radiation, which  
 1111 includes both longwave and shortwave radiation at the Earth's surface.



1112 Terrestrial  $R_N$  has four components: downwelling and upwelling shortwave radiation ( $R_G$  and  $R_R$ ),  
 1113 downwelling and upwelling longwave radiation ( $R_{L\downarrow}$  and  $R_{L\uparrow}$ ), respectively.

$$R_N = (R_G - R_R) + (R_{L\downarrow} - R_{L\uparrow}) \quad (B1)$$

1114 Out of these four terms mentioned in eq.(B1),  $R_G$  and  $R_{L\downarrow}$  are dependent on various factors such  
 1115 as geographic location, season, cloudiness, aerosol loading, atmospheric water vapor content and  
 1116 less on surface properties. On the other hand, the upwelling radiations in eq. (B1) strongly depends  
 1117 on the surface properties such as surface reflectance and emittance, land surface temperature, and  
 1118 soil water content (Zerefos and Bais, 2013).

1119 Instantaneous net radiation ( $R_{Ni}$ ) can be derived using eq. B2 as follows (Mallick et al., 2007):

$$R_{Ni} = R_{ns} - R_{nl} \quad (B2)$$

$$R_{ns} = (1 - \alpha_R) R_G \quad (B3)$$

$$R_{nl} = R_{L\downarrow} - R_{L\uparrow} \quad (B4)$$

1120 Where,  $R_{ns}$  is net shortwave radiation ( $W m^{-2}$ ),  $R_{nl}$  is net longwave radiation ( $W m^{-2}$ ).and  $\alpha_R$  is the  
 1121 broadband surface albedo shortwave spectrum.

1122 A WMO (World Meteorological Organization) shortwave radiation model (Cano et al.,1986)  
 1123 calibrated over Indian conditions (Mallick et al., 2007, 2009) was used to compute  $R_G$  using the  
 1124 following equation:

$$R_G = \tau_{sw} G_{sc} E (\sin\beta_e)^{1.15} \quad (B5)$$

1125 Where,  $\tau_{sw}$  is the is the global clear sky transmissivity for the shortwave radiation (0.7),  $G_{sc}$  is the  
 1126 solar constant ( $1367 Wm^{-2}$ ),  $\epsilon$  is the eccentricity correction factor due to variation in Sun-Earth  
 1127 distance and  $\beta_e$  is the sun elevation in degrees.

1128  $R_{L\downarrow}$  at any instance was calculated as follows:

$$R_{L\downarrow} = \epsilon_a \sigma (273.14 + T_A)^4 \quad (B6)$$

1129 Where,  $\sigma$  is the Stefan–Boltzmann constant ( $5.67 \times 10^{-8} \text{ Wm}^{-2}\text{K}^{-4}$ );  $T_A$  is the air temperature ( $^{\circ}\text{C}$ );  
1130  $\epsilon_a$  is the atmospheric emissivity.

1131 Atmospheric emissivity ( $\epsilon_a$ ) was computed using the following equation (Bastiaanssen et  
1132 al.,1998):

$$\epsilon_a = 0.85 - \ln\tau_{\text{sw}}^{0.09} \quad (\text{B7})$$

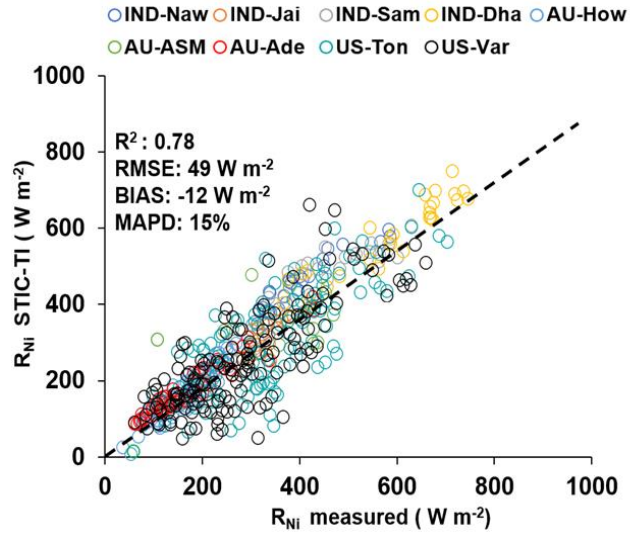
1133  $R_{L\uparrow}$  at any particular instance was calculated as follows:

$$R_{L\uparrow} = \epsilon_s \sigma (273.14 + T_s)^4 \quad (\text{B8})$$

1134 Where,  $\epsilon_s$  is the surface emissivity in thermal infrared (8 – 14  $\mu\text{m}$ ) spectrum and  $T_s$  is the land  
1135 surface temperature ( $^{\circ}\text{C}$ ).

## 1136 **B2: Evaluation of STIC-TI $R_{Ni}$**

1137 Comparison of the clear-sky  $R_{Ni}$  estimates with respect to *in situ* measurements revealed RMSE in  
1138  $R_{Ni}$  to the order of 27 – 72  $\text{W m}^{-2}$ , MAPD 8 –24%, BIAS (-67) – 50  $\text{W m}^{-2}$ , and  $R^2$  varying from  
1139 0.62– 0.90 across all the sites (Fig. B2, Table B2). Among the nine sites, a consistent  
1140 underestimation of  $R_{Ni}$  was noted in IND-Dha, US-Ton, and US-Var (with BIAS of -23  $\text{W m}^{-2}$ , -  
1141 61  $\text{W m}^{-2}$  and -67  $\text{W m}^{-2}$ ), whereas substantial overestimation of  $R_{Ni}$  was found in IND-Sam, IND-  
1142 Naw, and AU-ASM with a BIAS of 50  $\text{W m}^{-2}$ , 37  $\text{W m}^{-2}$  and 43  $\text{W m}^{-2}$ , respectively (Table B2).



**Figure B2:** Validation of STIC-TI derived  $R_{Ni}$  estimates with respect to *in situ* measurements in different ecosystems. The regression equation between modeled versus in-situ  $R_{Ni}$  is,  $R_{Ni}$  (STIC-TI) =  $0.78R_{Ni}$  (tower) + 58.92.

1143 **Table B2:** Performance evaluation statistics of clear-sky  $R_{Ni}$  estimates in nine different  
 1144 agroecosystems

Sites	Error statistics of clear-sky $R_{Ni}$ model estimates			
	$R^2$	BIAS ( $W m^{-2}$ )	RMSE ( $W m^{-2}$ )	MAPD (%)
IND-Jai	0.81	-9	32	8
IND-Naw	0.81	37	56	12
IND-Dha	0.81	-23	42	9
IND-Sam	0.64	50	67	15
US-Ton	0.68	-61	69	21
US-Var	0.62	-67	72	24
Au-How	0.87	7	27	15
AU-ASM	0.88	43	50	14
AU-Ade	0.90	11	27	16

1145 **Appendix C**

1146 **C1: Estimating SEB fluxes using STIC1.2 analytical model and thermal remote sensing data**

1147 STIC1.2 (Mallick et al., 2014, 2015a,b, 2016, 2018a) is a one-dimensional physically based SEB  
1148 model and is based on the integration of satellite LST observations into the Penman–Monteith  
1149 Energy Balance (PMEB) equation (Monteith, 1965). In STIC1.2, the vegetation–substrate  
1150 complex is considered as a single unit. Therefore, the aerodynamic conductances from individual  
1151 air-canopy and canopy-substrate components is regarded as an ‘effective’ aerodynamic  
1152 conductance ( $g_A$ ), and surface conductances from individual canopy (stomatal) and substrate  
1153 complexes is regarded as an ‘effective’ canopy-surface conductance ( $g_S$ ) which simultaneously  
1154 regulate the exchanges of sensible and latent heat fluxes (H and LE) between surface and  
1155 atmosphere. One of the fundamental assumptions in STIC1.2 is the first order dependence of these  
1156 two critical conductances on M through  $T_S$ . Such an assumption enabled an integration of satellite  
1157 LST in the PMEB model (Mallick et al., 2016). The common expression for LE and H according  
1158 to the PMEB equation is as follows:

$$LE = \frac{s\phi + \rho c_P g_A D_A}{s + \gamma \left(1 + \frac{g_A}{g_S}\right)} \quad (C6)$$

$$H = \frac{\gamma\phi \left(1 + \frac{g_A}{g_S}\right) - \rho c_P g_A D_A}{s + \gamma \left(1 + \frac{g_A}{g_S}\right)} \quad (C7)$$

1159 In the above equations, the two biophysical conductances ( $g_A$  and  $g_S$ ) are unknown and the  
1160 STIC1.2 methodology is based on finding analytical solutions for the two unknown conductances  
1161 to directly estimate LE (Mallick et al., 2016, 2018a). The need for such analytical estimation of  
1162 these conductances is motivated by the fact that  $g_A$  and  $g_S$  can neither be measured at the canopy  
1163 nor at larger spatial scales, and there is no universally agreed appropriate model of  $g_A$  and  $g_S$  that  
1164 currently exists (Matheny et al., 2014; van Dijk et al., 2015). By integrating  $T_S$  with standard SEB  
1165 theory and vegetation biophysical principles, STIC1.2 formulates multiple state equations in order

1166 to eliminate the need to use the empirical parameterizations of the  $g_A$  and  $g_S$  and also to bypass the  
1167 scaling uncertainties of the leaf-scale conductance functions to represent the canopy-scale  
1168 attributes. The state equations for the conductances are expressed as a function of those variables  
1169 that are mostly available as remote sensing observations and weather forecasting models. In the  
1170 state equations, a direct connection to  $T_S$  is established by estimating  $M$  as a function of  $T_S$ . The  
1171 information of  $M$  is subsequently used in the state equations of conductances, aerodynamic  
1172 variables (aerodynamic temperature, aerodynamic vapor pressure), and evaporative fraction,  
1173 which is eventually propagated into their analytical solutions.  $M$  is a unitless quantity, which  
1174 describes the relative wetness (or dryness) of a surface and also controls the transition from  
1175 potential to actual evaporation; which implies  $M \rightarrow 1$  under saturated surface conditions and  $M \rightarrow 0$   
1176 under extremely dry conditions. Therefore,  $M$  is critical for providing a constraint against which  
1177 the conductances are estimated. Since  $T_S$  is extremely sensitive to the surface moisture variations,  
1178 it is extensively used for estimating  $M$  in a physical retrieval scheme (detail in Appendix A3 of  
1179 Bhattarai et al., 2018; Mallick et al., 2016, 2018a). It is hypothesized that linking  $M$  with the  
1180 conductances will simultaneously integrate the information of  $T_S$  into the PMEB model. To  
1181 illustrate, we express the state equations by symbols,  $sv_1 = f \{c_1, c_2, c_3, v_1, v_2, v_3, v_4, sv_3, sv_5\}$ ;  $sv_2$   
1182  $= f \{v_4, sv_1, sv_5, sv_6\}$ ;  $sv_3 = f \{c_3, v_3, v_4, sv_4, sv_5\}$ ;  $sv_4 = f \{c_3, v_3, sv_1, sv_2, sv_7, sv_8\}$ . Here,  $f$ ,  $sv$ ,  $v$ ,  
1183 and  $c$  denote the function, state variables, input variables (5 input variables; radiative and  
1184 meteorological), and constants (3 constants), respectively. Here  $sv_1$  to  $sv_4$  are  $g_A$ ,  $g_S$ , aerodynamic  
1185 temperature ( $T_0$ ), evaporative fraction ( $\Lambda$ ), and  $sv_8$  is  $M$ . Given the estimates of  $M$ , net radiative  
1186 energy ( $R_{N_i} - G_i$ ),  $T_A$ ,  $R_H$ , the four state equations are solved simultaneously to derive analytical  
1187 solutions for the four state variables and to produce a surface energy balance “closure” that is  
1188 independent of empirical parameterizations for  $g_A$ ,  $g_S$ ,  $T_0$ , and  $\Lambda$ . However, the analytical solutions  
1189 to the four state equations contain three accompanying unknown state variables (effective vapor  
1190 pressures at source/sink height, and Priestley-Taylor variable), and as a result there are four  
1191 equations with seven unknowns. Consequently, an iterative solution was found to determine the  
1192 three additional unknown variables as detailed in this section above and also described in Mallick  
1193 et al. (2016, 2018a) and Bhattarai et al. (2018). The state equations of STIC are given below.

$$g_A = \frac{\phi}{\rho_{CP} \left[ (T_0 - T_A) + \left( \frac{e_0 - e_A}{\gamma} \right) \right]} \quad (C1)$$

$$g_S = g_A \frac{(e_0 - e_A)}{(e_0^* - e_0)} \quad (C2)$$

$$T_0 = T_A + \left( \frac{e_0 - e_A}{\gamma} \right) \left( \frac{1 - \Lambda}{\Lambda} \right) \quad (C3)$$

$$\Lambda = \frac{2\alpha s}{2s + 2\gamma + \gamma \frac{g_A}{g_S} (1 + M)} \quad (C4)$$

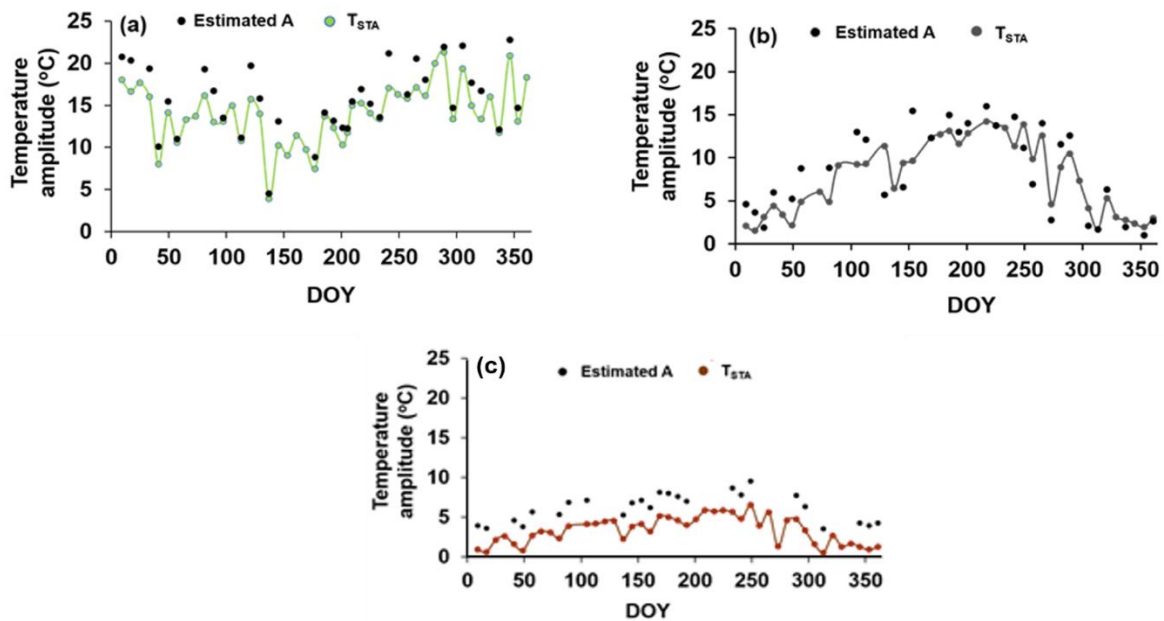
1194 Detailed derivations of these four state equations are given in Mallick et al. (2016). Given the  
 1195 values of  $M$ ,  $R_N$ ,  $G$ ,  $T_A$ , and  $R_H$  or  $e_A$ , the four state equations can be solved simultaneously to  
 1196 derive analytical solutions for the four unobserved variables and to simultaneously produce a  
 1197 ‘closure’ of the PMEB model that is independent of empirical parameterizations for both  $g_A$  and  
 1198  $g_S$ . However, the analytical solutions to the four state equations contain three accompanying  
 1199 unknowns;  $e_0$  (vapor pressure at the source/sink height),  $e_0^*$  (saturation vapor pressure at the  
 1200 source/sink height), and Priestley-Taylor coefficient ( $\alpha$ ), and as a result there are four equations  
 1201 with seven unknowns. Consequently, an iterative solution was needed to determine the three  
 1202 unknown variables (as described in Appendix A2 in Mallick et al. 2016). Once the analytical  
 1203 solutions of  $g_A$  and  $g_S$  are obtained, both variables are returned into eq. (13) to directly estimate  
 1204 LE.

1205 In STIC-TI, an initial value of  $\alpha$  was assigned as 1.26; initial estimates of  $e_0^*$  were obtained from  
 1206  $T_s$  through temperature-saturation vapour pressure relationship, and initial estimates of  $e_0$  were  
 1207 obtained from  $M$  as,  $e_0 = e_A + M(e_0^* - e_A)$ . Initial  $T_{0D}$  and  $M$  were estimated according to  
 1208 Venturini et al. (2008) as described in section 3.2, and initial estimation of  $G$  was performed from  
 1209 initial  $M$  using the equation sets eq. (2) – eq. (11). With the initial estimates of these variables;  
 1210 first estimate of the conductances,  $T_0$ ,  $\Lambda$ ,  $H$ , and LE were obtained. The process was then iterated  
 1211 by updating  $e_0^*$ ,  $D_0$ ,  $e_0$ ,  $T_{0D}$ ,  $M$ , and  $\alpha$  (using eq. A9, A10, A11, A17, A16 and A15 in Mallick et  
 1212 al., 2016), with the first estimates of  $g_S$ ,  $g_A$ ,  $T_0$ , and LE, and re-computing  $G$ ,  $\phi$ ,  $g_S$ ,  $g_A$ ,  $T_0$ ,  $\Lambda$ ,  $H$ ,  
 1213 and LE in the subsequent iterations with the previous estimates of  $e_0^*$ ,  $e_0$ ,  $T_{0D}$ ,  $M$ , and  $\alpha$  until the

1214 convergence of LE was achieved. Stable values of G, conductances, LE, H,  $T_0$ ,  $e_0^*$ ,  $e_0$ ,  $T_{0D}$ , M, and  
1215  $\alpha$  were obtained within ~25 iterations. The inputs needed for computation of  $LE_i$  (eq.C6) are air  
1216 temperature ( $T_A$ ), land surface temperature ( $T_S$ ), relative humidity ( $R_H$ ), net radiation ( $R_{Ni}$ ) and  
1217 soil heat flux ( $G_i$ ).

## 1218 Appendix D

1219 The temporal variation of estimated A and  $T_{STA}$  is shown in Fig. D1. The annual variations of  $T_{STA}$   
1220 in different ecosystem was found to be within the ranges of 1 - 4° C.



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1222 **Figure D1:** Temporal variation of A and  $T_{STA}$  in (a) AU-ASM (2013), (b) US-Ton (2014), (c) US-  
1223 Var (2014).

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1230 **Appendix E**

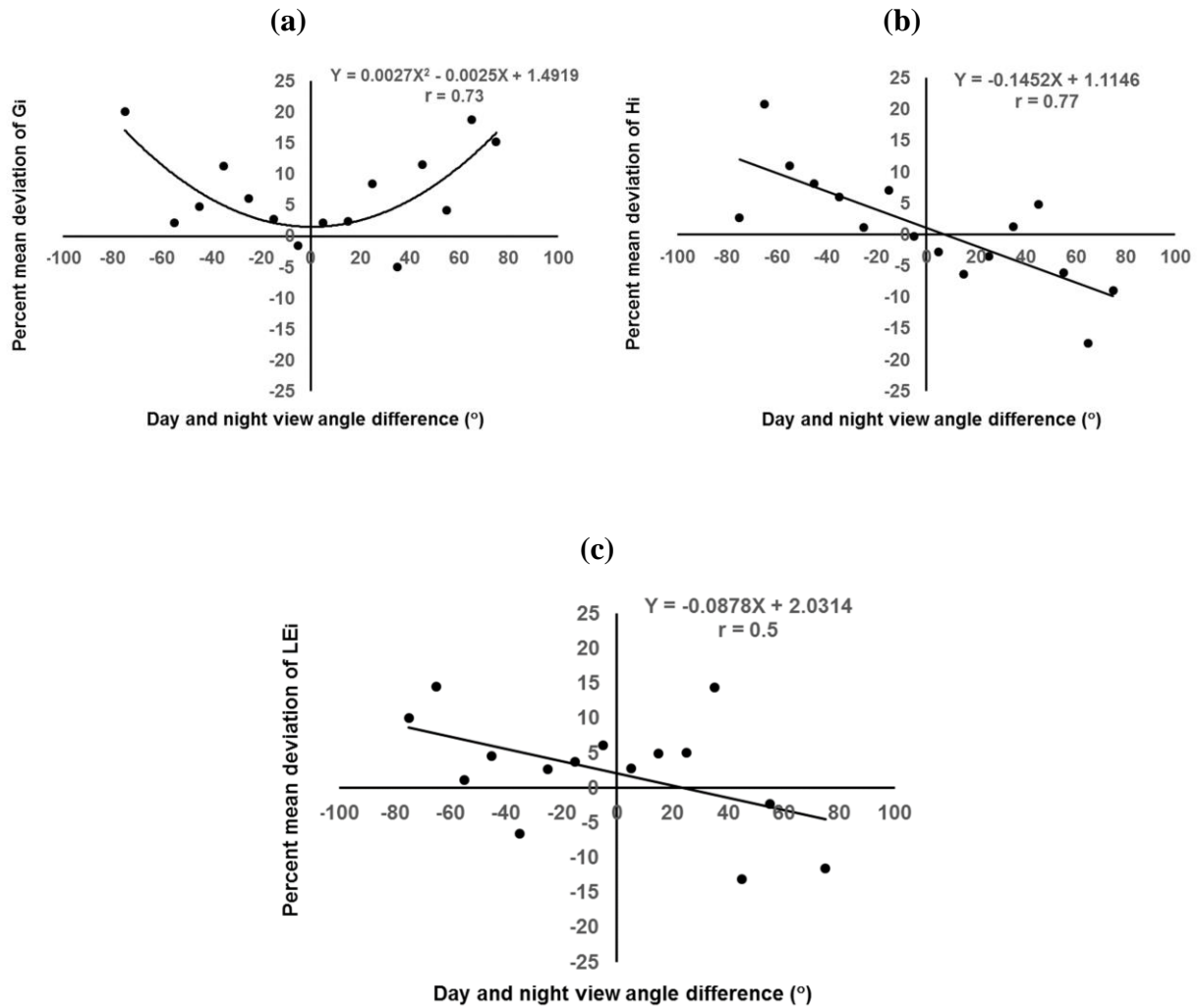
1231 **Table E1:** Soil textural properties and their values used in the present study (Murray and Verhoef,  
 1232 2007; Minasny et al., 2011; Anderson et al., 2007).

<b>Soil texture</b>	<b>Water retention Shape parameter (<math>\delta</math>)</b>	<b>Field capacity (vol/vol) (%) <math>\theta_{fc}</math></b>	<b>Wilting point (vol/vol) (%) <math>\theta_{wp}</math></b>	<b>Sand fraction (<math>f_s</math>)</b>	<b>Saturated soil moisture (vol/vol) (%) <math>\theta^*</math></b>
Sand	2.77	10	5	0.92	43
Loamy Sand	2.39	12	5	0.82	41
Sandy loam	2.27	18	8	0.58	41
Loam	2.20	28	14	0.43	43
Silty loam	2.22	31	11	0.17	45
Sandy clay loam	2.17	27	17	0.58	39
Clay loam	2.14	36	22	0.40	41
Silty clay loam	2.14	38	22	0.10	43
Sandy clay	2.11	36	25	0.52	38
Silty clay	2.12	41	27	0.06	46
Clay	2.10	42	30	0.22	38



1233 **Appendix F**

1234 Day-night view angle effect on errors of STIC-TI heat flux estimates from measurements is shown  
1235 in Figure F.



**Figure F1:** Dependence of STIC-TI model flux error in terms of mean percent deviation from measurements on day-night view angle difference of MODIS Aqua expressed as mean of  $10^\circ$  bin for (a)  $G_i$ , (b)  $H_i$ , and (c)  $LE_i$ .

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