



## The role of aerodynamic resistance in thermal remote sensing-based evapotranspiration models

Ivonne Trebs<sup>a,\*</sup>, Kaniska Mallick<sup>a,\*</sup>, Nishan Bhattarai<sup>b</sup>, Mauro Sulis<sup>a</sup>, Jamie Cleverly<sup>c,d</sup>, William Woodgate<sup>e,f</sup>, Richard Silberstein<sup>g,i</sup>, Nina Hinko-Najera<sup>h</sup>, Jason Beringer<sup>i</sup>, Wayne S. Meyer<sup>j</sup>, Zhongbo Su<sup>k</sup>, Gilles Boulet<sup>l</sup>

<sup>a</sup> Department of Environmental Research and Innovation, Luxembourg Institute of Science and Technology, Belvaux, Luxembourg

<sup>b</sup> School for Environment and Sustainability (SEAS), University of Michigan, Ann Arbor, USA

<sup>c</sup> School of Life Sciences, University of Technology Sydney, Broadway, NSW, Australia

<sup>d</sup> Terrestrial Ecosystem Research Network (TERN), College of Science and Engineering, James Cook University, Cairns, Qld, Australia

<sup>e</sup> CSIRO Land & Water, Canberra, ACT, Australia

<sup>f</sup> School of Earth and Environmental Science, University of Queensland, St Lucia, Australia

<sup>g</sup> Centre for Ecosystem Management, Edith Cowan University, Joondalup, WA, Australia

<sup>h</sup> School of Ecosystem and Forest Sciences, The University of Melbourne, Creswick, Australia

<sup>i</sup> School of Agriculture and Environment, University of Western Australia, Crawley, WA, Australia

<sup>j</sup> School of Biological Sciences, University of Adelaide, Adelaide, Australia

<sup>k</sup> University of Twente, Faculty of Geo-Information Science and Earth Observation (ITC), Enschede, the Netherlands

<sup>l</sup> CESBIO, Université de Toulouse, CNRS, CNES, UPS, IRD, INRAE, Toulouse, France

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### ABSTRACT

Aerodynamic resistance (hereafter  $r_a$ ) is a preeminent variable in evapotranspiration ( $ET$ ) modelling. The accurate quantification of  $r_a$  plays a pivotal role in determining the performance and consistency of thermal remote sensing-based surface energy balance (SEB) models for estimating  $ET$  at local to regional scales. Atmospheric stability links  $r_a$  with land surface temperature ( $LST$ ) and the representation of their interactions in the SEB models determines the accuracy of  $ET$  estimates.

The present study investigates the influence of  $r_a$  and its relation to  $LST$  uncertainties on the performance of three structurally different SEB models. It used data from nine Australian OzFlux eddy covariance sites of contrasting aridity in conjunction with MODIS Terra and Aqua  $LST$  and leaf area index (LAI) products. Simulations of the sensible heat flux ( $H$ ) and the latent heat flux ( $LE$ , the energy equivalent of  $ET$  in  $W/m^2$ ) from the SPARSE (Soil Plant Atmosphere and Remote Sensing Evapotranspiration), SEBS (Surface Energy Balance System) and STIC (Surface Temperature Initiated Closure) models forced with MODIS  $LST$ , LAI, and in-situ meteorological datasets were evaluated against flux observations in water-limited (arid and semi-arid) and energy-limited (mesic) ecosystems from 2011 to 2019.

Our results revealed an overestimation tendency of instantaneous  $LE$  by all three models in the water-limited shrubland, woodland and grassland ecosystems by up to 50% on average, which was caused by an underestimation of  $H$ . Overestimation of  $LE$  was associated with discrepancies in  $r_a$  retrievals under conditions of high atmospheric instability, during which uncertainties in  $LST$  (expressed as the difference between MODIS  $LST$  and in-situ  $LST$ ) apparently played a minor role. On the other hand, a positive difference in  $LST$  coincided with low  $r_a$  (high wind speeds) and caused a slight underestimation of  $LE$  at the water-limited sites. The impact of  $r_a$  on the  $LE$  residual error was found to be of the same magnitude as the influence of  $LST$  uncertainties in the semi-arid ecosystems as indicated by variable importance in projection (VIP) coefficients from partial least squares regression above unity. In contrast, our results for the mesic forest ecosystems indicated minor dependency on  $r_a$  for modelling  $LE$  ( $VIP < 0.4$ ), which was due to a higher roughness length and lower  $LST$  resulting in the dominance of mechanically generated turbulence, thereby diminishing the importance of buoyancy production for the determination of  $r_a$ .

\* Corresponding authors.

E-mail addresses: [ivonne.trebs@list.lu](mailto:ivonne.trebs@list.lu) (I. Trebs), [kaniska.mallick@gmail.com](mailto:kaniska.mallick@gmail.com) (K. Mallick).

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## 1. Introduction

Aerodynamic resistance (hereafter  $r_a$ ) expresses the efficiency of turbulent transport controlling the land-atmosphere (L-A) exchange of sensible heat ( $H$ ) and water vapor between the source/sink height within a vegetation canopy and a reference height above the surface. It is the pivotal link that connects evapotranspiration ( $ET$ ) with  $H$  through the surface energy balance (SEB) equation, and the estimation of  $r_a$  is central in thermal remote sensing of  $ET$  at local to regional scales (Bahir et al., 2017; Bhattarai et al., 2018; Kustas et al., 2007). Advanced understanding of L-A interactions is a prerequisite for accurate monitoring and predictions of Earth-system responses to drought, climate warming and surface drying. This is also one of the fundamental needs for developing effective mitigation strategies that minimize the socio-economic impacts of water scarcity caused by frequent droughts. Within this context, accurate estimation of the magnitude and variability of  $ET$  is critical for assessing the vegetation responses to drought and for developing knowledge of efficient water resources management (Anderson et al., 2011).

Contemporary SEB models use radiometric land surface temperature ( $LST$ ) and meteorological variables to derive  $H$  while estimating  $ET$  (or its energy equivalent, the latent heat flux  $LE$ ) as a residual SEB component (Chen and Liu, 2020). The  $r_a$  for momentum transfer ( $r_{aM}$ ) is an unobserved variable, and its estimation is commonly based on the Monin-Obukhov similarity theory (MOST), which requires aerodynamic roughness parameters, friction velocity ( $u_*$ ) and  $H$  as inputs (Foken, 2006). Major uncertainties of the MOST method are associated with the influence of complex/heterogeneous terrain, uncertainties in prescribing vegetation roughness and corrections for atmospheric stability (Holwerda et al., 2012; Sun et al., 2020; van Dijk et al., 2015; Zhou et al., 2012). Lee and Buban (2020) found that the Richardson number stability correction functions based on bulk meteorological variables yielded better agreement with field observations than using MOST relationships. These challenges are further exacerbated by the ambiguity in estimating the difference between  $r_{aM}$  and the  $r_a$  for heat transfer ( $r_{aH}$ ), whereby complexity is added due to the inequality of  $LST$  and the aerodynamic temperature ( $T_0$ ) (Paul et al., 2014).

$LE$  is typically overestimated by the contemporary SEB models under dry conditions (e.g., Gokmen et al., 2012; Gokool et al., 2020; Morillas et al., 2013; Pardo et al., 2014; Seneviratne et al., 2010; van der Kwast et al., 2009). Although this overestimation tendency has been addressed by revisiting the soil resistance formulation (Kustas et al., 2016; Li et al., 2019) and integration of an environmental stress factor or NDVI scaling factor for model calibration (Gokmen et al., 2012; Gokool et al., 2020; Pardo et al., 2014), operating SEB models in water-scarce ecosystems may also be subject to errors in the determination of  $r_{aM}$  and  $r_{aH}$ . In these ecosystems, variations in  $H$  and  $LE$  are strongly determined by the feedback-response relationships between soil moisture availability and biophysical resistances (Cleverly et al., 2013; Jarvis and McNaughton, 1986; Raupach, 2001). Since the magnitude of  $LE$  is small compared to  $H$ , the performance of SEB models is expected to be highly sensitive to the uncertainties in  $r_a$  (Gokool et al., 2020; Mallick et al., 2016). While the biophysical impact of  $r_a$  on the  $LST$  response to vegetation changes and Earth greening was investigated recently (Chen et al., 2020; Liao et al., 2018; Winckler et al., 2019), and the influence of the inverse Stanton number ( $kB^{-1}$ ) on SEB model performance has been discussed extensively (Boulet et al., 2012; Paul et al., 2014; Troufleau et al., 1997), the knowledge gap on the role of  $r_a$  for SEB model uncertainty has not yet been fully explored. Any attempt to advance the representation of L-A interactions within the SEB models is hindered due to the use of empirical functions to characterize the roughness and atmospheric stability components of  $r_a$ , which are generally not measurable at scales in which the remote sensing-based  $ET$  mapping is applied. Due to its fundamental importance in  $LST$ -based  $ET$  mapping and drought monitoring,  $r_a$  is a key variable that merits a detailed investigation to understand the extent of error propagation in  $ET$  estimates from different

SEB models.

The scientific objective addressed by this study is to analyze the dependency on  $r_a$  of the uncertainty in predicted instantaneous  $LE$  using three structurally different SEB models that use dissimilar approaches to retrieve  $r_a$ . We hypothesize that  $r_a$  largely controls the predictive uncertainty of SEB models, and its influence on the errors of instantaneous  $LE$  retrievals is potentially comparable to the impact of  $LST$ . This hypothesis is tested by exploiting the remotely sensed  $LST$  information in SEB models that are validated with in-situ eddy covariance (EC) observations from a range of contrasting ecosystems with different aridity of the OzFlux network in Australia (Beringer et al., 2016; Mallick et al., 2018a).

Section 2 sets out the methodology that includes a brief description of the models, input variables and statistical analysis. Section 3 describes the data sources used in the study. The results are presented in Section 4, while the discussion and conclusion are elaborated in Section 5 and 6, respectively.

## 2. Methodology

### 2.1. SEB models for estimating $ET$

$LST$  obtained from thermal infrared (TIR) remote sensing provides the key lower-boundary condition in SEB models for diagnostic estimates of  $LE$  and evaporative stress (Anderson et al., 2011; Chen and Liu, 2020). One-source SEB models treat the soil-vegetation complex as a single system, deriving lumped  $LE$  from the information of composite  $LST$  (Boegh et al., 2002; Su, 2002). Two-source SEB models treat the soil-vegetation complex independently and decompose  $LST$  into soil and vegetation temperatures whilst deriving the  $ET$  components (evaporation and transpiration) separately (Boulet et al., 2015; Kustas and Anderson, 2009). Both approaches are based on an appropriate expression of  $r_{aM}$  and  $r_{aH}$  for solving  $H$ , estimating  $LE$  as a residual in the SEB equation (Eq. (1)) (given net radiation ( $Rn$ ) and soil heat flux ( $G$ ) are known or estimated individually).

$$LE = Rn - G - H \quad (\text{W/m}^2) \quad (1)$$

The bulk formulation of  $H$  is based on the flux-gradient relationship:

$$H = \frac{\rho c_p (T_0 - T_a)}{r_{aH}} \quad (\text{W/m}^2) \quad (2)$$

where  $\rho c_p$  is the volumetric heat capacity of air ( $\text{J/K/m}^3$ ),  $T_0$  (K) is the aerodynamic temperature at the effective canopy source height at which energy fluxes arise and  $T_a$  (K) is the reference level air temperature. Despite substantial progress in global, regional and field scale  $ET$  mapping (Anderson et al., 2011; Bahir et al., 2017), implementation of SEB models is challenged by the uncertain specification of vegetation roughness and atmospheric stability variables for determining  $r_{aH}$  and also due to the empirical adjustments to accommodate for the inequalities between  $LST$  and  $T_0$  (Paul et al., 2014). Calculation of  $r_{aH}$  requires addition of an external resistance ( $r_{ex}$ ) to  $r_{aM}$ , which involves the  $kB^{-1}$  concept (Chen et al., 2019a, 2019b; Chen et al., 2013; Su, 2002):

$$r_{aH} = r_{aM} + r_{ex} \quad (\text{s/m}) \quad (3)$$

$$r_{ex} = \frac{1}{\kappa u_*} kB^{-1} \quad (\text{s/m}) \quad (4)$$

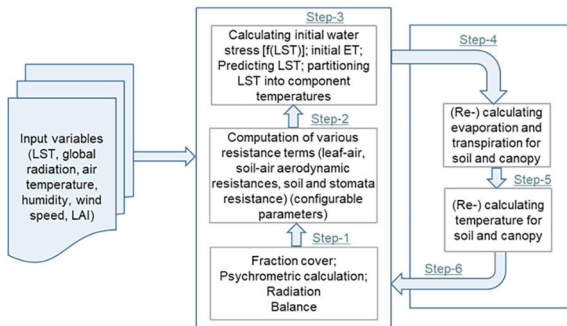
where  $\kappa$  is the von Kármán constant ( $=0.4$ ) and  $u_*$  is the friction velocity ( $\text{m/s}$ ). In Eq. (3),  $r_{aH}$  is greater than  $r_{aM}$ , i.e. momentum transport is more efficient than heat transport (Kustas et al., 2016). This implies that the source height for heat is lower than that for momentum, because heat is generated at the surface and its transfer is additionally controlled by molecular diffusion through the quasi-laminar sublayer (Verma, 1989). However, due to the use of  $LST$  instead of  $T_0$  (Eq. (2)),  $kB^{-1}$  is not

**Table 1**

Overview of  $r_{aM}$  ( $r_{aH}$ ) formulations used in three different SEB models. The symbols not mentioned in the main text are explained in the third column.

SEB model	Formulation of $r_{aM}$ ( $r_{aH}$ )	Symbols
SPARSE	$r_{aM} = \frac{\ln\left(\frac{z-d}{z_{0m}}\right)^2}{\kappa^2 u(1+R_{ib})^m}$ <p><math>m = 0.75</math> under unstable conditions and <math>m = 2</math> under stable conditions</p> $R_{ib} = \frac{5g(z-d)(T_0 - T_a)}{T_a u^2}$	<p><math>z</math>: measurement level of wind speed (m)  <math>d</math>: zero-plane-displacement height (m)  <math>z_{0m}</math>: aerodynamic roughness length for momentum transfer (m)  <math>u</math>: wind speed at measurement level (m/s)  <math>g</math>: standard acceleration due to gravity (9.81 m/s<sup>2</sup>)  <math>R_{ib}</math>: Richardson number (Choudhury and Monteith, 1988)</p>
SEBS	$r_{aH} = \frac{1}{\kappa L} \left[ \ln\left(\frac{z-d}{z_{0h}}\right) - \psi_h\left(\frac{z-d}{L}\right) + \psi_h\left(\frac{z_{0h}}{L}\right) \right]$ <p>with</p> $z_{0h} = \frac{z_{0m}}{\exp(kB^{-1})}$	<p><math>L</math>: Monin-Obukhov length (m)  <math>z_{0h}</math>: aerodynamic roughness lengths for heat transport (m)  <math>\psi_h</math>: universal function for sensible heat (Brutsaert, 1992, 1999)  <math>\theta_v</math>: potential virtual temperature at the measurement level (K)</p>
STIC	$L = \frac{\rho c_p u^2 \theta_v}{\kappa g H}$ $r_{aH} = \frac{\rho c_p \left[ (T_0 - T_a) + \left( \frac{e_0 - e_a}{\gamma} \right) \right]}{\phi}$	<p><math>e_0</math>: vapor pressure at the source/sink height (hPa)  <math>\gamma</math>: psychrometric constant (hPa K<sup>-1</sup>)  <math>\phi</math>: net available energy (W/m<sup>2</sup>)</p>

Estimation of  $T_0$  is based on finding an analytical solution of a host of state equations. Estimation of  $e_0$  is based on solving the saturation vapor pressure at the source/sink height and solving the vapor pressure deficit at the source/sink height of vegetation by combining Penman-Monteith and Shuttleworth-Wallace combination equations. Details are available in Mallick et al. (2016, 2018a).



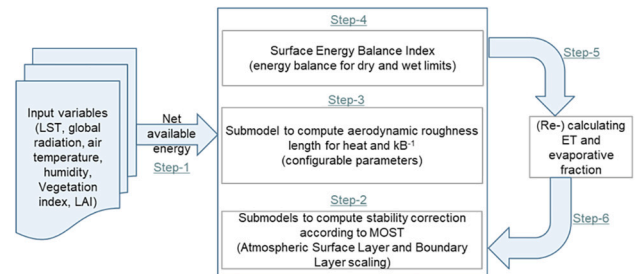
**Fig. 1.** Simplified flowchart of the SPARSE algorithm in retrieval mode. For a more detailed description see Boulet et al. (2015).

related to its original theoretical background, but it has become a purely empirical fitting parameter called radiometric  $kB^{-1}$  (Paul et al., 2014).

Despite the important role of  $LST$  in estimating  $ET$ , SEB models also require highly accurate  $r_{aM}$  and  $r_{aH}$ , but their role in governing the errors of modelled  $LE$  has received little attention to date. The three models employed in this study substantially differ in their structure, and, particularly, in their approaches to calculate  $r_{aM}$  and  $r_{aH}$  (see Table 1).

**2.1.1. SPARSE**

A new two-source  $ET$  model, the Soil Plant Atmosphere and Remote Sensing Evapotranspiration (SPARSE) model (Boulet et al., 2015; Saadi et al., 2018) tends to overcome the challenges associated with the inequality between  $T_0$  and  $LST$  (Fig. 1). SPARSE extends the original Two-Source Energy Balance (TSEB) model (Norman et al., 1995) in several aspects, notably by accounting for the effect of the vapor pressure deficit ( $VPD$ ). It linearizes the full set of energy budget equations and is based on the  $r_{aM}$  expression of Choudhury and Monteith (1988) using measured wind speed, and the correction for atmospheric stability based on the bulk Richardson number ( $R_{ib}$ ) that uses estimates of  $T_0$  (Table 1). It constrains the surface energy budgets of the main heat and vapor sources in soil and vegetation with the remotely sensed  $LST$  to



**Fig. 2.** Simplified flowchart of the SEBS algorithm. For a more detailed description see Su (2002).

retrieve instantaneous evaporation and transpiration rates. A layer (series) and a patch (parallel) version (Lhomme et al., 2012) of the model are available. SPARSE was operated in the retrieval mode where  $LST$  is an input (derived either from satellite observations or in-situ measurements in the thermal infrared domain). In its standard setup, SPARSE uses empirical relationships to derive roughness parameters from canopy height ( $h_c$ ) ( $z_{0m} = 0.13h_c$  and  $d = 0.65h_c$ ) for dense vegetation. These were modified to  $d = 0.6h_c$  for sites with sparse vegetation (Th. Foken, personal communication), for which  $z_{0m}$  was derived from EC data (see Table 3, Section 3.1) (Foken, 2017). The estimation of  $Rn$  in SPARSE is detailed in Boulet et al. (2015). Soil heat flux was calculated as a fraction of soil net radiation according to the time of day and ecosystem type. This approach showed comparable or even better results than the ones of e.g. Choudhury et al. (1987) or Su (2002) using LAI or fraction cover ( $F_c$ ) as additional scaling variables. The required input data to run SPARSE are  $LST$ , emissivity, surface albedo, view zenith angle ( $vza$ ), leaf area index (LAI),  $h_c$ , incoming solar radiation, wind speed, air temperature and relative humidity at a reference level.

To obtain consistent results and to understand the effects of  $r_a$  on  $LE$  uncertainties, simulations with the two other models (SEBS and STIC) were constrained using the net available energy ( $\phi$ ) derived from SPARSE. This simplifies disentangling the influence of modelled  $\phi$  which impacts  $LE$  by residual (Eq. (1)).

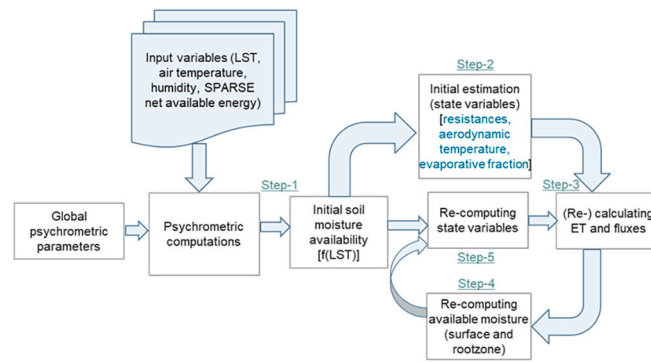


Fig. 3. Simplified flowchart of the STIC1.2 algorithm. For a more detailed description see Mallick et al. (2015).

### 2.1.2. SEBS

One-source models, such as the Surface Energy Balance System (SEBS) (Fig. 2) address the inequality between  $T_0$  and  $LST$  by introducing  $r_{ex}$  and the  $kB^{-1}$  concept (Chen et al., 2013; Su, 2002). SEBS derives the SEB components by treating the soil-vegetation composite as a single unit (Su, 2002; Su et al., 2001). It estimates  $H$  for the driest and wettest boundary conditions ( $H_{dry}$ ,  $H_{wet}$ ). Based on  $H_{dry}$ ,  $H_{wet}$  and actual  $H$ , relative evaporation ( $\Lambda_r$ ) and evaporative fraction ( $\Lambda$ ) are estimated by scaling the actual  $H$  with its dry and wet limits (details in Su, 2002).  $LE$  is derived through  $\Lambda$  and net available energy. Estimation of  $r_{aH}$  involves parameterization of the turbulent heat flux using MOST following an iteration procedure to derive  $u^*$ ,  $L$  and  $H$  by implementing the stability correction functions (Brutsaert, 1992, 1999) (Table 1). Like most one-source models, SEBS is based on the estimation of the  $kB^{-1}$  factor. For this study, a revised model version including modifications presented in González-Dugo et al. (2020) and Chen et al. (2013) was used. Because the main objective of the paper is to explore model dependency on  $r_a$ , instead of using the canopy momentum transfer model (Massman and Weil, 1999), we used constant  $z_{0m}$  and  $d$  values (see Table 3, Section 3.1) to assign identical aerodynamic parameters for SPARSE and SEBS. The other required input data are comparable to those of SPARSE.

### 2.1.3. STIC

The Surface Temperature Initiated Closure (STIC, version 1.2) model is a one-source non-parametric  $ET$  model (Fig. 3) (Mallick et al., 2015; Mallick et al., 2014; Mallick et al., 2018a; Mallick et al., 2016). It was developed to circumvent the uncertainties associated with  $LST$  versus  $T_0$  inequalities and MOST- $r_a$  parameterizations for satellite-based  $ET$  mapping (Bhattarai et al., 2018). STIC is a one-dimensional physically based SEB model based on integrating  $LST$  observations into the Penman-Monteith energy balance equation and finding analytical solutions for  $r_{aH}$  (Table 1) and canopy-substrate resistance ( $r_c$ ) that are independent of any empirical parameterizations. One of the fundamental assumptions in STIC is the first order dependence of  $r_{aH}$  and  $r_c$  on soil moisture through  $LST$ . By integrating  $LST$  with standard SEB theory, STIC formulates multiple state equations. These state equations are expressed as a function of those variables that are either directly available or deducible from remote sensing observations. Therefore, the equations can be solved algebraically to find analytical solutions of the resistances and  $T_0$ . Although most input variables for STIC are similar to those of SPARSE and SEBS, STIC does not require LAI and aerodynamic parameters ( $z_{0m}$  and  $d$ ).

### 2.2. Retrieval of input variables

Although most of the required input variables were directly measured at the flux tower sites (Section 3), additional quantities were also needed for the model runs. The calculation of time-variant surface emissivity ( $\epsilon$ ) to retrieve in-situ  $LST$  estimates was performed following Jimenez-Munoz et al. (2006):

$$\epsilon = \epsilon_{vi}F_c + \epsilon_{si}(1 - F_c) \quad (5)$$

where  $\epsilon_{vi}$  and  $\epsilon_{si}$  are band emissivity values for vegetation (0.99) and bare soil (0.96), respectively, and  $F_c$  is the fractional vegetation cover. The latter was derived according to:

$$F_c = 1 - e^{\left(\frac{-K \cdot LAI}{\cos(vza)}\right)} \quad (6)$$

where  $K$  is the attenuation coefficient of incoming radiation within the canopy (0.45), LAI is the leaf area index derived from MODIS LAI product (MCD15A2H) and  $vza$  is the MODIS view zenith angle.

The radiation balance was measured by pyranometer pairs (for shortwave components) and pyrgeometer pairs (for longwave components) mounted on the EC towers. Estimates of surface albedo to model net radiation were derived from in-situ upwelling and downwelling short wave radiation measurements. In-situ  $LST$  was computed from measured upwelling and downwelling longwave radiation covering the same spectral range using the Stefan-Boltzmann law (e.g. Chen et al., 2017):

$$LST_{in-situ} = \left(\frac{L\uparrow - (1 - \epsilon)L\downarrow}{\epsilon\sigma}\right)^{\frac{1}{4}} \quad (7)$$

where  $L\uparrow(W/m^2)$  is the upwelling longwave radiation,  $L\downarrow(W/m^2)$  is the downwelling longwave radiation,  $\epsilon$  is the surface emissivity,  $LST_{in-situ}$  (K) is the surface temperature and  $\sigma$  ( $W/m^2/K^4$ ) is the Stefan Boltzmann constant.

### 2.3. Statistical analysis

The following statistical metrics were used to evaluate the model performances for instantaneous  $LE$  at satellite overpass time:

Root mean Square Error ( $W/m^2$ ) :

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (LE_{mod} - LE_{obs})^2} \tag{8}$$

Mean Bias Error ( $W/m^2$ ) :

$$MBE = \frac{1}{n} \sum_{i=1}^n (LE_{mod} - LE_{obs}) \tag{9}$$

Mean Absolute Percentage Error (%) :

$$MAPE = \frac{1}{n} \sum_{i=1}^n \left| \frac{LE_{obs} - LE_{mod}}{LE_{obs}} \right| \tag{10}$$

Kling Gupta Efficiency :

$$KGE = 1 - \sqrt{(r-1)^2 + \left(\frac{\sigma_{mod}}{\sigma_{obs}} - 1\right)^2 + \left(\frac{\mu_{mod}}{\mu_{obs}} - 1\right)^2} \tag{11}$$

where the subscript ‘mod’ refers to modelled values and the subscript ‘obs’ refers to the observed values;  $r$  denotes the linear correlation between observations and simulations,  $\sigma$  denotes the standard deviation, and  $\mu$  represents the mean.  $KGE = 1$  indicates perfect agreement between simulations and observations, while a negative  $KGE$  indicates unsatisfactory model performance (for details see [Knoben et al., 2019](#)).

Furthermore, Partial Least Squares Regression (PLSR) was employed to identify fundamental relationships between the residual  $LE$  error and a host of variables. These were intermediate model variables (e.g.,  $\Phi$ ,  $r_{aM}$ ,

$r_{aH}$  and  $kB^{-1}$ ) as well as model input variables (e.g. LST). Regressions were made using the SIMPLS algorithm, which calculates PLS factors directly as linear combinations of the original variables ([de Jong, 1993](#)) after all variables were normalized. In order to quantify and present the relationship between the variables and the  $LE$  residual, we derived the Variable Importance in Projection (VIP) scores based on the normalized PLS weights, scores and loadings according to [Chong and Jun \(2005\)](#).

### 3. Datasets

#### 3.1. In-situ datasets

This study is based on high-quality EC and meteorological datasets for both model input and model evaluation from the regional Australian flux tower network OzFlux (<http://data.ozflux.org.au/portal/home.jsp>) that is funded by the National Collaborative Infrastructure Strategy (NCRIS) through the Terrestrial Ecosystem Research Network (TERN) platform (<https://www.tern.org.au/>) ([Beringer et al., 2016](#)). The three models were operated for the years 2011–2019 for a selection of nine OzFlux sites all over Australia including a wide range of ecosystem types, climates and aridity ([Table 2](#)). We used Level 3 datasets that were post-processed, corrected, but not gap-filled ([Isaac et al., 2017](#)).

Australia is a predominantly arid and semi-arid continent with substantial fluctuations in precipitation and primary production ([Cleverly et al., 2016](#)). In contrast, there are some mountainous rainforest locations where annual average precipitation exceeds 4000 mm ([Glenn et al., 2011](#)). The ecosystems in the Northern Territory (NT) of Australia (ASM, Stp, Dry, DaS, [Table 2](#)) are characterized by distinct wet and dry

**Table 2**

Summary showing general characteristics of the measurement sites of the Australian flux tower network used in this study. Model simulations were made for the period 2011–2019 (except GWW 2013–2019).

Aridity	Site	Lat/Lon	Ta (min-max) (°C)	P ( $\pm\sigma$ ) (mm)	Budyko aridity index mean (range)	World ecoregion
arid	Alice Springs Mulga (ASM)	–22.2828/133.2493	–0.8–43.4	302 (61)	31 (6–133)	Deserts and xeric shrublands
	Calperum (Cpr)	–34.0027/140.5877	–3.8–47.7	207 (66)	21 (8–40)	Mediterranean woodlands
	Great Western Woodlands (GWW)	–30.1913/120.6541	1.9–45.8	283 (52)	11 (5–22)	Mediterranean woodlands
semi-arid	Gingin (Gin)	–31.3764/115.7139	–0.14–43.3	560 (44)	8 (4–22)	Mediterranean woodlands
	Sturt Plains (Stp)	–17.1507/133.3502	4.4–45.4	581 (48)	7 (2–26)	Tropical grasslands
	Dry River (Dry)	–15.2588/132.3706	5.9–42.0	708 (43)	6 (2–12)	Tropical savannas
mesic	Wombat (Wom)	–37.4222/144.0944	–0.9–37.3	719 (46)	4 (1–6)	Temperate broadleaf forest
	Daly Uncleared (DaS)	–14.1592/131.3881	8.9–39.6	1116 (34)	4 (3–10)	Tropical savannas
	Tumbarumba (Tum)	–35.6566/148.1517	–5.5–33.7	914 (46)	1.6 (0.8–2)	Temperate broadleaf and mixed forest

**Table 3**

Summary showing specific characteristics of the measurement sites of the Australian flux tower network used in this study. The value of  $d$  was set to  $2/3h_c$  for dense vegetation and to  $0.6h_c$  for sparse vegetation (Th. Foken, personal communication). The values for  $z_{om}$  were set to  $0.13h_c$  for dense vegetation and calculated from Eqs. 2.67 and 3.1 in [Foken \(2017\)](#) for sparse vegetation. Mean values of the SEB closure were calculated at MODIS Terra and Aqua overpass times (see [Section 3.2](#)) for 2011–2019.

Site	canopy height (m)	LAI range ( $m^2/m^2$ )	$z_{om}$ (m)	$d$ (m)	SEB closure (%)
Alice Springs (ASM)	6.5	0.16–0.85	1.0	3.9	82
Calperum (Cpr)	3.0	0.17–0.66	0.21	1.8	93
Great Western Woodlands (GWW)	18.0	0.29–0.49	0.2	10.8	77
Gingin (Gin)	6.8	0.58–1.27	0.7	4.08	84
Sturt Plains (Stp)	0.5	0.15–1.35	0.065	0.325	92
Dry River (Dry)	12.3	0.7–2.0	1.2	7.38	78
Wombat (Wom)	23.0	2.2–4.9	2.5	13.8	82
Daly Uncleared (DaS)	16.4	0.66–2.5	2.0	9.84	91
Tumbarumba (Tum)	40.0	1.0–3.4	5.2	26.0	74

seasons and highly seasonal rainfall driven by monsoonal weather systems (Bowman et al., 2010). The sites located in the southern, south-eastern and south-western part of Australia (Cpr, GWW, Gin, Wom, Tum, Table 2) are affected by extra-tropical weather patterns and the wet season is in the winter (Jun-Aug) while the dry season is in the summer (Dec-Feb) (except at GWW, where rainfall is summer dominant for the past ten years).

The arid ecosystems toward central Australia are subject to very low rainfall amounts mainly occurring as occasional precipitation ( $P$ ) pulses, resulting in a very low top-soil water content ( $SWC < 20\%$ ) most of the time (Mallick et al., 2018a). They are characterized by strong surface heterogeneity and extremely low soil moisture coupled with high  $VPD$ .

By adopting the aridity classification as reported in Mallick et al. (2018a), we defined that sites with a mean Budyko aridity index ( $BAI = ET_{pot}/P$ ) greater than 10 are strongly water-limited (arid), which include ASM, Cpr, and GWW. The sites Gin, Stp, and Dry are considered as semi-arid (mean  $BAI = 5-10$ ). Sites with a mean  $BAI < 5$  are considered as energy-limited (mesic), i.e. Wom, DaS and Tum.

For model simulations, the half-hourly or hourly (for Tum only) in-situ data (including in-situ- $LST$ ) were interpolated to the timestamp of satellite overpass (see Section 3.2). Table 3 shows detailed characteristics of the measurement sites that includes LAI, estimated aerodynamic roughness parameters and mean values of the SEB closure, respectively. The statistical intercomparison of SEB model results against flux observations were performed by forcing the Bowen Ratio Energy Balance (BREB) closure adding energy to  $LE$  and  $H$  in proportion to the measured Bowen ratio (Mauder et al., 2020; Twine et al., 2000).

### 3.2. Remote sensing datasets

$LST$  is a key input variable for the three models employed in this study. The Moderate Resolution Imaging Spectroradiometer (MODIS), an instrument onboard NASA's Terra and Aqua polar-orbiting satellite platforms, provides daily  $LST$  at a spatial resolution of 1 km. Daily observations of MODIS Terra and Aqua  $LST$  (MOD11A1, MYD11A1, v006) were acquired from the Land Processes Distributed Active Archive Centre (LPDAAC) for the corresponding tower pixels according to the latitude and longitude provided in Table 2. This resulted in  $LST$ , emissivity, and corresponding  $vza$  values coincident with the MODIS Terra and Aqua overpass timestamp for the period 2011–2019. Data for  $vza > 40^\circ$  and cloud contaminated  $LST$ s were excluded from the analysis.

Furthermore, the MODIS Terra-Aqua combined 4-day LAI (MCD15A2Hv006) product with a spatial resolution of 500 m was used

as model input (Table 3) for estimating  $F_c$  (Eq. (6)) and calculating the  $kB^{-1}$  factor in SEBS (Chen et al., 2013; Su, 2002); the amount of net radiation intercepted by the canopy and the leaf-air aerodynamic resistance in SPARSE (Boulet et al., 2015). The extracted LAI values from the MCD15A2Hv006 product for each site (Table 3) were cross-checked with in-situ LAI measurements when available.

## 4. Results

The complete statistical results of modelled  $H$  and  $LE$  for all sites are presented in the Appendix (Tables A1-A6). For SPARSE, only results of the parallel resistance version of the model in the retrieval mode are shown, which is justified by the ecosystem types (often sparse vegetation). Simulated  $LE$  of the parallel model version compared better to the observations than that of the series model version for most of the sites. In some cases, model convergence was not achieved mainly due to high  $LST$  values, and these data were omitted from the analysis (see Tables A1 and A2).

For SEBS, in case the dry limits were reached (Mallick et al., 2018b), zero values of  $LE$  were rejected from further analysis (see Tables A3, A4). This is done to adapt with the structural uncertainties of SEBS in estimating relative evaporation ( $\Lambda_r$ ) under the dry limits. In SEBS,  $\Lambda_r$  is estimated by scaling the actual  $H$  with  $H$  for the driest ( $H_{dry}$ ) and wettest ( $H_{wet}$ ) conditions [ $\Lambda_r = 1 - (H - H_{wet})/(H_{dry} - H_{wet})$ ; and  $H_{dry} = Rn - G$ ] (Su, 2002). Any condition that produces  $H = H_{dry}$ , would tend to simulate  $\Lambda_r = 0$ , and  $LE$  will be consequently zero (Mallick et al., 2018b).

For STIC, no such rejection criteria are needed because of the structural characteristics of the model; and examples of iterative stabilization of STIC in different ecosystems are shown in previous studies (Mallick et al., 2015, 2016; Bhattarai et al., 2018).

In Section 4.1, the statistical results of the individual models are shown for  $H$  and  $LE$  using MODIS and in-situ  $LST$  as input. Sections 4.2–4.4 focus on the model results obtained using MODIS  $LST$  (Terra and Aqua) as input.

### 4.1. Model performance and intercomparison across sites with different aridity

For the SPARSE model, simulations using MODIS  $LST$  produced lower RMSE in instantaneous  $H$  and  $LE$  as compared to using in-situ  $LST$  at most of the sites (except for mesic ecosystems) (Fig. 4a,b). While the instantaneous  $H$  and  $LE$  from SPARSE showed lowest RMSE for the mesic sites ( $68-105 \text{ W/m}^2$ ), the RMSE for arid and semi-arid sites was

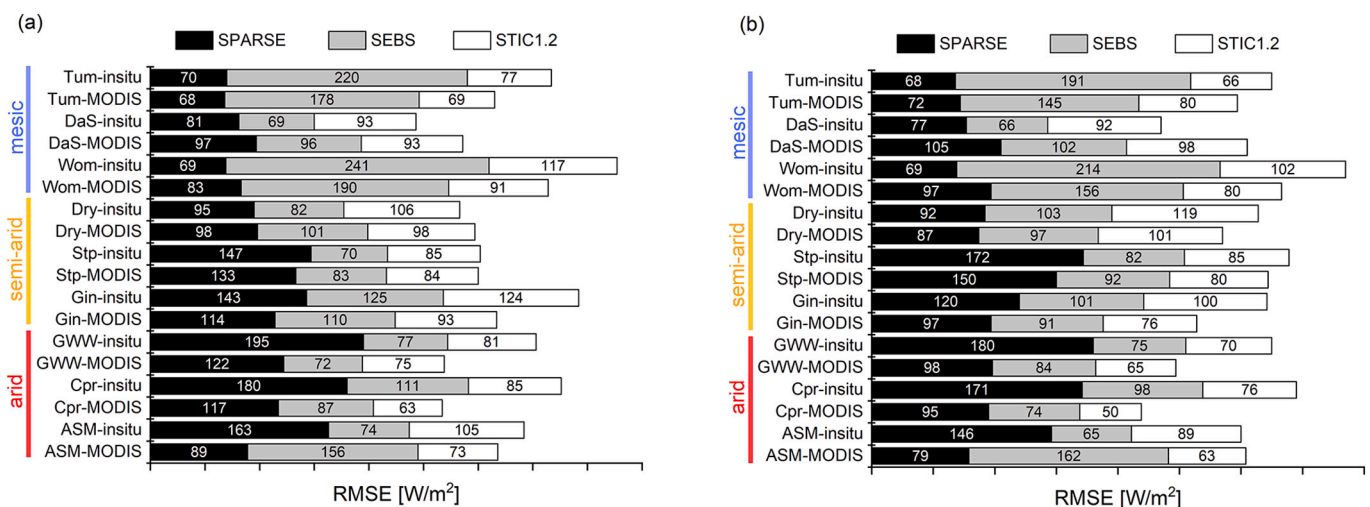
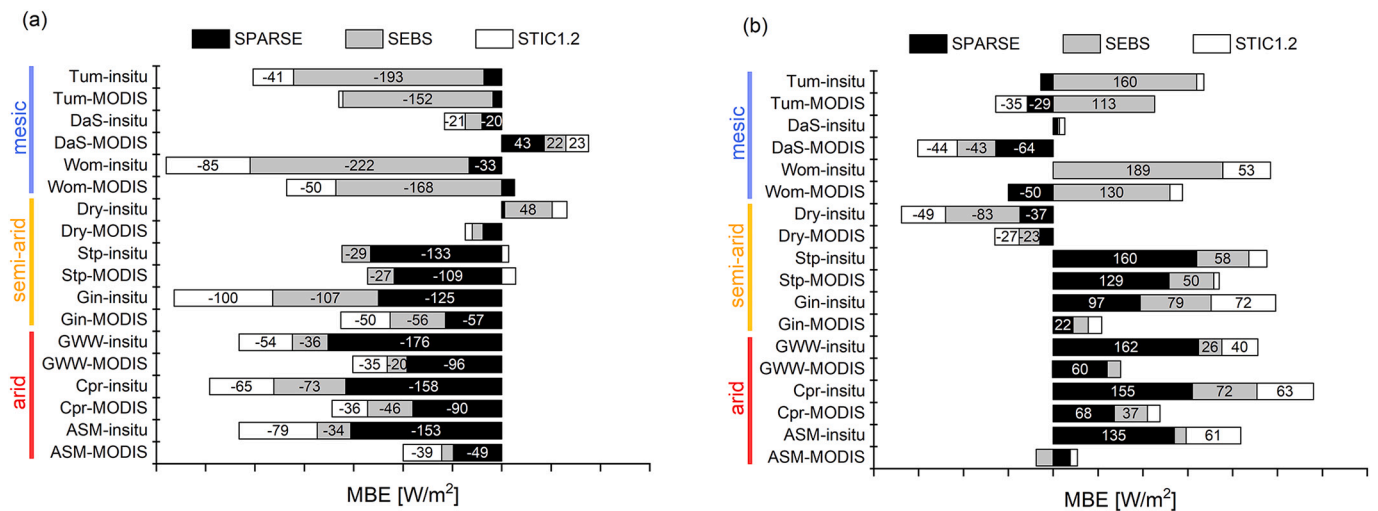


Fig. 4. Root Mean Square Error (RMSE) of the SPARSE (parallel version, retrieval mode), SEBS and STIC models for the instantaneous (a)  $H$  and (b)  $LE$  retrievals at satellite overpass times (MODIS Aqua and Terra) for nine sites of contrasting aridity in Australia using MODIS  $LST$  and in-situ  $LST$  as input. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

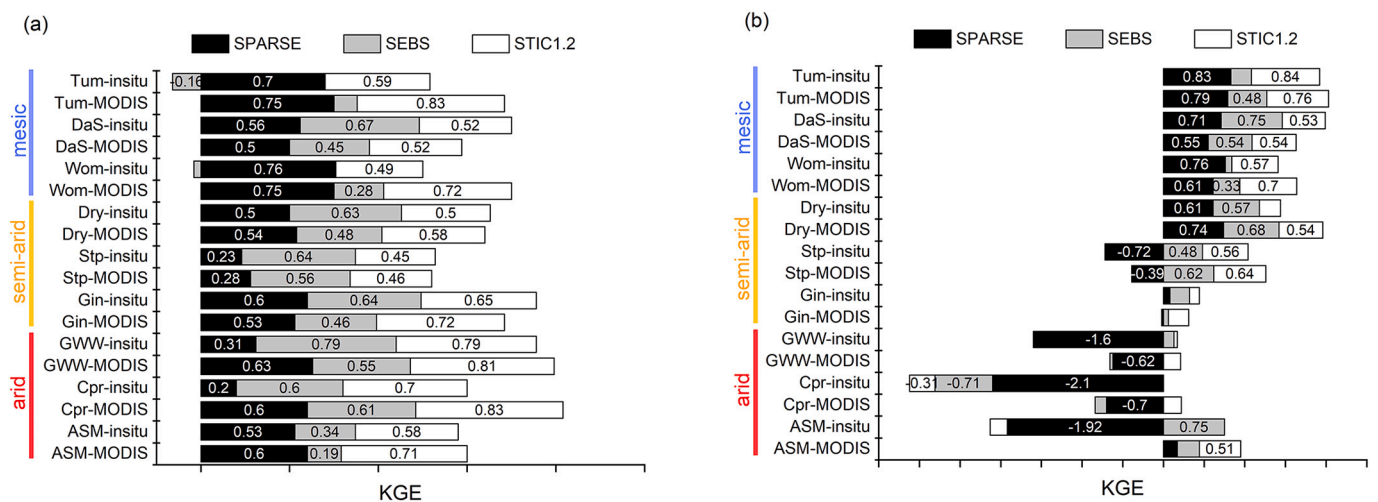


**Fig. 5.** Mean Bias Error (MBE) of SPARSE (parallel version, retrieval mode), SEBS and STIC models for instantaneous (a)  $H$  and (b)  $LE$  retrievals at satellite overpass times (MODIS Aqua and Terra) for nine sites of contrasting aridity in Australia using MODIS  $LST$  and in-situ  $LST$  as input. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

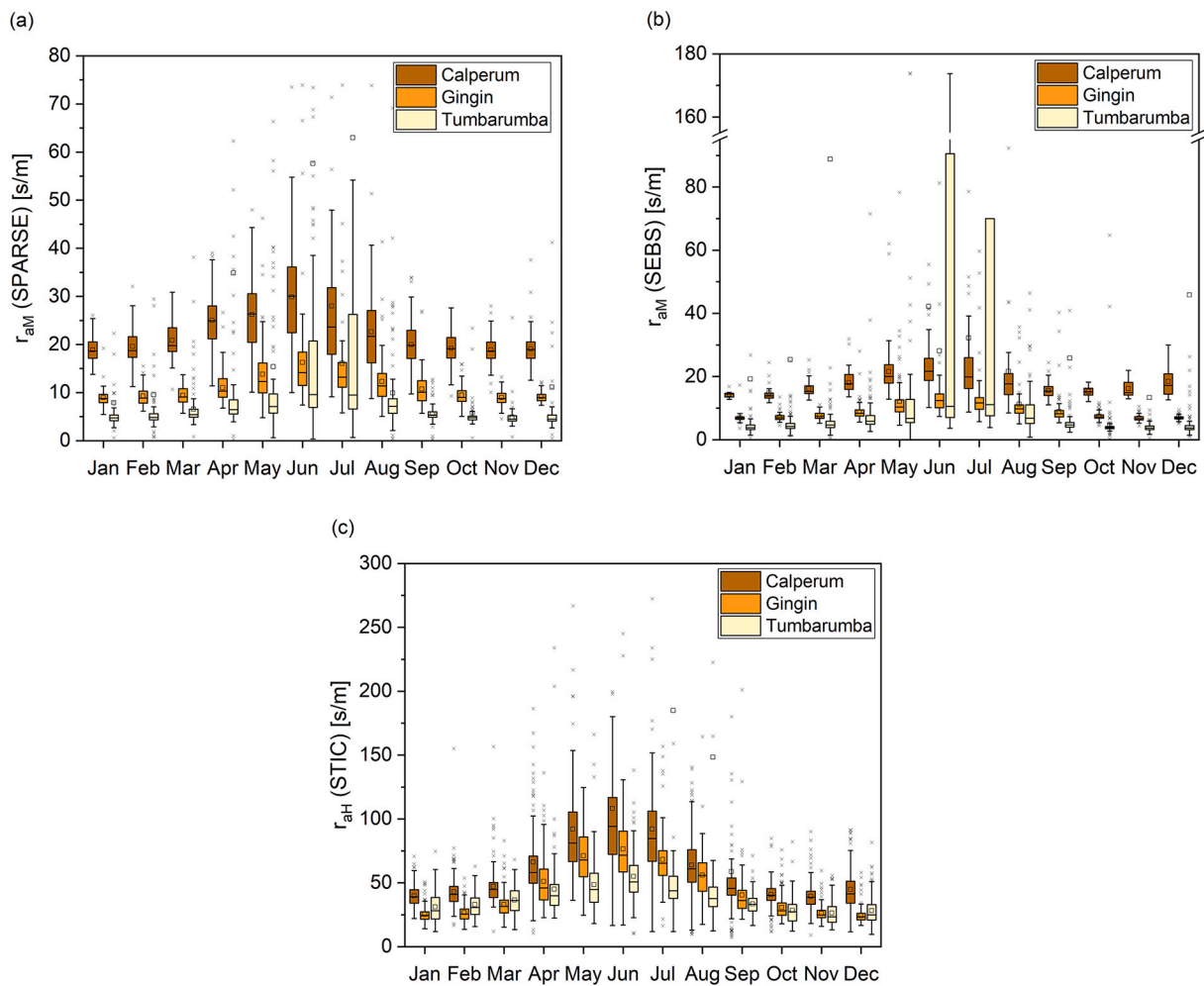
substantially higher (up to 195  $W/m^2$  for  $H$  and 180  $W/m^2$  for  $LE$ ), particularly when in-situ  $LST$  was used as input. The highest RMSE was found for the tropical grassland (Stp) and for one of the Mediterranean woodlands sites (GWW). The RMSE of SEBS exceeded that of SPARSE for all mesic sites (69–241  $W/m^2$  for  $H$  and 66–214  $W/m^2$  for  $LE$ ), while the RMSE of SEBS was lower than of SPARSE for arid and semi-arid sites, particularly when in-situ  $LST$  was used as model input (Fig. 4a,b). Instantaneous  $H$  and  $LE$  from STIC simulations resulted in lowest RMSE for the arid sites (63–105  $W/m^2$  for  $H$  and 50–89  $W/m^2$  for  $LE$ ) (Fig. 4a, b). The highest RMSE values ( $> 90 W/m^2$ ) from STIC for both  $H$  and  $LE$  were found for the savanna sites (Dry and DaS) as well as for Gin and Wom. Similar to SPARSE, the magnitudes of the RMSE from STIC were higher with in-situ  $LST$  for the majority of the sites. Overall, the RMSE was lower for STIC compared to the other two models and the magnitude of the RMSE for  $H$  and  $LE$  was comparable for all models.

Fig. 5 shows a significant underestimation (overestimation) of instantaneous  $H$  ( $LE$ ) by SPARSE for the arid (ASM, Cpr, GWW) and semi-arid sites (Gin and Stp, except Dry) as revealed by high negative MBE values ( $-49$  to  $-176 W/m^2$ ) for  $H$  (Fig. 5a) and high positive MBE values (22 to 162  $W/m^2$ ) for  $LE$  (Fig. 5b). This underestimation

(overestimation) persisted for sites with both sparse and dense vegetation (Stp) and is more pronounced when in-situ  $LST$  was used to simulate  $H$  and  $LE$ . In contrast, SPARSE slightly underestimated  $H$  and  $LE$  for most of the mesic sites (MBE values between  $-64$  and  $-20 W/m^2$ ) and model performance for  $LE$  improved with in-situ  $LST$  (MBE between  $-14$  and  $5 W/m^2$ ). The  $H$  and  $LE$  bias from SEBS simulations (Fig. 5a,b) was not only dependent on aridity but also on the ecosystem type. On average, SEBS underestimated (overestimated)  $H$  ( $LE$ ) for all sites except savanna ecosystems (Dry, DaS), where consistent overestimation of  $H$  and underestimation of  $LE$  was found (MBE of  $-23$  to  $-83 W/m^2$ ) (Fig. 5b). In contrast to SPARSE, SEBS substantially underestimated  $H$  and overestimated  $LE$  for mesic forest sites (Wom, Tum), which was more significant when in-situ  $LST$  was used as input (see Fig. 5a,b). Instantaneous  $H$  and  $LE$  from STIC revealed negative bias for  $H$  ( $-35$  to  $-100 W/m^2$ ) and positive bias for  $LE$  ( $6$ – $72 W/m^2$ ) for the arid and semi-arid ecosystems (except Dry), and a negative bias was found for both  $H$  and  $LE$  at the mesic ecosystems (MBE values between  $-21$  and  $-85 W/m^2$ ) (Fig. 5a,b). The results of STIC for the two savanna sites (Dry and DaS) were comparable to those of the other two models (negative bias for  $LE$ ). The overall performance of STIC was comparable to SPARSE, although



**Fig. 6.** Kling-Gupta efficiency (KGE) of SPARSE (parallel version, retrieval mode), SEBS and STIC models for instantaneous (a)  $H$  and (b)  $LE$  retrievals at satellite overpass times (MODIS Aqua and Terra) for nine sites of contrasting aridity in Australia using MODIS  $LST$  and in-situ  $LST$  as input. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



**Fig. 7.** Box-and-whisker plots showing seasonal variations of (a)  $r_{aM}$  simulated with the parallel version of the SPARSE model, (b)  $r_{aM}$  simulated with the SEBS model and (c)  $r_{aH}$  simulated with the STIC model using MODIS  $LST$  as input for three sites ( $z = 10$  m (Cpr),  $z = 15$  m (Gin),  $z = 70$  m (Tum)) of contrasting aridity in Australia. Note the different ranges of y-axis.

the mean bias for STIC was lower for arid and semi-arid sites but higher for the mesic forest sites.

KGE statistics for  $H$  and  $LE$  showed comparable values for SPARSE and STIC ( $KGE > 0.5$ ) that exceeded those of SEBS for the mesic sites (Fig. 6a,b). All KGE values were positive for  $H$  for the arid and semi-arid sites (Fig. 6a), while most values were negative for  $LE$  (Fig. 6b), which can be explained by the different magnitudes of  $H$  and  $LE$  at these sites (see Section 4.3). As the magnitude of  $H$  is large compared to  $LE$  under water-limited conditions, a small relative model error in  $H$  will propagate into a large relative error in  $LE$  (Payero et al., 2006) (see also MAPE values in Tables A1-A6). Although SPARSE results indicated positive KGE values for  $H$  ( $>0.2$ ) (Fig. 6a), very low and negative KGE (Fig. 6b) were found for  $LE$  at most of the arid and semi-arid sites. The KGE of SEBS for  $H$  ( $LE$ ) in the mesic sites varied between  $-0.16$  and  $0.67$  ( $0.08$  and  $0.75$ ). For the semi-arid sites, instantaneous  $H$  ( $LE$ ) by SEBS was simulated with moderate accuracy ( $KGE > 0.45$  ( $0.3$ )) and no major improvement in  $LE$  was found with in-situ  $LST$ . STIC revealed positive KGE values ( $>0.45$ ) for  $H$  at all sites, and for  $LE$  positive KGE values were also found at nearly all sites with MODIS  $LST$ , being highest for the mesic sites ( $0.53$ – $0.84$ ).

In general, the overestimation of  $LE$  coincided with a comparable underestimation of  $H$  suggesting that the impact of  $\phi$  obtained with SPARSE on the  $LE$  model bias was of minor importance. The overall performance of the three models to estimate instantaneous  $LE$  was substantially improved for sites with lower aridity, as indicated by KGE,

RMSE, MBE, MAPE and  $R^2$  values (Tables A1-A6) (except SEBS statistics for Wom and Tum). Moreover, forcing the models with in-situ  $LST$  did not yield any substantial improvement in the model performances at arid and semi-arid sites.

#### 4.2. Seasonal variations

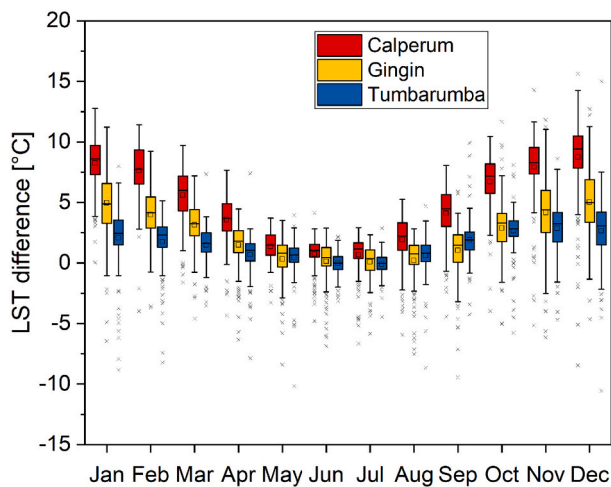
Results in Sections 4.2–4.4 focus on three sites in south, south-western, and southeastern Australia, namely Calperum (Cpr), Gingin (Gin) and Tumberumba (Tum), representing arid (Cpr) to semi-arid (Gin) and mesic (Tum) conditions.

##### 4.2.1. Seasonal variations of $r_{aM}$ and $r_{aH}$

The simulation of  $r_{aM}$  by SPARSE (Fig. 7a) showed an interquartile range (IQR) between 4 and 36 s/m and revealed a distinct difference in magnitude by a factor of two to three across sites, particularly during the dry season (Oct-Dec and Jan-Mar). The highest  $r_{aM}$  was found at Cpr as compared to the other sites, except during the wet season (Jun-Jul) when the difference between sites was less pronounced (Fig. 7a). Moreover, a strong inter-annual variation was found for all three sites. The largest values of  $r_{aM}$  were simulated during the wet season.

To gain more insight into the role of momentum transfer for SEBS,  $r_{aM}$  was calculated from  $r_{aH}$  (Table 1) according to Eqs. (3) and (4). Simulated  $r_{aM}$  by SEBS were lower than the  $r_{aM}$  of SPARSE, except during the wet season at Tum (Fig. 7b). SEBS  $r_{aM}$  exhibited an IQR between 14





**Fig. 8.** Box-and-whisker plots showing seasonal variations of the difference between MODIS *LST* and in-situ *LST* ( $\Delta LST$ ) for three sites of contrasting aridity in Australia. MODIS Terra and Aqua *LST* are combined in the analysis. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

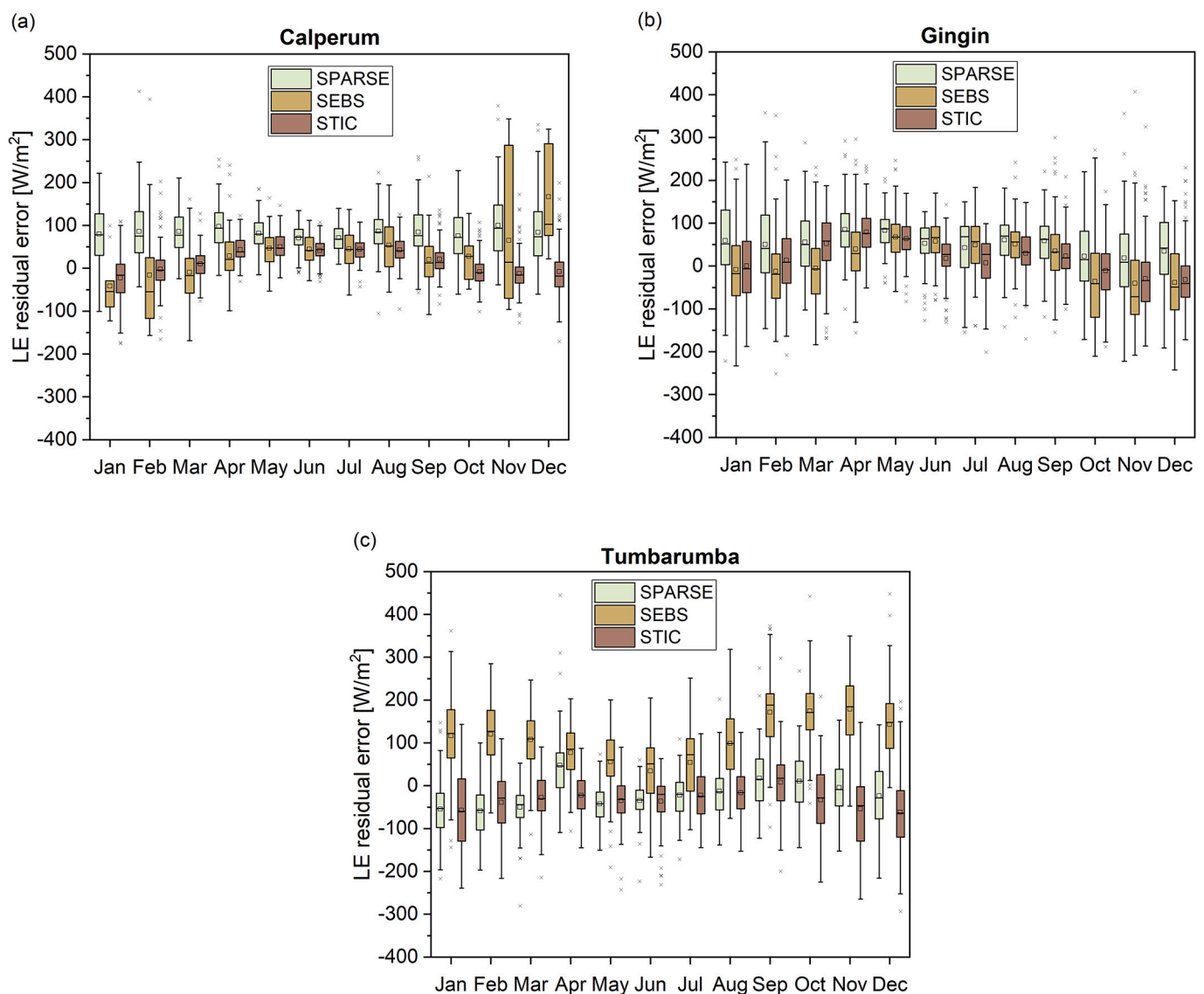
and 25 s/m for Cpr and between 6 and 14 s/m for Gin, with a marked seasonal variation. However,  $r_{aM}$  featured a stronger seasonality at Tum, with values mainly ranging between 3 and 90 s/m (IQR). Extremely high values were simulated for June and July (wet season) (Fig. 7b), when periods of a highly stable boundary layer under cloudy and misty conditions occur frequently.

As STIC derives an analytical solution of  $r_{aH}$  (Mallick et al., 2015, 2018a), the nature of  $r_{aH}$  simulated by STIC is different to that of SEBS (Table 1) and the retrieval of  $r_{aM}$  is not straightforward in STIC. Furthermore, the  $r_{aH}$  of STIC is not influenced by corrections involving the  $kB^{-1}$  factor because STIC directly computes the aerodynamic temperature (Mallick et al., 2016). STIC  $r_{aH}$  (Fig. 7c) also indicated substantial seasonality with an IQR between 20 and 120 s/m. Although the seasonal pattern of STIC  $r_{aH}$  is comparable to SPARSE, across site variation in simulated  $r_{aH}$  is lower for STIC as compared to  $r_{aM}$  of the other two models. The highest and lowest  $r_{aH}$  values are estimated for Cal and Tum, respectively.

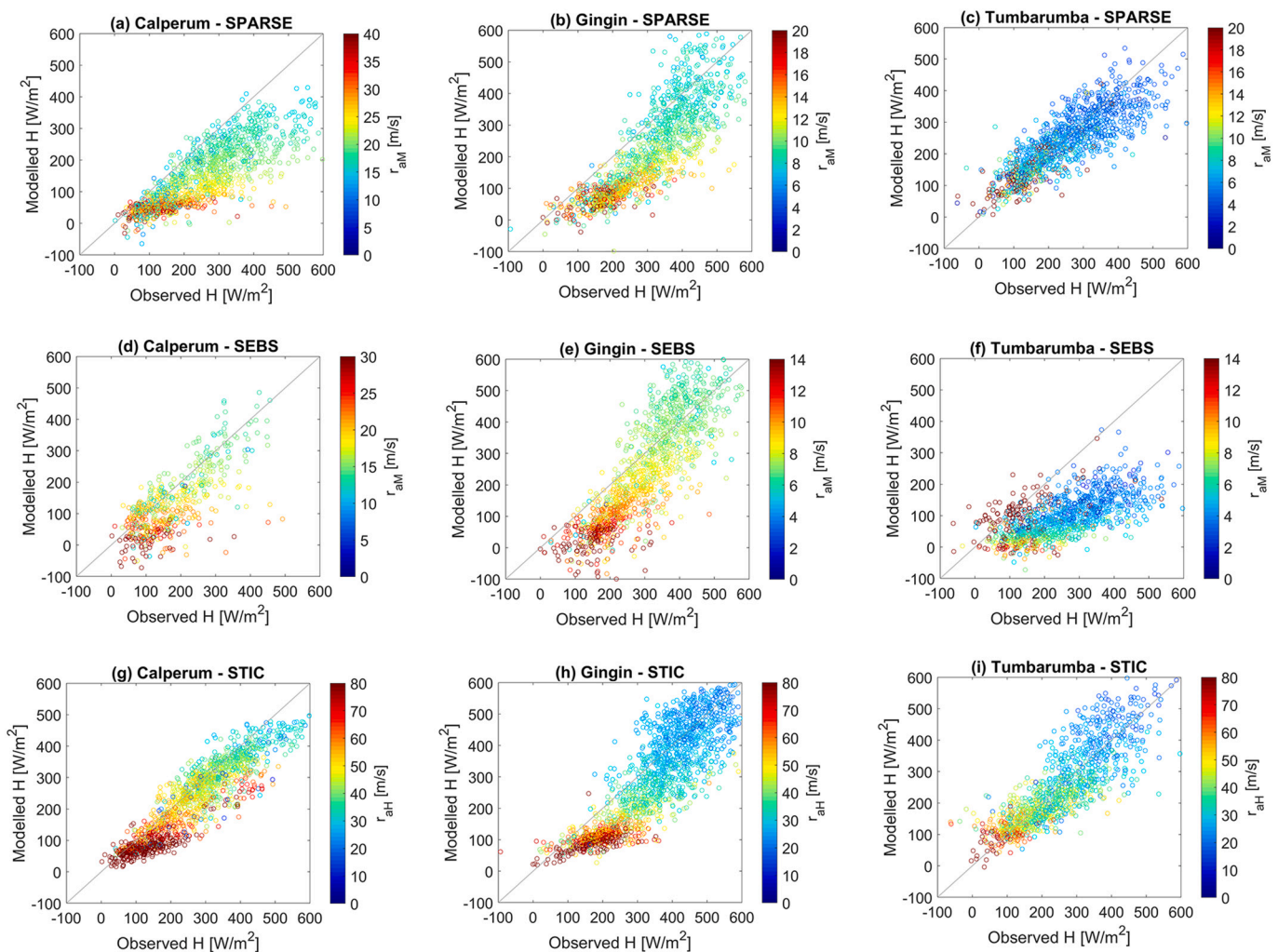
#### 4.2.2. Seasonal variations of the LST difference

The *LST* difference ( $\Delta LST$ ) (= MODIS *LST* – in-situ *LST*) is used as a proxy for the potential bias in MODIS *LST*. The relationship of  $\Delta LST$  to the *LE* residual error is compared to that of  $r_{aM}$  ( $r_{aH}$ ) in the following sections of the paper.

The seasonal variation of  $\Delta LST$  (Fig. 8) showed positive median  $\Delta LST$



**Fig. 9.** Box-and-whisker plots showing seasonal variations of the *LE* residual error (difference between modelled and observed *LE*) for SPARSE (parallel version), SEBS and STIC using MODIS *LST* as input at three sites of contrasting aridity in Australia (a) Calperum, (b) Gingin and (c) Tumbarumba.



**Fig. 10.** Scatter plots of modelled  $H$  versus observed  $H$  color-coded with  $r_{aM}$  for SPARSE (a-c), SEBS (d-f) and  $r_{aH}$  for STIC (g-i) for the representative arid (Cpr), semi-arid (Gin), and mesic (Tum) sites using MODIS  $LST$  as input to simulate  $H$  with the three models. Regression statistics are presented in [Tables A1, A3 and A5](#).

(1–10 °C), indicating MODIS  $LST$  to be higher than the in-situ values across all sites. This exceedance was most pronounced and had the largest seasonality for the arid site (Cpr) and declined with decreasing aridity (Gin and Tum, [Table 2](#)). The differences scaled with air temperature for each site (not shown for brevity) and were largest for the summer dry season (often  $> +5$  °C at Cpr and Gin), when soil moisture was extremely low ( $SWC < 5\%$ ). Differences were close to zero at Gin and Tum during the winter wet season (mainly June to August), when frequent precipitation causes increased soil moisture and when air temperature is at a minimum. In-situ  $LST$  exceeded MODIS  $LST$  only occasionally, mainly during the winter wet season. The lower  $\Delta LST$  during the wet season coincided with high  $r_{aM}$  and  $r_{aH}$  (see [Fig. 7](#)).

#### 4.2.3. Seasonal variations of the $LE$ residual error

The seasonal variation of the  $LE$  residual error revealed lowest values (median within  $-40$  and  $75$   $W/m^2$ ) and the lowest IQR ( $-75$  to  $100$   $W/m^2$ ) during the wet season for all three contrasting sites and all three models ([Fig. 9a-c](#)). As indicated by a large IQR, the variation of the  $LE$  residual error was highest during the dry season, ranging between  $280$   $W/m^2$  for SEBS at Cpr and  $-140$   $W/m^2$  for STIC at Tum. In general, the one-source models SEBS and STIC revealed the tendency to overestimate  $LE$  during the wet season and underestimate  $LE$  during the dry season at the water-limited sites (Cpr and Gin) ([Fig. 9a,b](#)). In contrast, SPARSE showed a consistent overestimation tendency of  $LE$  in nearly all months at Cpr and Gin, while in Tum the median residual error was often close to

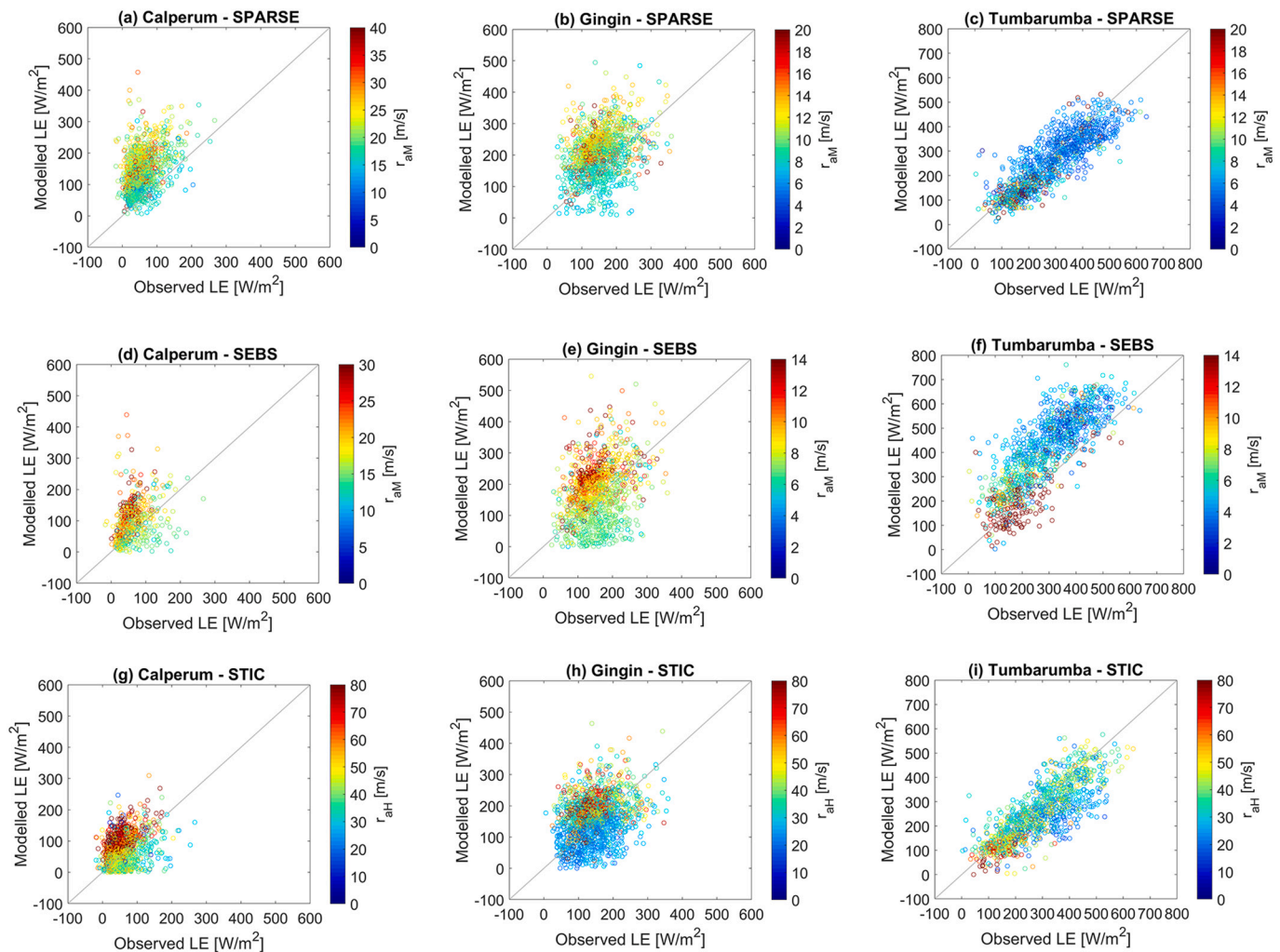
zero ([Fig. 9c](#)). STIC mainly underestimated  $LE$  in Tum during the dry season (IQR  $-140$  to  $25$   $W/m^2$ ), whereas SEBS showed a substantially large positive  $LE$  residual (IQR  $25$  to  $230$   $W/m^2$ ). Overall, for this mesic forest site, the largest variation amongst model results was found.

To summarize, turbulent transfer was lowest at the arid woodland site (Cpr) and highest at the mesic forest site (Tum), which is partly attributed to the different measurement heights ([Fig. 7](#)). [Figs. 7 and 8](#) reveal that a high  $\Delta LST$  coincided with low  $r_{aM}$  and  $r_{aH}$  during the dry season. The low or partly negative  $\Delta LST$  during the wet season coincided with an overestimation of  $LE$  at water-limited sites ([Fig. 9](#)).

#### 4.3. Dependency of the $H$ and $LE$ residual errors on $r_{aM}$ ( $r_{aH}$ ) and $LST$

Results for SPARSE in [Fig. 10a,b](#) and [Fig. 11a,b](#) indicate that underestimation of  $H$  and overestimation of  $LE$  is related to the magnitude of  $r_{aM}$  for the arid and semi-arid sites (Cpr and Gin). Underestimation (overestimation) of  $H$  ( $LE$ ) predominantly occurred at high  $r_{aM}$  (i.e., low wind speed), while a good agreement between modelled and observed  $H$  ( $LE$ ) or a slight overestimation (underestimation) was observed for low  $r_{aM}$  (i.e., high wind speed). This is indicated by values with high  $r_{aM}$  falling below (above) the 1:1 line and those with low  $r_{aM}$  falling close to or along the line in [Fig. 10a,b](#) and [Fig. 11a,b](#). This dependency was not visible in the mesic forest site (Tum), where no systematic over/underestimation was found ([Fig. 10c, 11c](#)).

The results of SEBS and STIC for the water-limited sites (Cal and Gin)



**Fig. 11.** Scatter plots of modelled  $LE$  versus observed  $LE$  color-coded with  $r_{aM}$  for SPARSE (a-c), SEBS (d-f) and  $r_{aH}$  for STIC (g-i) for the representative arid (Cpr), semi-arid (Gin), and mesic (Tum) sites using MODIS LST as input to simulate  $LE$  with the three models. Regression statistics are presented in Tables A2, A4 and A6.

revealed comparable patterns as found for SPARSE (Figs. 10d,e,g,h and 11d,e,g,h), although the  $LE$  underestimation for low  $r_{aM}$  and  $r_{aH}$  was more pronounced compared to SPARSE. At Tum, a minor dependency on  $r_{aM}$  was evident for SEBS (Figs. 10f and 11f), in which predominant underestimation (overestimation) of  $H$  ( $LE$ ) was found at low  $r_{aM}$  (i.e., high wind speed), in contrast to the pattern at the water-limited sites. This suggests that the substantial  $LE$  overestimation by SEBS at Tum is not caused by uncertainties in  $r_{aM}$ . For STIC, the dependency on  $r_{aH}$  was negligible at the mesic site (Tum) (Figs. 10i and 11i). Comparable patterns were found for the other sites listed in Table 2 (see Appendix, Fig. A1). The  $LE$  residual error for the semi-arid grassland site in northern Australia (Stp) also showed a strong relationship to  $r_{aM}$  and  $r_{aH}$  (see Fig. A1g,h,i). The dependencies on  $r_{aM}$  ( $r_{aH}$ ) were not significantly reduced when models were constrained with in-situ LST (see Appendix, Fig. A5, Tables A1-A6).

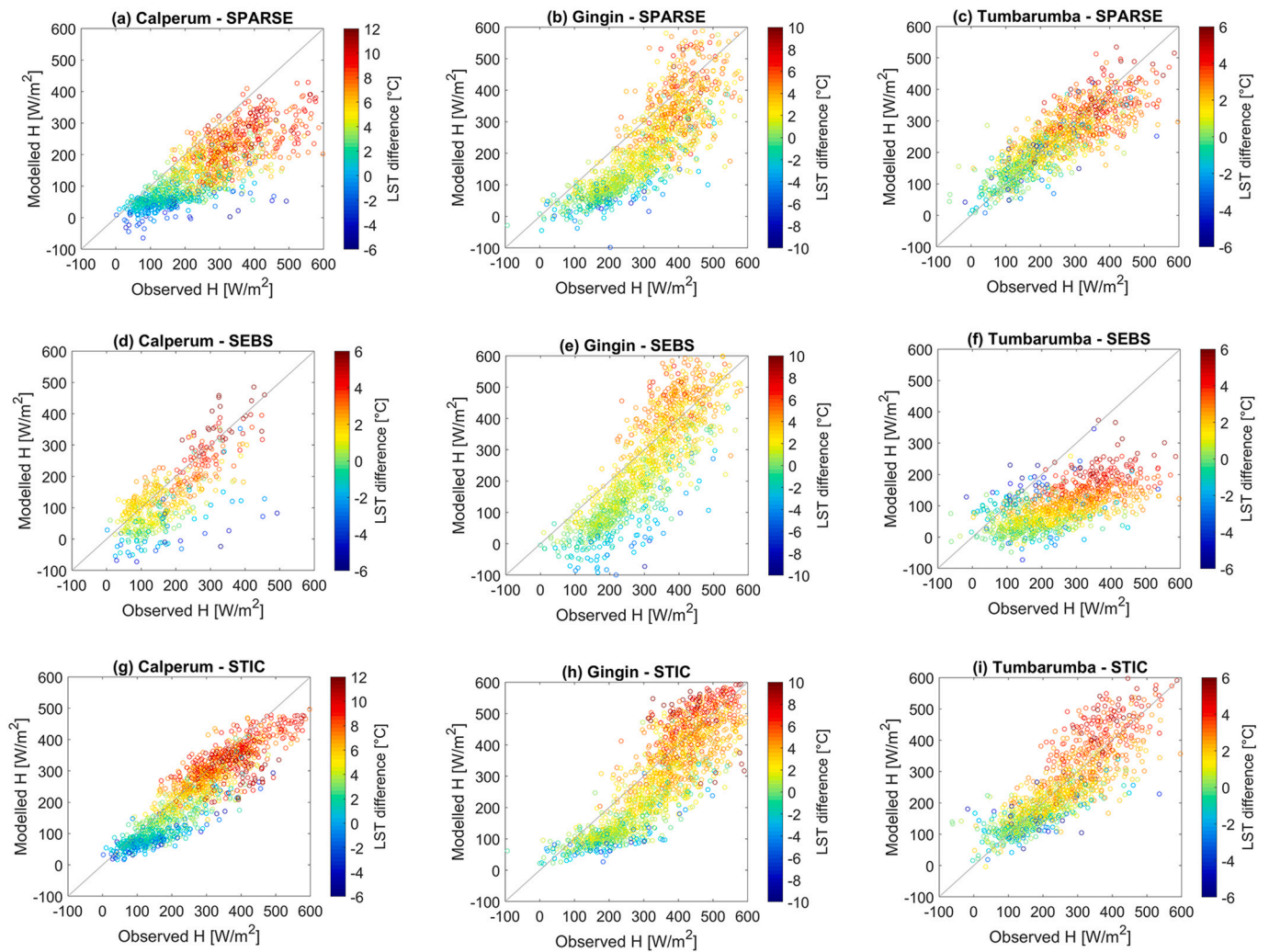
$H$  was slightly overestimated and  $LE$  was underestimated by all the three models at the water-limited sites (Cpr and Gin) when the difference between MODIS and in-situ LST was very high (Figs. 12 & 13 a,b,d, e,g,h). On the other hand, the underestimation (overestimation) of  $H$  ( $LE$ ) at these sites was largely associated with a  $\Delta LST$  near or below zero. For the mesic forest site (Tum), no substantial dependency on  $\Delta LST$  was observed for SPARSE (Figs. 12c and 13c), but the findings for SEBS and STIC were contrasting (Figs. 12f,i and 13f,i), i.e., a high  $\Delta LST$  coincided with underestimation (overestimation) of  $H$  by SEBS (STIC) and vice versa for  $LE$ . Similar findings from all models are confirmed for the other

sites presented in the Appendix (Fig. A2).

#### 4.4. Regression analysis

In order to substantiate our findings from the previous sections, the relationship between the residual error of  $LE$  as final model output and a host of variables (see Section 2.3) was investigated by performing a PLSR analysis (Fig. 14). These variables and corresponding modelled  $LE$  signals were clustered for each set of arid, semi-arid and mesic sites (Table 2). If the Variable Importance in Projection (VIP) score exceeds a value of 0.8, the variable plays an important role in determining the  $LE$  residual error. The results indicated that for all models  $\Delta LST$ ,  $r_{aM}$  (or  $r_{aH}$ ),  $VPD$  and  $F_c$  had a major impact on the  $LE$  residual error (Fig. 14). The influence of modelled  $\Phi$  on the  $LE$  residuals was of minor importance for SPARSE, but was important for SEBS (mesic sites) and for STIC (all sites). A detailed evaluation of the accuracy of modelled  $\Phi$  with SPARSE is presented in the Appendix (Fig. A3).

The most significant contribution of  $r_{aM}$  and  $r_{aH}$  to the residual  $LE$  error was found at the semi-arid sites, where it exceeded the influence of  $\Delta LST$  for SPARSE and STIC (Fig. 14b,h). Interestingly, for SEBS, the role of  $kB^{-1}$  was found to be one of the major determinants in controlling the residual  $LE$  error in the water-limited ecosystems (VIP = 1.1 to 1.2) (Fig. 14d,e) in addition to the critical impact of  $r_{aM}$  in semi-arid ecosystems. The role of  $r_{aM}$  or  $r_{aH}$  on model uncertainty was greatly diminished at the mesic ecosystems as shown in Fig. 14 (c,f,i). Overall,



**Fig. 12.** Scatter plots of modelled  $H$  versus observed  $H$  color-coded with the difference between MODIS  $LST$  and in-situ  $LST$  ( $\Delta LST$ ) for SPARSE (a-c), SEBS (d-f) and STIC (g-i) for the representative arid (Cpr), semi-arid (Gin), and mesic (Tum) sites using MODIS  $LST$  as input to simulate  $H$  with the three models. For SEBS, omission of data with high  $LST$  values due to the dry limit required a different scaling of the  $\Delta LST$  color bar for the site Cpr. Regression statistics are presented in Tables A1, A3 and A5.

the dependency of  $LE$  bias on  $r_{aM}$  in the water-limited ecosystems was slightly larger for the two-source model SPARSE as compared to the one-source models SEBS and STIC ( $r_{aH}$ ), which is also reflected in the PLSR results for  $H$  (Fig. A4).

## 5. Discussion

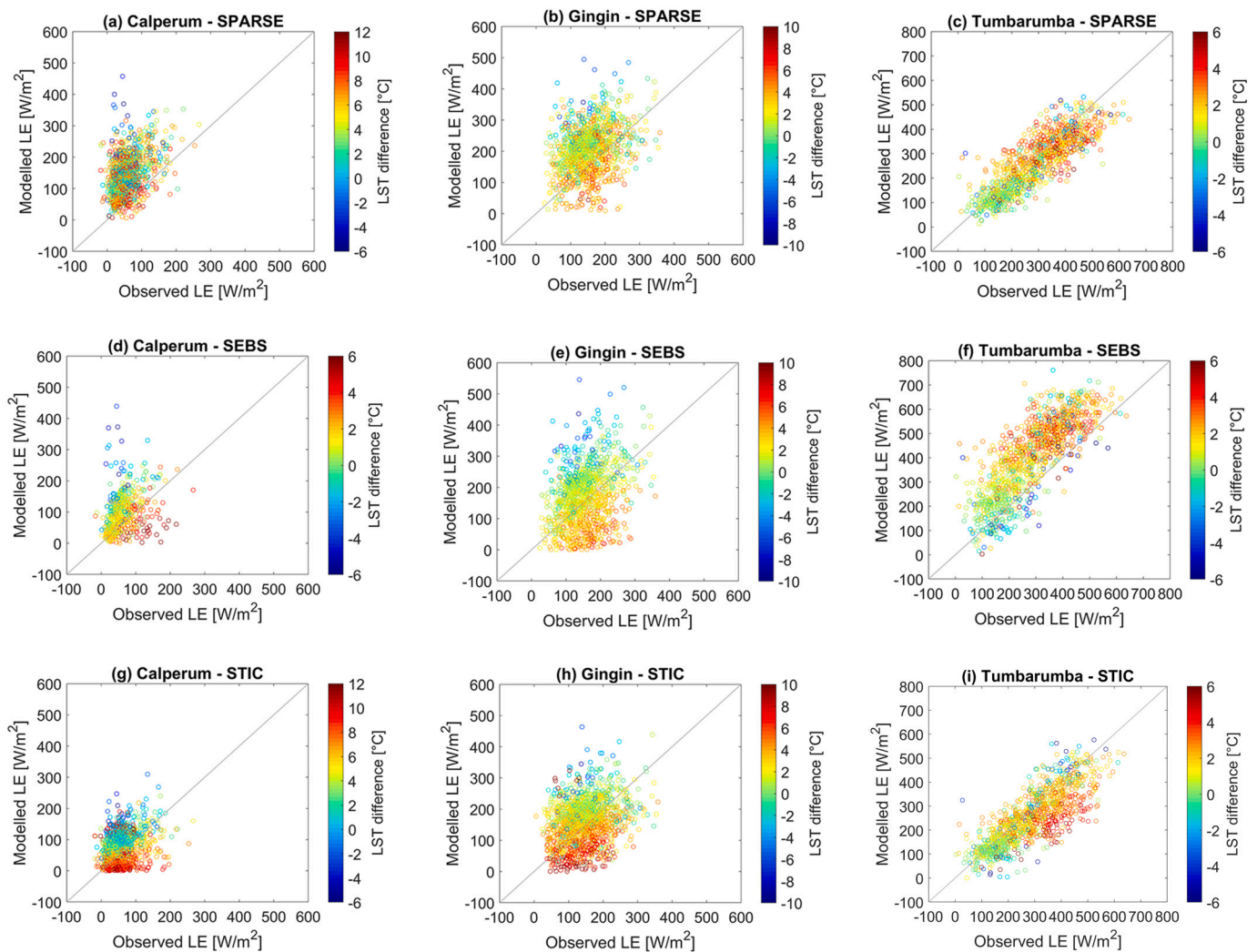
In general, our results at the water-limited sites provided support for our hypothesis, revealing that the influence of  $r_{aM}$  ( $r_{aH}$ ) on the instantaneous  $LE$  error is high in these ecosystems, where it can potentially be as large as the influence of uncertainties in  $LST$  (Fig. 14). Overestimation of  $LE$  by the models at the water-limited sites was found to coincide with high  $r_{aM}$  or  $r_{aH}$  (Fig. 7a,b, Fig. 9a,b) and is caused by an underestimation of  $H$ , which substantiates previous findings (Gokmen et al., 2012; Gokool et al., 2020; Morillas et al., 2013; Pardo et al., 2014; Seneviratne et al., 2010; van der Kwast et al., 2009). This reveals the tendency of underestimation (overestimation) of  $H$  ( $LE$ ) under low wind speeds resulting in high  $r_{aM}$  or  $r_{aH}$  (predominantly between June and August, see Fig. 7). Under such conditions  $\Delta LST$  was near zero or slightly negative (Fig. 8, Figs. 12 & 13), which implies that the substantial positive difference between MODIS  $LST$  and in-situ  $LST$  did not explain the positive model bias in  $LE$ . Instead, the positive  $\Delta LST$  caused a slight overestimation of  $H$ , and, subsequently underestimation of  $LE$  at the

water-limited sites (Figs. 12 & 13), prevailing mainly during the dry season (Fig. 8 & Fig. 9a,b).

In contrast, mesic forest sites (Tum and Wom) showed either no underestimation (overestimation) of  $H$  ( $LE$ ) (SPARSE and STIC) or the observed  $H$  underestimation ( $LE$  overestimation) indicated negligible dependency on  $r_{aM}$  or  $r_{aH}$  (SEBS), rejecting our hypothesis for these ecosystems. These ecosystems receive higher rainfall and have lower potential evaporative demand while retaining soil moisture more efficiently than sparse vegetation and grassland of arid and semi-arid ecosystems, which results in substantially higher SWC (Griebel et al., 2016; van Gorsel et al., 2016). Additionally,  $LST$  of forests is lower due to transpiration induced cooling, high surface roughness and strong turbulent mixing shown by low  $r_{aM}$  (Fig. 7) (Panwar et al., 2020).

### 5.1. Comparison of $r_{aM}$ between SPARSE and SEBS

In general,  $r_{aM}$  ( $r_{aH}$ ) cannot be directly measured in the field and is considered as an unobserved variable. In-situ  $r_a$  values are also obtained from friction velocity (or wind speed) and using MOST and Richardson number approaches (Banerjee et al., 2017; Liu et al., 2007), typically involving a constant  $kB^{-1}$  factor of two. Consequently, depending on the applied parameterization the “observed”  $r_{aM}$  or  $r_{aH}$  would be either comparable or different to the modelled  $r_{aM}$  or  $r_{aH}$ . Hence, in order to



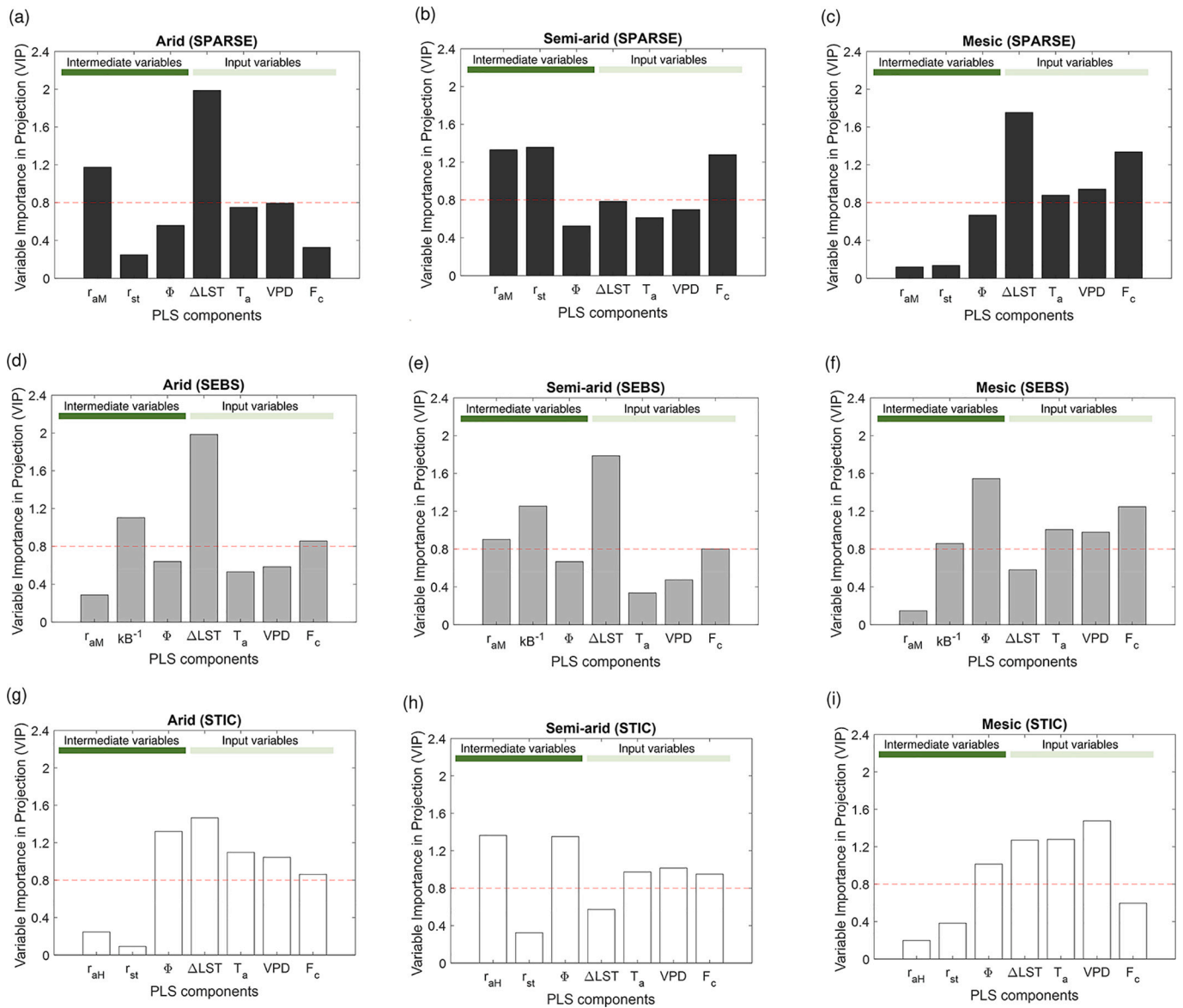
**Fig. 13.** Scatter plots of modelled  $LE$  versus observed  $LE$  color-coded with the difference between MODIS  $LST$  and in-situ  $LST$  ( $\Delta LST$ ) for SPARSE (a-c), SEBS (d-f) and STIC (g-i) for the representative arid (Cpr), semi-arid (Gin), and mesic (Tum) sites using MODIS  $LST$  as input to simulate  $LE$  with the three models. For SEBS, omission of data with high  $LST$  values due to the dry limit required a different scaling of the  $\Delta LST$  color bar for the site Cpr. Regression statistics are presented in Tables A2, A4 and A6.

coherently identify the structural uncertainties of the models, their computed  $r_{aM}$  values were compared between each other. As the estimation of  $r_{aH}$  in STIC is different from the methods applied in SPARSE and SEBS (Table 1), the computation of  $r_{aM}$  from STIC is not straightforward. Therefore, we only compared the  $r_{aM}$  derived by SPARSE and SEBS (see Eqs. (3) and (4)). Fig. 15a,b shows that SEBS computes lower  $r_{aM}$  values than SPARSE for the water-limited sites (Cpr and Gin). Relatively good agreement between the two models was found at high wind speeds (falling nearly along the 1:1 line in Fig. 15a,b) when mechanical turbulence production dominates (near-neutral conditions). However, large discrepancies under unstable conditions (Fig. 15, datapoints falling below the 1:1 line) are attributed to the different approaches to account for atmospheric stability in the two models. In contrast,  $r_{aM}$  estimates from the two models for the mesic site (Tum) compared relatively well (except some outliers, Fig. 15c).

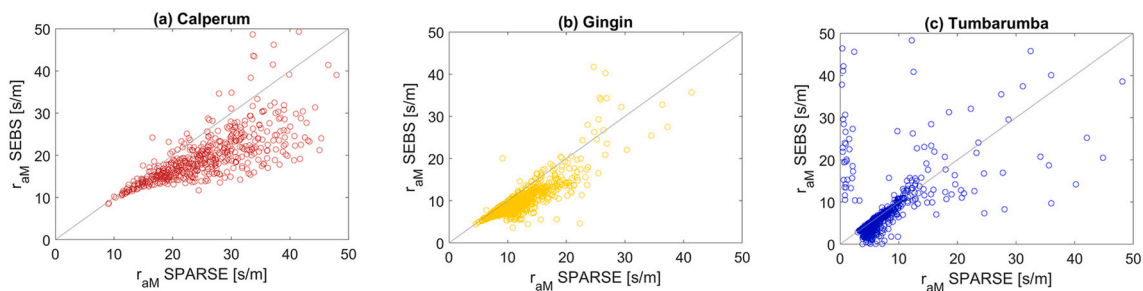
The stability correction term in  $r_{aM}$  is determined as a function of the Monin-Obukhov length scale ( $L$ ) in SEBS (Brutsaert, 1992, 1999) and by the bulk Richardson number ( $R_{ib}$ ) in SPARSE (Boulet et al., 2015) (Table 1). Both are computed through iteration either using  $H$  or aerodynamic temperature ( $T_0$ ), which directly depend on  $LST$  that strongly determines the buoyancy production near the surface. Accurate quantification of buoyant versus mechanical turbulence production

influences the stability correction and the magnitude of  $r_a$ . Hence, in both models,  $r_{aM}$  and  $LST$  are intrinsically linked through the stability correction term and aerodynamic feedbacks on  $T_0$ ,  $T_a$  and  $H$ . Although the discrepancies in  $r_{aM}$  between SPARSE and SEBS in Fig. 15 do not quantitatively explain the overestimation of  $LE$  by both models, it indicates substantial uncertainty associated with the empirical specification of  $r_{aM}$  that influences the model performance.

Additionally, seasonal effects on  $r_{aM}$  (Fig. 7) largely control the uncertainty in  $LE$ . During the winter wet season at Cpr and Gin, synoptic weather systems cause low wind speed conditions, thereby enhancing  $r_{aM}$  and the influence of the atmospheric stability correction terms. During winter, the subtropical ridge is at its northernmost position, away from southern Australia (Cai et al., 2011a), and subsidence on the western pole of the Southern Ocean reduces convection over Australia (Cai et al., 2011b), both of which thrust the southern Australian region into a calm wet season with low winds. Seasonal variations in SWC and humidity can also influence  $r_{aM}$  and stability in other arid or semi-arid locations (Cleverly et al., 2013). By example, at Cpr and Gin, SWC is always below 10% during wet and dry seasons, which limits evaporative cooling of the surface. In combination with low wind speeds, surface heating is intense and causes a strong surface layer stratification (Sun et al., 2020), which is not well represented by the stability correction



**Fig. 14.** Bar plots of the Variable Importance in Projection (VIP) scores for the residual error of  $LE$  involving  $r_{aM}$ ,  $r_{aH}$ ,  $KB^{-1}$  (SEBS), the stomata resistance ( $r_{st}$ ) (SPARSE & STIC), modelled  $\phi$  with SPARSE,  $LST$  difference ( $\Delta LST$ ), air temperature ( $T_a$ ), vapor pressure deficit (VPD) and  $F_c$  for SPARSE (a-c), SEBS (d-f) and STIC (g-i) for all the arid sites (clustered), semi-arid sites (clustered) and mesic sites (clustered) using MODIS  $LST$  as input to run the models. The dashed red line (VIP = 0.8) denotes the variable importance threshold. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



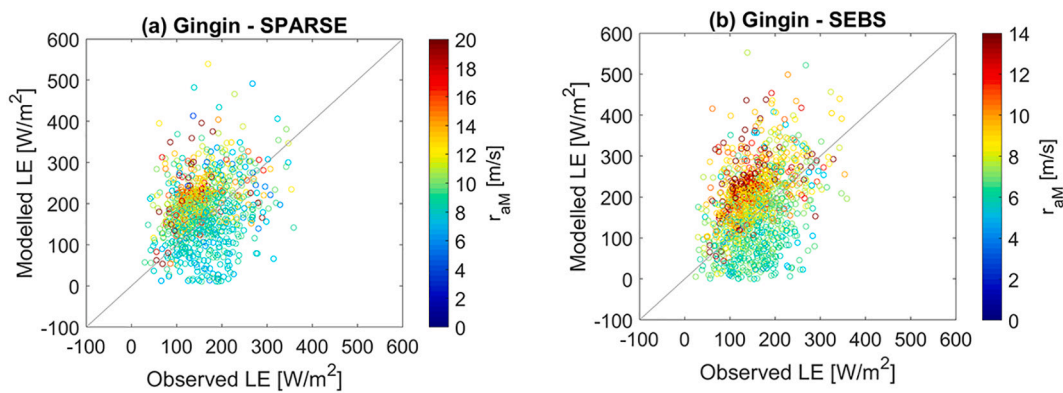
**Fig. 15.** Scatter plots of  $r_{aM}$  estimated by SEBS versus  $r_{aM}$  estimated by SPARSE for (a) Calperum, (b) Gingin and (c) Tumbarumba using MODIS  $LST$  as input to run the models.

terms. The identified differences in  $r_{aM}$  for both formulations are even higher in the shrubland and savanna ecosystems (ASM, Dry, DaS, not shown), at which, however, a negative bias in modelled  $LE$  was found for SEBS (Fig. 5).

## 5.2. Significance of model results

### 5.2.1. Empirical aerodynamic roughness parameters

The accurate representation of the aerodynamic parameters ( $z_{0m}$  and



**Fig. 16.** Scatter plots of modelled  $LE$  versus observed  $LE$  color-coded with  $r_{aM}$  for (a) SPARSE and (b) SEBS at the semi-arid site Gingin using MODIS  $LST$  and  $d = 2.5$  m and  $z_{0m} = 0.9$  m determined from vertical wind profiles as input to simulate  $LE$ . Regression statistics SPARSE:  $KGE = -0.07$ ,  $RMSE = 103$   $W/m^2$ ,  $MBE = -30$   $W/m^2$ ,  $MAPE = 64\%$ ,  $R^2 = 0.09$ ; SEBS:  $KGE = 0.08$ ,  $RMSE = 91$   $W/m^2$ ,  $MBE = 24$   $W/m^2$ ,  $MAPE = 55\%$ ,  $R^2 = 0.11$ .

$d$ ) is a key ingredient for obtaining good model performance. Due to the seasonal variations in LAI and ecosystem structure, seasonal variation of these parameters should ideally be obtained (Zhou et al., 2012), which is, however, quite complex for sparse heterogeneous ecosystems. The application of empirical parameterizations to derive time-variant values of  $z_{0m}$  and  $d$  based on LAI (e.g., expressions from Colaizzi et al. (2004) and Pereira et al. (1999)) generally degraded the model performance of SPARSE (results not shown for brevity) and are not suitable for these specific Australian ecosystems. Likewise, time-variant aerodynamic parameters calculated by SEBS using NDVI-based canopy height, LAI and the canopy momentum transfer sub-model (Section 2.1.2) were lower than experimentally derived values and increased the  $LE$  model bias (overestimation) for the arid and semi-arid sites. For these reasons, the study was performed with constant  $d$  and  $z_{0m}$  directly derived from EC measurements for both SPARSE and SEBS (see Table 3). For comparison, the only available measured vertical profiles of horizontal wind speed at the semi-arid site Gin allowed for the direct retrieval of  $d$  and  $z_{0m}$ , which resulted in  $d = 2.2$ – $2.9$  m and  $z_{0m} = 0.9$  m (personal communication, A. Kunadi). These values are different than the values presented in Table 3. Fig. 16a,b exemplarily shows simulations with the SPARSE and SEBS models with  $d = 2.5$  m and  $z_{0m} = 0.9$  m, from which the dependency of the  $LE$  residual error on  $r_{aM}$  is also evident.

While overall regression statistics did not improve significantly compared to the model runs with the original  $d$  and  $z_{0m}$  values (see Tables A2, A4), the MBE of SEBS increased slightly and the overestimation tendency of SPARSE was reversed (MBE changed from a positive to a negative value). This demonstrates the importance of accurate aerodynamic parameters for estimating  $LE$ , which are likely different from the standard empirical parameterizations in heterogeneous sparse ecosystems (e.g.  $d < 0.6h_c$ ). They also contribute to the accuracy of the stability correction functions and may vary with LAI and wind direction, making their quantification and application in SEB models extremely challenging.

### 5.2.2. Impact of the underlying soil and understory vegetation

For the two-source model SPARSE, the formulations of soil-air and canopy-air aerodynamic resistances may play an additional role in controlling the uncertainty of  $LE$ . Previous studies reported that novel soil parameterizations and explicitly incorporating the understory aerodynamic exchange significantly improves two-source model estimates of  $H$  and  $LE$  in the sparsely vegetated ecosystems (e.g. Li et al., 2019). Haghighi and Or (2015) developed a physically based model describing a soil resistance formulation for turbulent heat transport. Results show the enhancement of evaporative fluxes from bluff-rough surfaces relative to smooth flat surfaces under similar conditions. This new scheme has been successfully applied to semi-arid ecosystems where a meaningful reduction in the SEB flux retrieval error was found

(Haghighi and Kirchner, 2017). Considering these findings, it is likely that the underestimation (overestimation) of  $H$  ( $LE$ ) by SPARSE might be partly attributed to the representation of the soil-air or understory-air aerodynamic exchange. However, our results indicate that overestimation of  $LE$  is primarily related to exchanges above the aerodynamic level ( $r_{aM}$ ) and the associated buoyancy production intensity. This is supported by the fact that although some savanna sites (e.g. DaS) have sparse tree cover and substantial fluctuation in LAI between the dry and wet seasons (caused by dormant grass and bare soil patches) (Table 3),  $LE$  is not overestimated for these sites. On the other hand,  $H$  ( $LE$ ) is also underestimated (overestimated) substantially for the semi-arid grassland site Stp, where an understory is absent. This suggests a minor influence of the soil aerodynamic exchange parameterization of SPARSE in our study. Since the one-source models SEBS and STIC also overestimated  $LE$ , we conclude that a significant fraction of uncertainty in all models can be attributed to  $r_{aM}$  and  $r_{aH}$ .

### 5.2.3. Influence of radiometric $kB^{-1}$ in SEBS

The principal differences between observed and modelled  $LE$  of SEBS in the arid and semi-arid ecosystems are also due to  $kB^{-1}$  (Fig. 14d,e), which is a correction applied to circumvent the large differences between  $LST$  and  $T_o$  in such ecosystems. Here, the role of  $z_{0h}$  becomes critical, which is estimated empirically through the  $kB^{-1}$  factor (Paul et al., 2014). Despite the first order dependence of  $kB^{-1}$  on  $LST$ , radiation, and meteorological variables, no physical model of  $kB^{-1}$  is available (Paul et al., 2014; Bhattarai et al., 2018) and uncertainties in  $kB^{-1}$  estimation are propagated into  $z_{0h}$ . Overestimation (or underestimation) of  $z_{0h}$  would lead to an overestimation (underestimation) of  $r_{aH}$  in SEBS, which is reflected in the  $LE$  residual error. Bhattarai et al. (2018) obtained a logarithmic pattern and significant correlation between the  $LE$  residual error and  $kB^{-1}$ .

The underestimation (overestimation) of  $H$  ( $LE$ ) by SEBS for the mesic forest sites Wom and Tum might be associated with an overestimation of  $kB^{-1}$  and more specifically the canopy fraction of the  $kB^{-1}$  factor (Chen et al., 2019a). Chen et al. (2019a, 2019b) suggested that the overestimation of  $kB^{-1}$  for forest canopies in SEBS can be overcome by an improved column canopy-air turbulent transfer model that accounts for the momentum and heat transfer efficiency in different canopy vertical layers. While modification of the SEBS model is out of the scope of this study, this finding warrants future investigation using the SEBS model with an improved  $kB^{-1}$  parameterization for forest canopies.

### 5.2.4. $LST$ uncertainties

Water-limited ecosystems are more prone to mismatch of tower flux footprint and hemispherical radiometric footprint due to their heterogeneous vegetation composition as compared to the mesic ecosystems (Marcolla and Cescatti, 2018; Morillas et al., 2013; Vivoni et al., 2010).

We postulate that neither in-situ *LST* nor MODIS *LST* is representative of the EC footprint as in-situ *LST* is typically measured by longwave radiation sensors directly mounted at the tower at the same or at a lower level than the EC measurements. Consequently, the origin of the radiation signal is not representative of the total EC flux footprint (Marcolla and Cescatti, 2018). Although the selected Australian ecosystems are reasonably homogeneous within a distance of 1 km to the tower, MODIS *LST* and in-situ *LST* were often different, especially for arid and semi-arid ecosystems with sparse vegetation during the dry season (Fig. 8). Flux towers are generally shorter in these ecosystems (lower vegetation height) as compared to forests, and, thus shorter towers lead to smaller footprints of the net radiometer. Moreover, different MODIS viewing configurations at sites with large heterogeneity as well as atmospheric corrections may contribute to the discrepancies (Chen et al., 2017).

An additional reason for the discrepancy between MODIS and in-situ *LST* could be the surface emissivity values calculated by Eq. (5). In general, the derived values compared relatively well to MODIS broadband emissivities (ranging from 0.972 for arid heterogeneous sites to 0.983 for forests), which, however, do not represent seasonal variations. The dependency of soil emissivity on soil moisture and soil geological properties was not taken into account, and assuming that soil emissivity used in Eq. (5) could potentially be lower than 0.96 in shrubland and woodland ecosystems with high aridity (Jin and Liang, 2006), higher in-situ *LST* values would be derived which reduces the discrepancy with MODIS *LST*.

Given the absence of major improvements in the model results with in-situ *LST*, it appears that uncertainties in the empirical characterization of  $r_{aM}$  and  $r_{aH}$  tend to contribute substantially to the uncertainty in both SPARSE and SEBS. On the contrary, the theoretical assumptions in STIC, particularly the linearity of saturation vapor pressure versus temperatures to compute the psychrometric slopes and symmetrical assumptions in the advection-aridity hypothesis to obtain the closure equation of evaporative fraction tend to be the main source of uncertainty propagation in *LE* through  $r_{aH}$  (Mallick et al., 2015, 2016).

### 5.2.5. Accuracy of flux measurements

Another important aspect of our analysis is that the typical measurement error for *LE* of about 30 W/m<sup>2</sup> (Foken, 2017; Novick and Katul, 2020) is large compared to its absolute value in water-limited ecosystems. This introduces some uncertainty in our findings, as the accuracy of the EC method to derive *LE* is limited under these dry conditions when *H* is the dominating flux. Differences between modelled and observed *LE* may be partly attributed to the BREB-closure correction of *LE* observations. Mean values of the SEB closure at MODIS Terra and Aqua overpass times ranged from 74% to 93% (Table 3), which is comparable to values typically reported in the literature (Mauder et al., 2020). Mallick et al. (2018a) demonstrated that in the arid and semi-arid ecosystems, major corrections are generally observed in *H*, whereas correction in *LE* is negligible. Their study revealed significant correlations between the *LE* error statistics and BREB-closure corrections. In most of the arid and semi-arid sites, high MAPE and systematic RMSE in *LE* (>50%) was associated with low closure correction in *LE* (Mallick et al., 2018a).

### 5.2.6. Effect of modelled net available energy

Modelled  $\phi$  by SPARSE was slightly underestimated for most of the sites with MBE ranging from -40 W/m<sup>2</sup> (Tum) to -22 W/m<sup>2</sup> (Cal and DaS) (Fig. A3). Stp was the only site for which a small overestimation of  $\phi$  was found (MBE = 21 W/m<sup>2</sup>). In general, underestimation of  $\phi$  causes underestimation of *LE* (Figs. 4-6), which diminishes the effects of the underestimation of *H* due to high  $r_{aM}$  and  $r_{aH}$ . For SPARSE, modelled  $\phi$  did not significantly contribute to the *LE* residual error, while for SEBS  $\phi$  strongly influenced the *LE* residual error of mesic ecosystems (Fig. 14f). Due to the nature of the evaporative fraction equation in SEBS (see Section 4), the difference between  $\phi$  and modelled *LE* was marginal near the wet limit, which resulted in a substantial underestimation of *H* at the forest sites Wom and Tum (Fig. 5a, Fig. 10f). Any condition that

produces  $H \approx H_{wet}$  would tend to simulate substantially high relative evaporation ( $\Lambda_r \approx 1$ ) and *LE* will be consequently overestimated. Mallick et al. (2018b) reported a systematic linear relationship between the residual daily ET error with daily  $\Lambda_r$ .

Results obtained with STIC indicated strong influence of  $\phi$  on the *LE* residual error for all ecosystem types, which was comparable to the impact of  $r_{aH}$  for semi-arid ecosystems. The more predominant role of  $\phi$  in STIC can be explained by its use for the calculation of  $r_{aH}$  (see Table 1).

## 6. Conclusion

The representation of the aerodynamic resistance for momentum and heat ( $r_{aM}$  and  $r_{aH}$ ) determines the quality and consistency of thermal remote sensing-based surface energy balance (SEB) models for estimating *ET* (*LE*) in arid and semi-arid ecosystems and during drought. Moreover,  $r_{aM}$  ( $r_{aH}$ ) is tightly coupled with *LST* through both atmospheric stability and aerodynamic feedback, which implies that their interaction influences the accuracy of *ET* estimates. However, until now the pivotal role of  $r_{aM}$  and  $r_{aH}$  has been largely underexplored as most previous studies have focused on the role of the  $kB^{-1}$  factor. For the first time, this work provides insights into the uncertainties of three structurally different SEB models and their relationship to  $r_{aM}$  ( $r_{aH}$ ) and land surface temperature (*LST*) across a wide range of biomes and contrasting aridities. Evaluating the SEB models for the period 2011–2019 over nine Australian OzFlux sites using *LST* from both MODIS and in-situ observations as forcing led us to the following conclusions:

- The seasonality of  $r_{aM}$  ( $r_{aH}$ ) calculated with three SEB models mirrored the seasonal variation of the difference between MODIS *LST* and in-situ *LST*, which implies that in general, high  $r_{aM}$  ( $r_{aH}$ ) values coincide with a low *LST* difference and vice versa.
- Overall model performance to estimate instantaneous *H* and *LE* was relatively poor for arid and semi-arid sites with both sparse and dense vegetation, but it substantially improved for the mesic forest sites. While *LE* overestimation was attributed to inadequate accounting of soil and vegetation characteristics under water stress in previous studies (e.g., Gokool et al., 2020; Li et al., 2019; Kustas et al., 2016; Pardo et al., 2014), our results suggest that  $r_{aM}$  ( $r_{aH}$ ) is overestimated at arid and semi-arid sites, particularly under unstable conditions when thermally generated turbulent mixing dominates. For two water-limited sites in southern Australia, this is most predominant during the winter wet season when low wind speeds prevail. This caused an underestimation of *H*, and consequently overestimation of instantaneous *LE*. Low  $r_{aM}$  resulted in marginal underestimation of *LE*, which was associated with a positive *LST* difference during the dry season.
- The accurate specification of aerodynamic parameters to determine  $r_{aM}$  is very challenging for sparse and heterogeneous ecosystems and contributes to the uncertainty in *LE* estimates. Although STIC retrieves  $r_{aH}$  independently from any empirical parameterization, it also showed a comparable dependency of the model bias on  $r_{aH}$  as SEBS and SPARSE for water-limited ecosystems. PLSR analysis revealed that at the semi-arid sites the effect of  $r_{aM}$  ( $r_{aH}$ ) on the *LE* residual error can be of the same magnitude as the influence of uncertainties in *LST*. This dependency is not found for mesic forest ecosystems, where a high roughness length and low *LST* results in dominance of mechanically generated turbulence.
- As the magnitude of *H* becomes large compared to *LE* during drought, a small relative error in *H* due to uncertainties in  $r_{aM}$  or  $r_{aH}$  will propagate into a large relative error in *LE*. Our findings for dry Australian ecosystems question the accuracy with which instantaneous *LE* is modelled with current  $r_{aM}$  ( $r_{aH}$ ) specification approaches in the contemporary SEB models, which is likely related to inadequate stability correction functions and uncertain



approaches to determine aerodynamic roughness parameters. Hence, novel approaches to estimate  $r_{aM}$  ( $r_{aH}$ ) are required to enhance the performance of the SEB models in water-scarce environments.

**Author contributions**

IT and KM conceptualized the idea; IT organized the study and conducted SPARSE model simulations in consultation with GB; STIC and SEBS model simulations were made by KM and NB; IT made the data analysis in consultation with KM; IT wrote the first version of the manuscript; all authors contributed to discussions and corrections; IT and KM jointly finalized the manuscript.

**Declaration of Competing Interest**

None.

**Appendix A**

**Table A1**

Summary statistics of the SPARSE model performance (parallel version, retrieval mode) for the instantaneous  $H$  retrievals at satellite overpass times (MODIS Aqua and Terra) for nine sites of contrasting aridity in Australia. KGE: Kling-Gupta efficiency, RMSE: Root Mean Square Error, MBE: Mean Bias Error, MAPE: Mean absolute percentage error,  $R^2$ : Squared Pearson Correlation Coefficient, N: Number of data points retained for evaluation (LST<sub>mod</sub>: MODIS LST was used as input, LST<sub>insitu</sub>: in-situ LST was used as input).

Site	KGE	RMSE (W/m <sup>2</sup> )	MBE (W/m <sup>2</sup> )	MAPE (%)	R <sup>2</sup>	N
input	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )
Alice Springs	0.6 (0.53)	89 (163)	-49 (-153)	18 (42)	0.56 (0.73)	1094 (2201)
Calperum	0.6 (0.2)	117 (180)	-90 (-158)	39 (60)	0.65 (0.59)	1477 (1719)
Great Western Woodlands	0.62 (0.31)	122 (195)	-96 (-176)	35 (56)	0.68 (0.54)	1329 (1572)
Gingin	0.53 (0.6)	114 (143)	-57 (-125)	38 (45)	0.74 (0.74)	1707 (2057)
Sturt Plains	0.28 (0.23)	133 (147)	-109 (-133)	44 (52)	0.19 (0.3)	1923 (1982)
Dry River	0.54 (0.51)	98 (95)	-19 (3)	37 (41)	0.3 (0.28)	1487 (1494)
Wombat	0.75 (0.76)	83 (69)	13 (-33)	31 (25)	0.7 (0.77)	1307 (1374)
Daly Uncleared	0.5 (0.56)	97 (81)	43 (20)	43 (29)	0.28 (0.33)	1023 (1526)
Tumbarumba	0.75 (0.7)	68 (70)	-9 (-18)	33 (30)	0.68 (0.67)	1519 (1533)

**Table A2**

Summary statistics of the SPARSE model performance (parallel version, retrieval mode) for the instantaneous  $LE$  retrievals at satellite overpass times (MODIS Aqua and Terra) for nine sites of contrasting aridity in Australia. Detailed description see Table A1.

Site	KGE	RMSE (W/m <sup>2</sup> )	MBE (W/m <sup>2</sup> )	MAPE (%)	R <sup>2</sup>	N
input	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )
Alice Springs	0.17 (-1.92)	79 (146)	19 (135)	514 (1822)	0.28 (0.53)	1094 (2201)
Calperum	-0.7 (-2.1)	95 (171)	68 (155)	280 (564)	0.16 (0.14)	1477 (1719)
Great Western Woodlands	-0.62 (-1.6)	98 (180)	60 (162)	204 (435)	0.08 (0.07)	1329 (1572)
Gingin	-0.02 (0.08)	97 (120)	22 (97)	67 (93)	0.14 (0.17)	1707 (2057)
Sturt Plains	-0.39 (-0.72)	150 (172)	129 (160)	675 (837)	0.61 (0.69)	1923 (1982)
Dry River	0.74 (0.61)	87 (92)	-15 (-37)	70 (66)	0.56 (0.51)	1487 (1494)
Wombat	0.61 (0.76)	97 (69)	-50 (-0.1)	31 (25)	0.5 (0.63)	1307 (1374)
Daly Uncleared	0.55 (0.71)	105 (77)	-64 (5)	69 (76)	0.53 (0.52)	1023 (1526)
Tumbarumba	0.79 (0.83)	72 (68)	-29 (-14)	30 (30)	0.72 (0.73)	1519 (1533)

**Table A3**

Summary statistics of the SEBS model performance for the instantaneous  $H$  retrievals at satellite overpass times (MODIS Aqua and Terra) for nine sites of contrasting aridity in Australia. Detailed description see Table A1.

Site	KGE	RMSE (W/m <sup>2</sup> )	MBE (W/m <sup>2</sup> )	MAPE (%)	R <sup>2</sup>	N
input	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )
Alice Springs	0.19 (0.34)	156 (74)	-12 (-34)	48 (20)	0.1 (0.66)	146 (655)
Calperum	0.61 (0.6)	87 (111)	-46 (-73)	50 (40)	0.55 (0.57)	578 (1271)
Great Western Woodlands	0.55 (0.79)	72 (77)	-20 (-36)	30 (20)	0.59 (0.73)	429 (1121)
Gingin	0.46 (0.64)	110 (125)	-56 (-107)	44 (45)	0.72 (0.8)	1306 (1724)

(continued on next page)

**Table A3** (continued)

Site	KGE	RMSE (W/m <sup>2</sup> )	MBE (W/m <sup>2</sup> )	MAPE (%)	R <sup>2</sup>	N
input	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )
Sturt Plains	0.56 (0.64)	83 (70)	-27 (-29)	30 (25)	0.38 (0.5)	1027 (1391)
Dry River	0.48 (0.63)	101 (82)	-11 (48)	45 (49)	0.24 (0.53)	923 (987)
Wombat	0.28 (-0.04)	190 (241)	-168 (-222)	66 (83)	0.52 (0.67)	1110 (1112)
Daly Uncleared	0.45 (0.67)	96 (69)	22 (-17)	45 (26)	0.25 (0.47)	759 (1327)
Tumbarumba	0.13 (-0.16)	178 (220)	-152 (-193)	72 (81)	0.4 (0.23)	1375 (1378)

**Table A4**

Summary statistics of the SEBS model performance for the instantaneous *LE* retrievals at satellite overpass times (MODIS Aqua and Terra) for nine sites of contrasting aridity in Australia. Detailed description see [Table A1](#).

Site	KGE	RMSE (W/m <sup>2</sup> )	MBE (W/m <sup>2</sup> )	MAPE (%)	R <sup>2</sup>	N
input	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )
Alice Springs	0.27 (0.75)	162 (65)	-19 (13)	278 (106)	0.09 (0.65)	146 (655)
Calperum	-0.14 (-0.71)	74 (98)	37 (72)	128 (270)	0.07 (0.26)	578 (1271)
Great Western Woodlands	-0.04 (0.13)	84 (75)	15 (26)	94 (108)	0.08 (0.09)	429 (1121)
Gingin	0.06 (0.24)	91 (101)	17 (79)	54 (74)	0.09 (0.31)	1306 (1724)
Sturt Plains	0.62 (0.48)	92 (82)	50 (58)	154 (243)	0.72 (0.81)	1027 (1391)
Dry River	0.68 (0.57)	97 (103)	-23 (-83)	56 (47)	0.57 (0.74)	923 (987)
Wombat	0.33 (0.08)	156 (214)	130 (189)	65 (90)	0.55 (0.53)	1110 (1112)
Daly Uncleared	0.54 (0.75)	102 (66)	-43 (2)	48 (54)	0.58 (0.71)	759 (1327)
Tumbarumba	0.48 (0.25)	145 (191)	113 (160)	67 (81)	0.66 (0.67)	1375 (1378)

**Table A5**

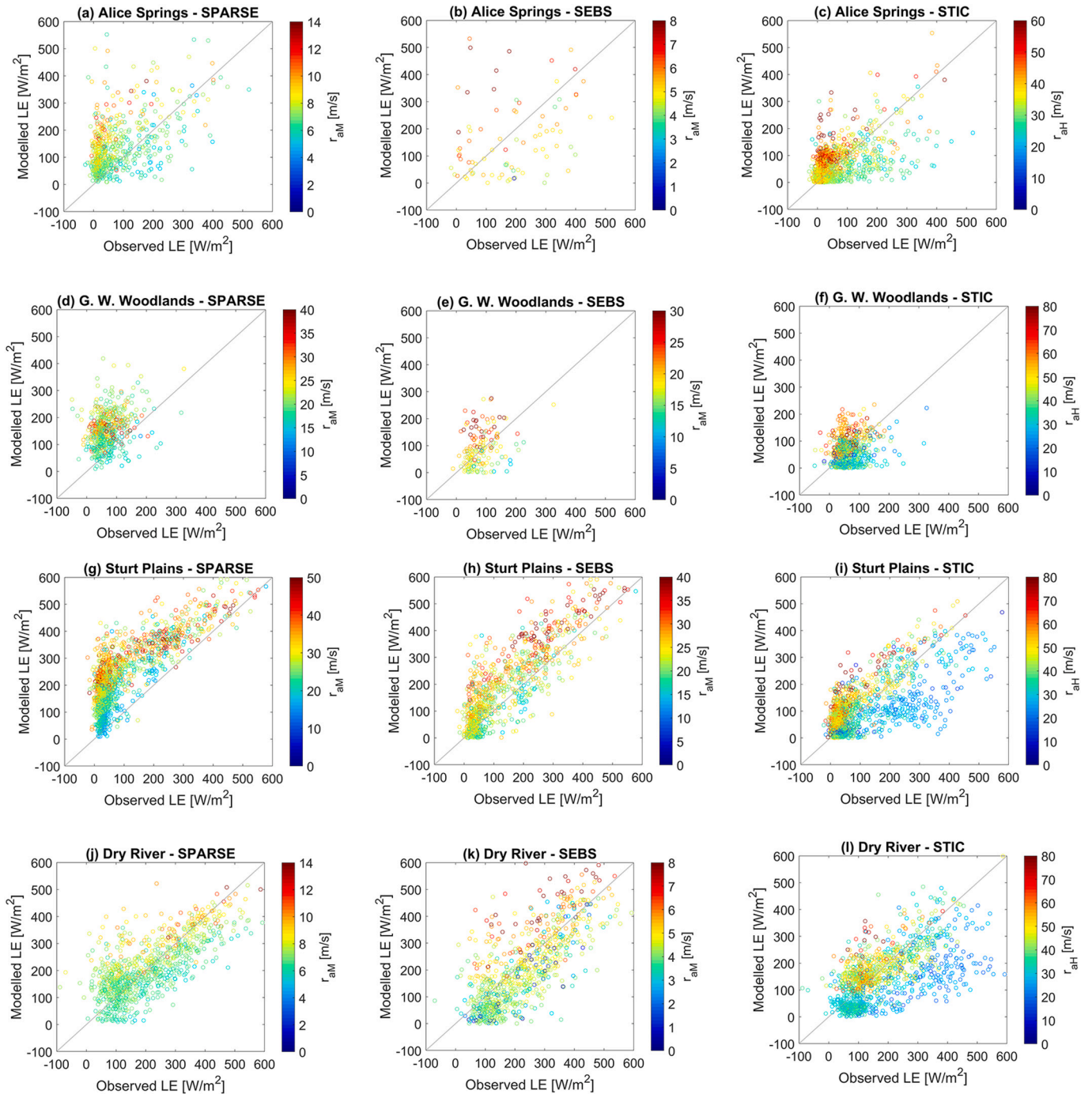
Summary statistics of the STIC model performance for the instantaneous *H* retrievals at satellite overpass times (MODIS Aqua and Terra) for nine sites of contrasting aridity in Australia. Detailed description see [Table A1](#).

Site	KGE	RMSE (W/m <sup>2</sup> )	MBE (W/m <sup>2</sup> )	MAPE (%)	R <sup>2</sup>	N
input	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )
Alice Springs	0.71 (0.58)	73 (105)	-39 (-79)	17 (25)	0.7 (0.71)	2228 (2228)
Calperum	0.83 (0.7)	63 (85)	-36 (-65)	22 (29)	0.83 (0.81)	1719 (1719)
Great Western Woodlands	0.81 (0.79)	75 (81)	-35 (-54)	18 (21)	0.71 (0.76)	1586 (1586)
Gingin	0.72 (0.65)	93 (124)	-50 (-100)	33 (41)	0.75 (0.71)	2068 (2068)
Sturt Plains	0.46 (0.45)	84 (85)	14 (7)	32 (33)	0.35 (0.29)	1984 (1984)
Dry River	0.58 (0.5)	98 (106)	-7 (15)	45 (52)	0.33 (0.26)	1814 (1814)
Wombat	0.72 (0.49)	91 (117)	-50 (-85)	38 (43)	0.65 (0.62)	1374 (1374)
Daly Uncleared	0.52 (0.52)	93 (93)	23 (-21)	38 (38)	0.31 (0.31)	1662 (1662)
Tumbarumba	0.83 (0.59)	69 (77)	-4 (-41)	37 (38)	0.7 (0.73)	1536 (1536)

**Table A6**

Summary statistics of the STIC model performance for the instantaneous *LE* retrievals at satellite overpass times (MODIS Aqua and Terra) for nine sites of contrasting aridity in Australia. Detailed description see [Table A1](#).

Site	KGE	RMSE (W/m <sup>2</sup> )	MBE (W/m <sup>2</sup> )	MAPE (%)	R <sup>2</sup>	N
input	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )	LST <sub>mod</sub> (LST <sub>in-situ</sub> )
Alice Springs	0.51 (-0.21)	63 (89)	8 (61)	407 (886)	0.31 (0.38)	2228 (2228)
Calperum	0.22 (-0.31)	50 (76)	14 (63)	144 (266)	0.11 (0.23)	1719 (1719)
Great Western Woodlands	0.21 (0.04)	65 (70)	-0.8 (40)	110 (151)	0.04 (0.1)	1586 (1586)
Gingin	0.25 (0.12)	76 (100)	15 (72)	54 (82)	0.08 (0.07)	2068 (2068)
Sturt Plains	0.64 (0.56)	80 (85)	6 (20)	300 (404)	0.5 (0.46)	1984 (1984)
Dry River	0.54 (0.26)	101 (119)	-27 (-49)	60 (59)	0.38 (0.2)	1814 (1814)
Wombat	0.7 (0.57)	80 (102)	14 (53)	29 (39)	0.53 (0.53)	1374 (1374)
Daly Uncleared	0.54 (0.53)	98 (92)	-44 (6)	55 (78)	0.38 (0.31)	1662 (1662)
Tumbarumba	0.76 (0.84)	80 (66)	-35 (8)	28 (27)	0.67 (0.76)	1536 (1536)



**Fig. A1.** Scatter plots of modelled  $LE$  versus observed  $LE$  color-coded with  $r_{aM}$  for SPARSE (left panel), SEBS (middle panel) and  $r_{aH}$  for STIC (right panel) for Alice Springs (a-c), Great Western Woodlands (d-f), Sturt Plains (g-i), Dry River (j-l), Wombat (m-o) and Daly Uncleared (p-r) using MODIS  $LST$  as input to run the models.

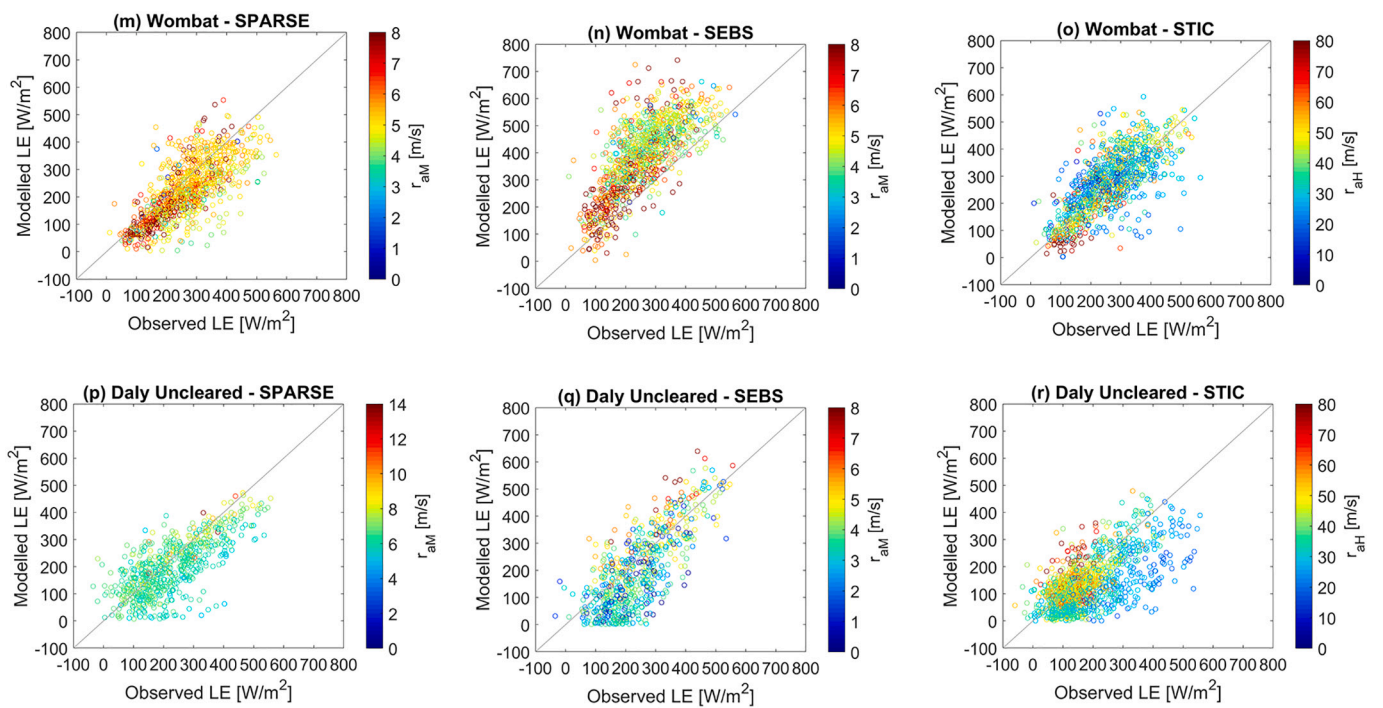
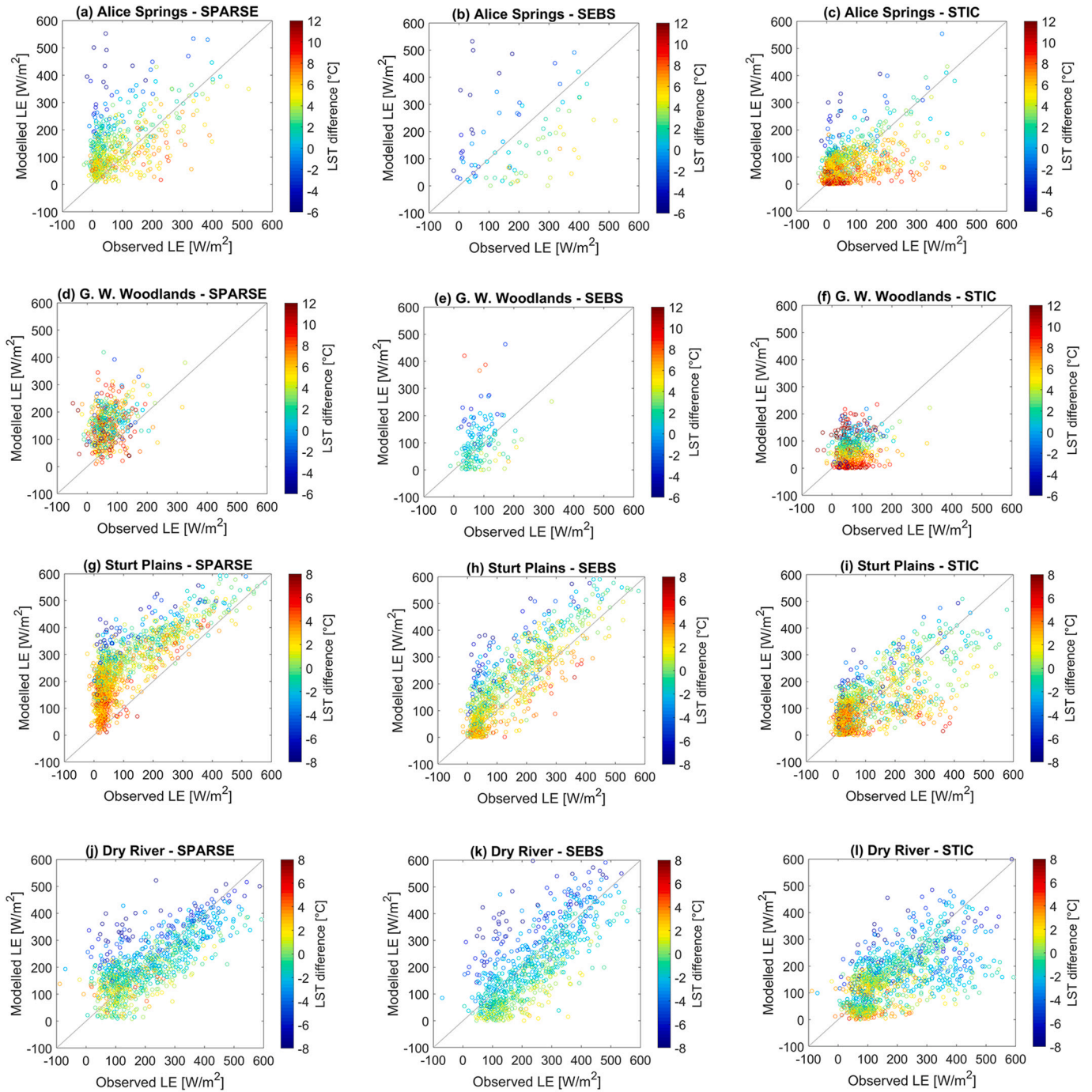


Fig. A1. (continued).



**Fig. A2.** Scatter plots of modelled *LE* versus observed *LE* color-coded with the difference between MODIS *LST* and in-situ *LST* for SPARSE (left panel), SEBS (middle panel) and STIC (right panel) for Alice Springs (a-c), Great Western Woodlands (d-f), Sturt Plains (g-i), Dry River (j-l), Wombat (m-o) and Daly Uncleared (p-r) using MODIS *LST* as input to run the models.

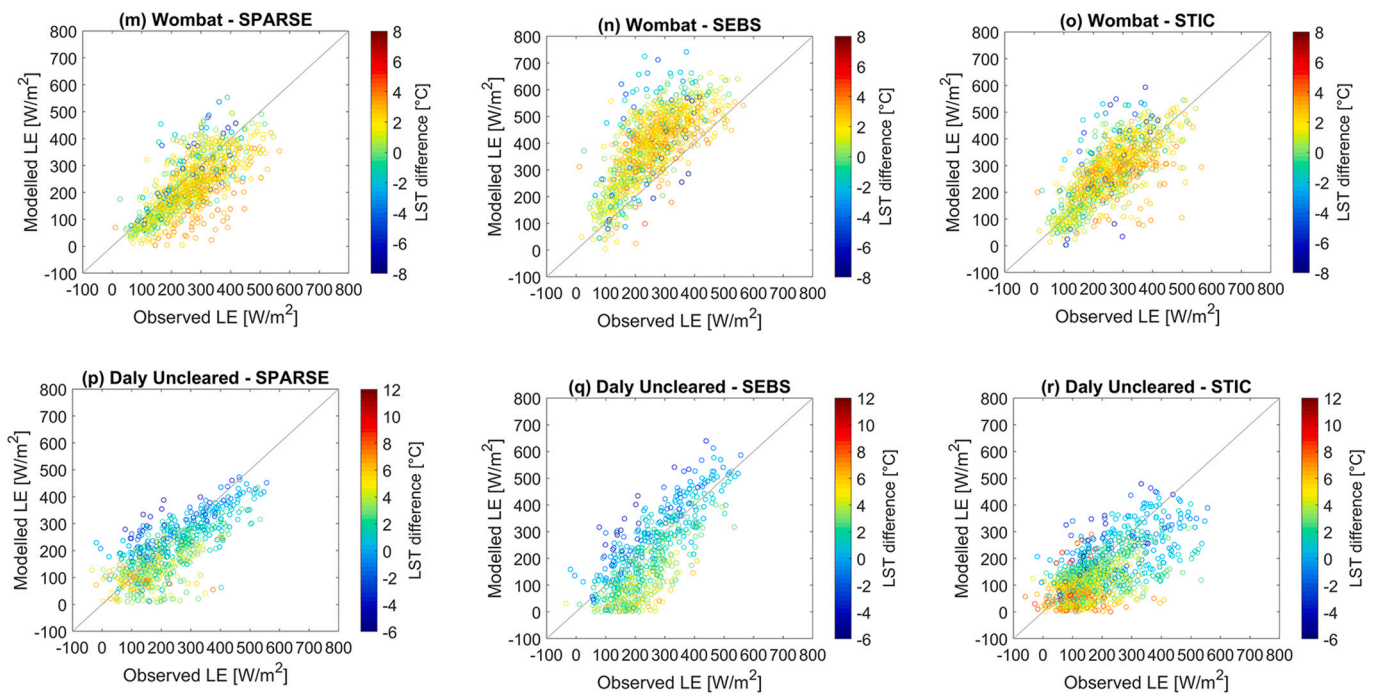
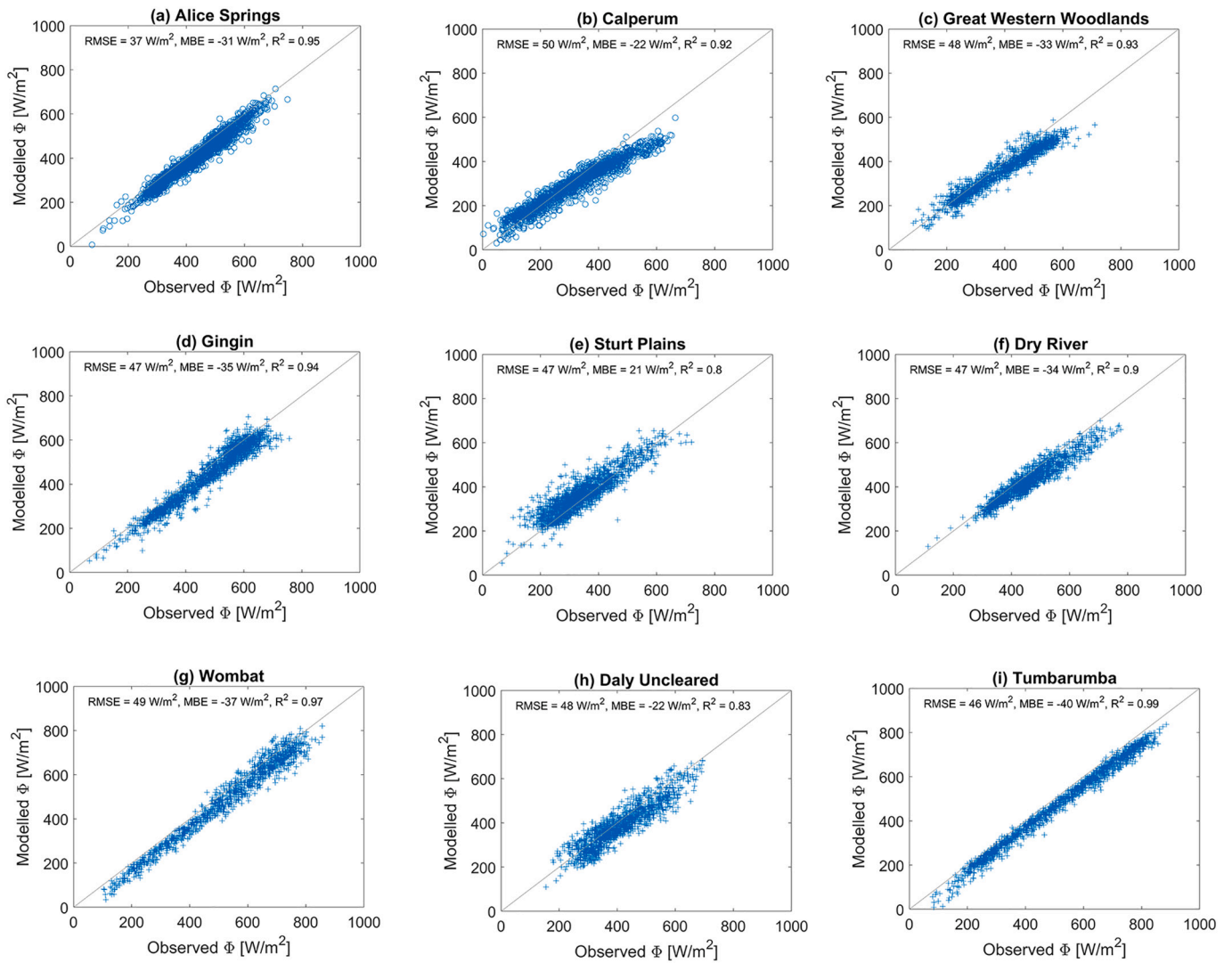
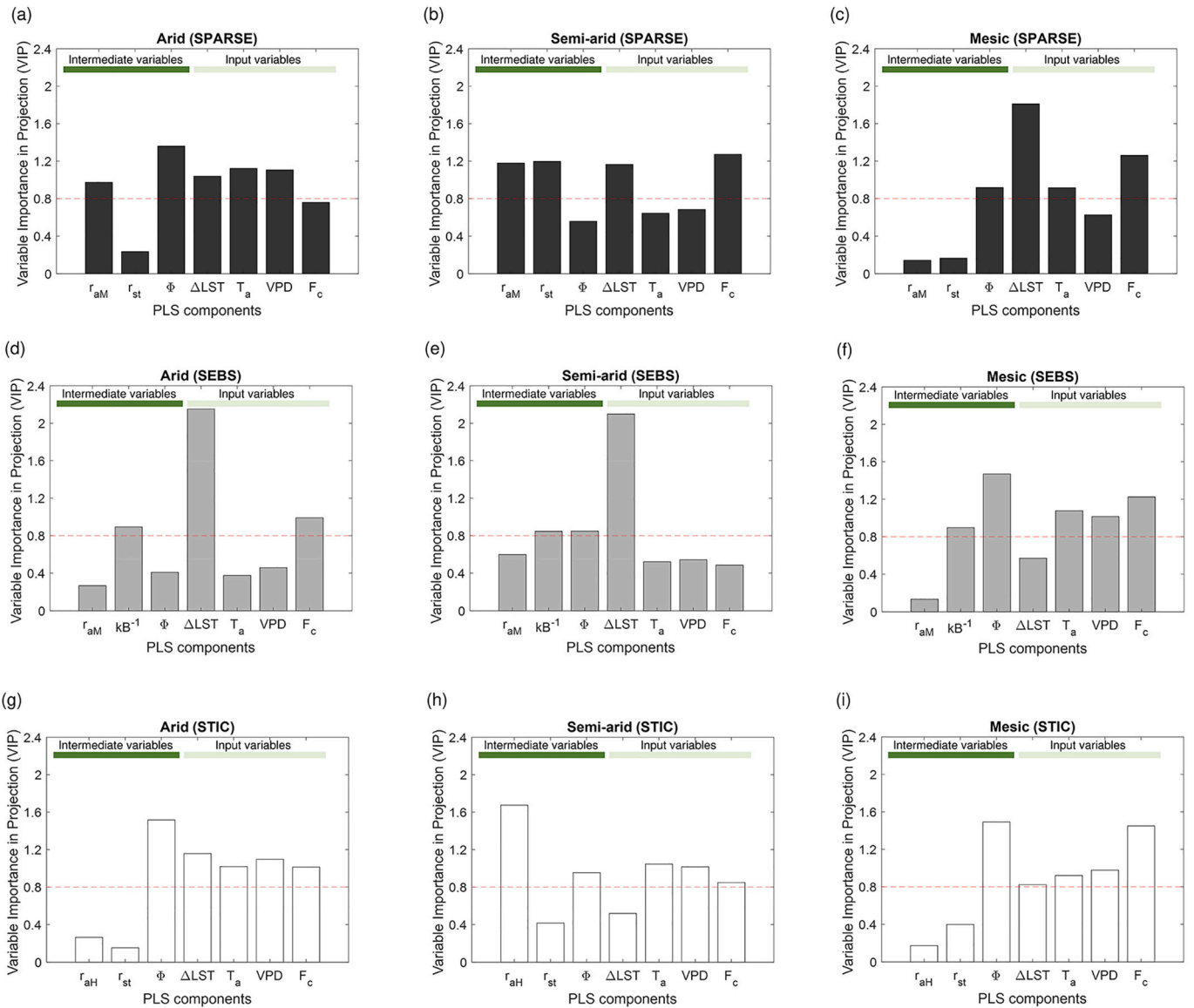


Fig. A2. (continued).

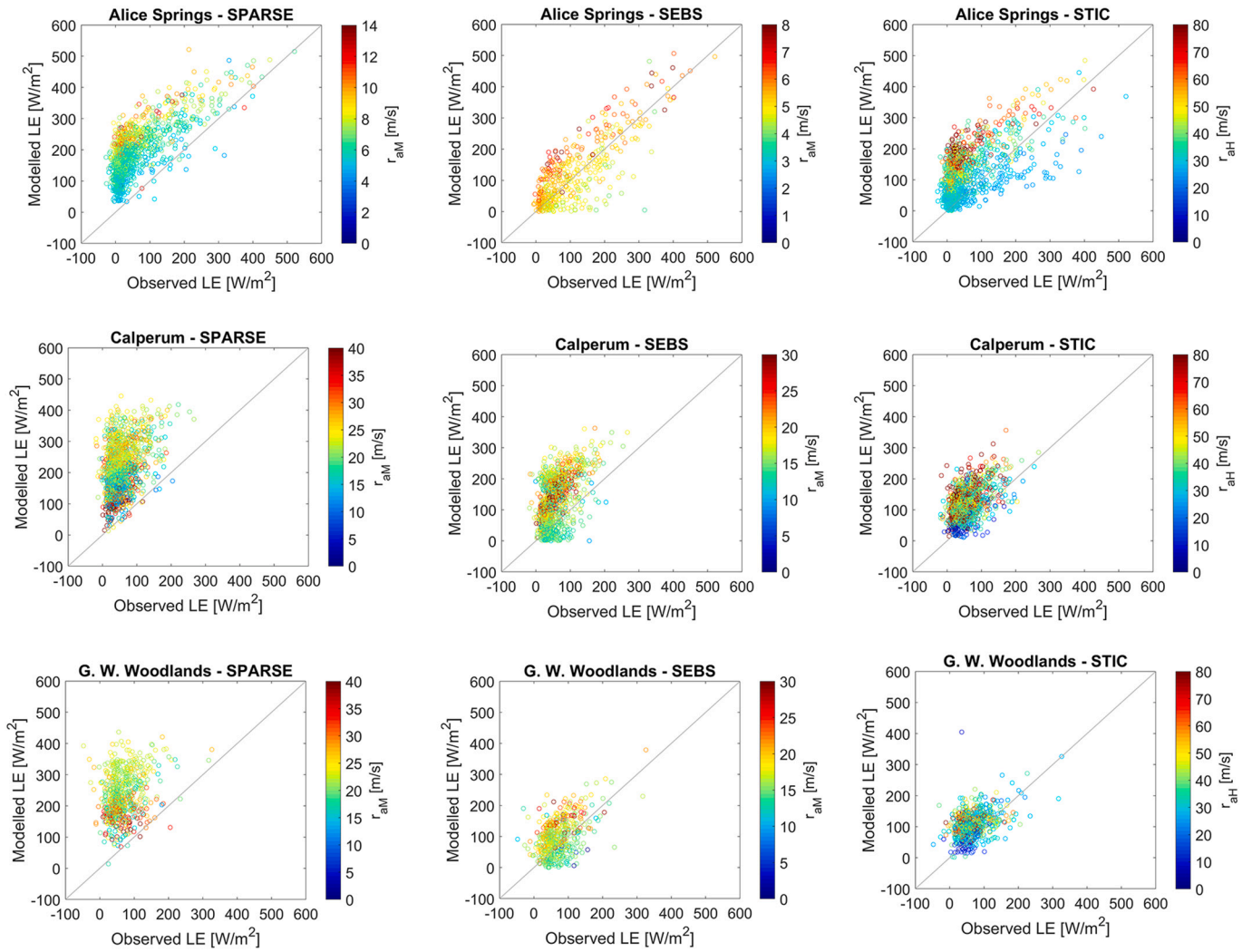


**Fig. A3.** Scatter plots of modelled net available energy ( $\Phi$ ) with SPARSE versus observed  $\Phi$  for (a) Alice Springs, (b) Calperum, (c) Great Western Woodlands, (d) Gingin, (e) Sturt Plains, (f) Dry River, (g) Wombat, (h) Daly Uncleared and (i) Tumarumba using MODIS LST as input to run the models.



**Fig. A4.** Bar plots of the Variable Importance in Projection (VIP) scores for the residual error of  $H$  involving  $r_{aM}$ ,  $r_{aH}$ ,  $kB^{-1}$  (SEBS), the stomata resistance ( $r_{st}$ ) (SPARSE & STIC), modelled  $\Phi$  with SPARSE,  $LST$  difference ( $\Delta LST$ ), air temperature ( $T_a$ ), vapor pressure deficit (VPD) and  $F_c$  for SPARSE (a-c), SEBS (d-f) and STIC (g-i) for all the arid sites (clustered), semi-arid sites (clustered) and mesic sites (clustered) using MODIS  $LST$  as input to run the models. The dashed red line (VIP = 0.8) denotes the variable importance threshold. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)





**Fig. A5.** Scatter plots of modelled *LE* versus observed *LE* color-coded with  $r_{aM}$  for SPARSE (left panel), SEBS (middle panel) and  $r_{aH}$  for STIC (right panel) for Alice Springs, Calperum, Great Western Woodlands, Gingin, Sturt Plains, Dry River, Wombat, Daly Uncleared and Tumarumba using in-situ *LST* as input to run the models.

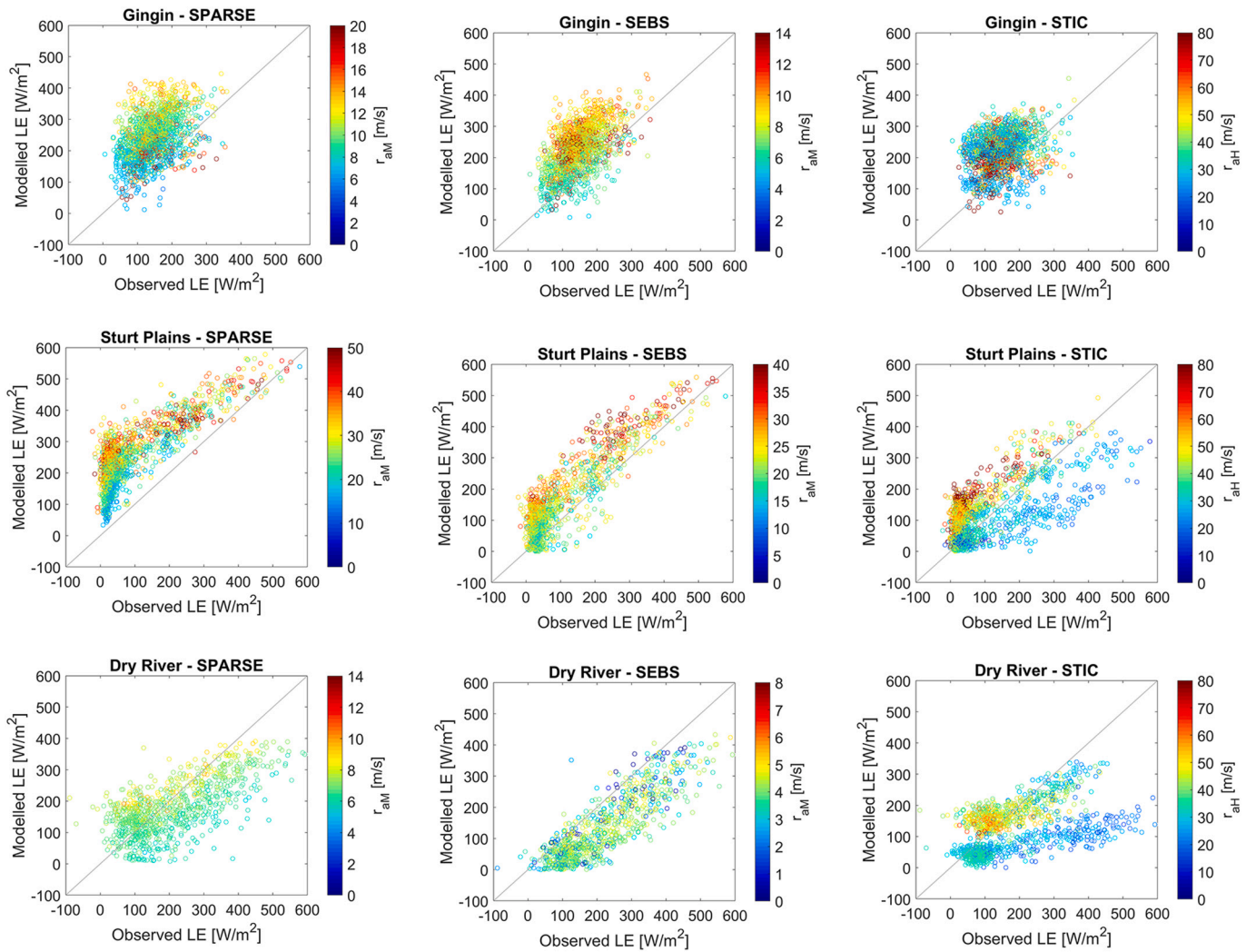


Fig. A5. (continued).

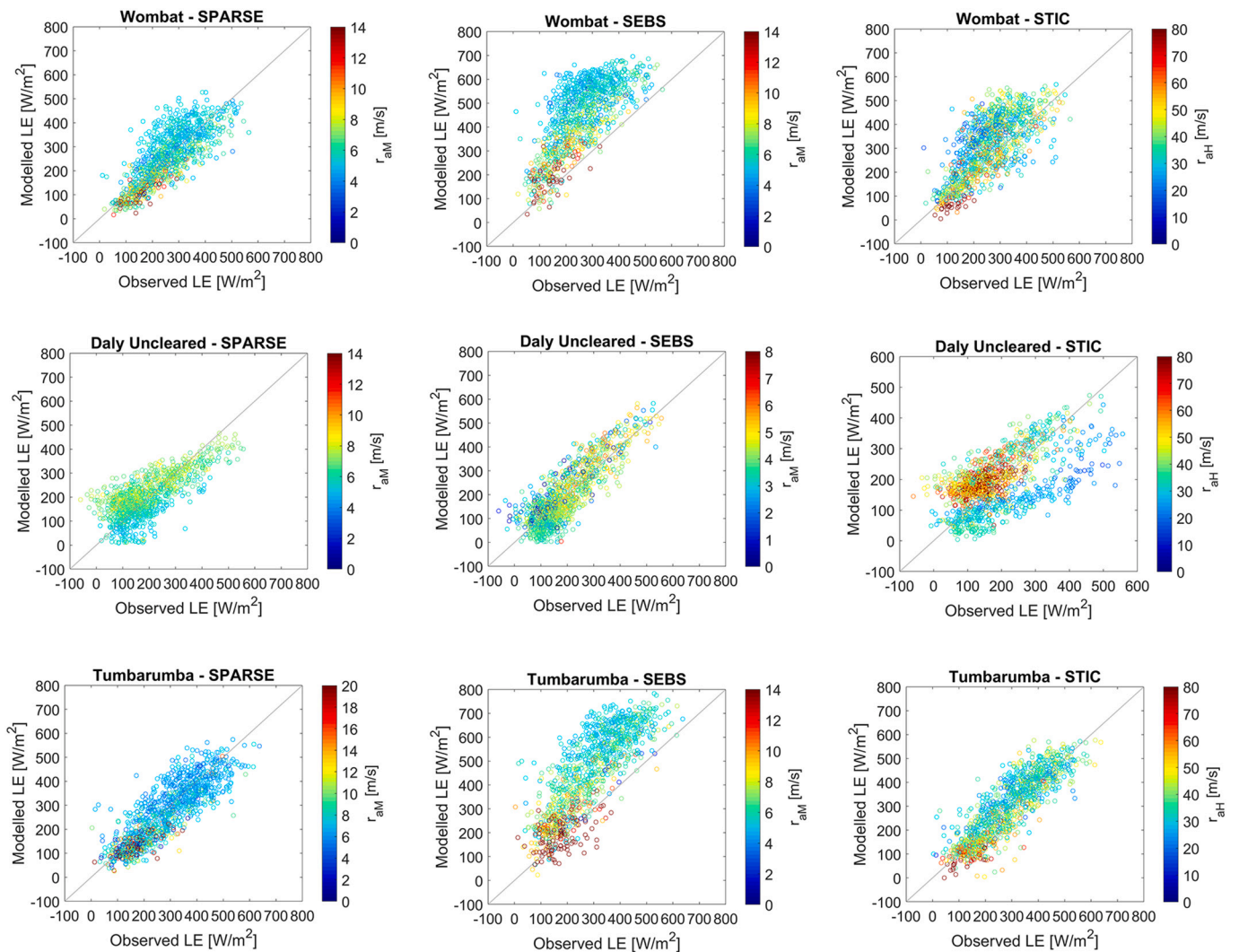


Fig. A5. (continued).

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