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# 1 Generating a 2-km, all-sky, hourly land surface temperature product

# 2 from Advanced Baseline Imager data

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- 7 Abstract

By characterizing high-frequency surface thermal dynamics at a medium spatial scale, 8 hourly land surface temperatures (LST), retrieved from geostationary satellite thermal infrared 9 10 (TIR) observations, shows great potential to be used across a range of scientific applications; however, cloud cover typically leads to data gaps and degraded retrieval accuracy in TIR LST 11 products, such as the official Advanced Baseline Imager (ABI) LST product. Studies have focused 12 on the LST gap reconstruction; however, most interpolation-based methods only work for a short-13 14 term cloud duration and are unable to adequately compensate for cloud effects, and traditional surface energy balance (SEB)-based methods are able to handle cloud coverage while they are not 15 16 feasible for use at night. Moreover, few studies have concentrated on recovering the abnormal retrievals of partial cloud pixels. In this study, an all-sky diurnal, hourly LST estimation method 17 based on SEB theory was proposed; the proposed method involved three major steps: 1) an original 18 spatiotemporal dynamic model of LST was constructed from ECMWF Reanalysis v.5 (ERA5); 2) 19 clear-sky ABI LST was then assimilated to the dynamic model to generate a continuous LST series; 20 3) the diurnal cloud effects were superimposed on cloudy time estimated by an innovative 21 22 optimization method from satellite radiation products. A 2-km, all-sky, hourly LST product was produced over the contiguous US and Mexico from July 2017 to June 2021. Validation was 23

conducted using ground measurements at 18 sites from Surface Radiation (SURFRAD) and core 24 AmeriFlux networks, and produced an overall root-mean-square error (RMSE) of 2.44 K, a bias 25 of -0.19 K, and an R<sup>2</sup> of 0.97 based on 408,300 samples. For clear-sky samples, the RMSE values 26 were 2.37 and 2.24 K for day and nighttime, respectively, which was a notable improvement over 27 the corresponding values of the official ABI LST product (2.73 and 2.86 K, respectively). The 28 RMSE values on cloudy-sky were 2.78 and 2.23 K for day and nighttime, respectively. The daily 29 mean LST by aggregating all-sky, hourly LST had an RMSE of 1.13 K and R<sup>2</sup> of 0.99. Overall, 30 31 this product showed reliability under consistent cloud durations, although it was slightly affected by surface elevation. The diurnal temperature cycle climatology of major land cover types was 32 33 also characterized. The product is freely available at: http://glass.umd.edu/allsky\_LST/ABI/.

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Keywords: land surface temperature, all-sky, diurnal temperature cycle, surface energy balance,
ABI, data assimilation

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#### 38 **1. Introduction**

The Intergovernmental Panel on Climate Change (IPCC) Sixth Assessment Report (AR6) 39 confirmed that the earth's climate has warmed 1.5 °C above pre-industrial levels, in a process 40 unequivocally resulting from human activities (Delmotte et al., 2018; Delmotte et al., 2021). Land 41 42 surface temperature (LST) drives the surface radiation and hydrological budgets, and is one of the 43 most important indicators for characterizing global climate change (Jia et al., 2020; Jin, 2004; Li et al., 2013; Liang et al., 2021). This radiative temperature at the terrestrial surface reflects the 44 surface equilibrium state, and hence, has been utilized for a variety of purposes, including air 45 temperature and heat flux estimates (Chen and Liu, 2020; Rao et al., 2019), drought monitoring 46

(Karnieli et al., 2010), permafrost mapping (Zou et al., 2017), urban heat island analysis (Hrisko
et al., 2020; Imhoff et al., 2010), and hazard risk detection (e.g., earthquakes, forest fire danger,
and parasites) (Blackett et al., 2011; Chuvieco et al., 2004; Neteler et al., 2011). Given the
spatiotemporal scale of such research and heterogeneity of LST, satellite remote sensing has
become the only feasible approach for measuring regional and global LST.

LST is well retrieved from thermal infrared (TIR) sensors onboard polar-orbiting platforms, 52 such as the Moderate Resolution Imaging Spectroradiometer (MODIS) on both Terra and Aqua 53 (Wan and Dozier, 1996; Wan and Li, 1997); however, because of the limited return times, MODIS 54 LST products cannot capture diurnal temperature cycles (DTCs). DTCs identify the high temporal 55 variability of LST, and play a vital role in advancing meteorological modeling (Orth et al., 2017), 56 downscaling (Zakšek and Oštir, 2012), and intra-day health exposure assessments from extreme 57 58 temperature events (Hrisko et al., 2020; Jiang et al., 2015). Studies have also revealed that DTCs 59 are influenced by plant stomatal closure; therefore, they can also be used to estimate plant water stress and evapotranspiration levels (Fensholt et al., 2011; Stisen et al., 2008). In addition, the 60 61 morning warming rate has been shown to be directly related to soil moisture status (Anderson et al., 2007; Piles et al., 2016; Van de Griend et al., 1985). Hence, geostationary (GEO) satellites 62 such as Geostationary Operational Environmental Satellites (GOES)-R Advanced Baseline Imager 63 64 (ABI) (Yu et al., 2008), Meteosat Second Generation (MSG) Spinning Enhanced Visible and InfraRed Imager (SEVIRI) (Freitas et al., 2009), and the Feng Yun meteorological satellites (Tang 65 et al., 2008), have become an optimal choice for observing sub-hourly LST across a wide spatial 66 coverage (Freitas et al., 2013). 67

However, cloud cover results in invalid pixels or degraded retrieval accuracy due to partial
cloud contamination, constricting LST applications, and limiting all-sky GEO LST products

available to the public. Therefore, LST-related analyses have focused strictly on clear-sky cases 70 71 (e.g., estimating urban air temperature from GOES-16 LST, Hrisko et al. (2020)), or postprocessing local temperature data by researchers (e.g., detecting coastal upwelling in the Mid-72 Atlantic Bight from gap-filled GOES-16 SST by DINEOF, Murphy et al. (2021)). Consequently, 73 there is an urgent need for an all-sky, hourly LST product using a more practical cloudy-sky GEO 74 LST estimation method. Different algorithmic methods have been developed to recover cloudy 75 76 pixel data in LST products (Mo et al., 2021; Wu et al., 2021), such as passive microwave (PMW) 77 data (Duan et al., 2017; Xu and Cheng, 2021; Yoo et al., 2020; Zhang et al., 2021), modeled data (Fu et al., 2019; Li et al., 2021; Long et al., 2020), mathematical interpolation (Neteler, 2010; 78 79 Zhang et al., 2022; Zhou et al., 2017), and surface energy balance (SEB) (Jia et al., 2021; Zeng et al., 2018). Although these proposed LST reconstruction methods are sensor-independent, they are 80 81 primarily designed for polar-orbiting satellites, and directly applying these methods to GEO LST 82 is not efficient and does not take adequate advantage of its higher temporal resolution. In comparison, cloudy-sky GEO LST estimation methods have not been well developed. 83

84 Limited studies have utilized PMW data for cloudy-sky GEO LST estimation because of its low spatiotemporal resolutions, in addition to the inherent physical property limitations of 85 microwave signals. Generally, LSTs have considerable diurnal variation, while global PMW data 86 87 can only be collected twice daily. Moreover, microwave signals are sensitive to surface emissivity, which can be highly affected by soil composition, moisture, and vegetation type; thus, the achieved 88 accuracies of PMW-derived LST vary by up to 6 K (Dash et al., 2002). Marullo et al. (2010) 89 generated gap-free, sea surface temperature (SST) data every 3 h by merging SSTs from the 90 Advanced Microwave Scanning Radiometer (AMSR) PMW and SEVIRI via optimal interpolation, 91 under the assumption that the SST biases at the overlapping passing times remained constant. Such 92

an assumption might be feasible for SSTs because of their relative spatiotemporal stability but
would not hold for LSTs. As precipitation has been successfully retrieved via a combination of
PMW and GEO data assimilation (Kidd et al., 2003; Ushio et al., 2009), PMW data still maintain
the potential for cloudy-sky GEO LST estimates (Holmes et al., 2015; Wu et al., 2021).

Simulated LSTs by land surface models are another auxiliary data candidate for filling 97 cloud gaps because of their continuous spatial coverage and high temporal resolution. Marullo et 98 al. (2014) fused clear-sky SSTs from the SEVIRI and Mediterranean Forecasting System to 99 generate gap-free, hourly SSTs using diurnal optimal interpolation across a moving temporal 100 window. Different model outputs have also been evaluated for filling invalid SST pixels (Nardelli 101 et al., 2015); however, the resulting accuracies of cloudy-sky results were highly reliant upon 102 simulation data, especially for continuous cloudy days, and no further correction was implemented 103 104 (Fablet et al., 2017). Dumitrescu et al. (2020) fused daytime hourly SEVIRI LSTs and modeled 105 skin temperature using multiple linear regression and generalized additive models, in addition to elevation, time, and solar radiation to improve GEO LST estimation under clouds. Inherently, 106 107 applying a clear-sky statistical model to cloudy cases introduces error, as the cloud cooling effect cannot be replicated by cloud-free samples. In addition, surface parameters (e.g., albedo and 108 109 vegetation coverage) also substantially influence LST, but have not been adequately accounted for. 110 Furthermore, few studies have focused on recovering ABI LST by combining satellite retrieval with model simulations. 111

Owing to the unique cycles, temporal interpolation based on a DTC model is the dominant method for missing GEO LST reconstruction. A DTC model is defined by a harmonic function during the day and an exponential function at night (Duan et al., 2012), of which parameters can be obtained by model simulation (Jin and Treadon, 2003), statistics (Aires et al., 2004; Ignatov

and Gutman, 1999), and physical interpretation (Göttsche and Olesen, 2009; Schädlich et al., 2001). 116 Parton and Logan (1981) initially created a DTC model to describe real-time temperature variation, 117 which was then developed for GEO brightness temperature (BT) or LST temporal interpolation 118 (Göttsche and Olesen, 2001; Inamdar and French, 2009; Inamdar et al., 2008; Jiang et al., 2006; 119 120 Udahemuka et al., 2008; Van den Bergh et al., 2007). Thereafter, DTC models were improved by introducing energy partitioning constraints (Gottsche and Olesen, 2009; Zhan et al., 2013; Zhan et 121 122 al., 2014), and Huang et al. (2014) proposed a generic, quasi-physical DTC framework based on 123 the SEB and heat conduction equations. Studies have also attempted to increase feasibility by reducing the quantity of DTC model parameters (Duan et al., 2014; Holmes et al., 2013), or 124 125 including additional data (e.g., spatially adjacent LST pixels or monthly mean) (Quan et al., 2014; Quan et al., 2018; Zhou et al., 2013). Accuracies and feasibilities of different DTC models have 126 127 been comprehensively evaluated and summarized by Duan et al. (2012) and Hong et al. (2018).

128 DTC-based models have clear mathematical formulas and are easily applicable; however, the equations cannot be resolved if enough clear-sky observations ( $\geq 4$ ) per day are not available. 129 Liu et al. (2017b) increased the clear-sky samples available to the DTC model by combining it 130 with a spatial inverse distance-weighted interpolation; however, such interpolation methods are 131 unreliable when cloud coverage has large spatiotemporal scales (Vinnikov et al., 2008). In addition, 132 133 DTC models determine interpolation accuracy, although model selection is difficult for various 134 study areas. Accordingly, Wu et al. (2019) utilized a convolutional neural network (CNN) to reconstruct the missing GEO LSTs from spatiotemporally adjacent pixels, a functional approach 135 for larger missing regions. Some other spatiotemporal interpolation methods were also designed 136 137 for GEO LSTs, such as reproducing kernel Hilbert space (RKHS) interpolator (Van den Bergh et al., 2007), multi-channel singular spectrum analysis (M-SSA) (Ghafarian et al., 2012), data 138

interpolating empirical orthogonal functions (DINEOF) (Beckers et al., 2014), and Fourier functions (Liu et al., 2017a). Ultimately, all spatiotemporal interpolation methods are affected by terrain complexity and referenced clear-sky pixels' distributions, as well as fill gaps with hypothetical "clear-sky" LSTs; however, cloud cooling (warming) effects on LST during the daytime (nighttime) cannot be ignored (Ermida et al., 2019). In addition, few studies have tested spatiotemporal interpolation methods using the ABI LST.

145 Considering the straightforward physical process, the SEB-based method represents one of the most promising solutions for cloudy-sky GEO LST estimation. Jin (2000) proposed an SEB-146 based method containing two primary steps: 1) reconstruct hypothetical LSTs based on 147 neighboring observed pixels, and 2) superpose the cloud effect corrections estimated from surface 148 insolation, air temperature, wind speed, and other variables. Essentially, it uses an interpolation 149 150 method before correcting the interpolated LSTs to realistic cloudy-sky LSTs based on SEB. Lu et 151 al. (2011) adjusted the algorithm for SEVIRI LST by utilizing only the temporal series. A combined diurnal cycle model of downward solar radiation (DSR) was designed to reconstruct 152 153 hypothetical LST values (Zhang et al., 2015b); however, the previous SEB-based methods remain restricted by the limitations of interpolation and only work when there are sufficient nearby clear-154 sky observations. In addition, local meteorological parameters are required, which considerably 155 156 limits their feasibility over larger spatial scales. More importantly, traditional SEB-based methods were driven by DSR, implying that the nighttime all-sky LST could not be obtained. The SEB-157 based method was also tested by Feng Yun-2D GEO LSTs, and a continuous DTC series was 158 generated assuming negligible nighttime cloud effects (Zhang et al., 2017). A revised SEB 159 algorithm was developed by Martins et al. (2019) for SEVIRI LST, where an iteration method was 160 employed by adjusting LST and turbulent heat fluxes to meet SEB during periods of cloud cover, 161

of which parameterization schemes of turbulent heat fluxes and radiation components were from
MSG/SEVIRI Satellite Application Facility on Land Surface Analysis (LSA-SAF) product suite;
however, heat flux estimation generally has higher uncertainty than LST retrieval, and thus in SEB
fitting step, the iteratively adjusted cloudy-sky LSTs could be affected by initial value and heat
fluxes' accuracy.

Furthermore, previous studies have rarely discussed pixel recovery and algorithm robustness toward cloud-contaminated pixels. Partially cloud-covered pixels can be retrieved, albeit with substantial bias (Ma et al., 2020; Yang et al., 2019), and accidentally interpolating or fusing contaminated pixels will introduce significant uncertainty to the filled results, thereby restricting the application of the current cloudy-sky GEO LST estimation algorithms.

Jia et al. (2021) estimated the cloudy-sky Visible Infrared Imaging Radiometer Suite 172 173 (VIIRS) LSTs by assimilating the noon clear-sky retrievals to a temporal LST evolving model, and simulated LSTs on cloudy days were corrected from satellite radiation products based on SEB. 174 By considering the importance and the scarcity of the all-sky GEO LST, here, the preliminary 175 algorithm was further refined to generate an all-sky, hourly LST product from GOES-16 ABI in 176 pursuit of three primary objectives: 1) design an innovative spatiotemporal dynamic model and 177 178 assimilation scheme to increase algorithm robustness and take full advantage of the high temporal resolution of ABI LST data; 2) propose a novel, diurnal cloud effect estimation method that can 179 recover complete DTCs, and calculate accurate daily mean LSTs; and 3) effectively recover 180 181 abnormally-retrieved LSTs mainly caused by partial cloud coverage. The first 2-km, all-sky, hourly LST product was produced from July 2017 to June 2021, and it was comprehensively 182 assessed over the contiguous US (CONUS) and Mexico. 183

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#### 185 **2. Data and methods**

186 *2.1 Data* 

This study assimilated the official ABI LSTs into a spatiotemporal dynamic model constructed by European Centre for Medium-range Weather Forecasts (ECMWF) Reanalysis v.5 (ERA5), and the cloud effects were primarily estimated by satellite products from ABI, Clouds and Earth's Radiant Energy Systems (CERES), MODIS, and Global LAnd Surface Satellite (GLASS). Eighteen ground sites from the Surface Radiation (SURFRAD) and core AmeriFlux networks were used for ground validation. Further information is provided below, where the basic input data are listed in Table 1, and the site metadata are presented in Table 2.

## 194 2.1.1 Satellite and reanalysis products

195 The official National Oceanic and Atmospheric Administration (NOAA) GOES-16 ABI LST was considered the target for all-sky diurnal LST estimates, while the GOES-16 ABI DSR 196 and cloud top temperature (CTT) were used to calculate the diurnal cloud radiative effect (CRE). 197 198 GOES-16 was launched in November 2016, and its LST product was retrieved using a splitwindow method (Yu and Yu, 2018). The longest set of NOAA ABI LSTs was available from mid-199 2017; thus, the all-sky diurnal LST from July 1, 2017, was released. It provides 10-km hourly LST 200 over North and South America (full disk), and 2-km hourly data (selected for the present study) 201 covering the CONUS and Mexico. The GOES-16 ABI LST reached its provisional maturity in 202 March 2018, achieving stable accuracy based on site validation (Yu et al., 2018). The GOES-16 203 ABI DSR product combines forward and backward algorithms to estimate reflection and 204 transmission, accounting for all major interactions of radiation between the atmosphere and surface. 205 Both the visible and infrared channels were utilized with other inputs (e.g., albedo and atmospheric 206 composition) to retrieve surface DSR (Laszlo et al., 2020). The NOAA officially released GOES-207

16 ABI CTT (Heidinger et al., 2010; Heidinger et al., 2020) is retrieved simultaneously with cloud
top height and pressure for each cloudy pixel, using an analytical model of infrared radiative
transfer embedded into an optimal retrieval methodology. The ABI observations for bands at 11,
12, and 13.3 µm were used to characterize cloud microphysical information. CTT was utilized to
estimate cloudy-sky downward longwave (DLW) radiation, and both atmospheric variables (DSR
and CTT) were interpolated bilinearly to align with the spatial scale of ABI LST data.

214 Cloud shortwave net radiative forcing is the difference between all-sky DSR and the theoretical clear-sky DSR, which is essential for the cloud cooling/warming effect estimation, thus 215 theoretical clear-sky DSR on cloudy times is required. The CERES clear-sky DSR product was 216 employed. Specifically, the CERES SYN1-deg product provides hourly, spatiotemporally 217 continuous surface radiation products by retrieving observations from both polar-orbiting and 218 219 GEO satellites (Kato et al., 2018). Based on the Fu-Liou radiative transfer theory (Fu et al., 1997), 220 the theoretical clear-sky DSR was obtained by removing the cloud impact estimates from multiple data sources, including microwave observations. 221

The CERES project aims to analyze the radiation budget at atmosphere and surface levels; thus, it retrieves the theoretical clear-sky DSR at cloudy times to estimate CRE. We directly take advantage of the CERES clear-sky DSR product, but use GOES-16 all-sky DSR rather than CERES all-sky DSR because the former has a higher spatial resolution. As clear-sky DSR has limited spatial heterogeneity, CERES clear-sky DSR was downscaled by bilinear interpolation.

Auxiliary input satellite data, such as a digital elevation model (DEM), were used for modeled LST downscaling (Danielson and Gesch, 2011). The VIIRS all-sky broadband emissivity (BBE) product was used to estimate the modeled clear-sky LST series, and was spectrally adjusted from the historical Advanced Spaceborne Thermal Emission and Reflection Radiometer Global

Emissivity Dataset (ASTER-GED) and MODIS land surface emissivity product (Wang et al., 231 232 2019). Cloudy pixels were replaced by the mean value of available adjacent grids within 2.5° of the same surface type. MODIS land cover data (MCD12Q1) (Sulla-Menashe and Friedl, 2018) 233 were used to select similar pixels in a spatial window, and aggregated (water, forest, low vegetation, 234 urban, and ice/snow) to increase classification accuracy. MODIS albedo (Schaaf et al., 2002) has 235 been widely employed in SEB-related studies (He et al., 2014; Jia et al., 2020). Here, surface 236 237 albedo was used for shortwave CRE calculation after a bilinear interpolation in cloudy time, and it was assumed that values would remain relatively stable in the neighboring days. The all-sky 238 GLASS leaf area index (LAI) was utilized for estimating energy partitioning (Liang et al., 2021). 239 240 All auxiliary data have a higher spatial resolution, and thus, have been aggregated to 2 km to match the dominant spatial scale used. 241

ERA5 (Hersbach et al., 2020) provides simulated hourly, clear-sky DLW and upward longwave (ULW) radiation for creating a clear-sky LST dynamic model, in addition to providing column water vapor (CWV) for DLW parameterizations. Clear-sky DLW and ULW were simulated by ERA5 for the same atmospheric and meteorological conditions as the corresponding representative scenario, but assuming clouds were absent. The all-sky ERA5 skin temperature was not used here, as reanalysis datasets primarily involve simulated clouds (Wang and Dickinson, 2013). The metadata for all input information are summarized in Table 1.

249 **Table 1.** Metadata for all-sky diurnal LST input.

Product	Variable	Spatial	Temporal	Usage
		resolution	resolution	
ABI	LST	2-km	hourly	clear-sky GEO LST
ERA5	clear-sky DLW and ULW	0.25°	hourly	LST dynamic model

VIIRS	BBE	1-km	daily	LST dynamic model, longwave CRE
GMTED2010	DEM	1-km	-	downscaling
MODIS	land cover type	500-m	yearly	neighboring pixel selection
ABI	DSR	0.25°	hourly	shortwave CRE
CERES	clear-sky DSR	1°	hourly	shortwave CRE
MODIS	surface albedo	500-m	daily	shortwave CRE
ABI	CTT	2-km	hourly	longwave CRE
ERA5	CWV	0.25°	hourly	longwave CRE
GLASS	LAI	500-m	daily	energy partitioning

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In addition, in order to demonstrate the advancement of the proposed all-sky diurnal LST, 251 we also included two available all-sky skin temperature reanalysis datasets for accuracy 252 comparison. As there were no available satellite-derived all-sky hourly LSTs over the CONUS 253 before this study, skin temperatures from ERA5-Land and North American Land Data 254 Assimilation System (NLDAS) were employed and validated by sites at different hours of a day 255 for accuracy comparison. ERA5-Land replays of the land component of the ERA5 climate 256 reanalysis with a finer spatial resolution (0.1°) at an hourly scale. NLDAS aims to provide spatially 257 258 and temporally consistent land surface model datasets by reanalyzing observations to support modeling activities. GOES surface brightness temperature is considered the essential forcing data 259 (Pinker et al., 2003). Hourly skin temperature with 0.125° resolution from the NLDAS Noah model 260 has been chosen in this study. Both reanalysis skin temperature data were downscaled to 2 km 261 based on elevation (Duan et al., 2017). 262

263 2.1.2 Ground measurements

Comprehensive validation using ground-based measurements is essential for the assessment and application of diurnal LST products. As widely distributed sites can encompass different climates and land cover types, 18 *in situ* sites from the SURFRAD (7) and core

AmeriFlux (11) networks were employed for the all-sky diurnal LST validation. SURFRAD was 267 established in 1993 through the support of the NOAA's Office of Global Programs, with an aim 268 to provide climate research with precise, continuous, long-term ground references of the surface 269 radiation records over the US (Augustine et al., 2000). It has been commonly utilized for surface 270 radiation product assessment (Jiang et al., 2018; Zeng et al., 2020; Zhou et al., 2018), and was thus 271 selected here to validate the SEB accuracy from satellite-based estimates. Core AmeriFlux sites 272 273 are flux towers providing timely, high-quality, and continuous data, with the basic objective to 274 ensure high-resolution data collection across a broad range of ecosystems and locations in the US. The sites utilized here included ULW and DLW observations (AmeriFlux, 2021), and ground 275 276 measured LSTs were computed using ULW, DLW, and all-sky VIIRS BBE by Eq. 1 in Jia et al. (2021), based on the Stefan–Boltzmann law. The site location map can be seen in Figure 1, with 277 278 site details listed in Table 2.



**Figure 1.** Distribution of the 18 sites with landcover types from Surface Radiation (SURFRAD) and Core



No.	Name	Lat. (°)	Long. (°)	Elev. (m)	Land cover	Period
1	BND	40.0519	-88.3731	230	cropland	2018–2021
2	FPK	48.3078	-105.1017	634	grassland	2018–2021
3	GWN	34.2547	-89.8729	98	pastureland	2018–2021
4	DRA	36.6237	-116.0195	1007	arid shrubland	2018-2021
5	PSU	40.7201	-77.9309	376	cropland	2018–2021
6	SXF	43.7340	-96.6233	473	grassland	2018–2021
7	TBL	40.1250	-105.2368	1689	grass and shrub	2018–2021
8	US-ARM	36.6058	-97.4888	314	cropland	2018–2021
9	US-Ho1	45.2041	-68.7402	60	forest	2018–2020
10	US-Los	46.0827	-89.9792	480	wetland	2018–2021
11	US-MMS	39.3232	-86.4131	275	forest	2018–2021
12	US-MOz	38.7441	-92.2000	219	forest	2018–2019
13	US-NC2	35.8030	-76.6685	5	forest	2018–2020
14	US-NE1	41.1651	-96.4766	361	cropland	2018–2020
15	US-Ro5	44.6910	-93.0576	283	cropland	2018-2021
16	US-SRM	31.8214	-110.8661	1120	woody savannas	2018–2021
17	US-Ton	38.4309	-120.9660	177	woody savannas	2018–2020

18	US-UMB	45.5598	-84.7138	234	forest	2018–2020

284 Site observations with low-quality flags in the raw records were filtered out during preprocessing. SURFRAD sites have a 1-min temporal resolution, and the raw ground observations were 285 286 extracted and averaged within a 15-min time window, centered on the satellite recording time. Core AmeriFlux sites have a 30-min temporal resolution, and only the site samples within the 15-287 288 min time window of satellite data acquisition were utilized for validation. Bias, root-mean-square 289 error (RMSE), and the coefficient of determination  $(R^2)$  were the validation indices used. The validation samples were extracted from the site locations, and sample accuracies of diurnal all-sky 290 LSTs and GOES-16 LSTs were compared during daytime and nighttime, from July 2018 to June 291 2021 after GOES-16 reached provisional maturity (Yu et al., 2018). As only SURFRAD sites have 292 1-min observations, they were employed for daily mean LST validation. In addition, only high-293 quality ground measurements that were fully observed  $(24 \times 60 \text{ high-quality records in a day})$  were 294 295 averaged to obtain the daily mean references.

### 296 2.2 Framework

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The conceptual flowchart of the proposed SEB-based, all-sky, hourly LST estimation method is shown in Figure 2; it can be divided into three primary steps: 1) an original spatiotemporal dynamic model of LST was constructed from ERA5 data; 2) after cleaning likely cloud-contaminated pixels, continuous LST series were reconstructed by assimilating the official clear-sky ABI LST to the dynamic model from spatial and temporal dimensions; and 3) diurnal cloud effects were superimposed on cloudy time estimated by an innovative optimization method from satellite radiation products.





**Figure 2.** Flowchart of the all-sky, hourly land surface temperature (LST) product generation from the Advanced Baseline Imager (ABI) data: DLW, downward longwave radiation; DSR, downward shortwave radiation; ULW, upward longwave radiation; CRE, cloud radiative effect; BBE, broadband emissivity; and  $\Delta T_s$ , cloud effects on LST.

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In the first step, a clear-sky LST dynamic model was built from ERA5 using a 3-D Kalman filter (KF). ERA5 released the simulated clear-sky ULW and DLW radiations, which are used for computing clear-sky LST combined with all-sky BBE (Wang et al., 2019). After downscaling, a spatiotemporal dynamic model was constructed for each pixel location using the simulated LST series (Section 2.3). Continuous simulations in clear-sky conditions rather than directly modeled skin temperatures were used in this study because the realistic cloud effects from the available radiation satellite products were superposed in the final step. ERA5 clear-sky fluxes are simulated by the real atmospheric condition so that they can still provide the LST variation signals caused
by near-surface meteorological changes (e.g., advective cold air movement).

In the second step, continuous LSTs were obtained by assimilating the official ABI LST to 319 the dynamic model. Before the assimilation, a partially cloud-contaminated pixel was identified 320 321 when: 1) its absolute difference with the corresponding simulated LST was significantly larger 322 (three standard deviations) than other days within  $\pm 15$  days, and 2) surrounding cloudy pixels 323 were >50% of the spatial window. Detected likely cloud-contaminated pixels were masked to be recovered. Subsequently, clear-sky ABI LSTs within a spatial window were assimilated into the 324 spatiotemporal dynamic model to correct the simulation (Section 2.4). After processing the 325 prediction from the corrected results, hypothetical clear-sky LSTs were reconstructed for missing 326 or likely cloud-contaminated pixels. 327

328 In the third step (Section 2.5), shortwave CRE was acquired from current land surface albedo and clear-sky/all-sky DSR satellite products. Estimating longwave CRE required cloudy-329 sky LST that is unavailable; therefore, it was assumed that the initial cloud effects ( $\Delta T_s$ ) were 0 K, 330 and the hypothetical LST was used for the initial CRE calculation. By converting total CRE to the 331 cloud heat effect after energy partitioning, an updated  $\Delta T_s$  was calculated, and the longwave CRE 332 was recomputed. To reduce the difference between the CREs of the two loops,  $\Delta T_s$  was adjusted 333 and iteratively reprocessed using the previous steps until the SEB was balanced. Subsequently, 334 optimal  $\Delta T_s$  was obtained and used to correct the hypothetical LST during cloudy periods. All-sky 335 336 diurnal LST was the combination of clear-sky LST in the second step and the estimated cloudy-337 sky LST in the third step.

### 339 2.3 Spatiotemporal dynamic model

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An original spatiotemporal dynamic model was designed to spatiotemporally characterize 340 the simulated clear-sky LST dynamics around a target pixel. The simulated clear-sky LST was 341 calculated from the ERA5 clear-sky longwave radiations and all-sky BBE (Wang et al., 2019), 342 according to the Stefan–Boltzmann law (Liang et al., 2010). To match the spatial scale, the 343 simulated LST was preliminarily downscaled to 2-km using elevational information (Duan et al., 344 2017), and the resulting spatiotemporal dynamic model was built within a 150-km spatial window, 345 centered on the target pixel (see Section 3.1), which can be mathematically represented as follows 346 (Eqs. 1–4): 347

$$LST_{c,t,d}^{t} = F_{c,t,d}^{t} \times LST_{c,t,d-1}^{t},$$
(1)

349 
$$F_{c,t,d}^{t} = 1 + \frac{1}{Z_{c,t,d} + \delta},$$
 (2)

$$LST_{c,t,d}^{s} = \sum_{1}^{N} w_{m,d} \cdot \left(F_{m,t,d}^{s} \times LST_{m,t,d}^{s}\right), \tag{3}$$

351 
$$F_{m,t,d}^{s} = 1 + \frac{1}{Z_{m,t,d} + \delta},$$
 (4)

The aforementioned equations hold true for target center pixel c, at time t (defined by the UTC 352 coordinate) of day d. The spatiotemporal dynamic model includes a temporal module  $(F_{c,t,d}^t; \text{Eqs.})$ 353 1 and 2) and a spatial module ( $F_{c,t,d}^s$ ; Eqs. 3 and 4).  $LST_{c,t,d}^t$  represents the prediction of the 354 temporal module, which is estimated from  $LST_{c,t,d-1}^{t}$ , i.e., the LST 24 h before, as the data in the 355 modeled series are most closely related to the same time on different days (TOD) (Marullo et al., 356 2014); thus, samples at the same TOD generally have similar simulated uncertainties, allowing for 357 358 corrections made by data assimilation to be easily passed on to the following days.  $Z_{c,t,d}$  is the difference between the simulated LSTs at t of d and d-1, and setting  $\delta = 0.01$  avoids a null 359 denominator.  $LST_{c,t,d}^{s}$  is the weighted average prediction from pixels of adjacent grids at time t of 360

day d (Eqs. 3, 4).  $Z_{m,t,d}$  represents the simulated LST difference between center c and one adjacent 361 pixel *m*. The spatial module  $(F_{m,t,d}^s)$  is activated only when there are valid neighboring ABI LSTs; 362 363 moreover, only the surrounding pixels with the same land cover as c were utilized for calculating  $LST_{c,t,d}^{s}$ , to minimize the bias caused by land cover differences (Nogueira et al., 2021). The MODIS 364 land cover data (MCD12Q1) were aggregated (water, forest, low vegetation, urban, and ice/snow) 365 to increase the classification accuracy. Therefore, the total number N equals the available clear-366 367 sky ABI pixels with the same land cover in the window, and the weight w was determined by the relative magnitude of inverse distance between each spatially adjacent pixel and c. The 368 spatiotemporal dynamic model was constructed with relative variation information of the 369 simulated LST, rather than the absolute magnitude, because the difference series can remove the 370 371 bias and keep the important dynamic modeling signals (Hong et al., 2021).

Before data assimilation is implemented, likely cloud-contaminated ABI LSTs need to be masked. It was assumed that the simulation might have higher uncertainty, but the modeling process was stable; thus, when a substantially abnormal difference between satellite retrieval and model simulation appeared near the clustered cloud pixels, it was more likely to be partially contaminated. After the spatiotemporal dynamic model was generated, and likely contaminated observations were removed, clear-sky ABI LSTs were assimilated into the modeling process, and the errors caused by model downscaling and predictions were corrected continuously.

379

380 *2.4 Data assimilation* 

381 KF is a data assimilation tool that uses discontinuous observations to correct model 382 prediction and modeling uncertainty, and ultimately obtains continuous and accurate estimations.

Each correction step is essentially the weighted average based on relative error magnitudes of 383 modeling and observation. For example, in Jia et al. (2021), LST time-evolving models are 384 corrected using satellite clear-sky LST retrievals, and formulate predictions on cloudy time based 385 on the corrected results. However, this preliminary scheme only utilized the temporal information. 386 In this study, A 3D-KF was proposed by revising the temporal KF, and a spatial module was 387 388 activated when the neighboring ABI LST was observed in a spatial window centered on pixel c. Adjacent, simulated LSTs were corrected first by corresponding ABI LSTs, and then LST at c 389 were predicted (Eqs. 3, 4). The spatial module helped the temporal module correct the predictions, 390 particularly when there were no observations at c, but neighboring ABI LSTs were available. The 391 392 temporal module of the 3D-KF was calculated according to Eqs. (5-8):

$$\widehat{LST_d^t} = A_{d-1}^t \widehat{LST_{d-1}} + \omega_{d-1}^t, \tag{5}$$

394 
$$\widehat{LST_d^t} = \widehat{LST_d^t} + K_d^t(LST_{d,c} - \widehat{LST_d^t}), \tag{6}$$

- 395  $K_k^t = P^-{}_d (P^-{}_d + R)^{-1}, \tag{7}$
- 396  $P_d = (I K_k^t) P_d^{-},$  (8)

where  $\widehat{LST_d^t}$  is the prior estimate of the temporal dynamic model  $(A_{d-1}^t, \text{ representing Eqs. 1, 2})$ 397 at center c on day d, from the previous filtered outcome  $\widehat{LST}_{d-1}$ . A symbol with – above indicates 398 that it is a prior prediction. And then the prediction error  $\omega_{d-1}^t$  is propagated to  $P_d^-$ . The initial 399 modeling error was calculated by referring to the corresponding ABILST at c, which did not affect 400 the overall accuracy because it is continuously corrected by observations, and the first computation 401 date is one month earlier than the starting date of the released product.  $\widehat{LST_d^t}$  is the corrected result 402 by filtering  $(K_d^t)$  the prior prediction  $(\widehat{LST_d^t})$  using the ABI retrieval  $LST_{d,c}$  (Eq. 6). The retrieval 403 error covariance R was set to 4 (Yu and Yu, 2020; Yu et al., 2019).  $K_d^t$  is based on the relative 404

405 magnitudes of  $P_d^-$  and R (Eq. 7), and the prediction uncertainty ( $P_d^-$ ) is then corrected to  $P_d$  by 406  $K_d^t$ , and *I* is a unit matrix (Eq. 8). More details can be found in Jia et al. (2021). The spatial module 407 is mathematically represented by Eqs. (9, 10):

408 
$$L\widehat{ST_{m,d}^s} = x_{m,d} + K_d^s (LST_{m,d} - x_{m,d}),$$
(9)

$$\widehat{LST_d^s}^- = \frac{\sum (A_d^s \widehat{LST_{m,d}^s} + \omega_d^s)}{N},\tag{10}$$

Eqs. 9–10 show that spatial KF  $(K_k^s)$  was implemented to assimilate surrounding clear-sky 410 retrieval  $(LST_{m,d})$  into spatially neighboring simulations  $(x_{m,d})$  with simulation error covariance 411 S, and the corrected spatial model prediction  $L\widehat{ST_{m,d}^s}$  was obtained at m with an error  $\omega_d^s$ .  $K_k^s$  is 412 calculated from S and R, similar to Eq. 7. The S was computed by referring to the ABI LSTs in the 413 spatial window and corrected to  $P_d^s$ , similar to Eq. 8. The predicted LST at c ( $\widehat{LST_d^s}^-$  in Eq. 10) 414 was computed by averaging predictions from all  $L\widehat{ST_{m,d}^s}$  in the spatial dynamic model  $(A_d^s)$ 415 representing Eqs. 3, 4), where N equals the available retrieved ABI LST, of which the prediction 416 error is  $P_d^{s-}$ . 417

418 On clear-sky conditions, the filtered LST estimate  $(\widehat{LST}_d)$  of c on d was the final clear-sky 419 LST output, by averaging the results from the temporal  $(\widehat{LST}_d^t, \text{Eq. 6})$  and the spatial  $(\widehat{LST}_d^s^-, \text{Eq. 420})$ 420 10) KF. Weights were based on the relative magnitude of the temporal and spatial module 421 uncertainties (Eq. 11).

422 
$$\widehat{LST}_{d} = \begin{cases} \frac{P_{d}^{S^{-}}}{P_{d}^{S^{-}} + P_{d}} \widehat{LST}_{d}^{t} + \frac{P_{d}}{P_{d}^{S^{-}} + P_{d}} \widehat{LST}_{d}^{s}^{-}, \text{ clear - sky} \\ \frac{P_{d}^{S^{-}}}{P_{d}^{S^{-}} + P_{-d}^{-}} \widehat{LST}_{d}^{t}^{-} + \frac{P_{-d}}{P_{d}^{S^{-}} + P_{-d}^{-}} \widehat{LST}_{d}^{s}^{-}, \text{ cloudy - sky} \end{cases}$$
(11)

423 On cloudy-sky conditions,  $\widehat{LST}_d$  is the reconstructed LST on cloudy-sky, the weighted 424 average from predictions from  $\widehat{LST}_d^{\overline{t}}$  (Eq. 5) and  $\widehat{LST}_d^{\overline{s}}$  (Eq. 10). Cloud effect ( $\Delta T_s$ ) correction is 425 required to convert the  $\widehat{LST}_d$  to final cloudy-sky LST output:  $LST_{cld} = \widehat{LST}_d + \Delta T_s$ .  $\Delta T_s$  is 426 introduced in Section 2.5.

The dynamic model with KFs was continuously processed for d+1 based on  $\widehat{LST}_d$ . The continuous LST series was reconstructed by 3D-KF, and the diurnal LST at clear-sky was essentially the weighted spatiotemporal fusion of ABI LSTs and model simulations. Further, the simulations during cloudy periods were also initially revised; however, the generated hypothetical LST required further correction by superposing the cloud effects based on SEB during day and nighttime.

433

### 434 2.5 Diurnal cloud effect

435 By reflecting the state of energy exchange, LST is an important component of the SEB (Eq.436 12):

 $R_n = DSR(1 - \alpha) + \varepsilon DLW - \sigma \varepsilon LST^4 = G + LE + H,$ (12)437 where  $R_n$  is the net radiation,  $\alpha$  is the surface albedo,  $\varepsilon$  is the broadband emissivity (BBE), and  $\sigma$ 438 439 is the Stefan–Boltzmann constant. The available energy is partitioned into ground heat (G), latent heat (LE), and sensible heat (H), and finally affects LST as the surface response. By following the 440 441 LSA-SAFs evapotranspiration algorithm (Arboleda et al., 2017), G was estimated by partitioning  $R_n$  according to LAI. The energy partitioning parameter is set to 0.15, 0.05, and 0.10 for rocks, 442 snow, and inland water, respectively (Jia et al., 2021). G can also be expressed using the 443 conventional force-restore method (Jin and Dickinson, 2000): 444

$$G = k_g \frac{\partial T}{\Delta h} = k_g \frac{LST - T_d}{\Delta h},\tag{13}$$

where  $k_g$  is the surface thermal conductivity (W·m<sup>-1</sup>·K<sup>-1</sup>), and  $\Delta h$  is the depth of the subsurface layer (0.1 m). By assuming that the subsurface layer temperature ( $T_d$ ) is insensitive to SEB, Eq. 13 can be revised as follows (Eq. 14):

445

449 
$$\frac{\partial G}{\partial LST} = \frac{\partial}{\partial LST} \left[ k_g \frac{LST - T_d}{\Delta h} \right] \approx \frac{k_g}{\Delta h}, \tag{14}$$

where  $\partial G$  can be considered the change in ground heat caused by cloud cover, partitioned from the CRE. Thus, after estimating  $k_g$ , the heat change can be converted to the corresponding cloud effect ( $\Delta T_s$ ). Essentially,  $k_g$  indicated the local sensitivity of LST response to the SEB. By taking advantage of the high temporal resolution of diurnal LST, a novel method for estimating  $k_g$  was created (Eq. 15):

$$k_g = \Delta h \frac{\overline{G_{noon}} - \overline{G_{sr}}}{\overline{LST_{noon}} - \overline{LST_{sr}}},$$
(15)

where  $\overline{G_{noon}}$  ( $\overline{LST_{noon}}$ ) and  $\overline{G_{sr}}$  ( $\overline{LST_{sr}}$ ) are the monthly (±15 days) averaged ground heat (clear-456 sky LST) at noon and sunrise, respectively. It was assumed that morning warming was primarily 457 due to the radiation budget; the continuous LST series was obtained from data assimilation, and G 458 was estimated from clear-sky radiation data with LAI. The monthly mean was utilized because the 459 surface property was assumed to be stable in closing days, while the DTC on any specific day 460 could be disturbed by meteorological conditions; thus, the difference in LSTs in Eq. 15 may be 461 too small to generate  $k_g$  accurately. Monthly averaging can therefore remove these disturbances. 462 Clear-sky heat and temperature series were chosen to estimate  $k_g$ , as clear-sky LSTs have a clearer 463 response to morning warming influenced by SEB. 464

465 Therefore, the primary objective of diurnal cloud effect estimation was to quantify the 466 diurnal CRE. CRE will be estimated by hourly cloudy-sky and clear-sky radiation fluxes in order

to quantify the impact toward LST from different cloud conditions. Previous studies aiming to 467 estimate cloudy-sky LST based on SEB have mainly built a linear relationship between DSR and 468  $R_n$  (Jin, 2000; Yu et al., 2014; Zeng et al., 2018). This is because shortwave net radiation is the 469 principal driving factor of daytime  $R_n$  (Jiang et al., 2018; Wang and Liang, 2009); however, 470 nighttime cloudy-sky LST cannot be recovered. Instantaneous longwave CRE has historically been 471 difficult to estimate in previous studies, as such cloudy-sky LSTs are a basic parameter. 472 Accordingly, an innovative optimization method was created here to determine the diurnal net 473 CRE by separating the hourly shortwave (CRE<sub>short-net</sub>) and longwave (CRE<sub>long-net</sub>) components. 474 CRE<sub>short-net</sub> can be easily calculated from surface albedo and the difference of ABI all-sky and 475 CERES clear-sky DSRs [Eq. 9 in Jia et al. (2018)], whereas CRE<sub>long-net</sub> needs to be estimated as 476 477 follows:

478  $CRE_{long-net} = (\varepsilon DLW_{cld} - \sigma\varepsilon (LST_r + \Delta T_s)^4) - (\varepsilon DLW_{clr} - \sigma\varepsilon LST_{clr}^4),$  (16) 479 where  $LST_r$  was reconstructed by the data assimilation step, and  $\Delta T_s$ ,  $DLW_{clr}$ , and  $DLW_{cld}$  were the 480 unknown variables.

Current DLW parameterizations are difficult to apply, as most existing satellite-based 481 482 algorithms depend on parameters that are not readily accessible from space (Cheng et al., 2019), such as the liquid water path, vapor pressure, and cloud base temperature. To this end, Wang et al. 483 (2020) developed a practical all-sky DLW parameterization scheme that employs available 484 satellite input data. By combining the CERES data, with MODerate resolution atmospheric 485 TRANsmission (MODTRAN) simulations, a global training database with approximately 55,664 486 records for cloudy-sky, and 62,806 for clear-sky conditions was constructed. This algorithm has 487 been used for hourly, all-sky DLW product generation (Letu et al., 2021). Based on the integrated 488 489 training samples, the relationship was built using a general parameterization scheme [Eqs. 1 and 2 in Wang et al. (2020)] and a random forest machine-learning scheme, separately. Two methods perform close accuracy, achieving greater levels of RMSE (~22 W·m<sup>-2</sup>) and feasibility over large regions compared to earlier studies. In the parameterizations, CWV was obtained from ERA5, and official CTT data is released by the GOES-16 product suite.

As cloudy-sky LST is required for calculating longwave radiative effect (Eq. 16), an 494 optimization method is necessary to obtain the best  $\Delta T_s$  to balance the energy in previous equations. 495 In the initial calculation,  $\Delta T_s$  was assumed to be 0 K in Eq. 16, and the initial CRE was computed. 496 After partitioning the CRE to ground heat through the LAI, an updated  $\Delta T_s$  was estimated using a 497 498 predetermined  $k_g$ ; thus, the CRE can be recomputed. By iteratively comparing the CRE differences and adjusting  $\Delta T_s$  (0.05 K in each iteration), the surface energy budget will become 499 balanced ( $|\Delta CRE_{long}| \le 20 \text{ W} \cdot \text{m}^{-2}$ ; see Figure 2). The threshold was not set to  $0 \text{ W} \cdot \text{m}^{-2}$ , as the DLW 500 parameterization RMSE was ~20 W·m<sup>-2</sup> (Wang et al., 2020). 501

502

# 503 2.6 Daily mean LST calculation

504 After retrieving the diurnal, all-sky LST, daily mean LST was readily calculated. To assess 505 its accuracy, it was validated by site measurement, and the accuracy statistics were compared with three other results: one was from the official ABI LSTs, where 24 clear-sky values are available 506 per day. The second is the daily mean from spline-interpolated 24 values in a day, and such 507 comparison will demonstrate if the diurnal hourly LST of the proposed product is representative 508 for daily-mean LST calculation, or whether users need to do the interpolation to obtain the daily 509 mean by themselves. Spline interpolation is a piecewise polynomial interpolation, and it can 510 accurately capture the variation details as we have 24 values in a diurnal cycle. 511

512 The second was the mean of two LSTs from Aqua (MYD11) at noon and midnight each day (Ouyang et al., 2012; Xing et al., 2021). This simple method has been commonly utilized in 513 LST applications, such as temporal upscaling (Chen et al., 2017), evapotranspiration (ET) 514 estimation (Yao et al., 2013), and permafrost monitoring (Zou et al., 2017). The last method 515 utilizes a DTC model to interpolate the four observations from Terra + Aqua (MOD11 + MYD11) 516 517 and obtain the daily mean LST. Based on a comprehensive review of DTC models (Hong et al., 518 2018), the GOT09 model (Göttsche and Olesen, 2009) was selected. By assuming day-to-day 519 change of residual temperature  $\delta T = 0$  and free attenuation time  $t_s$  = sunset time – 1, four unknown parameters were determined via the four observations of MOD11 + MYD11 in a day. More details 520 about GOT09 can be found at Eq. 2 in Hong et al. (2018). 521

522

# 523 **3. Results, analysis, and discussion**

### 524 *3.1 Configuration determination*

By assuming that 18 evenly distributed sites can represent the general surface conditions over CONUS, all-sky hourly LSTs were generated using different window sizes of the dynamic model (different schemes), and then the accuracies were compared to determine the optimal configuration. Owing to computational resource limitations, only samples from different schemes in 2019 (N = 148,008 in each scheme) were used in the test.



Figure 3. Overall accuracy (RMSE) of diurnal LSTs according to variable spatial window size for (a) clear-and (b) cloudy skies.

From Figure 3, it can be observed that the overall RMSE decreased when the spatial 533 window size increased from 0 to 150 km, especially at night (Figure 3a and 3b). By including the 534 spatial module, the nighttime cloudy-sky LST can improve the RMSE by ~0.4 K. Daytime LST 535 showed a smaller response for window size selection. Further, it was inferred that daytime LSTs 536 537 have stronger heterogeneity due to the SEB warming effect; thus, adjacent pixels at relatively farther locations may not benefit model correction, while larger spatial windows will substantially 538 increase computation time. Accordingly, based on the site assessments over the CONUS, a 150-539 km window size was selected for data production. 540



541

542 Figure 4. Overall accuracy (RMSE) during short-term cloud duration, with and without cloud effect543 correction, for the (a) daytime and (b) nighttime.

In order to check the necessity of cloud effect correction for short-term cloud duration 544 cases, corresponding analysis are shown in Figure 4. It indicates that cloud effects could be 545 546 neglected if the cloud coverage time was <2 h. The hypothetical clear-sky LST of 3D-KF during 547 short-term cloud coverage ( $\leq 6$  h) was tested, and the impacts of adding the estimated cloud effects 548 were analyzed. It was revealed that cases of cloud coverage <2 h may increase uncertainty after 549 adding the cloud effects during both the daytime and nighttime (Figure 4a and 4b). Previous research has demonstrated that the DTC interpolation model works well when the cloud duration 550 is <4 h (Göttsche and Olesen, 2001), as the LSTs in such circumstances may not be considerably 551 affected by clouds. Compared with the analysis in Figure 4, we determined that cloud effects were 552 ignored if coverage was <2 h in the production. Moreover, daytime hypothetical clear-sky LST 553 uncertainty increases with cloud duration (Figure 4a), and the cloud effect does well to address the 554 555 error accumulation. Following the basic configuration tests, the all-sky hourly LSTs were derived 556 and assessed.

557

## 558 3.2 Validation

The overall accuracy of the diurnal all-sky LST estimation using *in situ* measurements of the 18 field sites is shown in Figure 5. The validation results for the all-sky LSTs, and the official NOAA ABI LSTs were compared during daytime and nighttime from July 2018 to June 2021.





Figure 5. Density scatterplots of LST samples from (a) present study, daytime clear-sky; (b) present study,
nighttime clear-sky; (c) official ABI, daytime clear-sky; (d) official ABI, nighttime clear-sky; (e) present
study, daytime cloudy-sky; and (f) present study, nighttime cloudy-sky.

569

570 The resulting product from the present study had higher accuracies than the official NOAA 571 ABI clear-sky LST product, during both the daytime and nighttime. The daytime clear-sky samples of this study (Figure 5a) had an RMSE of 2.37 K (N = 85,565), whereas the corresponding official 572 ABI LST product had an RMSE of 2.73 K (Figure 5c). The nighttime clear-sky samples (Figure 573 5b) had an RMSE of 2.24 K (N = 92,179), whereas the official ABI LST product had an RMSE of 574 2.86 K (Figure 5d). The latter product included some cloud-contaminated samples, particularly at 575 576 night (Figure 5d), even all extracted samples of the NOAA ABI LST were marked as "goodretrieval" in the quality control flag. The contaminated pixels were distributed across Figures 5c 577 578 and d, thereby creating a larger negative bias in the clear-sky validations.

579 Daytime cloudy-sky samples had an RMSE of 2.78 K (N = 130,488; Figure 5e), and 580 cloudy-sky nighttime samples had an RMSE of 2.23 K (N = 100,068; Figure 5f). Based on all 581 hourly, all-sky LST samples, the overall RMSE was 2.44 K, with a bias of -0.19 K, and an  $R^2$  of 582 0.97 (N = 408,300). Likely cloud-contaminated cases identified in the data assimilation step were 583 validated in Figure 6, while the corresponding corrected results were also included for comparison.



#### 584

Figure 6. Scatterplot of likely cloud-contaminated samples from the official NOAA ABI and correctedresults.

587

588 Figure 6 indicates that the likely cloud-contaminated pixels were recovered well. The marked official NOAA ABI LST samples had an overall RMSE of 7.99 K, largely driven by the 589 590 negative bias of -5.58 K. Partially cloud-covered pixels typically have lower BT values than ground signals, resulting in abnormally cool LSTs in the images. Besides, some samples with 591 considerably positive bias were also detected, which might be caused by the difference of the 592 realistic surface emissivity and the climatological emissivity used in the GOES-16 LST production 593 (Yu and Yu, 2020), and BTs with low signal-noise-ratio could be another reason. Previous studies 594 generally ignored these disturbances that may introduce considerable uncertainties into the 595 596 interpolation results. Comparatively, the accuracy of the recovered samples from this study was substantially improved (RMSE = 3.57 K). It should be noted that some clear-sky pixels might be 597 included in Figure 6, but such misclassification won't affect the overall cloudy-sky LST estimation 598 accuracy, owing to the high tolerance toward long cloud duration (see Section 3.3). 599



Figure 7. Comparison of the RMSE for all sites, during the (a) daytime and (b) nighttime. The radius shows
RMSE values (unit: K), and exterior numbers represent the site order as indicated in Table 2.

600

The RMSE value comparisons for all the sites are shown in Figure 7. This suggests that 603 the all-sky LST derived here was more accurate than the NOAA ABI across nearly all sites. NOAA 604 605 ABI generally had larger RMSE patterns, especially at US-Ro5 (site 15) and US-UMB (site 18) during the nighttime (Figures 7b). Clear-sky samples of all-sky LST displayed relatively consistent 606 accuracy levels across both the daytime and nighttime. Further, the cloudy-sky estimation accuracy 607 was comparable to that of clear-sky LST estimates, but with a lower accuracy at TBL (site 7) and 608 US-SRM (site 16) during the daytime. Based on further analyses, high elevations of the two sites 609 might be the major reason that causes lower site surface representativeness (Figure 10c) and larger 610 611 estimation uncertainties (Figure 14a).



Figure 8. Comparison of the (a, b) RMSE and (c, d) Bias by hours in a day at (a, c) clear-sky and (b, d)
cloudy-sky. Samples have been converted to the local time of each site.

The clear-sky and cloudy-sky LSTs at different hours in a day have been assessed, of which accuracies have also been compared with two hourly all-sky LST reanalysis datasets (Figure 8) to highlight the superiority of the proposed data. As the only currently available all-sky LST driven by satellite retrieval over CONUS and Mexico, the proposed all-sky LST performs considerably better than the simulated datasets at different hours under both clear-sky and cloudy-sky. RMSEs of the present study vary between 2.0-3.1 K at different times with bias within ± 0.7 K, and RMSEs
at noon are relatively larger (Figure 8a and 8b) partly because the daytime surface is warmer that
may increase the surface heterogeneity issue of site validation (Ma et al., 2021; Yoo et al., 2018).
Reanalysis skin temperatures show a similar RMSE peak at noon; however, the uncertainty of
NLDAS is large at night, which is attributed to the substantial cold bias (Figure 8c and 8d) (Xia et
al., 2015). In comparison, ERA5-Land is more accurate than NLDAS, and even biased simulation
is still an issue (Nogueira et al., 2021).

Accuracies of hourly LST reconstruction from previous algorithms and products have been 628 summarized in Table 3. It shows the scarcity of hourly all-sky LST products, and the proposed all-629 sky hourly LST data perform high accuracy and advancement. It should be noted that some studies 630 utilized an assessment method by comparing reconstructed LST with the officially retrieved LST 631 632 values at artificial gaps. Such an assessment method has little surface heterogeneity issue, whereas 633 it may not reflect the realistic cloud effect. Moreover, it may overrate the accuracy and feasibility of interpolation-based methods because artificial gaps generally have considerably smaller 634 635 spatiotemporal scales than the realistic cloud, and they are essentially clear-sky LST series that have a smooth DTC curve while the cloudy-sky LST does not (Figure 10a). 636

637 **Table 3.** Accuracy summary of reconstructed hourly LST from previous studies.

Paper	Methodology	Outcome	Accuracy (RMSE)	Sensor	Reference data
Dumitrescu et al. (2020)	Fusion with ERA5 skin temperature	algorithm	2.46-3.35 K	MSG/SEVIRI	officially retrieved LST at artificial gaps

Liu et al. (2017b)	DTC model- based interpolation	algorithm	0.77-1.36 K	FY-2F	officially retrieved LST at artificial gaps
Wu et al. (2019)	CNN-based interpolation	algorithm	≤1 K	FY-2G and MSG/SEVIRI	officially retrieved LST at artificial gaps
Lu et al. (2011)	SEB	algorithm	5.11-5.55 K	MSG/SEVIRI	ground site measurement
Zhang et al. (2015a)	DTC model + SEB	algorithm	1.34-1.44 K	-	site measured LST at artificial gaps
Zhang et al. (2017)	SEB	algorithm	7 K	FY-2D	ground site measurement
Martins et al. (2019)	SEB	product	2.1-3.7 K	MSG/SEVIRI	ground site measurement

All-sky hourly LST provides a great opportunity for LST upscaling. The accuracy of daily
mean LST generated by this study was also evaluated and compared with traditional methods in
Figure 9.





Figure 9. Scatterplots of daily mean LSTs from: (a) directly averaging 24-h values, (b) spline interpolation
24-h values, (c) paired Aqua LSTs, and (d) 4-values (Terra + Aqua) DTC interpolation.

643

Figure 9 illustrates the daily mean LST accuracies, as estimated from the diurnal all-sky 646 LSTs, clear-sky NOAA ABI, two Aqua MODIS LSTs, and interpolated four Terra + Aqua MODIS 647 observations. By directly averaging 24 hourly values, diurnal all-sky LSTs provided high accuracy 648 649 estimates of the daily mean LSTs (RMSE = 1.13 K). Figure 9a shows that the daily mean of the all-sky LST is more accurate than the daily mean of the NOAA ABI for completely clear days 650 (RMSE = 1.39 K). NOAA ABI had a relatively larger negative bias (Figure 9a), and it was thus 651 inferred that its daily mean was influenced by cloud contamination. After spline interpolation, the 652 daily mean LST accuracies were not improved, and the correlated bias was only slightly corrected 653 (Figure 9b), indicating that users don't need to interpolate the 24 values for the temporal upscaling. 654

Daily mean LSTs from averaged MYD11 data (Figure 9c) had the largest RMSE (2.48 K).
After interpolating four observations from Terra and Aqua in a day using the DTC model (Section
2.6), the resulting daily mean had an RMSE of 1.53 K (N = 1250, Figure 9d), similar to what was
derived previously (Hong et al., 2018); however, the requirement of four observations per day
constrained its available sample number. In comparison, diurnal, all-sky LSTs showed superiority

when estimating daily mean LSTs, and thus has great potential for use in related applications
(Gallego - Elvira et al., 2016; Yao et al., 2013; Zhi-xia et al., 2011). Temporal analysis is shown



662 in Figure 10 at hourly and daily-mean scales.

Figure 10. Time series of hourly (a-d) and daily mean (e, f) LSTs at: (a, b, and e) BND and (c, d, and f)
TBL. Hourly LSTs were randomly selected from different seasons in 2020 and converted to local time.

670

The hourly and daily mean LST time series are shown in Figure 10 for representative sites 671 with relatively higher and lower accuracies. Hourly LST variations in Figure 10 a-d reveal that the 672 673 proposed all-sky LST well captured the realistic DTC no matter in clear days or cloudy days. Continuous cloudy days were also recovered, and the overall patterns were well matched (Figure 674 10a and 10b). Besides, these continuous cloudy cases also indicate the limitation of interpolation-675 based LST reconstruction methods as they have more various temporal patterns. Relatively larger 676 biases were found at TBL sites, especially at noontime (Figure 10c), partially due to the higher site 677 678 heterogeneity issue at noon.

Time series analysis of daily mean LSTs indicated that the all-sky LSTs were temporally 679 contiguous, and captured not only the general patterns but also the anomalous variations; in 680 addition, the accuracy underwent few changes over the years analyzed. The LST series at BND 681 maintained relatively high levels of accuracy, matching well with the ground-derived 682 measurements (Figure 10e). Comparatively, the LST series at TBL had the lowest accuracy of the 683 seven SURFRAD sites, revealing that all-sky LSTs were underestimated, especially in the 684 summers (Figure 10f). TBL site is at a relatively higher elevation surrounded by more complex 685 terrain, and the relatively lower surface representativeness of TBL may partly explain the larger 686 RMSE (Guillevic et al., 2014). The all-sky hourly LSTs were also mapped by randomly choosing 687 three images from three seasons in 2019 for comparison with the official NOAA ABI data. 688

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Apr. 29, 2019: 1600 (UTC)



Figure 11. Hourly LSTs (unit: K) for: (a, d, g) all-sky LSTs from the present study; (b, e, h) NOAA ABI
LST; and (c, f, i) the differences between the two.

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Figure 11 suggests that the SEB-based method effectively recovered the all-sky diurnal
LST patterns across different seasons, as well as the successful removal of cloud-contaminated
pixels. The all-sky LSTs in Figure 11a, 11d, and 11g match with the NOAA ABI (Figure 11b, 11e,

701 and 11h), and the estimated cloudy-sky LSTs are spatially continuous with the clear-sky pixels. In 702 addition, based on the differences of all-sky and NOAA ABI LSTs, considerably positive (dark 703 red) biases were observed along the edge of cloud patterns, as can be seen scattered in the central area of Figure 11f, and north-eastern area of Figure 11i. The partly cloud-covered pixels typically 704 had substantially cooler BTs than the pure surface signals, resulting in negative biases 705 706 reaching >20 K (Figure 6). Some mismatch appears at the west highland region partially due to 707 the larger estimation uncertainty (Figure 14a). A detailed analysis of the LST map at the middle 708 of the CONUS (Figure 11f) was illustrated in Figure 12.





Figure 12. Regional LST maps at the marked place in Figure 11(f): (a) all-sky LST, (b) NOAA ABI, (c)
pixels marked as likely cloud-contaminated, and (d) corresponding false-color image from red, nearinfrared, and blue bands.

Figure 12 indicates that all-sky LST can well capture the regional variation with good 714 715 spatial consistency. Compared with the clear-sky retrieval of NOAA ABI (Figure 12b), it can 716 reflect spatial details, no matter at clear-sky (bottom left, Figure 12a) or cloudy-sky (top left, Figure 12). Besides, Figures 12a and 12d illustrate various cloud effects of different clouds: cooling effect 717 718 is shown under thick cumulus in the middle, whereas cirrocumulus clouds have little cooling effect because they pass most solar energy through the atmosphere (top left, top right, and bottom right 719 in Figure 12d). However, Figure 12a has a smooth effect over the cloud recovered regions. This is 720 721 mainly due to the less spatial heterogeneity of cloudy-sky LST. In addition, 3D-KF might have 722 filtered some spatial texture after fusing the clear-sky retrieval with simulated LSTs. Texture information from adjacent days is not easily referred to when there is a long cloud duration. Figure 723

12c shows that the detected cloud-contaminated pixels are mainly around the cloud pixels; besides,

cloud contamination easily happens under the coverage of cirrocumulus (Figure 12d).

# 726 3.3 Impacts of cloud duration and surface elevation

Based on the assessment above, sensitivity analyses were performed to assess the
robustness of the generated all-sky LST product toward extreme cloud and local conditions.



Figure 13. Overall accuracy by cloud duration, during the (a) daytime and (c) nighttime; (b, d) display thecorresponding available sample numbers.

As continuous cloud duration for long periods may temporally detrimentally affect prediction accuracy until an observation is assimilated, the overall accuracy change with increasing cloud duration was quantified (Figure 13). The analyses revealed that both daytime and nighttime cloudy-sky LSTs maintained stable RMSEs. Notably, most observed cloud durations are less than 10 days, and the longer cloud duration cases that statistical numbers are less than 100 (<0.1% of the total number) were ignored (Figure 13b and 13d). Cloud duration information is included in the data quality mark, allowing users to perform quantitative analyses for specific regions orperiods they plan to use.



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Figure 14. Accuracy of each site under clear- and cloudy-sky conditions, as a function of (a) surface
elevation and (b) latitude.

The relationship between site accuracy by elevation is shown in Figure 14, revealing the correlation between accuracy and elevation. As elevation increases, as do terrain complexity and surface heterogeneity, creating difficulties for modeling simulations (Figure 14a). The impact of site latitude was also explored, as it determines the view zenith angle (VZA) of the NOAA ABI LSTs, and it has previously been found that as the VZA increases, retrieval accuracy may decrease (Yu et al., 2008). However, no such relationship was revealed here, leading to the conclusion that the all-sky LSTs produced over the CONUS all maintained relatively small VZAs (Figure 14b).

# 751 *3.4 Land cover-dependent DTC climatology*

DTC analyses were implemented to demonstrate that the all-sky LST product can successfully capture DTC variability. Climatological DTCs for different land cover types were characterized (Figure 15), and can potentially be used to quantify temperature feedbacks related 755 to landcover change, and the orbit drift correction of Advanced Very High Resolution Radiometer (AVHRR) LST data (Jin and Treadon, 2003). The climatological DTCs are the multiple years' 756 averages of DTC for different land cover types, which represent the general variation of DTC and 757 climatological feedback by ignoring meteorological disturbance in one specific year. 758



761 Figure 15. Climatological DTCs for different land cover types: (a) forest, (b) shrubland, (c) grassland, (d) 762 cropland, (e) urban, and (f) barren area.

Landcover type appears to be a major factor when determining DTCs, where forests 763 displayed the smallest diurnal temperature range (DTR), and barren areas had the largest DTR, 764 capable of reaching  $\geq$  30 K in summer. In addition, the temperature rise time of DTCs got delayed 765 from summer to winter as a result of the sunrise time change based on SEB. Barren areas had the 766 strongest response toward SEB, at both daily and seasonal scales, as local evapotranspiration is 767 limited, and most available surface energy is partitioned into sensible and ground heat. Notably, 768

geolocations (latitude and elevation) are also key factors influencing DTCs, and the cycle
differences for various land cover types may be in part affected by them, e.g., crops are mainly at
relatively high latitudes (Figure 1) and have smaller LSTs and DTCs.

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## 773 4. Conclusions

774 By characterizing high-frequency surface thermal dynamics at medium spatial scales, GEO 775 LSTs become invaluable for relevant studies; however, cloud coverage creates missing data and abnormal retrievals of these products, and there are few all-sky GEO LST products available to 776 the public. Methods for GEO LST recovery have been reviewed here, revealing the following 777 conclusions: the model fusion-based method is guaranteed gap-free, although the simulation on 778 cloudy days is rarely corrected effectively; interpolation-based methods have lower accuracy and 779 780 feasibility across larger cloud scales, nor can their results reflect realistic cloud effects on LSTs; and traditional SEB-based methods can estimate cloudy-sky LSTs, but the input requirements 781 severely constrain its application, particularly at nighttime. In addition, few studies have discussed 782 partial cloud contamination, an issue creating considerable uncertainty when interpolated. 783

Based on the SEB, a 2-km all-sky, diurnal hourly LST product over the CONUS and Mexico was created from July 2017 to June 2021. First, an original spatiotemporal dynamic model was built by ERA5, and GOES-16 ABI LST was then assimilated using 3D-KF. Finally, an innovative optimization method was proposed to estimate the diurnal cloud effects from multiple satellite radiation products, and partially cloud-contaminated pixels were also recovered.

The comprehensive assessment demonstrated the high accuracy and robustness of the allsky LSTs using 18 sites from SURFRAD and core AmeriFlux. The RMSE values of the generated

791 clear-sky samples for the daytime and nighttime were 2.37 and 2.24 K, respectively, which is a 792 notable improvement over the official NOAA ABI. Further, the cloudy-sky samples during the daytime and nighttime revealed RMSE values of 2.78 and 2.23 K, respectively. Accordingly, the 793 generated all-sky LSTs had an overall RMSE of 2.44 K, with a bias of -0.19 K and an R<sup>2</sup> value of 794 0.97 (N = 408,300), and RMSEs at different times in a day varied from 2.0 to 3.1 K. By simply 795 averaging the diurnal hourly LSTs, the accuracy of the daily mean LST increased (RMSE = 1.13) 796 797 K) compared to the daily means from paired Aqua LSTs and DTC model interpolation. Time series 798 analysis suggested high diurnal and interannual accuracy, and mapping analyses illustrated that the recovered cloudy-sky pixels had good spatial continuity across different seasons. Cloud-799 800 contaminated pixels, shown at the cloud edges of the official clear-sky ABI images, were also 801 recovered.

The sensitivity analyses indicated the robustness of the all-sky LSTs for different cloud and geolocation conditions. The proposed data have a high tolerance toward long cloud duration. Moreover, higher elevations may decrease the estimation accuracy of cloudy times, although the VZA had little impact on product accuracy over the study area observed. DTC analysis showed climatologically seasonal variations across different land cover types, demonstrating that the allsky hourly LST product was superior for characterizing DTC variability, and has great potential for future research use.

Ground validation and DTC analyses exhibited the readiness and robustness of this approach for further scientific application. The proposed method here is sensor-independent, and can potentially be implemented for other similar GEO LST products. Based on the results of the present study, all-sky diurnal air temperature and heat fluxes will be the focus of future research.

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## 827 Author contributions

S. Liang conceived the scope of this study; A. Jia processed the data; A. Jia, S. Liang, and D. Wang
interpreted the results; A. Jia wrote the manuscript. All authors contributed to the revision of the
article.

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## 832 Declaration of Competing Interest

833 The authors declare that they have no known competing financial interests or personal834 relationships that could have influenced the work reported in this paper.

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