Disaggregation of Remotely Sensed Land Surface Temperature: A New Dynamic Methodology

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KEY POINTS

- A dynamic methodology that disaggregates the controlling parameters rather than LSTs is proposed for DLST
- Diurnal and annual temperature cycle models are used to help DLST
- A modulation process that adds thermal details to coarse LSTs is incorporated

ABSTRACT

The tradeoff between the spatial and temporal resolutions of satellite-derived land surface temperature (LST) gives birth to disaggregation of LST (DLST). However, the concurrent enhancement of the spatio-temporal resolutions of LST remains difficult, and many studies disregard the conservation of thermal radiance between pre- and post-disaggregated LSTs. Here, we propose a new dynamic methodology to enhance concurrently the spatio-temporal resolutions of satellite-derived LSTs. This methodology conducts DLST by the controlling parameters of the temperature cycle models, i.e., the diurnal temperature cycle (DTC) model and annual temperature cycle (ATC) model, rather than directly by the LST. To achieve the conservation of thermal radiance between pre- and post-disaggregated LSTs, herein we incorporate a modulation procedure that adds temporal thermal details to coarse resolution LSTs rather than straightforwardly transforms fine-resolution scaling factors into LSTs. Indirect validations at the same resolution show that the mean absolute error (MAE) between the predicted and reference LSTs is around 1.0 K during a DTC; the associated MAE is around 2.0 K during an ATC, but this relatively lower accuracy is due more to the uncertainty of the ATC model. The upscaling validations indicate that the MAE is around 1.0 K and the normalized mean absolute error (NMAE) is around 0.3. Comparisons between the DTC- and ATC-based DLST illustrate that the former retains a higher accuracy, but the latter holds a higher flexibility on days when background low-resolution LSTs are unavailable. This methodology alters the static DLST into a dynamic way and it is able to provide temporally continuous fine-resolution LSTs; it will also promote the design of DLST methods for the generation of high-quality LSTs.

KEY WORDS

Land surface temperature; dynamic disaggregation; diurnal temperature cycle; annual temperature cycle; temperature cycle model; surface energy balance; and MODIS.

1. INTRODUCTION

Land surface temperature (LST), a variable that directly affects the longwave radiation emitting into the atmosphere, and the heat flux transferring downward into subsurface, is crucial to the net surface radiation and energy budget as well as a number of biogeochemical processes. As a physical relatively easy for precise measurements, LST has been becoming one of the many basic and important indicators for global climate change [*IPCC*, 2013].

Thermal infrared sensors onboard satellites convey a unique approach to sample LST in an effective and low-cost way. To cover the majority of the earth's surfaces, a satellite sensor with a lower spatial resolution usually samples the surface with a wider swath, therefore leading to a more frequent revisit, and *vice versa*. Such a sampling style initiates a tradeoff between the spatial and temporal resolutions among satellite-derived LSTs. This dilemma gives rise to the disaggregation of remotely sensed land surface temperature (DLST), which at least dates back to 1980s [*Dozier*, 1981]. The development of DLST continued but it experienced a slow development in the 1990s, due in part to the lack of satellite missions of thermal sensors within this period. Since the 2000s, DLST has again become the focus of researchers and has been experiencing a remarkable growth due to the availability of various spaceborne sensors that regularly sample LSTs (e.g., ETM+ and ASTER since 1999; MODIS since 1999 and 2002). In the recent decade, the significant growth has also been motivated by mounting requirements for monitoring surface evapotranspiration [*Anderson et al.*, 2012] and urban thermal environment [*Zhou et al.*, 2013], both regionally and globally. The past three-decade-long developments of DLST have resulted in a comprehensive literature survey by *Zhan et al.* [2013] and a generalization paradigm by *Chen et al.* [2014]. The recent years (2012-) have witnessed the further prosperity of DLST [*Bindhu et al.*, 2013; *Merlin et al.*, 2012; *Sismanidis et al.*, 2015; *Teggi and Despini*, 2014].

Throughout the development of DLST, most methods, except for a very few (e.g., *Inamdar et al.* [2008]) before 2012, usually disaggregated an instantaneous coarse LST into a fine-resolution one at a time − LST images at different time nodes were processed separately (hereafter this type of DLST is termed purely static). However, a notable feature of LST comes from its fast diurnal or annual dynamics − its variations are significant even within a short period (e.g., five minutes). The purely static DLST is thereby insufficient. Recent investigations have noticed this insufficiency and there exist three categories of approaches considering this dynamics.

The first approach considers the fast dynamics of LST by integrating land surface models (hereafter this approach is termed DLST_{LSM}) [*Mechri et al.*, 2014]. The DLST_{LSM} is relatively complex and not easy to implement at multiple spatial and temporal scales. The second approach directly disaggregates high-frequency thermal observations such as LSTs retrieved from geostationary satellites (hereafter termed $\text{DLST}_{\text{GEOS}}$), which already contain the information on LST dynamics [*Addesso et al.*, 2014; *Bechtel et al.*, 2012; *Inamdar and French*, 2009; *Keramitsoglou et al.*, 2013]. The $\text{DLST}_{\text{GEOS}}$ has been more or less integrated the diurnal dynamics of LST into DLST [*Zakšek and Oštir*, 2012]. Nevertheless, most of this type of approaches remain disaggregating LSTs statically, wherein temperature cycle models are not incorporated, and therefore the disaggregated LSTs are temporally inextensible. That is, LSTs are only disaggregated at the time nodes at which thermal observations are available. This becomes more problematic when temporally sparse LSTs (e.g., LST products obtained by Landsat series) need to be disaggregated at a time node between two transits, because the time gap between transits is large.

To overcome the structural complexity of the $DLST_{LSM}$ and the temporal inextensibility of the $DLST_{GEOS}$, the third approach makes a compromise between the previous two. It considers the fast dynamics of LST by resorting to temperature cycle models (hereafter it is termed $DLST_{TCM}$) − either by a diurnal temperature cycle (DTC) model [*Zhou et al.*, 2013] or an annual temperature cycle (ATC) model [*Weng et al.*, 2014]. The $DLST_{TCM}$ is relatively simple when compared with the $DLST_{LSM}$ while it becomes temporally extensible when compared with the $DLST_{GEOS}$. The $DLST_{TCM}$ has received more considerations recently and it can even be used to estimate subpixel component surface temperatures [*Quan et al.*, 2014a].

Though advancements have been made on the $DLST_{TCM}$, the following challenges remain. First, temperature cycle models in the $DLST_{TCM}$ were only used for fitting disaggregated LST time series; the information on surface physical properties contained in the controlling parameters of the dynamic models remains unexplored. LST is a variable regulated by both surface physical properties and atmospheric status, two facets that, respectively, control the local thermal heterogeneity and the large-scale thermal background of the surface-atmosphere interaction. Previous approaches that solely concentrate on LST but hardly pay close attention to the controls of LST dynamics are methodologically insufficient and, as a result, make the concurrent enhancement of the spatial and temporal resolutions difficult. Second, the success of the two benchmark DLST methods, i.e., *Kustas et al.* [2003] and *Agam et al.* [2007], can be attributable to the inclusion of the modulation process that aims to keep the approximate consistency of thermal radiance (usually approximated as LST) between pre- and post-disaggregated LSTs at a certain block of pixels [*Zhan et al.*, 2011]. Nevertheless, such a modulation process was ignored by many previous approaches that are based on temperature cycle models, making the pre- and post-disaggregated LSTs no longer consistent. Finally, previous $DLST_{TCM}$ was performed within either the DTC or the ATC − these two cycles were rarely investigated together. The DTC and ATC models are nevertheless interrelated because both of them are constructed based on the heat conduction equation when constrained by the surface energy balance (SEB) formula as boundary condition [*Zhan et al.*, 2014].

Facing these challenges, our current study continues to use temperature cycle models that have been adopted by the $DLST_{TCM}$ to solve the temporal inextensibility. To achieve the concurrent disaggregation of the spatial and temporal resolutions during a cycle, this study disaggregates the controlling parameters of temperature cycle models (e.g., thermal inertia) rather than the LSTs directly. In addition, this study incorporates the modulation process to keep the approximate consistency between pre- and post-disaggregated LSTs, while it parameterizes the SEB equation to investigate the DTC- and ATC-based DLST together.

We should clarify that this article is closely related to *Zhan et al.* [2013] and *Chen et al.* [2014]. The former is a comprehensive literature survey on DLST; the latter is a generalized paradigm and it identified the three basic principles underlying DLST. While this present paper intends to design a fully dynamic methodology (rather than a single method or algorithm) for practitioners to conduct DLST. We consider this dynamic methodology will be promising for promoting the generation of temporally continuous high-quality LSTs towards further enhancing the applications of DLST.

2. METHODOLOGY

This section firstly provides a brief introduction of steps used to perform a dynamic DLST, which is then followed by detailed explanations.

2.1. Method steps

The general flowchart is presented in **Figure 1**. The input data include sequential low-resolution LSTs ($\mathbf{T}_{low}$) and high-resolution scaling factors (i.e., $NDVI_{high}$ and $albedo_{high}$, high-resolution NDVI and albedo); the output are temporally continuous high-resolution LSTs ($\mathbf{T}_{high}$). We have the following six steps:

Step 1: Interpolate temporally discrete low-resolution LSTs (i.e., $\mathbf{T}_{low}$) using a temperature cycle model $f(\mathbf{X}_{low}, t)$, wherein $\mathbf{X}_{low}$ are the controlling parameters at the low resolution. It can be a DTC model given by Eq. (1) or an ATC model given by Eq. (2). This step corresponds to **Figure 1**a and it will be further explained in Section 2.2.

Step 2: Resample the available $NDVI_{high}$ and $albedo_{high}$ to obtain their low-resolution counterparts ($NDVI_{low}$ and $albedo_{low}$).

Step 3: Perform the statistical regression between $\mathbf{X}_{low}$ from **Step 1** and the resampled $NDVI_{low}$ and $albedo_{low}$ from **Step 2** using Eqs. (3) or (4) to obtain the coefficients **C**.

Step 4: Calculate the chosen parameters of the dynamic models at high-resolution (i.e., $\ddot{\mathbf{X}}_{high}$) and at low-resolution (i.e., $\ddot{\mathbf{X}}_{low}$), respectively, based on the statistical coefficients (**C**) from **Step 3** and scaling factors at high- and low-resolution. **Steps 3** and **4** correspond to **Figure 1**b and they will be explained in Section 2.3.

Step 5: Estimate the temporal thermal details derived from NDVI and albedo by subtracting $f(\ddot{\mathbf{X}}_{low}, t)$ from $f(\ddot{\mathbf{X}}_{high}, t)$.

Step 6: Combine the thermal details obtained from **Step 5** and the background low-resolution LSTs to obtain the disaggregated LSTs ($\mathbf{T}_{high}$) using Eq. (5). Note that background LSTs are set as the original low-resolution LSTs at times when observations are available. They can be estimated using $f(\mathbf{X}_{low}, t)$ once DLST needs to be performed at an arbitrary time. **Steps 5** and **6** correspond to **Figure 1**c and they will be explained in Section 2.4.

2.2. Dynamic modeling of LST by controlling parameters

Temperature cycle models are the prerequisite of a dynamic DLST. The majority of such models are derivatives of the solution to the heat conduction equation within semi-infinite media when constrained by a boundary condition given by the SEB equation. When the temporal domain is set as a day, a thermal-inertia-based DTC model (hereafter termed DTC-TI) can be obtained [*Huang et al.*, 2014]. Similarly, a simple solution to the heat conduction equation constrained by a harmonic variation of solar radiation, i.e., the sine function (hereafter termed ATC-SI), can be obtained once this temporal domain is set as an annual cycle [*Zhan et al.*, 2014].

2.2.1. *Thermal-inertia-based diurnal temperature cycle model (DTC-TI)*

To map the thermal inertia of land surfaces, many approaches were proposed based on remotely sensed LSTs [*Sobrino and El Kharraz*, 1999]. These approaches can be adapted to model the DTC [*Cracknell and Xue*, 1996]. This study adopts a DTC model (DTC-TI) simplified from *Zhan et al.* [2014], written as:

$$T_{\mathrm{s}}(t) = f_{\text{DTC-TI}}(T_{\mathrm{d}}, P, h, \sigma, t) = T_{\mathrm{d}} + \sigma(t - 0.5 \cdot t_{\mathrm{p}}) + \sum_{n=1}^{\infty} M(n) \cdot J(t) \qquad (1)$$

where $T_{\mathrm{s}}(t)$ represents the temporal LSTs. It is a function (i.e., $f_{\text{DTC-TI}}$) of the thermal inertia P, daily mean temperature T_{d}, the linear coefficient of upward fluxes, h, which is a measure of the surface-atmosphere interaction, and the day-to-day temperature change rate σ; t_p is the total seconds in a DTC (24×3600 s); and $M(n)$ and $J(t)$ are two intermediate functions of P, h, and T_d [*Zhan et al.*, 2014].

This study uses the DTC-TI rather than semiempirical DTC models, which divides the diurnal cycle into two relatively independent processes that separate around mid-afternoon [*Göttsche and Olesen*, 2001]. This is because the latter have at least five parameters and thus requires at least five observations per daily cycle to get a stable solution, which is hard to satisfy with the tandem polar-orbiting satellite-derived LSTs such as MODIS/LSTs. The number of parameters in some semiempirical models can be reduced to four when assuming the day-to-day LST difference is zero; this setting may however leads to large errors with only four observations during a DTC. By comparison, besides σ, only three parameters are required in the DTC-TI, facilitating the DTC modeling with only four observations. We need to clarify that both the DTC-TI and semiempirical DTC models are suitable for this dynamic DLST once there are adequate thermal observations per daily cycle.

2.2.2. *Annual temperature cycle model (ATC-SI)*

The ATC-SI is usually given by the following [*Bechtel*, 2012]:

$$T(t) = f_{\text{ATC-SI}}(T_a, T_y, \phi, t) = T_a + T_y \sin(2\pi t/365 + \theta) \quad (2)$$

where T_a, T_y, and θ are the annual mean, yearly amplitude, and phase shift of LST variations during an ATC. This simple ATC-SI uses the standard harmonic function to represent the ATC and disregards the short-period LST variations due to weather change [*Zhan et al.*, 2014]; it however has demonstrated its accuracy and usefulness in ATC modeling [*Bechtel*, 2015].

2.3. Quantification of the DTC and ATC parameters by scaling factors

For most previous DLST methods, the relationships between LSTs and optical reflectance (or the reflectance-based index such as NDVI) were quantified by a regression using samples (i.e., pixels) within an image [*Agam et al.*, 2007]. Similarly, herein for the DTC, we relate two of its parameters – daily mean temperature T_d and thermal inertia P – to the chosen scaling factors at the low resolution. A simple quadratic function is employed for this task, given as follows:

$$\begin{aligned}\mathbf{X}_{\text{DTC-low}} &= (T_\mathrm{d}, P)^T = \mathbf{C}\cdot\mathbf{K}_{\text{low}} \\ &= \begin{Bmatrix} c_{11}, c_{12}, c_{13}, c_{14}, c_{15}, c_{16} \\ c_{21}, c_{22}, c_{23}, c_{24}, c_{25}, c_{26} \end{Bmatrix} \cdot (1, \alpha_{\text{low}}, v_{\text{low}}, \alpha_{\text{low}} v_{\text{low}}, \alpha_{\text{low}}^2, v_{\text{low}}^2)^T\end{aligned} \quad (3)$$

where $\mathbf{X}_{\text{DTC}}$ is the vector of the two DTC parameters, written as $(T_\mathrm{d}, P)^T$, and the subscript 'low' means regression is performed at the low resolution; $\mathbf{C}$ is the coefficient vector $\begin{Bmatrix} c_{11}, c_{12}, c_{13}, c_{14}, c_{15}, c_{16} \\ c_{21}, c_{22}, c_{23}, c_{24}, c_{25}, c_{26} \end{Bmatrix}$, where the first and second rows represent the regression coefficients for T_d and P, respectively; and $\mathbf{K}$ is the scaling factor vector $(1, \alpha, v, \alpha\cdot v, \alpha^2, v^2)^T$, where α and v are the albedo and NDVI, respectively.

Albedo and NDVI have been shown capable of explaining the LST variations over heterogeneous areas [*Dominguez et al.*, 2011], as they are two of the most important controls that impact the surface energy budget and therefore the LST. It is natural that the daily mean LST (T_d) is related to albedo and NDVI. Physically, it is also expected that the thermal inertia P, a parameter to a certain extent that reflects the diurnal LST range [*Xue and Cracknell*, 1995], is also related to albedo and NDVI [*Duan et al.*, 2014], e.g., a pixel with a higher NDVI usually possesses a higher P. These statistical relationships and the associated significance analysis are further provided in Section 4.2.1. As in *Dominguez et al.* [2011], we employ the quadratic function rather than the linear one to quantify the complex relationships while rather than the high-degree polynomials to avoid over-fitting.

For the ATC, we again relate two of its variables – annual mean LST T_a and yearly amplitude T_y – to the scaling factors, given as follows:

$$\begin{aligned}\mathbf{X}_{\text{ATC-low}} &= (T_a, T_y)^T = \mathbf{C}\cdot\mathbf{K}_{\text{low}} \\ &= \begin{Bmatrix} c_{11}, c_{12}, c_{13}, c_{14}, c_{15}, c_{16} \\ c_{21}, c_{22}, c_{23}, c_{24}, c_{25}, c_{26} \end{Bmatrix} \cdot (1, \bar{\alpha}_{\text{low}}, \bar{v}_{\text{low}}, \bar{\alpha}_{\text{low}}\bar{v}_{\text{low}}, \bar{\alpha}^2_{\text{low}}, \bar{v}^2_{\text{low}})^T \end{aligned} \tag{4}$$

where $\mathbf{X}_{\text{ATC}}$ is the vector of the two ATC parameters, written as $(T_a, T_y)^T$. Note that currently $\bar{\alpha}$ and $\bar{v}$ are the annual mean albedo and NDVI, respectively, rather than the values on a specific day or in a short period as that for the DTC. T_a and T_y in the ATC model are comparable to T_d and P in the DTC model. They respectively denote the mean and amplitude of LST in a periodic cycle. It is therefore reasonable that T_a and T_y are also statistically related to NDVI and albedo. The statistical significance of such relationships during an ATC are illustrated in Section 4.2.2.

2.4. Prediction of high-resolution LSTs by adding sequential thermal details

A successful DLST requires the approximate conservation of thermal radiance (usually in the form of conservation of LSTs in simple cases). This indicates that the thermal radiance within a low-resolution pixel block should be equal to the mean of the thermal radiance of all the subpixels within this identical pixel block. To retain such a conservation, it is unsuitable to estimate high-resolution LSTs directly by multiplying high-resolution scaling factors by the associated coefficients (e.g., $T_{\text{high}} = a \cdot v_{\text{high}}$, where a is the linear coefficient between NDVI and LST). Rather, high-resolution LSTs should be estimated by a modulation process performed by adding low-resolution LSTs and thermal details (e.g., $T_{\text{high}} = T_{\text{low}} + a \cdot v_{\text{high}} - a \cdot v_{\text{low}}$) [*Kustas et al.*, 2003].

To keep the radiance conservation between pre- and post-DLST, this study uses a similar strategy in the dynamic methodology for disaggregating LSTs, which is given as follows:

$$\begin{cases} \mathbf{T}_{\text{high}}(t) = \mathbf{T}_{\text{low}}(t) + \left[f(\ddot{\mathbf{X}}_{\text{high}}, t) - f(\ddot{\mathbf{X}}_{\text{low}}, t) \right] \\ (\ddot{\mathbf{X}}_{\text{high}}, \ddot{\mathbf{X}}_{\text{low}}) = \mathbf{C} \cdot (\mathbf{K}_{\text{high}}, \mathbf{K}_{\text{low}}) \end{cases} \tag{5}$$

where $\mathbf{T}_{\text{high}}$ (t) and $\mathbf{T}_{\text{low}}$ (t) are the disaggregated high-resolution LSTs and background low-resolution LSTs, respectively; and $f(\cdot)$ is the temperature cycle model (i.e., the DTC or ATC models). Physically speaking, DLST by Eq. (5) can be perceived as a process by combining the background low-resolution LSTs and thermal details, which are derived as a function of the differences between the high- and low-resolution scaling factors (i.e., the high frequency details of scaling factors). Differing from the static DLST, in dynamic methodology temporal thermal details are retrieved. Note that although the incorporation of background LSTs is able to improve the accuracy of DLST, the radiance conservation is likely to be undermined at times when background LSTs are indirectly interpolated rather than directly observed [*Quan et al.*, 2014a].

2.5. Implementation details

(1) *Elimination of the grid effect*

The direct implementation of this dynamic DLST by Eq. (5) will suffer from a grid effect – disaggregated high-resolution LSTs will locally aggregate as a larger block with the size of the low resolution [*Zhan et al.*, 2013]. To overcome this issue, a low-pass filter, which is a mean filter with a window size of $R_{\text{low}}/R_{\text{high}}$ (i.e., the ratio between the low- and high-resolution), was adopted to smooth the background LSTs [*Anderson et al.*, 2011].

(2) *Determination of the parameters of the DTC-TI and ATC-SI at low-resolution*

As both the DTC-TI and ATC-SI are nonlinear, their associated parameters were solved by a nonlinear least square method. To fulfill this task, the '*lsqnonlin*' function in MATLAB (version: 2014b) was used, which by default employs the Levenberg-Marquardt algorithm for numerical iteration. Starting values for iteration as well as lower and upper boundaries are required for the model parameters before calculation. For the DTC model, the starting value vector for its four parameters, i.e., T_d (unit: K), P (unit: $J \cdot s^{-1/2} \cdot m^{-2} \cdot K^{-1}$), h (unit: $W \cdot m^{-2} \cdot K^{-1}$), and σ (unit: $K \cdot d^{-1}$), was given as (270, 2500, 20, 0). While the corresponding lower and upper boundary vectors were set as (250, 500, 5, −5) and (350, 6000, 50, 5), respectively. For the ATC model, the starting value vector for T_a (unit: K), T_y (unit: K), and θ (unit: rad), was given as (300, 10, 4); and the lower and upper boundaries were set as (250, 0, 0) and (350, 100, 2π), respectively.

(3) *Determination of the parameters of the DTC-TI and ATC-SI at high-resolution*

At high-resolution, T_d and P in the DTC model, and T_a and T_y in the ATC model can be decided by Eqs. (3) and (4) by substituting their subscripts with 'high'. By comparison, h, σ, and θ are more related to climate and weather conditions rather than surface scaling factors. These variables at the high-resolution were directly given as those corresponding values at low-resolution. This is reasonable because climate-related conditions are mostly similar across adjacent pixels.

2.6. Clarifications on methodology thoughts

Given the aforementioned flowchart and the associated explanations for this dynamic DLST, its implementation seems not easy. The thought of this study is nevertheless simple − it can be perceived as an extension of the classical transform-based (e.g., Principal-Component-Analysis (PCA) based or Intensity-Hue-Saturation based) methods for optical image fusion, which have been implemented for long in most commercial software on remote sensing image processing. Three steps are usually needed in such methods: (1) the low-resolution multispectral images are transformed into a new space by, say, the PCA. (2) The principle component is substituted by the high-resolution panchromatic image. (3) These new components are then transformed back to multispectral images with high-resolution by the inverse PCA.

By analogy, this methodology also contains three similar steps. For the first step, this study also makes a 'transform', not by a statistical way such as the PCA but by a dynamic model of LST (the DTC or ATC model) derived from the heat conduction equation when constrained by the SEB equation as the boundary condition. By this step, a set of 'components', say, T_a, T_y, and θ for the ATC model, are obtained. Second, the 'important components', are substituted with scaling factors. However, herein 'components' cannot be replaced by scaling factors directly, as they are physically different. A local regression within an image between 'components' and scaling factors is needed before this substitution. Third, the new 'components' are transformed back into LSTs by dynamic models. However, herein this inverse transform is further modulated by a procedure that aims to keeping the conservation of thermal radiance between low- and high-resolution LSTs. More discussions on the relations of the method thoughts between this methodology and previous methods will be given in Section 5.1.

3. STUDY AREA AND DATA

The study area covers the Beijing metropolis (see **Figure 2**), with an area of 80×80 km^2 and the center located at 39°54′23″ N, 116°23′29″ E. The Beijing metropolis is located in the northern tip of the North China plain. Its northern and western territories are mainly mountains, while cropland dominates the eastern and southern regions. This area was selected because of the following regards. (1) It contains relatively complex land covers including urban surfaces, cropland, and forests. (2) Its surface is characterized by high heterogeneity, facilitating the testing of the method performance. (3) Across an annual cycle, significant surface urban heat island (SUHI) when compared with its rural background has been observed over the Beijing metropolis [*Zhou et al.*, 2013], wherein DLST can be potentially useful for investigating the detailed spatio-temporal patterns of SUHI.

Four types of MODIS produces collected in 2012 were used and they include the 1-km MOD11A1 (1454 scenes of images) and MYD11A1 (1457 scenes of images), based on which daily LSTs and the associated acquisition times were extracted, 1-km MOD13A2 (92 scenes of images, NDVI was extracted), and 1-km MCD43B3 (181 scenes of images, the shortwave black-sky albedo was extracted). LSTs were frequently polluted by clouds, and only a small part of pixels has valid values for all the four transits during a DTC. To facilitate the diurnal modeling as well as to test the performance of the dynamic methodology within an entire annual cycle, composite rather than the original MODIS products were used hereafter as the basis for validations. To obtain composite products unaffected by clouds as much as possible, the associated MODIS LSTs were composited month-by-month [*Jin and Dickinson*, 1999], which is longer than the standard 8-day LST products. The associated ATC and DTC modeling were both based on these composite data. More discussions on the impacts of the use of composite products will be provided in Section 5.2.1.

4. VALIDATION

4.1. Validation strategy

Two strategies were used for validation (see **Figure 3**).

Strategy-1: The first is an indirect validation that compares the original 1-km MODIS LSTs with the LSTs simulated by replacing $\mathbf{X}$ with $\ddot{\mathbf{X}}$. For the DTC, this meant that T_d and P derived from Eq. (1) were substituted with those predicted from Eq. (3) based on the 1-km NDVI and albedo; for the ATC, it meant that T_a and T_y derived from Eq. (2) were substituted with those predicted by Eq. (4). Strategy-1 aims to judge whether this substitution leads to large errors in modeling of LSTs. This strategy is indicative for the performances of the DTC- and ATC-based DLST methods, because the accuracy of this substitution directly determines the final disaggregation accuracy. This strategy corresponds to Section 4.2.

Strategy-2: The second strategy was performed by the *upscaling-and-then-downscaling* method. It includes the following three steps. (1) The original 1-km MODIS LST image was upscaled into a coarser-resolution (e.g., 5 and 8 km in this study) image. (2) The upscaled low-resolution LST image was then disaggregated back into an image of 1-km resolution, during which the 1-km NDVI and albedo data were used as the scaling factors. (3) The disaggregated 1-km LST image was compared with the original 1-km MODIS LST image. This strategy is frequently employed for validating DLST methods, because high-resolution LSTs for comparison are not always available [*Agam et al.*, 2007; *Rodriguez-Galiano et al.*, 2012]. This strategy corresponds to Section 4.3.

The spatially derived mean absolute error (MAE) was used to assess the DLST accuracy, i.e., the differences between the disaggregated and reference LSTs. The MAE only provides an overall assessment; we therefore also presented the histograms as well as the spatial variations of the differences between the disaggregated and reference LSTs for a more detailed validation. In further consideration that both the MAE and histogram only offer an absolute comparison, this study additionally used the normalized MAE (NMAE) (calculated as the ratio between MAE and standard deviation), wherein the standard deviation was derived spatially based on the LSTs within the reference image.

Once adequate thermal observations are available within either a diurnal or an annual cycle, DLST can be performed based on either the DTC or the ATC model, which hereafter are termed the DTC- and ATC-based DLST, respectively. Validations within a DTC are provided in Sections 4.2.1 and 4.3.1, while those within an ATC are in Sections 4.2.2 and 4.3.2.

4.2. Validation at the same resolution

4.2.1. *Within a DTC*

The monthly variation of the statistical significance of the daily mean LSTs (T_d) and thermal inertia (P) against the scaling factors (i.e., NDVI and albedo) are provided in **Figure 4**a. These results show that both T_d and P generally have a close relationship with the scaling factors, with all the fitted significance level < 0.001. In detail, the r-square between thermal inertia and scaling factors is around 0.5 in most of the months except July, during which the r-square is 0.16. T_d is significantly related to the scaling factors from April to October, with the r-square greater than 0.6, whereas the associated r-square is relatively lower in winter and early spring (i.e., December through March).

The lower significance for thermal inertia during July is likely because of the heavy cloud cover in this period − the percent of pixels simultaneously cloud-free at the four transit times is only 7.84%. Such a small amount of cloud-free pixels, together with the associated precipitation (more clouds usually indicate more precipitation in July over Beijing), weakens the relationships between thermal inertia and the two scaling factors and probably contributes to the low r-square in July. Similarly for T_d, the lower significance in winter and early spring is due in part to that cloud-free LSTs in this period are also scarce − the percent of cloud-free pixels for these four months is only 12.4%, around half of the percentage in other months. Such a low significance may also be because the low NDVI values around winter are less capable of explaining T_d.

To show that whether or not a statistical relationship such as Eq. (3) to approximate T_d and P leads to high errors for the diurnal modeling, the accuracies of the modelled LSTs were assessed. The histograms of the modeled differences between the predicted and original MODIS LSTs at the four transit times are given by **Figure 4**b. In addition, the spatial variations of the MAEs between the predicted and reference LSTs for daytime and nighttime are shown in **Figure 5**. These assessments reveal that the accuracy is higher during nighttime than daytime, with the MAEs of 1.34 and 1.16 K for Aqua- and Terra-day, respectively, and 0.98 and 1.01 K for Aqua- and Terra-nig, respectively. The higher errors by day do not mean that DTC-TI is less suitable for modeling daytime LSTs; it is simply owing to the spatial variations of LST within the associated image, which have the following order when listed from the highest to lowest: Aqua-day, Terra-day, Terra-nig, and Aqua-nig. Further calculations demonstrate that the overall bias between the reference and prediction is only −0.01 K. These results suggest that the statistical relationship by Eq. (3) is acceptable for the diurnal modeling. The evaluations further illustrate the predicted LST errors at daytime (see **Figure 5**a) are generally unrelated to the land cover types (i.e., **Figure 2**); at nighttime however, the errors and land cover types are related (see **Figure 5**b), particularly for the urban and mountainous areas. This implies a lower performance of the two chosen scaling factors to explain the spatial variations of LSTs at nighttime. Such a phenomenon is probably because anthropogenic heat and urban street geometry outperform the albedo and NDVI in explaining the LST variations over urban areas during nighttime [*Quan et al.*, 2014b]. More discussions on the capability of scaling factors are provided in Section 5.2.1.

4.2.2. *Within an ATC*

The relationships between the two ATC model parameters (i.e., T_a and T_y) and the scaling factors (i.e., annual mean NDVI and albedo) at the four transit times are provided in **Table 1**a. These results indicate that both T_a and T_y are significantly related to the annual mean NDVI and albedo, with the mean r-squares of 0.73 and 0.60, respectively, all with the significance below the 0.01-level. Our results also confirm that θ is less significantly related to the scaling factors – its r-square on average is 0.25 lower than T_a and T_y. This is because according to its definition, the phase is more controlled by climate rather than land surface status. These assessments further elucidate that the statistical relationships are the most significant for Terra-day whereas the most irrelevant for Aqua-nig. This can be attributable to that NDVI and albedo play a greater role on determination of daytime T_a and T_y than nighttime ones.

To show that whether the statistical relationship given by Eq. (4) to approximate T_a and T_y results in high errors for the annual modeling, the histograms of the differences between the predicted and reference LSTs at the four transit times are offered in **Figure 6**. Interestingly, these four histograms demonstrate that the nighttime errors are generally Gaussian-distributed, while those daytime errors are not. They are characterized by a bimodal distribution, probably because of the differences between the aggregated monthly LSTs and those ATC-fitted ones. Calculations suggest that the MAEs are 2.35 and 1.14 K for the daytime and nighttime observations (see **Table 1** for details). These MAEs are not small for validations at the same resolution; however, most of these errors are derived from the ATC model, which simplifies the annual variations of LSTs as sinusoidal. For the mean MAE (1.74 K), 91% of its error (1.58 K) are from the ATC model rather than disaggregation, and the mean increment of MAE when combining the scaling factors and the associated regression coefficients to represent T_a and T_y is only 0.16 K. Indirectly, this minor increase of error indicates that the chosen scaling factors are able to explain LST variations by Eq. (4).

4.3. Validation through spatial upscaling

4.3.1. *Within a DTC*

Within a DTC, the monthly variations of the MAEs between the disaggregated and reference LSTs using the DTC-based DLST are given in **Figure 7**. The overall mean MAEs are 0.54 and 0.68 K for disaggregation from 8 and 5 to 1 km, respectively. The accuracy from 5 to 1 km is slightly higher than that from 8 to 1 km, owing to the lower resolution difference. These results also reveal that, judged by the MAE from 5 to 1 km, the annual mean disaggregation accuracy is generally lower during daytime than nighttime, with the decreasing accuracy order of Terra-nig, Aqua-nig, Terra-day, and Aqua-day, and with the mean MAEs of 0.45, 0.48, 0.56, and 0.69 K, respectively. During daytime, the accuracy is particularly lower in March and August. While during nighttime, the accuracy is notably lower in January. Additional assessments however indicate that this variation of accuracy is probably more due to the thermal contrast rather than the model performance. The associated NMAEs are

0.31, 0.32, 0.28, and 0.31 for Terra-day, Aqua-day, Terra-nig, and Aqua-nig, respectively. This low in-between difference of NMAE implies that the performance of this dynamic methodology at these four different times of day is similar. Evaluations further indicate that the monthly variations of the accuracy denoted by the NMAE is also low (**Figure 7**c).

The associated spatial variations of the annual mean MAEs between the reference and predicted LSTs are shown in **Figure 8**. The errors during daytime are higher than nighttime because of the greater spatial variations of LST in the former period, also evidenced by **Figure 7**. Under Strategy-2 when using background LSTs for modulation, the spatial patterns of LSTs at both daytime and nighttime becomes unrelated to the distribution of land cover types, especially when compared with those close relations as show in **Figure 5**b. Such a phenomenon confirms the validity of the modulation procedure for DLST. Though featured by an acceptable accuracy, the disaggregated LSTs are more fragmented especially during daytime, when compared to the reference LSTs (see **Figure 9**). This is probably owing to the use of the 1-km NDVI and albedo spatially aggregated from a finer spatial resolution (e.g., 250 m) as scaling factors, wherein no point spread function (PSF) was employed for the spatial aggregation. This fragmentation effect will weaken once a PSF is used for spatial aggregation [*Zhan et al.*, 2013].

4.3.2. *Within an ATC*

The monthly variations of the MAEs between the disaggregated and reference LSTs using the ATC-based DLST are provided in **Figure 10**. The mean MAEs of the four daily transits are 0.72 and 0.83 K for disaggregation from 5 to 1 km and from 8 to 1 km, respectively. Once more, the disaggregation accuracy is observed higher during daytime than nighttime, once judged from the MAEs. This observation is similar to that obtained via the DTC-based DLST.

Nevertheless, the month-by-month variations of accuracy derived from the ATC-based DLST are relatively lower than those DTC-based variations (see **Figure 11**). This is most likely due to that the ATC-based strategy performs DLST using all the data within an entire year, while the DTC-based strategy fulfills this process with only the temporally adjacent data. Though the ATC-based DLST holds a lower accuracy, it has a higher flexibility when compared with the DTC-based DLST. The DTC-based DLST can only be applied on the specific day when background low-resolution LSTs are of availability, otherwise DLST by this approach would be inapplicable. By comparison, the ATC-based DLST remains workable on days when background LSTs are unavailable, because they can be predicted once there are adequate background LSTs on the other days within an annual cycle [*Bechtel*, 2015]. This advantage becomes clearer, for example, when LSTs retrieved from infrequent satellite sensors (e.g., Landsat-8 TIRS) need to be disaggregated from ~100 m to 30 m on days when there is no thermal observations for the study area.

5. Discussion

5.1. Similarities and differences with previous DLST methods

As introduced in Section 1, the recent years have witnessed the progress of the spatio-temporal DLST, which stresses on the fast dynamics of LST at multiple time scales. This includes the use of geostationary LSTs [*Kolios et al.*, 2013; *Mecikalski et al.*, 2013; *Wu et al.*, 2015; *Zakšek and Oštir*, 2012], a temperature cycle (e.g., DTC or ATC) model [*Quan et al.*, 2014a; *Weng et al.*, 2014], a combination of geostationary LSTs and a DTC model [*Weng and Fu*, 2014; *Zhou et al.*, 2013], or a land surface model (LSM) [*Kallel et al.*, 2013; *Mechri et al.*, 2014].

Compared with the studies based on geostationary LSTs, the proposed methodology no longer requires hourly or sub-hourly background LSTs. We yet inherit the thought of *Zhou et al.* [2013] that DLST can be conducted through the controlling parameters of temperature cycle models rather than the LSTs. Parts of the DTC parameters in *Zhou et al.* [2013] were determined by land cover types. By contrast, this study resolves the DTC parameters by regression with scaling factors. In theory, the determination of DTC parameters by land cover types can be perceived as a kind of simple piecewise and discrete regression. We also inherit the thought of *Zakšek and Oštir* [2012], that a transform (i.e., PCA) is conducted in advance and DLST can be subsequently performed to the resultant parameters rather than the LSTs. By incorporating temperature cycle models, the 'transform' used herein is physically rather than statistically based (i.e., as denoted by the PCA). More importantly, our current study additionally emphasizes the importance of retaining the conservation of thermal radiance across spatial scales, as achieved by the modulation procedure.

This study is interlinked with *Quan et al.* [2014a] by merging neighborhood information to improve the dynamic modeling of LSTs. Neighborhood information within images has been illustrated effective to promote hyperspectral image processing for more than a decade [*Plaza et al.*, 2009]. This study nevertheless differs from *Quan et al.* [2014a] in two regards. First, its aim is DLST rather than diurnal modeling. Second, the use of scaling factors is more straightforward than using endmembers. While compared with the studies that assimilate a complex LSM with numerous variables as inputs, this methodology gives up the modelling of surface-atmosphere interaction but adopts a compromised solution through a highly simplified LSM. Such a simplification results in its incapability on cloudy days but it greatly reduces the number of inputs.

Compared with the spatio-temporal fusion of LSTs from multiple sources, this study is similar by integrating multi-source data with various resolutions. While differing from the fusion-based DLST, herein a series of temporal background LSTs and several fine-resolution scaling factors are integrated. Such a difference enables the possibility of generating LSTs with a resolution finer than the resolution of LST while equivalent to the resolution of scaling factors. In addition, dynamic models of LSTs were incorporated, which enables the generation of temporally continuous LSTs. We yet recognize that the fusion-based DLST is a good option for merging LSTs from multiple sources; a better way to improve DLST, therefore, may be from the integration of these two categories of methodologies.

5.2. Prospects and problems

5.2.1. *Prospects*

(1) *Prospects for generation of true temporally continuous high-resolution LSTs*

This study employed monthly composites of LSTs rather than LSTs per daily cycle for the aforementioned validations. The use of monthly composite data may likely affect the diurnal modeling especially at around sunrise. This is because the DTC model is usually constructed within a single daily cycle, while the sunrise moment, at which LST begins to rapidly increase, changes day by day (e.g., the sunrise difference is about 20 min within July in Beijing) and therefore control the LST dynamics [*Göttsche and Olesen*, 2001]. In addition, DLST through such a composition process only provides climatologically averaged high-resolution LSTs, i.e., the specific variations of the meteorological variables that disturb the LSTs within a month have been 'averaged'. We need to clarify in particular that the monthly composition herein only aims at testing the general applicability of the proposed dynamic methodology across an entire annual cycle. Such a composition nevertheless does not invalidate the application of this dynamic methodology in a single diurnal cycle. Practitioners just need to replace the monthly composite with instantaneous data, and true temporally continuous LSTs can be reproduced accordingly, once there are adequate valid LST pixels (i.e., under clear sky) for the four daily transits of MODIS LSTs.

(2) *Prospects for better scaling factors*

This study combined the NDVI and albedo as scaling factors. This is mostly suitable as indicated by the validations in Section 4, but it may be less feasible over areas where the NDVI and albedo are not the only controlling factors of LST. Nevertheless, this scenario barely undermines the steps of this methodology. For static DLST, various suitable scaling factors have been designed for particular areas. DLST over such areas may incorporate additional predictors related to local terrains (e.g., digital elevation model), land use/land cover, impervious percentage, multispectral reflectance (also including indices based on multispectral reflectance), and even high-resolution thermal radiance [*Bechtel et al.*, 2012; *Zhan et al.*, 2013]. Under this dynamic methodology, the previously designed predictors may be also applicable, and practitioners only need to update Eqs. (3) and (4) with the chosen predictors.

(3) *Prospects for relevant applications*

This dynamic methodology has prospects for enhancing relevant applications such as remote sensing of surface urban heat island and surface evapotranspiration. First, the generated fine-resolution LSTs guarantee such applications in relatively small regions. Second, the produced temporally continuous LSTs facilitate the temporal upscaling of surface fluxes or heat islands during a variety of time scales; they also provide climatically representative estimations than only with instantaneous observations.

5.2.2. *Problems*

(1) *Parameterization of the SEB*

The parameterization of diurnal or annual dynamics of LSTs into merely three or four controlling parameters is only applicable on ideal clear-sky days. Random weather other than clear-sky undermines the feasibility of these dynamic models. Long-term prevalence of clouds or precipitation will likely changes the standard temperature cycles within both a diurnal and an annual cycle. Nevertheless, this possibly imprecise parameterization hardly invalidates the steps given in Section 2. Under such scenarios, a dynamic model better representing LST variations is required, and DLST can be performed based on the controlling parameters of the new dynamic model under the similar framework.

(2) *Possible scale dependency of the relationships between the controlling parameters and scaling factors*

This study assumes that the relationships between the controlling parameters of temperature cycle models and the scaling factors are scale-independent. In other words, the relationships obtain at the coarse resolution are directly applied to the fine resolution without corrections. A recent research has shown that the '*scale effect*' are minimum across resolutions coarser than around 100 m [*Zhou et al.*, 2016], at which the current study was performed. This effect, however, may become significant once the resolution is finer than 100 m. Practitioners need to be careful at such fine resolutions. A recent study indicates that the support vector machine is able to partially suppress this effect [*Ghosh and Joshi*, 2014].

(3) *Errors of satellite-derived LSTs*

The accuracy of satellite-derived LSTs significantly depends upon the retrieval algorithm. The accuracy of most mature satellite-derived LST products is reported around 1−2 K over homogeneous surfaces, with an even lower accuracy over heterogeneous surfaces owing to surface thermal anisotropy [*Li et al.*, 2013]. The surface thermal anisotropy, together with other possible errors in the retrieved LSTs, affects the accuracies of the temperature cycle models and undermine all the procedures within DLST.

6. CONCLUSIONS

Aiming to the simultaneous enhancements of the temporal and spatial resolutions of LSTs, this study performed DLST by disaggregating the controlling parameters of the dynamic models of LSTs rather than the LSTs directly. A fully dynamic DLST methodology was accordingly designed. This dynamic methodology additionally incorporates the modulation procedure that injects temporal thermal details to the associated background low-resolution LSTs, rather than directly transforming the high-resolution scaling factors into LSTs. Under a unified framework, the two types of DLST (including the DTC- and ATC-based DLST) were also investigated and subsequently compared with each other.

The proposed methodology was validated by two strategies, including the indirect validation at the same resolution (Strategy-1) and the upscaling strategy (Strategy-2). Assessments indicate that, for both the DTC- and ATC-based DLST, the mean absolute errors (MAEs) between the disaggregated and reference LSTs are around 1-2 K. Comparatively, the DTC-based produces a relatively higher disaggregation accuracy, while the ATC-based possesses a higher flexibility for DLST in periods when there is no background LSTs.

This dynamic methodology is potentially able to produce temporally continuous LSTs with the resolution equivalent to that of the chosen scaling factors. Our study has been nevertheless trying to be methodological rather than single-method-specific. We recognize that the use of NDVI and albedo as scaling factors may not be the most appropriate for various terrains and land cover types, but this methodology can be easily extended once other scaling factors are used. Finally, this study hardly implies that DLST is capable of supplanting the airborne or spaceborne thermal missions in preparation. With the availability of mounting remote sensing data from multiple sources, DLST still has a long road to proceed.

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TABLES

Table 1. The r-squares between the two ATC model parameters and the annual mean NDVI and albedo at the four transit times are shown in (a), while (b) provides the MAEs between the predicted and reference LSTs.

Data type	(a) r-square*		(b) MAE (K)		
	T_{am}	T_{ya}	original**	predicted**	**increment**
Terra-day	0.79	0.67	2.24	2.31	**0.07**
Aqua-day	0.76	0.59	2.24	2.38	**0.14**
Terra-nig	0.70	0.61	0.89	1.13	**0.24**
Aqua-nig	0.68	0.51	0.95	1.15	**0.20**
Mean	0.73	0.60	1.58	1.74	**0.16**

* These correlations are all significant at the 0.01-level.

** ‘original’ denotes the MAEs between the ATC-fitted and original 1-km LSTs; ‘predicted’ represents the MAEs between the original LSTs and those predicted LSTs using scaling factors; and ‘increment’ is the difference between the ‘original’ and ‘predicted’.

FIGURE CAPTIONS

Figure 1. Flowchart followed to perform a dynamic DLST. The subscript 'high' and 'low' represent the resolution level. **T** denotes the LST; **X** is the chosen variable vector of a temperature cycle model $f(\cdot)$; **C** are the statistical coefficients between **X** and scaling factors (e.g., NDVI and albedo); and $\ddot{\mathbf{X}}$ is the estimated variable vector by combining scaling factors and statistical coefficients.

Figure 2. Land cover types around the Beijing metropolis (retrieved from MODIS land cover product MCD12Q1), including forest, shrubland, grassland, built-up, and cropland surfaces. Built-up areas locate at the center of the study area.

Figure 3. Strategies for validation. Strategy-1 is intended to verify the capability of scaling factors; and Strategy-2 is intended to validate the feasibility of the fitted relationships across different resolutions.

Figure 4. Annual variations of r-square fitted between the two DTC parameters (i.e., T_d and P) and the two scaling factors (i.e., NDVI and albedo) are shown in (a), all with the significance level < 0.001; and (b) shows the histogram of the differences between the reference and predicted LSTs at the four transit times.

Figure 5. Spatial variations of the MAEs between the reference and predicted LSTs for daytime (i.e., the average of Terra- and Aqua-day) and nighttime (i.e., the average of Terra- and Aqua-nig) across an annual cycle, wherein Strategy-1 was used.

Figure 6. Histograms of the differences between the reference and predicted LSTs at the four transit times.

Figure 7. Monthly variations of the MAEs and normalized MAEs (NMAEs) between the disaggregated and reference LSTs using the DTC-based DLST. (a) and (b) are the MAEs from 5 to 1 km and 8 to 1 km, respectively; and (c) are for the NMAEs.

Figure 8. Annual mean spatial variations of the MAEs between the reference and predicted LSTs for daytime and nighttime, wherein Strategy-2 was used.

Figure 9. The disaggregation of the upscaled MODIS (5 km) to the resolution of 1 km in September. (a), (b), (c), and (d) are the LSTs of Terra-day, Aqua-day, Terra-nig, and Aqua-nig.

Figure 10. Monthly variations of the MAEs between the disaggregated and reference LSTs using the ATC-based DLST. (a) and (b) are for 5 to 1 km and 8 to 1 km, respectively.

Figure 11. Comparisons of the mean MAEs (averaged from the four daily transits) between using the DTC- and ATC-based DLST. (a) and (b) are from 5 to 1 km and 8 to 1 km, respectively.