Examining the impacts of urban biophysical compositions on surface urban heat island: A spectral unmixing and thermal mixing approach

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A B S T R A C T

Land surface temperature (LST) is a central parameter for surface urban heat island (SUHI) studies, in which thermal remote sensing plays a key role. Traditionally, normalized difference vegetation index (NDVI), percent green vegetation (%GV), and percent impervious surface area (%ISA), have been widely applied to examine the impacts of land cover compositions on SUHI. Urban thermal pattern, however, is a complicated physical phenomenon involving a series of environmental factors, and it is insufficient to employ only one indicator for the explanation of the SUHI phenomenon. Therefore, considering different thermal properties of various land cover compositions, this study proposed a two-step physically based method, the spectral unmixing and thermal mixing (SUTM) model, to examine the impacts of typical land cover compositions on urban thermal pattern. The performance of SUTM was compared with those of linear and non-linear (quadratic) regression models with NDVI, %GV, and %ISA as individual independent variables. Results indicate that SUTM outperforms all regression models, with the lowest root mean square error (2.89 K) and mean absolute error (2.11 K). Moreover, when the accuracy was assessed at five interval levels of percent impervious surface area, it indicates that SUTM performs consistently well in both rural and urban areas. Comparatively, NDVI and %GV-based regression models perform well in rural areas, but poorly in urban areas, whereas %ISA-based models perform well in urban areas, but relatively poor in rural areas. This study found that soil, including both moist and dry soil, has significant impacts on modeling SUHI.

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1. Introduction

Due to rapid population growth and migration, urbanization has taken place globally at an unprecedented rate, and it is likely to continue in upcoming several decades according to the most recent analysis and projections in the United Nations report (2012). During the process of urbanization, a direct environmental consequence is the modification of land surfaces. A large amount of natural lands have been, or will be, converted to various developed lands (e.g. commercial, industrial, transportation, and residential lands), within which impervious surfaces are a major composition. Subsequently, this conversion results in the alteration of physical properties of land surfaces, including soil moisture, material heat capacity, conductivity, albedo, and emissivity, etc., which leads to the decrease of evaportranspiration (Chudnovsky et al., 2004; Friedl, 2002; Shoshany et al., 1994). As a result, one of the most significant environmental impacts is the change in urban land surface temperature (LST) and atmospheric temperature, which significantly affects urban internal microclimatology, surface energy change, anthropogenic heat discharge, building energy consumption, atmospheric pollution, and human thermal comfort (Lu & Weng, 2006; Sarrat et al., 2006; Voogt & Oke, 2003). When observed at a large geographical scale, such urban–rural surface temperature variation is well known as the surface urban heat island (SUHI) phenomenon, and has been extensively documented in a number of studies based on a variety of remote sensing platforms and sensors since the 1970s (Chandler, 1976; Oke, 1982; Quattrochi & Goel, 1995; Quattrochi & Luvall, 1999).

Among existing studies, two major categories of methods have been developed to examine UHI phenomenon. The first category involves the simulation of UHI phenomenon and its spatial pattern using governing equations for fluid mechanics or atmosphere (e.g. energy balance equation, etc.) with in-situ measurements or laboratory experimental data. Major simulation models include energy balance models (Oke et al., 1999; Tong et al., 2005) and dynamic numerical simulation methods (Cendese & Monti, 2003; Saitoh et al., 1996; Tominaga et al., 2008). Models under the second category quantitatively examine the relationships between LST and spectral indicators generated from remotely sensed data. Linear regression models have been widely adopted to explore the empirical relationships between LST and various metrics of socio-economic or biophysical factors, such as population density and distribution (Weng et al., 2006; Xiao et al., 2008), intensity of human activity (Elvidge et al., 1997), geometry of street canyon (Bottény & Unger, 2003; Eliasson, 1996), land use and land cover (LULC) type and change (Amiri et al., 2009; Li et al., 2009), normalized difference vegetation index (NDVI) (Carlson et al., 1994; Gallo et al., 2006; Bodén & Unger, 2003; Eliasson, 1996).
vegetation abundance (Weng et al., 2004, 2011), impervious surface abundance (Imhoff et al., 2010; Yuan & Bauer, 2007), and landscape metrics (Li et al., 2011; Zhou et al., 2011), etc. On the other hand, nonlinear statistical models have also been employed to characterize the intensity and magnitude of UHI. Such models include Gaussian model (Streutker, 2002, 2003), nonparametric kernel convolution model (Rajasek & Weng, 2009a, 2009b; Weng et al., 2011), and association rule mining technique (Rajasek & Weng, 2009c).

Currently, although many spectral indices have been extracted from remotely sensed data for analyzing UHI phenomenon, they are still insufficient to fully characterize urban thermal characteristics and patterns (Weng et al., 2004). One reason could be that, although an individual spectral index is able to quantify certain characteristics of land surface property, a comprehensive characterization is still of great necessity because of the variety of thermal properties associated with different urban biophysical compositions (Friedl, 2002). In particular, Roberts et al. (2012) pointed out that the background substrates of vegetation could impact the urban LST. In their research, with similar vegetation cover, pixels with significantly different LSTs were discerned due probably to different background substrates (e.g. moist or dry soil) that having apparently different thermal properties. In other words, although a variety of aforementioned spectral metrics are argued to have potentials to characterize urban LST characteristics, these methods hardly consider the impacts of soil, which, however, is regarded as one of the most important land compositions in urban and suburban regions (Ridd, 1995). Therefore, it is necessary to perform a comprehensive examination on the impacts of urban biophysical compositions on UHI effects, with which the impacts from thermal properties of different urban biophysical compositions and their fractional land covers are taken into consideration (Friedl, 2002). In an attempt to solve this problem, we proposed a physically based method, the spectral unmixing and thermal mixing (SUTM) model, to examine the interplay between urban LST and various land cover compositions. Specifically, the first step of this model is to estimate subpixel land cover abundance through a fully constrained spectral mixture analysis (SMA) technique. Then the urban thermal pattern is modeled as a mixture of thermal characteristics of land cover components weighted by their respective abundances. The resultant LST estimates were then compared with those derived by linear and nonlinear regression models with NDVI, percent green vegetation (%GV), and percent impervious surface area (%ISA), respectively.

The remainder of this paper is organized as follows. The next section introduces the study area and data. Section 3 describes the methods employed for retrieving LST from Landsat Enhanced Thematic Mapper Plus (ETM+) imagery. Further, Section 4 re-examines the relationship between LST and land surface characteristics, and argues the necessity of incorporating the impacts of moist and dry soil into modeling LST. The development of the proposed SUTM model is detailed in Section 5, and its accuracy assessment and comparative analysis are described in Section 6. Results of SUTM and comparative analyses are reported in Section 7. Finally, discussion and conclusions are provided in Sections 8 and 9, respectively.

2. Study area and data

Four counties in Wisconsin, USA, including Washington, Ozaukee, Milwaukee and Waukesha, were selected as the study area (see Fig. 1). Located in Southeast Wisconsin, these four counties cover a land area of 3784 km² and have a population about 1.6 million (U.S. Census Bureau, 2010). According to the surveys of Southeastern Wisconsin Regional Planning Commission (SEWRPC) and US Census Bureau, the average growth rates of population and household number have reached approximately 3.5% and 7% since 1980 (SEWRPC, 2010; U.S. Census Bureau, 2010). This trend of development is believed to continue in upcoming several decades based on the analysis and projection with historic socio-economic data (SEWRPC, 2004a, 2004b). The most recent SEWRPC land use data shows that there are a variety of land uses within these four counties, including residential, commercial, civic (e.g. government services, hospital and educational institutes, etc.), transportation, industrial, agricultural, water, and other rural open lands, such as wetland, woodland, barren land, etc. (SEWRPC, 2000). Specifically, major urbanized areas are found within and around the City of Milwaukee in the Milwaukee County where more than 60% of population of this region inhabits. An apparent outward development trend can be discerned from the City of Milwaukee and along state and interstate highways.

A cloud-free Landsat ETM+ image acquired on July 9, 2001 was obtained, and rectified to a Universal Transverse Mercator (UTM) projection with WGS84 datum and UTM zone 16. The multispectral optical bands, including visible, near-infrared (VNIR) (i.e. bands 1 to 4) and shortwave infrared (SWIR) bands (i.e. bands 5 and 7), of this image were utilized for spectral unmixing for fractional land covers. The digital numbers (DNs) of multispectral bands were then converted to at-satellite reflectance according to the work of Markham and Barker (1986) and Landsat 7 science data user’s handbook (Irish, 2000). In addition, thermal band DN were employed to retrieve LST for further analysis and modeling, and the retrieval process is detailed in the next section. Note that although the original thermal band of ETM+ image was obtained at a 60-m spatial resolution, its final product was resampled to 30-m resolution to be consistent with the spatial resolution of other multispectral bands (U.S. Geological Survey, 2010). The 2001 Landsat ETM+ image was adopted to be consistent with the land use/land cover classification and imperviousness percentage data from the 2001 National Land Cover Dataset (NLCD). For a better appreciation of development and accuracy assessment of the 2001 NLCD data, readers can refer to the studies conducted by Yang et al. (2001), Yang et al. (2003) and Homer et al. (2004). Besides, for LST retrieval, we also collected weather data from the University of Wisconsin-Milwaukee field station and zenith wet delay estimate data (DeMets, 2012), respectively.

3. LST retrieval

In order to obtain accurate LST values, we adopted the mono-window algorithm (MWA) developed by Qin et al. (2001), which accounts for the impacts of emissivity and atmosphere using both remotely sensed thermal data and meteorological data. The formulation of LST can be expressed as follows.

\[ T_s = \frac{a_0(1-C_b-D_b) + (b_0(1-C_b-D_b) + C_b + D_b)T_a-D_bT_a)}{C_b} \]  

(1)

with

\[ C_b = \varepsilon_b T_b \]  

(2)

\[ D_b = (1-T_a)(1+(1-\varepsilon_b)T_b) \]  

(3)

where \( a_0 = -67.355351 \) and \( b_0 = 0.458606 \) are model constants; \( \varepsilon_b \) is the emissivity for Landsat ETM+ thermal band 6; \( T_a \) is the atmospheric transmittance for Landsat ETM+ thermal band 6 on the image acquisition date; \( T_a \) is the effective mean atmospheric temperature; and \( T_b \) is the brightness temperature for Landsat ETM+ thermal band 6. To retrieve LST data using Eq. (1), parameters \( \varepsilon_b, T_a, T_b \), and \( T_s \) should be predetermined respectively (Okwem et al., 2011), and the details of deriving these parameters are described in the following subsections (see Fig. 2).

3.1. Determination of emissivity (\( \varepsilon_b \))

We adopted the NDVI thresholds method, which considers different impacts of distinct land cover types (e.g. water, vegetation, bare land, and others). In order to get accurate LST values, we adopted the mono-window algorithm (MWA) developed by Qin et al. (2001), which accounts for the impacts of emissivity and atmosphere using both remotely sensed thermal data and meteorological data. The formulation of LST can be expressed as follows.
soil, and impervious surface), proposed by Sobrino et al. (2001) to
determine emissivity. Prior to the calculation using this method, an
iterative self-organizing data analysis (ISODATA) (Tou & Gonzalez,
1974) unsupervised classification was performed to obtain water
pixels, the emissivity of which was then assigned as 0.990 (Okwen
et al., 2011; Snyder et al., 1998). Fully vegetated pixels (with an
NDVI greater than 0.5) were assigned to an emissivity of 0.985. Similarly,
non-water pixels with NDVI less than 0.2 are considered as non-
vegetated land covers, and 0.972 is assigned as the emissivity of these
pixels (Snyder et al., 1998; Sobrino et al., 2004). Finally, pixels with
NDVI greater than 0.2 and less than 0.5 are considered as mixed pixels
including various degrees of vegetation and non-vegetation (such as
bare soil and impervious surfaces). Emissivity of these mixed pixels
was then calculated as follows (Carlson & Ripley, 1997; Sobrino &
Raissouni, 2000; Sobrino et al., 2004).

$$\varepsilon_{\text{mix}} = \varepsilon_v p_v + \varepsilon_n (1 - p_v) + C_i$$  (4)
where \( p_v = (NDVI - NDVI_{\text{min}}) / (NDVI_{\text{max}} - NDVI_{\text{min}}) \) \(^2\)

\[
C_i = (1 - e_n) (1 - p_v) F e_v
\]

(6)

where \( NDVI_{\text{min}} \) and \( NDVI_{\text{max}} \) are the NDVI values for non-vegetation and full vegetation, respectively; \( p_v \) is the scaled NDVI; \( e_n \) and \( e_v \) are emissivities of vegetation and non-vegetation, respectively; \( F = 0.55 \) is a shape factor considering geometrical distribution (Sobrino et al., 1990).

3.2. Determination of atmospheric transmittance (\( \tau_0 \))

Atmospheric transmittance \( (\tau_0) \) was determined through constructing a linear regression model with water vapor content \( (w) \) as the independent variable (Qin et al., 2001).

\[
\tau_0 = a \cdot w + b
\]

(7)

where \( a \) is the slope of the transmittance regression model; \( b \) is the intercept, both of which are determined according to different atmospheric conditions including air temperature and water vapor content (listed in Table 1); and \( w \) is water vapor content.

The water vapor content \( w \) was estimated based on its proportional relationship with the GPS microwave signal delay during the propagation process from GPS satellites to ground-based GPS receivers (Bevis et al., 1992; Hogg et al., 1981; Resch, 1984). More details about the development of GPS meteorology can be referred to the works of Bevis et al. (1992) and Bevis et al. (1994). Water vapor content \( (w) \) can be derived by the estimation of atmospheric integrated water vapor \( (IWV) \) based on GPS meteorology (see Eq. (8)).

\[
IWV = \rho \cdot PW = \rho \cdot ZWD \cdot II
\]

(8)

with

\[
II = \frac{10^6}{\rho \cdot R_v \cdot (k_2/T_m + k_3)}
\]

(9)

where \( \rho \) is the density of liquid water; \( PW \) is precipitable water vapor; \( ZWD \) is an observed zenith wet delay measured from ground-based GPS receivers; \( k_2 \) and \( k_3 \) are physical constants from the atmospheric refractivity, as suggested by Rocken et al. (1995), \( k_2 = 22 k m^{-1} \) and \( k_3 = 3.739 \times 10^{5} K m^{-1} \) were adopted; \( R_v = 461.495 J kg^{-1} K^{-1} \) is the specific gas constant for water vapor. \( T_m \) is the weighted mean temperature of the atmosphere (Askne & Nordius, 1987; Bevis et al., 1992; Tregoning et al., 1998), which can be defined as follows.

\[
T_m = \frac{\int (P_v/T) dz}{\int (P_v/T^2) dz}
\]

(10)

where \( T \) is temperature, and \( P_v \) is the partial pressure of water vapor. For simplification, an empirical linear regression model was also proposed by Bevis et al. (1992) using the following expression.

\[
T_m = 70.2 + 0.72 \cdot T_0
\]

(11)

Table 1

<table>
<thead>
<tr>
<th>Atmospheric condition</th>
<th>Coefficients</th>
<th>Model coefficients</th>
</tr>
</thead>
<tbody>
<tr>
<td>Profiles</td>
<td>Water vapor (g cm(^{-2}))</td>
<td>a</td>
</tr>
<tr>
<td>High air temperature (35 °C)</td>
<td>0.4–1.6</td>
<td>–0.08007</td>
</tr>
<tr>
<td>Low air temperature (18 °C)</td>
<td>0.4–1.6</td>
<td>–0.09611</td>
</tr>
</tbody>
</table>

where \( T_0 \) is near-surface air temperature acquired from field measurements.

3.3. Determination of effective mean atmospheric temperature (\( T_a \))

To determine the effective mean atmospheric temperature \( (T_a) \), we adopted the regression model developed by Qin et al. (2001) for the summer season of mid-latitude regions, as the Landsat image was acquired in July and Southeast Wisconsin is located in the mid-latitude area (see Eq. (12)).

\[
T_a = 16.0110 + 0.92621 \cdot T_0
\]

(12)

where \( T_0 \) is near-surface air temperature in \( K \) acquired from field measurements.

3.4. Brightness temperature (\( T_\beta \)) calculation

For the at-satellite brightness temperature conversion from thermal band DNs, we followed the transformation equations according to the works of Markham and Barker (1986) and Landsat 7 science data user’s handbook (Irish, 2000) as follows.

\[
T_\beta = \frac{K_s}{\ln \left( \frac{L_s}{L_\min} + 1 \right)}
\]

(13)

with

\[
I_\lambda = \frac{L_{\max} - L_{\min}}{Q_{\max} - Q_{\min}} (DN - Q_{\min}) + L_{\min}
\]

(14)

where \( T_\beta \) is the effective at-satellite brightness temperature in degrees Kelvin (\( K \)); \( K_s = 666.09 W cm^{-2} sr^{-1} \) is calibration constants for the Landsat 7 ETM+ thermal band; \( I_\lambda \) is the spectral radiance received by the Landsat sensor; \( Q_{\min} \) and \( Q_{\max} \) are the minimum and maximum DN values (1 and 255 for Landsat ETM+ imagery), respectively; \( L_{\min} \) and \( L_{\max} \) are the detected spectral radiance that are scaled to \( Q_{\min} \) and \( Q_{\max} \) respectively; \( DN \) is the grey level digital value; and \( \lambda \) is the wavelength.

4. Re-examining the relationship between urban LST and land surface characteristics

With the retrieved LST image for the study area, we examined the relationship between urban LST and land surface characteristics. In particular, we re-examined two categories of major UHI indicators, namely (1) vegetation indicators, including NDVI and percent green vegetation abundance (%GV), and (2) percent impervious surface area (%ISA), to characterize urban LST patterns in the study area. Further, we performed a comprehensive examination on the relationship between LST and land cover compositions, according to which we proposed a new method to model SUHI phenomenon comprehensively.

4.1. Vegetation indicators: NDVI and green vegetation abundance

The surface temperature-vegetation index (TVX) feature space (see Fig. 3) was generated to examine the relationship between NDVI and LST with 10,000 random sample pixels. In addition, clusters of typical land cover types were highlighted with circles in different colors. The TVX has been well documented in a number of studies since the 1980s (Amiri et al., 2009; Gillies et al., 1997; Lambin & Ehrlich, 1996; Nemani & Running, 1989; Nemani et al., 1993). It has proven to effectively reflect the moisture content of soil and vegetation, and characterize the impacts of land surface properties on evapotranspiration (Hope & McDowell, 1992). Through a careful examination of the TVX triangle as illustrated in Fig. 3, we found that the vertices of the TVX triangle...
represent different land cover compositions with apparently different thermal characteristics. Vegetation occupies the upper left vertex of the TVX triangle with higher NDVI values and relatively lower LST values. The lower left vertex, with the lowest NDVI values of both NDVI and LST, is dominated by moist soil and water. The lower right vertex, with the lowest NDVI values and highest LSTs, is occupied by dark impervious surfaces. Next to the dark impervious surface cluster, dry soil and bright impervious surfaces are with relatively high LSTs and low NDVI values. As a summary, this analysis indicates that the nonlinear relationship between LST and NDVI is majorly due to the apparent LST values of these materials, such as vegetation, asphalt, concrete, bare soil/rocks, and water, etc., are with significantly different thermal properties (Chudnovsky et al., 2004; Jensen, 2000; Quattrochi & Ridd, 1994, 1998). In rural areas, major land covers generally include vegetation, dry soil and wet objects (i.e. moist soil and water). Among them, dry soil has the highest diurnal LST, followed by vegetation, and moist soil (if water is ignored). Comparatively, in urban areas, there are more manmade materials and less bare soil, and major land covers include vegetation and various types of impervious surfaces. Among these materials, dark impervious surfaces (e.g. asphalt in parking lots and roofs, etc.) are proven as the warmest urban elements with the highest LST, followed by bright impervious surfaces (e.g. concrete) and vegetation (Chudnovsky et al., 2004; Jensen, 2000; Quattrochi & Ridd, 1994, 1998). Note that dry soil and bright impervious surfaces share very similar thermal properties (Jensen, 2000), as well as almost identical spectral characteristics (Powell et al., 2007; Wu, 2004). Therefore, these two materials can be grouped into a class of “high albedo materials”. When accounting for both rural and urban areas, four land cover compositions with apparently different thermal properties, including vegetation, moist soil, high albedo material, and dark impervious surface, are appropriate to model urban LST.

4.3. Land cover compositions

Through analyzing the respective relationships between LST and NDVI, LST and %GV, and LST and %ISA, we found that it is inappropriate to model urban LST using just a single metric (Li et al., 2011; Yuan & Bauer, 2007). In fact, water and moist soil may significantly impact the negative linear correlation between vegetation indicators (i.e. NDVI or %GV) and LST; and the existences of dark impervious surfaces, moist and dry soil may dramatically influence the positive linear correlation between %ISA and LST. To solve this problem, it is necessary to consider the thermal properties of all land cover compositions, because different materials, such as vegetation, asphalt, concrete, bare soil/rocks, and water, etc., are with significantly different thermal properties (Chudnovsky et al., 2004; Jensen, 2000; Quattrochi & Ridd, 1994, 1998). In rural areas, major land covers generally include vegetation, dry soil and wet objects (i.e. moist soil and water). Among them, dry soil has the highest diurnal LST, followed by vegetation, and moist soil (if water is ignored). Comparatively, in urban areas, there are more manmade materials and less bare soil, and major land covers include vegetation and various types of impervious surfaces. Among these materials, dark impervious surfaces (e.g. asphalt in parking lots and roofs, etc.) are proven as the warmest urban elements with the highest LST, followed by bright impervious surfaces (e.g. concrete) and vegetation (Chudnovsky et al., 2004; Jensen, 2000; Quattrochi & Ridd, 1994, 1998). Note that dry soil and bright impervious surfaces share very similar thermal properties (Jensen, 2000), as well as almost identical spectral characteristics (Powell et al., 2007; Wu, 2004). Therefore, these two materials can be grouped into a class of “high albedo materials”. When accounting for both rural and urban areas, four land cover compositions with apparently different thermal properties, including vegetation, moist soil, high albedo material, and dark impervious surface, are appropriate to model urban LST.

5. Spectral unmixing and thermal mixing (SUTM)

Through analyzing the relationship between LST and land surface characteristics, we have found that four major land cover compositions, i.e. vegetation, moist soil, high albedo material, and dark impervious surface, have illustrated apparently different thermal properties. Therefore, we developed a two-step SUTM approach to model urban LST with these four land cover compositions. The first step of SUTM is to quantify the fractions of these four materials by spectral unmixing using the Landsat multispectral reflectance image. Second, with representative LST value of each land cover selected in the TVX feature space in Fig. 3, urban LST is modeled by thermal mixing. The scheme of SUTM is illustrated in Fig. 5, and its details are described in following subsections.
5.1. Spectral unmixing

In order to estimate the abundance of each land cover composition, we applied a constrained linear SMA model (Roberts et al., 1998; Wu, 2004; Wu & Murray, 2003). Linear SMA model assumes that the reflectance of each pixel is a linear weighted sum of reflectance of various homogeneous land cover types (called endmembers) (Adams et al., 1995; Roberts et al., 1998; Smith et al., 1990). The specific model of linear SMA with full constraints can be formulated as follows:

\[ R_b = \sum_{i=1}^{N} f_i R_{b,i} + e_b \]  \hspace{1cm} (15)

subject to

\[ \sum_{i=1}^{N} f_i = 1 \text{ and } f_i \geq 0 \]  \hspace{1cm} (16)

where \( R_b \) is the reflectance for each band \( b \) of the remote sensing image; \( N \) is the total number of endmembers; \( f_i \) is the resultant fraction of endmember \( i \); \( R_{b,i} \) is the reflectance of endmember \( i \) in band \( b \); and \( e_b \) is the model residual.

In this step, three spectral endmembers, i.e. vegetation, high albedo material (including dry soil and bright impervious surfaces), and low albedo material (including moist soil and dark impervious surfaces), were first selected from the feature space scatterplot of the principal component analysis (PCA) components 1 and 2 (see Fig. 6). Note that although the thermal properties between moist soil and dark impervious surfaces are completely different, these two land cover compositions are always confused due to their spectral similarity (Jensen, 2000; Lu & Weng, 2004, 2006; Small, 2001; Wu & Murray, 2003). Therefore, it would be problematic if these two spectrally confused endmembers are directly utilized in the spectral unmixing. To overcome this spectral confusion, we first grouped moist soil and dark impervious surface into a class of “low-albedo materials” for spectral unmixing, and then separated the derived fractions from each other using the 2001 NLCD land cover classification data. With the spectra of these three spectral endmembers, a fully constrained linear SMA was applied to the Landsat ETM+ reflectance imagery to obtain the fraction of each endmember.

With the resultant fraction of the “aggregated” low-albedo materials, the 2001 NLCD land cover classification data was employed as a mask to further separate moist soil from dark impervious surfaces.

5.2. Thermal mixing

LST is dependent on both the composition and quantity of land covers (Friedl & Davis, 1994). Various forms of surface temperature mixing have been applied as a critical component of different models for the studies of evapotranspiration, soil moisture, temperature variation, and relationship between vegetation and remote sensing vegetation indices, etc., with spatial resolutions ranging from coarse (1.1 km for Advanced Very High Resolution Radiometer (AVHRR) imagery) and medium resolution (30 m for Landsat TM/ETM+ imagery) to very high resolution (<2 mm for microbolometer imagery) (Becker & Li, 1990a, 1990b; Boegh et al., 1999; Friedl & Davis, 1994; McCabe et al., 2008; Norman et al., 1995; Price, 1990). According to these existing studies, the principle of linear mixing for surface temperature can be expressed as follows.

\[ T_s = \sum_{i=1}^{N} f_i T_i + e \]  \hspace{1cm} (17)

subject to

\[ \sum_{i=1}^{N} 1 \text{ and } f_i \geq 0 \]  \hspace{1cm} (18)

where \( T_s \) is land surface temperature; \( T_i \) is representative LST of endmember \( i \); \( e \) is the model residual. Therefore, the LST value of each pixel can be estimated with the known values of \( f_i \) and \( T_i \), where fractions of each land cover composition \( f_i \) have been estimated in the previous subsection. To obtain representative thermal endmember \( (T_i) \), the TVX feature space was utilized for thermal endmember selection (see Fig. 3). With the obtained \( f_i \) and \( T_i \), the modeled LST was derived as the summation of thermal endmembers weighted by their respective fractions. One should note that, as illustrated in Fig. 5, spectral unmixing and thermal endmember selection
are two relatively independent processes, both of which are implemented respectively for the final step of thermal mixing.

In addition, it is worth noting that, following the SUTM mechanism, with independently gauged LST value for each land cover composition, LST of the whole study area can be modeled without the help of thermal remote sensing imagery. In this paper, although LST is derived from the conversion of the Landsat ETM + TIR band, the adoption of the Landsat thermal image is only to facilitate the demonstration of the mechanism of the proposed SUTM method. To estimate LST based on this mechanism during revisit interval period or on the revisit day but with poor weather conditions, in-situ LST measurements from ground-based thermal instruments can be employed alternatively as thermal endmembers, while the fraction of each land cover can be assumed unchanged.

6. Comparative analysis and accuracy assessment

With 10,000 randomly sampled pixels (out of a total number of about 4 million pixels) selected as training data, three ordinary least squares (OLS) linear regression models, as well as three nonlinear quadratic polynomial models, were constructed with NDVI, %GV, and %ISA as the single independent variable respectively. NDVI was calculated using the reflectance of the red and near infrared bands of the Landsat ETM + image (i.e. bands 3 and 4); %GV was obtained through SMA detailed in Section 5; and %ISA was obtained directly from the 2001 NLCD percent impervious surface data. Specific coefficients for all OLS linear regression and quadratic polynomial models are reported in Table 2.

To assess the accuracy of the LST estimates, two accuracy metrics, root mean square error (RMSE) and mean absolute error (MAE), were employed. These metrics can be expressed as follows.

\[
\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (LST_i - \hat{LST}_i)^2}
\]

\[
\text{MAE} = \frac{1}{N} \sum_{i=1}^{N} |LST_i - \hat{LST}_i|
\]

where \(\hat{LST}_i\) is the estimated LST for pixel \(i\); \(LST_i\) is the actual LST of pixel \(i\) retrieved from the Landsat ETM + thermal image; \(N\) is the total number of pixels of the Landsat ETM + image. Both RMSE and MAE are measures of precision, and quantify the relative estimation error at the pixel level. To investigate the performance of SUTM with different degrees of urban development, those two error metrics were also calculated for five groups with different levels of impervious surface percentages (e.g. 0–20%, 21–40%, 41–60%, 61–80%, and 81–100%).

7. Results

7.1. SUTM method

As the first step of SUTM, SMA was implemented to obtain fractions of three land covers, i.e. vegetation, high albedo materials, and low albedo materials. Subsequently, moist soil and dark impervious surfaces were separated from the low albedo fraction image through the post-processing step using the reclassified 2001 NLCD land cover data. The resultant fraction images of vegetation, high albedo materials, moist soil, and dark impervious surfaces are shown in Fig. 7. Note that although vegetation, bright and dark impervious surfaces could be digitized on aerial photos by visual examination, the identification of moist and dry soil is very difficult. Therefore, unlike traditional SMA studies, we did not perform an accuracy assessment of the derived fractions of endmembers. Fig. 7A indicates that vegetated lands, including dense and sparse woodlands and grass lands, are dominant in rural areas. Comparatively, bright dry soil with high albedo was found scattered in rural areas, while bright impervious surfaces were found mainly in developed areas (e.g. the City of Milwaukee and its neighboring cities) (see Fig. 7B). In addition, moist soil with low albedo was found as the substrate layer and mixed with vegetation in agriculture lands, grasslands, forestlands, and wetlands (see Fig. 7C). Dark impervious surfaces, such as asphalt in parking lots and roads, etc., were identified primarily in developed areas, particularly in the central business district (CBD) areas in the City of Milwaukee (see Fig. 7D).

In the second step of SUTM, the representative thermal endmembers were manually selected from the vertices and bases of the TVX triangle followed by careful visual examinations of the Landsat ETM + image. The representative LST value for each endmember was then calculated as the expected value of the selected samples for simplicity, and they were then acquired as follows: 299.3 K for moist soil, 300.4 K for vegetation, 309.5 K for high-albedo materials and 315.4 K for dark impervious surfaces, respectively. With the derived fraction \(f_i\) of each land cover composition and their representative LST value \(T_i\), the LST of each pixel was then estimated using the thermal mixing approach (see Fig. 8B). When compared with the retrieved LST image (Fig. 8A), the estimated image has a similar overall spatial pattern. Specifically, pixels with lower LSTs (with darker grey tone) were found in non-developed areas, in which forest, agriculture, and wetlands are dominant land covers. Comparatively, pixels with higher LST (displayed with light grey to white tone) are in developed areas, such as CBD, highways, and airports, etc., and also in rural area with dry soil. Besides, pixels in residential areas where vegetation was mixed with different manmade materials (e.g. bright/dark impervious surfaces) were shown in a grey to dark grey tone, indicating the existence of medium LSTs. A difference map (Fig. 9A) and a scatterplot (Fig. 10A) between the estimated and retrieved LST values also indicate a satisfactory estimation with SUTM. In particular, no obvious under- or over-estimation of LST can be discerned in the study area. In addition to visual comparisons, accuracy measurements also verified the similarity between the SUTM-modeled LST and the retrieved LST (see Table 3). Table 3 indicates that the overall error for the whole study area is quite low, with 2.885 K for RMSE and 2.114 K for MAE. Further, it also shows that lower RMSEs and MAEs are found in less-developed areas where impervious surface fraction is less than 60%, whereas higher RMSEs and MAEs are found in developed areas with relatively higher percentage of impervious surfaces (i.e. higher than 60%). This observation could be probably due to the larger variations of thermal properties of different impervious surfaces with various anthropogenic materials than those of natural materials dominated by vegetation.

7.2. NDVI

The results of the linear regression analysis with NDVI as the single independent variable are displayed in Fig. 8C, and the LST difference map and the scatterplot between the LST derived from the NDVI-based linear regression model and retrieved LST are illustrated in Figs. 9B and 10B respectively. Visual comparisons indicate that the NDVI-based linear regression model significantly underestimate LSTs
in developed lands, such as commercial, residential, and transportation land uses, etc., and slightly over-estimate LSTs in rural areas. This is probably due to the ignorance of the impacts of moist soil in rural areas. Further quantitative analysis presented in Table 3 indicates that the overall accuracy is lower than that of the proposal SUTM method, with an RMSE of 3.277 K and MAE of 2.647 K. Moreover, it also shows that the performance of this model is relatively well in rural areas, but poor in urban areas (with percent impervious surface area greater than 20%) (see Table 3). This is probably due to the nonlinear relationship between NDVI and LST, in particular when the NDVI approaches zero (see Fig. 3). Further, this model also underestimates LSTs in urban areas, and slightly overestimates LSTs in rural areas (see Figs. 9B and 10B). Besides, when compared with the linear regression model, the NDVI-based polynomial model performs slightly better in rural areas, low-density, and medium-density developed areas (e.g. %ISA less than 80%), but leads to much worse estimation in highly developed areas with %ISA more than 80% (with a RMSE of 6.67 K and MAE of 5.71 K, as shown in Table 3). This result suggests that, although improved performance in less developed areas can be observed, the nonlinear polynomial model severely underestimates LST in urban areas, and consequently it still cannot effectively model the relationship between LST and NDVI. Due to a similar performance when compared with linear regression models, the scatterplots between the retrieved LST and the LST derived from the polynomial models are not included.

7.3. Percent green vegetation (%GV)

Similar to NDVI, %GV was also employed as the single independent variable to model LSTs with linear regression analysis (see Table 2). The results are reported in Fig. 8D, and the LST difference map and the scatterplot are reported in Figs. 9C and 10C respectively. They indicate that the performance of %GV is similar to that of NDVI, which underestimates LSTs in developed lands and slightly overestimates LSTs in rural lands as well. Its precision is also comparable to that obtained from the NDVI model, with an overall RMSE of 3.319 K and MAE of 2.635 K. In addition, the quadratic polynomial regression model generated similar results (see Table 3). Therefore, no significant differences were found between the performances of %GV-based regression models and those of their NDVI-based counterparts.

7.4. Percent impervious surface area (%ISA)

Finally, we estimated the LSTs using the linear regression model with %ISA as the single independent variable (see Table 2), and the results are shown in Fig. 8E. In addition, LST difference map and the
scatterplot between the estimated and retrieved LSTs are shown in Figs. 9D and 10D, respectively. Results indicate that although LSTs were modeled appropriately in developed lands, severe underestimations were found in rural areas in the western, southern and southwestern parts of the study area, where are dominated by forest and agricultural lands, particularly lands covered by dry soil. Table 3 further confirms that this model performs the worst in terms of two accuracy metrics (i.e. 3.691 K for RMSE and 2.847 K for MAE) for the whole study area. Such poor estimation may be due to the severe underestimation of LST of dry soil, slight underestimation of the LST of vegetation, and slight overestimation of the LST of impervious surfaces. Comparatively, the performance of this model is better in urban areas and relatively poorer in rural areas, which is due likely to the LST variability of materials with vastly different thermal properties, e.g. vegetation, moist and bare soil, and their mixtures. In addition, although slight improvements in areas with all development levels can be discerned (see Table 3), the performance of the %ISA-based polynomial model is still very close to its linear regression counterpart, both of which are poorer than that of the SUTM model.

8. Discussion

Results from this research show that the usage of a single spectral metric as the only indicator for characterizing SUHI is insufficient, because they fail to characterize the considerably large thermal variability of various land cover compositions. As can be observed in the TVX space in Fig. 3, several important parameters, such as the amount and nature of vegetation, thermal properties of soil and its moisture content, all play important roles in surface energy exchange (Avissar & Verstraete, 1990; Brutsaert, 1982; Friedl, 2002; Garratt, 1992; Gillies et al., 1997; Quattrochi & Ridd, 1998; Stull, 1988). In addition to these factors, various thermal properties of anthropogenic materials in developed areas should be taken into considerations. Unfortunately, only one aspect is considered and compared individually in most traditional remote sensing-based LST/SUHI studies, and consequently leads to the unsatisfactory explanation of the mechanisms of urban thermal patterns. For instance, when vegetation indicator (i.e. NDVI or %CV) is solely utilized as the factor in the scatterplot (see Fig. 3), it is observed that with a zero or negative value, the variance of LST at that range is extremely high. In other words, land cover with such a low value of vegetation indicator could be a variety of potential non-vegetation compositions, including moist soil, dry soil, bright and dark impervious surfaces, as well as their mixtures. These materials possess significantly distinct thermal properties, which are very difficult to be characterized only by NDVI (Li et al., 2011; Xian & Crane, 2006; Yuan & Bauer, 2007). Similarly, when only %ISA is taken into account, it is found that, in rural areas with %ISA less than 20%, the LST could vary from 295 K to 330 K in our study site. The reason is similar: there are various possibilities of land covers with low %ISA values, including vegetation, moist and dry soil, as well as their mixtures, all of which have completely different thermal properties as well (see Fig. 4). In addition, although the impact of soil moisture on SUHI is regarded as a potential cause of temperature variation (Roberts et al., 2012), this factor has rarely been considered in existing LST/SUHI research. Soil moisture, however, is shown to have significant impacts on LST in our study site.

In addition to the ignorance of the impacts of soil and its moisture, another difficulty lies on the derivation of fractional covers according to their thermal properties. In this research, considering spectral and thermal characteristics of land cover compositions, we employed spectral unmixing to solve this problem. Specifically, five major land compositions with significantly different thermal properties, i.e. vegetation, bright and dark impervious surfaces, moist and dry soil, were taken into account and initially grouped into three classes based on their spectral features. Individual abundance of each composition is then derived using linear SMA, followed by a post-processing of segmentation for individual abundances of moist soil and dark impervious surfaces. Note that, although this approach is applicable in most cases, there might be an exception, i.e. a very small number.
of mixed pixels with cool objects (e.g. metals and water body) were regarded as impervious surfaces with higher LST values because of their spectral characteristics. Such confusion could result in LST overestimation in our study area. Through incorporating subpixel land cover information, SUTM can provide a more comprehensive and realistic representation of urban surface complexity, and therefore generate a more satisfactory modeling result, an expectation proposed by Voogt and Oke (2003). Overall, the traditional binary interplay between LST and a single spectral indicator is extended to multiple interplays between LST and the amount and thermal properties of various land biophysical compositions through SUTM.

It is unsurprising that SUTM can significantly outperform other empirical models. Empirical models like OLS linear regression with individual spectral indices as the explanatory variable only suggest a negative relationship between LST and vegetation indicator (i.e. NDVI or %GV), as well as a positive relationship between LST and impervious surfaces. These models, however, cannot provide a comprehensive explanation of the complicated mechanism of SUHI. Furthermore, although subpixel vegetation and impervious surface information are two widely adopted spectral indicators for LST analysis, it is very difficult to combine both indices to improve statistical modeling of urban thermal pattern due to their significantly negative correlation, which can result in severe multicollinearity, particularly when a multivariate regression model is applied. Besides, as examined and illustrated in this study using quadratic polynomial model, even nonlinear statistical models cannot appropriately characterize the complex nature of the SUHI phenomenon. On the contrary, as a physically based method with explicit physical meanings, SUTM is able to effectively demonstrate the interaction mechanism between LST and land cover compositions. Different from empirical models emphasizing on the well-known negative or positive relationship of LST with only one certain land cover type, the proposed method

Fig. 9. LST Difference maps (subtraction of the retrieved LST from modeled LST) using (A) SUTM, (B) NDVI-based linear regression model, (C) GV-based linear regression model, and (D) ISA-based linear regression model.
takes into consideration the thermal variability of different typical materials, particularly the within-class thermal variations, including the difference between moist soil and dry soil, and between bright impervious surfaces and dark impervious surfaces. Therefore, it provides a more in-depth understanding of the roles of land surface characteristics played in urban thermal pattern.

Another important topic in SUHI studies is the selection of remote sensing images. As demonstrated in this research, with a medium spatial resolution, Landsat imagery provides adequate spatial and spectral information for deriving land biophysical compositions and their respective thermal properties, which can be further incorporated into modeling the interaction mechanism between land cover compositions and urban thermal patterns. The major limitations of Landsat imagery for SUHI research, however, could be (1) relatively complicated process of LST retrieval, and (2) low temporal resolution (with a revisit interval of approximately 16 days for Landsat ETM+ and 18 days for Landsat TM). In contrast, with a much coarser spatial resolution, Moderate-resolution Imaging Spectroradiometer (MODIS) imagery lacks sufficient detailed urban/rural spatial surface information. Its considerably higher temporal resolution, however, allows it to be more readily available for examining “temporal dynamics of urban thermal landscapes” (Weng, 2009), such as intra- and inter-annual change of spatial patterns of energy fluxes in urban areas, and temporal variation of energy fluxes in urban areas.

Table 3
Accuracy measures of different models: the proposed SUTM model, three OLS linear regression models with NDVI, %GV and %ISA as individual independent variables, and three polynomial models with the same spectral indicators.

<table>
<thead>
<tr>
<th>Metric</th>
<th>Imp%</th>
<th>SUTM (°K)</th>
<th>Linear regression models</th>
<th>Polynomial models</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>NDVI (°K)</td>
<td>%CV (°K)</td>
<td>%ISA (°K)</td>
</tr>
<tr>
<td>RMSE</td>
<td>0–20</td>
<td>2.783</td>
<td>2.954</td>
<td>3.071</td>
</tr>
<tr>
<td></td>
<td>41–60</td>
<td>2.911</td>
<td>4.232</td>
<td>3.909</td>
</tr>
<tr>
<td>Overall</td>
<td>2.885</td>
<td>3.277</td>
<td>3.319</td>
<td>3.691</td>
</tr>
<tr>
<td>MAE</td>
<td>0–20</td>
<td>2.048</td>
<td>2.379</td>
<td>2.41</td>
</tr>
<tr>
<td></td>
<td>21–40</td>
<td>2.299</td>
<td>3.171</td>
<td>2.97</td>
</tr>
<tr>
<td></td>
<td>41–60</td>
<td>2.165</td>
<td>3.733</td>
<td>3.417</td>
</tr>
<tr>
<td></td>
<td>81–100</td>
<td>2.911</td>
<td>4.388</td>
<td>4.864</td>
</tr>
<tr>
<td>Overall</td>
<td>2.114</td>
<td>2.647</td>
<td>2.635</td>
<td>2.847</td>
</tr>
</tbody>
</table>

%GV: percent green vegetation; %ISA: percent impervious surface area.
magnitude and density of SUHI phenomenon, etc. Therefore, to overcome respective limitations for a wide range of applications, more efforts are necessary to incorporate multi-temporal with multi-source remotely sensed thermal data (Weng, 2009).

9. Conclusions

Considering different thermal properties, composition and quantity of various land covers, this study proposed a two-step physically based SUTM model to explore the impacts of interaction of different typical land cover compositions on LST. Analyses of the LST modeling results derived from SUTM and comparisons with linear and quadratic polynomial regression models using three individual spectral indicators suggest two major conclusions.

First, SUTM has proven as a practical method toward integrating fractional land cover components and their respective thermal end-members for LST estimation according to the linear thermal mixing mechanism. Specifically, SUTM performs the best when compared to empirical models for examining urban thermal pattern, with the lowest RMSEs and MAEs. The overall RMSE of SUTM is approximately 2.89 K, far less than those of the NDVI-, %GV-, and %ISA-based models. Similar results were also obtained in MAEs for the examination of the overall performance.

Second, when the accuracy was assessed at five development levels with different percent impervious surface area, results indicate that SUTM consistently outperforms the other models. With SUTM, no obvious under- or over-estimations can be found in rural or urban areas. Comparatively, NDVI-based and %CV-based regression models perform relatively well in rural areas, and poor in urban areas (e.g. with %ISA greater than 20%), majorly due to the nonlinear relationship between NDVI (%CV) and LST. On the contrary, %ISA-based regression model performs relatively well in urban areas, and poor in rural areas, majorly because of the impacts of dry soil. The proposed SUTM method has achieved a much better LST modeling result as it takes into consideration the apparently different thermal properties of various typical biophysical compositions.

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References


