Comparative analysis of urban reflectance and surface temperature

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Received 4 March 2005; received in revised form 18 October 2005; accepted 20 October 2005

Abstract

Urban environmental conditions are strongly dependent on the biophysical properties and radiant thermal field of the land cover elements in the urban mosaic. Observations of urban reflectance and surface temperature provide valuable constraints on the physical properties that are determinants of mass and energy fluxes in the urban environment. Consistencies in the covariation of surface temperature with reflectance properties can be parameterized to represent characteristics of the surface energy flux associated with different land covers and physical conditions. Linear mixture models can accurately represent Landsat ETM+ reflectances as fractions of generic spectral endmembers that correspond to land surface materials with distinct physical properties. Modeling heterogeneous land cover as mixtures of rock and/or soil Substrate, Vegetation and non-reflective Dark surface (SVD) generic endmembers makes it possible to quantify the dependence of aggregate surface temperature on the relative abundance of each physical component of the land cover, thereby distinguishing the effects of vegetation abundance, soil exposure, albedo and shadowing. Comparing these covariations in a wide variety of urban settings and physical environments provides a more robust indication of the global variability in these parameter spaces than could be inferred from a single study area. A comparative analysis of 24 urban areas and their non-urban peripheries illustrates the variability in the urban thermal fields and its dependence on biophysical land surface components. Contrary to expectation, moderate resolution intra-urban variations in surface temperature are generally as large as regional surface heat island signatures in these urban areas. Many of the non-temperate urban areas did not have surface heat island signatures at all. However, the multivariate distributions of surface temperature and generic endmember fractions reveal consistent patterns of thermal fraction covariation resulting from land cover characteristics. The Thermal-Vegetation (TV) fraction space illustrates the considerable variability in the well-known inverse correlation between surface temperature and vegetation fraction at moderate (< 100 m) spatial resolutions. The Thermal-Substrate (TS) fraction space reveals energetic thresholds where competing effects of albedo, illumination and soil moisture determine the covariation of maximum and minimum temperature with illuminated substrate fraction. The dark surface endmember fraction represents a fundamental ambiguity in the radiance signal because it can correspond to either absorptive (e.g. low albedo asphalt), transmissive (e.g. deep clear water) or shadowed (e.g. tree canopy shadow) surfaces. However, in areas where dark surface composition can be inferred from spatial context, the different responses of these surfaces may still allow them to be distinguished in the thermal fraction space.

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Keywords: Urban; Landsat; Reflectance; Thermal; Temperature; Heat island; Spectral mixture analysis

1. Introduction

The urban climate is of interest for at least three reasons. (1) It has a direct impact on approximately half of the world’s population. (2) Its dynamics are, to some extent, predictable. (3) It may be possible to influence it, for better or worse, with specific land use patterns. Regional mesoscale dynamics are known to be influenced by land cover differences between urban areas and the hinterlands on their peripheries (e.g. Avissar, 1996; Avissar & Verstraete, 1990; Bornstein & Lin, 2000). Understanding and predicting these dynamics requires an understanding of the spatial and temporal variations of the surface energy balance and physical properties. This, in turn, requires synoptic observations of surface conditions and estimates of energy fluxes from remotely sensed measurements. Urban reflectance properties are strong determinants of environmental conditions in the urban environment. Surface reflectance is a first order determinant of energy flux but reflectance is also influenced by factors such as moisture availability and temperature. The relationship between surface temperature and reflectance provides information about both the surface properties (e.g. composition, emissivity) as well as...
processes (e.g. evapotranspiration, latent and sensible heat flux) that are key determinants of surface energy balance. For this reason, considerable effort has been devoted to understanding the factors that influence the relationship between surface temperature and optical reflectance. To date, most effort has been focused on using estimates of vegetation cover to constrain evapotranspiration (e.g. Carlson & Buffum, 1989; Carlson et al., 1995, 1981, 1990; Gillies & Carlson, 1995; Gillies et al., 1997; Goward et al., 1985, 2002; Price, 1982, 1984, 1990), and emissivity (Kahle et al., 1980; van de Griende & Owe, 1993; Valor & Caselles, 1996). The covariation of surface temperature with albedo is also used to constrain surface energy balance (e.g. Menenti, 1993; Roerink et al., 2000; Menenti et al., 1989).

The recognition that albedo and vegetation cover impact surface energy flux has lead to a variety of methods to extract synoptic surface parameters from remotely sensed imagery (see Dash et al., 2002 for a recent review). However, methods that rely on vegetation indices (e.g. NDVI) as proxies for surface properties must contend with a nonlinear dependence on areal vegetation fraction (Asrar et al., 1985; Elmore et al., 2000; Small, 2001) and the fact that difference indices are not associative (Price, 1990). It has also been shown that vegetation indices are influenced by underlying soil reflectance (Huete, 1986; Huete et al., 1985).

In addition to albedo and vegetation cover, surface energy fluxes are also strongly influenced by soil properties and surface roughness. Roughness affects both advective cooling and shadowing while soil properties influence moisture availability and emissivity. Moreover, soil reflectance is known to change with moisture content thereby changing the energy partition between latent and sensible heat flux. In order to decouple the effects of vegetation cover, soil properties (e.g. albedo, emissivity), surface conditions (e.g. moisture content) and surface illumination on synoptic thermal imagery, it is necessary to incorporate more information from the coincident surface reflectance measurements. One obvious option would be to combine the vegetation cover and albedo approaches referred to above but vegetation indices and albedo are not independent. Linear transformations of multispectral imagery (e.g. Jackson, 1983; Kauth & Thomas, 1976) contain more information than vegetation indices and provide greater separation of vegetation and soil reflectance but the resulting greenness and wetness bands are still not generally independent. There is, however, another option. Linear mixture models provide an alternative approach that can deconvolve the competing influences of vegetation cover, substrate properties (both pervious and impervious) and surface shadowing on both aggregate reflectance and surface temperature measurements. Recent analyses of diverse global collections of Landsat ETM+ imagery suggest the existence of a global mixing space in which >90% of multispectral image variance can be described as linear mixtures of three independent spectral endmembers (Small, 2004, 2005). These analyses reveal a consistency in spectral mixing processes in a wide variety of both developed and undeveloped landscapes. A simple three endmember mixture model can resolve ETM+ spectra into estimates of areal fractions of rock and soil substrate, vegetation and dark surface components with RMS errors less than 0.04 reflectance units in >95% of 30,000,000 spectra (Small, 2004). Additional endmembers can be added to accommodate important characteristics of specific mixing spaces. Rock and soil Substrate, Vegetation, and non-reflective Dark surfaces represent three fundamental physical components of a wide variety of landscapes and they have distinct influences on surface energy flux. Understanding how these components simultaneously influence surface temperatures at moderate (30 m) spatial scales could resolve some ambiguities in our current understanding of surface energy fluxes in urban areas and their non-urban hinterlands.

The objective of this analysis is to investigate the relationship between optical reflectance properties and surface energy balance in a diverse range of urban settings and non-urban peripheries. The approach is to quantify the relationship between surface temperature and biophysical land surface fractions (SVD=Substrate, Vegetation and Dark surface) at moderate spatial scales for a wide variety of developed and undeveloped landscapes and to determine which characteristics of the reflectance and surface temperature covariation are consistent across the range of different environments. A three endmember linear mixture model is inverted with a single suite of generic global endmembers to yield directly comparable estimates of vegetation, substrate and dark surface fractions for 24,000,000 Landsat ETM+ spectra in 24 diverse urban settings and their rural peripheries. The covariation of surface temperature with substrate, vegetation and shadow fractions in these thermal fraction spaces is determined by physical properties such as moisture content, surface roughness and emissivity. While most studies to date have focused on individual study sites, a comparative analysis of these thermal fraction spaces under a range of environmental conditions for different landcover mosaics can highlight consistencies in the relationship between surface temperature and different biophysical components of the landscape. It is not feasible to field validate such a diverse collection of study sites (without generous funding) but the spatial resolution of the ETM+ sensor makes it possible to infer many of the land cover types from spatial context within the image. The strategy is to use a wide variety of urban settings, landscapes and environmental conditions to quantify consistencies in the relationship between reflectance properties and surface temperature.

2. The spectral mixture model

Simple linear mixture models can be used to quantify reflectance properties on the basis of fundamental biophysical components of the land surface. Spectral Mixture Analysis (SMA) provides a methodology whereby an observed radiance is modeled as a linear mixture of spectrally pure endmember radiances. Linear mixture models are based on the observation that, in many situations, radiances from surfaces with different endmember reflectances mix linearly in proportion to area within the IFOV (Johnson et al., 1983; Singer, 1981; Singer & McCord, 1979). This observation has made possible the development of a systematic methodology for spectral mixture analysis (Adams et al., 1993; 1986; Gillespie et al., 1990; Sabol
et al., 1992; Smith et al., 1990) in which land surface reflectance variations are represented by a set of endmember fraction images describing spatial variations in the areal abundance of each endmember. Although the physical process represented by the mixture model corresponds to the measurement of a mixed radiance within the sensor IFOV, the model can also be applied to exoatmospheric reflectances because the calibrations are linear. If a limited number of spectrally distinct endmembers can be found it is often possible to define a mixing space within which mixed pixels can be described as linear mixtures of the endmembers. Given sufficient spectral resolution, a system of linear mixing equations can then be defined and the best fitting combination of endmember fractions can be estimated for each of the observed reflectance spectra. The solution to the linear mixing problem can be cast as a linear inverse problem in which the system of mixing equations is inverted to yield estimates of the endmember fractions that best fit the observed mixed reflectances (Adams et al., 1986; Boardman, 1993; Boardman & Kruse, 1994; Settle & Drake, 1993; Smith et al., 1990). It is important to note that even when the surface within the IFOV is not actually a mixture of the model endmember materials, it can be represented as such a mixture if it lies within the bounds of the mixing space. Because the methodology provides a general physical representation of mixed reflectances, it has proven successful for a wide variety of quantitative applications with multispectral imagery (e.g. Adams et al., 1993, 1986; Elmore et al., 2000; Pech et al., 1986; Roberts et al., 1998; Smith et al., 1990).

The feasibility of the linear mixture model depends on the topology of the spectral mixing space in which the observed spectra reside. The mixing space is the N-dimensional cloud of image pixels corresponding to all of the image spectra to be represented by the mixture model. The mixing space can be represented graphically as scatterplots of the various band combinations corresponding to different 2D projections of the N-dimensional cloud. The dimensionality of the problem can be reduced by focusing on the dimensions of the mixing space that contain the majority of the image variance. A principal component transformation can be used to reorient (rotate) the mixing space and provide quantitative estimates of the variance accounted for by each principal component (PC). Principal component analyses of Landsat and Ikonos imagery indicate that >90% of image variance can generally be represented with the three primary PCs of the mixing space (Small, 2003, 2004, Fig. 1. Global composite spectral mixing space. Orthogonal projections of three primary principal components of the 30 sub-scene ETM+ composite from Small (2004). Gray shading indicates scatterplot pixel density. The Side view shows the two primary dimensions accounting for >90% of the variance with a triangular mixing space bounded by Vegetation, Substrate and Dark spectral endmembers. The prominent spur extending from the Low albedo endmember corresponds to Reefs and shallow seafloor. The End view shows the tapering of the mixing space approaching the Vegetation endmember and the divergence resulting from nonlinear mixing along the gray axis spanning the Dark and Substrate endmembers. The Top view also highlights the increasing divergence approaching the Substrate endmember(s). Endmember spectra correspond to dense green vegetation, SWIR reflective rock and soil substrates and the Rayleigh scattering associated with very low albedo surfaces like clear water, deep shadow, dark soils and rocks. Lighter gray spectra correspond to binary mixtures along the straight edges of the mixing space extending from the Dark to the Vegetation and Substrate endmembers.
2005). This allows us to represent the topology of the mixing space with three orthogonal projections of the three primary PCs. In the case of Landsat imagery, the 3D mixing space has a triangular topology which suggests that the mixed reflectances contained within can be represented by a three endmember mixing model (Fig. 1).

The limited number of spectral endmembers that are distinguishable by broadband sensors generally corresponds to basic biophysical land surface types. These endmembers can be illustrated with a sufficiently diverse mixing space such as the global 3D mixing space shown in Fig. 1. The apexes of the mixing space correspond to the spectral endmembers while the mixed pixel reflectances lie within a convex hull circumscribing the apexes (Boardman, 1993). The reflectance vectors residing at the three primary apexes of the global mixing space are shown in Fig. 1d. These endmember spectra correspond to high albedo rock and soil Substrate, Vegetation and non-reflective Dark surfaces. The three endmember linear mixture model describing the global mixing space is henceforth referred to as the SVD model. The triangular topology of the global ETM+ mixing space (Small, 2004) shown in Fig. 1 is very similar to that of many urban areas worldwide (Small, 2002a,b) because urban areas are spectrally diverse. The straight edges bounding the Dark surface endmember indicate that binary mixing between the Dark and Vegetation endmembers is strongly linear. The mixing continuum between the Dark and Substrate endmembers also appears to be linear in the side view but the end view of the mixing space reveals convexity in the third dimension suggesting a small degree of nonlinear mixing along this “gray axis”. The concave edge of the mixing space between the Vegetation and high albedo Substrate endmembers is consistent with the linear model although the concavity suggests that all mixtures of these two endmembers contain some amount of the Dark endmember also.

In this analysis a three endmember linear mixture model is inverted 24,000,000 times using a single set of generic global SVD endmembers (Fig. 1) to provide Substrate, Vegetation and Dark surface fraction estimates for each mixed pixel in each

Fig. 2. Endmember fractions and RMS error for the ETM+ three endmember linear mixture model for the New York metro area. Higher fractions (and error) are indicated by lighter shading. A 2% linear stretch has been applied to each image. Spatially contiguous areas of higher (∼ 0.02) RMS error correspond to an exposed soil that is not represented by the three endmember model. 99% of the pixels in the image have RMS error less than 0.015 reflectance units. Note the neighborhood scale variations in vegetation abundance.
image. The three component linear mixture model is given in continuous form by:

\[ R(\lambda) = f_S E_S(\lambda) + f_V E_V(\lambda) + f_D E_D(\lambda) \]  

where \( R(\lambda) \) is the observed radiance profile, a continuous function of wavelength \( \lambda \). The \( E(\lambda) \) are the spectra corresponding to the substrate (S), vegetation (V) and dark (D) endmembers. The corresponding endmember fraction estimates we seek are \( f_S, f_V \), and \( f_D \). For simplicity, this model does not accommodate the cloud, snow/ice or submarine reflectance limbs of the global mixing space. However, the mixture model need not be limited to the SVD endmembers and could theoretically accommodate up to three additional endmembers. In practice, however, the inherent dimensionality is generally less than the full six dimensions and observed reflectance can usually be accurately represented with the three SVD endmembers (Small, 2004). In some cases, region specific mixture models using local endmembers may be more appropriate for individual studies. For this analysis the generic global endmembers are used to facilitate comparison of the endmember fractions in different settings. Estimating endmember fractions using both global and local endmember suites provides both region specific endmember fractions which may be more accurate and global fractions that can be compared to other locations.

Endmember fractions are estimated with a constrained least squares inversion following the procedure described in detail by (Small, 2001). An example of the Substrate, Vegetation and Dark endmember fractions, as well as the RMS error for New York are shown in Fig. 2. The only significant error is associated with areas having distinct soil types as would be expected when only a single high albedo substrate endmember is used. In spite of the larger errors for some soils, 99% of the pixels in the NYC image have RMS error less than 0.015 reflectance units indicating that even the misfit soil areas can be represented with the generic global endmembers. In both global and local analyses, RMS error generally diminishes with increasing fractions of Dark and Vegetation endmembers. This indicates that the inverse problem is well posed with respect to vegetation and dark fraction estimation. Despite the larger errors for some high albedo substrates, RMS error is generally less than 0.02 reflectance units, suggesting that the 3 endmember linear model is still capable of replicating the observed mixed reflectances quite closely.

While RMS error will always expose a poorly posed model or endmember, estimate accuracy must be determined through validation. Vegetation fraction estimates for the New York subscene were validated with Quickbird imagery and generally agree to within 10% for fractions greater than 0.1 (Fig. 3). A detailed validation by Small and Lu (in press) indicates that the observed scatter in Fig. 3 is consistent with a combination of 3% to 6% estimation error and a 17 m subpixel misregistration of the Landsat to the Quickbird image.

It is important to note that the substrate and vegetation fractions correspond to the illuminated areas within the GIFOV. Illuminated vegetation and substrate fractions will generally be lower than actual areal fractions because some fraction of their surfaces will be shadowed at various scales by surface roughness and illumination angle. This same caveat applies to vegetation indices. This may partially explain the nonlinearity in which NDVI saturates above \( \sim 0.7 \) as even fully closed canopies generally have some degree of internal shadowing within and between crowns. Although vegetation fractions estimated from TM and ETM+ data with mixture models are linear with respect to measured vegetation fraction, they should not necessarily scale with volumetric metrics such as Leaf Area Index because the sensor generally detects only illuminated surface. In spite of the shadow caveat, the dark surface fraction provides valuable information precisely because it is sensitive to shadow. In areas where overall albedo can be assumed constant (e.g. agriculture, some forests), the shadow fraction

Fig. 3. Measured versus estimated vegetation fractions for the New York validation site (Small and Lu, 2006). Measured fractions are calculated from 2.8 m Quickbird estimates integrated to 30 m. Estimated fractions are derived from Landsat ETM+ estimates co-registered to the resampled Quickbird image. Circles show median estimated fractions and bars show InterQuartile Ranges in 1% bins. Darker pixels correspond to larger numbers of 30 m samples. Medians are within 5% for fractions greater than 10%. The observed scatter about the 1:1 line is consistent with a 3% to 6% estimation error combined with a 17 m spatial misregistration between the ETM+ and Quickbird images.

Fig. 4. (A) Visible/Infrared false color composites for 24 cities worldwide. Each subscene is 30 x 30 km. Red/Green/Blue = ETM+ bands 7/4/2. Each image is displayed with a 2% linear stretch. (B) Endmember fraction composites for 24 cities. R/G/B = Substrate/Vegetation/Dark surface endmember fractions with a 2% linear stretch. Note inter city and intra city variability in relative fraction distributions. (C) Surface temperature images for 24 cities. Color scale ranges from black and cooler to warmer colors with increasing temperature. Each scene is displayed with a 2% linear stretch. Note that while many urban cores have higher temperatures than surrounding areas, some cities are indistinguishable from surrounding areas and some cities are actually cooler than surrounding areas. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
Fig. 4 (continued).
Fig. 4 (continued).
could provide a scale-dependent measure of surface roughness. This has obvious applications for surface energy budgets as surface roughness has a strong influence on advective cooling of the land surface. Large variations in shadowing occur in urban areas and have a noticeable impact on environmental conditions. Significantly higher (~20%) shadow fractions are evident in the canyons of midtown and lower Manhattan relative to other parts of New York (Fig. 2).

Resolving the mixed reflectance into spectral endmember fractions makes it possible to compare diverse environments on the basis of distributions of illuminated vegetation, rock and soil substrate, and nonreflective dark surface. While these are only generic endmembers (not specific types of vegetation or rock or soil), they are representative of three distinct types of spectra that correspond to three of the most commonly observed scene elements found on Earth. Rock and soil substrate, vegetation and non-reflective dark surfaces (shadow, water, asphalt, lava, etc.) are the fundamental biophysical components of an enormous range of landscapes. The energetic response of each component to radiation and emission is governed by different physical processes. Separating their fractions at pixel scales allows the different processes to be accommodated proportionally in energy balance models. However, a fundamental ambiguity still exists with respect to albedo of permeable and impermeable surfaces. Because permeability is not an optical property, optical reflectance alone cannot generally distinguish permeable and impermeable surfaces. Similarly, broadband optical sensors like ETM+ cannot generally distinguish between low albedo absorptive surfaces (like fresh asphalt or basalt), transmissive surfaces (like water) and non-illuminated surfaces (shadows) of individual pixels on the basis of reflectance alone. This is because a non-reflective surface does not provide the sensor with a sufficient upwelling radiance signal to indicate what is happening to the downwelling radiance that is not being reflected. Hence a water-saturated soil can be effectively indistinguishable from an illuminated fresh basalt flow or even a high albedo surface (permeable or impermeable) in deep shadow. Fortunately, these surfaces have very different thermal responses so a comparison with coincident surface temperature measurements can help distinguish them. This is discussed in greater detail below.

3. Endmember fractions and surface temperature

This analysis quantifies the relationship(s) between surface temperature and vegetation, substrate and dark surface fractions for a diverse collection of 24 urban/rural settings worldwide. Each 1000×1000 pixel ETM+ subscene was chosen on the basis of land cover heterogeneity, cloud cover, data availability and spectral diversity. Most of these subscenes were also used in the detailed spectral mixture analysis described by Small (2005). Endmember fractions are estimated using a simple three endmember linear mixture model with the generic global Substrate, Vegetation and Dark surface (SVD) endmember spectra used by Small (2004). The resulting fractions and errors are not significantly different from those obtained using the global urban endmembers from the 2005 analysis (which was actually conducted in 2002) as the endmember suites are almost identical. Each subscene is shown as both a visible/infrared false color composite and an endmember fraction composite in Fig. 4. No radiometric normalization was applied because the analysis focuses on the topology of the thermal fraction spaces but does not compare them quantitatively. It is also important to acknowledge the effects of seasonality on both the reflectance and the surface temperature. The geographic diversity of the subscenes is intended to incorporate the effects of the seasonal and climatic variability but these factors cannot be explicitly addressed with the limited data set used here.

Surface temperature is represented as at-sensor brightness temperatures derived from the ETM+ low gain thermal band as described in the Landsat Data Users Handbook (1999). Landsat’s mid-morning overpass time is less than optimal for imaging the thermal field responsible for maintaining an urban heat island but it does provide the time coincident response of the land surface to solar radiation. The 60 m surface temperature estimates are resampled to 30 m for coregistration with the ETM+ exoatmospheric reflectance spectra. No atmospheric correction was applied and no emissivity calibration was attempted because the ancillary data required for accurate corrections are not available for most of the locations and dates. Speculative corrections are of questionable value. The expected uncertainty introduced by emissivity differences is less than 1.4 K for mid latitude summer acquisitions (Dash et al., 2002). The most obvious effect of emissivity differences will correspond to differences in the physical properties of the three endmember types so the effect of a correction could change the size of the thermal fraction space somewhat but it should not change the shape of the thermal fraction space. Thermal images for each subscene are shown in Fig. 1c.

In urban settings Landsat images both the reflected radiance field and the emitted thermal field as mixed pixels. Fractal analyses of ETM+ surface temperatures and vegetation fractions in an urban setting suggest an operational scale of 120 m for the surface temperature field (Weng et al., 2004) so the 60 m pixels are conceivably oversampling the dominant spatial structure of the temperature field. The fact that the thermal imagery is spatially correlated at pixel scales is consistent with the suggestion that the operational scale is coarser than the 60 m pixel size. However, it is known that the individual elements contributing to the thermal field are generally smaller than the GIFOV of the thermal sensor (Voogt & Oke, 2003). Correlation analyses of high spatial resolution imagery from a variety of urban settings worldwide consistently show characteristic spatial scales of 20 to 30 m for urban reflectance variations (Small, 2003). This suggests that the spatial variations of urban vegetation cover that dominate the thermal field occur at a spatial scale significantly coarser than the characteristic scale observed for reflectance. In reality both the reflectance and thermal fields are being imaged as mixed pixels but the 30 m spatial resolution and the use of mixture models provides constraints on the biophysical surfaces that contribute to the mixed reflectance and composite thermal signature. This is consistent with the use of generic SVD...
Fig. 5. Thermal-Vegetation fraction spaces for 24 cities. All plots span the full fraction range (0–1) on the abscissa and a common temperature range of 275–325 K on the ordinate. Warmer colors indicate exponentially greater numbers of pixels. Note that the temperature range of most individual cities is small compared the range spanned by all of the cities. For this reason, stretching the temperature range to accommodate each city would better highlight the temperature variation with each fraction.
endmembers because substrate and vegetation have very different spectral characteristics (SWIR bright vs VIS absorptive and NIR bright) and energetic responses (absorption vs transpiration) and both are modulated by shadow at a wide range of scales.

The relationships between each endmember fraction and the surface temperature are shown in thermal fraction space scatterplots. The effects of solar radiation differences are immediately apparent when surface temperature is plotted against vegetation fraction at a common scale. Fig. 5 indicates that the range of temperatures spanned by most of the individual subscenes is significantly less than the overall range spanned by the collection of 24 subscenes. Plotting all the spaces at the same scale highlights differences among the overall temperatures of the study sites but it does not facilitate comparison of the thermal fraction spaces because the individual temperature ranges are compressed. For this reason, all thermal fraction spaces are plotted using a common fraction range but an individually scaled temperature range to highlight the covariation between the endmember fraction and the surface temperature. Thermal fraction spaces for substrate, vegetation and dark surfaces are shown in Fig. 6.

4. Thermal fraction spaces and energy balance

Consistencies in the covariation of surface temperature with each endmember fraction illustrate the energetic consequences of areal tradeoffs in biophysical endmembers with different reflectance properties. Continuous gradients in aggregate mixed reflectance arise from gradual changes in vegetation type, abundance and canopy closure, variations in albedo and moisture content of pervious surfaces and surface texture and shadowing of all illuminated surfaces. Therefore, consistent changes in the maximum and minimum temperatures with the relative amount of each endmember fraction can highlight the physical conditions and properties that influence the surface temperature and energy partition. Clustering of pixels within the thermal fraction space also constrains the homogeneity or heterogeneity of the land cover properties in the corresponding pixels. For instance, the dispersion of the broad clusters associated with most forests contrasts the sharp clusters associated with water surfaces because the reflectance and surface temperature of water bodies is generally much more homogeneous (at scales <100 m) than the variations in illuminated vegetation and shadow in forests with varying degrees of canopy roughness and closure. Consistencies in the covariation of surface temperature with endmember fractions can be parameterized to describe changes and differences in the relationship under different physical conditions. To date, most effort has focused on parameterizing the covariation of surface temperature and vegetation cover to constrain evapotranspiration rate and soil moisture (e.g. Carlson et al., 1981; Gillies & Carlson, 1995; Goetz, 1997; Goward et al., 1985, 2002; Price, 1982, 1990), air temperature (e.g. Moran et al., 1994; Prihodko & Goward, 1997) and stomatal resistance (Nemani & Running, 1989). It is clear that all of these factors can influence surface energy balance of vegetated landscapes but it is not necessarily obvious how much influence each factor has under different circumstances. With only two variables (temperature and vegetation abundance), it is not generally possible to distinguish the relative influence of three or more factors. Considering additional variables add dimensions to the parameter space. This makes it possible to distinguish among greater numbers of factors if the factors can be inferred from the reflectance and spatial context (i.e. land cover type) of the corresponding pixels in the image. Covariation of surface temperature with substrate, vegetation and dark surfaces can potentially distinguish among three different factors. Comparing these covariations in a wide variety of physical environments provides a better indication of the global variability in these parameter spaces than could be inferred from a single study area.

Variation of surface temperature with illuminated substrate fraction in Fig. 6A illustrates how physical properties and processes influence the surface energy balance. Overall, land surface temperatures increase with substrate fraction but the maximum and minimum temperatures generally increase at different rates. In each of the thermal substrate fraction spaces (Fig. 6A) the maximum temperature initially increases with substrate fraction but then diminishes at higher fractions. Minimum temperatures of land surfaces (warmer and brighter than water) generally increase monotonically with substrate fraction. Maximum and minimum temperatures converge at the highest substrate fractions which are associated with intermediate temperatures while the highest temperatures are associated with intermediate substrate fractions. In most of the subscenes, the lowest temperatures are associated with water. It is hypothesized that the initial temperature increase in the main trend results from decreasing shadow and vegetation fractions with increasing fractions of illuminated substrate because substrates generally heat up faster than vegetation or water. Beyond a critical point, however the maximum temperature decreases with greater substrate fraction. This could be explained by increases in the aggregate albedo of the mixed pixel. At a constant substrate fraction maximum temperatures are expected to correspond to illuminated dry low albedo surfaces—either relatively dark soil or impervious

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Fig. 6. (A) Thermal-Substrate fraction spaces for 24 cities and surrounding areas. Warmer colors indicate exponentially greater numbers of pixels. All fractions are plotted over the full range but each temperature range is stretched to illustrate its variation with fraction. Maximum temperatures initially increase with greater substrate fraction but then decrease with increasing albedo as energy flux shifts from absorption to reflection. Arrows showing trends of max and min temperatures are subjective illustrations. (B) Thermal-Vegetation fraction spaces for 24 cities and surrounding areas. Warmer coloring indicates exponentially greater numbers of pixels. All fractions are plotted over the full range but each temperature range is stretched to illustrate its variation with fraction. In each case, maximum temperature decreases monotonically with increasing vegetation fraction while minimum temperature is stabilized by soil moisture and shadow. (C) Thermal-Dark surface fraction spaces for 24 cities and surrounding areas. Warmer coloring indicates exponentially greater numbers of pixels. All fractions are plotted over the full range but each temperature range is stretched to illustrate its variation with fraction. There is no consistent variation of temperature with dark fraction because this fraction represents contrasting effects of both shadowing and low albedo surfaces.
surface. Because the substrate endmember is relatively bright at all wavelengths, increasing the substrate fraction in a mixed pixel increases the aggregate albedo thereby reducing the net radiation flux as more downwelling radiation is being reflected and less absorbed. Hence the decrease of surface temperature with increasing substrate fraction can result from a progressive shift from energy absorption to reflection with increasing albedo which is presumably related to SWIR brightening. At constant substrate fraction minimum temperatures are expected to be associated with moist surfaces. The increase in minimum temperature is influenced by changes in soil moisture and a progressive increase in sensible heat flux as evaporation and diminishing shadow increase the radiation flux to the moist substrate until the maximum and minimum temperatures converge at maximally illuminated (and dry) substrate.

There is a fundamental ambiguity in the characterization of substrate reflectance. Changes in soil composition (at constant moisture level) can be indistinguishable from changes in soil moisture (for constant soil composition). However, given sufficient variability this ambiguity can be resolved with coincident surface temperature because the effects of soil composition and soil moisture have opposite energetic consequences. That is, soils that are darker because of higher moisture content have greater heat capacity than dry soils of equivalent albedo. Reflectance alone cannot resolve this ambiguity.

Variation of surface temperature with illuminated vegetation fraction illustrates the well-known negative correlation in which the highest vegetation fractions are associated with low temperatures (Fig. 6B). This relationship is discussed at length in the works cited above. In some cases water bodies have significantly lower temperatures than fully vegetated surfaces but in most cases the highest vegetation fractions have temperatures close to that of the shallower water bodies. Although the modal trend (red in Fig. 6B) and maximum temperature consistently diminishes with increasing vegetation fraction, the minimum temperature of land surfaces (warmer than water) often remains nearly constant with increasing vegetation fraction. In two cases (Quito and Kathmandu) the minimum temperature increases significantly with vegetation fraction. This suggests that the temperature of the vegetation canopy is significantly warmer than the underlying substrate and or shadow in some places. In four cases (Beirut, Damascus, Kabul, San Francisco) the minimum temperature decreases significantly with increasing vegetation fraction. The decrease in maximum temperature is expected as canopy closure increases illuminated vegetation fraction at the expense of warmer exposed soil. Since transpiring vegetation is generally near thermal equilibrium with ambient air temperature and moist soil has a greater heat capacity than air it makes sense that increasing canopy closure would reduce aggregate surface temperature in mixed pixels. Previous studies refer to the upper and lower bounds of this distribution as either the warm and cold edges (Gillies & Carlson, 1995) or the dry and wet edges (Lambin & Ehrlich, 1996; Sandholt et al., 2002) respectively. In areas where a wide range of soil and water distributions is present (e.g. wetlands) the minimum temperature changes little with increasing vegetation fraction as fully saturated soil has sufficient heat capacity to absorb incoming radiation and maintain quasiequilibrium by evaporation. In arid and semiarid environments there may be insufficient soil moisture to approach the heat capacity of water so the minimum temperature is not only significantly higher than water but also decreases with increasing vegetation (and shadow) fraction at rates comparable to the maximum temperature. In these cases, the variation in temperature at a constant vegetation fraction is presumably due more to differences in shadow and substrate fraction between closed and open canopies respectively.

Variation of surface temperature with dark surface fraction shows no consistent trend or pattern. This is a result of the low albedo ambiguity discussed previously. In many cases the temperature increases with dark fraction but in several cases it decreases and in some cases the distribution shows two separate trends simultaneously. This is to be expected because the dark endmember can represent either water, shadow or low albedo surface (permeable or impermeable). When the dark endmember represents water the surface temperature is generally low because of water’s high heat capacity and thermal inertia. When the dark endmember represents absorptive low albedo surface the temperature increases with dark fraction because greater area of absorptive surface is exposed. When the dark endmember represents shadow the surface temperature is strongly influenced by the other fractions in and adjacent to the pixel. Shadows within vegetation canopies are generally significantly cooler than shadows on substrate like rock and soil because vegetation offsets absorptive heating by transpiration. These covariations can be illustrated by comparison of two different types of urban development in two contrasting environments. In spite of this ambiguity, the thermal-dark fraction space can be informative because the alignment of pixels into limbs in the thermal fraction space can highlight differences between the competing effects of albedo and shadows and moisture. Two contrasting urban settings illustrate the consistencies and differences observed among the thermal fraction spaces.

4.1. Calgary and Cairo

Calgary provides an example of a relatively young, dispersed urban center in a cool temperate environment. At the transition from the North American Great Plains to the foothills of the Canadian Rocky Mountains, Calgary has a humid microthermal climate (Koppen Dbf). The native landcover transitions from Aspen grove boreal forest with diverse soil types to a mixed prairie grassland characterized by dark, well drained Chernozemic soils (MacMillan, 1987). Most native landcover in the study area has been replaced by agriculture, suburban residential development, and a variety of intrauurban industrial and commercial centers. Fig. 7 illustrates the strong contrast and sharp gradients between the residential, industrial and commercial areas within the city and the agricultural areas on the periphery. The study area is traversed by the Bow River and wetland tributaries in the Elbow Valley and Fish Creek. The
agricultural areas contain a wide variety of crops (wheat, barley, rye, flax, canola, oats) in various states of vegetation canopy cover and soil moisture. Intraurban variations in reflectance correspond to differences in urban vegetation in residential areas and differences in shadow fraction and illuminated substrate in commercial corridors and industrial areas. The surface temperature shows a classic urban heat island configuration with a higher temperature polycentric core surrounded by a lower temperature periphery. While vegetation fraction exerts the dominant thermal influence, strong variations in urban albedo in sparsely vegetated areas also have a noticeable impact on the surface temperature. The thermal fraction spaces reveal the effect of each endmember fraction on the surface temperature. The initial increases in temperature with substrate fraction correspond to increasing exposure of substrate with diminishing vegetation fraction — both in residential and agricultural areas. The maximum surface temperatures correspond to dark soil and impervious surface. As the substrate fraction and aggregate albedo increases further the energetic shift from absorption to reflection results in a decrease of maximum temperature. As increasing fraction of moist soil is illuminated the minimum temperature increases with exposed substrate fraction as the sensible heat increases relative to the latent heat removed by evaporation. The core of the thermal vegetation fraction space is partially a mirror image (about \( T \) axis) of the core of the thermal substrate fraction space (except for water) because the main trend is dominated by the gradation from fully illuminated vegetation to mixtures of illuminated vegetation, substrate and shadow. The thermal dark fraction space shows a nearly isothermal gradation from fully illuminated vegetation to vegetation canopy with shadow. As the fraction of illuminated substrate begins to increase, the overall surface temperature increases correspondingly. This is consistent with the expectation that vegetation is nearly in thermal equilibrium with the surrounding air (and hence shadows) but that the higher heat capacity of the underlying substrate results in an increase in surface temperature as greater fractions of substrate are illuminated.

The Cairo/Giza conurbation provides a contrasting example of a relatively old but still growing urban center in an arid environment. The strong albedo contrast between the urban area and the surrounding agricultural land cover is highlighted in a false color composite (upper right) that shows different vegetation and fallow soil reflectances. The SVD endmember fraction composite (lower left) shows relative fractions of the three generic endmembers. Surface temperature variations (lower right) highlight the surface urban heat island associated with the built up area and the cooler surrounding areas. Image acquired September 9, 1999.
environment. The climate classification is low latitude hot desert (Koppen BWh). The cities flank the Nile River at the transition from the Nile delta to the uplands of the northwestern Sahara desert. The dark, fine grained alluvial soils of the delta contrast strongly with the high albedo Eocene chalk and limestone of the Mukatim desert to the south. The moisture content of these contrasting substrates is also markedly different as the desert substrate is either impermeable or dry and the agricultural areas on the delta are generally saturated from the over irrigation necessary to offset salinization of the poorly drained soils (Hamdi & Abdelhafez, 2001). An excellent summary of the land use, land cover and reflectance properties around Cairo is given by Rashed et al., 2001. The color composite images in Fig. 9 show the strong contrast between the agricultural areas on the delta to the northwest, the built up urban area near the center and the desert to the southeast. In this case the city and outlying villages on the delta are associated with surface temperatures intermediate between those in the agricultural areas and those in the desert. Although the desert has considerably higher albedo, than the urban or agricultural areas, it has relatively high surface temperatures. This suggests that the lower aggregate surface temperatures of the built up areas may be associated with a greater degree of shadowing as well as a difference in the albedo of the building materials. The thermal fraction space plots in Fig. 10 reveal a structure distinctly different from that seen in Calgary — as well as some important similarities. As in the previous example, maximum temperature increases with illuminated substrate fraction from fully illuminated vegetation through decreasing canopy closure to intermediate fractions of substrate, vegetation and shadow in the developed areas. The moisture and the low albedo of the delta soils have contrasting effects on the surface temperature so the pronounced thermal maximum is followed by only a slight decrease in surface temperature before the transition to the slightly cooler high albedo desert substrates beyond ~0.4. Most of the land area follows the shadowed minimum temperature trend toward the dry bright substrates. In this case, there is a distinct difference between the low albedo of the delta soils and the higher albedo desert substrate to the southeast of the city. This is highlighted by the two distinct trends in the thermal dark fraction space and in the

Fig. 8. Thermal fraction spaces and characteristic reflectance spectra for Calgary. Variation of surface temperature with substrate fraction (upper left) shows increasing maximum temperature with increasing substrate illumination followed by diminishing maximum temperature with increasing albedo as energy flux shifts from absorption to reflection. Variation of surface temperature with vegetation fraction (upper right) shows temperature diminishing with increasing vegetation fraction. Variation of surface temperature with dark fraction (lower left) shows increasing surface temperature associated with the simultaneously increasing fractions of substrate and decreasing fractions of vegetation seen in the main trends of the other two thermal fraction spaces. Characteristic spectra (lower right) show the pronounced effect of SWIR brightening. Image acquired August 23, 2000.
wide range of temperatures associated with the unvegetated limb of the main trend on the thermal vegetation fraction space. The strong contrast is also apparent in the characteristic spectra.

5. Implications

5.1. Urban diversity and consistency

Despite great environmental, socioeconomic and historical diversity, the 24 cities considered in this analysis illustrate several consistent characteristics of the influence of reflectance properties on urban energy balance and environmental conditions. The endmember fraction composites in Fig. 4B highlight the diversity in urban reflectance—both within and among individual cities. The endmember composites condense six bands of reflectance information into three fundamental components that more clearly indicate the dominant biophysical component(s) as primary colors. This simplifies the representation of land cover in much the same way that a thematic classification does but accommodates the continuous gradations that thematic classifications cannot. In most of the 24 false color infrared images (Fig. 4A) the built up urban areas can be easily distinguished by an experienced analyst but the distinction is less apparent in the fraction composites. This is because many of the recognizable characteristics of urban areas are textural as well as spectral. The comparison highlights the difference in the core reflectance characteristics of different cities. This diversity is also apparent in the thermal signatures in Fig. 4C. Note that many of the cities are not associated with a stereotypical surface urban heat island signature. In most cases the intra-urban variations are as great as the urban-rural temperature difference. Predawn and mid-afternoon thermal images would show the surface heat island more clearly but the overall patterns would not be radically different from the mid-morning images. As expected, some cities are associated with higher surface temperatures than their more densely vegetated peripheries. However, many cities are more difficult to distinguish because of both urban vegetation and sparsely vegetated peripheries. In arid environments (e.g. Kabul, Damascus) cities often result in
Fig. 10. Thermal fraction spaces and characteristic reflectance spectra for Cairo. Variation of surface temperature with substrate fraction (upper left) shows steadily increasing minimum temperature with substrate fraction (bottom arrow) and rapidly increasing maximum temperature with substrate fraction followed by slightly diminishing maximum temperature as the albedo increases and energy flux shifts from absorption to reflection. Variation of surface temperature with vegetation fraction (upper right) shows the thermal gradient at lower temperatures (<309 K) as vegetation fraction decreases from agricultural to urban areas. Variation of higher (>309 K) temperatures with dark fraction (lower left) also mirrors the effect of SWIR brightening seen in the substrate plot above. Characteristic spectra (lower right) illustrate the considerable increase in SWIR brightness associated with the desert substrate.

Fig. 11. Schematic illustrations of thermal fraction spaces and dependence of bounding temperature trends on moisture, albedo and shadow. Crossover threshold temperature ($T_x$) and substrate fraction ($S_x$) values indicate energetic transition points where competing physical factors heating and cooling the surface balance each other. The corresponding thermal-dark fraction space (not shown) represents the contrasting effects of both shadow and albedo and does not have an analogous characteristic structure.
“cool islands” if they have higher vegetation and shadow fractions than the surrounding deserts. In spite of this diversity, the 24 study areas have a number of similarities in their thermal fraction spaces. In addition to the well-known covariation of surface temperature with illuminated vegetation fraction, there is also a complementary covariation of surface temperature with illuminated substrate fraction. It is important to refer explicitly to illuminated fractions because vegetation and substrate surfaces both have roughness-dependent shadowed fractions as well. These are accommodated by the dark surface endmember and modulate the aggregate reflectance and surface temperature of the vegetation and substrate surfaces as the illumination and shadows shift over the course of the day.

5.2. Energetic constraints and considerations

The mixed reflectance properties of a pixel provide multiple constraints on the factors influencing the aggregate surface energy flux through the covariation of surface temperature and endmember fractions. Three different processes are illustrated by the changes in maximum and minimum temperature with increasing substrate fraction (Fig. 11a). The initial increase in maximum temperature is hypothesized to result from the initial exposure and heating of substrate at low fractions while the subsequent decrease in maximum temperature results from diminishing thermal radiation flux as the aggregate broadband albedo increases with substrate fraction in dry and fully illuminated substrate. The increase in minimum temperature with increasing substrate fraction is hypothesized to result from increasing exposure of wet or partially shadowed substrate. If these hypotheses are correct, at least four threshold parameters can be derived from the thermal-substrate fraction plot to supplement the slope-related parameters often derived from thermal-vegetation fraction plots. The values of these four threshold parameters are determined by the two crossover points of the three trends of maximum and minimum temperature with increasing substrate fraction. The threshold crossover substrate fraction, \( S_x \), is the fraction at which the maximum temperature \( T_{x\text{H}} \) occurs and corresponds to the point where increasing exposure of substrate fraction to illumination causing increasing absorptive heating balances the decreasing sensible heat flux (surface temperature) that results from the increasing albedo and greater reflectance of incoming energy as the illuminated substrate fraction continues to increase. The rate at which the albedo of pervious surfaces increases (and energy absorption decreases) is determined, in part, by the rate of evaporation of soil moisture. Drying of soils generally results in increasing albedo which decreases the net radiation flux thereby modulating the evaporation by limiting the energy available to drive further evaporation. The threshold crossover temperature, \( T_x \), occurs at the maximum substrate fraction \( S_{x\text{H}} \) and is the temperature at which the decreasing sensible heat flux associated with increasing aggregate albedo is balanced by the increasing heat flux associated with diminishing shadow and soil moisture and increasing exposure of the substrate fraction. These trends, crossover points and phenomena are summarized schematically in Fig. 11. The slopes and crossovers of these trends represent the limiting effects of albedo, soil moisture and shadow on the aggregate surface temperature. In locations where the substrate is soil of uniform color and roughness, differences in temperature may correspond predictably to soil moisture. Testing this assertion and the predictive power of the relationship is beyond the scope of this study but is currently the focus of a separate investigation. If the assertion proves correct, it may be possible to use the slopes and crossovers of the bounding trends to estimate moisture in the presence of varying vegetation cover.

Parameterizing covariations of soil moisture, vegetation and surface energy balance with complementary endmember fractions representing energetically distinct components of the land surface has potential applications for hydrologic, ecologic and climate models. This analysis highlights consistent variations in both maximum and minimum temperature as well as the modal trends of the distributions. In the schematic examples used here subjective linear trends are used to illustrate these covariations. However, some of the trends and distributions appear to have bilinear or even nonlinear covariations so it is not necessary to represent them with linear trends in all cases. Ultimately, the linearity of the trends in different locations might itself be used as a constraint in the appropriate process model. A detailed analysis of the individual covariations is beyond the scope of this study but it is apparent that different methodologies could be developed to fit both linear and nonlinear functions to the bounds of the distributions. The analysis shows that distinguishing illuminated vegetation and substrate from shadow and other non-reflective surfaces provides additional degrees of freedom to distinguish competing effects of other surface characteristics in addition to vegetation fraction. Representing surface reflectance with endmember fractions derived from mixture models also eliminates the need to use linearized vegetation indices as proxies for vegetation fraction. A further benefit of the spectral mixture analysis is the ability to distinguish areas of nonlinear mixing where multiple scattering is likely to complicate the surface energy fluxes. The RMS error of the mixture model could be used to flag pixels where nonlinear mixing violates the linear mixture model and may also nullify simplifying assumptions about the surface energy flux model. All of these benefits derive from the fact that the mixture model makes use of multiple dimensions of information in the mixed reflectance signal.

Acknowledgements

This research was supported by the NASA Socioeconomic Data Applications Center (SEDAC), the Doherty Foundation and the Environmental Protection Agency STAR program. This work was supported by the U.S. Environmental Protection Agency’s National Center for Environmental Research (NCER) STAR Program, under Grant R-828733. Disclaimer: Although the research described in this presentation has been funded in part by the U.S. Environmental Protection Agency, it has not been subjected to the Agency’s required peer and policy review and therefore does not necessarily reflect the views of the Agency and no official endorsement should be inferred.
Copious thanks to Rob Gillies, Dale Quattrochi, Anton Seimon and Ian McCubbin for helpful discussions.

References


