Estimating Heat Storage in Urban Areas Using Multispectral Satellite Data and Machine Learning

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Abstract

1

A satellite-derived hysteresis model is presented for estimate heat storage in urban areas. Storage heat flux, one of the dominant terms in the urban surface energy budget (USEB), is largely unknown despite its critical relationship to various urban environmental processes. This study introduces a novel technique for quantifying heat storage by relating multispectral satellite radiances and geophysical properties to ground-truth residual heat storage computed with flux instruments. Gradient-boosted regression trees serve as the method of maximizing the relationship between satellite data and flux measurements. Several flux networks are used to train and validate the model over varying land cover types, which strengthens the robustness of the model. The model performs well under variable weather conditions such as cloudy rainy days. In comparison with other studies, the RMSE and MAE values were found to be lower than some ground-to-ground studies, and is one of few satellite-derived methods that computes direct comparison over a range of different land cover types.

Keywords: Heat Storage, GOES-16, Machine Learning, Radiance, Heat

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1 1. Introduction and Background

Heat storage has been cited as a major contributor to the urban heat 2 island phenomenon due to increased thermal conductivity and heat capac-3 ity of impervious surfaces in cities (Grimmond et al., 1991; Oke, 1988; Ra-4 mamurthy and Bou-Zeid, 2017; Roth and Oke, 1994; Taha, 1999). Several 5 studies conclude that heat storage (ΔQ_s) is one of the dominant terms in 6 the urban surface energy budget, in some cases amounting to 40% or more 7 of the net radiation (Bonacquisti et al., 2006; Coutts et al., 2007; Grimmond and Oke, 2002; Offerle et al., 2006; Oke et al., 1999). Heat storage is also 9 significant as a proxy for other fluxes. For example, anthropogenic heat may 10 be difficult to measure, but it can be derived using energy balance closure if 11 each of the other terms has been measured or calculated (Nitis et al., 2017; 12 Offerle et al., 2005; Olivo et al., 2017; Wilson et al., 2002). Despite its signif-13 icance, there is no standard for calculating ΔQ_s ; instead, five common meth-14 ods can be found scattered throughout the literature: the energy balance 15 residual method (RES), the objective hysteresis model (OHM), the thermal 16 mass scheme (TMS), the town energy balance (TEB), and the element sur-17 face temperature method (ESTM) (Chrysoulakis et al., 2018; Grimmond and 18 Oke, 1999; Kerschgens and Kraus, 1990; Lindberg et al., 2020; Lipson et al., 19 2017; Masson, 2000; Oke and Cleugh, 1987). There are varying degrees of 20 agreement between the different methods, as outlined in the Roberts et al. 21 (2006) article, which reinforces the claims that there is no standard routine 22 for measuring or calculating heat storage. 23

Much of the progress associated with urban heat storage has been lim-24 ited to sparsely distributed eddy covariance instruments mounted on flux 25 towers (Nordbo et al., 2012). Flux towers are great tools for measuring 26 accurate fluxes within a given footprint, but they also give rise to incom-27 plete spatial representations over heterogeneous areas due to the separation 28 between sites (Feigenwinter et al., 2018; Kanda et al., 2006; Ramamurthy 29 and Pardyjak, 2011). Some satellite methods remedy this by combining 30 satellite-derived surface temperatures with NDVI-based relationships (Kato 31 and Yamaguchi, 2005a; Parlow, 2003) that are capable of representing the 32 urban form, however, nearly all are time-restricted by satellite overpass pe-33 riods (Kato and Yamaguchi, 2007; Rigo and Parlow, 2007; Tsuang, 2005). 34 This results in poor statistical significance and sparse diurnal distribution of 35 data points, giving an incomplete picture of spatially-distributed urban heat 36 storage. Fortunately, with the release of two new state-of-the-art geosta-37 tionary satellites (GOES-16 and GOES-17) from the National Oceanic and 38 Atmospheric Administration (NOAA), the time between satellite observa-30 tions has finally become competitive with ground-based instruments (Schmit 40 and Gunshor, 2020). 41

In the present study, two methods are used to calculate heat storage: the residual method (RES) and a satellite-derived hysteresis model. The residual method acts as a ground-truth training and validation tool for the hysteresis model, something that is ordinarily done for the objective hysteresis model (OHM) proposed in the literature (Arnfield and Grimmond, 1998; Meyn and Oke, 2009; Pearlmutter et al., 2005). The GOES-16 satellite radiance data serves as the primary input variable to the model, while land cover and ⁴⁹ geography-specific properties act as peripheral inputs to characterize each ⁵⁰ satellite pixel. The inclusion of satellite radiance avoids many of the short-⁵¹ comings associated with applying the traditional objective hysteresis model ⁵² (OHM) to satellite data, such as the non-Lambertianity of urban materi-⁵³ als and the difficulty in quantifying the temporal hysteresis of net radiation ⁵⁴ (Herold et al., 2004; Roberts et al., 2012).

Gradient-boosted regression trees (GBRTs) are are used to statistically 55 train and validate the satellite and geographic inputs against ground resid-56 ual heat storage. Similar machine learning algorithms have been broadly 57 demonstrated as approaches to correlating multivariate systems in Earth-58 atmosphere interactions (Camps-Valls, 2009; DeFries and Chan, 2000; Lary 59 et al., 2016; Novack et al., 2011; Yoo et al., 2018). Similar methods have been 60 implemented for ground-to-satellite relationships involving aerosols (Just et al., 61 2018), shortwave radiation (Yang et al., 2018b), water vapor (Just et al., 2019; 62 Lee et al., 2019), soil moisture (Wei et al., 2019), among others. 63

One of the major challenges facing the development of satellite energy 64 balance estimates in urban areas is the lack of validation points. As a way 65 to combat this, the NYS Mesonet (Mesonet, 2020), National Ecological Ob-66 servatory Network (NEON) (Network, 2020b), and Ameriflux (Ameriflux, 67 2020) networks all serve as ground-based instruments used for training and 68 validating the satellite hysteresis algorithm. The GBRT model uses the wide 69 range of geophysical properties from ground stations to develop an accurate 70 and versatile characterization of heat storage in cities. The proposed method 71 overcomes many of the issues plaguing satellite algorithms such as dropped 72 pixels during cloudy periods, inaccurate material properties of urban surfaces, and statistically insignificant analyses. And it does so by approaching
the problem from a multi-network, statistical viewpoint. The benefits of this
method will be discussed in great detail during the presentation of results.

First, this paper outlines the methods used in quantifying heat storage in 77 urban areas using satellite data. This includes description of heat storage and 78 how it is traditionally measured and modeled with the hysteresis approach, 79 presentation of the GBRT algorithm, and methods for downscaling the re-80 sulting product. Then, New York City is introduced as the test area for the 81 summer of 2019, where summertime was chosen as a particular point of in-82 terest because of the potential for heat storage to provide information about 83 extreme heat events and urban heat island phenomena (Golden, 2004; Sailor, 84 2014; Zhou and Shepherd, 2010). By the end of this study, a diurnal urban 85 heat storage product will be posited, implemented, and validated. As a con-86 sequence of using all 16 bands of the GOES-16 satellite (wavelengths from 87 0.47µm - 13.3µm), all-weather periods are also captured, including clouds 88 and precipitation - which are often caveats when developing satellite-based 80 algorithms (Chrysoulakis et al., 2018; Middel et al., 2012). 90

Several methods proposed here are new and novel, particularly in relation to the temporal resolution of the satellite radiance data. The multispectral satellite hysteresis model challenges the status quo in surface energy budget estimates by narrowing the temporal capabilities of a widely recognized deficiency in the research area, thus, resulting in an application of heat storage that has potential implications in weather modeling, predictions of energy use, and the partitioning of energy across heat fluxes in urban environments.

98 2. Methodology

99 2.1. Satellite Hysteresis Model

The temporal hysteresis between net radiation and heat storage has been 100 widely cited (Anandakumar, 1999; Grimmond et al., 1991; Järvi et al., 2014; 101 Roth and Oke, 1994; Sun et al., 2013; Wang, 2014). Unfortunately, nearly all 102 studies that employ the objective hysteresis model (OHM) use ground-based 103 correlations to approximate heat storage. This leads to issues in spatial reso-104 lution, as many towers are located far from one another. For the few studies 105 that employ the OHM with satellite data, they first derive net radiation and 106 then implement land cover-based coefficients from the literature (Rigo and 107 Parlow, 2007). The direct implementation of the OHM to satellite data is 108 highly inaccurate due to uncertainty associated with quantifying net radia-109 tion. Satellite-derived net radiation can carry errors greater than the largest 110 errors given in heat storage studies, making the direct implementation of the 111 traditional OHM to satellite data unfavorable. The proposed multispectral 112 method instead uses satellite radiances to avoid amounting errors associated 113 with first deriving net radiation and OHM coefficients. 114

The traditional objective hysteresis model (OHM) was first developed by Camuffo and Bernardi (1982) and is often attributed to Grimmond et al. (1991), which is stated below for a given surface type:

$$\Delta Q_s = a_1 Q^* + a_2 \frac{dQ^*}{dt} + a_3 \tag{1}$$

where a_1, a_2, a_3 represent coefficients relating to different land cover types (i.e. urban, forest, crop), Q^* is net radiation, and the derivative is typically computed on an hourly basis. The satellite-derived hysteresis model is proposed below, where spectral radiances are used as the dominant input variables in place of net radiation. Land cover and geophysical properties are also used directly in the model, which leads to the following multi-variate satellite hysteresis relationship:

$$\Delta Q_s = f(t_h, L_i, dL_i/dt, g_j, e, \phi, \lambda) \tag{2}$$

where L_i designates a spectral radiance band of the GOES-16 satellite, re-125 placing Q^* as the hysteresis variable. The index *i* represents each satellite 126 band, spanning 1-16. The variable t_h is the local time in hours, from 0-23. 127 The land cover input, labeled g_j , is determined using the most recent itera-128 tion of the National Land Cover Database (NLCD 2016)- a static database 129 consisting of 20 land cover types, only 16 of which are present outside of 130 Alaska and used in this study. The NLCD parameter g_j ranges from 0-1131 and represents the fraction of each land cover class within a corresponding 132 satellite pixel. The sum of all NLCD components over subscript j must sum 133 to 1. The elevation, latitude, and longitude are also included in the model 134 and are labeled e, ϕ , and λ , respectively. The variables that are input to 135 the model are: 16 radiance bands, 16 radiance time derivatives, 20 NLCD 136 classes, latitude, longitude, elevation, and hour of day. This amounts to 56 137 variables used for training residual heat storage flux from ground stations. 138

A process flow diagram for the satellite hysteresis model is given in Fig. 1. The diagram represents each required data source and how it is used in the hysteresis model. The input data and process flow mimic the general sequence used in machine learning algorithms - where known parameters and variables are used as inputs, and desired variables are used for training and



Figure 1: Schematic diagram of the data sources, the derived variables, and how the process of developing and validating the model is carried out

validation. The inputs used specifically in the hysteresis model are both stationary (land cover, latitude, longitude, elevation) and non-stationary (satellite radiance). This combination of stationary and non-stationary information will aid in the extrapolation to areas where ground stations do not exist.

148 2.2. Residual Heat Storage

The surface energy budget can be used to solve for heat storage as a residual between the heat sources and sinks under energy balance closure assumptions (Oke, 1988; Piringer et al., 2002; Sun et al., 2013, 2017b):

$$\Delta Q_s = Q^* - (Q_H + Q_{LE}) \tag{3}$$

where ΔQ_s denotes the storage heat flux, Q^* is the all-wave net radiation, 152 and Q_H and Q_{LE} represent the sensible and latent heat fluxes, respectively. 153 The residual heat storage derived above is a straightforward method and is 154 often used when radiometers and eddy covariance instruments are available 155 to measure the remaining fluxes (Ferreira et al., 2013; Roberts et al., 2020). 156 The anthropogenic heat flux (Q_F) is often omitted under the assumption 157 that either the error associated with models for Q_F are larger than its con-158 tribution to the energy budget (Parlow et al., 2014; Sun et al., 2017a), or 159 the eddy covariance instruments are believed to capture most of the radia-160 tive, conductive, and convective components of the anthropogenic release. 161 (Grimmond and Oke, 2002). 162

The sensible and latent heat fluxes are observed using closed-path eddy covariance systems fitted with gas analyzers and 3-D ultrasonic anemometers (Balogun et al., 2009). Net radiation is measured using net radiometers, taking components of incoming and outgoing shortwave and longwave radiation in balance (Ando and Ueyama, 2017). Two networks were used, the NYS Mesonet and National Ecological Observatory Network (NEON); thus, varying models of instrumentation can be found across all sites.

The flux data was acquired every half hour for comparison with each corresponding satellite pixel, which was time-aligned with the flux measurement down to a 2.5 minute window (resulting from the 5-minute satellite interval). The satellite pixels for each of the 16 bands were available regardless of weather impacts, whereas the flux stations would remove periods of

¹⁷⁵ extreme wind or rain automatically.

176 2.3. Gradient Boosted Regression Trees (GBRT)

Gradient-boosted regression trees (GBRTs) were selected based on their 177 performance with multivariate systems and their ability to handle nonlinear-178 ities without overfitting (Kedem et al., 2012). The GBRT algorithm used 179 here is similar to the method developed by Ke et al. (2017), wherein the dif-180 ference between variable and observation is calculated as a 'loss function' and 181 broken into parts, called trees. The number of trees is determined by the in-182 crease in accuracy for subsequent added trees. For example, if the increase in 183 number of trees decreases the error down by a certain amount, then another 184 tree is added, and the partitioning continues. If an asymptote in accuracy 185 is reached, then the adding of trees ceases (Friedman, 2001; Mason et al., 186 2000). The accuracy for GBRTs here is calculated using the least-squares 187 method. For the gradient boosting aspect, pseudo-residuals are computed as 188 the gradient of the loss function and used at each time step to increase the 189 prediction capabilities of the model (Friedman, 2002). 190

Using GBRTs, the 16 satellite radiances, the 16 satellite radiance time 191 derivatives, and land cover and geography-specific properties will be trained 192 with the residual heat storage, as stated in Eqn. 2. The goal is to create 193 a robust algorithm that uses not only the radiance data relayed from the 194 satellite, but also the contribution of land cover and other phenomena. By 195 using land cover-specific parameters, the hysteresis algorithm will uncover 196 potential relationships between satellite data and ground properties, making 197 it easier to use the algorithm in uncalibrated areas. GBRTs are sensitive 198 to overfitting, and as a result, independent stations will be used to assess 199

the true performance of the model. Training size will also be varied as a way to explore the time-series dependence of the model and asses the peak performance of the model (Robinzonov et al., 2012; Schonlau, 2005).

Python's Scikit-learn library (Pedregosa et al., 2011) is used to implement 203 the gradient-boosted regression tree method outlined above (Prettenhofer 204 and Louppe, 2014). For training and validation, the residual heat storage 205 flux is partitioned in time and across 34 flux stations over the summer of 206 2019. The stations are then separated into testing and validation groups, 207 where some stations are reserved for independent verification of the model. 208 The data was partitioned in time as a percentage of total data points for 209 each station to be inputted into the GBRT algorithm. For example, if a 210 station has 1000 valid data points, a training size of 80% uses 800 data 211 points for training and 200 data points for validation. Training periods are 212 partitioned sequentially as a way to optimize the algorithm for real-world 213 implementation. Using the sequential partition allows the data to be used 214 in a similar method for an operational product, where the training can be 215 done continuously with data as it is updated in time. This may enable real-216 time calibration and perhaps improve the overall accuracy of the model in 217 the long-term. The stations are randomly shuffled when trained, meaning 218 the errors can vary from training to training. This helps diversify the model 219 with different inputs and test the stability and overfitting artifacts, if any, 220 present in the model. 221

222 2.4. Downscaling Routine

A simple downscaling routine is proposed that requires no further tools or training to the machine learning algorithm. The downscaling takes the available parameters: NLCD, geography, satellite radiances; and uses the
higher spatial resolution parameters to create higher resolution maps of heat
storage. The proposed scaling takes the 2-km native algorithm (chosen based
on the dominant resolution of 12 of the 16 radiance bands) and outputs a
320-m product.

The NLCD and digital elevation model both have the advantage of 30-230 m spatial resolution. The 30-m resolution, therefore, dictates the smallest 231 resolution possible for the algorithm, assuming the downscaling procedure 232 functions accurately and linearly, without introducing considerably large er-233 rors. The downscaling proposed here follows a similar method used in vari-234 ous satellite algorithms relating to meteorology (Busch et al., 2012; Mascaro 235 et al., 2010; Ranney et al., 2015). Three types of algorithms can be found for 236 downscaling satellite products: satellite-to-satellite methods, methods that 237 use geoinformation data, and model-based models (Mitraka et al., 2015; Peng 238 et al., 2017). One or a combination of the aforementioned methods can be 230 seen across the literature for accurately downscaling satellite data. 240

The downscaling presented here hinges on the hypothesis that the heat 241 storage relies heavily on land cover fraction, meaning the machine learning 242 model will respond to the higher resolution inputs without change to its 243 accuracy. And since there is no comparative satellite with higher spatial res-244 olution and similar temporal or spectral resolution - the satellite-to-satellite 245 method is not employable here. Of course, a higher resolution satellite could 246 be used while available over its specific overpass times, and this is perhaps the 247 most commond method of downscaling, however, since the model used here is 248 a multi-spectral approach, the satellite comparison would require downscal-249

ing first in the spectral domain, which is outside the scope of this particular 250 study. The model-based method is also difficult to employ in this particular 251 case due to lack of high-resolution ground networks for model training and 252 the lack of a standard for comparison with numerical models. Consequently, 253 geoinformation data is the method that will be used to downscale the model. 254 These geostatistical assumptions may break down when compared with 255 flux towers, due to the flux tower footprint in urban areas measuring from 256 0.5km - 2km across the literature (Bergeron and Strachan, 2011; Feigenwin-257 ter et al., 2017; Kotthaus and Grimmond, 2012, 2014; Velasco et al., 2005, 258 2009), however, this will be assessed during the presentation of results in 259 later sections. 260

261 2.5. Error Metrics

The hysteresis model given in the forthcoming analysis uses standard statistical methods to assess its performance against ground station residual flux data. The following metrics are given in relation to the comparison between model storage heat flux and ground-truth station heat storage flux derived as a residual (Laurent et al., 1998; Singh and Irmak, 2009; Şahin, 2012):

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (\Delta Q_{s,i,model} - \Delta Q_{s,i,station})^2}$$
(4)

$$MAE = \frac{1}{N} \sum_{i=1}^{N} |\Delta Q_{s,i,model} - \Delta Q_{s,i,station}|$$
(5)

$$MBE = \frac{1}{N} \sum_{i=1}^{N} (\Delta Q_{s,i,model} - \Delta Q_{s,i,station})$$
(6)



Figure 2: Flux station locations and land cover map for New York City mapped from the National Land Cover Database (NLCD).

$$R^{2} = 1 - \frac{\sum_{i} (\Delta Q_{s,i,model} - \Delta Q_{s,i,station})^{2}}{\sum_{i} (\Delta Q_{s,i,station} - \overline{\Delta Q_{station}})^{2}}$$
(7)

where RMSE represents the root-mean-square error, MAE is the meanabsolute error, MBE is the mean bias error, and R^2 is the coefficient of determination, sometimes called the model efficiency. These four metrics were chosen as a way of normalizing the comparisons in the literature - which use a varying amount of the relationships given above.

273 3. Geography and Data Selection

274 3.1. Study Area

The study area contains a grid of 16x24 GOES-16 satellite pixels at the 276 2-km scale, resulting in a total of 384 pixels in the NYC region for the native 277 satellite-derived algorithm. A total of 34 stations were used for the analysis:

20 from NEON, 10 from Ameriflux, 3 from the NYS Mesonet, and 1 from the 278 City College of New York. The observation period spanned June - August 279 2019, and the geographic spread of the stations was limited to the bounds 280 of the CONUS (continental United States). All of the stations were trained 281 for different percentages of the available data, whereas the particular urban 282 analytics are focused on the four urban sites located in New York City. Figure 283 2 shows the four NYC flux stations plotted atop the NLCD map of NYC. 284 The study area is dominated by open water and developed land cover, both 285 of which can be observed in Fig. 2. 286

287 3.2. Surface Flux Stations

Three networks are used for analysis: the National Ecological Observa-288 tory Network (NEON), the Ameriflux network, and the New York State 289 Mesonet. For each of the networks, fluxes are derived using the eddy-290 covariance method (Network, 2020a). NEON sites use Campbell Scientific 291 CSAT-3 sonic anemometers and Li-Cor LI-7200 gas analyzers mounted atop 292 vertical towers. The raw data are used to generate 30-minute turbulent flux 293 data products for sensible and latent heat fluxes. Net radiation is derived 294 using components of incoming and outgoing shortwave and longwave radia-295 tion, acquired with Hukseflux NR01 net radiometers. A total of 21 NEON 296 sites are, for the most part, non-urban and will help decouple vegetative 297 components of land cover in urban sites produced by the NYS Mesonet. 298

Ameriflux core sites are used in conjunction with the NEON sites and employ flux towers and gas analyzers similarly from Campbell Scientific and Li-Cor (Ameriflux, 2020). Nine stations are used from the Ameriflux network, most of which are non-urban. The Ameriflux sites were introduced as a way of diversifying the training and validation of the satellite algorithm. Similar to the NEON network, sensible and latent heat fluxes, along with net radiation were acquired at 30-minute intervals to produce the heat storage residuals.

The final ground network is the NYS Mesonet. NYS Mesonet stations use 306 Kipp & Zonen CNR4 net radiometers and Campbell Scientific CSAT3A 3D 307 ultrasonic anemometers and EC155 gas analyzers. The instrumentation lo-308 cated on the NYS Mesonet sites also record sensible, latent, and 4-component 309 radiation every thirty minutes. Three NYS Mesonet sites are used, all of 310 which are specifically urban and are located within New York City. An ad-311 ditional flux tower is located in Manhattan at the City College of New York 312 (CCNY), which is identical to the NYS Mesonet instruments but is not main-313 tained by the NYS Mesonet. This results in a total of 34 ground flux stations 314 for the analysis. The urban sites will serve as the test bed for the satellite 315 routine and will be used as performance benchmarks for the machine learning 316 routine. 317

318 3.3. GOES-16 Satellite Data

The Geostationary Operational Environmental Satellite-R Series (GOES-R) renamed GOES-16 upon reaching its operational orbit, is used as the weather satellite for comparison with ground-based residual heat storage fluxes acquired from the flux networks NEON and NYS Mesonet. The raw spectral radiance data is acquired from the Advanced Baseline Imager (ABI) in a data product called L1b (Level 1b), which are openly available to anyone on the Google BigQuery database.

The units associated with L1b spectral radiances are $[W \cdot m^{-2} sr^{-1} \mu m^{-1}]$. GOES-16 scan mode 3 is used and results in one observation of the continental United States (CONUS) every five minutes, for each of the 16 bands.
This allows a temporal alignment accuracy of 2.5 minutes between groundbased flux stations and corresponding satellite pixels. The spatial resolution
between neighboring pixels depends on the chosen band, but vary roughly
0.5 km - 2.0 km (Group and Program, 2017).

333 3.4. Land Cover and Digital Elevation Model

The U.S. Geological Survey recently published its fifth National Land 334 Cover Database (NLCD), designated the NLCD 2016. The contiguous U.S. 335 (CONUS) NLCD 2016 product is used here, which is produced at 30-m spa-336 tial resolution and contains 16 land cover classes (Jin et al., 2019; Wickham 337 et al., 2014; Yang et al., 2018a). The classes are divided into the following 338 categories: open water; perennial ice/snow; developed: open space, low in-339 tensity, medium intensity, and high intensity; barren land (rock/sand/clay); 340 forest: deciduous, evergreen, mixed; shrub/scrub; grasslands/herbaceous; 341 pasture/hay; cultivated crops; wetlands: woody and emergent herbaceous. 342 Refer to Fig. 2 for the NLCD breakdown in New York City. The NLCD 343 2016 incorporates four urban categories (developed classes) and will serve as 344 the determination of urbanization for given satellite pixels. 345

Along with the 16 NLCD classes, a digital elevation model (DEM) will be added as part of the classification of each satellite pixel. The Shuttle Radar Topography Mission (SRTM) is run by the U.S. Geological Survey and publishes a freely available, 30-m resolution, elevation product that spans the entire contiguous U.S. (Elkhrachy, 2018). Latitude and longitude coordinates dictate the elevation across a given satellite pixel, and is used in the machine learning algorithm to capture the sensitivity of heat storage to changes in elevation and as well as land class. This is commonly done for satellitebased assessments of evapotranspiration or thermodynamic processes at the Earth's surface (Cheng et al., 2011; Semmens et al., 2016; Xian and Crane, 2006; Zhou et al., 2014). Both the DEM and NLCD are at much higher resolution than the satellite, which will aid in the downscaling of the final satellite algorithm.

359 3.5. Relationship Between Satellite Bands and Residual Heat Storage

The hypothesis of this research hinges on the correlation between satel-360 lite radiance and ground station residual heat storage. If net radiation is 361 derived using satellite radiances throughout the literature (Bisht and Bras, 362 2010; Carmona et al., 2015; Hou et al., 2014; Jin et al., 2011), then an ap-363 plication of raw radiances, without the intermediary routine for predicting 364 net radiation, may suffice for approximating of heat storage directly. Partic-365 ularly, with the high temporal resolution of the 16 satellite bands covering 366 the visible, near-infrared, and infrared wavelengths (Schmit et al., 2018) -367 the correlation between satellite radiances and heat storage should be high. 368 Figure 3 demonstrates the correlation between ground station and nearest 369 satellite pixel for an urban area (Brooklyn, NY), where the correlation be-370 tween variables is defined as (Benesty et al., 2009; Inglada, 2002): 371

$$\operatorname{Corr} = \frac{\sum_{k=1}^{N} (\Delta Q_{s,k} - \overline{\Delta Q_s}) \cdot (L_{\lambda,k} - \overline{L_{\lambda}})}{\sqrt{\sum_{k=1}^{N} (\Delta Q_{s,k} - \overline{\Delta Q_s})^2} \cdot \sqrt{\sum_{k=1}^{N} (L_{\lambda,k} - \overline{L_{\lambda}})^2}}$$
(8)

The shortwave bands can be seen to negatively correlate with the heat storage flux during the daytime, which is expected due to the influence of direct solar irradiation. During the nighttime, the shortwave bands have



Figure 3: Correlation between ground station residual heat storage flux and nearest satellite pixel for each GOES-16 band. The shortwave bands are negatively correlated to the heat storage flux during the daytime, and minimally correlated during the nighttime; whereas the longwave bands are positively correlated to the storage flux during the daytime and negatively correlated during the nighttime. These correlations are essential to the hypothesis that radiance bands can be used to calculate heat storage flux.

almost no correlation to the heat storage, as expected, due to the opposite reasoning proposed in the previous sentence. For longwave bands, there is high correlation during the nighttime and daytime. Longwave bands are positvely correlated to the storage flux during the daytime and negatively correlated during the nighttime. These correlations reinforce the original hypothesis that the GOES-16 radiance bands can be used to calculate heat storage flux - the primary motivator going forward in this research.



Figure 4: RMSE as a function of training size for the training dataset and independent dataset. The training dataset and independent dataset have also been divided into the training period and validation period as well. We see the decrease in RMSE as a function of increased training size for the validation periods, as expected.

382 4. Results and Discussion

383 4.1. Training and Validation

Neither training nor validation were uniform across the swath of available 384 stations due to the variability of local meteorological conditions (high winds, 385 heavy rain) and complications with instrumentation, both of which cause 386 drops in data. This results in differing amounts of points per station over 387 the full testing period. Figure 4 shows the average RMSE for training and 388 validation periods, where the training dataset is a unique set of 21 ground 389 stations taken from all three networks, while the independent dataset is a 390 separate unique set of 13 ground stations from each of the three networks. 391

Dataset	Period	# Stations	Mean # Points	RMSE
Training	Training	21	2927	55.8
Training	Validation	21	326	52.6
Independent	Training	13	2594	63.7
Independent	Validation	13	289	60.5

Table 1: Division of training and validation data for the analysis over summer 2019.

The profiles given in Fig. 4 exhibit expected behavior as the training size 392 changes. The training dataset carries the lowest error during the training 393 period, which is most likely due to overfitting - a common artifact of GBRT 394 algorithms (Kedem et al., 2012). Similarly, the error in the validation period 395 is also lower than that of the independent dataset. The independent dataset 396 does, however, demonstrate consistent error across the range of training sizes, 397 indicating that the training is somewhat stable in training size, with a slight 398 decrease in error as the training size increases. 399

Considering the results of Fig. 4, 90% of the data was selected for training
and 10% was reserved for validation. It would be valid to select any training
size over 80%, as that point marks the approximate asymptote in training and
validation error. The independent dataset experiences similar phenomena,
with less variability, indicating a more accurate prediction of the model's true
performance in relation independent ground stations (or satellite pixels).

Statistics relating to the satellite-derived GBRT model for heat storage at 90% training are given in Table 1. A resulting argument can be made regarding the performance of the satellite hysteresis model , stating that the 2-km spatial model carries errors on the order of 60-65 W·m⁻², when



Figure 5: Scatter for NYC flux stations and the model performance using GOES-16 satellite.

compared with ground-based residual heat flux. This, of course, has only
been posited for the summer of 2019, and the validity of this statement is
contingent upon further validation across multiple seasons.

413 4.2. The Case Study of New York City

In Fig. 5, four scatter plots are given for each of the urban stations in New York City, exclusively for the validation period. Two of the urban stations were used during training (BLKN and CCNY), while the other two were not (QUEE and STAT). For all four stations, the RMSE values were below 60 $W \cdot m^{-2}$ and the MAE were below 43 $W \cdot m^{-2}$. The average value for both RMSE and MAE in the urban region were 49 and 34 $W \cdot m^{-2}$, respectively.



Figure 6: Temporal reconstruction of ΔQ_s using the satellite hysteresis model.

⁴²⁰ The average MBE was 7.6 W·m⁻², and the average R^2 was 0.83. All four ⁴²¹ performance metrics are well within the ranges cited across the literature ⁴²² (Roberts et al., 2006).

Investigation of Fig. 6 shows the temporal reconstruction of the same set of validation data given in Fig. 5. The array of temporal reconstructions is capable of tracking the diurnal profile of ΔQ_s quite well, something that has not been demonstrated in the contemporary satellite research (Chrysoulakis et al., 2018; Kato and Yamaguchi, 2007; Parlow, 2003; Rigo and Parlow, 2007). The satellite hysteresis model is also capable of approximating heat storage during rainy and cloudy periods, another capability lacking in the satellite literature. On the 22nd, 23rd, and 28th of August, historical weather
records for the NYC area show rainy and cloudy conditions, which is exhibited in Fig. 6 by the lower amplitudes of heat storage.

For most of the diurnal cycle, the model is able to recreate the trend of 433 heat storage for each of the sites. What varies most with the model is its abil-434 ity to capture the full-scale amplitude of both the daytime maximums and 435 the nighttime minimums. For the Queens station (QUEE), the daytime satel-436 lite heat storage peaks are smaller than the station residuals, and during the 437 nighttime the opposite can be observed. For the Staten Island (STAT) sta-438 tion, the daytime peaks are somewhat over-predicted by the satellite, which 439 can also be concluded by looking at the statistical bias. 440

Since both QUEE and STAT were omitted from the training dataset, we can hypothesize that the satellite-derived ΔQ_s may have a positive bias for less urban stations (STAT island is only about 60% developed in land cover class), and has a more tempered response in amplitude both during the daytime and nighttime for more urban areas (observed for QUEE, where the land cover class is nearly 100% developed). However, more urban stations are needed to fully verify this claim.

Something to note is that both training stations, BKLN and CCNY, are each nearly 100% urban, meaning that each of the stations and satellite pixels have different responses despite similar classifications in land cover. This is an important observation and one that increases the confidence of the model's ability to capture varying responses over urban environments where ground stations are unavailable for comparison. Although the error associated with QUEE is higher than the other three stations, it is well within the range of errors cited across the literature for ground-based OHM methods, indicating
that the satellite routine is a viable approach to quantifying heat storage.
The errors will also be explored in subsequent sections, once the downscaling
routine has been introduced.

459 4.3. Downscaling from 2-km to 320-m

The ubiquity of water surrounding the land masses of New York City 460 results in a particular obstacle for development of the satellite algorithm. The 461 issue arises when training the algorithm, where the lack of ground stations 462 over water creates a weakness for pixels that contain certain amounts of 463 water. As a consequence, pixels with a water fraction greater than 0.05 (5%) 464 were dropped. And with the satellite-derived heat storage outputting data at 465 a native 2-km resolution, many of the pixels in the study area were dropped. 466 As a way to both increase the number of satellite pixels in the small 467 window of NYC and avoid dropping so many pixels due to water content -468 a downscaling routine was developed. The downscaling takes the satellite 469 algorithm from 2-km to 320-m, which results in fewer dropped pixels and 470 a better representation of the distribution of heat storage in cities. This is 471 specifically important for coastal cities where water surrounds highly urban 472 areas. 473

As explained in Section 2.4, the native resolution of the satellite-derived heat storage is 2-km, set by the dominant spatial resolution of the radiance bands. Here, the downscaling is set to 320-m, which increases the resolution of the NYC grid to 100x150. The implementation of the downscaling algorithm is validated for QUEE and STAT, with a decrease in RMSE of $5.4 \text{ W}\cdot\text{m}^{-2}$ for QUEE and 0.3 W·m⁻² for STAT. This is shown in Fig. 7.



Figure 7: Downscaling performance for STAT (left) and QUEE (right) sites. The downscaling from 2-km to 320-m resulted in a decrease in RMSE ($5.5W \cdot m^{-2}$) for the QUEE pixel and no change in RMSE for the STAT pixel, partially validating the accuracy of the downscaling procedure.

The same was observed for both BKLN and CCNY stations as well, where 480 their errors never deviated more than 2 $W \cdot m^{-2}$ when comparing the 2-km 481 pixel to the 320-m downscaled value. A sensitivity analysis was done for 482 neighboring pixels surrounding each ground station, and similar results were 483 found for the adjacent pixels, where marginal variability was found due to 484 land cover changes. The results presented henceforth will be on the 320-m 485 satellite-derived heat storage using the GBRT method and the downscaling 486 presented here. 487

488 4.4. Spatial Representation of Heat Storage

A spatial representation of heat storage using the satellite hysteresis 489 model is given in Fig. 8 for both midday and midnight periods on Au-490 gust 24th, 2019. The data has been downscaled as per the routine given in 491 the previous section, resulting in a resolution of 320-m, rather than 2-km. A 492 spatial filter has also been implemented based on water content: any pixel 493 with more than 5% water is omitted. Additionally, any pixel that exists out-494 side the range [-200,600] W·m⁻² is also omitted. This is based on the average 495 maxima and minima observed over several standard deviations. 496

The first and perhaps most obvious inference is that the native 2-km pixels 497 have overwhelmingly influenced each downscaled pixel. The distribution of 498 color in the spatial domain seems to be dominanted by each underlying 2-499 km pixel, giving the squared-off artifact in both plots in Fig. 8. This is 500 likely due to the priority of each variable in the GBRT model, i.e., time and 501 radiance bands take precedent over land cover and elevation. This, simply 502 put, indicates that the model is more sensitive to macro changes in geography, 503 rather than local changes in geography, perhaps due to viewing angle of the 504 satellite or large changes in elevation. 505

The transition between positive and negative fluxes is also visible in the spatial representations of heat storage. Sunrise, for example, is captured on the 27th of August in Fig. 9a, where the storage is largely varied throughout the city. The sunrise on that day was observed at 6:18 a.m., indicating a possible delayed effect in heat storage for certain areas. The same can be observed a few hours after peak heating at 5:30 p.m., in Fig. 9b, where the release of heat (negative storage) is seen for some pixels, while positive



Figure 8: (a) Daytime representation of heat storage, ΔQ_s on Aug. 24 at 12:00 EDT.. (b) Nighttime representation of heat storage on Aug. 24 at 01:30 EDT.



Figure 9: (a) Heat storage after sunrise (07:30 EDT on Aug. 27) capturing the variability of the city's response to heating of its surface. (b) The inversion of heat storage (zero-crossing point) is shown just after sunset on Aug. 27 at 18:30 EDT.

⁵¹³ storage is seen for others. This indicates another possible spatial delay.

The standard deviation of ΔQ_s across valid pixels is also observed to vary throughout the day. The midday spatial distribution of heat storage varies up to $\pm 65 \text{ W} \cdot \text{m}^{-2}$, and the nighttime down to $\pm \text{ W} \cdot \text{m}^{-2}$. These values, on average, amount to 15-20% of the relative amplitudes of ΔQ_s . The largest variability occurs during the transitional periods given in Fig. 9, at sunrise and a few hours after peak heating.

520 4.5. Comparisons with Literature

A statistical comparison between satellite-derived heat storage algorithms 521 is nearly impossible as no identifiable studies have used an approach that 522 validates their model directly against ground station values. Therefore, no 523 satellite-to-satellite performance comparison is possible. This is likely due 524 to the lack of measurement standards for heat storage, and moreover, a 525 consequence of ground station sparseness in urban areas. One thing that is 526 investigated in the literature is the fraction of net radiation occupied by heat 527 storage. This is not valid in our case as net radiation is a component in the 528 residual method and, accordingly, used to train the model. 529

One definite advantage of the GBRT-based method is that it avoids a 530 common pitfall associated with satellite algorithms in urban areas, namely, 531 the handling of non-Lambertian surfaces. This is likely due to the inclusion of 532 multispectral data, which may handle some of the urban heterogeneity issues 533 in reflected radiation (de Almeida Castanho et al., 2007; Hamedianfar and 534 Shafri, 2015). Moreover, the temporal resolution of the satellite also permit-535 ted a large statistical comparison between model and ground stations, which 536 also contributes to the uniqueness and stability of the algorithm. MODIS 537 comparisons, for example, are limited to two comparison points per day along 538 the diurnal cycle. 539

A more appropriate evaluation of the satellite hysteresis model is through comparison with studies that calculate statistics based on ground-to-ground measurements. As mentioned in the introduction, there are four methods used for calculating heat storage in the relevant literature: the residual method (RES), the objective hysteresis model (OHM), the thermal mass

Table 2: Comparison between satellite-derived hysteresis model and the objective hysteresis model derived from ground net radiation data for various cities. Results from this study are in bold and are taken from the downscaled comparison with the nearest NYC ground station. The table is ordered by increasing RMSE.

Site/Description	# Points	R^2	RMSE
Los Angeles, CA (suburban) ^a	424	0.92	29.0
Mexico City (city center) ^a	61	0.96	33.6
Brooklyn, NY (urban)	345	0.92	39.5
Manhattan, NY (urban)	$\boldsymbol{229}$	0.91	45.0
Vancouver, Canada (industrial) ^a	312	0.88	48.9
Queens, NY (urban)	397	0.87	53.7
Staten Island, NY (suburban)	379	0.65	53.9
Miami, FL (suburban) ^a	204	0.79	61.9
Vancouver, Canada (suburban) ^a	464	0.67	62.9
Sacramento, CA (suburban) ^a	222	0.56	66.0
São Paulo city, Brazil (suburban) ^a	353	0.69	74.1
Chicago, IL (suburban) ^a	163	0.56	83.3
Marseille, France (city center) ^b	192	0.70	94.8
Tucson, AZ (suburban) ^a	75	0.75	107.4

^aGrimmond and Oke (1999)

^bRoberts et al. (2006)

scheme (TMS), and the town energy balance (TEB). One widely recognized paper by Roberts et al. (2006) compiles a comparison of all four methods into one study, and includes an error analysis for the OHM, TMS, and TEB against the RES method. It also agglomerates other studies in an effort to corroborate its statistics. Those errors are used here as a guide, in part, to assess the results produced by the satellite hysteresis model.

Table 2 shows the comparison between 14 different heat storage calculations by hysteresis model, four of which contain the satellite-derived results from NYC. Overall, the New York City stations: Queens (QUEE), Brooklyn (BKLN), Manhattan (CCNY), and Staten Island (STAT), all outperform 7 of the 10 stations in root-mean-square error. This is quite remarkable, particularly for the independently verified stations STAT and QUEE. All four NYC stations are also validated with more data points than 6 out of 10 stations. These statistics are an indication that the satellite-derived heat storage is a viable model against the ground-based OHM.

As for the town energy balance (TEB) method, the same study uses 560 Marseille, France as a test site. The TEB estimated a mean hourly RMSE 561 between TEB and RES of 79 $W \cdot m^{-2}$. Another evaluation of the TEB was 562 done by Masson et al. (2002) for Mexico City and Vancouver, which managed 563 mean RMSE values of 39 and 87 $W \cdot m^{-2}$, respectively. A third experiment 564 carried out in the city of Basel, Switzerland compared two different imple-565 mentation schemes for the TEB and found RMSE values of 64 and 70 $W \cdot m^{-2}$. 566 Resolutely, it is fair to say that the satellite-derived hysteresis model outper-567 forms the town energy balance. 568

For the previous study in Marseille, the final calculative method for heat 560 storage is examined: the thermal mass scheme (TMS). The RMSE between 570 RES and TMS was measured to be $109 \text{ W} \cdot \text{m}^{-2}$ - quite a large error when com-571 pared to the satellite hysteresis model. Heat storage derived by thermal mass 572 scheme and objective hysteresis model are most suited for satellite data due 573 to incorporation of thermal properties rather than aerodynamic properties. 574 Thus, the dilemma described above regarding inability to compare satellite 575 methods arises again for the TMS. As a result, very few studies have errors 576 associated with the RES method. 577

Building information is often used as an input to urban storage mod-578 els, such as the town energy balance (TEB) or element surface temperature 579 method (ESTM). Building height and building area fraction information were 580 deliberately excluded in the proposed satellite hysteresis model, due to the 581 limitations in training, where the majority of the ground stations either do 582 not contain buildings or lack building information. Thus, training with build-583 ing information would be very limited and likely result in further overfitting 584 in the GBRT model. This is where the national land cover database's four 585 urban categories become important, as they account for the range of urban-586 ization in the ground networks ranging from open space to high intensity 587 urban development. 588

Another important aspect of quantifying heat storage, either from the 589 satellite or surface perspective, is the accurate accounting of anthropogenic 590 heat flux. A wide range of studies have developed algorithms for deter-591 mining anthropogenic heat flux using traffic information, population density, 592 fuel economies, among others (Sailor and Lu, 2004). For the proposed mul-593 tispectral hysteresis model, it is assumed that the anthropogenic heat flux is 594 inherent in the measurement of conductive, convective, and radiative fluxes 595 captured by eddy covariance instruments placed in the urban areas (Grim-596 mond and Oke, 2002). This is based on observations made in several cities 597 that argue that the majority of the anthropogenic influence is outputted as 598 sensible heat flux (Kato and Yamaguchi, 2005b; Olivo et al., 2017; Sailor, 599 2011). This assumption may result in under-prediction of heat storage, but 600 it is difficult to quantify by how much, and is designated as an area for future 601 research. 602

The lack of studies comparing satellite-derived heat storage to ground stations is a motivating factor for other future works relating to satellite-derived heat storage. It is likely that in the future, the thermal mass scheme will be implemented using satellite data, notably due to the temporal resolution advancements of the GOES-16 and GOES-17 satellites. For now, the comparison between satellite-derived heat storage and ground stations remains chiefly neglected.

⁶¹⁰ 5. Conclusion

A multispectral hysteresis model was introduced as a way to predict heat 611 storage flux in urban areas using land cover and geographic properties con-612 tained within satellite pixels. The model bridges the divide between single-613 point ground measurements and spatially-distributed satellite approxima-614 tions, with direct validation - something nonexistent in the peered literature. 615 A gradient-boosted regression tree (GBRT) method was used to train input 616 variables against a series of ground flux stations. The satellite hysteresis 617 model outperformed many of the ground-to-ground hysteresis models, indi-618 cating that the satellite method may be an improved, more robust method 619 for calculating heat storage flux. 620

The error associated with the urban satellite hysteresis model was among the best inhen compared with other studies in the research field. For all four urban stations, the independently validated, 320-m spatially downscaled, average RMSE value was found to be $48.0 \text{ W} \cdot \text{m}^{-2}$, the average mean-absolute error (MAE) was found to be $33.8 \text{ W} \cdot \text{m}^{-2}$, the average mean bias error (MBE) was $9.3 \text{ W} \cdot \text{m}^{-2}$, and the mean R^2 , 0.84. The satellite-derived heat storage is also able to recreate spatial patterns in heat storage that were not previously possible, specifically in relation to the full diurnal cycle. Because the algorithm was independently trained and validated, its accuracy and ability to recreate hourly approximations of heat storage is noteworthy and unprecedented.

Another accomplishment of the satellite hysteresis model is its ability to 632 capture all-weather profiles. We saw for several periods that the satellite 633 radiances were able to capture cloudy and rainy days, which permitted the 634 calculation of tempered heat storage despite limited solar irradiance. The 635 captured heat storage under rainy weather is something that has not been 636 observed in the literature. One hypothesis is that the machine learning algo-637 rithm is able to relate the diminishment of radiance amplitude to the decrease 638 in heat storage. It could also be true that some of the radiance bands are 639 capturing minimal radiation beyond the clouds, however, this has not been 640 verified or studied at length, and remains a topic for future exploration. 641

Lastly, the maintained accuracy of the approximation of heat storage un-642 der downscaled conditions proves that the algorithm is capable of component 643 analysis and needs to be explored to the fullest extend. In summary, accurate 644 quantification of the spatial distribution of heat storage in built environments 645 has been an open question that, if resolved, will open a wide range of oppor-646 tunities in closing the surface energy balance. Temporal, spectral, and spatial 647 resolutions of new generation geostationary satellites are making this quan-648 tification a closer reality. This may enable significant advances in weather 649 and climate modeling for accurate prediction of UHI, for urban planning, 650 and for relationships between thermal responses of urban environments and 651

energy demands. This contribution is a first major step in this direction.

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