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Evaluation of the OPTRAM Using Sentinel-2 Imagery to Estimate Soil Moisture in Urban Environments.

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A B S T R A C T

The determination of soil moisture is a crucial issue for various purposes, including hydrological, climatological, and agricultural studies. Over the past few decades, several distinct remote sensing approaches have been developed. One recent development is the Optical TRApezoil Model (OPTRAM). This approach is similar to the traditional TOTRAM, but it replaces the LST index (thermal band) with the STR index, which is calculated using the SWIR band. Numerous studies have demonstrated the effectiveness of OPTRAM in predicting soil moisture. However, the capability of OPTRAM to estimate soil moisture in urbanized areas has not yet been fully recognized. To address this gap, we conducted tests in the Rio Claro municipality, where land use and occupation vary significantly. By utilizing Sentinel-2 multispectral images, we constructed the NDVI-STR space, estimated soil moisture, and compared it with field measurements. The values of R^2, MAE, and RMSE for the OPTRAM-derived soil moisture at urbanized of Rio Claro were 0.92, 0.0196, and 0.1413, respectively. These results demonstrate a high level of representativeness for the soil moisture estimates Furthermore, the freely distributed Sentinel-2 satellite images has a spatial resolution that is well-suited to the dimensions of the target areas in the evaluated scene.

Keywords: Remote sensing, Soil moisture, groundwater recharge, urban hydrology, Sentinel-2.

Avaliação do OPTRAM Usando Imagens do Sentinel-2 para Estimar a Umidade do Solo em Ambientes Urbanos.

R E S U M O

A determinação da umidade do solo é uma questão crucial para vários propósitos, incluindo estudos hidrológicos, climatológicos e agrícolas. Nas últimas décadas, várias abordagens distintas de sensoriamento remoto foram desenvolvidas. Um desenvolvimento recente é o Modelo Óptico TRApezoidal (OPTRAM). Esta abordagem é semelhante ao TOTRAM tradicional, mas substitui o índice LST (banda térmica) pelo índice STR, que é calculado usando a banda SWIR. Numerosos estudos demonstraram a eficácia do OPTRAM na previsão da umidade do solo. No entanto, a capacidade do OPTRAM de estimar a umidade do solo em áreas urbanizadas ainda não foi totalmente reconhecida. Para abordar essa lacuna, realizamos testes no município de Rio Claro, onde o uso e a ocupação da terra variam significativamente. Utilizando imagens multiespectrais do Sentinel-2, construímos o espaço NDVI-STR, estimamos a umidade do solo e a comparamos com as medições de campo. Os valores de R2, MAE e RMSE para a umidade do solo derivada do OPTRAM em áreas urbanizadas de Rio Claro foram 0,92, 0,0196 e 0,1413, respectivamente. Esses resultados demonstram um alto nível de representatividade para as estimativas de umidade do solo. Além disso, as imagens de satélite do Sentinel-2 distribuídas gratuitamente têm uma resolução espacial bem adequada às dimensões das áreas-alvo na cena avaliada.

Palavras-chave: Sensoriamento remoto, Umidade do solo, recarga de águas subterrâneas, hidrologia urbana, Sentinel-2.

Introduction

Water is an essential resource that underpins life on Earth and significantly impacts human well-being, economic opportunities, and social stability (UNICEF, 2019). The interdependence between society and water resources is fundamental for ensuring sustainable development and maintaining social equilibrium. As a vital component of the global hydrological cycle, water influences a wide range of activities, from public health and economic growth to environmental conservation. Adequate access to these services is intrinsically linked to human development, as improvements in water access are correlated with increases in the Human Development Index (HDI) (Amorocho-Daza, Zaag, & Sułnik, 2023). Therefore, efficient management of water resources is critical for advancing social development and ensuring long-term sustainability.

Access to clean and safe water is a cornerstone of public health. Contaminated water sources can lead to the spread of waterborne diseases, which have significant health implications for communities, particularly in developing regions. Ensuring reliable access to potable water reduces the prevalence of diseases such as cholera, dysentery, and typhoid fever. Improvements in water quality and sanitation infrastructure are directly correlated with reductions in mortality rates and improvements in overall health outcomes (WHO, 2017). The importance of water for maintaining health underscores the necessity of robust water management systems that safeguard water quality and availability.

Water plays a crucial role in various economic sectors, including agriculture, industry, and energy production. In agriculture, water is essential for irrigation, which supports crop growth and food security. Efficient water use in agriculture can enhance productivity, reduce costs, and promote sustainable farming practices. For industries, water is used in various processes, such as cooling, cleaning, and manufacturing. Adequate water supply is necessary for maintaining industrial operations and supporting economic growth. Moreover, water resources are integral to energy production, particularly in hydroelectric power generation. Hydropower plants rely on water flow to generate electricity, contributing to energy security and reducing reliance on fossil fuels. The economic benefits of water extend to tourism and recreation, as clean and accessible water bodies attract visitors and support local economies. Thus, the effective management of water resources is vital for sustaining economic opportunities and promoting development across various sectors.

Water scarcity can lead to social tensions and conflicts, particularly in regions where resources are limited or unevenly distributed. Competition for water resources can exacerbate existing social inequalities and create conflicts between different user groups, including agricultural, industrial, and domestic consumers. Cooperative water management policies are essential for addressing these challenges and promoting equitable access to water resources. Collaborative approaches that involve stakeholders from various sectors and communities can help mitigate conflicts and ensure that water resources are managed in a fair and sustainable manner (Pereira & Cuellar, 2015).

The availability of water also impacts social cohesion and quality of life. Inadequate access to water can lead to social exclusion and marginalization, particularly in underserved communities. Improved water access is associated with increased social equity, as it enables communities to participate more fully in economic and social activities. Ensuring equitable water distribution and access is essential for fostering social inclusion and improving overall quality of life.

The interactions between human activities and hydrological cycles require a socio-hydrological approach, which provides a more holistic understanding of these relationships. This approach integrates social, economic, and environmental factors to assess how human actions impact water systems and how these systems, in turn, affect society (Chang et al., 2022). By considering both human and natural components, the socio-hydrological approach enables more comprehensive water resource management and supports the development of strategies that address both current and future challenges.

Effective water management must balance ecological sustainability with human demands. The hydrological cycle, which includes processes such as precipitation, evaporation, and groundwater recharge, is critical for sustaining ecosystems and human civilizations. Inadequate management can lead to environmental degradation, such as reduced water quality, habitat loss, and biodiversity decline. For instance, over-extraction of groundwater can lead to the depletion of aquifers, while pollution from agricultural runoff and industrial discharges can compromise water quality.

To address these challenges, water management strategies must prioritize ecological sustainability by protecting natural water systems and promoting responsible water use. This includes implementing practices that conserve water resources, reduce pollution, and restore degraded ecosystems. The goal is to ensure that water resources are available for both current and future generations while maintaining the health and integrity of natural systems (Schaeffer-Novelli & Cintrón-Molero, 2018).

Adopting a resilient approach to water management is essential for ensuring long-term sustainability. Resilience refers to the capacity of water systems to withstand and adapt to changes, such as population growth, climate variability, and environmental stresses. Resilient water management strategies focus on enhancing the adaptability of water systems by incorporating flexible and adaptive practices.

This includes promoting water conservation, investing in infrastructure improvements, and adopting innovative technologies for water treatment and distribution. Additionally, fostering community engagement and collaboration can enhance the resilience of water management systems by incorporating local knowledge and addressing diverse needs. By building resilience into water management practices, societies can better navigate uncertainties and challenges while ensuring the sustainability of water resources.

Water management faces a range of challenges driven by population growth, accelerated economic development, and climate change. The 20th century saw a significant increase in water consumption due to these factors. Rapid population growth has led to higher water demand for domestic, agricultural, and industrial use. Agricultural intensification, including increased irrigation and the use of fertilizers and pesticides, has further heightened water consumption and pollution. Simultaneously, urbanization has transformed water consumption patterns, with more people living in cities and contributing to increased water demand and altered runoff patterns (Clark & Wu, 2016; Tundisi, 2003). In Brazil, this trend has resulted in substantial demographic growth and urbanization, placing additional pressure on water resources and management systems (Carmo et al., 2014).

Soil moisture is a critical parameter in the hydrological cycle, despite representing only a small fraction of freshwater resources (~0.15%). It serves as an important water reservoir and influences various hydrological processes, including runoff, infiltration, and evaporation. Soil moisture plays a vital role in agriculture, as it directly impacts plant growth and crop yield. Adequate soil moisture levels are necessary for optimal plant health and productivity (Green et al., 2019; Cui et al., 2020; Wang et al., 2021). In addition to its agricultural significance, soil moisture is essential for drought index assessments, which are used to evaluate and manage drought conditions. Accurate soil moisture measurements are crucial for understanding drought severity and implementing effective drought mitigation strategies (Ghulam et al., 2007; Ajaz et al., 2019; Xu et al., 2020; Arif & Susena, 2024). Monitoring soil moisture also supports hydrological modeling and ecosystem assessments, contributing to better water resource management and climate risk management.

In urban areas, monitoring soil moisture is critical due to its influence on hydrological processes, vegetation, and climate resilience. Urbanization can alter natural water flow patterns, leading to increased runoff and reduced infiltration. Accurate soil moisture data is essential for hydrological modeling, which helps in predicting water flow and availability in urban environments (Schatffitel et al., 2020; Koltsidas et al., 2023). Understanding soil moisture dynamics in urban areas also supports ecosystem property assessments, including vegetation health and land cover changes. Soil moisture mapping can help correlate vegetation patterns with surface temperature, providing valuable insights for climate risk management and urban planning (Gonchrova et al., 2020; Eldridge et al., 2021; Cui et al., 2021). Urbanization significantly impacts soil moisture dynamics, making it essential to incorporate soil moisture data into hydrological models. Studies have shown that integrating soil moisture measurements improves the accuracy of runoff predictions, reinforcing urban water management strategies (Fidal & Kjeldsen, 2020; Huang et al., 2023). In urban gardens and agricultural settings, proper soil management can enhance water retention capacity, which is crucial for maintaining plant health under climate stress conditions. Improving soil quality and moisture levels can support agricultural productivity and resilience (Lin et al., 2018; Dixit et al., 2024).

Various methods are available for measuring soil moisture, each with its own advantages and limitations. Traditional field methods include neutron scattering, gamma attenuation, time domain reflectometry (TDR), soil resistivity sensors, thermal dissipation blocks, heat flux sensors, and tensiometric techniques (Su et al., 2014). While these methods provide accurate measurements, they have limited spatial coverage and are not suitable for large-scale studies. To overcome these limitations, remote sensing techniques have been developed for monitoring soil moisture at watershed and regional scales. Satellites such as the Soil Moisture and Ocean Salinity (SMOS) and Soil Moisture Active Passive (SMAP) have been instrumental in providing large-scale soil moisture data (Kerr et al., 2001; Entekhabi et al., 2010). However, these satellites have limited spatial resolution, which restricts their ability to detect small-scale variations in soil moisture.

Recent advancements in remote sensing techniques have greatly improved the ability to monitor soil moisture with higher spatial resolution, offering more accurate and detailed information essential for a range of applications, from agriculture to urban planning. Among these advancements is the Thermal-Optical Trapezoidal Model (TOTRAM), which utilizes remote sensing data to estimate soil moisture. TOTRAM is an innovative model that estimates soil moisture by analyzing the relationship between land surface temperature (LST) and a vegetation index (VI). It operates on the principle that soil moisture affects both the thermal and optical properties of the land surface. By correlating variations in LST and VI, TOTRAM can infer soil moisture content. The effectiveness of TOTRAM has been validated through various studies. Bai et al. (2019) applied the model across different ecological settings and confirmed its accuracy and reliability in diverse climatic conditions. Pandey et al. (2021) demonstrated TOTRAM's ability to capture soil moisture variations in agricultural landscapes, emphasizing its usefulness in precision agriculture. Additionally, Wang et al. (2021) further validated the model's performance across different regions, supporting its effectiveness in varying environmental contexts.

Despite its strengths, TOTRAM relies on thermal sensors to measure LST, which presents limitations. Thermal sensors are not available on all satellites, such as Sentinel-2, which only carries optical sensors. Additionally, LST measurements can be influenced by atmospheric factors such as wind speed, air temperature, and humidity, which can introduce variability into the soil moisture estimates (Mallick et al., 2009; Sadeghi et al., 2017; Bababeian et al., 2018). These factors can affect the accuracy of TOTRAM's soil moisture estimates, particularly in environments with significant atmospheric variability.

To address the limitations of the Thermal-Optical Trapezoidal Model (TOTRAM), the Optical Trapezoidal Model (OPTRAM) was developed. OPTRAM improves soil moisture estimation by utilizing shortwave infrared (SWIR) bands, providing an alternative to thermal sensors. Unlike TOTRAM, which depends on thermal measurements, OPTRAM relies solely on optical data, which are available from a broader range of satellites, including Sentinel-2.

This model estimates soil moisture by analyzing SWIR reflectance and its correlation with soil moisture content. OPTRAM has demonstrated significant promise in delivering consistent and reliable soil moisture estimates. Research has shown that OPTRAM effectively leverages SWIR bands to provide accurate soil moisture estimates across various environmental conditions. Studies by Ambrosone et al. (2020) confirm that OPTRAM enhances its effectiveness in different settings, while Chen et al. (2020) highlight its capability to monitor soil moisture with high spatial resolution, making it particularly suitable for both urban and agricultural applications. Further validation by Dubinin et al. (2020) underscores the model's robustness in diverse climatic regions, supporting its broad applicability. Yao et al. (2022) and Pandey et al. (2023) also support the model's reliability and effectiveness, demonstrating its utility in providing accurate soil moisture estimates using optical remote sensing data. Sentinel-2, with its 10-meter spatial resolution, enhances the accuracy of soil moisture measurements compared to lower-resolution satellites like Landsat, which has a 30-meter resolution. This higher resolution allows for more detailed and precise monitoring, particularly valuable in environments with significant spatial variability.

Estimating soil moisture in urban areas presents unique challenges due to land-use variability and mixed pixels. Urban areas often feature a mix of land uses, including buildings, water bodies, native vegetation, and agricultural plots. This variability can impact the accuracy of remote sensing estimates, as mixed pixels may represent a combination of different land covers. In the municipality of Rio Claro, São Paulo state, Brazil, the high land-use variability creates additional challenges for soil moisture estimation. Mixed pixels in remote sensing data can lead to inaccuracies in soil moisture measurements, highlighting the need for validation with field data. By comparing remote sensing estimates with ground-based measurements, researchers can assess the accuracy of soil moisture models and address potential issues related to mixed pixels. The objective of this study was to evaluate the effectiveness of OPTRAM in estimating soil moisture in an urban environment, specifically in the municipality of Rio Claro. By utilizing Sentinel-2 imagery and comparing the results with field data, the study aimed to assess the model's performance and address challenges associated with urban land use. This investigation is crucial for understanding the applicability of remote sensing techniques in diverse land-use scenarios and improving soil moisture monitoring in urban settings.

Materials and methods

This study was conducted in the municipality of Rio Claro, located in the state of São Paulo, in the Southeast region of Brazil. To assess soil moisture using the OPTRAM method, Sentinel-2 satellite images from the European Space Agency's (ESA) Copernicus Program were employed. The images were obtained throughout the study period.

As described later in this article, the empirical correlation for the study area involved comparing in situ soil moisture measurements with images produced by the Sentinel-2 satellite.

From the Sentinel-2 images, two indices were generated: NDVI and STR. Additionally, a supervised classification of the same satellite images resulted in a land use and land cover map, where areas classified as “impervious” were used as a mask to avoid misinterpretations when applying the OPTRAM index.

The in-situ moisture data were collected on days and times that coincided with the Sentinel-2 satellite's orbital passes, aiming to ensure correlation between field data and estimated data, with preference given to days with little or no cloud cover.

Figure 1 presents the flowchart that outlines the methodological approach adopted for the case study, focusing on soil moisture estimation at the urban area of the municipality of Rio Claro.

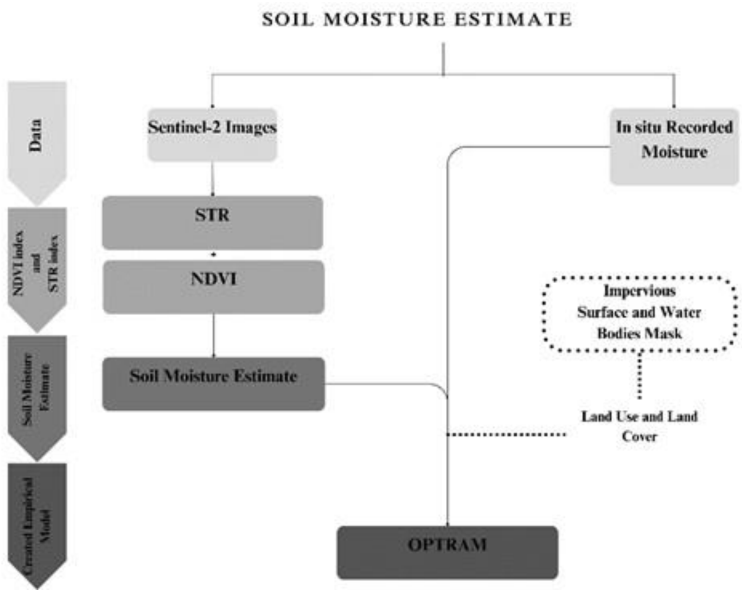

Figure 1 - Flowchart of the Methodological Approach for Soil Moisture Estimation at the Urban Area of Rio Claro Municipality

In Figure 1, the flowchart illustrates the steps followed to develop the empirical model used to estimate soil moisture in the urban area of Rio Claro. Initially, the in-situ field data and estimates derived from Sentinel-2 images were used as the foundation for constructing a statistical analysis aimed at identifying a possible empirical correlation.

From the Sentinel-2 images, the NDVI, an index that identifies vegetation pixels, and the SWIR band (band 12), which was resampled using the

Sentinel Application Platform (SNAP) software to adjust its spatial resolution from 20 to 10 meters, were used as parameters to develop the OPTRAM empirical model. A land use map was also created, from which polygons were generated to serve as masks, to avoid errors in moisture estimates in areas classified as impervious surfaces and water bodies. Finally, moisture maps were generated to illustrate the soil moisture estimates based on the OPTRAM model.

Study site

The Rio Claro municipality is in the central portion of Sao Paulo State, located in southeastern Brazil (Figure 2). The selected area is located in the eastern region of the urban region of Rio Claro, where land use and occupation are complex and variable. While a large portion is composed of impervious areas (concrete and asphalt), some portions are covered by native or reforested vegetation, bare soil and grass cover. With respect to the geology, most of the study area is covered by the Rio Claro Formation, while siltstone of the Corumbataí Formation, diabases of the Serra Geral Formation and Quaternary alluvial deposits occur in minor parts. The Rio Formation is composed of clayey, fine- to medium-grained sandstone. Most samples were collected from the Rio Claro aquifer, where several previous hydrogeological studies were conducted (e.g., Oliva, 2006; Nogueira and Kiang, 2015; Neto et al., 2016; Gonçalves et al., 2019).

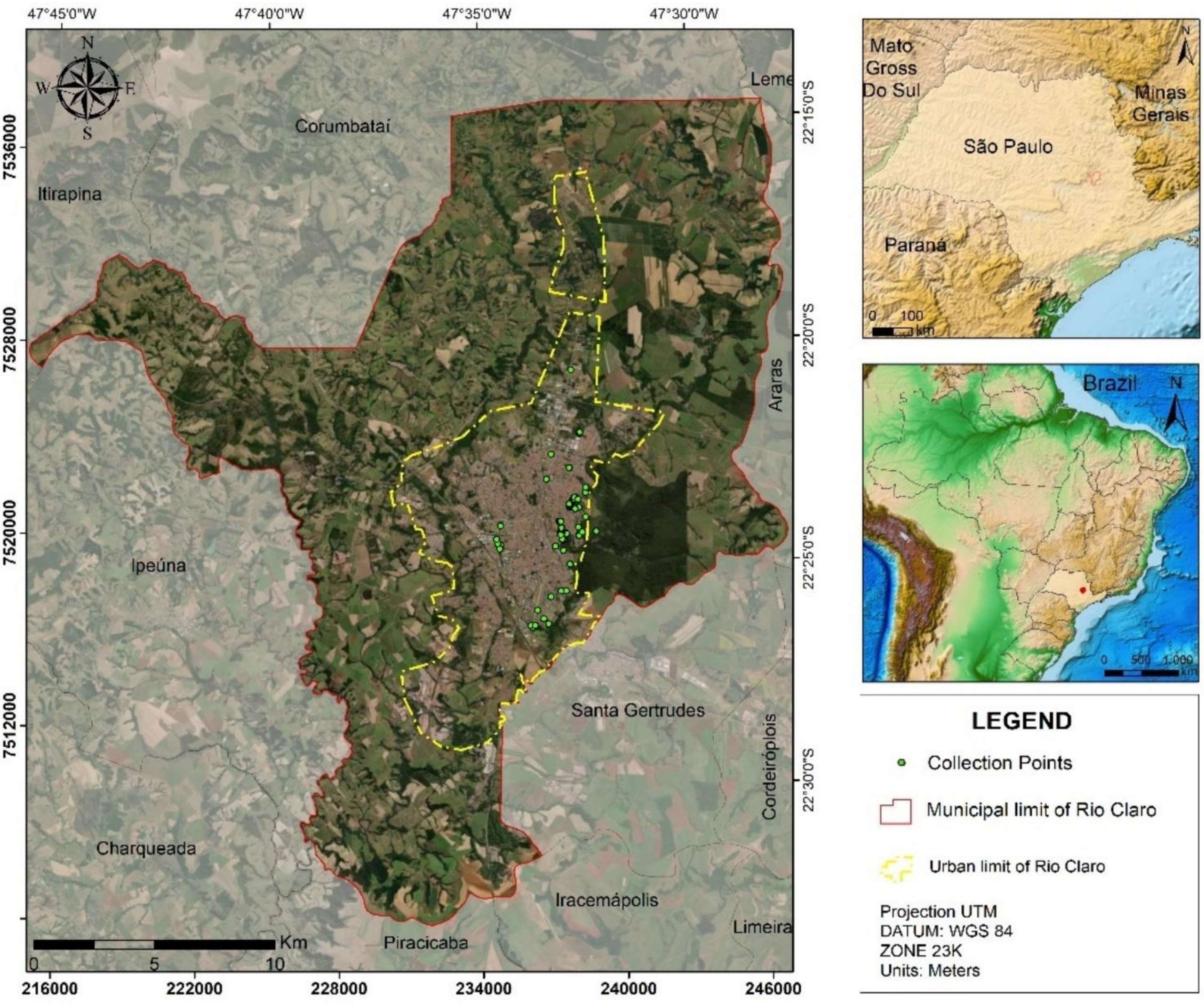

Figure 2 – Location of the Rio Claro municipality, where the study site is located. The locations where the soil samples were collected for soil-moisture determination are also presented.

The optical trapezoid model (OPTRAM)

As an alternative to the TOTRAM method, Sadeghi et al. (2017) developed the OPTRAM, a novel approach based on optical sensors of multispectral satellites. Similar to the well-established TOTRAM, the OPTRAM approach is based on a graphical approach by plotting the vegetation index (NDVI) against an index related to soil moisture. The normalized difference vegetation index, a parameter related to vegetation robustness, is calculated as follows.

$$NDVI = \frac{(NIR-Red)}{(NIR+Red)} \quad (1)$$

Instead of the thermal data used in the TOTRAM, the OPTRAM uses the STR, a new parameter proposed by Sadeghi et al. (2015). The deduction of STR was based on the Kubelka–Munk, two-flux, radiative-transfer theory, which describes the diffuse reflectance from a uniform, optically thick, absorbing, and scattering medium (SADEGHI et al., 2015). Under this physically based approach, the STR is obtained from SWIR by Eq. 2.

$$STR = \frac{(1-SWIR)^2}{(2SWIR)} \quad (2)$$

Based on the assumption described by Sadeghi et al. (2015), the soil moisture (W) is linearly related to STR, following the relation described by Eq. 3.

$$W = \frac{STR-STR_d}{STR_w-STR_d} \quad (3)$$

where STR_d represents the STR to dry soil (W=0) and STR_w represents the STR to wet soil (W=1).

To obtain the estimates of soil moisture, the computed pixel values of the NDVI and STR from cloudless images are plotted in a scatterplot graph, in which the points are distributed within an envelope resembling a trapezoid, similar to those illustrated in Figure 3.

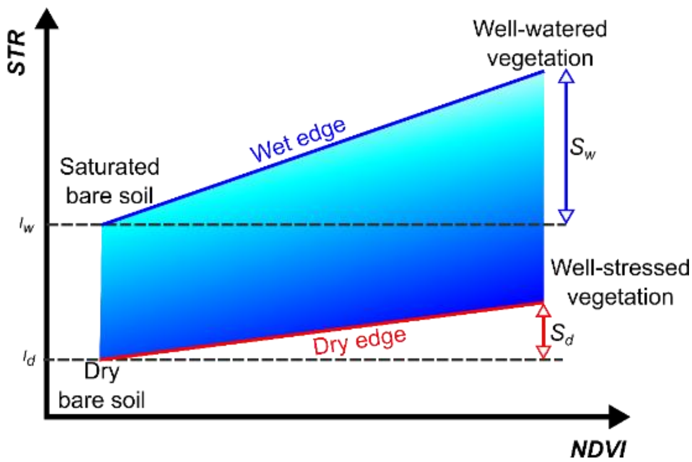

Figure 3 – Illustration of the conceptualized OPtical TRApezoid Model (OPTRAM) produced by plotting the STR against NDVI pixel values obtained from the optical sensor (Sadeghi et al., 2017).

As illustrated in Figure 3, the four corners of the trapezoid represent four distinct conditions, in which a low NDVI and low STR represent dry bare soil, a low NDVI and high STR represent saturated bare soil, a high NDVI and low STR represent well-stressed vegetation, and a high NDVI and STR represent well-watered vegetation. Additionally, the upper and lower edges of the trapezoid are composed of wet and dry lines (see Figure 3), obtained empirically from the analysis of the trapezoidal graph, and are described by Eqs. 4 and 5, respectively.

$$STR_d = i_d + s_d NDVI \quad (4)$$

$$STR_w = i_w + s_w NDVI \quad (5)$$

Finally, W is obtained by combining Eqs. 3 to 5, producing Eq. 6.

$$W = \frac{id + S_d NDVI - SRT}{i_d - i_w + (S_d - S_w) NDVI} \quad (6)$$

Data acquisition and processing

Our analysis was carried out using imagery from Sentinel-2, a multispectral satellite from the Copernicus Programme. The Sentinel-2 mission is composed of a constellation with two twin satellites (Sentinel-2A and Sentinel-2B) that methodically obtain spectral imagery from the Earth's surface. The set of Sentinel-2 bands, their central wavelengths, and spatial resolution are listed in Table 1.

Table 1 – Bands of Sentinel-2, central wavelengths, and spatial resolution of Sentinel-2 imagery. Source: European Space Agency (ESA).

Sentinel-2 bands	Central Wavelength (nm)	Spatial resolution (m)
Band 1 - Coastal aerosol	442.7	60
Band 2- Blue	492.4	10
Band 3 - Green	559.8	10
Band 4 - Red	664.6	10
Band 5 - Vegetation red edge	704.1	20
Band 6 - Vegetation red edge	740.5	20
Band 7 - Vegetation red edge	782.8	20
Band 8 - NIR	832.8	10
Band 8A - Vegetation red edge	864.7	20
Band 9 - Water vapor	945.1	60
Band 10 - SWIR - Cirrius	1373.5	60
Band 11 - SWIR	1613.7	20
Band 12 - SWIR	2202.4	20

The Sentinel-2 satellite is managed by the European Community and the European Space Agency (ESA). The downloaded images at Level-1C provide top-of-atmosphere (TOA) reflectance values without radiometric and geometric corrections. Because the reflectance is presented in the form of digital numbers (DNs), it should first be converted to physical values of reflectance by dividing it by a rescaling factor known as Quantification_value, according to Equation 7. The Quantification_value (Qv) is presented in metafiles that accompany the acquired Sentinel-2 imagery.

$$Reflectance = DN/Qv \qquad (7)$$

Then, the original images containing TOA reflectance at Level 1C were corrected to the bottom-of-atmosphere (BOA) utilizing the Sen2Cor (Version 2.8) processor, developed by Telespazio VEGA Deutschland GmbH on behalf of the ESA (MALENOVSKÝ et al., 2012). The conversion of TOA at Level 1C to BOA at Level 2A was performed by atmospheric, terrain, and cirrus correction.

The NDVI calculation was conducted by Eq. 1 using Band 4 (red) and Band 8 (infrared). To calculate the STR, we initially resampled Band 12 (SWIR band) to 10 m and then used Equation 2. We processed images from August 2020 to July 2021, and the NDVI and STR pixel values were extracted and plotted to obtain a trapezoidal diagram. By manually adjusting the wet and dry edges, we obtained the values of S_d, S_w, I_d, and I_w.

Supervised classification

Due to the high variability in land use and land cover in the study area, a supervised classification was performed to create a land use and land cover map, distinguishing impervious surfaces (concrete and asphalt) and water bodies from permeable areas (native vegetation, reforestation, pastures, exposed soil, and sugarcane plantations). Using a true color RGB composition, the classification was carried out in QGIS software (version 3.22.7) based on data collected on 06/13/2021. The Orfeo Toolbox (OTB) extension, developed by the French Space Agency (CNES), was employed for this task, whose applications are well-documented, as noted by Cresson et al. (2018), Grizonnet et al. (2017), and Inglada and Christophe (2009).

Five land use classes were established: water bodies, forests, grasslands and pastures, agriculture, exposed soil, and urbanization. The classification utilized the TrainImagesClassifier algorithm from OTB, which processes image and vector data pairs for training. The class training was performed using the Random Forest machine learning algorithm, which constructs multiple decision trees and determines the final class based on the majority classification of individual trees.

The resulting raster image was converted into a vector file, transforming pixel values into points. Finally, permeable areas were removed, leaving only impervious surfaces and water bodies, which were converted into vector polygons and used as a mask to prevent misclassification of moisture in the respective soils.

Soil characterization and moisture measurement

To test the suitability of the soil-moisture estimation produced by the OPTRAM at the study site, we collected 52 soil samples to determine the soil moisture collected between July 2021 and January 2022. The date for in situ soil-moisture measurement was planned to coincide with the satellite visit. All sample soils were collected at depths of 5 to 10 cm at points representative of the outcropping geological units in the study area. At each sampling location, we collected three different points with distances between 2 and 3 meters apart from each other to reduce problems with sample representativeness. All soil samples collected were stored in hermetically sealed pots and immediately taken to the lab.

In the lab, approximately 10 grams of soil samples were weighed in triplicate, placed in capsules, placed in an oven and left at 70 °C to dry. After 48 hours, these samples were removed and newly weighed. The mass difference between the humid sample and after drying represents the amount of water in the soil samples and was used to calculate the soil moisture.

Assuming the water density is equal to 1 g/cm^3, the water volume (V_w) was obtained by subtracting the mass of humid soil (M_{hs}) by dry soil (M_{ds}).

$$V_w = M_{hs} - M_{ds} \quad (8)$$

The volume of dry soil (V_s) was obtained by dividing the mass of dry soil by bulk soil density (ρ), as described by Eq. 9. In our analysis, we utilized a bulk soil density equal to 1.4 g/cm^3.

$$W = \frac{M_{ds}}{\rho} \quad (9)$$

Finally, the volumetric soil moisture was determined according to Eq. 10. Then, we computed the average and standard deviation of triplicate samples.

$$W_{field} = \frac{V_w}{V_s} \quad (10)$$

To verify the adequateness of OPTRAM estimation in response to soil granulometry, we measured the particle-size distribution of representative samples using a QIPIC® particle-size and shape analyzer.

Model validation

To measure the representativeness of soil moisture estimated by the OPTRAM, we compared it with field data using three distinct metrics: the determination coefficient (R^2), the mean absolute error (MAE), and the root mean square error (RMSE), described in Eqs. 11, 12, and 13, respectively, to N observations.

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(W_{field,i} - W_{OPTRAM,i})^2}{\sum_{i=1}^{n}(W_{field,i} - \bar{W}_{field})^2} \quad (11)$$

$$MAE = \frac{1}{N}\sum_{i=1}^{N}(W_{field} - W_{OPTRAM}) \quad (12)$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(W_{field} - W_{OPTRAM})^2} \quad (13)$$

where $\bar{W}_{field}$ represents the average value of W measured in the field.

Results

Land and use occupation map

The land use and land cover produced by Sentinel-2 images (Figure 4) show the spatial distribution of different surface cover types. Rio Claro, a small to medium-sized city in Brazil, is characterized by diverse land use and land cover, with urbanized areas bordered by native/reforested vegetation and monoculture agriculture. The urban class consists of impervious zones, made up of concrete, rooftops, and asphalt.

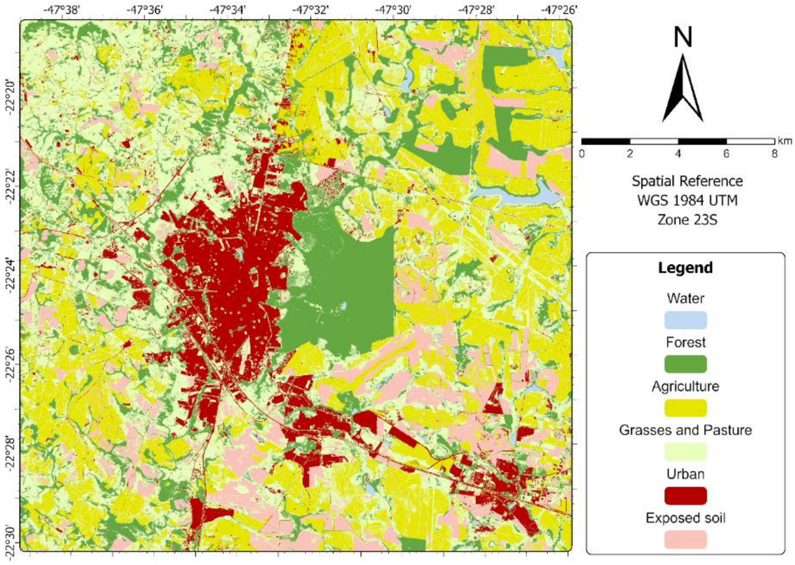

Figure 4 – Land and use occupation of Rio Claro municipality.

Soil-moisture estimation by the OPTRAM

Analyzing the scatterplot of processed NDVI and STR values (Figure 5), we empirically determined the dry and wet edge limits of trapezoidal STR-NDVI, following the methodology described by Sadeghi et al. (2017). Based on the established limits, we conducted the OPTRAM parameterization, achieving I_d, I_w, S_d, and S_w values of 0, 0.6, 2.55, and 14, respectively.

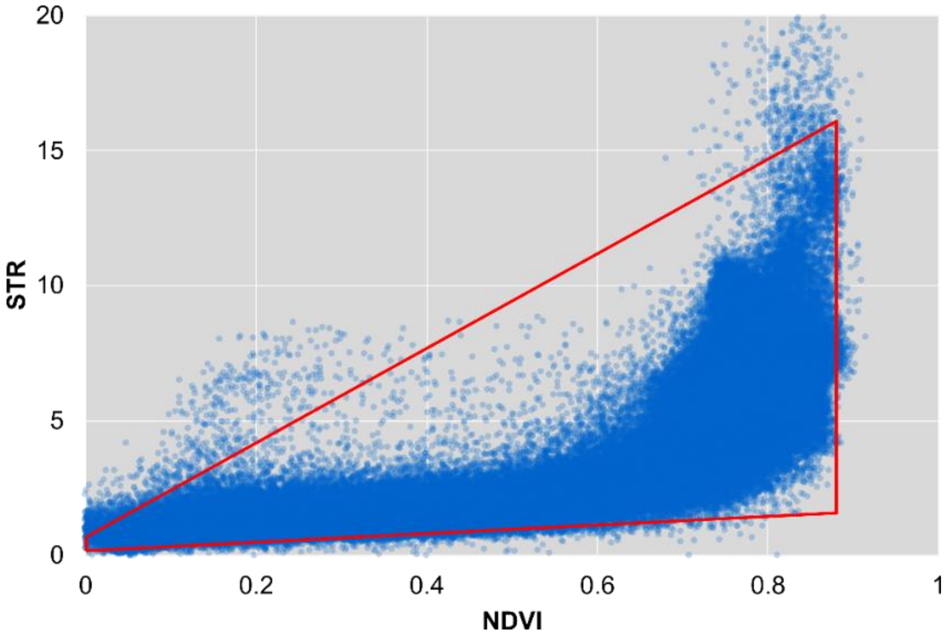

Figure 5 – Scatterplot of the STR and NDVI pixel values, forming the trapezoidal STR-NDVI space with Sentinel-2 imagery from August 2020 to January 2022. The dry and wet edges were empirically delineated by manual adjustments.

Figure 6 illustrates the particle-size distribution curves of some soil types found at the study site, ranging from silty clay to fine to medium grains. While the sandy soils are associated with the Rio Claro Formation, silty clay and sandy clay are associated with siltstones of the Corumbataí Formation and diabases of the Serra Geral Formation, respectively.

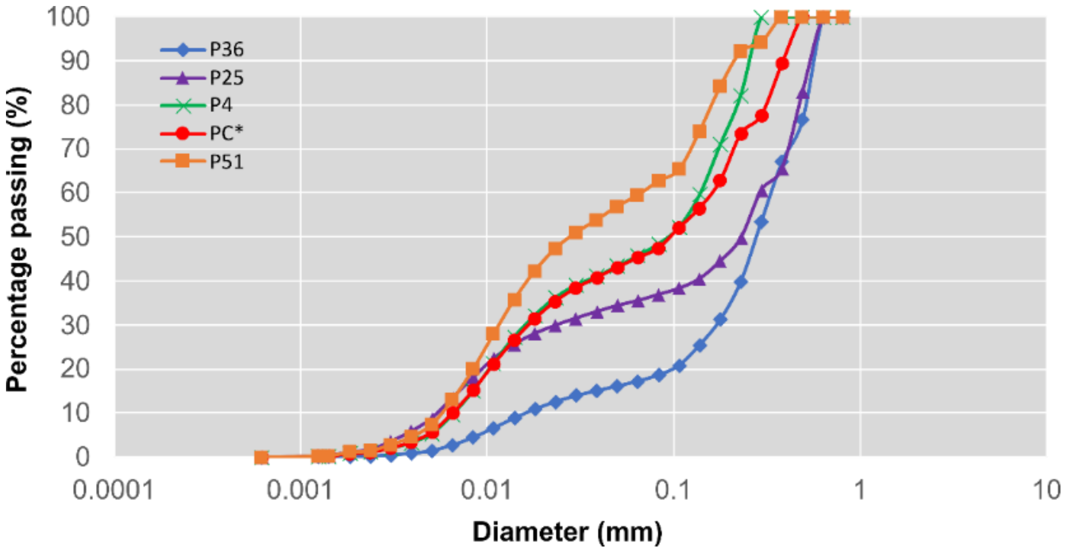

Figure 6 – Particle-size distribution curves of five representative soil types in which the soil moisture was measured in the lab.

Comparison between field- and OPTRAM-derived soil moisture

The values of soil moisture measured in the field had a broad variation, ranging from 0.057±0.006 to 0.865±0.061, reflecting the period of sampling conducted during the dry and wet seasons. The coefficient of variation of soil moisture varied between 5.55 and 17.73%, demonstrating the relative homogeneity of soil moisture at the sampling sites. The scatterplot of measured and estimated soil moisture is depicted in Figure 7, displaying good agreement between both. The values of R^2, MAE and RMSE were 0.92, -0.0196, and 0.1413, respectively. We did not find significant differences in the representativeness of soil moisture derived from the OPTRAM approach, which was not impacted by soil type.

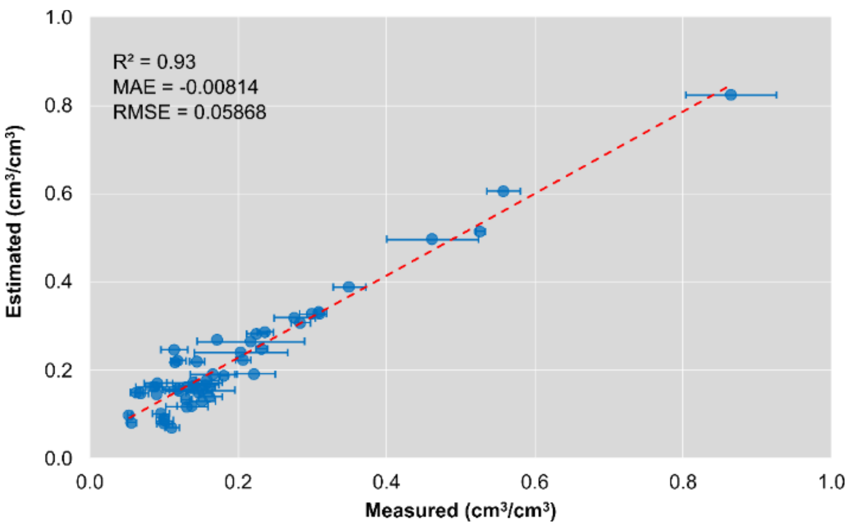

Figure 7 – Scatterplot of the soil moisture measured in the field and that obtained by the OPTRAM at the study site. The horizontal error bars represent the standard deviation of triplicates.

Time series of soil moisture

To evaluate the seasonal variation in soil moisture over two hydrological years, we used the OPTRAM to create a monthly time series of soil moisture between January 2020 and November 2021 using the NDVI and STR data retrieved from Sentinel-2 images. Some representative estimated soil-moisture maps are presented in Figure 8.

The highest soil-moisture values were observed along the streams and densely vegetated areas, followed by irrigated zones in agricultural zones. Moreover, strong variation in soil moisture was observed over time, with the highest and lowest values observed between March 2021 and November 2021, respectively. On the other hand, low values were observed during the dry season (April to October), with the lowest values observed in August. Within and around urban areas, the temporal variability of soil moisture was very distinct.

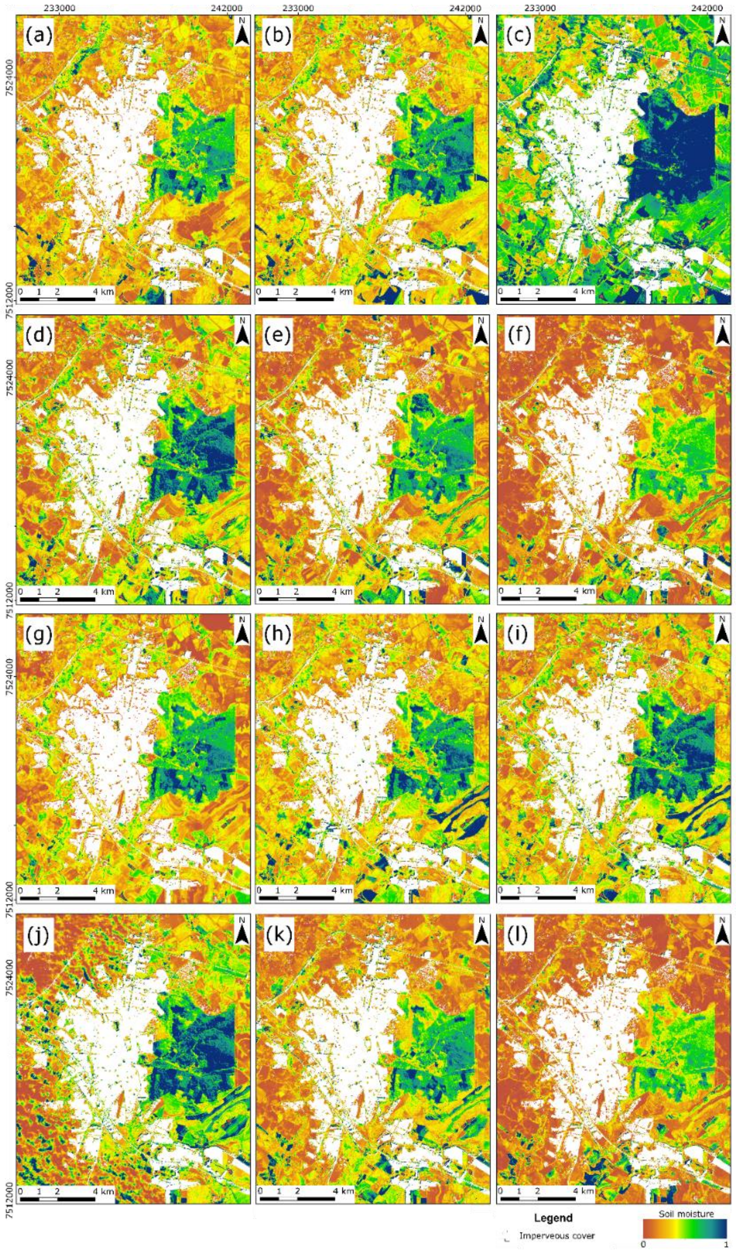

Figure 8 – Maps of estimated soil moisture in distinct periods: a) January 2020; b) March 2020; c) May 2020; d) July 2020; e) September 2020; f) November 2020; g) January 2021; h) March 2021; i) May 2021; j) July 2020; k) September 2021; and l) November 2021.

Discussion

The determination of soil moisture is essential for hydrological, climatological, and agricultural studies. In recent decades, various Remote Sensing techniques have been developed, such as the Optical Trapezoid Model (OPTRAM). This approach, which uses the STR index calculated with the SWIR band instead of the traditional LST (thermal band), has proven effective in predicting soil moisture in several studies. However, its application in urban areas remains underexplored.

This study aimed to fill that gap by testing OPTRAM in the municipality of Rio Claro, São Paulo, where land use and occupation vary. Using multispectral images from Sentinel-2, the NDVI-STR space was constructed to estimate soil moisture, and the data were compared with field measurements. The results, measured by R^2, MAE, and RMSE, indicate that OPTRAM provides representative estimates, even in urbanized areas. Furthermore, the spatial resolution of Sentinel-2 images proved adequate for the size of the studied areas.

Urbanization significantly affects natural hydrogeological conditions, increasing surface runoff, floods, and reducing groundwater recharge (e.g., Oudin et al., 2018; Gori et al., 2019; Sheldon et al., 2019; Raj & Rawat, 2023). One of the main effects of urbanization is the proliferation of impermeable surfaces, hindering infiltration and groundwater recharge (e.g., Erickson & Stefan, 2009; Braud et al., 2013; Lamichhane & Shakya, 2020). Additionally, excessive runoff overwhelms drainage systems, resulting in urban flooding (Bilgiç & Baba, 2022; Shaikh et al., 2023). Therefore, monitoring urban hydrology, especially in the face of land use changes, is crucial for urban planning and policy formulation.

Infiltrated water, stored as soil moisture, is a critical parameter in groundwater management. However, estimating it remains a technical challenge. OPTRAM, validated by several studies, mainly in watersheds (e.g., Ambrosone et al., 2020; Chen et al., 2020; Dubinin et al., 2020; Sadeghi et al., 2023), emerges as a promising approach. Our study is pioneering in applying OPTRAM to urbanized areas, showing that it can generate realistic soil moisture estimates even in small-scale urban areas with complex land use. This opens new possibilities for consistent soil moisture monitoring in urban and understudied environments.

Several cities in Brazil have experienced rapid urban expansion in recent decades (e.g., Ahmed et al., 2021), impacting hydrological processes, but few studies have investigated this relationship. The application of OPTRAM, using Sentinel-2 imagery, offers a new way to monitor these changes, aiding research on the effects of climate change and urbanization consequences. Additionally, the soil moisture time series obtained through OPTRAM can be used to calibrate numerical simulations of groundwater recharge and evapotranspiration, providing more accurate predictions.

Interestingly, despite the geological variability and soil type at the study site (siltstones, diabase, sandstones, and sandy sediments), OPTRAM provided consistent soil moisture estimates. This suggests that soil grain size did not significantly impact the results. Figure 4, with Id, Iw, Sd, and Sw values in the NDVI-STR space, illustrates how these geological variations were overcome to provide reliable estimates across all soil types.

However, as in other studies, we found discrepancies in the reported R^2 values. Dubinin et al. (2020) obtained $R^2 = 0.96$, while Ambrosone et al. (2020) reported R^2 of 0.54, and Chen et al. (2020) between 0.1 and 0.5. These variations likely result from different land use conditions, sensor resolution, and field measurement methods. Sadeghi et al. (2017) showed that OPTRAM can be applied using both Sentinel-2 and Landsat 8 OLI, but for our study, Sentinel-2 was more suitable due to its spatial resolution and 5-day revisit time, superior to Landsat-8 OLI, which has a 15-day cycle.

We observed a rapid soil moisture response to rainfall events, as illustrated in Figure 8. Unlike previous studies, such as Teramoto et al. (2018), which showed seasonal NDVI behavior correlated with groundwater levels, we did not identify a clear seasonal variation in soil moisture. Instead, our analysis highlighted short-term responses to precipitation events, with soil moisture increasing shortly after rainfall and decreasing rapidly due to infiltration and evapotranspiration.

Despite Sentinel-2's potential for reliably estimating soil moisture in urban areas, a significant limitation is cloud cover. During rainy periods, when soil moisture is higher, cloud presence hinders data collection via OPTRAM. This constraint still needs to be overcome to improve the accuracy of estimates during these critical conditions.

Conclusions

In this study, the OPTRAM model was employed to estimate soil moisture in an urban area of Rio Claro, SP, using Sentinel-2 satellite images. The primary objective was to assess the effectiveness of OPTRAM in an urban environment characterized by diverse land use and land cover, a topic that has been underexplored in the literature. The comparison between the remote sensing estimates and the field-collected data demonstrated OPTRAM's capability to capture soil moisture dynamics in urban areas.

The results show that even in complex urban settings, OPTRAM can provide accurate soil moisture estimates, which can significantly contribute to hydrological monitoring in urbanized areas. Moreover, this data can serve as essential parameters in hydrological models aimed at predicting shallow aquifer behavior and assessing the impacts of climate change on water resource availability. The application of OPTRAM thus fills an important gap in the study of soil moisture in urban zones, proving to be a valuable tool for water resource management and sustainable planning.

These findings indicate that OPTRAM, in addition to its proven use in rural areas, can also play a crucial role in urban areas, aiding in the calibration of hydrological models and forecasting the long-term effects on aquifers, even in contexts with diverse land use. In this way, OPTRAM establishes itself as a reliable tool for soil moisture monitoring, with great potential to improve water management strategies in the face of climate change and urban growth.

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