

UNIVERSIDADE FEDERAL DE VIÇOSA

**Investigating Brazilian agriculture with Sentinel-5P: TROPOMI's potential for
characterizing the plant-animal-atmosphere system**

Humberto Paiva Fonseca
Doctor Scientiae

**VIÇOSA - MINAS GERAIS
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HUMBERTO PAIVA FONSECA

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characterizing the plant-animal-atmosphere system**

Thesis submitted to the Applied
Meteorology Graduate Program of the
Universidade Federal de Viçosa in partial
fulfillment of the requirements for the
degree of *Doctor Scientiae*.

Adviser: Gabrielle Ferreira Pires

Co-adviser: Marcos Heil Costa

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I dedicate this thesis to four people, my parents,
my sister and my beloved wife.

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“Science explains the past and warns about the approaching future.”
(Eiichiro Oda)

ABSTRACT

FONSECA, Humberto Paiva, D.Sc., Universidade Federal de Viçosa, October, 2025.
Investigating Brazilian agriculture with Sentinel-5P: TROPOMI's potential for characterizing the plant-animal-atmosphere system. Adviser: Gabrielle Ferreira Pires. Co-adviser: Marcos Heil Costa.

This study tackles a dual challenge for large-scale tropical agriculture under climate change: maintaining the competitiveness of highly mechanized systems while measuring and mitigating emissions at decision-relevant spatiotemporal scales (from field to national levels). It integrates Sentinel-5P/TROPOMI observations along two complementary axes. Axis 1 processes solar-induced fluorescence (SIF) time series to infer soybean phenology and operational metrics (planting/harvest intensity and synchrony), including daily mechanized-area peaks $>100,000$ ha day⁻¹ in Central-West hubs. These phenological landmarks are validated across scales (official databases, higher-resolution imagery, agrometeorological indices) and tested for sensitivity to interannual climate variability, revealing stress signals and phenological delays during La Niña in southern Brazil. Axis 2 quantifies agricultural emissions using top-down CH inversions and leverages tropospheric NO anomalies to infer NO patterns over pastures, with implications for indirect NO via deposition. The analyses distinguish pasture conditions (degraded vs. intensified), identify hotspots aligned with production structure (e.g., Center–South livestock corridors), and quantify uncertainties from transport, retrieval errors, and management heterogeneity. Together, the axes form an observational framework linking agricultural logistics (phenology, operational windows, potential productivity) to atmospheric trace-gas accounting, supporting more transparent inventories, targeted mitigation, and adaptive management. Methodological contributions include: (i) operationalizing SIF-based crop phenology at continental scale; (ii) integrating TROPOMI hyperspectral products for sectoral CH and NO diagnostics; and (iii) proposing comparable metrics across regions and seasons for continuous monitoring of climate risk and environmental performance.

Keywords: SIF; TROPOMI; soybean phenology; agricultural mechanization; CH; NO; indirect NO; top-down inversions; degraded pastures; climate variability; Brazil.

RESUMO

FONSECA, Humberto Paiva, D.Sc., Universidade Federal de Viçosa, outubro de 2025. **Investigando a agricultura brasileira com o Sentinel-5P: potencial do TROPOMI para caracterizar o sistema planta-animal-atmosfera.** Orientadora: Gabrielle Ferreira Pires. Coorientador: Marcos Heil Costa.

Este estudo enfrenta dois desafios da agricultura tropical em larga escala sob mudança do clima: manter a competitividade de sistemas mecanizados e medir/mitigar emissões em escala útil à decisão (do talhão ao nacional). Para isso, integra dados orbitais do Sentinel-5P/TROPOMI em dois eixos. No Eixo 1, séries de SIF são usadas para inferir a fenologia da soja e métricas operacionais da safra (intensidade e sincronia de plantio/colheita), validadas com bases oficiais, imagens de maior resolução e índices agrometeorológicos, além de avaliar a sensibilidade à variabilidade interanual (ex.: atrasos e sinais de estresse em anos de La Niña no Sul do Brasil). No Eixo 2, o estudo estima emissões por inversões top-down de CH e utiliza anomalias de NO troposférico para inferir padrões de NO em pastagens, discutindo implicações para NO indireto por deposição. As análises distinguem pastagens degradadas e intensificadas, mapeiam hotspots coerentes com a estrutura produtiva e explicitam incertezas (transporte atmosférico, erros de retrieval e heterogeneidade de manejo). Em conjunto, os eixos conectam logística agrícola (fenologia e janelas operacionais) com contabilidade atmosférica de gases-traço, apoiando inventários mais transparentes, mitigação direcionada e manejo adaptativo.

Palavras-chave: SIF; TROPOMI; fenologia da soja; mecanização agrícola; CH; NO; NO indireto; inversões “top-down”; pastagens degradadas; variabilidade climática; Brasil.

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1. General Introduction

Climate change poses a two-sided challenge to Brazilian agriculture: safeguarding the competitiveness of highly mechanized production systems while simultaneously measuring and mitigating emissions with spatiotemporal granularity commensurate with decision-making at multiple scales, from farm to nation. In large tropical economies such as Brazil, where intensive agricultural mosaics coexist with extensive pasturelands, knowing when and how production occurs, and where and when emissions arise, has become a prerequisite for food security, climate diplomacy, and a productive transition. The livestock sector, in particular, accounts for a substantive share of the country's agricultural emissions and rests on a continent-scale herd, which amplifies both responsibility and the opportunity for methodological leadership (Molossi et al., 2023; Robinson et al., 2014; SEEG, 2024). In short, consistently capturing crop phenology and quantifying emissions across vast, heterogeneous landscapes remains challenging due to regional management differences, climate variability, and data gaps, demands that call for frequent observation with continental coverage. High-revisit orbital platforms therefore come to the fore, enabling near-real-time monitoring of coupled plant–animal–atmosphere systems.

Among high-revisit orbital platforms, the TROPOspheric Monitoring Instrument (TROPOMI) aboard Sentinel-5P provides a uniquely operational lens for agriculture: within a single instrument, it combines near-daily, quasi-global coverage of vegetation physiological signals and atmospheric trace-gas columns. On the surface side, TROPOMI enables retrievals of Solar-Induced Chlorophyll Fluorescence (SIF), which is directly linked to photosynthetic activity; on the atmospheric side, it observes the column-averaged dry-air mole fraction of methane (XCH_4) and the column of nitrogen dioxide (XNO_2), anchoring emission and reactivity estimates. This convergence, offering spatial resolution compatible with agricultural landscapes and temporal continuity—creates an observational frame connecting phenology, cropping logistics, and emissions accounting, thereby underpinning forecasting and risk management at continental scale (Veefkind et al., 2012; Köhler et al., 2018; Guanter et al., 2021; Lorente et al., 2022; Verhoelst et al., 2021).

In vegetation monitoring, notably vegetation indices, suffer saturation at high biomass and uncertainty in detecting critical phenological events, especially toward the end of the season, which constrains the accuracy of operational calendars. SIF, observable with TROPOMI, emerges as a physiological proxy of the photosynthetic apparatus that is less prone to saturation and thus more consistent for inferring large-scale phenology and productivity (Huete et al., 2002; Jiang et al., 2008; Köhler et al., 2018; Guanter et al., 2021). With daily mapping and moderate resolution, TROPOMI enables continental-scale integration of physiological signals from annual crops with direct applications in forecasting and risk management.

The same orbital platform also sustains an atmospheric perspective on agro-pastoral systems. Observed XCH_4 columns feed top-down inversions that adjust simulated fluxes and expose discrepancies in bottom-up inventories, revealing consistent subnational hotspots (e.g., landfills, oil-and-gas, and agro-pastoral areas) (Jacob et al., 2022; Nesser et al., 2024). These patterns, anchored in herd density and management practices, often persist even after observation-based corrections, indicating underestimation and spatial heterogeneity that traditional methods frequently obscure.

For reactive nitrogen, tropospheric NO_2 anomalies above pasturelands, isolated by contrast with upwind natural areas, allow estimation of soil NO_x emissions via a box-model approach using atmospheric parameters (wind speed, boundary-layer height, deposition, and chemical lifetime) (Huber et al., 2020). A fraction of this NO_x is subsequently removed by wet and dry deposition, enriching soils with nitrogen that microbial processes can convert to N_2O via nitrification/denitrification; this indirect pathway is recognized in the IPCC Guidelines (2006; 2019 Refinement) and can be quantified using conservative conversion and deposition factors (Verhoelst et al., 2021; IPCC, 2019). This chain closes the loop between atmospheric chemistry and soil biogeochemistry in tropical pastoral systems.

Coordinating the two axes, SIF for phenology and CH_4/NO_x for emissions—offers analytical and practical gains. Sowing and harvest rhythms, when synchronized to enable a second season crop, modulate water use, fertilization, and pest and disease pressure; in turn, these management choices and pasture condition (degraded vs. intensified) reverberate through emissions and nitrogen reactivity. In

La Niña years, for example, southern Brazil exhibits substantial hydrological perturbations and yield declines, with potential indirect effects on management practices and, consequently, on gas fluxes (Nóia-Júnior et al., 2020; Pilau et al., 2020). Integrating these diagnostics in a timely manner enables targeted mitigation (territorial and practice prioritization) and evidence-based adaptation.

We propose a framework in which a single data constellation (TROPOMI) simultaneously feeds: (i) operational soybean calendars for forecasting, logistics, and risk zoning; and (ii) robust atmospheric accounting of CH₄ and NO_x/indirect N₂O for inventories, targets, and policy. By coupling crop physiology and atmospheric chemistry through the same orbital lens, we advance toward more transparent and spatially explicit inventories, high-leverage mitigation, and integrated management of tropical agriculture—from field to national scale (Spera et al., 2020; Zhang et al., 2021; Rey-Pommier et al., 2024).

CHAPTER 1. Functioning of the Sentinel-5P TROPOMI Sensor for SIF Retrieval and Methane Quantification

The Sentinel-5 Precursor (Sentinel-5P) mission, launched on 13 October 2017 by the European Space Agency (ESA), represents a fundamental milestone in the global observation of atmospheric composition and biogeochemical surface processes. As the first Copernicus atmospheric chemistry mission capable of delivering kilometre-scale daily observations worldwide, Sentinel-5P fills the observational gap between heritage sensors such as SCIAMACHY, GOME-2 and OCO-2, while providing unprecedented information regarding trace gases, aerosols, cloud properties and biospheric signals embedded in top-of-atmosphere radiances. Its sole instrument, the TROPOspheric Monitoring Instrument (TROPOMI), integrates advanced optical engineering, state-of-the-art detectors and sophisticated spectral retrieval algorithms to retrieve a wide array of atmospheric constituents, including nitrogen dioxide (NO_2), ozone (O_3), carbon monoxide (CO), formaldehyde (HCHO), aerosols, and, crucially for agricultural and climatic applications, Solar-Induced Chlorophyll Fluorescence (SIF) and atmospheric methane (XCH_4). These two products, derived from the instrument's Near-Infrared (NIR) and Short-Wave Infrared (SWIR) bands, respectively, have transformed our capacity to investigate terrestrial carbon dynamics, agricultural productivity, greenhouse-gas emissions and atmospheric inversion processes.

TROPOMI operates in a Sun-synchronous orbit at approximately 824 km altitude, with a local equator crossing time near 13:30. This geometry maintains quasi-constant solar zenith angles from day to day, minimizing radiometric inconsistencies and facilitating temporal comparability across seasons and latitudes. The instrument observes Earth using a wide field of view (108°), generating an across-track swath of approximately 2600 km,

enabling daily global coverage. The observational geometry involves view angles spanning -35° to $+35^\circ$ across track, which affect the atmospheric optical path, radiance levels, surface anisotropy retrievals and signal-to-noise ratios (SNR). The detector's resolution is approximately 3.5×7 km for UV–VIS channels and $\sim 7 \times 7$ km for the SWIR channels used for methane retrieval (though the NIR SIF band was improved to 3.5×7 km after algorithm updates). These resolutions represent more than an order-of-magnitude improvement over previous global methane sensors and enable high-resolution SIF mapping suitable for regional agricultural studies.

TROPOMI uses a push-broom design, in which a linear detector array captures all across-track positions simultaneously. Incoming sunlight reflected by the surface and atmosphere enters the telescope, where it is collimated and split into four spectral modules: UV (270–320 nm), UVIS (320–500 nm), NIR (675–775 nm) and SWIR (2305–2385 nm). Each module contains dedicated optics, gratings and detectors (silicon CCDs for UV–NIR and HgCdTe for SWIR), allowing simultaneous multi-spectral acquisition. The instrument is thermally stabilized to prevent spectral drift; even a shift smaller than 0.01 nm can bias narrow-band absorption retrievals. TROPOMI includes internal calibration sources—white-light lamps, LEDs, laser diodes and periodic lunar observations—to maintain radiometric accuracy and spectral alignment throughout the mission. Detector calibration also includes correction for dark current, hot pixels, non-linear detector response, spectral smile and keystone effects.

The fundamental measurement recorded by TROPOMI is the top-of-atmosphere radiance (LTOA), described by the radiative-transfer equation (Equation 1):

$$L_{\text{TOA}}(\lambda) = [\rho_s(\lambda) E_{\text{sun}}(\lambda) T_{\text{down}}(\lambda) T_{\text{up}}(\lambda) + L_{\text{atm}}(\lambda)] R_{\text{inst}}(\lambda) + \epsilon(\lambda), \quad \text{Eq. 1.1}$$

where $\rho_s(\lambda)$ represents the bidirectional reflectance of the surface; $E_{\text{sun}}(\lambda)$ is the extraterrestrial solar irradiance; T_{down} and T_{up} represent downward and upward atmospheric transmission; $L_{\text{atm}}(\lambda)$ accounts for atmospheric path radiance from Rayleigh and Mie scattering as well as multiple-scattering interactions; $R_{\text{inst}}(\lambda)$ is the spectral instrument response function; and $\epsilon(\lambda)$ accounts for electronic noise, quantization artefacts and calibration residuals. Modelling LTOA requires high-precision radiative-transfer simulations such as LIDORT, VLIDORT or SCIATRAN, which approximate multiple scattering, angular geometry, bidirectional reflectance distribution functions (BRDF), gas absorption and aerosol interactions.

SIF retrieval in TROPOMI relies primarily on the high-resolution structure of the O₂ A-band (759–770 nm) in the NIR module. Solar-induced chlorophyll fluorescence is a weak emission (0.5–2% of the total radiance in the NIR) produced by the chlorophyll antennae during the dissipation of excess energy not used in photochemistry. Because the O₂ A-band contains strong, narrow absorption features, it allows separation of the reflected radiance from the smooth spectral shape of fluorescence. Classical two-band FLD (Fluorescence Line Discrimination) methods are insufficient for the moderate spectral resolution of TROPOMI (~0.25 nm), so enhanced approaches are used, including 3-FLD, improved FLD (iFLD), singular-value-decomposition FLD (SVD-FLD), and nonlinear spectral fitting techniques that model fluorescence explicitly as an additive smooth component (Equation 2):

$$T_{\text{down}}(\lambda) T_{\text{up}}(\lambda) + L_{\text{atm}}(\lambda)] R_{\text{inst}}(\lambda) + \epsilon(\lambda), \quad \text{Eq. 1.2}$$

where $P(\lambda)$ is a low-order polynomial representing the background reflectance, SIF is the retrieved fluorescence amplitude, $f(\lambda)$ represents the theoretical fluorescence shape, and $\sigma_j(\lambda)$ denote absorption cross-sections of O_2 and interfering gases. Retrieval windows typically include 740 nm and 757–771 nm, producing SIF740 and SIF760 products, the latter being more sensitive to atmospheric absorption and the former more robust over bright soils. The retrievals are highly sensitive to clouds, aerosol loadings, surface anisotropy and instrument noise, so quality filtering is essential.

Methane retrieval from the SWIR band (2305–2385 nm) uses the IMAP-DOAS algorithm, a physically constrained differential-absorption approach that simultaneously fits absorption by CH_4 , H_2O , CO_2 and CO , along with surface albedo, aerosol properties and atmospheric scattering. The measured spectrum can be expressed as (Equation 3):

$$I(\lambda) = I_0(\lambda) \exp \left[- \sum_i \sigma_i(\lambda) S_i \right] \rho(\lambda) + \delta(\lambda), \quad \text{Eq. 1.3}$$

where $\sigma_i(\lambda)$ are laboratory absorption cross-sections, S_i are slant columns of gases, $\rho(\lambda)$ is the surface reflectance and $\delta(\lambda)$ is the residual term. Retrievals rely on Jacobians describing sensitivity to perturbations in gas concentration, surface reflectance and atmospheric state (Equation 4):

$$K_{ij} = \frac{\partial I(\lambda_i)}{\partial S_j}. \quad \text{Eq. 1.4}$$

The inversion is solved iteratively (e.g., using Levenberg–Marquardt), optimizing the match between simulated and observed radiances. Because SWIR retrievals are strongly influenced by clouds, water vapour, aerosols and BRDF effects—particularly in humid tropical regions—strict quality filtering ($qa_value \geq 0.5$ or ≥ 0.8 for scientific inversions) is required. In tropical environments such as Brazil, high humidity reduces SWIR SNR, and biomass-burning aerosols introduce spectral correlations that can degrade CH_4 retrievals if not properly accounted for.

The combined use of SIF and CH_4 from TROPOMI is especially powerful for agricultural and land-atmosphere studies. SIF provides a biophysical tracer of gross primary productivity (GPP), reflecting photosynthetic electron transport rates and canopy-level physiological status. Methane, in contrast, traces biogenic emissions from enteric fermentation in ruminants, anaerobic decomposition of organic matter, flooded soils and anthropogenic activities such as manure management. In tropical grazing systems, SIF signals reflect seasonal biomass dynamics, pasture degradation and recovery, water-stress cycles and canopy greenness patterns, while CH_4 retrievals can map the spatial distribution of cattle herds and manure-related emissions. When combined with bottom-up inventories (Tier 1–3), cattle density maps (e.g., FAOSTAT, MapBiomass), soil moisture datasets and atmospheric inversion models, TROPOMI becomes a central tool for quantifying emission drivers and validating sectoral emission factors in tropical agricultural regions. TROPOMI CH_4 datasets are widely used in atmospheric inversions using frameworks such as GEOS-Chem adjoint, TM5-4DVar, and WRF-Chem 4DVar. Equation 5.

$$y = H(x) + \eta \quad \text{Eq. 1.5}$$

The assimilation relates observations y to the model state x through the observation operator H , which simulates radiances or XCH_4 at the instrument's geometry. The observation error covariance matrix R must incorporate spatially and temporally varying uncertainties, including biases related to aerosols, BRDF and atmospheric humidity. Experience from inversion studies shows that adding TROPOMI data significantly reduces posterior uncertainty in emission estimates, particularly in regions where previous satellite coverage was sparse (Amazon, Cerrado, Sub-Saharan Africa).

Validation of TROPOMI products is conducted using ground-based FTIR networks such as TCCON, airborne campaigns, OCO-2 and GOSAT comparisons, flux-tower measurements for SIF, and radiometric calibration procedures involving lunar observations. Methane products demonstrate random errors of approximately 10–15 ppb per pixel and systematic biases of 5–10 ppb depending on surface type and atmospheric conditions. SIF validation relies heavily on flux towers and ecosystem models such as SCOPE, SiB4 and BETHY, demonstrating strong correlation between SIF760 and GPP in a wide range of ecosystems.

Despite its unparalleled capabilities, TROPOMI has inherent limitations. The spectral range does not include the red fluorescence peak at 685 nm, limiting direct comparison with hyperspectral sensors. Spatial resolution, though superior to previous atmospheric sensors, remains coarse for small agricultural fields. Humid tropical atmospheres reduce SWIR sensitivity, and bright soils or strong BRDF in savanna ecosystems can bias retrievals. Aerosol events—such as Amazonian biomass burning—introduce both spectral interference

and geometric complications. Nonetheless, robust filtering, cross-calibration procedures and data-assimilation frameworks mitigate many of these constraints.

The impact of TROPOMI on Earth observation is transformative. For the first time, it is possible to observe near-real-time global patterns of diffuse methane emissions and monitor terrestrial photosynthesis at kilometre scale. This synergy between atmospheric composition and biospheric function has opened new avenues in modelling the Earth system, improving inventories, identifying emission hotspots, and informing agricultural and climate policies. In tropical countries such as Brazil—where agricultural expansion, ruminant emissions and climatic variability are globally significant—TROPOMI provides an unprecedented dataset for integrated analyses of vegetation productivity, greenhouse-gas emissions, land degradation and atmospheric chemistry. As new missions such as CO2M, FLEX, GOSAT-GW and MethaneSAT emerge, TROPOMI will remain a foundational reference and complementary source, continuing to shape scientific understanding of the coupled plant–animal–atmosphere systems of the Earth.

CHAPTER 2. Solar-Induced Fluorescence reveals critical characteristics of intensive large-scale agriculture in Brazil

2.1. Introduction

Brazil has established itself as a global leader in soybean production, with output increasing by more than 300% over the past two decades, reaching approximately 167 million tons in 2024, which corresponds to around 40% of total global production (CONAB, 2025; USDA, 2025; IBGE, 2024). This significant expansion, driven by advances in genetics, mechanization, and land use, emphasizes the strategic need to improve crop monitoring systems, particularly phenological tracking, in light of increasing climate variability (Dias et al., 2016; da Silva Gundim et al., 2023; Bigolin and Talamini, 2025; Thomasz et al., 2024).

Despite significant advancements, precise, large-scale monitoring of crop phenology remains a challenge, particularly in tropical regions. This limitation hinders adaptive responses to climate risks (Fatima et al., 2021; Rezaei et al., 2023; Yuan et al., 2024). A comprehensive understanding of phenological parameters is crucial not only for predicting the impacts of climate change on agricultural productivity but also for adapting management practices to ensure the resilience of agricultural systems under evolving environmental conditions. While numerous global studies have aimed to understand the physiological responses of crops to climate change (Rezaei et al., 2023; Liu et al., 2022; Xiao et al., 2021), such research remains in its early stages within the Brazilian context.

Understanding the duration of phenological phases is essential for crop growth modeling, water management, pest control, and adaptation to climate change. Models such as DSSAT and APSIM use these data to predict productivity, enabling farmers and researchers to optimize management practices (Timlin et al., 2024; Holzworth et al., 2018). Irrigation

strategies are strongly influenced by phenology, as water demand varies according to the crop's development stage (Zhang et al., 2020). Similarly, plant health control relies on knowledge of phenological cycles for the efficient application of pesticides and integrated pest management strategies (Ashfaq et al., 2024; Gvozdenac et al., 2022). Climate change has altered crop phenological patterns, affecting the duration of the growth cycle and, consequently, agricultural productivity, requiring the adaptation of more resilient cultivars to thermal and water stress (Liu et al., 2020a; Agnolucci et al., 2020).

Field data on the crops' phenological stages are generally neglected in most countries, mainly due to their high operational costs (USDA, 2017). The USA is one of the few countries that collect phenological data released by the National Agricultural Statistics Service (NASS, <https://www.nass.usda.gov/>). These data are collected from field observations (approximately 3,600 observations annually) and aggregated at the district (multiple counties) and state levels. In Brazil, crop progress monitoring is carried out by the Companhia Nacional de Abastecimento (CONAB, <https://www.conab.gov.br/>) and is only released at the state level. At the same time, Brazil lacks a consolidated PhenoCam network that could provide high-frequency, site-scale phenological observations to complement field surveys and remote-sensing products; by contrast, in the U.S. and other developed countries such networks are routinely integrated into biome and agricultural monitoring (Richardson et al., 2018; Moon et al., 2021; Browning et al., 2021). In both cases, more data is needed for more in-depth research into cultivation conditions, as they have low spatial (from tens to thousands of km²) and temporal (weekly) resolution.

Over the last twenty years, advances in remote sensing have been fundamental in mitigating the need for in situ data on vegetation phenology. More specifically, the Moderate Resolution Imaging Spectroradiometer sensor (MODIS, on board the Terra and Aqua satellites) made it possible to monitor phenology with high temporal (daily or near daily

revisit) and spatial (250, 500, and 1000 meters) resolution through products such as MCD43A4 (Zhong et al., 2016; Diao et al., 2020; Fonseca et al., 2022) and MOD09A1/MYD09A1 (Sakamoto et al., 2013; Liu et al., 2020b).

In general, these methods rely on traditional vegetation indices (VIs) time series, such as the Normalized Difference Vegetation Index (NDVI) and Enhanced Vegetation Index (EVI). However, more recent studies revealed that VIs show great uncertainty in retrieving vegetation phenology, especially at the end of the growing season (Gao & Zhang, 2021; Shen et al., 2024; Kato et al., 2021). This may occur as VIs saturate with increasing leaf biomass and in multilayered vegetation (Huete et al., 2002). New remote sensing tools, like solar energy-induced chlorophyll fluorescence (SIF) from the Tropospheric Monitoring Instrument (TROPOMI) sensor, could fill this gap and allow more accurate phenological metrics. SIF - a weak electromagnetic signal emitted by excited chlorophyll molecules upon absorption of photosynthetically active radiation in the red to near-infrared range (650-800 nm) with two peaks centered around 685 and 740 nm - is a powerful proxy for photosynthesis, linked to electron transport in the light reactions of photosynthesis (Köhler et al., 2018; Fang et al., 2025), and therefore is a more consistent measurement of photosynthesis when compared to VIs (which relate photosynthesis to the amount of chlorophyll measured by the red and infrared bands). TROPOMI is a spectrometer on the Sentinel-5 Precursor satellite, launched in October 2017. It has allowed many studies about vegetation from SIF, such as the identification that the dry season is becoming longer in the Amazon (Doughty et al., 2019), and indication that low temperatures are hard on winter crops (Wu et al., 2024). SIF data has been collected for at least 10 years through the SCIAMACHY (Khosravi et al., 2015), GOSAT (Joiner et al., 2011), and OCO-2 (Yu et al., 2019) sensors, but TROPOMI allows, for the first time, mapping SIF daily, and with moderate spatial resolution pixels (7 x 7.5 km) (Köhler et al., 2018).

This study aims to evaluate the potential of SIF as a proxy variable for characterizing phenological events and predicting crop yield in large-scale agricultural systems, with a specific focus on soybean cultivation in Brazil. In particular, this research assesses the accuracy and sensitivity of the SIF signal in detecting key phenological stages, in comparison to traditional vegetation indices (VIs), across multiple spatial scales (state, municipality, and field level), to support the improvement of agricultural monitoring models and contribute to the development of operational tools for precision agriculture.

2.2. Materials and Methods

This methodology encompasses a set of approaches developed to characterize the phenological phases of soybeans based on remote sensing data. We created a phenological observation system that works through four steps: I) pre-processing SIF-TROPOMI data, which includes filling in missing data and filtering to eliminate data contaminated by clouds, changes in management, aerosols, and the atmosphere; II) masking for soybean cropland using the area fraction method with data from MapBiomass (Souza et al., 2020); III) modeling and characterizing phenological data; and IV) validating and mapping phenological data. This methodological flowchart is presented in Figure 1.1, and methodological details will be explained throughout the Section.

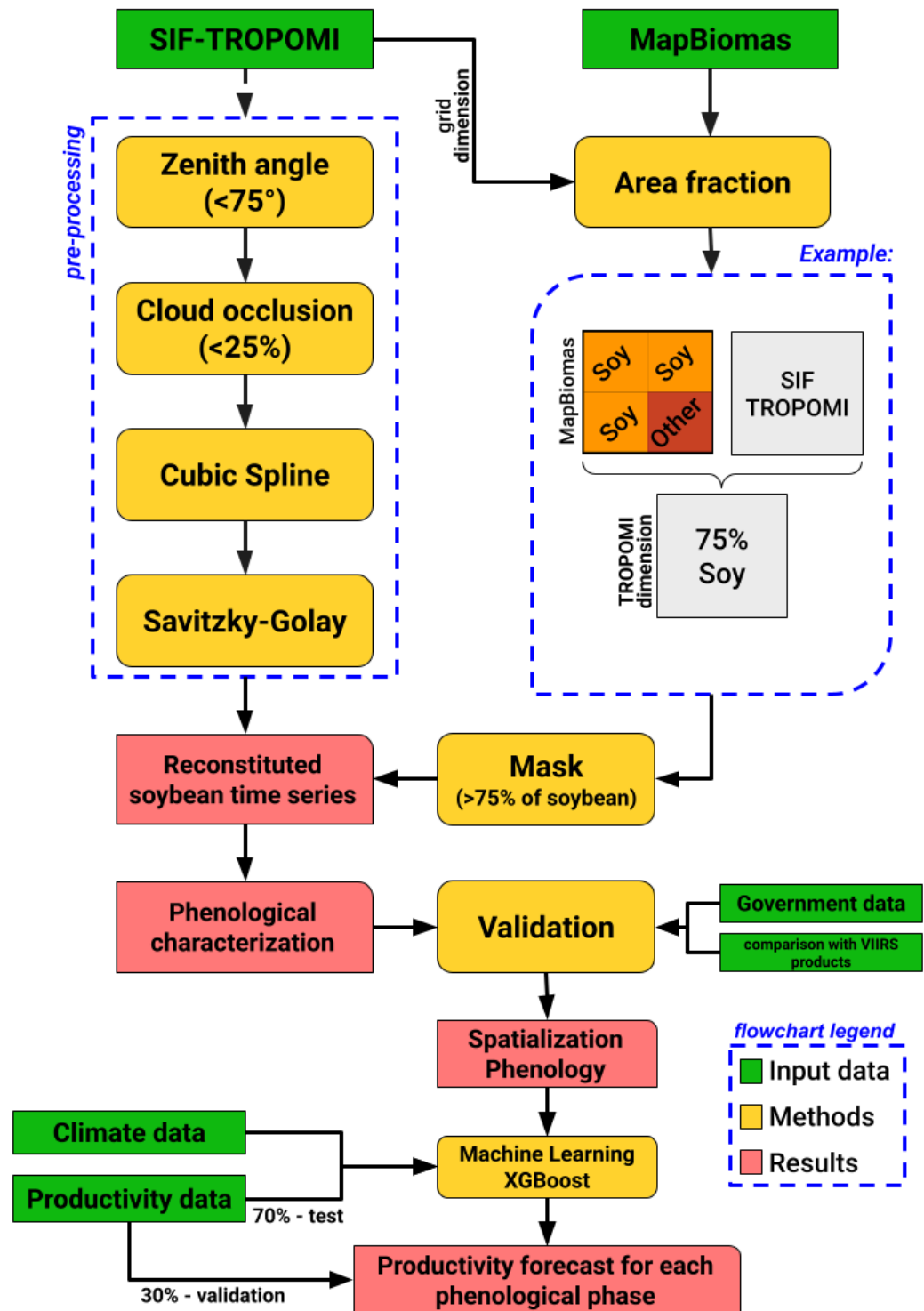


Figure 2.1. Methodological flowchart for phenological observation using SIF-TROPOMI.

2.2.1. Study Area

The study area includes the four largest soybean-producing regions in Brazil (Figure 1.2): Southern, Southeast, Center-West, and the expanding agricultural frontier known as MATOPIBA, which comprises the states of Maranhão, Tocantins, Piauí, and Western Bahia. Together, these regions produced approximately 116 million metric tons (Mt) of soybeans in 2022, representing about 96% of Brazil's total production and 31% of global production (IBGE, 2024; USDA, 2024).

The Southern region accounted for approximately 25 Mt of soybeans in 2022 (20% of national production), with a planted area of around 13 million hectares (ha) and an average yield of 2,272 kg.ha⁻¹. This production generated an estimated revenue of US\$ 12 billion (IBGE, 2024).

The Southeast region, responsible for about 10% of national production (~12 Mt in 2023; IBGE, 2024), stands out for its high yields, exceeding 3,500 kg.ha⁻¹. This performance is primarily attributed to significant investments in technology and irrigation, particularly in the northwestern part of Minas Gerais.

The Midwest region leads soybean production in Brazil, contributing approximately 47% of the national total (~56.4 Mt in 2023; IBGE, 2024). High productivity levels, above 3,200 kg.ha⁻¹, are driven by the availability of fertile land and continuous advancements in agricultural technology, especially in Mato Grosso, the country's top-producing state.

The MATOPIBA region accounts for around 12% of national soybean production (~14.4 Mt in 2023; IBGE, 2024), with an average yield of approximately 3,000 kg.ha⁻¹. Expansion in this region is largely driven by the increasing cultivation area, particularly in

Maranhão and Tocantins, along with significant investments in agricultural technology, including irrigation, which contribute to high yields.

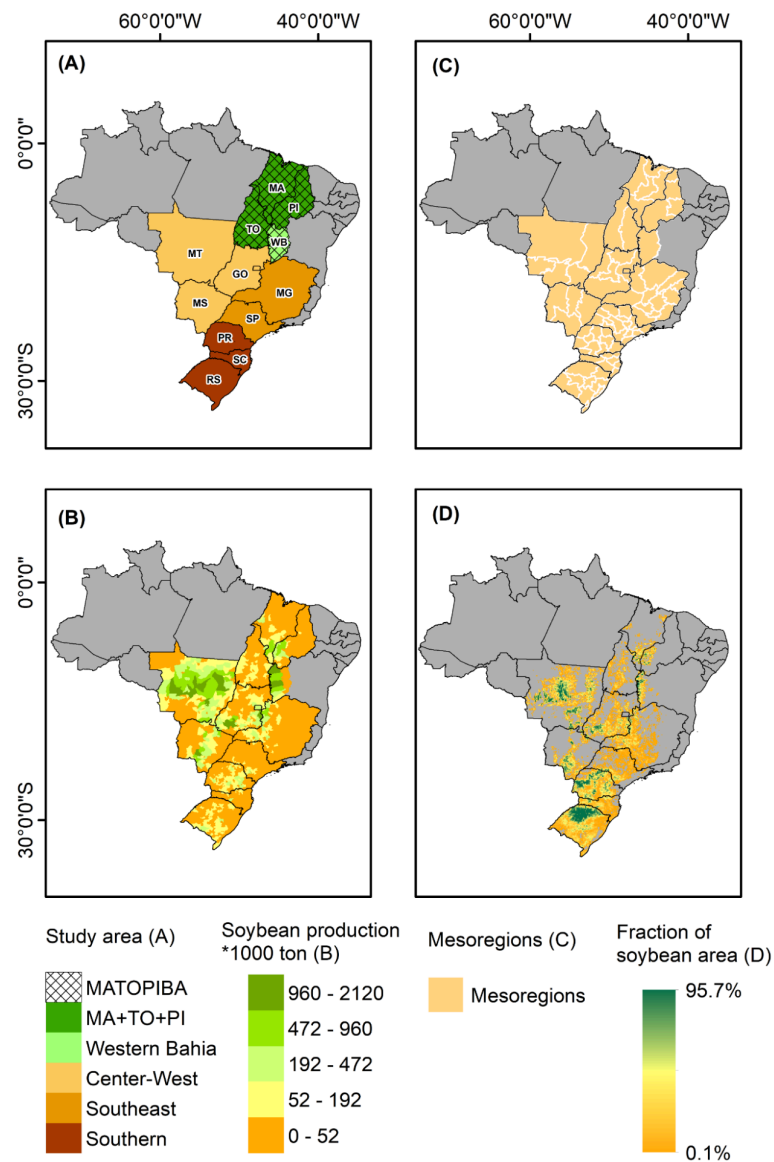


Figure 2.2. Location of the Center-West, MATOPIBA, South and Southeast regions in Brazil (A); municipal soy production based on IBGE data (B); mesoregions of Brazil (C) fraction of TROPOMI pixel land area planted with soybeans (D). Abbreviations of the Brazilian states: GO) Goiás, MA) Maranhão, MG) Minas Gerais, MS) Mato Grosso do Sul, MT) Mato Grosso, PI) Piauí, PR) Paraná, RS) Rio Grande do Sul, SC) Santa Catarina, SP) São Paulo, TO) Tocantins, WB) Western Bahia.

2.2.2. Land use data

We relied on the MapBiomas platform (*Mapeamento Anual do Uso e Cobertura da Terra no Brasil* – <https://mapbiomas.org>) for our land use and land cover data from 2019 to 2022. This platform, known for its supervised classifications using machine learning algorithms from 30 m spatial resolution Landsat data, was instrumental in distinguishing different seasonal crops such as soybeans, sugarcane, and cotton.

We applied a resampling technique to adjust the pixel dimensions from the MapBiomas dataset to match those of the TROPOMI dataset. To achieve this, we calculated the ratio between the area of MapBiomas pixels belonging to a specific class (e.g., soybean) that are found within the area of a TROPOMI pixel and the total number of MapBiomas pixels within that same TROPOMI pixel area. Figure 1.2D presents the soybean area fraction (AF).

2.2.3. SIF-TROPOMI reflectance and pre-processing methods

TROPOMI is a Differential Optical Absorption Spectrometer on board the Sentinel-5 Precursor (S5P) satellite of the European Space Agency (ESA). S5P flies at an altitude of 824 km in a near-polar, sun-synchronous orbit (equatorial crossing at ~13:30 local solar time), with a repeating cycle of 17 days at nadir (227 orbits) and a footprint size of 7 km along the trail and 3.5–7 km across (3.5 km at nadir and 15 km off-nadir). TROPOMI's wide coverage range (~2600 km) enables retrieval of gridded data with 100% daily global coverage for latitudes greater than $\pm 7^\circ$. TROPOMI was initially designed to monitor atmospheric gases (CO , CH_4 , O_3 , NO_2 , and SO_2), cloud properties, and aerosols. To carry out such measurements, TROPOMI operates using four spectrometers, from ultraviolet to shortwave infrared (UV-VIS, 270 nm – 495 nm; NIR, 675 nm – 775 nm; SWIR, 2305 nm – 2385 nm).

TROPOMI also allows, as secondary data, the recovery of sun-induced fluorescence from a window of the electromagnetic spectrum of 743-758 nm (van Hees et al., 2018; Hu et al., 2018; Goldberg et al., 2021; Van Kempen et al., 2021; Reshi et al., 2024) . In this ~15 nm window, there is minimal interaction between radiation and gases present in the atmosphere, allowing the retrieval of SIF by resolving the optical depth of the Fraunhofer lines in the solar spectrum (Köhler et al., 2020; Guanter et al., 2021;; Bai et al., 2024)

We applied specific exclusion criteria to ensure the quality of the data. First, we removed S5P passes with a zenith angle greater than 75° and pixels with more than 25% cloud cover, following the procedures described in Köhler et al. (2018) and Guanter et al. (2021). Throughout the time series, we aimed to have at least 75% of pixels available for analysis, so we discarded stacks of pixels with more than 25% missing data.

To handle missing or masked values, we employed cubic-spline interpolation. Additionally, we addressed noisy data, which often results from clouds (cloud cover ranging between 0.1% and 25%) and adverse weather conditions during the time series, applying a weighted Savitzky-Golay filter. This filtering process enhanced the stability of the input data in the subsequent fit model, particularly when dealing with fluctuating SIF values.

2.2.4. Retrievals of phenological metrics

We used the Phenofit package (Kong et al., 2022), developed for the R programming language, to retrieve the phenological transition dates of seasonal soybeans. We fine-tuned the SIF curves using four phenological models based on the dual logistic function described by Zhang et al. (2003), Beck et al. (2006), Gu et al. (2009), and Elmore et al. (2012). The adjustment functions are presented in Table 1. Methods that use the dual logistic function are

widely used to monitor the phenological development of crops over time, especially crops with relatively short harvests, such as soybeans (Diao, 2020).

Table 2.1. Fine-tuning functions of phenological curves using Zhang, Beck, Emore, and Gu methods. Where: t corresponds to each day of the SIF time series; mn and mx are the minimum and maximum values of y (y corresponds to the SIF value); SOS and EOS correspond to the start and end of the growing season, respectively. rsp and rau are, respectively, the green up and senescence rate; t_0 is the turning point of vegetation green up and senescence; m_7 is the summer green-down parameter; $c1$ and $c2$ are the shape parameters of the Gu logistic.

Function	References
$f(t) = \frac{mx-mn}{1+e^{-rsp(t-sos)}} + mn, t \leq t_0$ $f(t) = \frac{mx-mn}{1+e^{rau(t-eos)}} + mn, t > t_0$	Zhang et al. (2003)
$f(t) = mn + (mx - mn) \cdot \left(\frac{1}{1+e^{(-rsp(t-sos))}} + \frac{1}{1+e^{rau(t-eos)}} - 1 \right)$	Beck et al. (2006)
$f(t) = mn + (mx - m_7 t) \cdot \left(\frac{1}{1+e^{-rsp(t-sos)}} - \frac{1}{1+e^{-rau(t-eos)}} \right)$	Elmore et al. (2012)
$f(t) = mn + \frac{a_1}{[1+e^{-rsp(t-sos)}]^{c_1}} - \frac{a_2}{[1+e^{-rau(t-eos)}]^{c_2}}$	Gu et al. (2009)

Phenological cycles in crops refer to the sequential stages of plant development that occur throughout a growing season, each characterized by specific physiological and morphological changes. For soybean, these cycles are typically divided into vegetative stages (V) and reproductive stages (R). The vegetative stages encompass germination, seedling establishment, and successive leaf development, while the reproductive stages include

flowering (e.g., full bloom, R2), pod development (e.g., beginning pod, R3), seed filling, and maturation.

After adjusting the SIF curves, we proceeded to recover the phenological transition dates, which consisted of estimating the critical point of a time series in which there is a change from one phenological stage to another. In this study, we used four methods to retrieve phenological transition dates: threshold-based, derivative-based, inflection-based (or Zhang-based), and Gu-based methods (Figure 1.3).

The threshold-based method identifies the critical transition point of phenological phases based on arbitrary user-defined thresholds (White et al., 2009). Limits for phenological characterization can be defined using absolute values (e.g., SIF of $1 \text{ mW/m}^2/\text{sr/nm}$) or relative values (e.g., a percentage of the SIF curve amplitude; White et al., 1997). Due to the difference in vegetation's biochemical and biophysical structures, the absolute limits defined for phenological stage extractions in a specific region may not be suitable in large regions (Diao, 2020). Thus, due to the geographic extension of our study area, we used relative thresholds of 20% and 50% of the curve amplitude to recover two phenological transition dates, called start of season (SOS) and end of season (EOS) (Figure 1.3A).

The derivative-based method describes crop development progress based on identifying change points in the first derivative of the time series (Diao, 2020). Fluctuations in SIF values are associated with abrupt changes in photosynthetic activity, which may indicate the phenological transition of vegetation from one stage to another (Diao, 2020). Therefore, the inflection points identified in the derivative of the vegetative development curve are used to characterize phenological events. The derivative-based method, similar to the threshold-based one, allows the estimation of three phenological transition dates. The SOS and EOS are defined when the first derivative of the curve reaches the absolute maximum and

minimum value, respectively. The Peak of the Season (POS), in turn, was defined when the maximum SIF of the curve was reached (Figure 1.3B).

The inflection-based method recovers the phenological transition from the local maxima and minima of the rate of variation of the SIF curve, which indicates when the crop cycle transitions from one approximately linear stage to another. This method allows estimating four transitions: green up (beginning of photosynthetic activity), maturity (the moment in which the leaf area is at its maximum), senescence (photosynthetic activity and the green leaf area begin to decrease rapidly), and dormancy (the physiological state when the activity becomes close to zero). Greenup and maturity correspond to the moment when the rate of change of curvature reaches local maximums during the upward direction of the SIF curve. In turn, senescence and dormancy correspond to the moment when the rate of curvature variation reaches local minima during the downward direction of the SIF curve (Figure 1.3C). This method is less stable than the others, as it requires a SIF time series with two local maxima and two local minima values of the rate of change of curvature, a requirement that might not be always satisfied (Kong et al., 2022).

The Gu-based method allows recovering the phenological transition from four lines fitted to the SIF curve. The first line intercepts the local minima (called the baseline), corresponding to the start and end of the growing season; the second line intersects the maximum SIF value. The baseline and maximum lines define the slope of two lines tangent to the SIF curve (recovery and senescence lines). The intersections of the recovery and senescence lines with the baseline and maximum lines define four phenological metrics: update date (UD), stabilization date (SD), initial downturn date (DD), and recession date (RD) (Figure 1.3D).

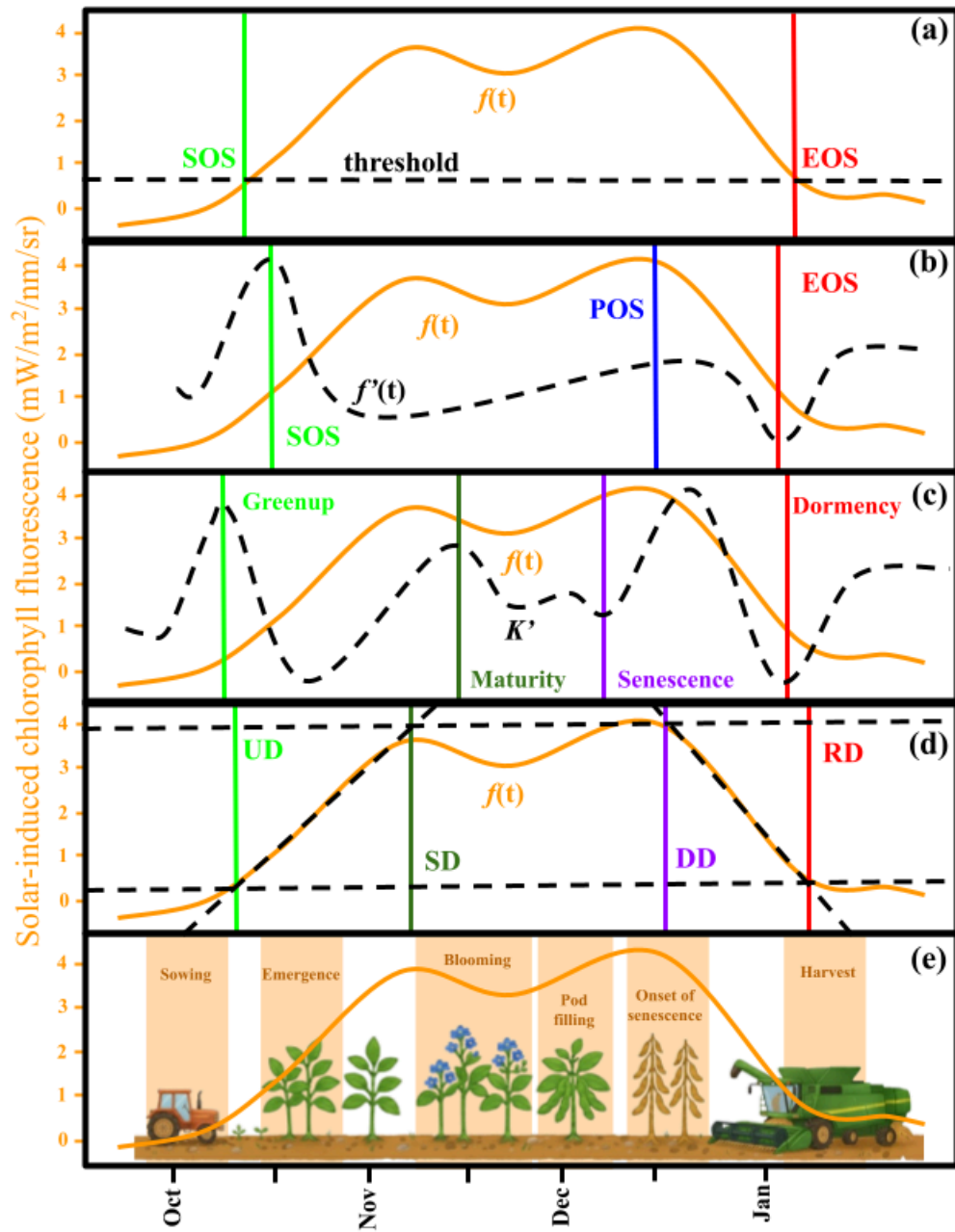


Figure 2.3. Schematic of the vegetation phenology extraction methods. a) dynamic threshold-based method; b) derivative method; c) inflection method; d) Gu's method; e) summary of the phenological stages.

Finally, we determine the sowing date (Doy_{sow}) from the emergence date (SOS; greenup; update date), by applying a modified version of the method for calculating biological

days based on degree days by Soltani and Sinclair (2012), as presented in Fonseca et al. (2022). This method assumes that the plants must accumulate pre-defined temperature units ($CTU^{sow-emg}$) from sowing until crop emergence ($Doy_{emergency}$), according to the crop's energy needs (Equation 1).

$$Doy_{sow} = Doy_{sow-emg} - \frac{CTU^{sow-emg}}{\sum_{Doy=1}^k DTU} \quad \text{Eq. 2.1}$$

Where: $CTU^{sow-emg}$ ($^{\circ}C$) is the cumulative growing degree-day required for the transition from seeding to emergence (here assumed as $70^{\circ}C$), k is the day of the year on which the cumulative growing degree-day required for the transition from sowing to emergence is reached, and DTU is the daily temperature unit ($^{\circ}C.day^{-1}$), calculated as in Equation 2.

$$DTU = (TP1D - TBD) * tempfun \quad \text{Eq. 2.2}$$

Where: $TP1D$ is the lowest optimum temperature for crop growth ($21^{\circ}C$), TBD is the crop basal temperature ($10^{\circ}C$), and $tempfun$ is the relative development response of crops to temperature.

The temperature function ($TempFun$, Figure 1.4) represents the physiological response of the crop as a function of mean air temperature (TMP). No development occurs when TMP is below the base temperature (TBD) or above the upper critical temperature (TCD), indicating thermal conditions limiting growth. Between TBD and $TP1D$, a positive linear response is observed, reflecting a progressive increase in the development rate. The function reaches its maximum value within the range from $TP1D$ to $TP2D$, indicating the optimal

temperature for plant development. From TP2D to TCD, there is a linear decline in the response, characterizing the inhibitory effect of supra-optimal temperatures.

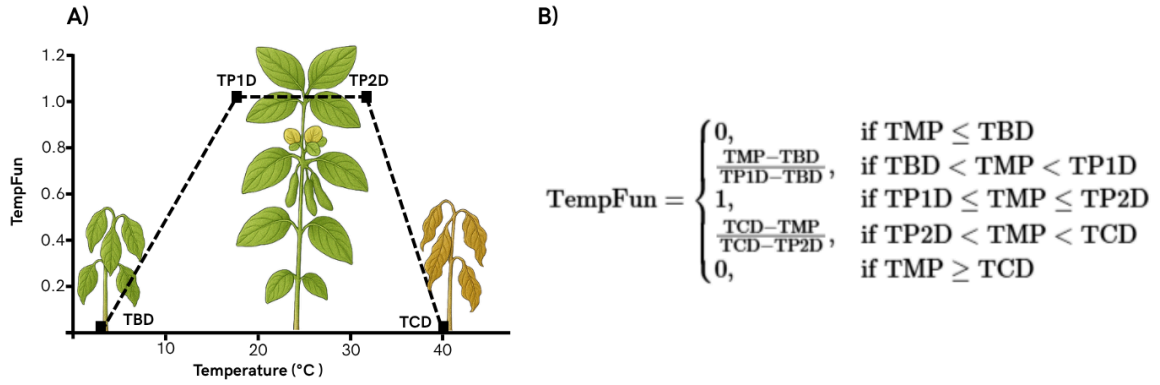


Figure 2.4. Functional response to temperature for plant growth.

Where: TMP is the daily average air temperature (°C), calculated as the average of four observations (night and day) of the MOD11A1 (MODIS-Earth) and MYD11A1 (MODIS-Aqua) products; TP2D is the lowest ideal temperature for crop development (36 °C); and TCD is the maximum temperature (ceiling) at which the plant develops (43 °C).

2.2.5. Validation through government data and VIIRS data

Where available, near-surface phenological observations from the PhenoCam network provide a gold-standard reference for validating satellite-derived land-surface phenology, offering intra-daily canopy RGB imagery from which Gcc-based transition dates (SOS/POS/EOS) are derived under standardized quality-control protocols (e.g., Richardson et

al., 2018). In Brazil, however, such near-surface networks are largely absent or remain underutilized; accordingly, we validated our results using a multiscale strategy leveraging independent datasets at the state, municipality, and agricultural (farm/field) levels.

At the state level, we used monitoring data from the National Supply Company (CONAB), which provides weekly reports on soybean planting and harvesting, including the percentage of planted area and the state-wide average transition dates between phenological stages. We calculated the average of the SIF calendar pixels for each state and compared them with CONAB data.

At the municipal level, we employed the Agroclimatic Risk Zoning (ACRZ - is a planning tool that identifies suitable planting periods and regions by analyzing climate, soil, and crop requirements to reduce agricultural risk), published annually by the Ministry of Agriculture, which defines the ideal soybean planting period for each municipality based on soil type and climate. We evaluated ACRZ planting dates with climate risk below 20%, comparing them with those from the SIF calendar. Three soil types with distinct water retention capacities (<35 mm, 35-55 mm, >55 mm), as mapped by IBGE, were considered.

At the farm level, we validated phenological transition dates using high-spatial-resolution imagery. We visually identified planting/emergence and harvest using images from Planet Labs (<10 m), Sentinel-2 (10 m), and CBERS-4A (resolutions varying from 2 m to 16 m), which enable monitoring of the soybean vegetative cycle. Approximately 20,000 soybean fields were delineated across 10 sub-regions, allowing comparisons of mean, maximum, and minimum values with SIF results. This multiscale approach provided a robust validation of soybean phenological data in Brazil.

Additionally, we conducted a comparative analysis between SIF products and phenological metrics derived from traditional vegetation indices. To assess the consistency of

these datasets, we calculated the coefficient of determination (R^2) and the mean difference using the two approaches. Soybean phenological metrics were obtained following the methodologies outlined in Section 2.4, but in this case, we utilized the Normalized Difference Vegetation Index (NDVI) derived from the VNP09GA product of the Visible Infrared Imaging Radiometer Suite (VIIRS). The VNP09GA product offers a daily revisit time with a spatial resolution of 500 meters.

Furthermore, we used global land surface phenology metrics from the VNP22Q2 product, which derives phenological metrics using the Enhanced Vegetation Index (EVI2). VNP22Q2 is a 500m-resolution product generated using VIIRS Daily Nadir BRDF-Adjusted Reflectance (NBAR). Its production is based on the Hybrid Piecewise Logistic Model (HPLM) and the Land Surface Phenology Detection (LSPD) algorithm (Zhang et al., 2020; Liu et al., 2022b).

2.2.6. Predicting Soybean Yield Using Physiological and Meteorological Parameters with Machine Learning

We also assess whether soybean yield could be predicted based on the crop's physiological conditions at two specific phenological time steps: (i) from emergence to maturity and (ii) from emergence to grain filling.

The predictive framework uses physiological (SIF) and weather data (cumulative mean precipitation derived from CHIRPS and maximum, minimum, and mean temperature data obtained from VIIRS). All datasets were aggregated at the municipal level to ensure compatibility with the official soybean yield records from SIDRA/IBGE.

To model soybean yield, we employed Extreme Gradient Boosting (XGBoost), a robust machine learning algorithm known for its efficiency in handling complex and nonlinear relationships in large datasets. The model was trained using the compiled dataset, with soybean yield as the dependent variable and physiological and weather data as predictors.

2.3. Results

The SIF time series reveal clear and regionally distinct patterns of soybean development in Brazil, providing both scientific and operational insights. In the following sections, we first examine phenological trajectories across major producing regions (Section 3.1). Next, we analyze the degree of sowing synchronization and mechanization demand in double-cropping systems (Section 3.2). We then evaluate the influence of climatic variability and extreme events on interannual dynamics (Section 3.3). Finally, we explore how these signals translate into yield forecasting potential (Section 3.4). Together, these results position SIF as a decision-support variable for agricultural monitoring in Brazil.

2.3.1. Results of SIF models and curves

We estimated the timing of four phenological stages (emergence, blooming, pod filling, and harvest) across states and regions in the 2018–2022 time series (Figure 1.5). These estimates were derived using four curve-smoothing approaches (Zhang et al., 2003; Beck et al., 2006; Gu et al., 2009; Elmore et al., 2012), applied consistently to each phenophase. The results show a strong overall convergence among methods, with median differences typically below one week for most states. Nonetheless, some

regions exhibited larger divergences, particularly for later stages (pod filling and harvest), where discrepancies occasionally exceeded 20–30 days. This variability reflects differences in sensitivity of the curve-smoothing approaches to crop cycle length and local management practices.

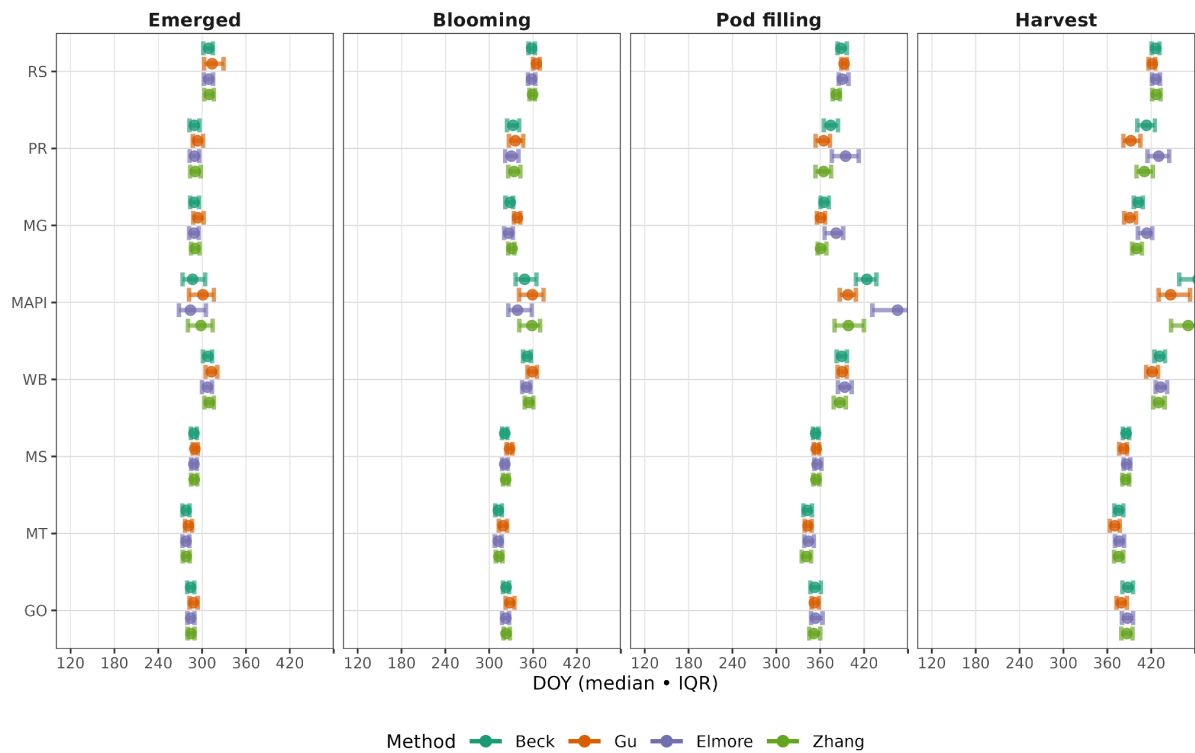


Figure 2.5. Median day of year (DOY) estimates and interquartile ranges (IQR) for soybean phenological stages (emergence, blooming, pod filling, and harvest) across Brazilian states and regions during 2018–2022. Estimates were obtained using four curve-smoothing approaches: Beck et al. 2006, Gu et al. 2009, Elmore et al. 2012, and Zhang et al. 2003.

We found that the double cropping system; characterized by two distinct peaks within the same agricultural year in the SIF (Solar-Induced Chlorophyll Fluorescence) time series; was detectable in the states of Mato Grosso, Mato Grosso do Sul, and Goiás (Figure 1.6). The first crop cycle exhibits a green-up phase in September and October, followed by senescence in January, coinciding with its harvest and the subsequent sowing of the second crop. The

maximum SIF peak of the second crop was approximately 20% lower than that of the first cycle. This difference may be attributed to two primary factors: (1) not all soybean producers in the region adopt the second-crop system, potentially resulting in an underestimation of the second peak's SIF maximum; and (2) the cessation of the rainy season in these states around mid-March to April, which limits water availability and negatively impacts the vegetative vigor of the second harvest (Liebmann et al., 2007; Brumatti et al., 2020;).

Additionally, Figure 1.6 reveals pronounced interannual variability in both the first and second cropping cycles across the 2018–2022 period, with marked differences among states. For the first crop cycle, variability is particularly evident in the timing and amplitude of the green-up phase. For example, in Mato Grosso (A) and Mato Grosso do Sul (B), the 2021 and 2022 seasons show slightly delayed and attenuated first-cycle peaks compared to the sharper, earlier peaks observed in 2019 and 2020. Such shifts likely reflect anomalous precipitation patterns or delays in sowing operations associated with climatic variability, including La Niña events that can alter rainfall onset and distribution. Similarly, Goiás (C) exhibits a narrower and lower first-cycle peak in 2021, suggesting a more constrained vegetative development that year.

The second crop cycle also demonstrates substantial interannual differences in both peak height and duration. Notably, in Mato Grosso and Mato Grosso do Sul, the second-cycle peak in 2021 and 2022 appears not only lower but also slightly shifted later in the season, potentially due to shortened rainy seasons and reduced soil moisture availability during critical growth stages from March to April. In contrast, years with more regular precipitation patterns (e.g., 2019–2020) support more robust second-cycle peaks, indicating more favorable growing conditions. States like Minas Gerais (D) and the MA+TO+PI cluster (F) display even greater interannual variability, with broader standard deviation bands, suggesting

heterogeneous management practices and stronger sensitivity to climatic fluctuations. Meanwhile, Paraná (H) exhibits consistently well-defined seasonal cycles with lower variability, likely reflecting more uniform agroclimatic conditions and management practices. These patterns underscore the influence of interannual climatic variability, especially rainfall distribution, on crop phenology and productivity across the Brazilian Cerrado and Southern regions.

In addition, climatic differences between regions play a crucial role in the viability and development of a second crop. In Mato Grosso, Mato Grosso do Sul, and Goiás, the rainy season starts earlier and lasts longer, creating more favorable conditions for planting a second crop soon after the soybean harvest. These regions also tend to experience higher cumulative rainfall and slightly lower evapotranspiration rates during the transition period between harvests, which helps maintain the soil moisture levels necessary for the establishment and growth of the second crop (Arvor et al., 2014; Spangler et al., 2017).

In contrast, in the western region of Bahia, the rainy season tends to end earlier, and rainfall distribution is more irregular. These factors shorten the window available for the second crop and increase the risk of water stress during critical growth stages of a second crop. Higher temperatures and reduced humidity in the post-soybean period also limit the success of a second crop cycle. These climatic limitations, combined with strategic decisions by producers, likely explain why the second harvest is not clearly captured in the SIF signal for Western Bahia (Pousa et al., 2019; Bazame et al., 2019; Marengo et al., 2022).

Moreover, Figure 1.6 suggests notable differences in the SIF growth rate during the first cropping cycle between states practicing double cropping and those with predominantly single-season systems. In Mato Grosso (A), Mato Grosso do Sul (B), and Goiás (C), the first-cycle SIF curve exhibits a steeper ascent during the green-up phase

(September–October), indicating rapid canopy development and strong early-season photosynthetic activity; likely a result of management practices aiming to maximize the window for the second crop. By contrast, states such as Minas Gerais (D), West of Bahia (E), and MA+TO+PI (F) show more gradual green-up phases with broader, less pronounced peaks, consistent with a single cropping cycle where planting dates are often spread over longer periods to accommodate climatic heterogeneity. This difference in growth rate highlights the role of intensive management in double-cropping systems, where precise sowing schedules and input use are optimized to ensure a rapid vegetative establishment, enabling the timely sowing of the subsequent crop despite climatic constraints.

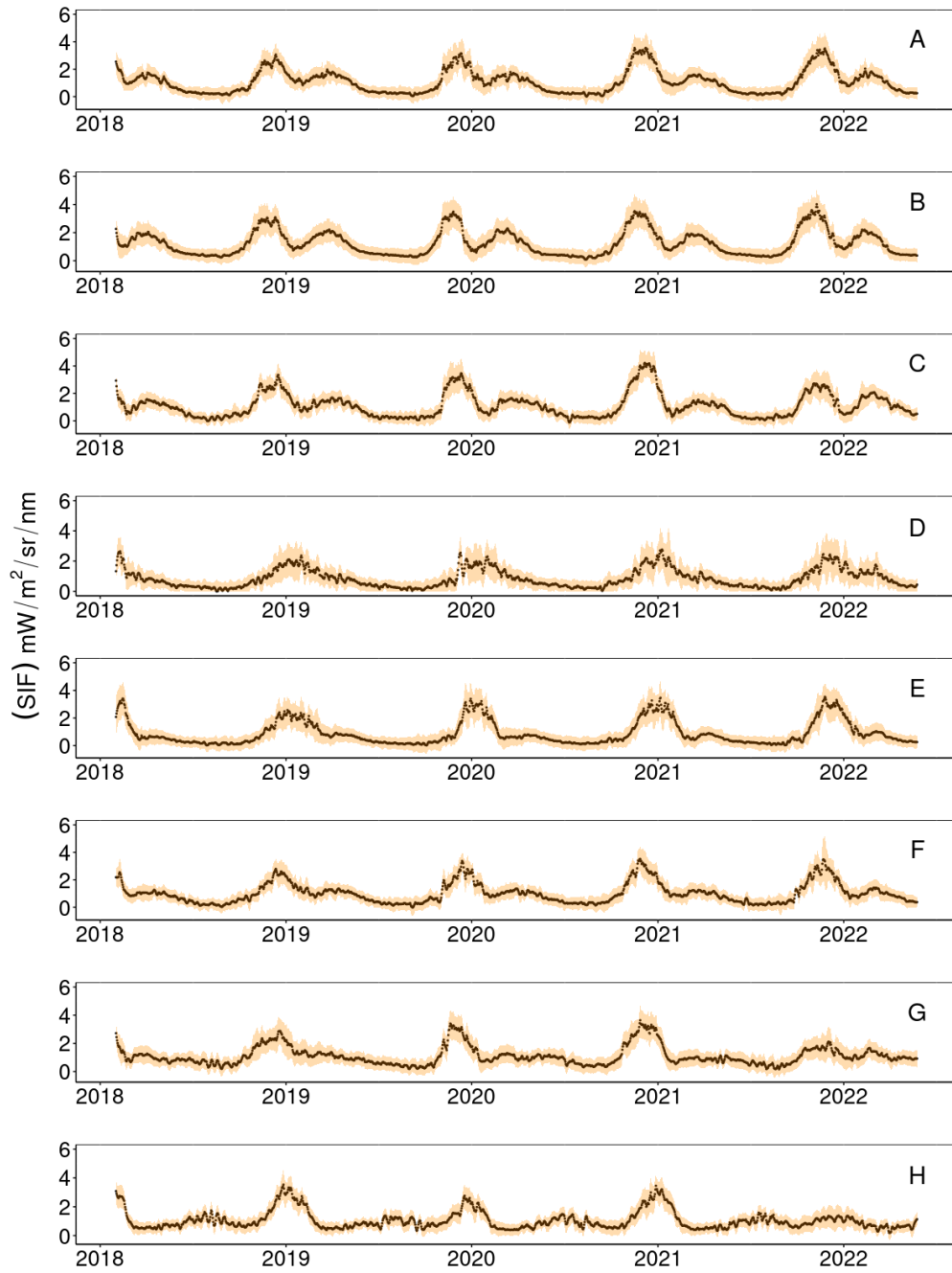


Figure 2.6. SIF curves from 2018 to 2022 for A) Mato Grosso; B) Mato Grosso do Sul; C) Goiás; D) Minas Gerais; E) West of Bahia; F) MA+TO+PI; G) Rio Grande do Sul; H) Paraná. The black line represents the average of the pixels and the yellow area represents the standard deviation.

Furthermore, for southern Brazil (Rio Grande do Sul and Paraná), the SIF curve shows a substantial decline in the 2021/2022 agricultural year. During this agricultural year, the SIF in the POS period for soybeans was approximately 90% lower than in previous years. This fact explains the absence of phenological transition dates for these states this year (Figure 1.6G-H), that might have related to the La Niña climate phenomenon that significantly impacted the 2021/22 soybean harvest in southern Brazil, resulting in significant productivity losses due to severe drought and irregular rainfall. Studies indicate that, in the Cascavel region (PR), production loss reached 72% due to water deficiency in the critical period of the crop (Unioeste, 2022). In Rio Grande do Sul, the drought drastically reduced productivity, with some areas registering only 13 bags per hectare, resulting in negative gross margins (CNA, 2022). The Brazilian Agriculture and Livestock Confederation and the National Agriculture Society reported that, as a result of these adverse weather conditions, the initial estimate of soybean production in Brazil was reduced to 125.47 million tons, representing a drop of approximately 9% compared to the previous harvest (SNA, 2022).

As recovering the data for the second crop proved to be a complex task - both in the processing part and at the time of validation due to the unavailability of the data - we chose not to present it in our results; however, they are available upon request.

Figure 1.7, represents the state of Mato Grosso, and shows the relationship between the sowing date of the first cropping season and the photosynthetic activity [SIF] of the second season. In panel A, areas with higher SIF at the peak of the second season (shown in green; $SIF-POS-SH > 3$) tend to concentrate first-season sowing between early September and early October. In contrast, areas with lower SIF in the second season (shown in red; $1.5 \leq SIF-POS-SH < 3$) exhibit later sowing in the first season, peaking in late October. Panel B illustrates how these differences in sowing timing translate into distinct seasonal SIF patterns: areas with earlier sowing maintain higher SIF values throughout the second season,

particularly during the critical period between February and March, suggesting greater photosynthetic activity and yield potential. Conversely, areas with later sowing show lower average SIF values and greater variability during this period. These results indicate that producers who adopt earlier sowing management in the first season can advance second-season planting, enabling a potentially more productive second harvest.

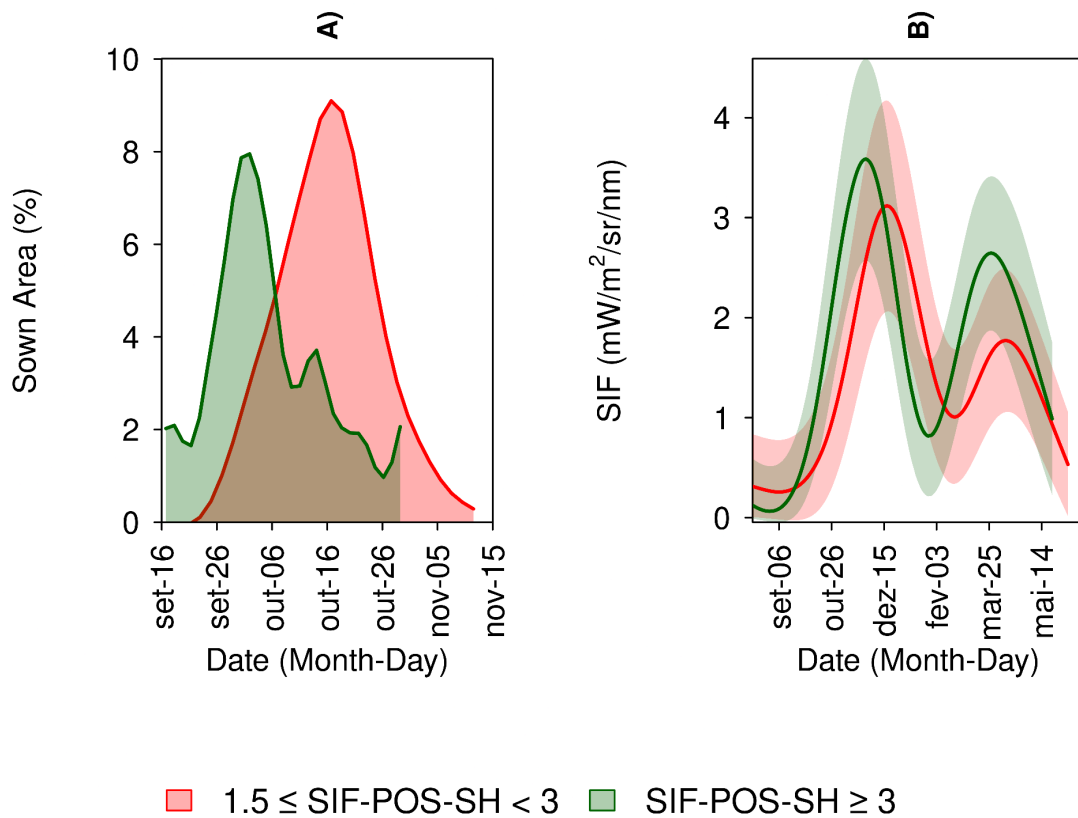


Figure 2.7. Distribution of sowing dates (A) and seasonal dynamics of Solar-Induced Fluorescence (SIF) (B) for soybean areas classified according to SIF values at the Pick of the Season (POS) during the second crop.

2.3.2. Spatiotemporal characterization of soybean phenology

The results for Brazil indicate that, on average, soybean emergence occurred around October 26, varying from mid-September in Mato Grosso to early May in the MA+TO+PI

region. Flowering took place on November 30, followed by pod filling on December 13 and harvesting on February 4, with Mato Grosso starting the harvest earlier, on January 16 (Figure 8 and Figure 1.9). Additionally, we observed that soybean sowing occurred, on average, on October 16.

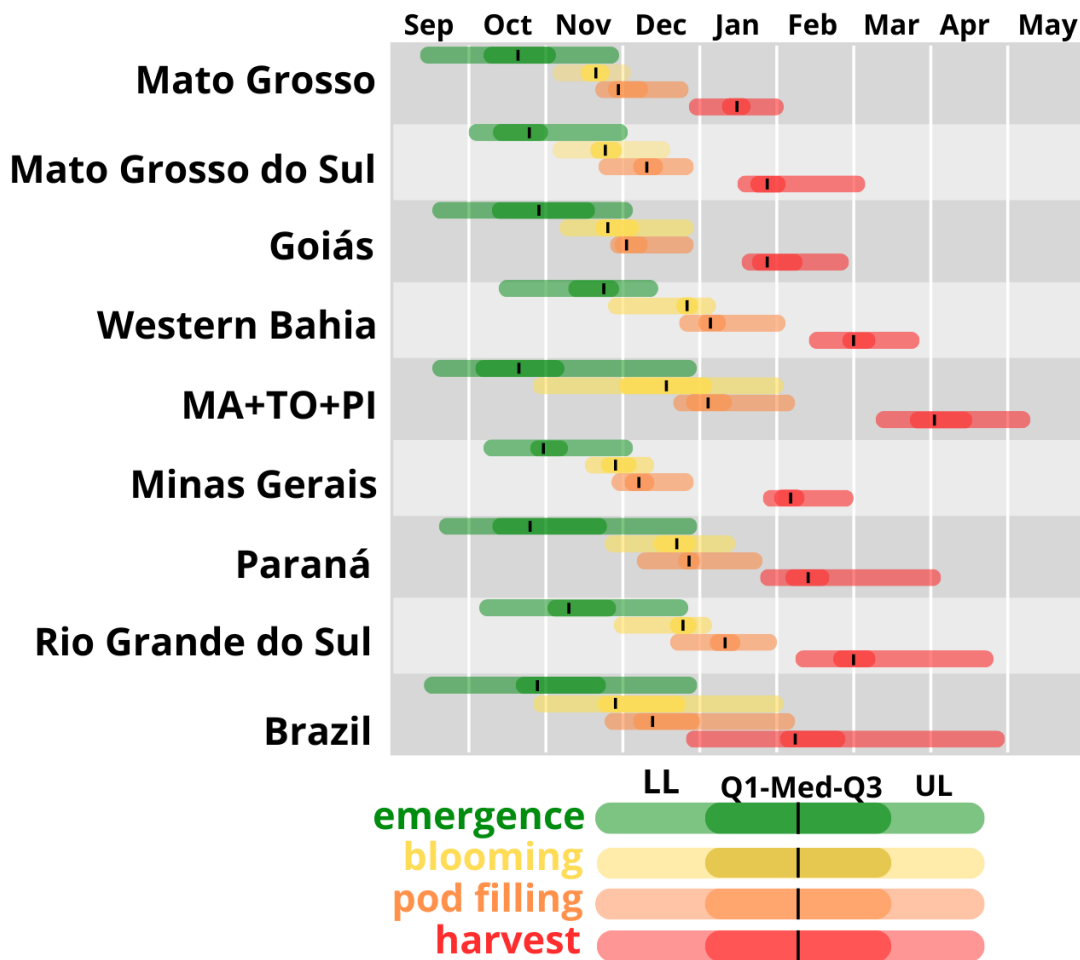


Figure 2.8. Soybean phenological calendar. LL = Lower Limit, Q1-Q3 = First Quartile to Third Quartile, UL = Upper Limit.

For most of the cultivated land (approximately 98%), sowing occurs within 1–11 days after the sanitary break. In Brazil, the sanitary break typically lasts between 60 and 90 days,

with average dates ranging from mid-June to mid-September, depending on the state. This variability reflects regional phytosanitary regulations designed to interrupt the soybean lifecycle and reduce the incidence of pests such as *Phakopsora pachyrhizi* (Asian soybean rust).

The median duration of the soybean growth cycle in Brazil spans 108 [± 9] days, encompassing the period from sowing to harvest. Southern states exhibit prolonged cycles, notably Paraná with a duration of 116 [± 12] days and Rio Grande do Sul with a cycle lasting 120 [± 7] days. In contrast, the Central-West states manifest shorter growth cycles, with Mato Grosso and Mato Grosso do Sul both registering at 100 [± 20] days, and Goiás presenting a cycle of 97 [± 10] days.

A discernible west–east and north–south gradient in soybean sowing dates was detected in the study region (Figure 1.9). In Mato Grosso, sowing typically began around October 11th [± 11 days], reflecting the earliest regional start. In contrast, the last states to begin sowing were Rio Grande do Sul (October 31st [± 12 days]) and Western Bahia (October 30th [± 7 days]). It is important to note that planting large farms usually takes 2–3 weeks, so these dates represent regional averages or the start of sowing windows. In approximately 20% of the pixels, it was impossible to recover all phenological stages due to several factors: 1) large temporal variability; 2) subpixel cloud contamination; and 3) errors in the phenological retrieval models.

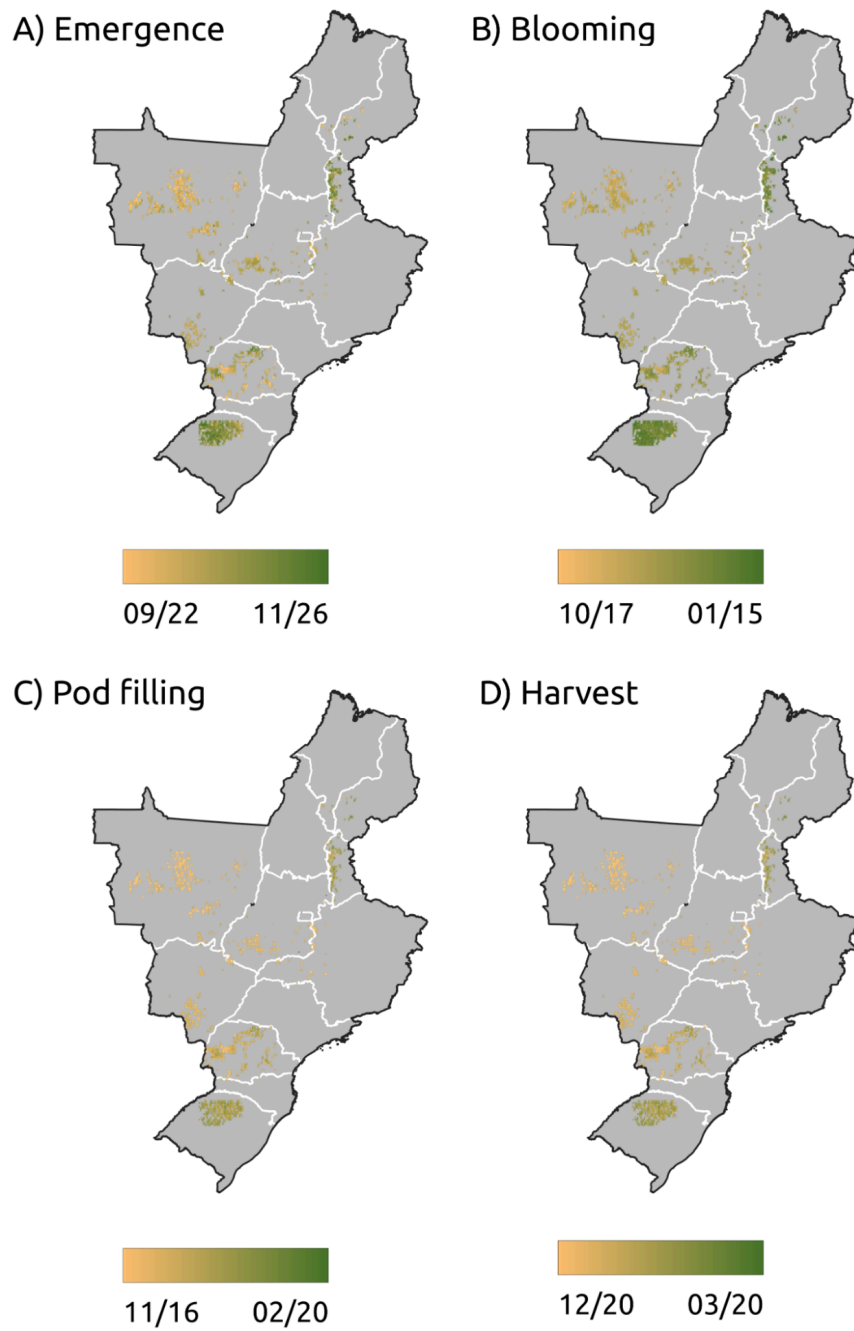


Figure 2.9. Spatial distribution of the average dates that soybean reached each phenology phase (A) emergence, (B) blooming, (C) pod filling, and (D) harvest.

Figure 1.10 shows the distribution of soybean planted area (in hectares) across Brazil's main producing states between September and December. The graphs (Figure 1.10) reveal marked differences in planting calendars among regions. In Mato Grosso (A), the planting profile is highly defined and concentrated, with a sharp peak in October surpassing 100,000 hectares per day. This pattern indicates strong synchronization of planting operations to exploit the onset of seasonal rains and ensure the viability of the second crop (safrinha). Such intense concentration imposes high technological demands: meeting this daily planting capacity would require thousands of machines operating in sync. On peak days, the state would need approximately 10,000–20,000 small planters (~2–4 ha/h/machine), 5,000–10,000 medium (~4–7 ha/h/machine), or 3,000–5,000 large planters (~8–12 ha/h/machine). This exemplifies the level of mechanization and logistical coordination required in the region, with MT operating between 3,000 and 20,000 machines simultaneously.

Mato Grosso do Sul (B) and Goiás (C) also exhibit October planting peaks but with smaller planted areas and a slightly wider distribution, indicating a longer planting window. Nevertheless, the figures are substantial: in MS, a peak around 50,000 hectares/day would demand between ~1,500 and 10,000 planters daily. In GO, with a peak of approximately 30,000 hectares/day, between ~1,000 and 6,000 machines would be needed per day. These estimates highlight the importance of having modern, high-capacity machinery and well-planned mechanized operations to ensure planting occurs within the ideal climatic window.

Minas Gerais (D) shows lower values, with a modest peak in October, indicating smaller planted area and less intensive operations, which translates to lower peak machinery demand. In Western Bahia (E), planting is later, with the peak shifted to November. This delay

reflects local climatic characteristics, where the consistent onset of rains occurs later, requiring differentiated planning for acquiring and deploying agricultural machinery.

Southern states, Paraná (G) and Rio Grande do Sul (F), display distinct patterns with more prolonged planting windows. Rio Grande do Sul stands out with a high peak between November and December, while Paraná shows a more evenly distributed planting period between October and November. These patterns reflect the region's more varied climatic conditions and rainfall regimes, where a longer planting window partly reduces peak machinery demand but requires flexibility and continuous maintenance of equipment.

Finally, the Maranhão, Tocantins, and Piauí group (H) shows much lower total planted area and no clear peak of concentration, suggesting less intensive practices or greater temporal dispersion of planting operations, resulting in correspondingly lower demands on the machinery fleet.

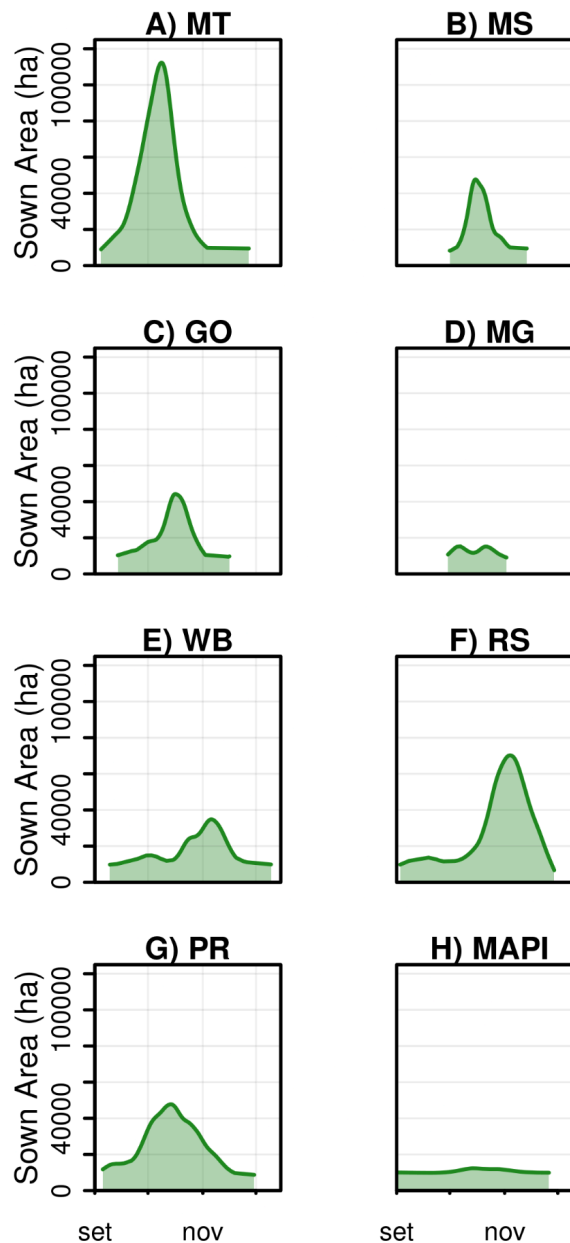


Figure 2.10. Monthly distribution of soybean sown area (ha) from September to December in Brazilian states. Density curves represent the area sown per month for each state or region: (A) Mato Grosso (MT), (B) Mato Grosso do Sul (MS), (C) Goiás (GO), (D) Minas Gerais (MG), (E) Western Bahia (WB), (F) Rio Grande do Sul (RS), (G) Paraná (PR), and (H) Maranhão, Tocantins, and Piauí (MAPI).

We evaluated the accuracy of state-level SIF-derived soybean phenological dates by comparing them with official data from CONAB (Table S2 and Figure S1). The results

demonstrate higher accuracy during early phenological stages in Mato Grosso (MT), Mato Grosso do Sul (MS), Goiás (GO), and western Bahia (BA). For the emergence stage (VE), the mean difference between SIF estimates and CONAB's calendar data was approximately 7 ± 4 days, and this discrepancy did not appear to depend on the total cultivated area in each state. In contrast, other states exhibited larger differences, occasionally exceeding 30 days. Moreover, there were insufficient CONAB records to validate the emergence stage in the southern states (Paraná [PR], Santa Catarina [SC], and Rio Grande do Sul [RS]) as well as in Maranhão, Tocantins, and Piauí (MA, TO, and PI).

Regarding the harvest stage (H), the average difference between SIF-derived dates and CONAB data was 13 ± 3 days. When the harvested area represented less than 20% of the total cultivated area (as observed in western BA), the discrepancy could reach up to 50 days. This substantial difference is likely attributable to the low or absent photosynthetic activity at harvest time, which limits the sensitivity of SIF to detect phenological transitions at the state scale. Additionally, the SIF-derived harvest dates exhibited a more linear and uniform temporal pattern compared to CONAB's field-based reports, suggesting that satellite-derived estimates may smooth out the inherent spatial and temporal variability of harvest operations. Notably, when the harvested area exceeded 50% of the total cultivated area, the agreement between SIF and CONAB improved substantially, with an average difference of 7 ± 5 days.

For intermediate phenological stages such as flowering (R2) and pod formation (R4), which are also included in CONAB's reporting, the average differences between SIF estimates and official data were 5 ± 1 and 4 ± 2 days, respectively. These results indicate that SIF time series can reliably characterize not only early and late stages, but also mid-season phenological transitions, supporting its potential as a complementary tool for large-scale crop monitoring.

The CONAB field data were compared with the phenological calendar derived from traditional vegetation indices (e.g., NDVI and EVI). We observed that the VNP 09GA and 22Q2 products are less accurate than SIF, with mean differences exceeding 15 days for sowing and 20 days for harvesting (Figure S2). In the MA+TO+PI region, the NDVI-VNP09GA showed higher accuracy (MD = 9 days) than SIF (MD = 26 days), possibly due to the VIIRS spatial resolution of 500 m, which reduces interference.

We also computed SIF data at the municipal level and compared them with the ACRZ database (Figure S1), which considers only sowing dates. The average difference between the calendars was 8 ± 2 days, with 60% of soybean-producing municipalities exhibiting a variation of less than 10 days. Notably, WB (100% of municipalities), MT (71% of municipalities), GO (62.5% of municipalities), and MS (58% of municipalities) showed differences of less than 10 days (Figure S1). Municipalities with the highest degree of agreement between data from the SIF and ACRZ calendar have pixels displaying $AF > 80\%$ and high soybean production. The Central-Eastern region of MT exhibited the smallest difference, with an average of 4 days.

Comparisons between SIF-scale and high-resolution images (Planet, Sentinel-2, and CBERS-4A) demonstrate that errors between sowing dates derived from SIF data and the ACRZ calendar are smaller when the fraction of soybean area (AF, calculated from MapBiomas as described in Section 2.2) within the TROPOMI pixel is higher. At the Brazilian level, the average difference between SIF and high-resolution-derived sowing dates was six days when $AF > 80\%$. Conversely, when AF was between 50% and 60%, the average difference increased to 14 days (outliers excluded, Table 2). The states with the poorest performance were MA+TO+PI and Minas Gerais, regardless of AF. High-resolution imagery was used to identify sowing and harvest dates directly, providing the reference for comparison.

Table 1.2. Mean difference and standard deviation between emergence and [harvest] dates estimated from SIF data and those identified in high-resolution imagery (Planet, Sentinel-2, CBERS-4A). Results are stratified by the fraction of soybean area (AF) within the TROPOMI pixel, as calculated from MapBiomass (Section 2.2). High-resolution images provide the reference sowing and harvest dates for comparison.

States	50%<AF<60%	60%<AF<70%	70%<AF<80%	80%<AF
Mato Grosso	11±7 [17±5]	7±2 [14±6]	7±2 [13±7]	5±1 [10±3]
Mato Grosso do Sul	10±7 [13±4]	9±2 [13±4]	8±5 [11±6]	7±3 [13±6]
Goiás	8±5 [18±5]	5±1 [12±4]	8±3 [9±10]	4±4 [9±8]
Western Bahia	7±3 [20±15]	6±3 [10±9]	6±4 [14±3]	1±5 [5±9]
MA+TO+PI	27±20 [—]	25±10 [20±12]	— [—]	12±8 [—]
Minas Gerais	18±12 [—]	14±9 [4±11]	12±9 [12±7]	— [—]
Rio Grande do Sul	16±9 [19±8]	11±5 [17±8]	9±6 [13±4]	6±3 [9±9]
Paraná	14±6 [22±11]	9±5 [18±9]	9±4 [7±4]	4±5 [8±1]

1.3.4. Crop yield forecast based on phenology

Figure 1.11 presents soybean yield forecasts generated from phenological and meteorological data at two distinct phenological stages. At the VE-R2 stage ($R^2 = 0.19$), the predictions exhibit high dispersion relative to the 1:1 line, with low explanatory power, reflecting the limitations of information available early in the crop cycle. In contrast, at the VE-R4 stage ($R^2 = 0.75$), the forecasts align much more consistently with observed values, demonstrating substantially higher accuracy as additional phenological data are incorporated.

The variation in the coefficients of determination across stages clearly illustrates the incremental value of phenological monitoring throughout the cycle: the low R^2 at VE-R2 indicates that early-season forecasts carry high uncertainty, which is critical for agricultural risk management since early decisions must account for this limitation. Conversely, the high R^2 at VE-R4 suggests that continuous monitoring reduces uncertainty and improves estimate precision, making it especially useful for logistical planning such as storage and marketing.

Moreover, the distribution patterns shown in the plots highlight this difference in performance. In VE-R2, the color distribution is fragmented and scattered, signaling low overall model robustness at this initial stage. In VE-R4, there is a dense concentration along the 1:1 diagonal, indicating that the model can reliably capture even regional variations in yield with greater confidence.

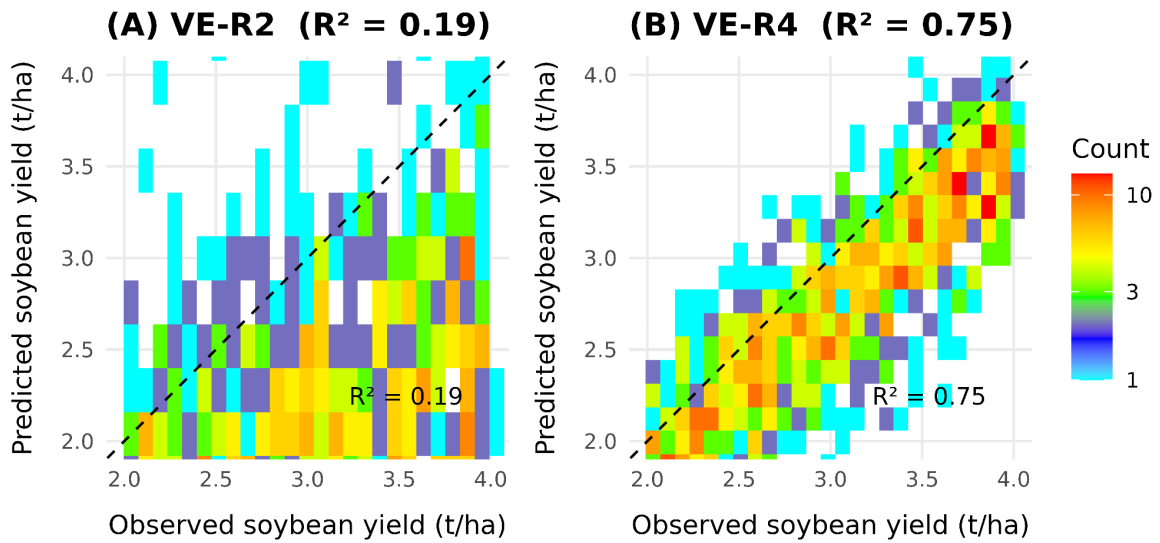


Figure 2.11. Model performance for predicting soybean yield using phenological and meteorological variables. Predicted versus observed values (SIDRA/IBGE) for VE-R2 (A) and VE-R4 (B), with improved accuracy close to H.

2.4. Discussion

Solar-Induced Chlorophyll Fluorescence (SIF) represents a paradigm shift in agricultural monitoring, offering a direct and physiologically grounded measure of photosynthetic activity that fundamentally surpasses the limitations of traditional vegetation indices. While NDVI and EVI remain useful for general vegetation monitoring, their tendency to saturate under high biomass, their sensitivity to canopy structure and soil background, and their poor performance in reproductive phases have long constrained their utility for intensive, large-scale agriculture. In contrast, our results show that SIF provides not only unprecedented accuracy in detecting phenological transitions but also the ability to translate these transitions into operational insights with direct value for Brazilian agriculture. By capturing the true dynamics of crop vigor and stress, SIF enables the construction of precise regional calendars,

the anticipation of yield potential, and the mapping of management intensity at a scale and resolution never before achieved. These qualities establish SIF as the most advanced and strategic tool currently available for understanding and managing crop systems in Brazil.

The clear detection of two distinct SIF peaks in Mato Grosso, Mato Grosso do Sul, and Goiás confirms the intensive adoption of double-cropping systems in these states (Brumatti et al., 2020; Pires et al., 2016). These regions benefit from an earlier and longer rainy season, enabling producers to carry out highly synchronized sowing in September and October, ensure harvest of the first crop cycle in January, and establish a second crop before the end of the rainy season (Zheng et al., 2019). This is reflected in our SIF curves for the first cycle, which show rapid green-up phases, evidencing deliberate management strategies — such as intensive mechanization (for example, in Mato Grosso, we estimated the number of agricultural machines required to vary daily from ~20,000 in the worst scenario to ~3,000 in the best scenario for sowing operations) and input use, to maximize initial vegetative development. Beyond a scientific finding, this quantification of sowing synchronization and machine demand offers practical insights for planning fleets, fuel supply, labor allocation, and logistical chains in one of the world's largest agricultural frontiers.

In contrast, regions such as Western Bahia and the Maranhão-Tocantins-Piauí (MA+TO+PI) cluster showed single, flatter SIF peaks with more distributed planting periods over time. This indicates systems less favorable to second-crop cultivation, with the use of long-cycle cultivars to maximize yield in a single harvest. The irregular and later onset of rains, combined with the early end of the wet season, restricts the viability of second cropping in these areas (Brumatti et al., 2020; Pires et al., 2016). These climatic limitations demand differentiated management strategies and highlight regional disparities in the potential for agricultural intensification. Such spatial differences are also evident in our results showing an

east–west gradient of up to 13 days in sowing dates across Western Bahia (Fonseca et al., 2022), underscoring the need for locally adapted planting calendars and cultivar selection.

It is also important to emphasize the marked interannual variability captured by the SIF time series, which is strongly linked to climatic anomalies. The sharp reduction in SIF values observed in Southern Brazil (Rio Grande do Sul and Paraná) during the 2021/2022 season aligns with the severe drought conditions caused by the La Niña phenomenon (Santos & Lima, 2020; Zheng et al., 2019). These events led to dramatic yield losses exceeding 70% in some areas (CNA, 2022; Unioeste, 2022), underlining soybean’s high sensitivity to rainfall variability. ENSO cycles influence not only total rainfall amounts but also their temporal distribution, altering the planting window and the duration of the phenological cycle (Zheng et al., 2019). The interannual shifts we identified in the timing and amplitude of the green-up phase in the SIF curves reinforce the need for adaptive management strategies and risk mitigation, including the selection of more drought-tolerant cultivars and greater flexibility in planting schedules. Such information is directly applicable to Brazil’s Agroclimatic Risk Zoning (ZARC), where SIF can complement climate and soil-based models with physiological evidence of crop stress and yield losses.

Notably, this reduction is associated with the occurrence of a La Niña event characterized by a sea surface temperature anomaly in the Niño 3.4 region of approximately $\sim 1^{\circ}\text{C}$ during the productive period (CPC/NOAA). According to Hamed et al. (2023), sustained negative ENSO anomalies of about -1.5 standard deviations (SD) tend to lead to reductions of approximately -0.4 SD in soybean production. Although the anomaly observed in 2021/2022 was somewhat more moderate, the recorded decline in production (about -0.3 SD, considering the region's historical variability of 15 Mt with peaks of 20 Mt) remains consistent with this relationship pattern.

The superior capacity of SIF compared to traditional vegetation indices (NDVI, EVI) to capture these phenological transitions is evident in our results, where SIF-derived dates showed better agreement with CONAB, ACRZ, and high-resolution imagery data across different phenological stages. Unlike VIs, which saturate at high biomass levels and can be confounded by soil background and canopy reflectance (Huete et al., 2002; Zhang et al., 2023), SIF directly traces photosynthetic activity, enabling more reliable detection of the onset, peak, and end of the growing season (Köhler et al., 2018). This advantage is particularly relevant for reproductive stages, where vegetation indices often fail to capture dynamics accurately (Yang et al., 2022). Our results are consistent with Leng et al. (2022), who demonstrated SIF's ability to monitor drought-induced declines in photosynthesis in dryland ecosystems, reinforcing its utility in capturing stress-induced variations in soybean phenology.

Additionally, our analysis of yield forecasting models showed that incorporating phenological data significantly improves prediction accuracy as the season progresses, with an increase in R^2 from 0.19 at the VE–R2 stage to 0.75 at VE–R4. This result aligns with findings by Richetti et al. (2018), who showed that integrating phenological and climatic data enhances yield estimation models. Such improvements are crucial for logistical planning (storage, transportation, and marketing), credit allocation, and export strategies in highly mechanized, export-oriented systems such as those in Mato Grosso (Dias et al., 2016).

Despite these advantages, important limitations remain. The accuracy of phenological estimates derived from SIF depends on the fraction of soybean area within the satellite pixel (AF). We found higher errors in regions with low AF values, such as MA+TO+PI and parts of Minas Gerais, reflecting challenges posed by mixed-pixel effects and landscape heterogeneity (Fonseca et al., 2022; Chen et al., 2018). Additionally, cloud contamination during critical

phases and the moderate spatial resolution ($\sim 7 \times 3.5$ km) of TROPOMI limit field-scale precision. Future missions such as ESA's FLEX satellite, with ~ 300 m resolution (Köhler et al., 2018), promise to overcome these limitations, enabling operational monitoring at sub-municipal or even field levels.

In light of these findings, integrating SIF data with traditional vegetation indices, high-resolution imagery, and field observations represents a robust pathway for operational phenological monitoring. Multi-source approaches can support precision agriculture, inform agroclimatic zoning, anticipate mechanization peaks, and underpin adaptation strategies for climate change. Given the projected increase in rainfall variability and the occurrence of extreme events in the context of climate change (Rattis et al., 2021), building more resilient agricultural systems will require not only improved monitoring but also targeted investments in irrigation, mechanization, and the development of cultivars adapted to local conditions.

These advantages make SIF not only a scientific breakthrough but also a strategic variable for agricultural management in Brazil, with transformative potential for both research and practice. By generating robust, regionalized calendars and linking them to yield forecasts, SIF bridges the gap between physiological crop monitoring and the operational demands of a global agricultural powerhouse. Specifically, SIF can support:

- **Government planning and policy:** strengthening the Agroclimatic Risk Zoning (ZARC) with physiological indicators, improving national food security monitoring, and providing scientific evidence for climate adaptation policies. This contributes directly to risk management frameworks, insurance programs, and long-term strategies for sustainable intensification.

- **Farm-level decision-making:** guiding cultivar choice according to regional sowing windows, supporting the timing of irrigation and pest management, and informing adaptive responses to climate anomalies such as delayed rainfall onset or prolonged droughts. The capacity to anticipate stress and phenological shifts enhances farmer resilience and profitability.
- **Agroindustry and export logistics:** allowing better anticipation of planting and harvest flows, which in turn informs storage infrastructure planning, transportation logistics, and contract negotiations in international markets. In highly synchronized production regions such as Mato Grosso, where planting peaks can exceed 100,000 hectares per day, SIF reveals the extraordinary mechanization requirements, directly informing machinery allocation, fuel supply, and labor management.
- **Financial and insurance sectors:** reducing uncertainty in yield forecasting and enabling more accurate assessment of credit and insurance risk. By incorporating real-time physiological indicators, SIF can enhance the transparency and reliability of crop monitoring systems, with implications for agricultural finance and investment.

Taken together, these applications underscore that SIF is not merely a novel remote-sensing metric but a decision-support variable capable of reshaping how Brazil manages its agricultural frontier under climate variability and global market pressures. Its integration into operational monitoring systems represents a step forward in aligning scientific innovation with the urgent needs of a sector that is simultaneously a driver of economic growth, food security, and climate vulnerability.

Future research should prioritize extending SIF time series, refining algorithms for cloud filtering and phenological extraction, and increasing field validation data collection across different Brazilian agroecological zones. Additionally, exploring the relationships among sowing dates, cultivar selection, cycle duration, and yield could further enhance the value of satellite-derived phenological monitoring in supporting the sustainable intensification of Brazil's soybean sector.

2.4. Conclusions

The findings of this study unequivocally demonstrate that Solar-Induced Chlorophyll Fluorescence (SIF) is not merely an incremental improvement over traditional vegetation indices but a fundamental leap forward in agricultural monitoring. By directly capturing photosynthetic activity, SIF delivers physiologically grounded and highly sensitive estimates of key soybean phenological events, overcoming the chronic limitations of indices that saturate at high biomass or fail during reproductive stages. This methodological advance translates into strategic value for one of the world's largest and most dynamic agricultural systems: Brazilian soybean cultivation.

Our results show that SIF not only reconstructs the full phenological cycle with unprecedented precision but also exposes the management strategies and regional contrasts that define Brazilian agriculture. The ability to detect synchronized sowing and double-cropping in the Center-West, quantify the extraordinary mechanization demands in Mato Grosso, and reveal vulnerabilities to climatic extremes such as La Niña-induced drought in the South confirms that SIF operates simultaneously as a scientific diagnostic and a management tool.

Moreover, when integrated with meteorological data and machine learning, SIF enables progressively accurate yield forecasts, with predictive capacity rising sharply as the season advances (R^2 from 0.19 to 0.75). This directly supports operational decisions at multiple scales: from government agencies designing risk zoning and food security strategies, to farmers optimizing cultivar choice, irrigation, and pest control, to agribusiness and exporters anticipating harvest flows, storage capacity, and logistical bottlenecks. Financial and insurance sectors also stand to benefit, as SIF provides a transparent, physiology-based metric to reduce uncertainty in risk assessment.

Taken together, these results establish SIF as a strategic decision-support variable, capable of reshaping how Brazil monitors, plans, and adapts its agricultural frontier under the pressures of climate variability and global market demand. While challenges remain — including mixed-pixel effects and the moderate spatial resolution of TROPOMI — the imminent arrival of next-generation missions such as ESA's FLEX will further enhance the spatial granularity of SIF monitoring, consolidating its role in operational systems.

In conclusion, SIF should be regarded not only as a novel scientific indicator but as a cornerstone of next-generation agricultural intelligence. By bridging physiological monitoring with practical applications, SIF paves the way for a more resilient, efficient, and adaptive agricultural sector in Brazil. Its integration into monitoring platforms represents a critical step toward sustainable intensification, ensuring that Brazil can continue to expand its global leadership in soybean production while confronting the escalating challenges of climate change.

CHAPTER 3. Quantification of CH₄, NO_x, and N₂O emissions from Brazilian livestock using top-down methods and TROPOMI satellite data

3.1. Introduction

The intensification of climate change represents a growing threat to environmental stability, food security, and human health on a global scale. Human activities have already raised the planet's temperature by approximately 1.1 °C above pre-industrial levels, and projections suggest that this threshold may be surpassed within the next two decades, even under moderate mitigation scenarios (IPCC, 2023). Greenhouse gases (GHGs) are the primary drivers of this warming, with carbon dioxide (CO₂), methane (CH₄), and nitrous oxide (N₂O) being the most significant in terms of radiative forcing (Friedlingstein et al., 2023; NOAA, 2024).

Among GHGs, methane warrants particular attention due to its high global warming potential (GWP = 27.2 over 100 years, IPCC AR6, 2021) and relatively short atmospheric lifetime (~12 years), making it a strategic target for short-term mitigation actions (Saunois et al., 2020; Ocko et al., 2021). Global CH₄ emissions are estimated to have reached 580 Tg/year in 2022, with approximately 40% originating from agriculture, notably from ruminant enteric fermentation and manure management (Jackson et al., 2020; Crippa et al., 2021; Tubiello et al., 2022).

The livestock sector plays a particularly critical role in GHG emissions in tropical countries such as Brazil, India, and Indonesia, which are characterized by large cattle herds and extensive pasturelands. In these contexts, emissions are exacerbated not only by herd size but also by the predominance of extensive and heterogeneous production systems, low productive efficiency, and limited technological intensification. Widespread pasture degradation, inadequate manure management, reliance on low-quality forage, and the limited adoption of mitigation strategies—such as strategic supplementation, genetic improvement,

and crop-livestock-forest integration—further intensify enteric and indirect emissions. In addition, significant spatial variability in emission rates reflects regional disparities in land use, technological adoption, and institutional capacity for implementing climate policies (Herrero et al., 2021; Tubiello et al., 2022; Thornton & Herrero, 2010).

Brazil occupies a central position in this debate. The country hosts the world's largest commercial cattle herd, with approximately 234.4 million head in 2024 (IBGE, 2025), predominantly raised in extensive systems on natural or cultivated pastures. According to SEEG (2024), livestock accounts for nearly 70% of national agricultural emissions and over 20% of the country's total gross emissions. Methane emissions from enteric fermentation alone exceed 26 Mt CH₄/year, potentially reaching up to 849 Mt CO₂eq/year when considering the variability estimated by atmospheric inversion techniques (this study; Maasakkers et al., 2022).

In addition to methane, agricultural systems emit substantial quantities of nitrogen oxides (NO_x = NO + NO₂), particularly from pasture soils subject to compaction, fertilization, and intense hydrological fluctuations (Butterbach-Bahl et al., 2013; Liu et al., 2021). Although short-lived in the atmosphere, NO_x contributes to ozone formation and is rapidly oxidized into soluble products such as nitric acid (HNO₃) and nitrate (NO₃⁻), which are deposited into soils. Atmospheric deposition of NO_x serves as an indirect source of N₂O, as the reactive nitrogen deposited can be microbially transformed through nitrification and denitrification processes—especially in clay-rich tropical soils experiencing wet-dry cycles (Reis et al., 2023; Zhang et al., 2024). Recent studies estimate global agricultural soil N₂O emissions at approximately 3.0 to 4.0 Mt N₂O/year, with a rising trend and Brazil among the top contributors in the developing world (Tian et al., 2020; Xu et al., 2023; Silva et al., 2024).

Historically, national GHG inventories have been developed using bottom-up methodologies, which rely on agricultural statistics combined with emission factors. However, such approaches often overlook spatial and seasonal heterogeneity, and are limited by uncertainties in input data, lack of local measurements, and low sensitivity to anomalous or localized changes. In contrast, top-down approaches based on atmospheric observations and inverse modeling have gained prominence, offering independent and spatially explicit estimates that help identify discrepancies and gaps in official inventories (Bergamaschi et al., 2018; Chevallier et al., 2022; Thompson et al., 2022).

In this context, satellite remote sensing has emerged as a transformative tool. Earlier missions such as SCIAMACHY (aboard Envisat), GOSAT (Greenhouse Gases Observing Satellite), and OCO-2 (Orbiting Carbon Observatory-2) significantly contributed to trace gas monitoring, albeit with limited spatial resolution ($\sim 10\text{--}100$ km) and less frequent coverage. The TROPospheric Monitoring Instrument (TROPOMI), aboard the Sentinel-5P satellite, represents a substantial advance, offering improved spatial resolution (up to 5.5×7 km), near-daily revisit frequency, and heightened sensitivity for detecting CH_4 , NO_2 , CO , and other pollutants at regional and subnational scales (Lorente et al., 2021; Hu et al., 2023). This capacity allows for more precise identification of emission hotspots and supports evidence-based policymaking. When integrated with atmospheric transport models such as GEOS-Chem, TROPOMI has proven essential for flux inversion applications and the assessment of underestimated sectoral emissions (Maasakkers et al., 2019; Varon et al., 2022; Scarpelli et al., 2022).

Given this scenario, there is growing consensus in the literature regarding the need to incorporate satellite atmospheric observations and inverse modeling techniques into national inventories to enhance accuracy, spatial resolution, and transparency. The convergence of remote sensing, atmospheric modeling, and agronomic expertise is now regarded as a key

frontier in advancing climate policy within the agricultural sector (Butterbach-Bahl et al., 2023; IPCC, 2023; Ogle et al., 2022). In this context, this study aims to quantify CH₄, NO_x, and N₂O emissions associated with Brazilian agriculture, with an emphasis on assessing potential differences between low and high productivity pasturelands, as well as to compare these top-down estimates with bottom-up national inventories (e.g., the Brazilian National GHG Inventory and the SEEG) to assess potential biases and discrepancies.

3.2. Material and methods

3.2.1. Study area

Cattle ranching represents the primary activity within Brazil's agribusiness sector. In 2024, the national cattle herd reached a historic milestone of 234.4 million head, reflecting a 4.3% increase compared to the previous year (IBGE, 2025). The geographical distribution of the herd reveals significant regional disparities. The Central-West region stands out as the main cattle-producing area, hosting 77.2 million head (32.9% of the national total), supported by extensive pasturelands and favorable edaphoclimatic conditions (IBGE, 2025). The Northern region follows, with 60.6 million head (25.9%), particularly in the state of Pará, which holds the second-largest cattle herd in the country. The Southeast (38.9 million), Northeast (33.2 million), and South (24.3 million) regions complete the national landscape, each characterized by distinct production systems. At the state level, Mato Grosso leads with 34.2 million head, followed by Pará (24.7 million) and Goiás (24.4 million), while Minas Gerais is notable for its contributions to both beef and dairy production (IBGE, 2025).

A critical component underlying the productivity and sustainability of cattle ranching in Brazil is the quality of pasturelands. Pastures occupy more than 150 million hectares of the national territory, constituting the largest land use category in the country (MapBiomass,

2023). However, a significant portion of these areas exhibits signs of degradation. According to MapBiomas data, approximately 56% of Brazilian pastures present some degree of degradation, ranging from moderate to severe, with the most affected regions being the Amazon and Cerrado biomes. These degraded pastures compromise forage availability, reduce animal performance, and exert pressure for the expansion of new grazing areas, often at the expense of native vegetation.

In contrast, areas with well-managed pastures, particularly those incorporating rotational grazing, integrated crop-livestock-forest systems (ILPF), or improved forage species, demonstrate higher productivity and resilience. The implementation of sustainable intensification practices has shown potential to recover degraded lands and increase carrying capacity without further land conversion. Notably, states like Mato Grosso do Sul, Minas Gerais, and Paraná have been at the forefront of adopting such practices, leading to improvements in both animal productivity and environmental performance (MapBiomas, 2023; Embrapa, 2022).

Regarding dairy cattle farming, Brazil produced approximately 34.6 billion liters of milk in 2022, representing a 1.6% decline relative to the previous year. This decrease is primarily attributed to rising production costs, which disproportionately affect small-scale producers. The regional distribution of milk production shows a relatively balanced share between the South (33.8%) and Southeast (33.6%), while the Northeast has expanded its participation, accounting for 16.5% of national output. Minas Gerais remains the leading milk-producing state, responsible for 27.1% of total national production.

3.2.2. TROPOMI instrument applied to the detection and quantification of atmospheric gases

The TROPOspheric Monitoring Instrument (TROPOMI) is a Differential Optical Absorption Spectrometer (DOAS) onboard the Sentinel-5 Precursor (S5P) satellite, launched by the European Space Agency (ESA). Operating at an altitude of 824 km in a near-polar, sun-synchronous orbit with equatorial overpass at approximately 13:30 local solar time, the satellite completes a 17-day repeat cycle (227 orbits). TROPOMI features a ground footprint of 7 km along track and a swath width that varies from 3.5 km at nadir to 15 km at the edge of the swath. Its wide swath (~2,600 km) enables near-daily global coverage, with full coverage above $\pm 7^\circ$ latitude and over 95% coverage in other regions.

TROPOMI is designed for the monitoring of various atmospheric constituents, including carbon monoxide (CO), methane (CH₄), ozone (O₃), nitrogen dioxide (NO₂), and sulfur dioxide (SO₂), as well as for the retrieval of aerosol and cloud properties. The instrument includes four spectrometers covering the ultraviolet to shortwave infrared regions (UV-VIS: 270–495 nm; NIR: 675–775 nm; SWIR: 2305–2385 nm). Methane column concentrations are retrieved using the 2.3 μm absorption band (SWIR), with a spatial resolution of 5.5×7 km (improved from the previous 7×7 km until August 2019), allowing for global daily coverage.

Data processing is carried out by the Netherlands Institute for Space Research (SRON) using the RemoTeC retrieval algorithm, which also estimates surface reflectance, atmospheric scattering, and additional parameters such as surface pressure, vertical CH₄ profiles, retrieval quality, and albedo in the NIR and SWIR bands. The data are made publicly available on the Amazon Web Services (AWS) cloud with a short latency. The operational data series began in May 2018 with Version 1 and transitioned to Version 2 in July 2021. Comparisons with 19 stations from the TCCON network reported a global mean bias of -2.7 ppb in Version 1.3.0,

which was reduced to 5.6 ppb in Version 2.2.0; within the ± 10 ppb threshold considered suitable for regional inversion applications. To ensure data quality, only land pixels with a quality assurance value ≥ 0.5 are used, excluding observations with SWIR albedo < 0.05 or total albedo > 0.85 .

3.2.3. Analytical inversion

To estimate methane emissions from observations made by the TROPOMI sensor, we employed the Integrated Methane Inversion model (IMI v1.0), operating on cloud computing infrastructure via Amazon Web Services (AWS) with an EC2 c5.9xlarge instance with 36 CPUs, 128 GB of RAM and 10 TB of EBS/S3 storage. The IMI model is an analytical inversion framework based on GEOS-Chem, a three-dimensional chemical transport model (CTM), which functions as the forward model in the inversion process. This model simulates the atmospheric distribution of methane based on prescribed emissions, accounting for the physical and chemical processes that govern the transport and transformation of the gas in the atmosphere. By comparing the simulated methane fields with column-averaged methane concentrations retrieved from TROPOMI, we derived methane emissions using Bayesian inversion techniques.

The GEOS-Chem model, as described by Bey et al. (2001), is driven by meteorological fields from the Goddard Earth Observing System (GEOS), provided by NASA's Global Modeling and Assimilation Office (GMAO). These datasets integrate satellite and ground-based observations with numerical modeling to provide a comprehensive and up-to-date representation of the atmospheric state. In this study, we used the GEOS-FP product, which features 72 vertical levels (aggregated to 47 levels for computational compatibility) and a horizontal resolution of $0.25^\circ \times 0.3125^\circ$.

For the boundary conditions, the Brazilian territory was subdivided into 20 scenes, each representing spatial emission blocks to be optimized during the inversion process. This spatial discretization was implemented to reduce computational demands. A 5-degree buffer was applied to each scene to adequately capture boundary conditions and account for atmospheric transport across adjacent regions. Finally, the scenes were merged into a single domain, with edge data filtered to smooth the transitions and minimize boundary artifacts.

The forward simulation using the GEOS-Chem model is combined with TROPOMI observations through a Bayesian inverse analysis to infer methane emissions. This process involves assigning weights to prior estimates and their associated uncertainties, assuming a probability density function with normally distributed error, and minimizing a scalar cost function (Eq. 1).

$$J(x) = (x - x_A)^T S_A^{-1} (x - x_A) + \gamma (y - Kx)^T S_O^{-1} (y - Kx) \quad \text{Eq. 3.1}$$

In this cost function, x represents the vector of emissions to be estimated, while x_a corresponds to the *a priori* emissions derived from emission inventories. The Jacobian matrix (K_x) describes the sensitivity of column-averaged methane concentrations (XCH_4), as observed by the TROPOMI sensor (y), to variations in emissions, as simulated by the GEOS-Chem model. The observational error covariance matrix for TROPOMI (S_o) was assumed to be 15 ppb, based on the default values provided by the IMI. The matrix S_a represents the covariance associated with uncertainties in the *a priori* emissions, and γ is the regularization factor.

To incorporate uncertainties in the inversion parameters, a grid search was performed over different ranges for S_a and γ , including recommended values from IMI and previous

studies. Based on this analysis, an ensemble inversion was conducted using various parameter combinations, and the resulting mean values were used to estimate the final emissions.

Through the analytical solution of Equation 2, we obtained the optimal a posteriori estimate, as well as the associated error covariance matrix (Equation 3) and the averaging kernel matrix (Equation 4) for each ensemble member. The sensitivity of the estimate to the true values is described by the averaging kernel matrix, whose trace represents the degrees of freedom for the estimate.

$$\hat{x} = x_A + (\gamma K^T S_O^{-1} K + S_A^{-1})^{-1} \gamma K^T S_O^{-1} (y - K x_A) \quad \text{Eq. 3.2}$$

$$\hat{S} = (\gamma K^T S_O^{-1} K + S_A^{-1})^{-1} \quad \text{Eq. 3.3}$$

$$A = I_n - \hat{S} S_A^{-1} \quad \text{Eq. 3.4}$$

The posterior state vector is obtained by the analytical solution in Eq. (2). In this Gaussian Bayesian (Gauss–Markov) formulation, x is the emission state vector to be inferred and $\hat{x}$ is its posterior estimate; x_a is the prior (a priori) state; y is the observation vector (e.g., satellite retrievals); and K is the Jacobian (sensitivity) matrix whose element K_{ij} gives the change in observation y per unit change in state element x_i (i.e., $\partial y / \partial x_i$). The matrices S_o and S_a are the error covariance matrices for observation and prior errors, respectively; they weight the relative trust placed in data versus prior knowledge, including error correlations if

specified. Some applications include a scalar tuning parameter γ that rescales either S_o or S_a to explore the effect of assumed errors; such regularization choices can be probed systematically with an inversion ensemble. The posterior error covariance (Eq. 3) then provides a closed-form quantification of uncertainty in $\hat{x}$. Misspecification in the cost-function setup (e.g., error variances, assumed correlations, representativeness, or sampling) can be evaluated by varying γ , the prior emissions, and the subset/weighting of observations and examining the spread of resulting posteriors. Information content is summarized by the averaging kernel matrix in Eq. (4), A , which describes how changes in the true state map into changes in the posterior estimate; here I_n is the $n \times n$ identity matrix and $tr(A)$ is the degrees of freedom for signal (DOFS), i.e., the number of independent pieces of information supplied by the observations about the state vector. The diagonal elements of A (“averaging kernel sensitivities”) indicate, for each grid cell or state element, the fraction of the posterior driven by observations rather than the prior: values near 0 imply the posterior reverts to the prior, whereas values near 1 indicate strong observational constraint largely independent of the prior. In practice, we implement the matrix operations in Eqs. (2)–(4) with sparse linear algebra, making the optimization inexpensive relative to constructing K .

3.2.4. Prior Emissions

The *bottom-up* emissions used as prior information in this study are shown in Figure 2.1. For all years analyzed, we adopted fossil fuel emissions (oil, gas, and coal) for the year 2018 based on the Global Fuel Exploitation Inventory v2 (GFEI; Scarpelli et al., 2022). Other anthropogenic emissions ; primarily related to livestock and waste management ; were obtained from the EDGAR v6 database, also for 2018 (Monforti Ferrario et al., 2021). Natural emissions from wetlands were extracted from the WetCHARTs v1.2.1 model (Bloom et al.,

2017). Additionally, we incorporated emissions from termites and geological seepage (Varon et al., 2022), as well as biomass burning emissions from the GFED v4 dataset (Randerson et al., 2018).

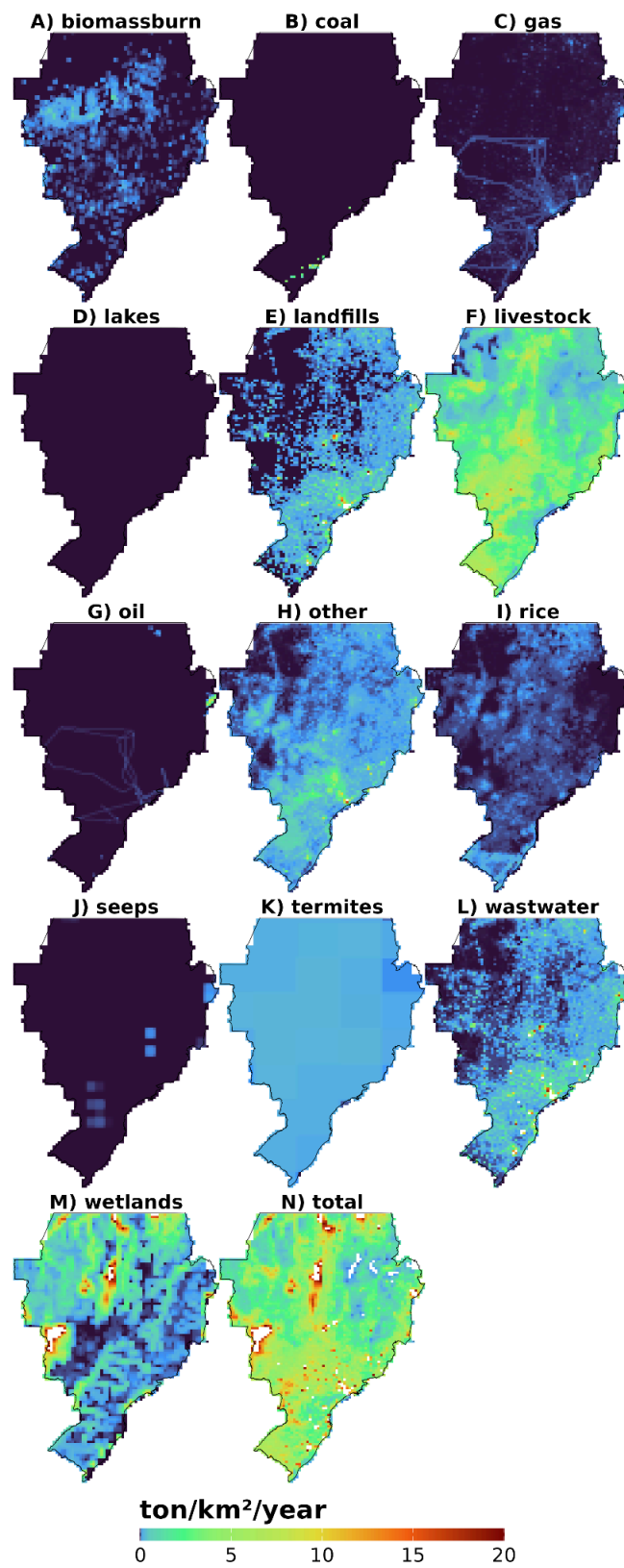


Figure 3.1. Prior Emissions Estimates

To perform the inversion using TROPOMI data, we aggregated the observations to a moderate spatial resolution, aiming to reduce the influence of small-scale transport errors (Maasakkers et al., 2022). We estimated observational errors to range between 15 and 19 ppb, based on the standard deviation of the mismatch between the prior model and the observations.

To assess the sensitivity of the inversions and to quantify associated uncertainties, we built an ensemble of simulations varying model inputs, assumptions, and configurations. This ensemble included:

- A. Uniform scaling of the prior emissions by 50%, 100%, 150%, 200%, and 250%;
- B. Aggregation of observations at spatial resolutions of 0.1° , 0.2° , and 0.5° ;
- C. Application of an optimal regularization factor $\gamma = 0.25$, obtained via L-curve analysis (Hansen, 2000), along with sensitivity tests using $\gamma = 0.1$ and $\gamma = 0.5$;
- D. Consideration of both normal and log-normal error distributions (Maasakkers et al., 2019);
- E. Use of different TROPOMI filtering strategies, including filtering by $Q_a = 1$;
- F. Optimization of boundary conditions on both monthly and annual bases;
- G. Analyses with and without the application of the standard SWIR-surface albedo correction to TROPOMI data;
- H. Assumption that aggregated observational errors follow either the Central Limit Theorem or remain constant with the number of aggregated observations.

3.2.5. NO_x emissions estimates

Nitrogen oxide (NO_x = NO + NO₂) emissions from pasture soils were quantified through the integration of satellite observations and atmospheric modeling. The study utilized data from the TROPOMI sensor, specifically tropospheric column densities of nitrogen dioxide (NO₂). Daily observations were filtered to include only pixels with a quality flag (*flag_value*) of ≥ 0.75 , thereby excluding measurements affected by clouds or low data quality. Only days with at least 30 valid pixels and a minimum spatial coverage of 25% within the region of interest were retained for analysis.

Soil moisture data were obtained from the SMAP (*Soil Moisture Active Passive*) satellite, which provides high-temporal-resolution measurements of volumetric soil moisture (VSM) in the top ~5 cm of the soil. To ensure measurements corresponded to exposed soil surfaces, pixels with vegetation water content exceeding 5 kg/m² were excluded.

Daily meteorological variables, including wind speed and direction, were extracted from the ERA5 reanalysis (ECMWF), corresponding to the TROPOMI overpass time. Precipitation data were sourced from the CHIRPS dataset. Anthropogenic NO_x emissions were derived from the EDGAR (Emissions Database for Global Atmospheric Research) inventory.

3.2.6. Estimation of NO₂ Enhancement

To isolate the signal associated with soil emissions, we estimated NO₂ enhancement as the difference between the mean NO₂ concentrations over pasture areas and those over

adjacent upwind regions that are predominantly natural or forested, according to the prevailing wind direction. We excluded days with winds primarily originating from urban or industrial centers from the analysis.

3.2.2.3.2. Box Model for Emission Estimation

We applied a box model as a simplified approach to estimate the NO_x emission rate from soil (in this case, pasturelands) using satellite-derived observations. This model treats the area of interest as an atmospheric “box” in which emissions accumulate and are balanced by inflows, outflows, and chemical losses of the compound.

$$E_{soil} = \frac{U \cdot \Delta NO_2}{L} + V_d \cdot \frac{NO_2}{Z_{PBL}} + \frac{NO_2}{\tau} - E_{EDGAR} \quad \text{Eq. 5}$$

Where:

- U is the average wind speed (m.s^{-1});
- ΔNO_2 is the enhancement of the NO₂ column (molecules.m^{-2});
- L is the distance between the pasture and reference domains (m);
- V_d is the deposition velocity of NO₂ (m.s^{-1});
- Z_{PBL} is the height of the planetary boundary layer (m);
- τ is the NO_x lifetime, assumed to vary throughout the year (minimum of 3 to 7 hours in summer and maximum of 15 hours in winter);
- E_{EDGAR} represents anthropogenic NO_x emissions according to the EDGAR inventory.

3.2.7. Estimating Indirect N₂O Emissions Derived from Atmospheric Deposition of NO_x in Pasturelands Used for Livestock Production

Nitrogen oxides (NO_x), comprising nitric oxide (NO) and nitrogen dioxide (NO₂), are short-lived atmospheric pollutants that, upon emission, undergo oxidation and transformation into soluble species such as nitric acid (HNO₃), nitrate (NO₃⁻), and nitrite (NO₂⁻). These reactive nitrogen compounds can be removed from the atmosphere through wet deposition (precipitation) or dry deposition, contributing to the accumulation of reactive nitrogen in soils.

Once deposited in the soil, this nitrogen may be microbially converted into nitrous oxide (N₂O) via nitrification and denitrification pathways. According to the Intergovernmental Panel on Climate Change (IPCC) guidelines, these emissions are classified as indirect sources of N₂O, as they result from nitrogen initially released into the atmosphere in a different form.

To estimate the nitrogen load associated with NO_x emissions, we apply a conversion factor that reflects the proportion of nitrogen's molar mass relative to the average molar mass of nitrogen oxides (primarily NO and NO₂). This approach enables us to quantify the contribution of atmospheric NO_x deposition to soil nitrogen inputs and, subsequently, to indirect N₂O emissions from pasture-based livestock systems.

$$N(t) = \text{NO}_x(t) \times \text{Conversion Factor for N} \quad \text{Eq. 3.6}$$

We adopt a standard conversion factor of 0.304 kg N per kg of NO_x emitted, based on the average molar mass of nitrogen oxides (primarily NO and NO₂). This factor allows us to estimate the amount of reactive nitrogen associated with NO_x emissions that could potentially be deposited onto terrestrial ecosystems.

However, not all emitted NO_x is deposited onto soils. A significant portion remains in the atmosphere, where it may be further transformed into other compounds or transported across regions before deposition occurs. To account for this, we apply a deposition fraction (*fd*) that reflects the proportion of emitted NO_x expected to be deposited locally or regionally.

As recommended by the IPCC Tier 1 methodology, we base our choice of *fd* on available literature and global default values, acknowledging the uncertainties inherent in atmospheric transport and chemical transformation processes. This approach ensures that our estimates of indirect N₂O emissions remain conservative and scientifically grounded.

$$N_{\text{deposited}}(t) = N_{\text{total emitted}}(t) \times fd \quad \text{Eq. 3.6}$$

A portion of the nitrogen deposited onto soils is microbially converted into nitrous oxide (N₂O) through biogeochemical processes such as nitrification and denitrification. To quantify this conversion, we apply a specific emission factor that represents the fraction of deposited nitrogen ultimately emitted as N₂O–N.

This deposition-to-emission factor, defined in the IPCC guidelines as EF_{5(g)}, accounts for the proportion of atmospherically deposited nitrogen that is transformed into N₂O–N under typical soil conditions. By incorporating EF_{5(g)} into our calculations, we are able to estimate the indirect N₂O emissions resulting from NO_x deposition in pasture ecosystems.

This approach provides a standardized and conservative framework to assess indirect greenhouse gas emissions, ensuring consistency with international reporting protocols.

$$N_2O-N(t) = N_{\text{deposited}}(t) \times EF5g \quad \text{Eq. 3.7}$$

Finally, we convert the estimated amount of nitrogen in nitrous oxide form ($\text{N}_2\text{O-N}$) into the corresponding mass of N_2O . This step is essential to express emissions in terms of the actual greenhouse gas emitted, as required for standardized reporting and comparison with global inventories.

To perform this conversion, we apply a molecular weight ratio between N_2O and nitrogen (N). Specifically, since the molecular weight of N_2O is 44 g/mol and that of N (in N_2O) is 28 g/mol, we multiply the amount of $\text{N}_2\text{O-N}$ by a factor of $44/28 \approx 1.571$.

This conversion allows us to present our final estimates of indirect N_2O emissions from NO_x deposition in terms that are directly compatible with international climate reporting standards, such as those established by the IPCC.

$$\text{N}_2\text{O}(t) = \text{N}_2\text{O-N}(t) \times \frac{M_{\text{N}_2\text{O}}}{M_{\text{N}}} = \text{N}_2\text{O-N}(t) \times \frac{44}{28} \quad \text{Eq. 3.8}$$

3.3. Results

The results obtained reveal substantial discrepancies among the different methane emission estimation approaches, with particular emphasis on a systematic underestimation in the *a priori* inventories (Figure 2.2.). The aggregated *a posteriori* emission estimate for the analyzed states amounts to approximately 17.5 Mt CH_4 /year, with an uncertainty range between 15.2 and 23.2 Mt CH_4 /year, reflecting the variability associated with the atmospheric inversion process.

In the state of Mato Grosso (MT), for instance, emissions corrected through inversion reach approximately 3.8 Mt CH_4 /year (ranging from 3.1 to 4.5 Mt CH_4 /year), whereas the *a priori* inventories and SEEG estimates report values of 2.1 Mt and 2.4 Mt CH_4 /year, respectively ; representing an increase of about 80% compared to the initial estimates.

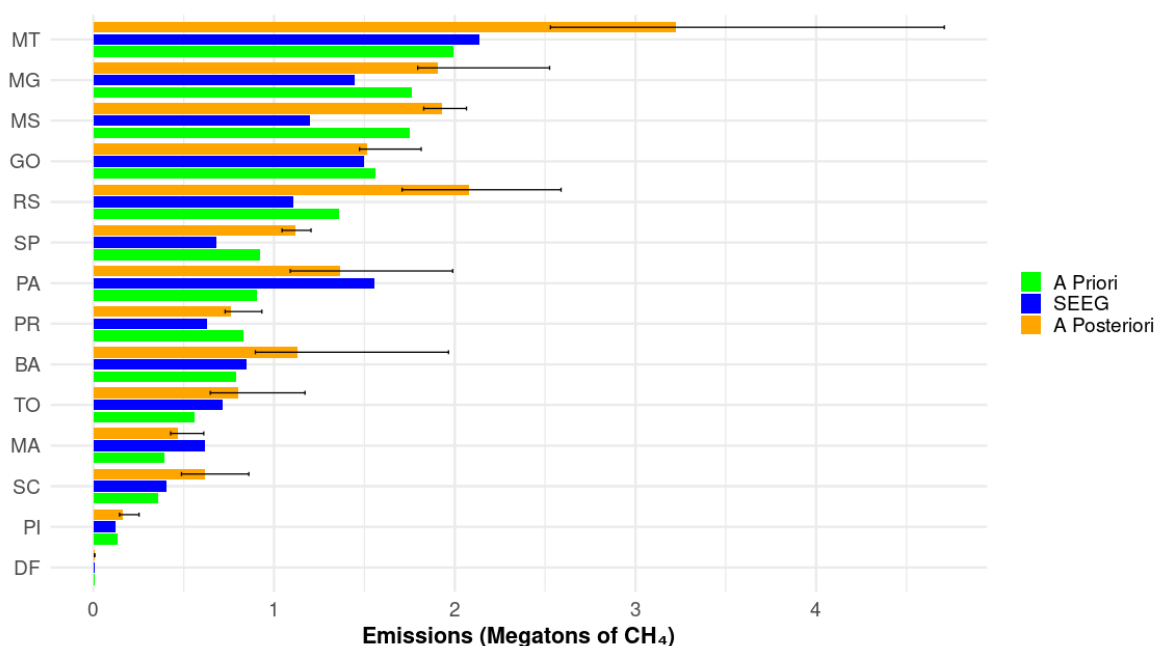


Figure 3.2. Comparison of Methane (CH₄) Emission Estimates by Brazilian State: A Priori Inventories, SEEG, and Atmospheric Inversion Adjustments (A Posteriori).

Figure 2.2A illustrates the spatial distribution of scale factors, which represent the degree of adjustment required for the a priori simulated fluxes to align with atmospheric concentrations observed by the TROPOMI sensor. The highest values (>2.5) are concentrated in the northwestern region of Mato Grosso and southern Santa Catarina, suggesting that actual emissions in these areas may be more than twice the initially estimated values. The presence of these hotspots underscores the limitations of traditional inventories, particularly in regions with intense livestock activity.

Figure 2.2B presents the adjusted (a posteriori) emissions, revealing that the areas with the highest emission intensities coincide with zones of high cattle density and show a strong spatial correlation with the correction factors. Notable examples include the mesoregion of Sinop (MT) and southern Santa Catarina, where values exceed 20 t CH₄/km²/year.

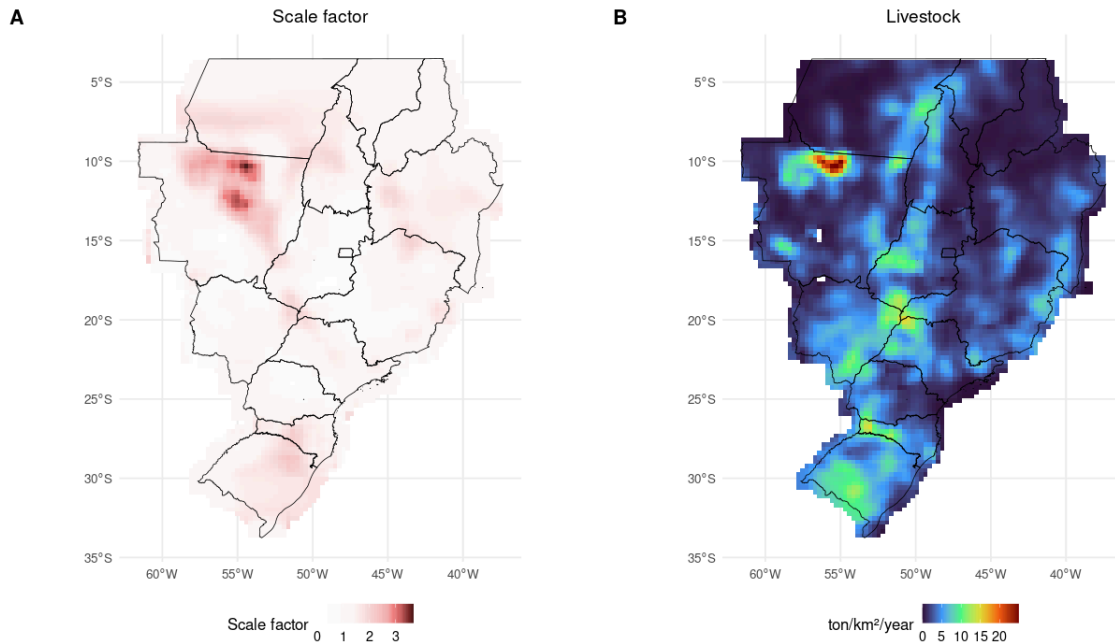


Figure 3.2. Spatial distribution of the scale factor (A) and livestock methane emissions (B).

The discrepancies between estimation approaches highlight methodological limitations of traditional inventories, such as underreporting of cattle numbers, imprecise spatial allocation of herds, and omission of emissions related to inefficient management practices. The spatial overlap between the highest scale factors and the peaks of corrected emissions further reinforces the robustness of atmospheric inversion as a diagnostic tool.

The spatial distribution of emissions consistently mirrors the patterns of cattle density in Brazil. Central-West and Southeast states, such as Mato Grosso (32.7 million head), Minas Gerais (23.8 million), and Goiás (23.2 million), not only harbor the largest cattle stocks but also exhibit the highest CH_4 emission estimates; demonstrating a direct relationship between livestock intensity and emission magnitude. In contrast, Northeastern states such as Piauí (1.7 million) and Maranhão (4.7 million) present systematically lower emissions across all three

estimation approaches. This pattern may reflect both a smaller cattle population and satellite detection challenges, including higher cloud cover, more heterogeneous land use, and difficulties in atmospheric modeling in regions with low source density.

Figure 2.2B also reveals robust regional patterns in a posteriori methane emissions, with two prominent hotspots: the mesoregion of Sinop (MT) and the tri-border area between Goiás, Minas Gerais, and Mato Grosso do Sul. In both regions, emission levels exceed 20 t CH₄/km²/year, even after correction based on observed atmospheric concentrations.

In the Sinop mesoregion, the municipality of Alta Floresta alone holds approximately 705,000 head of cattle, followed by Guarantã do Norte (397,000), Colíder (297,000), and Sinop (186,000) (IBGE, 2025). These municipalities collectively account for over 1.5 million cattle in a relatively compact area, marked by the predominance of extensive production systems and frequent use of degraded pastures (MapBiomas, 2025). The high herd density, coupled with rapid agricultural expansion and the persistence of unsustainable management practices, significantly contributes to the elevated emission levels observed; even after inversion-based adjustments.

Another critical zone is the tri-border region encompassing Goiás, Minas Gerais, and Mato Grosso do Sul, where municipalities such as Itajá (GO), Iturama (MG), and Paranaíba (MS) form a continuous corridor of high emissions. Together, these three municipalities house approximately 1.1 million head of cattle (IBGE, 2025) and share similar structural characteristics: well-established pasturelands, partial crop-livestock integration, and a production chain oriented toward fattening and slaughter.

Figure 2.3 displays the spatial distribution of specific enteric methane emissions per animal, expressed in kg CH₄/head/year, with a notable concentration in the South-Central region of Brazil. The estimates were derived by multiplying the emission factors adjusted through

atmospheric inversion by the local cattle density, allowing for the identification of regional patterns influenced by the prevailing production systems.

The results reveal substantial spatial variability, with values ranging from less than 50 kg CH₄/head/year in areas dominated by extensive grazing systems to over 150 kg CH₄/head/year in regions characterized by intensive dairy production. Notably, southern Minas Gerais, western Santa Catarina, and northern Rio Grande do Sul exhibit values exceeding 125 kg CH₄/head/year, with localized hotspots surpassing 150 kg/animal/year; indicating critical areas in terms of specific emission intensity.

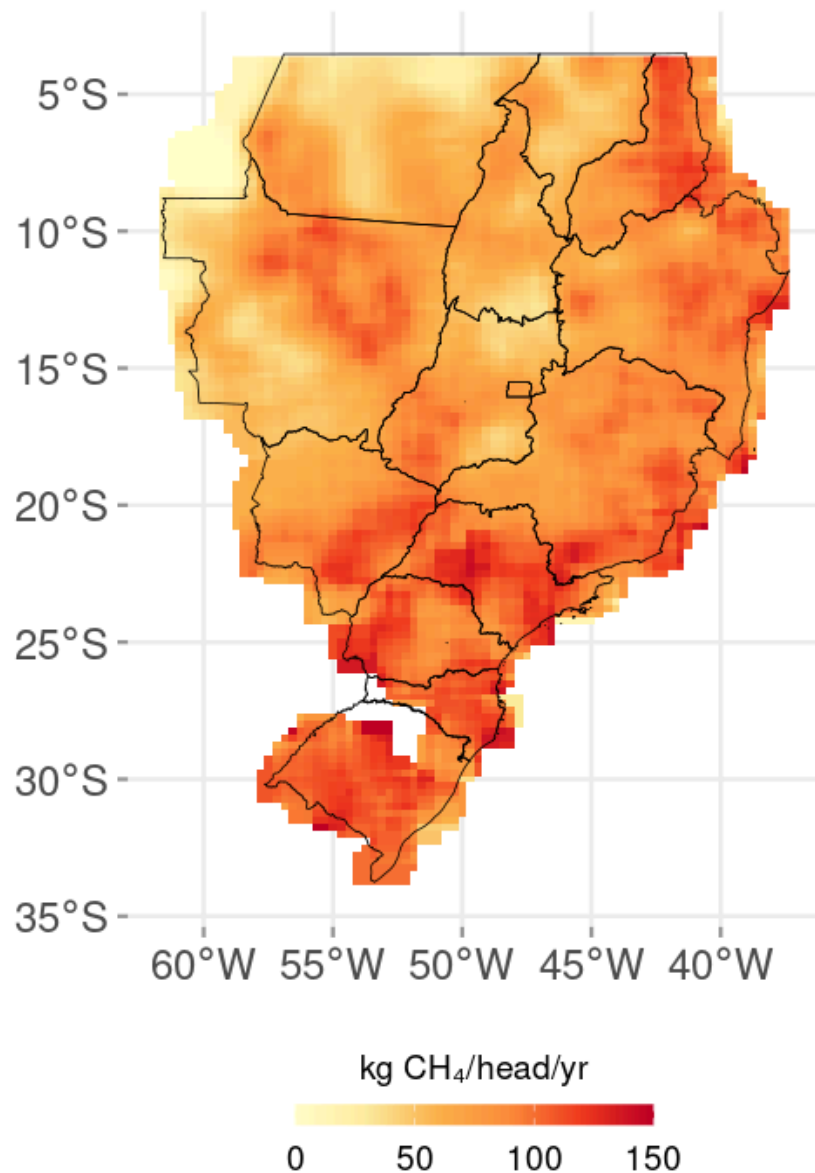


Figure 3.3. Enteric methane emission intensity per cattle head in Central and Southern Brazil (kg CH₄/head/year).

The South and Southwest mesoregions of Minas Gerais encompass municipalities such as Passos, Bambuí, and Patos de Minas, which are historically dedicated to specialized dairy production. In these areas, the values observed in Figure 2.3 range from 130 to 160 kg CH₄/head/year, reflecting not only the high density of lactating cows but also the increased nutritional demands of high-yielding herds. According to data from SIDRA/IBGE (2023), the

state of Minas Gerais hosts approximately 9.7 million head of cattle, of which 2.3 million are lactating cows, with average daily milk yields exceeding 15 liters per animal in several microregions.

In western Santa Catarina, municipalities such as Chapecó, Concórdia, and Xaxim exhibit values ranging from 120 to 150 kg CH₄/head/year, as shown in Figure 2.3.. This region is characterized by a highly technified dairy production model, involving intensive use of silage and concentrated feed supplementation. While these practices enhance productivity, they also lead to increased specific enteric methane emissions per animal.

The state of Mato Grosso (MT), which holds the largest cattle herd in the country with 32.7 million head (SIDRA/IBGE, 2023), exhibits a distinct emission pattern. The predominance of extensive beef cattle systems, based on low-digestibility native pastures, results in moderate specific emissions, ranging from 60 to 110 kg CH₄/head/year across most of the state. However, a localized increase in specific emissions is observed in the northern mesoregion, particularly around municipalities such as Sinop, Sorriso, and Lucas do Rio Verde, where values approach 120 to 130 kg CH₄/head/year. This pattern may reflect the growing adoption of semi-intensive systems, feedlots, and the rehabilitation of degraded pastures; developments often associated with the ongoing agricultural modernization in the region.

3.3.2. *Comparative emissions with biomass*

The relationship between pasture biomass and methane emissions exhibits distinct responses when assessed per head (Figure 2.4.A) versus per unit area (Figure 2.4.B). In Figure 2.4.A, specific emissions (kg CH₄ head⁻¹ yr⁻¹) cluster in two high-density domains: (i) moderate biomass (~12–16 t ha⁻¹) with ~80–90 kg CH₄ head⁻¹ yr⁻¹, and (ii) higher biomass (~22–26 t ha⁻¹), where values stabilize at similar or slightly higher levels. This nonlinearity is

consistent with the joint effects of intake and forage quality: at intermediate biomass, greater fiber fraction and lower digestibility enhance ruminal H_2 production and methanogenesis; as biomass increasingly reflects corrective management (balanced fertilization, higher-yielding cultivars, rotational grazing), diet quality and digestive efficiency improve and CH_4 per head tends to plateau.

In Panel B, areal fluxes ($kt\ CH_4\ km^{-2}\ yr^{-1}$) peak between $\sim 15\text{--}24\ t\ ha^{-1}$, indicating that rising biomass sustains higher stocking rates; thus, even if per-head emission stabilizes, the product “number of animals $\times$ per-animal emission” intensifies emissions per unit area. Mechanistically, biomass acts both as a proxy for forage quality (modulating CH_4 per head) and as a carrying-capacity indicator (modulating CH_4 per area), reconciling the apparent contrast between panels.

State-level trajectories reveal regional modulation. In Minas Gerais (MG), per-head emissions increase with biomass (from ~ 87 up to $\sim 107\ kg\ head^{-1}\ yr^{-1}$), aligning with values commonly reported for dairy systems; however, areal emissions remain comparatively stable, suggesting that stocking adjustments and management practices buffer landscape-level fluxes. In Mato Grosso (MT) and Pará (PA), per-head CH_4 is lower, consistent with predominantly beef systems, yet areal emissions diverge: MT shows relatively constant areal fluxes with increasing biomass, while PA exhibits pronounced increases driven by high stocking in specific municipalities. Notably, São Félix do Xingu (PA), which holds the country’s largest cattle herd (>2 million head), displays per-head emissions within reference ranges for beef ($\sim 61\ kg\ head^{-1}\ yr^{-1}$), but very high areal fluxes (on the order of $10^3\ kt\ CH_4\ km^{-2}\ yr^{-1}$ in our raster-derived metrics), reflecting strong production intensification. In Paraná (PR), improvements in forage quality across the nation’s leading dairy belt coincide with lower per-head CH_4 and some of the highest areal peaks, consistent with elevated animal density and

sustained pasture productivity. In São Paulo (SP), the raised arc of specific CH₄ at mid-range biomass and an areal peak near ~18–22 t.ha⁻¹ are consistent with consolidated intensification; the next frontier is reducing emission intensity per product (CH₄ per kg of milk/meat) via supplementation and precision herd management.

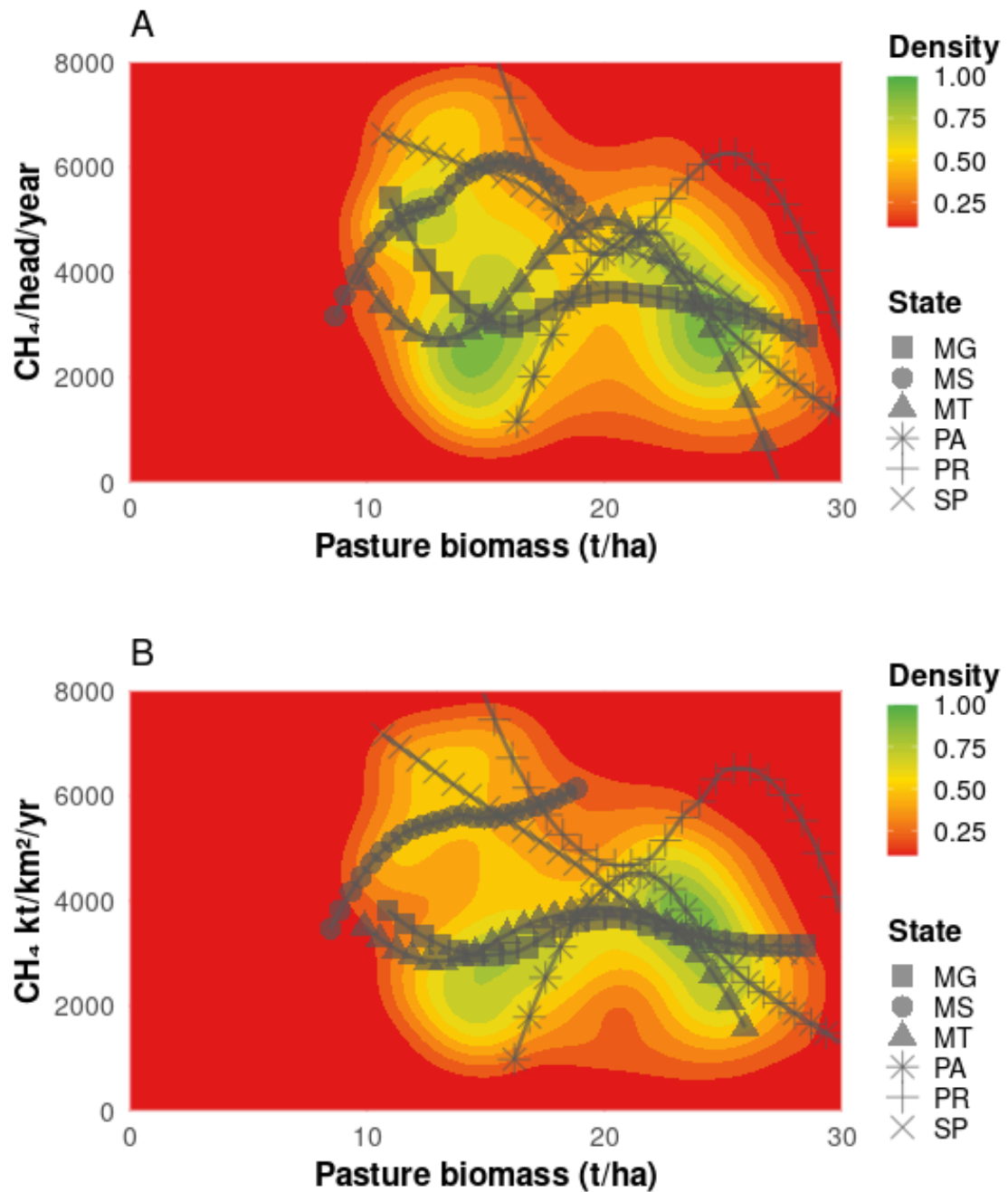


Figure 3.4. Relationship between methane emissions and pasture biomass. Panel A: Specific methane emissions per head ($\text{kg CH}_4 \cdot \text{head}^{-1} \cdot \text{yr}^{-1}$) as a function of pasture biomass ($\text{t} \cdot \text{ha}^{-1}$). Panel B: Methane emissions per area ($\text{kt CH}_4 \cdot \text{km}^{-2} \cdot \text{yr}^{-1}$) as a function of pasture biomass ($\text{t} \cdot \text{ha}^{-1}$).

3.3.1. General NO_x Emissions Behavior

Our data indicate that, in most of the states analyzed, non-degraded pastures exhibit higher greenhouse gas (GHG) emissions compared to degraded ones (Figure 2.5.). This pattern is observed, for example, in Mato Grosso do Sul (+135.35 kg/km²/year), Pará (+102.26 kg/km²/year), Paraná (+183.80 kg/km²/year), and Rio Grande do Sul (+49.96 kg/km²/year). The greatest absolute difference was found in Paraná. In these states, we observe a trend of livestock intensification in well-managed areas, which increases emissions mainly due to enteric fermentation and the application of nitrogen fertilizers; a significant source of nitrous oxide (N₂O), a GHG with a high global warming potential.

The highest total emissions, for both degraded and non-degraded pastures, were recorded in the state of São Paulo (1,286.00 and 1,258.46 kg/km²/year, respectively), reflecting the high technological level of livestock systems in the state, characterized by intensive use of inputs, partial confinement, and integrated production systems. Although the difference between the two pasture types in São Paulo is small (−27.54 kg/km²/year), the absolute volume of emissions reinforces the role of highly productive regions as significant emission centers.

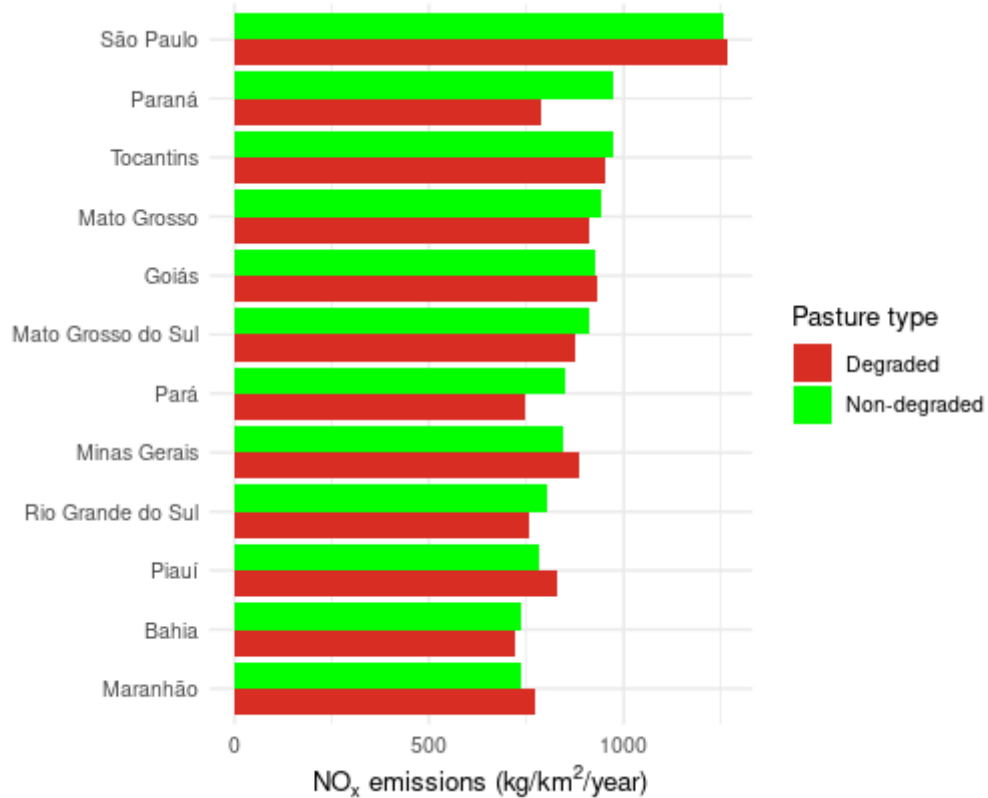


Figure 3.5. NO_x emissions associated with degraded and non-degraded pastures in selected Brazilian states (kg/km²/year).

2.3.2. Trend Reversal in Minas Gerais and Other States

In contrast to the pattern observed in states with intensified livestock systems, Minas Gerais exhibited higher emissions in degraded pastures (885.50 kg/km²/year) than in non-degraded ones (845.08 kg/km²/year), with a difference of −40.42 kg/km²/year. Similar patterns were identified in Maranhão (−40.71 kg/km²/year), Paraíba (−58.93 kg/km²/year), and Piauí (−45.75 kg/km²/year).

We attribute this trend reversal to a combination of socioeconomic and technical factors. In many regions of these states, especially in smallholder properties, degraded areas continue to be used beyond their carrying capacity, resulting in overstocking and, consequently, higher emissions per unit area. Soil compaction, reduced water infiltration, and

loss of vegetation cover promote anoxic conditions that may intensify the emission of GHGs such as methane (CH_4) and N_2O , particularly in clay-rich, poorly drained soils. Furthermore, the lack of pasture restoration practices and the limited adoption of technologies contribute to the degradation process and the intensification of emissions in economically marginalized areas.

3.3.3. Temporal considerations on pasture use and management

The variation in emission patterns among states suggests that degradation status alone is not sufficient to determine emission levels; it is also essential to consider how these areas are managed. Technified pastures, even when non-degraded, may present high emission levels due to intensive nitrogen fertilizer use and high stocking rates. Conversely, degraded areas may maintain high animal loads due to the socioeconomic needs of producers, further exacerbating their contribution to the GHG balance.

The temporal analysis of monthly nitrogen oxide (NO_x) emissions by pasture type reveals a recurring seasonal pattern across several Brazilian states (Figure 2.5). Emissions tend to increase during the transition from the end of the rainy season to the beginning of the dry period, particularly between May and August. This behavior suggests a direct influence of soil hydrological conditions and microbial dynamics, both of which are closely associated with water availability and livestock management practices (Silva et al., 2024; Zhang et al., 2024).

During the dry season, soil moisture progressively declines, resulting in enhanced aeration and increased oxygen diffusion through soil pores. These more aerobic conditions favor the nitrification process, in which ammonium (NH_4^+) is converted into nitrate (NO_3^-), releasing nitrogen oxides (especially NO) as intermediate byproducts (Silva et al., 2024).

Therefore, even in the absence of rainfall, the reduction in soil moisture alone creates favorable conditions for increased NO_x emissions.

Additionally, isolated rainfall events at the onset of the dry season or occasional irrigation can trigger a phenomenon known as the rewetting pulse effect (also referred to as the drying–rewetting effect or Birch effect). This phenomenon involves the rapid reactivation of the soil microbial community following a dry period, intensifying organic matter mineralization and nitrogen transformation processes (Zhang et al., 2024). As a result, there is an abrupt and temporary increase in NO_x emissions, which can peak shortly after these rewetting events.

We observed that this seasonal pattern is particularly evident in states such as Goiás, Mato Grosso, Mato Grosso do Sul, Tocantins, and Pará, which experience significant increases in emissions from June to August. These states are characterized by pronounced seasonal climates with well-defined dry seasons, which intensify both soil oxygenation and the effects of moisture pulses (Silva et al., 2024). In contrast, in states with less marked seasonal contrasts or higher residual soil moisture; such as São Paulo, Paraná, and Minas Gerais; the fluctuations in emissions are less pronounced.

Our findings indicate that NO_x emissions from pasturelands are highly sensitive to soil moisture dynamics. The combination of dry soil, increased oxygen availability, and rewetting pulses constitutes a key mechanism behind seasonal emission intensification. These dynamics must be considered in national emission inventories and the development of mitigation strategies for the agricultural sector (Silva et al., 2024; Zhang et al., 2024).

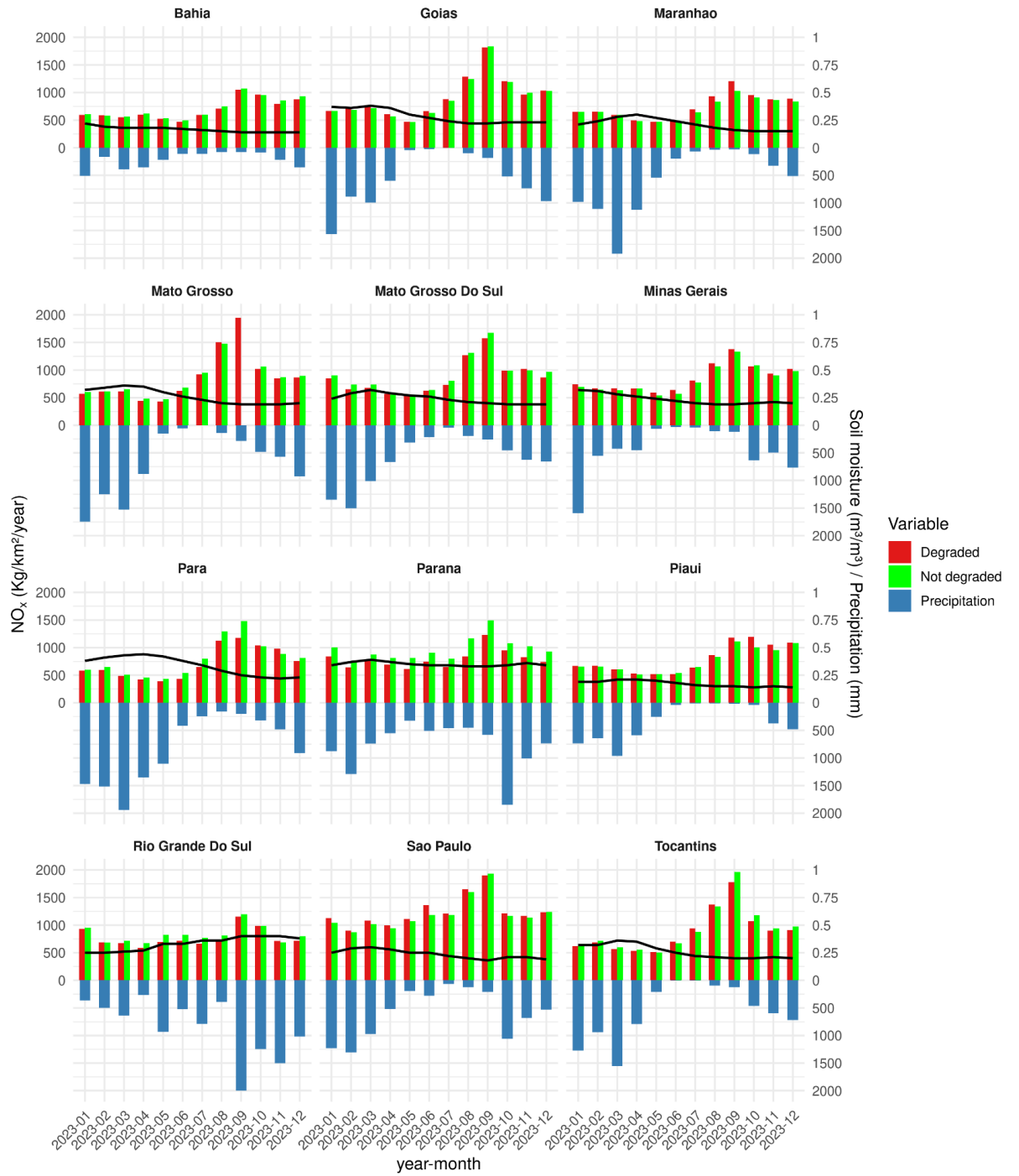


Figure 3.5. Monthly variation of NO_x emissions in degraded and non-degraded pastures, precipitation, and soil moisture in selected Brazilian states

3.3.4. Indirect N_2O emissions from Brazilian pasturelands

Figure 2.6 presents the distribution of estimated nitrous oxide (N_2O) emissions from pasturelands across different federative units of Brazil, revealing marked spatial heterogeneity. Higher emission levels are predominantly observed in states with extensive pasture areas and greater cattle herd densities, particularly in the Central-West and Northern regions.

The state of Mato Grosso stands out as the leading emitter, followed by Pará and Minas Gerais. This predominance can be attributed to a combination of factors, including the vast land area devoted to livestock production, high stocking rates, and the adoption of management practices that enhance nitrogen mineralization in soils. These factors increase the availability of reactive nitrogen, which, under favorable edaphoclimatic conditions, promotes the microbial processes of nitrification and denitrification; the primary pathways for N_2O formation (Butterbach-Bahl et al., 2013; IPCC, 2019).

States such as Goiás, Bahia, and São Paulo occupy intermediate positions, reflecting the regional significance of livestock farming, albeit with varying degrees of intensification and use of nitrogen fertilizers. Conversely, federative units in the South and Northeast, such as Rio Grande do Sul, Piauí, and Maranhão, showed the lowest estimated emissions among those analyzed. This may be associated with both the smaller extent of pasturelands and edaphoclimatic conditions that are less conducive to N_2O production, such as soils with lower organic matter content or more limiting hydrological regimes (Reis et al., 2023).

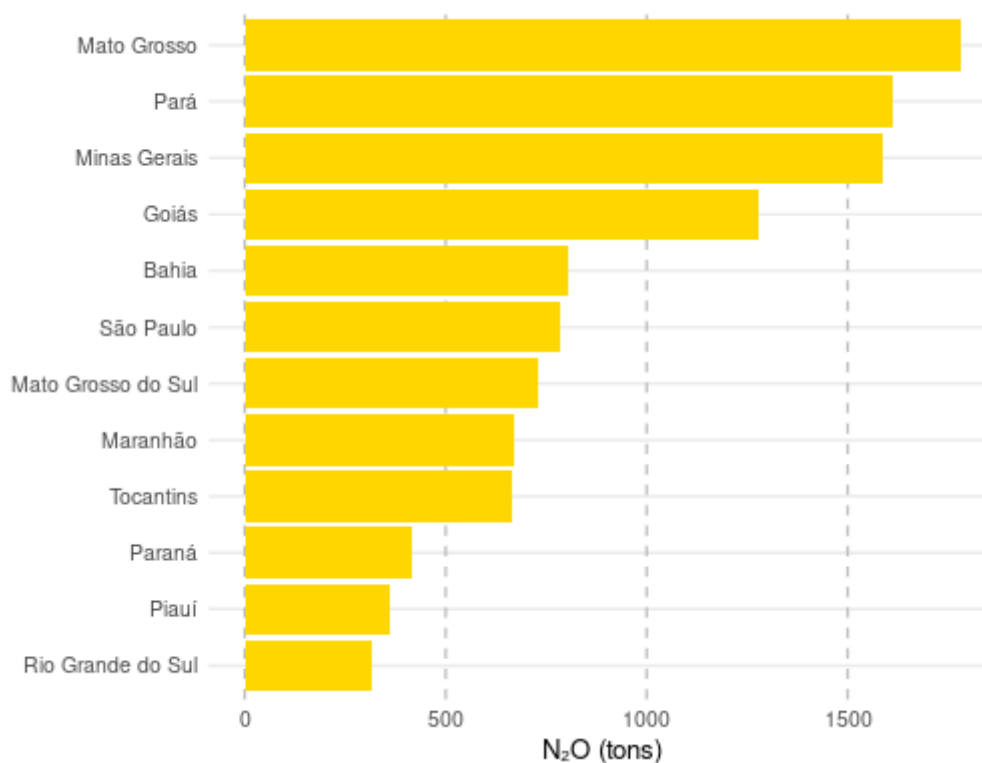


Figure 3.6. Total nitrous oxide (N₂O) emissions by the Brazilian state (in tons).

3.4. Discussion

Methane emission estimates derived from atmospheric inversion techniques indicate that the Brazilian livestock sector is responsible for approximately 26.7 Mt CH₄/year, with a range between 22.3 and 31.2 Mt CH₄/year. Considering the global warming potential (GWP) of methane as 27.2 (according to the IPCC AR6), this corresponds to an emission range of approximately 607 to 849 Mt CO₂eq/year, with a mean value of 726 Mt CO₂eq/year. When combined with nitrous oxide (N₂O) emissions; estimated at approximately 42.5 thousand tonnes per year, or 11.6 Mt CO₂eq/year using a GWP of 273; the total contribution of the national livestock sector reaches nearly 738 Mt CO₂eq/year (ranging from 618.6 to 860.6 Mt CO₂eq/year). These figures position livestock production as one of the leading sectoral sources of greenhouse gas (GHG) emissions in Brazil, underscoring the urgent need for

integrated mitigation strategies that encompass both animal management and land use practices.

When comparing GHG emission estimates for Brazilian livestock derived from atmospheric inversion with those reported in national inventories, a significant discrepancy becomes evident; highlighting the need to improve current estimation methodologies. According to the *Sistema de Estimativas de Emissões e Remoções de Gases de Efeito Estufa* (SEEG), the Brazilian agricultural sector emitted approximately 617 Mt CO₂eq in 2023, accounting for 27% of the country's gross emissions.

The results of this study reveal striking differences between conventional inventory-based estimates of enteric methane emissions and those adjusted using atmospheric inversion data from the TROPOMI sensor. In certain states, such as Mato Grosso, this discrepancy reaches up to an 80% increase over prior inventory estimates, reinforcing growing evidence that conventional methodologies may substantially underestimate the true emissions from the livestock sector (Maasakkers et al., 2022; Zhang et al., 2021).

The spatial distribution of scale factor corrections and adjusted emissions underscores the importance of regional heterogeneity in production systems. Regions such as the Sinop mesoregion (Mato Grosso) and southern Santa Catarina exhibited correction factors exceeding 2.5 times the initial estimates, indicating critical hotspots associated with high cattle density and suboptimal management practices. These findings align with previous research indicating that areas with intensive production systems; yet lacking full implementation of mitigation technologies; tend to exhibit higher per-animal emission intensities (Mapfumo et al., 2022; Herrero et al., 2021).

A particularly notable pattern is the divergence in emission profiles between extensive beef cattle systems and more technified dairy operations. While the former generally produce

moderate specific emissions (60–110 kg CH₄/head/year), the latter may exceed 150 kg CH₄/head/year in areas such as southern Minas Gerais and western Santa Catarina. This pattern reflects the higher digestibility of dairy diets and the elevated metabolic demands of high-yielding cows, as described by Hristov et al. (2023).

The substantial variability in emissions can also be partially attributed to pasture conditions. Degraded pastures, characterized by low forage availability and digestibility, often result in reduced animal productivity but not necessarily lower emissions per unit area. In states such as Minas Gerais, higher emissions were observed in degraded pastures; likely a consequence of overstocking and inadequate management, a common scenario among smallholders (Reis et al., 2023; Dias et al., 2020).

Moreover, the findings regarding NO_x and N₂O emissions highlight the significance of indirect emissions in livestock systems. The seasonality observed in NO_x emissions, with peaks between May and August, emphasizes the role of edaphoclimatic conditions and rewetting pulses in shaping GHG dynamics, consistent with the frameworks proposed by Zhang et al. (2024) and Silva et al. (2024). These results indicate that mitigation strategies must consider not only pasture type but also hydrological regimes and extreme events that affect soil microbial processes.

Finally, the application of inversion modeling based on TROPOMI data proved to be a valuable tool for refining national emission estimates and identifying priority regions for mitigation interventions. These findings support recent calls for greater incorporation of atmospheric observations into national GHG inventories, as advocated by the IPCC (2019) and Butterbach-Bahl et al. (2023).

In summary, pasture biomass is a primary system control: dietary improvement reduces or stabilizes emissions per head, while gains in carrying capacity can raise emissions

per area. Effective mitigation therefore requires three coordinated, state-sensitive fronts: (i) forage quality via recovery and balanced fertilization; (ii) seasonally calibrated stocking to prevent transient biomass surpluses from translating into higher areal fluxes; and (iii) sustained focus on product-level intensity, ensuring that territorial productivity gains do not expand the CH₄ footprint. Read jointly, the two panels trace a transition from “more pasture” to “the right pasture, in the right amount, at the right time.”

3.5. Conclusions

This study provides an integrated, satellite-constrained assessment of greenhouse-gas emissions from Brazilian livestock by combining TROPOMI-informed analytical inversions for CH₄ with NO₂-based diagnostics of soil NO_x and an IPCC-consistent accounting of indirect N₂O from atmospheric deposition. *A posteriori* methane emissions sum to ~26.7 Mt CH₄ yr⁻¹ (22.3–31.2 Mt CH₄ yr⁻¹), with pronounced regional hotspots (e.g., Sinop/MT and the Goiás–Minas Gerais–Mato Grosso do Sul corridor) and systematic upward corrections over prior inventories—reaching ~80% in some states. When expressed in CO₂-equivalent terms (GWP₁₀₀ for CH₄ = 27.2) and combined with our indirect N₂O estimate (~42.5 kt N₂O yr⁻¹; ~11.6 Mt CO₂e yr⁻¹), the sectoral total approaches ~738 Mt CO₂e yr⁻¹, underscoring livestock as a dominant and policy-relevant source. We also document clear contrasts between extensive beef systems (lower per-head CH₄ intensity) and technified dairy regions (>150 kg CH₄ head⁻¹ yr⁻¹ in parts of MG/SC), as well as a robust seasonality in NO_x consistent with drying–rewetting pulses.

Beyond quantification, our results point to concrete avenues for mitigation and monitoring. Scale-factor patterns and *a posteriori* fluxes highlight priority geographies where interventions (diet quality and supplementation, manure handling, pasture rehabilitation, and

integrated crop–livestock systems) are likely to yield the largest returns. The seasonal amplification of NO_x between late wet and early dry seasons suggests timing-aware management (e.g., fertilization and stocking decisions) and targeted verification during hydrologic transition periods. These outcomes argue for embedding satellite-constrained top-down estimates within national inventories to improve spatial detail, detect bias in bottom-up factors (herd allocation, emission factors), and enable more transparent, near-real-time MRV of livestock emissions.

Methodologically, the framework is robust yet its uncertainties are explicit: inversion results depend on prior fields, boundary conditions, transport errors at mesoscale, observational screening, and assumptions about NO_x lifetime, deposition fractions, and $\text{EF}_5(\text{g})$ for indirect N_2O . Cloud contamination, source co-location (e.g., biomass burning, fossil CH_4), and limited in-situ constraints remain challenges. Addressing these will require co-designed bottom-up data (fine-grained herd and productivity maps; manure management and fertilization practices), expanded ground/airborne validation, and multi-species inversions that jointly leverage CH_4 – NO_2 – CO to improve source attribution.

Looking forward, coupling this atmospheric lens with additional Earth-observation streams can tighten attribution from “where” to “why.” Time-series L/S-band SAR (canopy structure/biomass proxies and surface moisture) together with routine soil-moisture products can mechanistically link management, hydrology, and emissions—especially during drying–rewetting transitions. Higher-resolution and next-generation hyperspectral missions for CH_4/NO_2 will help resolve sub-mesoregion sources, quantify mitigation outcomes at facility/pasture scales, and track interannual variability tied to climate modes. As these data streams mature, a unified, observation-driven system that reconciles top-down and bottom-up

estimates can underwrite Brazil's sectoral targets with greater confidence and temporal responsiveness.

In sum, satellite-constrained inversions reveal that Brazilian livestock emissions are larger and more heterogeneous than suggested by conventional inventories, but also more *actionable*: the same observations that expose the problem delineate where, when, and how to intervene. This integrated framework—linking atmospheric measurements, transport modeling, and agronomic context—offers a scalable pathway to credible MRV and targeted mitigation, aligning productivity, environmental integrity, and climate policy.

4. General conclusions

We conclude that it is feasible to integrate, in an operational and continent-wide manner, the productive dynamics of highly mechanized tropical agriculture with the atmospheric accounting of trace gases within a single, physically coherent observational and analytical framework, using one and the same orbital platform. By jointly constructing time series of sun-induced chlorophyll fluorescence (SIF) for phenological calendars and derivation of mechanization metrics with hyperspectral orbital observations of CH₄ and NO₂ anomalies (a proxy for NO_x with implications for indirect N₂O), we establish a measurable nexus between when and how production occurs and where and when emissions take place. The outcome is a set of indicators that are comparable across regions and seasons, with sufficient granularity to inform decisions from field to national levels and, at the same time, compatible with sectoral inventories via top-down approaches and their consistency with bottom-up estimates.

On the biophysical axis, we demonstrate that SIF robustly recovers soybean phenological calendars and quantifies the synchrony and intensity of planting and harvest windows, circumventing the typical saturation of spectral indices under dense canopies. From these series, we infer operational mechanization metrics—including daily peaks exceeding 100,000 ha·day⁻¹ in hubs of Brazil's Central-West—characterize interannual variations associated with climatic extremes, and reveal early-warning capability by anticipating physiological changes relevant for crop forecasting on lead times of weeks. This architecture is supported by multiscale validation (state–municipality–field), explicit uncertainty quantification, and spatial adaptation/transfer strategies (domain adaptation) to accommodate management heterogeneity.

On the atmospheric axis, we integrate orbital measurements into top-down CH₄ inversions and use NO₂ anomalies to infer NO_x patterns over agro-pastoral landscapes, making explicit the role of pasture condition—degraded versus intensified—in determining emission intensity. We identify persistent hotspots and spatial contrasts consistent with the biogeophysical logic of enteric fermentation and soil nitrogen reactivity, and we show that pasture restoration and sustainable intensification shift the system toward lower emission ranges per unit of product. By aligning phenological schedules with emissive cycles, we open a path to synchronized production–emission metrics suitable for performance-oriented, transparent MRV (measurement, reporting, and verification) systems.

Methodologically, three contributions stand out. First, the operationalization of SIF as a master axis for phenology and physiological risk at continental scale, with multiscale validation and tractable uncertainty. Second, atmospheric inversions capable of closing regional CH₄ budgets and informing NO_x/N₂O proxies without violating the system's physicochemical coherence. Third, the harmonization of phenological metrics with trace-gas

dynamics, enabling comparable dashboards across biomes, seasons, and management regimes, and structuring a reproducible pipeline that is scalable to other land-use systems.

The practical implications are direct: (i) more realistic crop forecasts via anticipated physiological alerts; (ii) adaptive management based on climatic risk, supporting optimal windows for water and nitrogen management; (iii) targeted mitigation that prioritizes areas and pathways with the lowest marginal abatement cost; (iv) reconciliation between bottom-up inventories and top-down estimates, increasing the credibility of territorial and sectoral reporting; and (v) the design of policy instruments, credit, zoning, public procurement, traceability—anchored in high spatiotemporal-resolution observational evidence.

In the near term, the field is poised to move from a still-fragmented diagnosis to dense, coherent, and truly operational agro-atmospheric observation. On the biophysical front, dedicated global SIF missions (e.g., FLEX) and visible–NIR/SWIR hyperspectral imagers (e.g., CHIME), in synergy with VSWIR+TIR sensors (e.g., SBG), will enable estimation of functional traits (chlorophyll, foliar nitrogen, LMA), more robust tower–airborne–orbit scale transfer to calibrate SIF, and multi-season phenological calendars with predictive power weeks ahead of structural changes detectable by classical VIs. L/S-band SAR constellations will add cloud-insensitive series for canopy structure, aboveground biomass, and surface moisture, opening space for SIF–SAR fusion in pastures and perennial crops. On the greenhouse-gas front, the CO2M constellation should deliver anthropogenic CO₂ with co-observation of CH₄/NO₂, enabling multi-gas inversions and reconciliation of territorial inventories; platforms such as GOSAT-GW will enhance sensitivity to regional CO₂/CH₄ columns; spaceborne CH₄ lidar (e.g., MERLIN) will improve detection under challenging radiative conditions; and high-resolution facility-scale hyperspectral mappers (e.g., Carbon Mapper/Tanager) will permit plume “zoom-ins,” closing the loop between broad screening,

fine diagnosis, and regional inversions. This configuration will reduce uncertainties, quantify super-emitters, and align mitigation with levers offering the highest return per tonne abated.

In sum, as new sensors expand spatial, temporal, and spectral resolution, the proposed axis evolves from diagnosis to precision governance: more transparent inventories, high-return mitigation, and productive resilience to climate variability and change. The scientific ambition realized here, connecting the pulse of photosynthesis to greenhouse-gas fluxes with physical coherence and decision utility, lays a solid foundation for public policies and private strategies that treat competitiveness and climate responsibility not as competing goals, but as inseparable dimensions of the same future-oriented project.

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