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Estimates of Annual Carbon Dioxide Fluxes from the Soil of Spruce Forests of the Ural-Carbon Carbon Supersite based on Incomplete Time Series using Classical Regression Approaches and Machine Learning

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Abstract—The annual flux of carbon dioxide from soils across different biomes plays a key role in global climate models and terrestrial carbon cycle analysis. However, there are significant gaps in such research at a regional scale. Due to the high labor intensity of obtaining daily soil respiration indicators, various modeling methods are used. In this work, based on 2760 measurements of soil respiration in spruce forests of the Ural-Carbon carbon supersite (Middle Urals), carried out in the fall of 2021 and from April to October 2022, using classical regression approaches and machine learning, annual soil respiration indicators were estimated. We also investigated the dependence of the results on the complexity of the model (number of predictors) and the methods used (random forest model extrapolation and combined approaches for estimating winter CO_2 fluxes). The "simplified" model with seven predictors showed only a slight decrease in accuracy compared to the full model with 21 predictors ($R^2 = 0.89$, $MSE = 0.22$ vs. $R^2 = 0.92$, $MSE = 0.31$). Remote sensing-based predictors contributed more to model accuracy than field data. While initial results varied across methods, incorporating literature-based winter respiration values into the random forest model and averaging combined-approach estimates yielded consistent annual soil respiration values: 830.3 ± 6.4 and 851.6 ± 8.0 g C/m^2 year, respectively.

Keywords: CO_2 emissions, carbon cycle, machine learning, forest ecosystems, carbon supersites, environmental factors

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INTRODUCTION

Accurate estimates of climate-active gas fluxes are important for analyzing and predicting changes in the carbon cycle [1]. The magnitude of these flows can vary considerably depending on the type of landscape. However, for many regions of Russia there is still no data on annual carbon dioxide emissions.

To assess carbon dioxide emissions from soil, two main methods are used: chamber and, indirectly, the eddy covariance method. The chamber method allows measurements to be made on a larger scale, but it does not provide daily data coverage throughout the year, especially when using non-stationary chambers. An additional challenge is estimating winter carbon dioxide emissions, which can reach a quarter of the annual volume [2].

To address data scarcity, mathematical modeling is used. Transitioning from discrete measurements to annual flux estimates involves both traditional regression models and machine learning methods. Among these, the Random Forest (RF) algorithm outperforms classical regression and neural networks in accuracy. However, machine learning models often incorporate an excessive number of predictors, reducing interpretability. Thus, developing simple yet highly accurate models remains a priority.

A key limitation of the RF algorithm is its poor extrapolation capability beyond the training data range—particularly for winter measurements, which are often unavailable. To solve this problem, models are proposed that calculate the annual flow based on data from the warm period of the year [3, 4]. Such models, based on classical regression approaches, demonstrate high coefficients of determination (0.81–0.95), but they were created on different data sets, and we did not find comparative studies of their performance conducted on the same data.

Thus, on the one hand, there is a pressing problem of obtaining estimates of annual greenhouse gas fluxes from soils of different biomes, and on the other hand, there is the problem of the lack of complete data series throughout the year and different ways of solving it. Therefore, the goal of our work is to estimate the amount of annual CO_2 emissions using different approaches (including machine learning) from the soil of spruce forests of the Ural-Carbon carbon supersite (Middle Urals) in 2022.

MATERIAL AND METHODS

Research Area

In order to establish a monitoring system and obtain adequate estimates of greenhouse gas flows in the country, two federal projects for monitoring the carbon balance were launched: Carbon Supersites and the Key Innovative Project of National Importance "The national system for monitoring the dynamics of climatically active substances in terrestrial ecosystems of the Russian Federation." A program to create a carbon supersites network was launched in 2021. Each supersite is a area with a relief, vegetation, and soil cover characteristic of the region. These sites are intended for conducting scientific research, developing infrastructure, and testing technologies for monitoring the balance of climate-active gases in natural ecosystems [5]. The Ural-Carbon carbon supersite is located in the Sverdlovsk region and consists of two areas located on opposite slopes of the Urals (western and eastern) and including forests typical for these macroslopes (spruce and pine, respectively). The study area (coordinates of the center 57.036389° N, 59.552222° E) is located in the southern taiga, within the ridge of residual mountains of the axial part of the Middle Urals and its western slope, on a watershed, floodplain terrace with a terrace-like slope and a section of the Chusovaya river valley. According to physico-geographical zoning, this territory belongs to the Middle Urals low-mountain region dominated by dark coniferous forests, with soils including sod-podzolic, mountain brown forest, and sod-meadow types [6]. The climate of the study area is continental, moderately cold, and humid. The average air temperature is 0.3°C, snow cover is established in late October–early November and thaws by mid-April; the average length of the growing season is 109 days (from May 20 to September 7) [7].

Experimental Design

The research was conducted in mature dark coniferous forests (80--110 years old) dominated by spruce (60%) and fir (30%), with minor components of pine (10%), birch, and larch [8]. In the study area selected three clusters (Fig. 1). Each cluster contained two sites positioned at different terrace levels along the riverbank–upper and lower terraces with an elevation difference of 25–27 m. On each site, three sample plots (Plot) of 5 × (15–20) m (65–100 m^2) were established, extending in different directions from the relative center of the site. A total of 18 sample plots were established, in each of which measurements were taken at 10 random points. The points were no closer than 1 m from large tree trunks and avoided the gaps of the tree stand [9].

Emission measurements were conducted three times in 2021 (August 26 (only 1 cluster), September 22 and October 12) and 13 times from May 18 to November 1, 2022, every 10–16 days (mostly 14 days). A total of 16 rounds of measurements were conducted. In each round, work was carried out between 9:00 and 17:00. To minimize diurnal variation effects, we randomized the site visitation order across measurement rounds. A total of 2760 measurements were carried out (10 measurements on each of the 18 sample plots for 15 complete rounds (one incomplete)).

CO_2 Emission Measurement

CO_2 flow rate from the soil surface was measured using a closed dynamic chamber method [10] using a Li-8100A field gas analyzer (Li-Cor biosciences, United States). Then, 5–10 min before the measurement, stainless steel rings with a diameter of 10.5 cm and a height of 5 cm were installed and buried 3 cm into the soil; the green parts of the plants were precut. Next, the device's camera was placed on the ring. The time of one measurement was 1 min.

At the same time, the soil temperature was measured using an Omega 88311E soil temperature probe, included in the respirometer kit, with an accuracy of 0.1°C (OMEGA Engineering, United Kingdom), and the volumetric soil moisture was measured using a ThetaProbe ML2 sensor (Delta-T devices, United Kingdom), connected to the gas analyzer control unit, with an accuracy of 0.1%. Measurements of soil humidity and temperature were carried out near the respiration measurement point at a depth of 5 cm. Air temperature was also measured using a temperature sensor built into the gas analyzer chamber.

Data Analysis

Statistical processing was performed in the R v 4.1.2 software. In all cases, the statistical unit was considered to be the sample plot, i.e., the average value of ten measurements on the sample plot in one round. This value was used as the daily average, since due to significant microscale variability in the forest with a large number of measurement points, the emission determined at a specific moment did not differ significantly from the daily average [11].

Data preparation. Predictors measured in-situ and Earth remote sensing data were used for modeling. Remote data on soil and air temperature and soil moisture, as well as NDVI, based on the products of the MODIS spectrometer from the Terra and Aqua

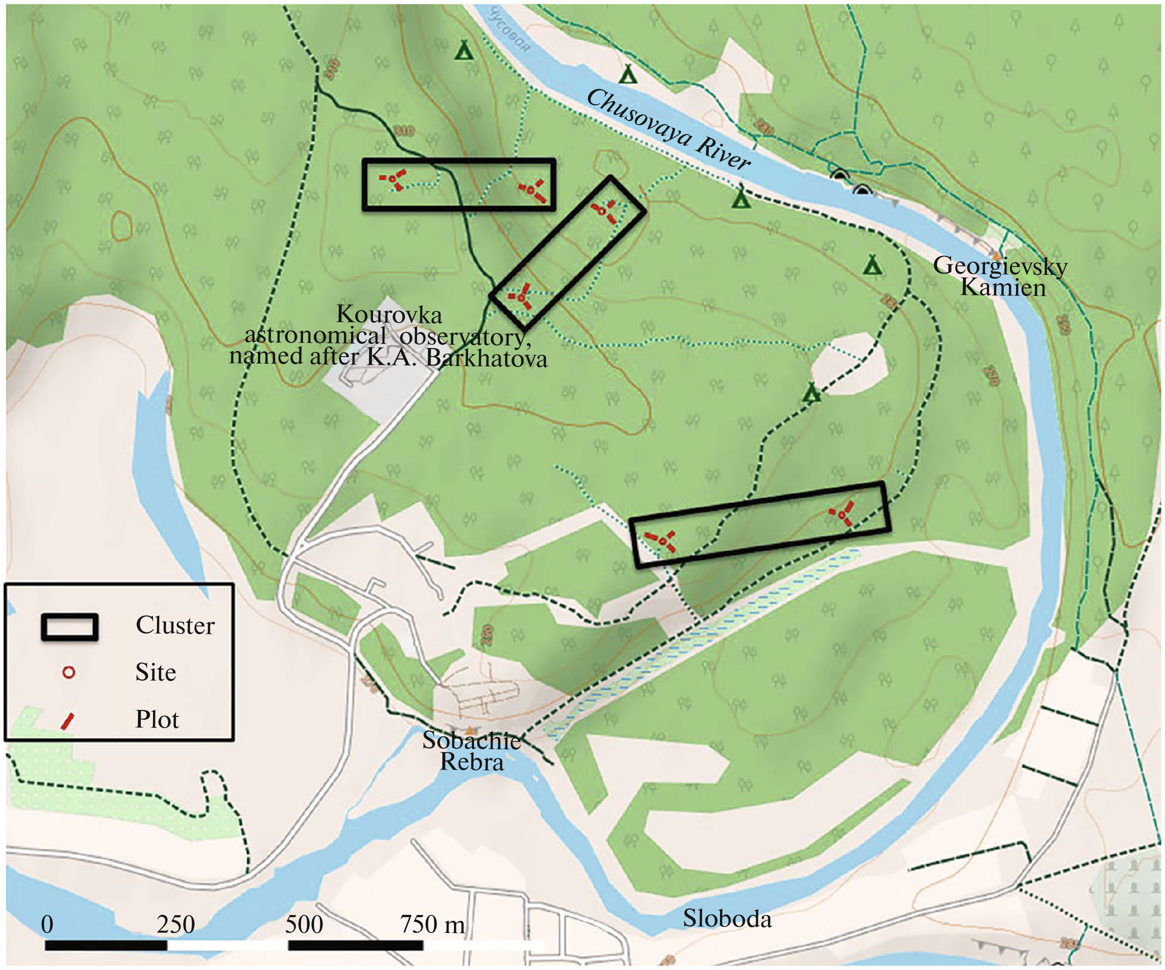

Fig. 1. Layout of test plots: Cluster—cluster, Site—area, Plot—sample plot.

satellites for 2022, were obtained using the VEGA-Science service [12] (Table 1).

Additionally, the Standardized Precipitation Evapotranspiration Index (SPEI) [13] from the global database (http://spei.csic.es) was used [14]. It shows how dry the studied period was relative to the norm over the past several decades (in this database – from 1950 to 2022). The index value [–0.99, 0.99] is an

Table 1. List of predictors used

Predictor	Description	Note
Soil temperature	Soil temperature at a depth of 5 cm	Measured in close proximity to the measurement point
Air temperature	Air temperature	
Soil moisture	Volumetric soil moisture at a depth of 5 cm	
Cluster	Cluster number	See Fig. 1
Position	Upper or lower terraces	
Soil temperature (remote)	Soil temperature at a depth of 10 cm	According to remote sensing data, resolution 1 km
Air temperature (remote)	Air temperature	
Soil moisture (remote)	Soil moisture at a depth of 10 cm	
NDVI	Normalized differential vegetation index, usually correlates well with total aboveground phytomass	Product MYD09Q1, resolution 250 m
SPEI 1–12	Drought index for 1–12 months preceding measurements	From the SPEI Global Drought Monitor database, spatial resolution 0.5°

indicator of normal moisture conditions, [1.00, 1.49]/[−1, −1.49] is moderate waterlogging/drought, >1.50 /<−1.50 is severe waterlogging/drought.

Remote temperature and humidity data were taken at 6-h intervals. However, these values are the product of algorithm calculations based on two direct daily satellite measurements, so we used their daily average values.

In the case of NDVI, we had a set of values of 1, 4, and 8-day composite images. Multi-day composite images are intended to reduce the impact of cloudiness on NDVI determination, but the study area may have over 200 cloudy days, so there are still gaps in the data. To obtain a series of daily NDVI values, we filled in missing data with the average of adjacent values and then averaged all three series (1, 4, and 8 day). Outside the growing season (before April 20 and after September 30), due to inadequately strong NDVI fluctuations (due to a large number of cloudy days), the lowest values at the boundary of the growing season were used, which was about 0.69. This is the minimum value that was in our training set, so values below this did not affect the result due to the operating principle of decision trees, on which the RF algorithm is based.

The selection of predictors was carried out using the "Boruta" package [15] and correlation analysis. This feature selection method leverages the Random Forest (RF) algorithm's capability to evaluate variable importance through an innovative permutation approach. The algorithm operates by creating multiple shadow predictors—artificial variables generated by randomly shuffling the values of each original predictor. Through iterative model building, the algorithm compares the predictive performance between models containing genuine predictors and those incorporating these shadow variables. By systematically evaluating these differences across numerous iterations, the algorithm calculates standardized *Z*-scores that quantify each predictor's statistical significance and relative importance.

Calculation of annual flows. In the first step, to estimate annual fluxes based on field measurements of soil respiration using the RF algorithm ("randomForest" package [16]), we created two models: "full" (using all variables) and "simplified" (only with selected predictors). Model hyperparameters—including the number of decision trees and the maximum features considered for node splitting—were optimized through a grid search procedure. Model performance was evaluated using 5-fold cross-validation implemented in the "caret" package [17], with validation metrics focusing on the coefficient of determination (R^2) and the mean squared error (MSE) between predicted and observed values. This dual-metric assessment ensured robust evaluation of both predictive accuracy (via R^2) and precision (via MSE) across the dataset.

The resulting models were used to estimate annual CO_2 fluxes from the soil in two ways:

(1) Extrapolation based on daily data on the values of selected predictors.

(2) A combined approach using a random forest model and one of two models:

(2.1) A model for calculating annual emissions based on determining the contribution of soil respiration during the summer period and average annual temperature [4].

(2.2) A model based on emission calculations for periods with temperatures above 5°C [3].

When assessing annual flows, the statistical unit was the "plot," i.e., with each method we obtained six values of annual flows, which allowed us to assess the spatial variation of the results.

The annual flux values from the global Soil Respiration Database v. 5.0 (SRBD) [18]). We selected values obtained for forests north of 55° N using infrared gas analyzers (IRGAs): in the entire northern hemisphere (n = 170) and only in Russia (n = 39). To estimate the effect of winter emissions on the calculated annual flux, we took winter respiration values from a study of a spruce forest in Canada [19], because it was similar in climate and the paper provided a formula by which we could calculate the emission rate for soil temperatures of 0, −1, −3, and −5°C (0.13–0.16 g (C–CO_2)/m^2 days) (with further decrease in temperature the indicators did not change). We added these calculated values to the training set and estimated the annual flow.

The data on carbon dioxide emission rates, field temperatures of soil and air, and soil moisture used in the article are available in the depository [20].

RESULTS

Field Measurements

Soil respiration ranged from 1.52–9.81 g (C–CO_2)/m^2 day and had a pronounced seasonal dynamic with maximum values in mid-July. Due to the dry weather that set in during the second half of the summer, we observed relatively low values of the CO_2 emission rate from the soil, even at soil temperatures higher than in early July.

The soil temperature during the measurements varying in the range of 3.2–24.2°C, air temperature—4.2–29.0°C, and soil moisture—8.3–61.7% (Fig. 2). Remotely sensed temperature data were in good agreement with field data, but field-measured air temperatures were consistently higher than the daily average calculated from remote sensing data. In contrast to temperature, field data on soil moisture were less consistent with remote sensing.

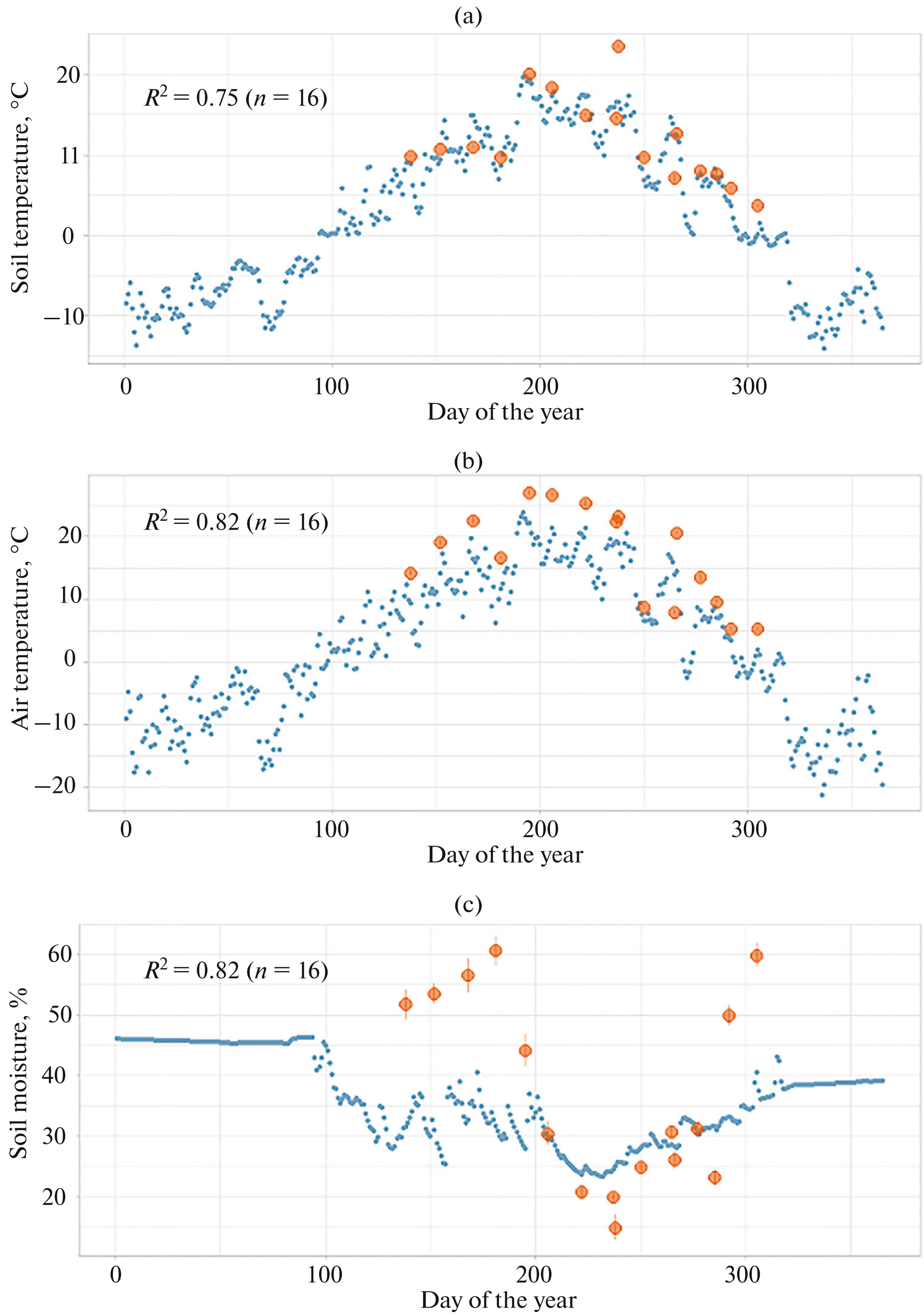

Fig. 2. Dynamics of soil temperature (a), air temperature (b), and soil moisture (c) throughout the year.

Selection of Predictors

Analysis of the features importance using the Boruta method showed that the importance of the "sample plot" factor (Plot) was lower than that of the shadow predictors (Fig. 3a). The "Position" and "Cluster" factors showed marginally higher importance but still overlapped with shadow predictor boundaries. Therefore, we decided to exclude these variables from the "simplified" model. The greatest influence on the accuracy of the model was exerted by air and soil temperature, as well as soil moisture. Moreover, remote sensing data were of greater significance than field-measured parameters; field and remote sensing data highly correlated with each other (Fig. 4). Therefore, we excluded field measurements of temperature and humidity to create a model with

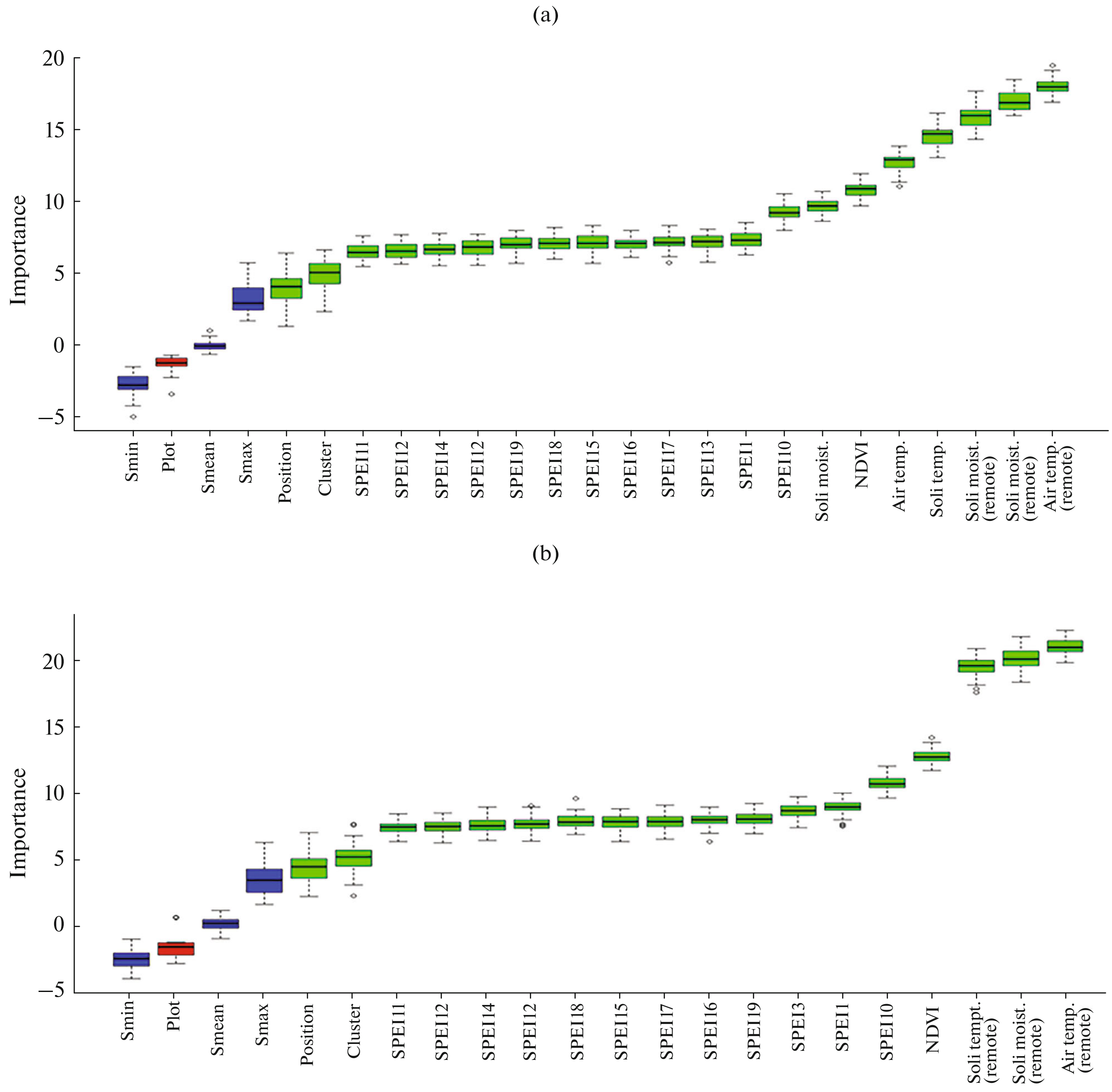

Fig. 3. Importance of predictors estimated by the Boruta algorithm: (a) all predictors, (b) predictors measured in the field were excluded. Smin, Smean, Smax—shadow predictors.

fewer predictors. The NDVI index had a smaller impact on accuracy, and the importance of the SPEI index was approximately at the same level, with the exception of SPEI10. After excluding field observations, the differences in the significance of the SPEI indices became more noticeable (Fig. 3b). For the simplified model of 12 predictors, we retained three SPEI indicators: for 1, 3, and 10 months. Thus, for the "simplified" model we selected only predictors based on remote sensing data: air and soil temperature, soil moisture, NDVI and the SPEI1, SPEI3, and SPEI10 indices.

Annual CO_2 Fluxes

The full and simplified models demonstrated comparable performance in both annual dynamics and accuracy metrics (Fig. 5, Table 2); annual values of CO_2 emissions for each approach did not differ when using both models. However, the results of different approaches differed significantly from each other (see Table 2). When evaluating the model supplemented with literature data on winter respiration, the annual emission value with direct extrapolation was 830.3 ± 6.4 g C/m^{2}year, i.e., the initial model overestimated the annual results by almost 1.4 times. When averaging

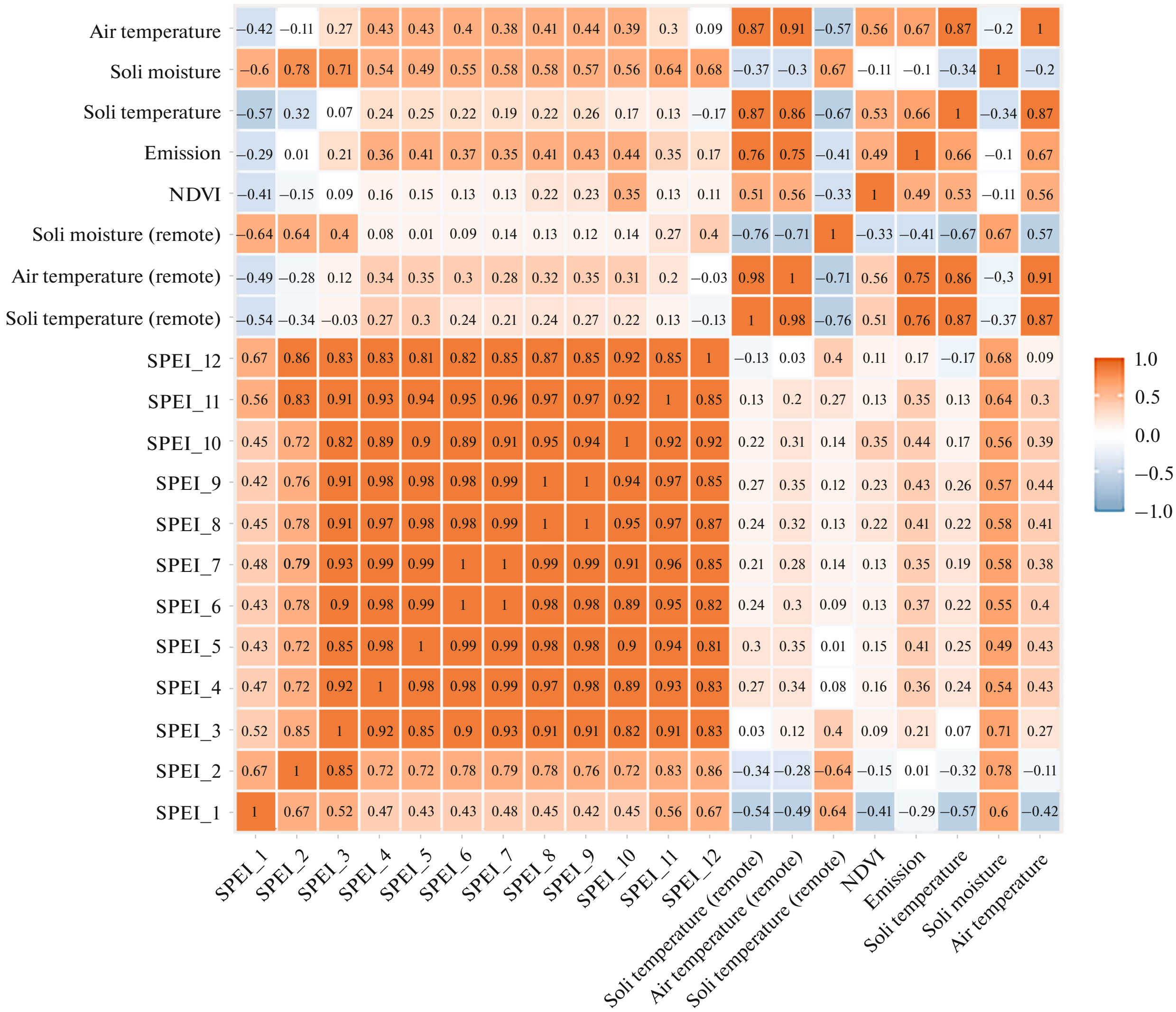

Fig. 4. Correlations of predictors with each other and with soil respiration rate.

the results of approaches based on classical regression, the annual flux was 851.6 ± 8.0 g C/m^{2}year. We found no significant differences between the calculation results and the SRBD data.

RESULTS AND DISCUSSION

Field Measurements

The obtained absolute values of soil respiration (1.52–9.81 g (C–CO_2)/m^2 day) were close to the values that are usually recorded for temperate latitude forests: up to 4.5 ± 0.8 [21], 2.9 ± 0.7 [22], 4.6–11.7 [23], 3.6–4.6 [24], and 1.3–14.4 [9, 25]. Seasonal dynamics characterized by maximum CO_2 emissions in the summer months was similar to the dynamics described for the southern taiga [26] and the northern taiga forests of Eastern Siberia [24] and Central Siberia [27]. In the second half of summer (between 220 and 240 days), despite the highest soil temperatures of the year (over 15°C), low humidity was the reason that soil respiration values hardly rose above 5 g (C–CO_2)/m^{2}day, although even at low temperatures but higher soil moisture, the respiration rate reached this value and even exceeded it. It is known that at extreme values of soil moisture (too low or too high), the absolute indicators of soil respiration decrease and its temperature sensitivity changes [10, 28]. Furthermore, despite its low correlation with the carbon dioxide emission rate, soil moisture had high “significance” for the model’s accuracy. This can be interpreted as a fact of its strong influence on soil respiration at certain points in time. Therefore, we conclude that soil respiration during the summer drought of 2022 was limited by its moisture content, and not by temperature, which was also noted in other studies [28].

Table 2. Comparison of annual soil CO_2 emissions from the forests of the Ural-Carbon carbon supersite (g C/m^2 year), estimated using different approaches and literature data (mean ± standard deviation, $n = 6$)

Approach	Model used	
	full $R^2 = 0.92$, $MSE = 0.22$	simplified $R^2 = 0.89$, $MSE = 0.31$
Direct extrapolation	1187.31 ± 45.03	1152.86 ± 7.83
Based on summer emission	966.99 ± 49.32	965.99 ± 10.35
Based on emission at $T > 5°C$	737.11 ± 27.73	737.15 ± 5.55
According to SRBD	All forests north of 55° N 751.85 ± 477.29 ($n = 170$)	Forests of the Russian Federation north of 55° N 687.35 ± 273.42 ($n = 39$)

SRBD—Soil Respiration Database [18].

Evidently, due to the dry summer conditions, spatial variability in CO_2 emissions was lower than temporal variability, as demonstrated by the minimal contribution of spatial predictors ("Cluster," "Position," "Plot") to the model's accuracy.

Selection of Predictors

In developing our simplified model, we intentionally prioritized temporal predictors through a selection process that balanced statistical metrics (predictive contribution and multicollinearity) with mechanistic interpretability of their effects on soil CO_2 efflux rates. The inclusion of SPEI1 accounts for immediate antecedent moisture conditions, effectively buffering against disproportionate respiration pulses following rewetting after drought episodes [10]. SPEI3's significance corroborates known hydrological legacy effects, particularly the demonstrated impact of spring soil moisture on annual carbon fluxes [2]. However, our current single-year analysis necessarily limits temporal inference—while SPEI3 may currently reflect measurement-date effects, multiyear data could reveal its stronger association with interannual May condi-

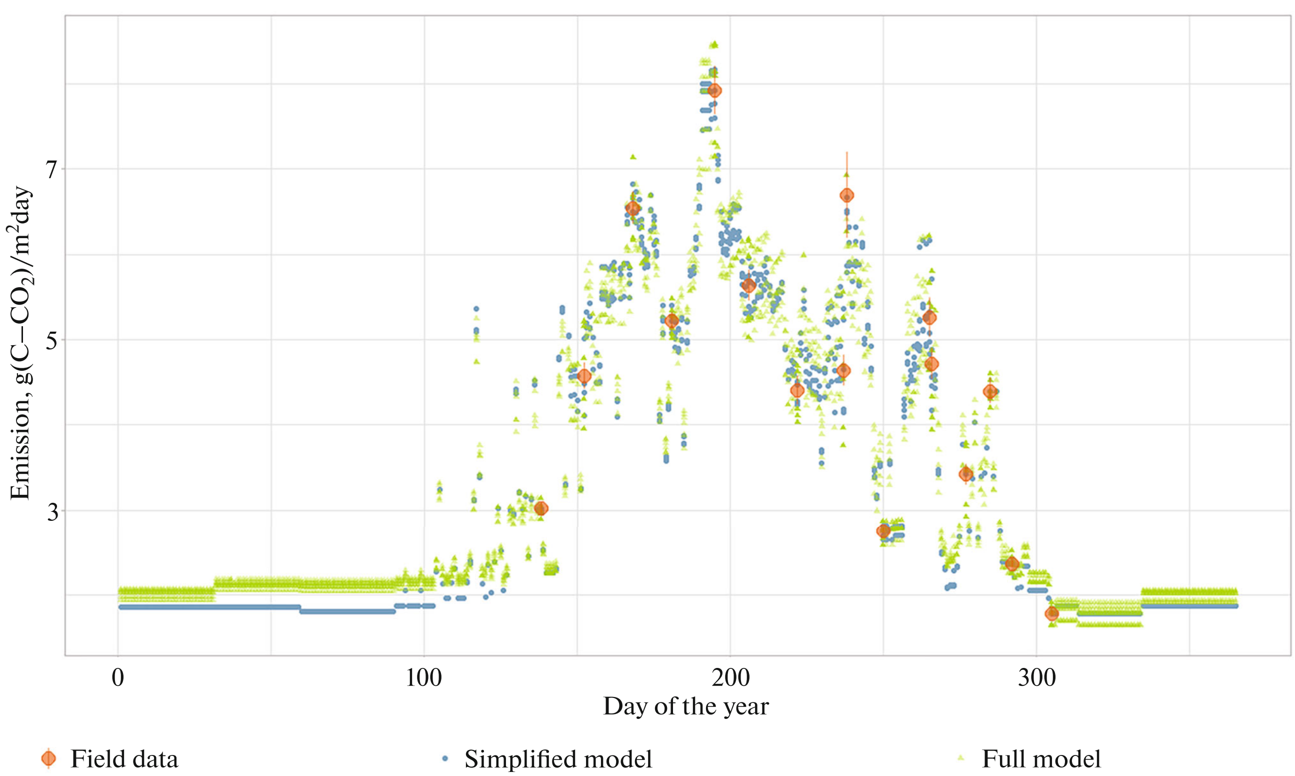

Fig. 5. Dynamics of soil respiration throughout the year.

tions. It is also likely that the high importance of SPEI10 is associated with the analysis of data for essentially one year, and when analyzing long-term dynamics it will be replaced by SPEI12 (i.e. what was the humidity level of the year preceding the measurements), similar to what we showed for the pine forests of the Middle Urals [25].

Annual Flows

Both the full and simplified models of the dependence of the soil emission rate on environmental factors based on an RF turned out to be higher in accuracy than the model for pine forests of the Middle Urals with a comparable set of predictors ($R^2 = 0.77$, $MSE = 0.8$) [25]. Their quality was also superior to a local model based on the RF algorithm for mountain forests in the southern Rocky Mountains ($R^2 = 0.44$, $MSE = 0.8$) [29] and a global scale model of northern hemisphere forests with a higher R^2 (up to 0.86, $MSE = 2.16$) [30].

The difference in the estimates of annual CO_2 fluxes from the soil obtained using different approaches is interesting. We can conclusively state that direct extrapolation of the RF model beyond its training data range led to overestimation. The point is the principle of operation of decision trees, used as a basis for this algorithm: when splitting by the extreme value of the predictor in the training sample, the algorithm assigns the same value of the target variable to the entire set located beyond this extreme point [31]. For example, in our model, the rate of soil respiration was the same at all soil temperatures below 3°C, which naturally does not correspond to reality at all, because at low soil temperatures, its respiration is especially sensitive to it and quickly decreases with decreasing temperatures [19, 32]. Winter CO_2 fluxes can vary by an order of magnitude while remaining quantitatively small (e.g., 0.5 g $C-CO_2/m^2$/day [33] or 0.2–0.3 at 0°C, decreasing to ~0.05 at −3°C [34]). This explains why incorporating literature-derived winter fluxes significantly improved model accuracy compared to direct extrapolation.

The more difficult question to answer is which of the two combined approaches gives values closer to reality? Each of them is essentially a classical regression model that takes into account only temperature, ignoring changes in other factors and having its own sources of uncertainty. They are based on a large amount of data: Soil Breathing in Russia [4] and the global SRBD database [3], but do not have absolute accuracy ($R^2 = 0.95$ and $R^2 = 0.81$, respectively), i.e., in each specific year the calculation results of these approaches may deviate from the ideal regression dependence by which they are described. Therefore, averaging the results of different approaches can have an ensemble effect, where the average of the different forecasts is closer to the true values than each individual forecast.

The strong agreement between field and remote sensing temperature data, coupled with satellites' greater predictive contribution, recommends prioritizing satellite data for soil respiration modeling. Beyond methodological advantages, this approach would standardize flux estimations across regions while minimizing instrumentation errors and observer bias.

CONCLUSIONS

In 2022, the CO_2 flux from soils of the dark coniferous forest at our carbon monitoring site showed no statistically significant increase compared to average values recorded for forests north of 55°N latitude. While these preliminary results require further validation, our study yielded several important methodological insights.

(1) Spatial variability within the our monitoring site proved minimal, with spatial factors contributing negligibly to model accuracy.

(2) Remote sensing data for soil and air temperatures demonstrated strong agreement with field measurements. Satellite-derived variables not only enhanced model precision but also offer standardized data acquisition across research teams.

(3) Direct Random Forest extrapolation without winter respiration data systematically overestimated annual fluxes. This bias can be mitigated either through minimal winter sampling or by employing combined methodological approaches.

(4) Predictor selection enabled development of a more interpretable model without compromising predictive performance, through retention of only the most significant environmental variables.

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ETHICS APPROVAL AND CONSENT TO PARTICIPATE

This work does not contain any studies involving human and animal subjects.

CONFLICT OF INTEREST

The author declares that he has no conflict of interest.

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