



Technical note: Soil MIR-FTIR spectral signatures reveal a measurable link to soil greenhouse gas flux potential

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Abstract. The growing reliance on nature-based solutions for climate change mitigation has increased the need for robust methods to assess soil greenhouse gas (GHG: CO₂, CH₄, N₂O) emissions. A key challenge is the upscaling of site-specific observations to improve predictions of the spatial distribution and magnitude of soil GHG fluxes. Upscaling is hindered by the laborious, costly, and time-consuming nature of soil flux measurements at the scale needed to generate sufficiently large datasets. Fourier-transform infrared (FTIR) spectroscopy is a cost-effective, high-throughput method that has demonstrated its ability to predict soil physicochemical properties. Since the magnitude of soil GHG fluxes is strongly influenced by these properties, FTIR may also serve as a basis for predicting soil GHG fluxes. In this study, we evaluated whether FTIR calibration models can be developed to predict soil GHG fluxes and organic matter decomposition rates directly from mid-infrared spectra. FTIR calibration and cross-validation were performed using soil samples collected across 20 wetland study sites in six European countries and linked to measured soil GHG fluxes and decomposition rates at the corresponding sampling sites. The results demonstrated that FTIR can be calibrated to reliably predict soil decomposition rates and heterotrophic respiration standardised at a given soil temperature. For decomposition rates, the root mean square error (RMSE) of FTIR-predicted values was 0.01 dd⁻¹, corresponding to approximately 17–53% of the interquartile range of observed rates. For heterotrophic respiration, the RMSE of 18 mg CO₂-C m⁻² h⁻¹ corresponded to 21–64% of the interquartile flux range. The findings also indicate FTIR's potential to identify biogeochemical risk areas or potential hotspots of CH₄ and N₂O emissions, effectively mapping the substrate-driven 'ultimate' controls even when 'proximate' environmental triggers (e.g., water table fluctuations) are absent.



1 Introduction

Fourier-transform infrared spectroscopy (FTIR) measures the absorption of infrared radiation by chemical bonds within the analysed material, thereby producing spectra that reflect the sample's chemical and physical properties. FTIR of the mid-infrared (MIR) region is widely used to characterise various organic and inorganic materials. Infrared soil spectra can be acquired near-instantaneously and contain detailed information on soil organic matter composition, mineralogy, and physicochemical characteristics (Stenberg et al., 2010; Rossel et al., 2016). Specifically, MIR-FTIR captures the fundamental vibrations of functional groups (e.g., aliphatic C-H, amide N-H, and carboxyl C=O) that serve as the primary substrates and catalysts for microbial metabolism. By integrating these diverse chemical signals into a single spectral signature, FTIR provides a 'metabolic fingerprint' of the soil's capacity for carbon and nitrogen turnover.

The increasing availability of large spectral libraries and advances in chemometric modelling have expanded the applicability of FTIR spectroscopy in environmental research and monitoring. In recent decades, the FTIR techniques have become increasingly applied in soil science due to their rapid, non-destructive, and cost-effective analytical potential (e.g., Margenot et al., 2023). Current MIR-FTIR techniques have been shown to have the ability to quantify soil organic carbon, total nitrogen, texture, pH, cation exchange capacity, bulk density, moisture content, and concentrations of various macro- and micronutrients, often with sufficient accuracy for large-scale soil assessment and monitoring applications (Sanderman et al., 2020; Mammadov et al., 2024; Kandel et al., 2018; Knox et al., 2015). This is particularly relevant in heterogeneous wetland ecosystems, where direct flux measurements are difficult to upscale.

Alongside soil properties and soil health indicators, there is a growing demand to quantify and map soil greenhouse gas (GHG) fluxes, particularly carbon dioxide (CO₂), methane (CH₄), and nitrous oxide (N₂O) fluxes, given their critical role in assessing the impacts of soil type and land use on climate change (Li et al., 2024). However, direct measurements of soil GHG fluxes are labour-intensive and time-consuming. A further challenge lies in spatial upscaling, the limited number of observations across space and the development of higher-tier approaches for estimating emissions. Despite increasing efforts in emission monitoring, soil GHG emission estimates still rely on emission factors; i.e. simplified coefficients that represent average emissions per unit area or activity, which are insufficient to capture the spatial and temporal variability of soil GHG fluxes. In addition, existing models are constrained by limited input data and validation. Consequently, the development of alternative (time-, labour- and cost-efficient) methods for evaluating soil GHG fluxes is urgently needed.

Easily measurable and widely recognised environmental drivers, such as soil temperature and moisture, are commonly used to model temporal variability in soil GHG fluxes and can often successfully describe short-term emission dynamics at individual sites (Davidson and Janssens, 2006; Hao et al., 2025; Reichstein et al., 2003). Temperature and soil moisture are the primary factors controlling variability in soil CO₂ flux and substantially influence CH₄ and N₂O fluxes (Schaufler et al., 2010; Hao et al., 2025). However, their applicability for broader spatial upscaling remains limited. While these factors can explain temporal fluctuations in fluxes, they are poor predictors of GHG magnitudes across different soils and ecosystems. Soil microbial activity and the magnitude of resulting soil GHG fluxes are strongly controlled by soil physicochemical



properties, including organic matter composition, nutrient availability, pH, texture, and hydrological characteristics, which regulate microbial activity and biogeochemical processes that produce and consume GHGs (Le Mer and Roger, 2001; Conant et al., 2011; Hénault et al., 2012). Higher concentrations of biogenic elements (e.g. nitrogen, phosphorus, potassium, calcium, and magnesium), combined with a more neutral soil pH, increase nutrient availability, which is associated with higher soil GHG emissions (Butlers et al., 2025). Although an increasing number of studies have demonstrated quantifiable relationships between soil physicochemical properties and soil GHG fluxes, the available datasets remain relatively limited for robust large-scale prediction approaches. One of the main constraints is that comprehensive soil characterisation substantially increases study costs and analytical workload, particularly when combined with the large number of spatially distributed GHG monitoring replicates required to capture landscape-scale variability adequately.

Due to its versatility, rapid analytical throughput, and cost-effective soil screening capabilities, FTIR spectroscopy may have substantial potential to address challenges associated with soil GHG emission assessment and spatial upscaling. Since FTIR spectroscopy can characterise a wide range of soil properties (Artz et al., 2008) that regulate microbial activity and biogeochemical processes responsible for GHG production and consumption, it may provide opportunities to reduce the dependence on labour-intensive conventional soil analyses through spectral data-based gap-filling approaches, or potentially even through calibration of soil spectral signatures in relation to the expected magnitude of soil GHG fluxes. Therefore, we posed the research question of whether mid-infrared spectral signatures of soil contain measurable information about soil decomposition and GHG fluxes. The objective of this study was to evaluate whether diffuse reflectance mid-infrared Fourier-transform spectroscopy can be directly linked to measured soil decomposition rates and GHG fluxes and whether spectral information alone may provide a basis for rapid assessment of soil GHG flux potential.

2 Materials and methods

2.1 Study sites

The study was conducted at 20 study sites (Figure 1) across six European countries (Belgium, Estonia, Spain, Finland, France, and Latvia) during 2024–2025. The sites represented a broad range of wetland ecosystems with mineral and organic soils distributed across Europe's latitudinal gradient, including temperate, hemiboreal, boreal, and subarctic climatic regions. The study network included rewetted peatlands, drained peatlands, peat extraction areas, riparian wetlands, treatment wetlands, wet forests, agricultural peatlands, and near-natural peatland ecosystems exposed to contrasting hydrological conditions, nutrient status, vegetation composition, and land-use histories (Table A1).

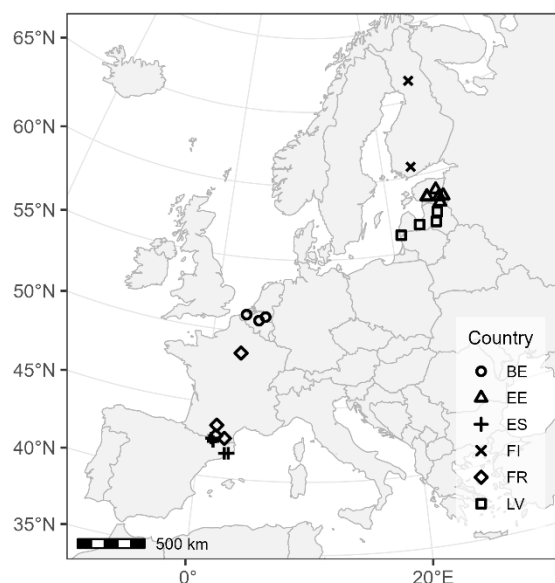


Figure 1: Locations of the study sites in Belgium (BE), Estonia (EE), Spain (ES), Finland (FI), France (FR), and Latvia (LV)

2.2 Data collection

2.2.1 Soil and greenhouse gas sampling

GHG fluxes were monitored at each study site using the closed, opaque-chamber method (Hutchinson and Livingston, 1993). Prior to GHG monitoring, soil measurement points were established using the trenching (root exclusion) technique (“Trench”) described by Bond-Lamberty et al. (2011) to characterise soil CO₂ heterotrophic respiration (HR), while separate measurement points with intact vegetation were used for CH₄ and N₂O flux measurements, with CO₂ measured as a secondary variable. Due to slight differences in sample plot designs, soil GHG fluxes were monitored in up to six replicates per measurement point type, with measurements conducted at least monthly across all seasons (spring, summer, autumn, winter), alongside parallel soil temperature measurements at a depth of 15 cm. Soil samples for laboratory analyses were collected during spring and summer to ensure comparable environmental conditions across the latitudinal gradient and were taken from the 0–10, 10–20, and 20–40 cm soil layers adjacent to the GHG monitoring points. Detailed information on soil GHG emission monitoring and soil sampling methodology is provided by Butlers et al. (2025). Separate scientific teams in each participating country were responsible for field measurements, sample collection, and initial processing of GHG monitoring data following a harmonised protocol.

Soil samples air-dried at a temperature below 40 °C were sent to the ISO 17025 certified laboratory of the Latvian State Forest Research Institute “Silava” for further FTIR analysis (detailed in Section 2.4). Once at least 12 consecutive months of soil GHG monitoring data had been collected for a given site, pre-processed datasets containing measured HR (mg CO₂–C m^{–2} h^{–1}) and N₂O and CH₄ fluxes (μg m^{–2} h^{–1}) were received from the research teams.



2.2.2 Soil decomposition rate and incubation-derived N₂O emission variables

Soil organic matter decomposition rates were assessed using the cotton strip assay, a standardised method widely applied as a proxy for microbial decomposition activity in soil (Latter et al., 1988; Latter and Howson, 1977). Unprimed cotton fabric strips were inserted vertically into the topsoil layer (approximately 10–12 cm deep) near the soil GHG monitoring and sampling points. The cotton strips were incubated in situ for multiple retrieval intervals, ranging from 2 to 12 weeks. During in-situ incubation, degradation of cellulose by soil microorganisms and soil fauna reduced the tensile strength of the cotton material. After retrieval, strips were cleaned, dried, and analysed for tensile strength loss using a tensiometer. The remaining tensile strength relative to unburied reference strips was used to estimate decomposition rates using an exponential decay function (Bärlocher et al., 2020). Decomposition rates were temperature-corrected and expressed in degree days (dd⁻¹), enabling comparison across sites with differing climatic conditions (Escarmena et al., *in review*).

Separate soil samples were collected from 0-10 cm soil layer within 5 m of the cotton strip setup to evaluate denitrification potential using the acetylene block assay and N₂O flux using laboratory soil incubation experiments following the protocol outlined in Crestey-Chury et al., 2026. Briefly, 20 mL of soil samples were incubated under anaerobic conditions (N₂-flushing) with excess nitrate (20 mL of 100 mg N L⁻¹ KNO₃). N₂O emission rates and denitrification potential were measured using a G200 N₂O Analyser (Geotech, QED Environmental Systems Ltd., Coventry, UK) with and without acetylene added to the headspace (10% v/v).

2.3 Greenhouse gas data preprocessing

The GHG emission data from the sites were grouped and linked to the nearest soil sampling point. Before assigning GHG emission values to specific soil samples, the data were processed differently for each GHG. Mean measured fluxes for CH₄ and N₂O were calculated for each monitoring point. In contrast, HR data were standardised by fitting regression models between measured CO₂ fluxes and corresponding soil temperature measurements. Each dataset was visually inspected, and exponential regression was applied when it provided a better fit to the observed relationship; otherwise, linear regression was used. The resulting site-specific models were then used to estimate soil CO₂ flux at standardised soil temperatures of 10 °C (HR10), 15 °C (HR15), and 20 °C (HR20). In rare cases where no clear relationship between HR and soil temperature was detected, mean measured HR values were assigned to the HR10 category, as the average soil temperature observed during the measurement period in these cases was close to 10 °C.

Similarly, when direct HR measurements were unavailable, CO₂ fluxes measured at points with intact vegetation were multiplied by 0.5 (Bond-Lamberty et al., 2004; Hanson et al., 2000) and then processed as HR datasets. This recalculation was performed because the use of data representing HR is crucial for FTIR calibration, as the spectral signature reflects the soil matrix's intrinsic organic matter pools, which drive heterotrophic processes, rather than the transient flux of recent photosynthates associated with autotrophic root respiration. GHG flux values were assigned to respective soil sampling points



collected from different depths (0–10, 10–20, and 20–40 cm), as well as to combined 0–20 cm soil samples composed of the 0–10 and 10–20 cm layers. These processed GHG values are further referred to as “measured” GHG fluxes.

2.4 FTIR calibration

150 Mid-infrared diffuse reflectance infrared Fourier transform spectroscopy (hereafter FTIR) was performed using a Bruker
INVENIO-S spectrometer (Bruker Optik GmbH, Ettlingen, Germany) equipped with an HTS-XT microplate reader accessory
and a liquid-nitrogen-cooled MCT detector, operating in the spectral range of 4000–400 cm^{-1} (instrument specification and
measurement settings are provided in the Supplementary Material). Spectral acquisition and subsequent calibration
development were performed using OPUS 8.5 software (Bruker), including the integrated QUANT module for partial least
155 squares (PLS) regression modelling.

Air-dried soil samples sieved to <2 mm particle size were placed into microplate sample cups in three replicate subsamples.
Samples were compressed in the cups using a matching-diameter steel rod (Seybold et al., 2026). The acquired interferograms
were Fourier transformed into absorbance spectra. Processed GHG fluxes (Section 2.3) and incubation-derived variables
(Section 2.2.2) were assigned to the acquired MIR spectra, and calibration models were developed using PLS regression.
160 Several calibration models were developed for each variable and soil-layer pair by testing different combinations of
preprocessing methods and spectral regions. Preprocessing approaches included no preprocessing, constant offset elimination,
straight-line subtraction, vector normalisation, min–max normalisation, multiplicative scatter correction, first- and second-
order derivatives, and combinations of derivatives with normalisation or scatter correction. Spectral regions were selected
automatically by the OPUS software using built-in optimisation approaches that iteratively identify combinations of spectral
165 regions and minimise prediction error. All calibration versions were evaluated using cross-validation implemented in the OPUS
software, where repeated calibration and validation cycles were performed by systematically excluding subsets of spectra from
model fitting and using them for validation. During subsequent cycles, excluded spectra were returned to the calibration subset
while different spectra were used for validation until all samples had been validated. To identify the best-performing model
for each variable-soil-layer pair, the performance of calibration versions was evaluated using the coefficient of determination
170 (R^2), root-mean-square error of cross-validation (RMSECV), and residual prediction deviation (RPD). The outputs of the best-
performing models (measured and FTIR-predicted values are provided in the Supplementary Material) were selected for
further detailed analysis.

2.5 Statistical analysis for calibration evaluation

The calibration performance of the FTIR models was evaluated using soil-sample-averaged FTIR-predicted values derived
175 from replicate FTIR measurements. Model performance was assessed using the coefficient of determination (R^2), Lin’s
concordance correlation coefficient (CCC), root mean square error (RMSE), mean absolute error (MAE), bias, RPD, and ratio
of performance to interquartile distance (RPIQ). The relationship between measured and FTIR-predicted values was assessed
using Pearson correlation analysis, from which R^2 and associated p -values were obtained. Lin’s concordance correlation



coefficient (CCC) was used to evaluate both the strength of correlation and the agreement between measured and predicted values relative to the 1:1 relationship, thereby accounting for both precision and systematic deviations from perfect agreement. CCC values range from -1 to 1 , with values approaching 1 indicating stronger agreement between measured and predicted values (Lin, 1989). RMSE was used to quantify the overall magnitude of prediction error, with greater sensitivity to larger errors. MAE was calculated as the mean absolute difference between predicted and measured values and therefore represents the average magnitude of prediction error irrespective of its direction. In contrast, bias was calculated as the mean signed difference between predicted and measured values and was used to evaluate systematic over- or underestimation by the models. RPD was calculated as the ratio between the standard deviation of measured values and RMSE, whereas RPIQ was calculated as the ratio between the interquartile range (difference between the 75th and 25th percentiles) of measured values and RMSE. Higher RPD and RPIQ values indicate improved predictive performance relative to the variability of the measured dataset. RPD values were interpreted according to commonly used soil spectroscopy criteria, where values below 1.5 indicate poor predictive performance, values between 1.5 and 2.0 indicate suitability for rough screening, values between 2.0 and 2.5 indicate good quantitative predictive ability, and values above 2.5 indicate very good to excellent model performance (Chang et al., 1986). To provide a relative measure of prediction uncertainty, RMSE values were evaluated against the interquartile range of measured values (Q3–Q1).

3 Results

Cross-validation of the emission prediction models revealed varying performance across the analysed GHG variables (Figure A1, Table A2). The best predictive performance was achieved for HR. Depending on the soil layer and standardised temperature level, RMSE values for HR prediction models ranged from 21 – 47% of the lower measured flux range (Q1) to 46 – 156% of the upper concentration range (Q3). The best-performing model was obtained for HR10 predicted using soil samples from the 20 – 40 cm layer (Figure 2), where RMSE corresponded to 21 – 64% of the interquartile concentration range. The model also demonstrated strong agreement between measured and FTIR-predicted values, with an R^2 of 0.81 and a concordance correlation coefficient (CCC) of 0.90 . The low model bias (0.07 mg CO₂–C m^{–2} h^{–1}) indicated minimal systematic over- or underestimation of flux. The predictive performance of this model was further supported by an RPD of 2.3 , indicating good suitability for quantitative prediction. The model performance indicates that FTIR allows prediction of expected CO₂ flux at a soil temperature of 10 °C with an error of around 15 mg CO₂–C m^{–2} h^{–1} (Figure 3, panel b), which translates into a mean relative error of $33.7 \pm 42.2\%$ (Figure 3, panel a).

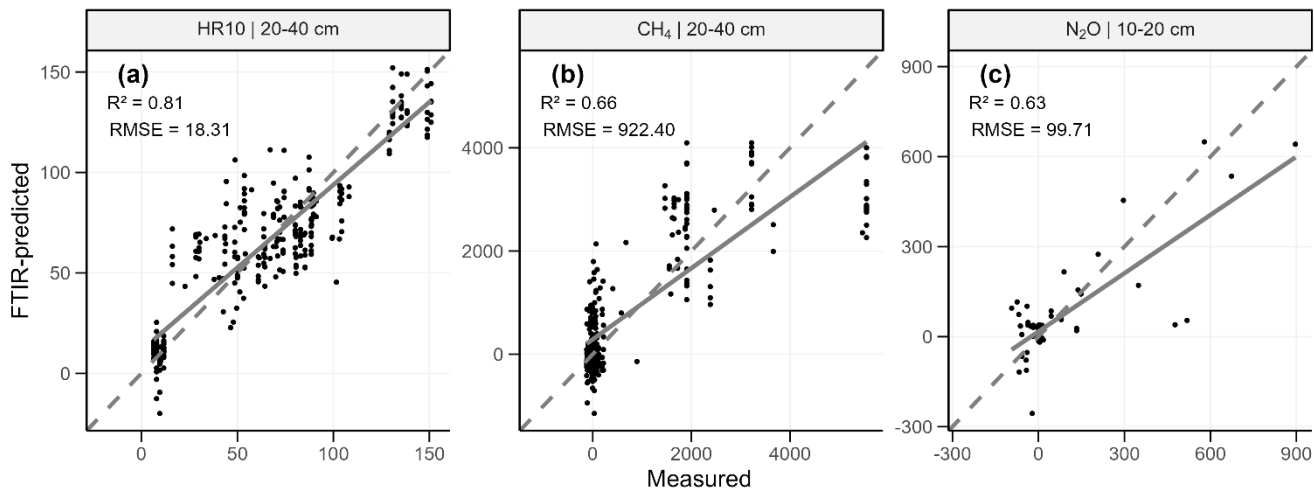


Figure 2: Field observed versus FTIR-predicted soil greenhouse gas emission (HR in $\text{mg CO}_2\text{-C m}^{-2} \text{ h}^{-1}$; CH_4 and N_2O in $\mu\text{g m}^{-2} \text{ h}^{-1}$) values for different soil layers. Panels (a) and (b) show heterotrophic respiration and CH_4 emissions predicted from spectra of the 20–40 cm soil layer, respectively, while panel (c) shows N_2O emissions predicted from spectra of the 10–20 cm soil layer. Points represent soil sample-averaged predicted values derived from replicate FTIR measurements. Solid lines represent linear regression fits, and dashed lines indicate the 1:1 relationship corresponding to perfect agreement between measured and predicted values. Separate panels are shown for each greenhouse gas and for the corresponding soil layer that provides the best calibration performance.

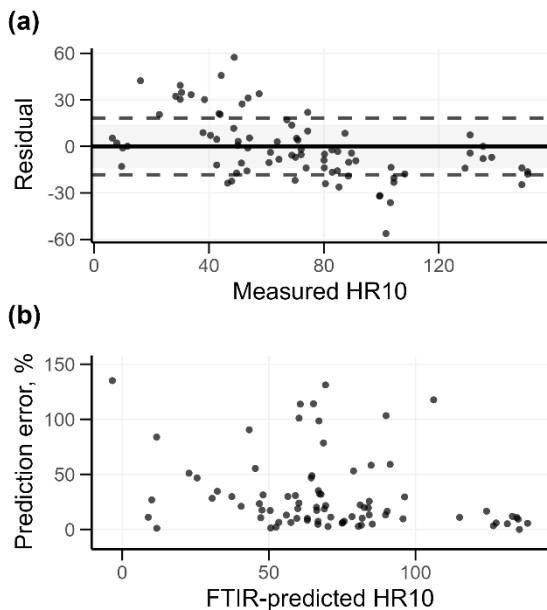


Figure 3: Diagnostic error plots for FTIR-predicted gas HR10 ($\text{CO}_2\text{-C m}^{-2} \text{ h}^{-1}$) by the 20–40 cm soil depth. (a) Prediction residuals (FTIR-predicted – measured) relative to measured fluxes; shaded areas and dashed lines define the calculated MAE and RMSE metrics,



respectively. (b) Relative prediction error (residual/measured) plotted against FTIR-predicted. Data points reflect averaged replicates for identical observed inputs to avoid noise from instances where the same measured HR10 values are assigned to multiple soil samples.

The predictive performance for CH₄ was weaker compared with that of the HR models. Although RMSE in the upper concentration range (Q3) remained comparatively moderate at 55%, prediction uncertainty in the lower concentration ranges was substantially higher, with relative prediction error reaching several orders of magnitude. The best-performing CH₄ prediction model was also obtained using the 20–40 cm soil layer. However, this model demonstrated lower predictive performance, with an R² of 0.66, a CCC of 0.80, and a MAE of 620 µg CH₄ m⁻² h⁻¹, indicating it was insufficiently reliable for quantitative prediction of CH₄ flux. Calibration of the N₂O prediction models using field measurement data was also unsuccessful, with both RMSE and MAE exceeding the interquartile range of measured fluxes multiple times across all soil layers, indicating very high prediction uncertainty and insufficient predictive reliability for quantitative application.

In contrast to field-measured N₂O fluxes, FTIR demonstrated a moderate ability to predict incubation-derived N₂O emissions (Figure 4). The best-performing model achieved an RMSE of 21 nmol N₂O hr⁻¹ g⁻¹, corresponding to an error of 32% at the upper concentration range (Q3). However, at low emission levels, the prediction error exceeded 100% of the measured values. Prediction accuracy improved with increasing emission rates, whereas substantial scatter at lower values indicates reduced precision near the lower end of the observed range. The resulting RPD of 1.7 suggests the model may be suitable for screening applications, but the current version lacks sufficient accuracy for quantitative prediction.

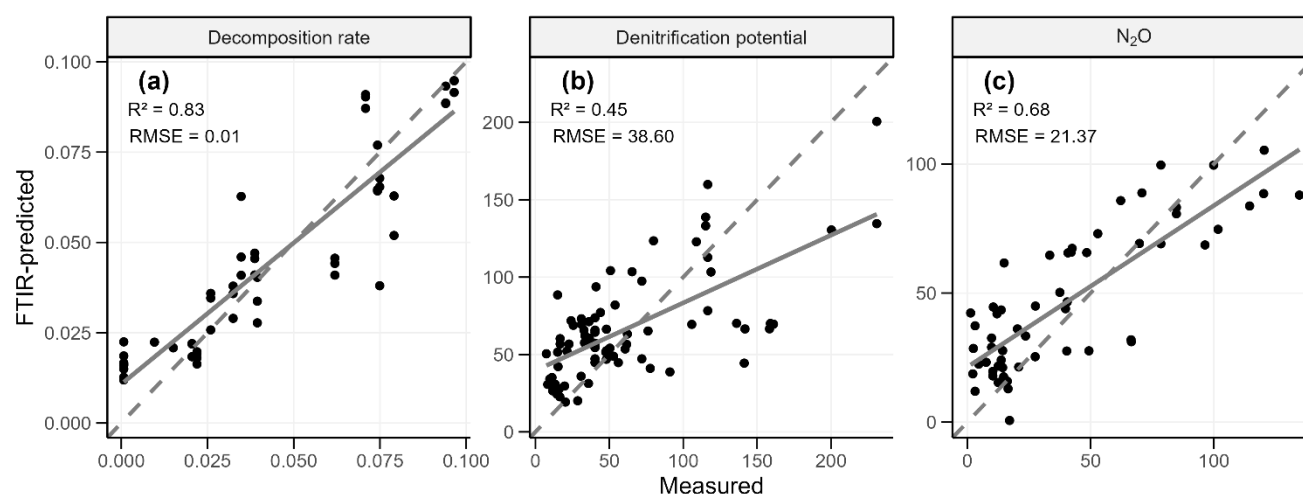


Figure 4: Observed decomposition rate (a, dd⁻¹), denitrification potential (b, nmol N₂O hr⁻¹ g⁻¹) and N₂O emissions (c, nmol N₂O hr⁻¹ g⁻¹) determined by soil incubation experiments versus FTIR-predicted values. Points represent soil sample-averaged predicted values derived from replicate FTIR measurements. Solid lines represent linear regression fits, and dashed lines indicate the 1:1 relationship corresponding to perfect agreement between measured and predicted values. Separate panels are shown for each variable.



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Calibration of denitrification potential prediction models was unsuccessful. The regression line deviated substantially from the 1:1 relationship, indicating strong systematic bias in the predictions. Most measured values were clustered below approximately 50 nmol N₂O hr⁻¹ g⁻¹, while the corresponding RMSE reached 38 nmol N₂O hr⁻¹ g⁻¹, resulting in insufficient discrimination between low and high denitrification potentials and poor predictive performance (Figure 4). The wide scatter of data points across the observed range further reflects high prediction uncertainty and limited agreement between measured and predicted values.

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In contrast, the decomposition rate showed promising calibration results (Figure 4). Strong statistical agreement between measured and FTIR-predicted values was demonstrated by a high coefficient of determination ($R^2 = 0.83$) and a low RMSE of 0.01 dd⁻¹. The regression line was close to the 1:1 relationship, which indicates limited systematic bias in the predictions. A slightly increased scatter of points at higher decomposition rates suggests some variability in prediction accuracy towards the upper end of the observed range. This corresponded to a prediction error ranging from 17% to 53% across the measured values' interquartile range. Furthermore, the RPD value of 2.4 indicated good quantitative predictive ability, suggesting considerable potential for FTIR-based assessment of soil organic matter decomposition activity.

4 Discussion

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4.1 Heterotrophic respiration

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This study aimed to evaluate whether diffuse reflectance mid-infrared Fourier-transform spectroscopy can predict soil GHG fluxes. The results showed particularly strong potential for predicting soil CO₂ flux. The HR calibration delivered strong predictive performance, even though the calibration dataset combined directly measured HR with approximated HR values derived from ecosystem respiration values. This likely added uncertainty to the reference dataset, which was reflected in calibration execution. Still, the predictive performance suggested that the used MIR spectral signatures effectively captured information about soil properties and biogeochemical processes that affect HR.

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Additional support for this interpretation came from the successful calibration of soil organic matter decomposition rates. Decomposition is one of the key processes that control soil carbon turnover (Conant et al., 2011) and is closely linked to microbial activity, which produces CO₂ in soils (Kuzyakov, 2006). The strong agreement between measured and FTIR-predicted decomposition rates indicates that MIR spectra contain information related to the physicochemical characteristics of soils that govern organic matter decomposition, enabling indirect assessment of decomposition rates. This observation provides mechanistic support and a proof of concept for using FTIR to predict soil GHG fluxes. The finding aligns with the established relationships between decomposition activity and soil properties, including organic matter content, carbon concentration, C:N ratio, pH, nutrient availability, and other factors that affect microbial activity (Davidson and Janssens, 2006; Schmidt et al., 2011; Lehmann and Kleber, 2015).

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While soil physicochemical and biogeochemical properties govern the magnitude of fluxes that can be expected from a soil (Smith et al., 2018), instantaneous fluxes at any given time are strongly influenced by transient environmental factors, such as temperature, oxygen availability, and hydrological conditions (Davidson and Janssens, 2006; Smith et al., 2018), which may vary independently of the soil physicochemical properties captured by FTIR spectra. This interpretation is supported by our approach to calibration, which uses temperature-standardised HR data, with CO₂ emissions normalised to defined soil temperatures before calibration. Therefore, the FTIR models developed should be considered to predict the soil GHG emission potential, defined as the expected magnitude of fluxes under prevailing site conditions shaped by long-term soil development and management, rather than instantaneous GHG fluxes at a specific point in time.

Interestingly, the best predictive performance for HR was achieved using spectra from deeper soil layers (20–40 cm) rather than from the topsoil (0–20 cm), where CO₂ production would intuitively be expected to be greatest. One possible explanation is that the deeper soil layer represents more stable inherent soil properties that control carbon turnover (Tenhovirta et al., 2026) and are less influenced by transient environmental variability. Furthermore, the superior performance of the 20–40 cm layer suggests that deep-soil MIR signatures integrate the 'legacy' of long-term carbon accumulation and stabilisation. While surface layers are more metabolically active, their spectral signals may be 'noisier' due to fresh, un-decomposed litter, whereas the deeper layers provide a more consistent baseline of the soil's ultimate greenhouse gas potential.

4.2 CH₄ and N₂O fluxes

The model performed less well in predicting measured field fluxes of CH₄ and N₂O. However, measurable relationships between observed and FTIR-predicted values were detected, suggesting that the soil spectral signature contains information associated with factors that regulate these fluxes. This interpretation is supported by the successful prediction of incubation-derived N₂O flux under controlled laboratory conditions, where the influence of short-term environmental variability was minimised (Bedford et al., 2006). The poorer predictive performance observed for the field-measured CH₄ and N₂O fluxes is therefore likely due to the episodic, process-driven nature of these fluxes, which depend on short-term environmental conditions (Le Mer and Roger, 2001; Smith et al., 2018) not explicitly captured in soil spectral signatures, particularly at low flux levels where emissions are more strongly controlled by environmental conditions rather than stable soil properties. This represents the 'proximate-ultimate' driver decoupling: while MIR spectra accurately quantify the soil's ultimate capacity to produce CH₄ or N₂O (e.g., via total N or anaerobic carbon pools), the proximate timing of the flux is governed by stochastic variables like water table height or sudden nitrate pulses. Future calibrations may therefore benefit from a hybrid approach, weighting spectral potential with real-time moisture data.

In addition, prediction performance differed among soil layers. CH₄ prediction performed better when calibrated using deeper soil layers, whereas N₂O prediction performance was highest for the intermediate layer at 10–20 cm depth. The strongest N₂O prediction performance by this layer may indicate that this soil depth better reflects the biogeochemical zone where the availability of substrates for nitrification and denitrification, aeration status, and nitrogen cycling processes most strongly influence N₂O production potential (Jahangir et al., 2012). Surface layers may be too strongly affected by transient



environmental conditions and recent litter inputs, while deeper layers may contain weaker nitrogen-related spectral signatures relevant to N₂O generation. These observations are consistent with current understanding of soil GHG production processes, as different soil layers encode distinct physicochemical and biogeochemical information (Tenhovirta et al., 2026) relevant to specific GHG pathways. Deeper soil layers are more closely associated with hydrological conditions and anaerobic processes that influence CH₄ production (Mcnicol et al., 2026; Conrad, 2020; Le Mer and Roger, 2001). In contrast, topsoil properties are more strongly linked to microbial nitrogen transformations under aerobic conditions that govern N₂O flux (Robertson and Groffman, 2015).

The current results should not be interpreted as evidence against the appropriateness of FTIR for assessing CH₄ and N₂O emission potential. The prediction performance could be improved with larger datasets combined with a more structured approach that encompasses a wider range of short- and long-term environmental conditions, ecosystem types, management status and emission magnitudes. Calibration data were limited, and model performance may have been further limited by the inclusion of mineral and organic soils within the same calibration data set. These soil groups differ substantially in their physicochemical properties, organic matter composition, and biogeochemical processes, potentially introducing additional complexity into the calibration procedure. Future studies should investigate whether different calibration models for mineral and organic soils, or for their specific layers, would enhance predictive performance. Nevertheless, even in its current form, the method shows potential to identify soils associated with elevated emission risk. It may serve as a practical screening tool for locating CH₄ and N₂O emission hotspots.

4.3 Validation and potential applications

The developed and evaluated prediction models were not validated using an independent external dataset. Although cross-validation provides a useful assessment of model performance, it may overestimate predictive accuracy compared with external validation (Wold et al., 2001). Nevertheless, the reliability of the reported performance metrics is supported by the substantial environmental heterogeneity represented in the calibration dataset, which included samples from multiple European countries encompassing mineral soils, highly decomposed organic soils, and peat soils. The high diversity in the dataset suggests that the observed relationships are not limited to a narrow set of soil types or site conditions.

To ensure the reliability and practical applicability of the developed HR prediction models, future studies should validate them on independent datasets. For CH₄ and N₂O, the potential of FTIR to identify emission hotspots and, potentially, to support quantitative emission prediction should be further investigated using substantially larger calibration and validation datasets. Thus, the current results support continued development towards a practically applicable FTIR-based method for assessing soil GHG emission potential.

A robustly calibrated and independently validated method could enable high-throughput, cost-effective FTIR-based mapping of soil HR potential and GHG emission hotspots. Such an approach could be implemented either through dedicated soil inventory campaigns or by integration into existing soil monitoring and inventory programmes. A particular advantage of the method is its potential to utilise already georeferenced soil samples stored in soil archives and spectra libraries (Tóth et al.,



2013; Rossel et al., 2016; Id et al., 2025), thereby leveraging existing resources to generate new information on soil GHG emission potential without requiring extensive additional field measurements. This approach bridges the gap between point-scale chamber measurements and landscape-scale modelling. By integrating these spectral proxies into global initiatives such as the Open Soil Spectral Library (OSSL), we can initialise Earth System Models with spatially explicit 'metabolic starting points,' thereby significantly reducing the uncertainty associated with current carbon turnover assumptions in wetland ecosystems.

The resulting maps could support the identification of areas at risk of elevated GHG emissions, facilitating the targeted climate change mitigation measures and the more efficient allocation of monitoring resources. In addition, they could also help prioritise research efforts by identifying sites with the greatest potential for carbon loss from soil through decomposition and other GHG emissions.

5 Conclusions

This study demonstrated that diffuse reflectance mid-infrared Fourier-transform infrared (FTIR) spectroscopy contains measurable information on soil GHG fluxes and associated biogeochemical processes. The most successful calibration was achieved for soil heterotrophic respiration standardised to a defined temperature, where predictive models showed good quantitative performance despite the soil heterogeneity represented in the calibration dataset. Successful prediction of soil decomposition rates further supported the interpretation that MIR spectra capture information about soil carbon turnover processes that underlie CO₂ production. The ability of FTIR to predict both decomposition rates and heterotrophic respiration suggests that soil spectral signatures reflect the biological processes that drive soil carbon cycling, providing mechanistic support and proof of concept for its use in assessing soil CO₂ flux.

Prediction of field-measured CH₄ and N₂O fluxes was less successful. However, the observed relationships between measured and FTIR-predicted values, together with the successful prediction of incubation-derived N₂O emissions, indicate that soil spectral signatures contain information related to the factors regulating these fluxes. The weaker predictive performance is likely attributable to the episodic nature of field-measured CH₄ and N₂O fluxes, which makes it difficult to derive representative reference emission values for FTIR calibration from limited temporal monitoring data.

The results suggest that FTIR spectroscopy has considerable potential as a rapid and cost-effective method for assessing soil GHG flux potential, i.e. the capacity of a soil to act as a source or sink of GHGs under specific environmental conditions determined by soil physicochemical and biogeochemical characteristics. Further improvements may be achieved through larger calibration datasets, separate calibrations for contrasting soil groups or layers, the development of more advanced approaches for deriving representative reference emission values from field measurements, and independent external validation. While CO₂ fluxes were standardised to defined temperature conditions before calibration, CH₄ and N₂O calibrations relied on mean measured fluxes. Future studies thus may improve predictive performance by developing approaches that better account for the episodic nature and environmental controls of CH₄ and N₂O fluxes when deriving reference values for FTIR calibration.



We propose that 'GHG Flux Potential' be formally recognised as a standardised soil trait, analogous to Cation Exchange Capacity or Soil Organic Carbon. By using standardised temperature (e.g., HR10), we move from reporting what the soil emitted on a specific day to reporting what the soil is capable of emitting, a metric that is far more valuable for long-term climate sensitivity mapping and regional upscaling. Following further developments, FTIR could support a high-throughput and cost-effective approach for the quantitative prediction of soil GHG emission potential and the identification of GHG emission hotspots, thereby contributing to the development of soil monitoring, GHG assessment, and climate change mitigation frameworks.

Data availability

Measured and FTIR-predicted values used to produce the results presented are provided in the Supplementary Material.

Author contributions

ABu conceptualised the research, prepared the methodology, curated the data, and prepared the original draft; ZAZ operated the FTIR and performed calibration; ABā and JP provided critical review; AL, KS, TL, JT, FS acquired funding. NC and RD conducted incubation lab experiments. KS, TS, JJ, TL, JT, LE, SP, and FS participated in soil sampling and GHG data collection from Estonia, Finland, France, and Spain, and reviewed the manuscript. LE, NP, SP, FS, and TL conducted cotton strip assay measurements.

Competing interests

The authors declare no conflicts of interest.

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climate change mitigation targets in Latvia's land use, land-use change, and forestry (LULUCF) sector for reducing greenhouse
395 gas (GHG) emissions and promoting carbon dioxide (CO₂) sequestration in forest management.

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Appendix

Country	Site	Coordinates	Soil type	Description
Finland	Kivalo	66°20'21.1"N, 26°36'25.5"E	Peat soil	Drained peatland forest. Partly herb-rich type II, partly V. myrtillus type II drained peatland forest site type. Mixed spruce & birch stand. Spruce is the dominant tree.
Finland	Lettosuo	60°38'35.0"N, 23°57'35.8"E	Peat soil	Drained peatland forest. Vaccinium myrtillus type II drained peatland forest site. Mixed pine-dominated stand.
Estonia	Laiuse	58°47'26" N, 26°31'45" E	Peat soil	Open peatland. Vegetation includes common heather (<i>Calluna vulgaris</i>), Hare's-tail cottongrass (<i>Eriophorum vaginatum</i>), crowberry (<i>Empetrum nigrum</i>), Scots pine (<i>Pinus sylvestris</i>), polytrichum mosses, and sedges (<i>Carex</i> spp.).
Estonia	Kuresoo	58°28'28.43" N, 25°12'30.26" E	Peat soil	Open peatland. Dwarf bog pine trees, forest floor vegetation includes patches of hummocks, wet cotton grass. Sphagnum moss is dominant (Salm et al., 2012).
Estonia	Ess-soo	57°54'53" N, 26°41'51" E	Peat soil	Open peatland. Natural revegetation dominated by cranberry, crowberry (<i>Empetrum nigrum</i>), Hare's-tail cottongrass (<i>Eriophorum vaginatum</i>), common heather (<i>Calluna vulgaris</i>), and white beak-sedge (<i>Rhynchospora alba</i>).
Latvia	Kengi	57° 19' 21.8" N, 26° 4' 12.9" E	Peat soil	Reforested farmland. Reforested with black alder (<i>Alnus glutinosa</i> (L.) Gaertn). Hemiboreal vegetation zone.
Latvia	Kaigu	56° 42' 47.0" N, 23° 36' 25.7" E	Peat soil	Agroforestry plantation. Blueberry and cranberry plantations, Scots pine (<i>Pinus sylvestris</i> L.), hemiboreal vegetation zone (Bārdule et al., 2024).
Latvia	Plavi	56° 41' 37.9" N, 25° 41' 17.1" E	Peat soil	Drained peatland forest. Characterised by a birch stand. Afforested with silver birch (<i>Betula pendula</i> Roth). Hemiboreal vegetation zone (Butlers et al., 2025).
Latvia	Rucav	56° 13' 48.5" N, 21° 7' 26.1" E	Peat soil	Agroforestry and reforested farmland. Hybrid poplar, reforested with spruce (<i>Picea abies</i> (L.) Karst.). Hemiboreal vegetation zone.
Belgium	Zuidleie Valley	51° 9' 16.1" N, 3° 16' 6.3" E	Peat soil	Open peatland. Molinia (<i>Molinia caeruleae</i>) meadow.
Belgium	Zwarte Beek	51° 5' 27.7" N, 5° 19' 21.5" E	Peat soil	Floodplain with partially buried peat. Quacking fen.
Belgium	Dyle Valley	50° 49' 10.8" N, 4° 38' 46.6" E	Alluvial soil	Alluvial floodplain with buried peat. Dominated by Alopecurion, Calthion (<i>Calthion palustris</i>), Common reed (<i>Phragmites australis</i>).
France	Rampillon	48° 32' 19.3" N, 3° 3' 46.6" E	Alluvial soil	Constructed wetland receiving agricultural runoff. Dominated by blue rush (<i>Juncus inflexus</i>), common reed (<i>Phragmites australis</i>), vernal water-starwort (<i>Callitriche palustris</i>), and sedge (<i>Carex riparia</i>) (Lebrun et al., 2019; Mander et al., 2021).
France	Confluent	43° 31' 19.5" N, 1° 24' 54.0" E	Alluvial soil	Floodplain. Gallery forests of white willow are often accompanied by black poplar and oxyphyllous ash (Kanaan et al., 2025).



Country	Site	Coordinates	Soil type	Description
France	Bernadouze	42° 48' 00" N, 1° 25' 12" E	Peat soil	Mountain open peatland. The site is characterized by the presence of scattered dwarf pines and ashes in the driest patches, while in the wetter, lower-lying areas pioneer willows, dwarf juniper, and thorn bushes occur (Garisoain et al., 2024).
France	Col de Jau	42°41'19.7"N, 2°14'02.4"E	Peat soil	Mountain open peatland. Dominated by different Sphagnum and vascular plant species. single dominant Sphagnum species is <i>S. warnstorffii</i> (Kanaan et al., 2025).
Spain	Estanyeres	42° 36' 26.3" N, 1° 3' 30.8" E	Peat soil	Mountain open peatland. Rich fen with <i>Carex davalliana</i> (Ninot et al., 2025).
Spain	Rubió	42° 24' 39.6" N, 1° 14' 17.5" E	Peat soil	Mountain open peatland. Acidic fen of <i>Carex nigra</i> (Ninot et al., 2025).
Spain	Tordera	41° 42' 44.5" N, 2° 43' 21.6" E	Alluvial soil	Floodplain. Mixed forest of <i>Quercus robur</i> and <i>Fraxinus angustifolia</i> (Poblador, 2018)
Spain	Cànoves	41° 40' 57.5" N, 2° 21' 20.3" E	Alluvial soil	Riparian forest intermittently receiving secondary-treated wastewater. Dominated by <i>Alnus glutinosa</i> accompanied by <i>Platanus x Hispanica</i> , <i>Fraxinus excelsior</i> and <i>Ulmus minor</i> . Abundant macrophytes such as <i>Carex</i> (Escarmena et al., 2025, 2024).

Table A1: Summary of all study sites, including the country, name of the site, coordinates, soil type, and a brief description of the wetland type and vegetation.

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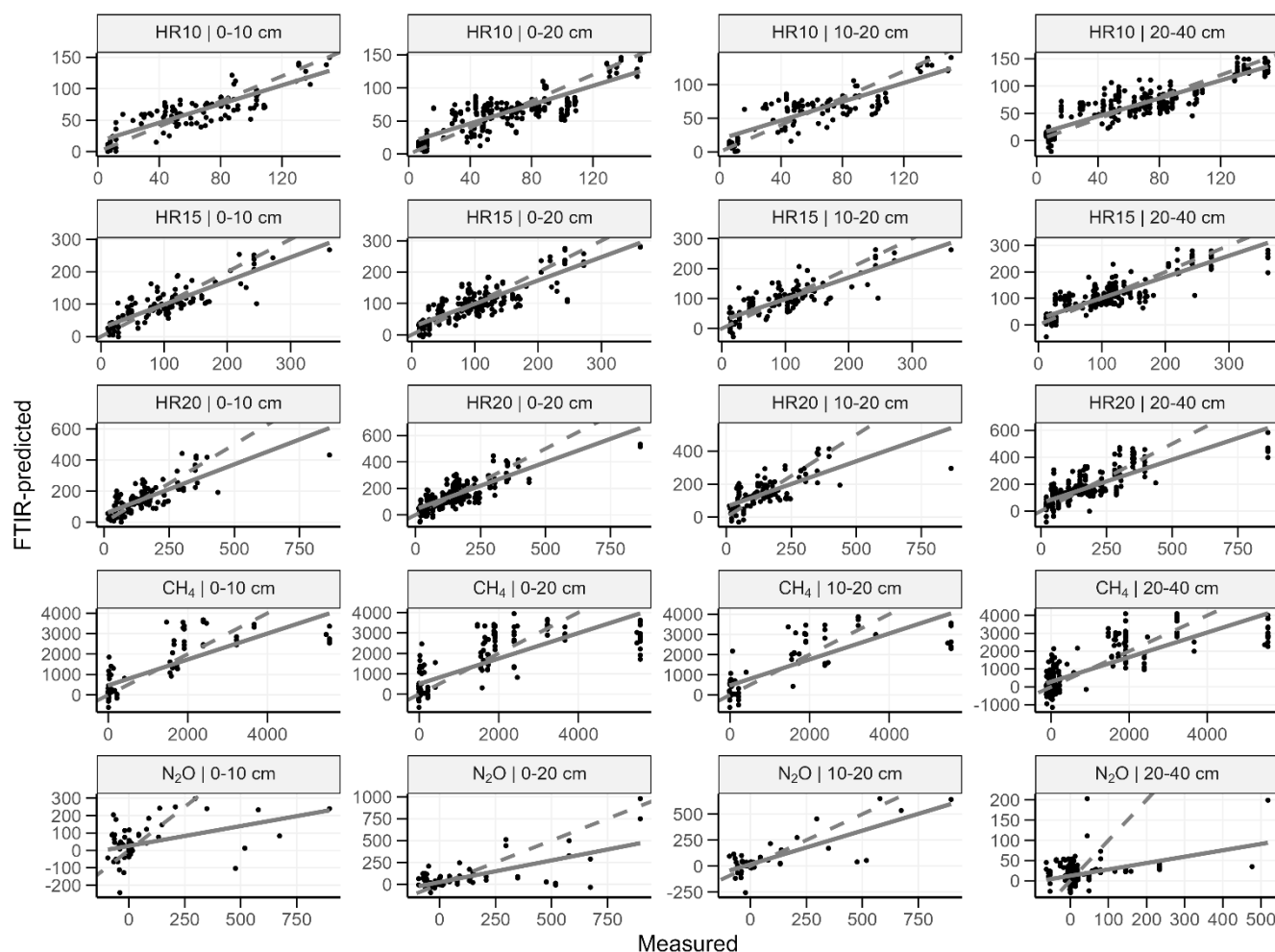


Figure A1: Measured versus FTIR-predicted soil heterotrophic ($\text{CO}_2\text{-C m}^{-2} \text{ h}^{-1}$) respiration, CH_4 and N_2O ($\mu\text{g m}^{-2} \text{ h}^{-1}$) emissions for different soil layers. HR10, HR15, and HR20 correspond to heterotrophic respiration at soil temperatures of 10, 15, and 20 °C, respectively. Points represent soil sample-averaged predicted values derived from replicate FTIR measurements. Solid lines represent linear regression fits, and dashed lines indicate the 1:1 relationship corresponding to perfect agreement between measured and predicted values. Separate panels are shown for each greenhouse gas-soil layer combination, with independently scaled axes to improve visualisation of differences in prediction performance across variables and layers.



Parameter	Layer	n	IQR	R ²	CCC	RMSE	MAE	Bias	RPD	RPIQ
CH ₄	0-10 cm	87	9...1906	0.63	0.77	1020.06	657.83	-3.83	1.64	1.86
CH ₄	0-20 cm	172	9...1906	0.61	0.76	1046.94	647.9	12.03	1.6	1.81
CH ₄	10-20 cm	85	9...1906	0.62	0.77	1031.68	660.04	4.18	1.63	1.84
CH ₄	20-40 cm	286	-13...1650	0.66	0.8	922.4	620.28	13.48	1.71	1.8
HR10	0-10 cm	116	42...86	0.72	0.84	19.24	15.62	0.31	1.89	2.27
HR10	0-20 cm	230	43...87	0.7	0.82	20.06	15.91	-0.16	1.82	2.2
HR10	10-20 cm	114	43...87	0.68	0.81	20.7	16.55	-0.04	1.78	2.13
HR10	20-40 cm	287	28...89	0.81	0.9	18.31	13.89	0.07	2.29	3.28
HR15	0-10 cm	118	43...122	0.72	0.84	35.77	26.82	-0.64	1.9	2.19
HR15	0-20 cm	234	43...121	0.73	0.84	35.24	27.19	-0.19	1.92	2.21
HR15	10-20 cm	116	43...121	0.67	0.81	38.69	29.14	-0.89	1.74	2
HR15	20-40 cm	284	35...135	0.78	0.88	36.39	26.11	0.16	2.13	2.75
HR20	0-10 cm	116	66...186	0.59	0.76	76.23	53.38	-0.42	1.56	1.59
HR20	0-20 cm	232	62...185	0.67	0.81	68.84	50.97	-0.33	1.73	1.78
HR20	10-20 cm	116	54...180	0.5	0.69	83.82	53.77	-1.71	1.42	1.51
HR20	20-40 cm	284	66...201	0.6	0.76	87.9	57.93	0.84	1.58	1.54
N ₂ O	0-10 cm	87	-18...4	0.18	0.36	148.75	76.27	-7.89	1.11	0.14
N ₂ O	0-20 cm	172	-4...4	0.47	0.65	119.26	60.9	1.64	1.38	0.07
N ₂ O	10-20 cm	85	0...5	0.63	0.78	99.71	56.47	0.11	1.66	0.04
N ₂ O	20-40 cm	277	1...13	0.15	0.27	54.9	28.95	-1.45	1.09	0.22
DR	0-10 cm	53	0.02...0.07	0.83	0.9	0.01	0.01	0	2.44	4.19
DP	0-10 cm	77	25.6...77.7	0.45	0.61	38.6	30.1	4.96	1.34	1.35
N ₂ O*	0-10 cm	57	12.5...66.4	0.68	0.78	21.4	17.5	6.2	1.69	2.52

Table A2: Performance metrics of FTIR calibration models across different soil layers. HR10, HR15, and HR20 correspond to heterotrophic respiration (CO₂-C m⁻² h⁻¹) at soil temperatures of 10, 15, and 20 °C, respectively. DR = decomposition rate (dd⁻¹); DP = denitrification potential (nmol N₂O hr⁻¹ g⁻¹); N₂O* = N₂O emissions measured during laboratory incubation (nmol N₂O hr⁻¹ g⁻¹); CH₄ and N₂O in µg m⁻² h⁻¹. Model performance was evaluated using soil sample-averaged predicted values derived from replicate FTIR measurements. Metrics include the coefficient of determination (R²), Lin's concordance correlation coefficient (CCC), root mean square error (RMSE), mean absolute error (MAE), bias, residual prediction deviation (RPD), and ratio of performance to interquartile distance (RPIQ). Interquartile range (IQR) represents the range between the first (Q1) and third (Q3) quartiles of measured values. Higher values of R², CCC, RPD, and RPIQ indicate improved predictive performance, whereas lower RMSE, MAE, and absolute bias values indicate lower prediction error.