Estimating the mineralizable form of organic carbon (OC) in bio-based fertilizers using non-destructive spectroscopy techniques

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Abstract

The estimation of organic carbon (OC) mineralization is desirable for both agronomic and environmental reasons. To estimate the rate of mineralization, the NIR and MIR spectroscopy has been used in past, which link the rate of mineralization with the composition of biobased fertilizers. The current study evaluate the potential of NIR and MIR spectroscopy in combination with machine learning techniques to estimate the mineralizable form of OC to CO_2. Carbon mineralization from 85 different potential soil organic amendments (composts, manures, plant residues and biosolids) was quantified under controlled environmental conditions over a 547-day incubation period. Cumulative mineralization of organic carbon from the amendments was fitted to a two-pool exponential model. A wavelength selection method followed by partial least squares regression was adapted to estimate the fast-decomposing pool (C_f) and slow decomposing pool (C_s). The Cf and Cs values has been estimated with coefficient of determination value (R2=0.94) and root mean square error (RMSE=19.17). The obtained result suggests that NIR and MIR spectroscopy has the potential estimate and quantify the plant available for form of diverse set of biobased fertilizers.

Objectives

- To Quantify the mineralization form of OC to CO_2 using NIR and MIR spectroscopy
- Application advanced machine learning techniques to improve the estimation

Sensor Technologies

- Visible Near Infrared (Vis-NIR)
- Mid Infrared (MIR)

Material and Method

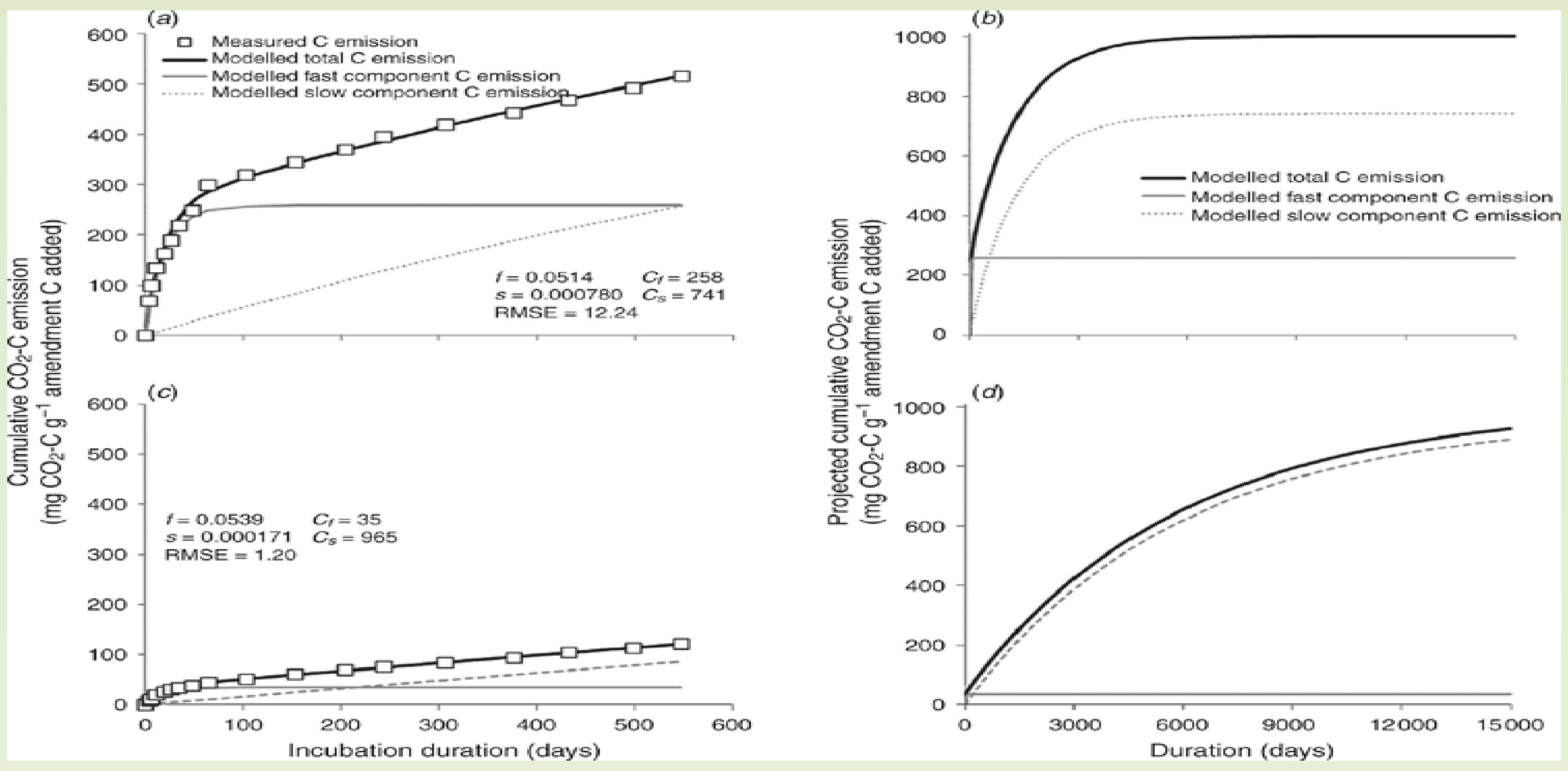

Fig 1. Measured and modelled cumulative CO_2 -C emission from organic amendments exhibiting high (a) and low (c) CO_2 -C emission over the duration of the incubation. Projected cumulative mineralisation beyond the incubation duration derived for the same high (b) and low (d) CO_2 -C emitting amendments.

$C_{min}(t) = C_f\left(1 - e^{-ft}\right) + C_s\left(1 - e^{-st}\right)$ (1)

When t=0, $C_{min}(0) = 0$, and when t=∞ equation 1 become:

$C_{min}(\infty) = C_f(1-0) + C_s(1-0) = C_f + C_s$ (2)

Hence summation of C_f and C_s gives total mineralized OC

Where $C_s = 1 - C_f$

Fitted two-pool first order exponential decay model

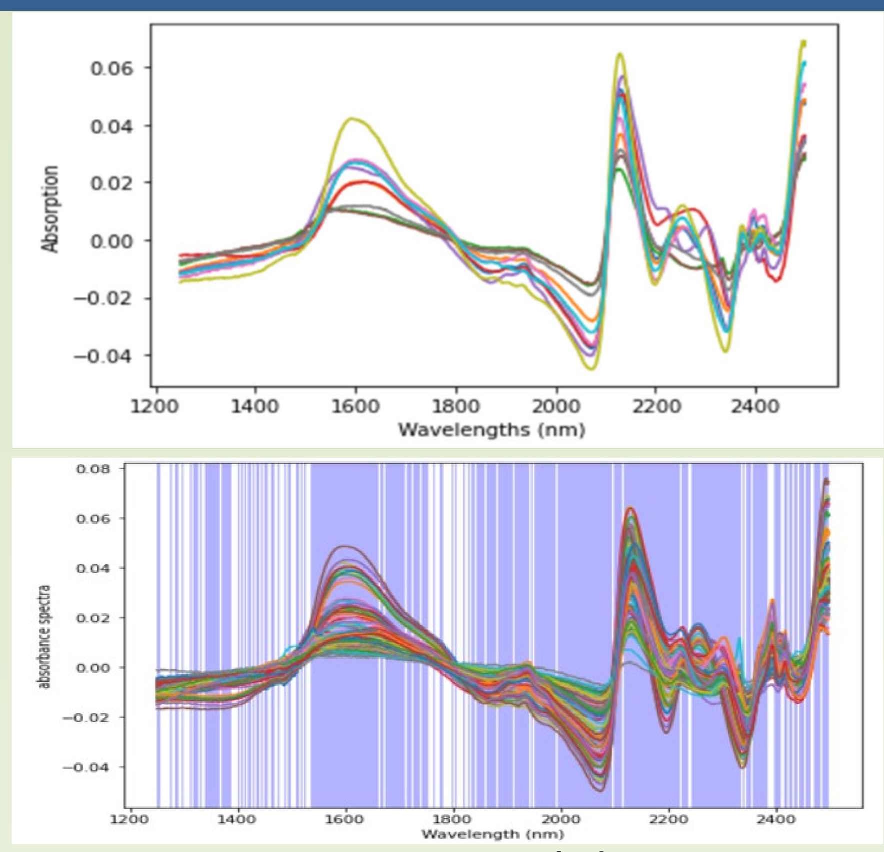

Fig 2. NIR spectral data

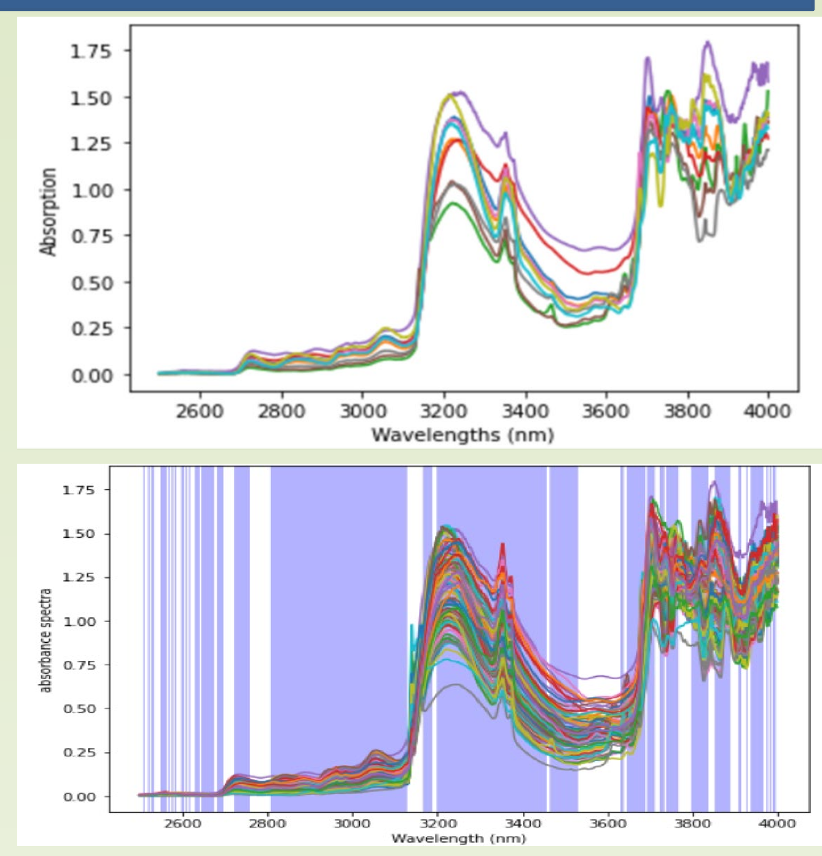

Fig 3. MIR spectral data

```
a=1
W(:,a)=X'*Y;
    W(:,a)=W(:,a)/norm(W(:,a));

    T(:,a)=X*W(:,a);

    P(:,a)=X'*T(:,a)/(T(:,a)'*T(:,a));

    Q(a,1)=Y'*T(:,a)/(T(:,a)'*T(:,a));

    X=X-T(:,a)*P(:,a)';

    Y=Y-T(:,a)*Q(a,1);

    W=W*(P'*W)^(-1);
a=a+1
    B=W*Q;
    Y=XB+E
```

Algorithm 1 Wavelength selection algorithm

H

1: Fit PLS model on NIR/MIR spectral data and optimize the number latent variables
2: Find all the regression coefficients(B)
3: Arrange B in descending order
4: Select λ_i corresponding to first entry of B i.e b_i
5: Fit PLS and find RMSE -> choose this as a reference
6: **procedure** WAVELENGTH SELECTION(λ_i)
7: Fit PLS on $b_i(k)$ corresponding wavelength where $k = 2$
8: **if** $RMSE(k) <= RMSE(k-1)$ **then**
9: Select wavelength
10: k=k+1
11: Repeat step 7
12: **else**
13: **if** $RMSE(k) > RMSE(k-1)$ **then**
14: Discard wavelength
15: Stop
16: Print all the selected wavelengths

Algorithm for wavelength selection and PLS

Results

Statistic	NIR Spectra Cf	f	Cs	s	MIR Spectra Cf	f	Cs	s
R^2	0.94	0.42	0.94	0.15	0.92	0.37	0.91	0.11
RMSE	19.17	0.018	19.17	0.000142	23.56	0.026	23.56	0.00024

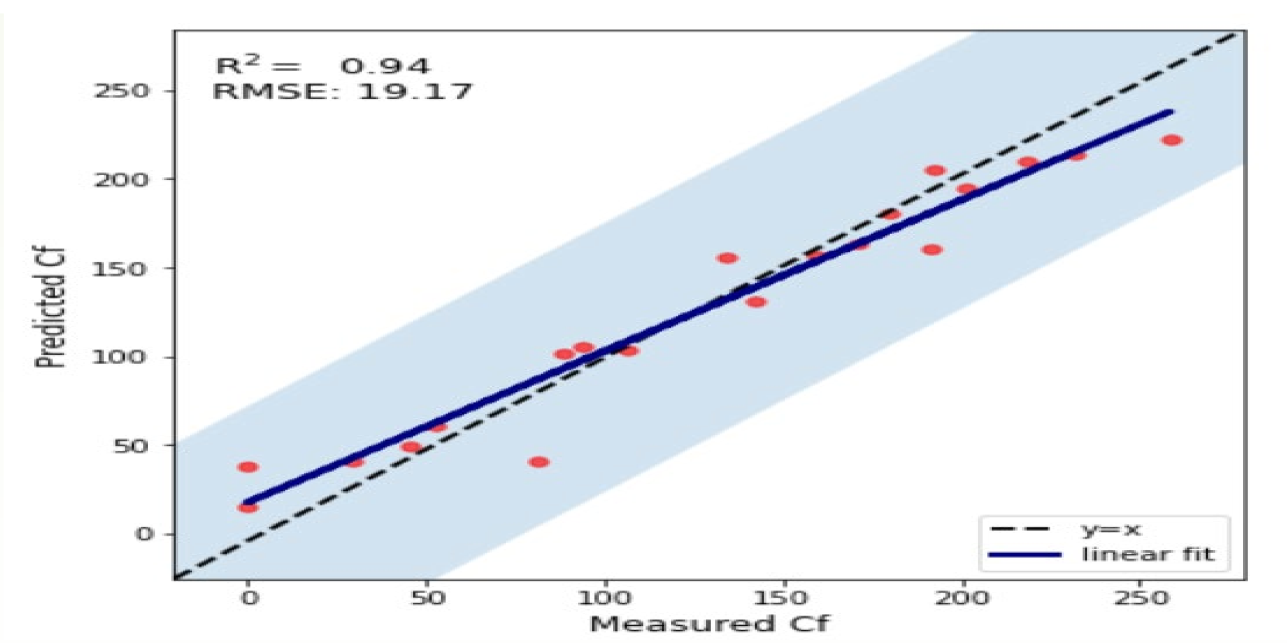

Fig 4. predicted vs actual fast-decomposing pool (C_f)

Conclusion

The potential of near infrared and mid-infrared spectroscopy for the estimation of the rate of OC mineralization to CO_2 from biowaste has been evaluated in the current study. Based on our obtained results, the following conclusions are made.

1) NIR and MIR Spectroscopy have the potential to predict rate of mineralization.
2) NIR and MIR in combination with machine learning can be a useful tool to predict the mineralizable form of OC.
3) In future more experiment will be performed to quantify the amount of nitrogen which will be eventually transformed to plant available form.

The results obtained in this study are beneficial for evaluating both the agronomical as well environmental effects of bio-based fertilizers.

References

1. J. Baldock, C. Creamer, S. Szarvas, J. McGowan, T. Carter, and M. Farrell, “Linking decomposition rates of soil organic amendments to their chemical composition,” Soil Research, 2021.
2. Patrick Kiiti Mutuo, Keith D. Shepherd, Alain Albrecht, Georg Cadisch, “Prediction of carbon mineralization rates from different soil physical fractions using diffuse reflectance spectroscopy”, Soil Biology and Biochemistry, 2006.

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