

Supplementary information

Combining a coupled FTIR-EGA system and in situ DRIFTS for studying soil organic matter in arable soils

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For the optimization of the FTIR-EGA and in situ_T DRIFTS systems, purge rate, heating rate, and calibration range were investigated in order to obtain the optimal operating conditions. Figure S1 shows the effect of purge rate of the heating chamber and gas cell. At low purge rate the CO₂ concentration is more than twice as high and the residence time of the gas in the system is much longer, as seen by the lack of a decrease of the curve upon reaching the end of the programmed heating at 700°C. The change in heating rate from 10 to 68°C also produced a marked change in the evolved gas profile (Figure S2). An increase in both the peak temperature of maximum CO₂ evolution was found and also an increase in the absorbance values. Figure S3 shows the effect of the two extreme heating rates on the change in relative intensity of the mid-infrared peak at 1620 cm⁻¹ (COO=/C=C). The lower heating rate seems to produce a greater overall increase in this peak area and likewise at the end of the programmed heating increase, the intensity of the peak has not declined as much as compared to 68°C min⁻¹ possibly indicating the formation and retention of more thermal recalcitrant C which justified our use of the higher heating rate. Figure S4 shows the linear range of the FTIR-EGA gas cell calibration with NaHCO₃ and also shows the “overflow” or non-linear area where the absorbance values no-longer respond linearly to an increase in C content of the sample. Additionally if any of the variables are changed in the experimental setup (heating rate, purge rate, purge gas), then a new calibration must be developed.

Figure S1. Effect of flow rate (synthetic air) on evolved gas profile of CO₂ as measured by FTIR-EGA of bulk soil from Kraichgau site. Sample was heated from 25 to 700°C at 68°C min⁻¹ under synthetic air purge.

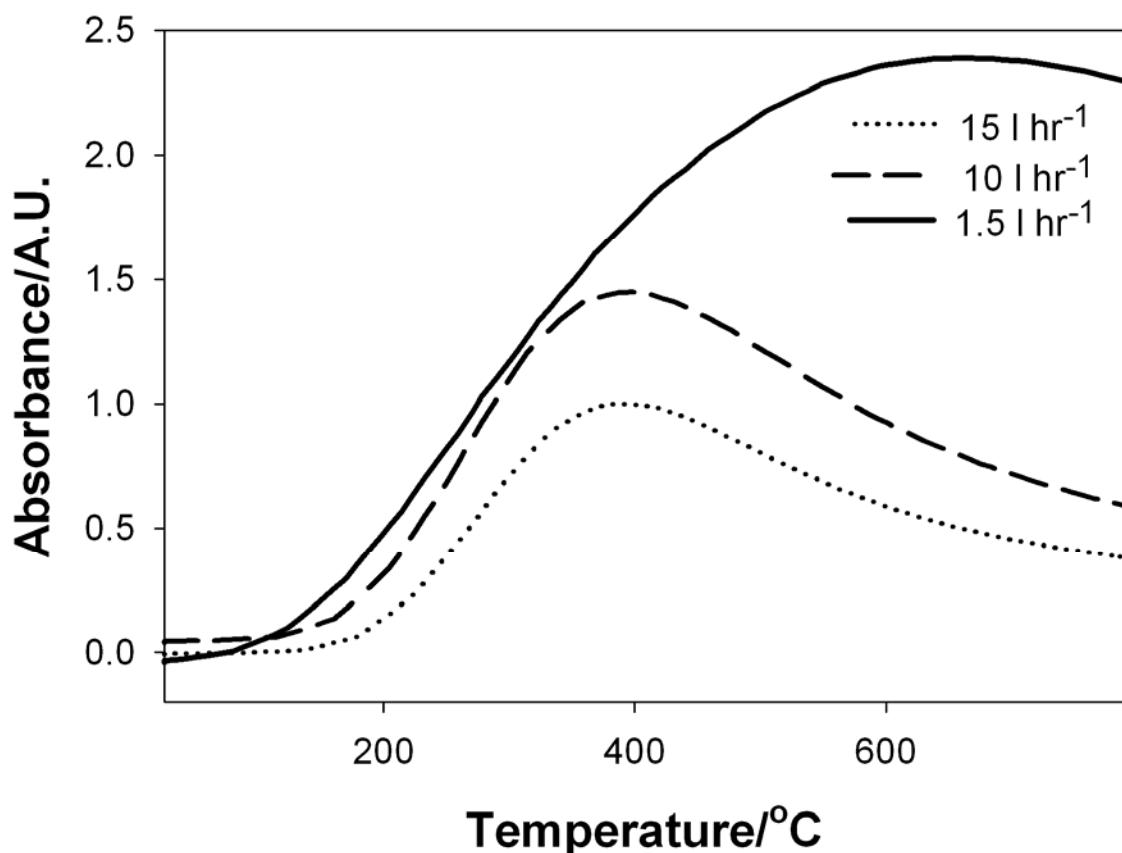


Figure S2. Effect of heating rate on evolved gas profile of CO₂ as measured by FTIR-EGA of bulk soil from Kraichgau site heated from 25 to 700 °C under synthetic air purge.

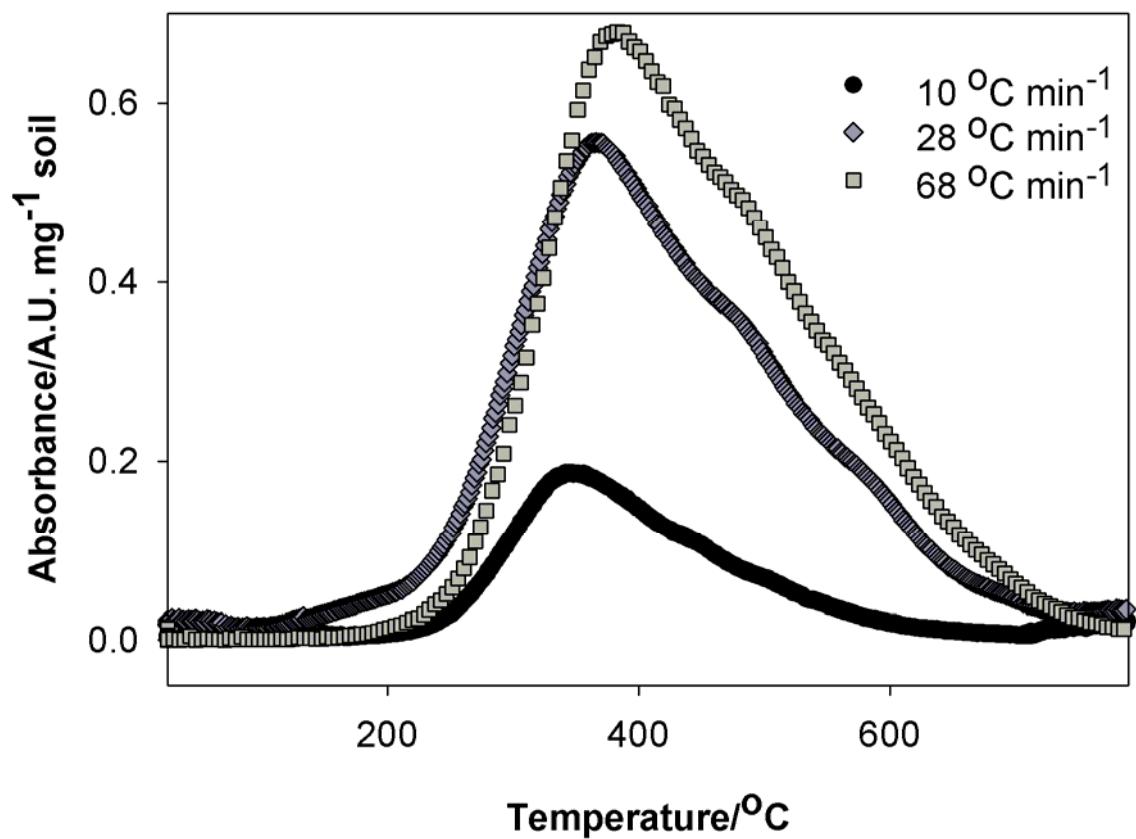


Figure S3. *In situ* DRIFTS of effect of heating rate on vibrational intensity change of peak at 1620 cm^{-1} (COO-/C=C) of bulk soil samples heated from 25 to 700°C under synthetic air purge.

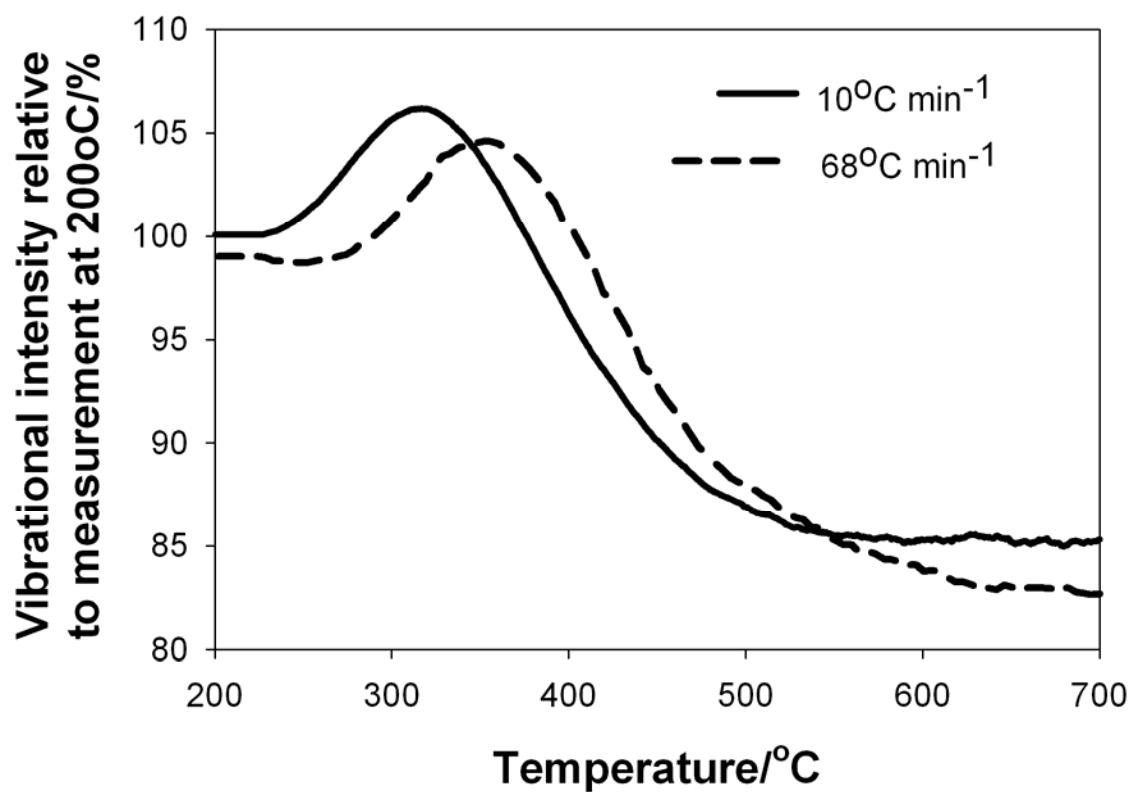


Figure S4. Extended range of NaHCO_3 standard showing no-linear response with increasing C content under synthetic air purge.

