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Discussions

Interactive comment on "Combining a coupled FTIR-EGA system and in situ DRIFTS for studying soil organic matter in arable soils" *by* M. S. Demyan et al.

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This is a high quality study, and the introduced technique, a coupling of FTIR-EGA and in situ DRIFT seems to hold potential to rapidly assess SOM quality. Most importantly, it holds promise to provide us with information on the strength of bonding of SOM constituents. I support publication of the present paper but I do have some ideas for its improvement. Most importantly, a further elucidation of the observed evolution of the DRIFT spectra with temperature is needed. To really get this new approach accepted an important requirement is that more than two samples are investigated. Other elements like a soil incubation experiment, the assesment of the effect of chemical oxidation, and a strictly statistical deconvolution of the couled data FTIR-EGA DRIFT are of lesser importance.

The authors here present an alternative technique to gather temperature resolved information on SOM composition. Over the past 40 years HR Schulten and P Leinweber have thoroughly developed pyrolysis field-ionization MS, i.e. temperature resolved analytical pyrolysis with soft ionization. This technique has amply been used to study the thermal stability of specific individual (soil) OM molecular markers and these efforts have resulted in the formulation of a conceptual model linking SOM biochemistry to thermal stability and biodegradability. This wealth of information cannot be overlooked. To better interpret the FTIR-EGA in situ DRIFT data (4.2), more analogies could be made to previous findings. (e.g. P15386. & Table 2: In fact Py-FIMS has been applied on clay fractions originating from two treatments of the Static Fertilization experiment at Bad Lauchstadt - Mertz et al., 2005 Organic Geochemistry). Py-FIMS analysis of soils has revealed general trends in organic compound class distribution. Phenols and lignin monomers increase in relative abundance with progressing decomposition stage, while the contributions of lignin dimers and alkyl aromatics decrease. Labile N-containing compounds and carbohydrates, representing products of microbial synthesis (Leinweber and Schulten, 1995), are enriched in clay size separates. This model should be referred to in the discussion.

The DRIFT technique yields an overall, yet coarse picture on C-speciation – not a detailed recording of ion intensities of individual SOM components (lignin monomers, peptides, pentose- and hexose units, fatty acids, sterols,. . .). This is a limitation of the technique and should be recognized in the text. On the other hand this may be compensated for by a (low?) cost of analysis and a (high?) sample throughput. Could the authors make a comparison with Py-FIMS?

P 15386 Thermal stability cannot be seen independently from the soil mineral phase. It is the intimate association of SOM with soil minerals which primarily affects thermal stability. Clay% and contents of Feox and Alox are of importance. This should also be made clear in the introduction.

15391 L4 ‘Synthetic air was used as the purge and carrier gas of the system’. Just what is synthetic air? This is a crucial point which needs to be specified. Does this gas contain any oxygen – this would be a major drawback because in that case combustion of the OM cannot be excluded – unlike in pyrolysis, which occurs in the absence of oxygen. While it seems acceptable to postulate that bonding strength may relate to thermal energy required for cleavage in an atmosphere absent of oxygen, I don’t know whether this assumption still holds in the case of combustion. It should be made very clear to the reader that this important difference exists with temperature resolved pyrolysis. I’m not familiar with EGA so I may be wrong, just like other readers could be. So please explain if this possibility of combustion is realistic or not. P15400 L3-5 This seems a bold statement to start the discussion with. At this point it has not been demonstrated yet that the technique is sensitive to changes in the quality and composition of organic matter.

P15401 L25 Lignin is always thermostable in case of Py-FIMS (around 550°C) – bound or unbound to minerals – occluded in aggregates or free. Thermal stability of bulk SOM therefore can strongly depend on its proportion of lignin, which is strongly depending on the nature of OM inputs (lignin-rich woody materials vs green above ground plant materials). Thermal stability of a bulk soil rich in lignin therefore tells little about the bonding strength of SOM constituents or on their proneness to microbial decomposition.

P15398 L 26 The decrease of C-H signals between 220 and 300°C may originate from the loss of ‘free’ fatty acids.

P15402 Fig 7 & Table 4 I’m not in favor of attempting to deconvolute the DRIFTs peak into artificial components. Interpretation of these components may always remain speculative and I would myself choose to omit this exercise from the present paper. If the authors stay with there convoluted components, more than two soils should be included to make general statements of distinct SOM pools. At least, I would ask to make an analogy to the conceptual model by Schulten & Leinweber, 1999, Eur J Soil Sci 50) These authors found that volatilization of mineral bound OM requires higher temperatures than unbound OM to enable thermal bond cleavage. They identified three thermal classes: i) unbound undecomposed plant fragments relatively rich in aliphatics; ii) a thermally labile fraction containing N-containing compounds and carbohydrates associated with humified OM and iii) thermally stable mineral bound OM.

P15402 l20 I don't think the microbial biomass is large enough to explain differences in component 1. l24-28 Speculative, delete.

4.4 This section is out of focus and I suggest to delete this entire part. Why should we at all be interested in the effect of hypochlorite on thermal stability? Other parts of the present study are far more important. The complete data received by coupled FTIR-EGA and DRIFTS on two soils needs to be further investigated. The paper would have really been stronger if more samples were analyzed by coupled FTIR-EGA and DRIFTS and it is not clear why so few samples were included. I would ask to expand the analysis made in 4.2. You need to attempt to better explain (Fig 7a) the temperature patterns in the DRIFT spectra. A statement like '. . .which lends evidence to different organic compounds being decomposed at different temperatures.' (lines 13-14) is insufficient.

15383 L 9-14, very long sentence

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