Exploratory study of infrared spectral signatures of a range of forest, agricultural and artificialized soils from the North-East of France

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Context and objectives

Artificialized soils encompass a large **diversity** of soils depending both on the environmental conditions and the history of land uses. In particular, these soils can contain original mixtures of constituents of natural and anthropic origin. Studying these soils requires to investigate their diversity and variability and to develop an approach to compare and classify them.

Vibrational spectroscopies are used in soil science as they provide rapid and cost-effective analyses giving molecular information about inorganic and organic soil constituents [1]. Coupled with chemometrics approaches (*e.g.* [2]), they can be used to estimate some soil properties and/or to classify soils [3].

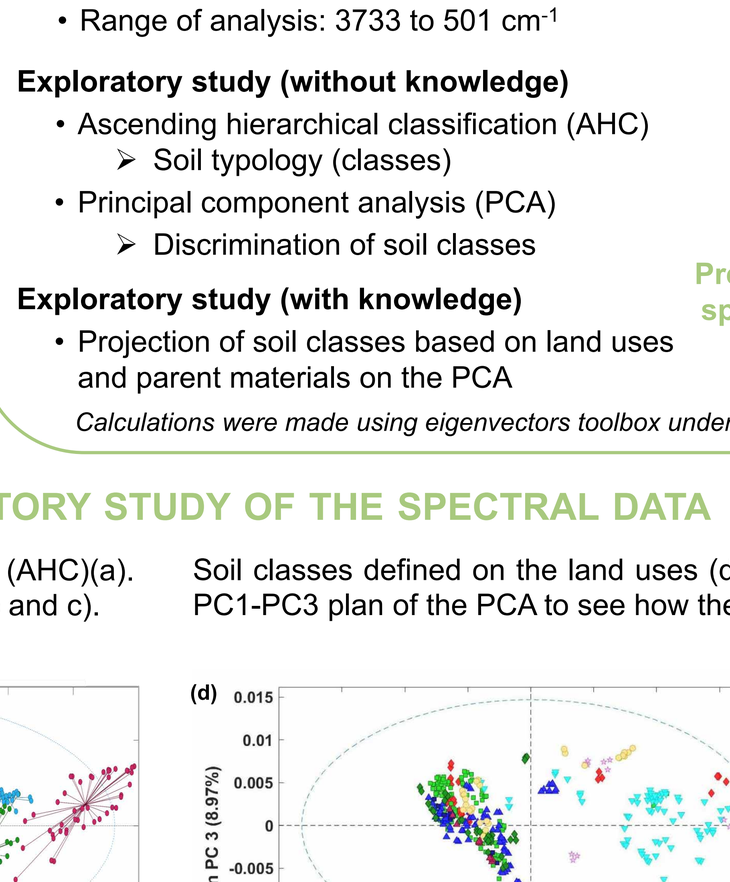
This study aims at exploring the **potential of mid-infrared (mid-IR) spectroscopy** to:

1. **Differentiate** soils depending on the history of land uses;
2. Propose a soil **typology** at the regional scale;
3. Define **markers** of human activities.

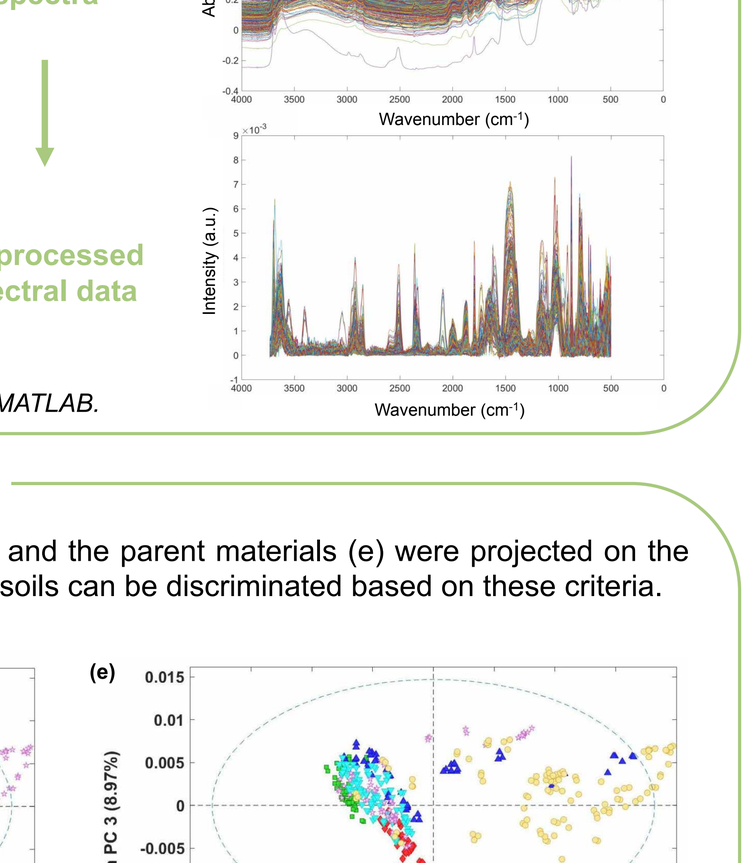
Soil samples

A set of **150 samples** of surface soils collected in the North-East of France in the framework of different research projects and monitoring sites was selected in order to have a **range of soils** developed on various **parental materials** with varying **history of land uses**.

Diversity of land uses



Diversity of parental materials



Data acquisition

Preparation of the soil samples

- Sampling at the surface (5 to 30 first cm)
- Air-drying and sieving at 2 mm
- Grinding and storage in a desiccator

Acquisition of mid-infrared spectra

- Mid-infrared Fourier Transform Spectrometer Bruker Vector 22
- Diffuse reflectance mode
- Soil samples diluted at 15% in KBr
- Scans from 400 to 4000 cm^{-1} with a resolution of 2 cm^{-1}
- Acquisition of 4 spectra per sample
- Data selection (150 samples x 3 = 450 spectra)

Spectral data analysis

Spectral data preprocessing

- Baseline correction (Whittaker filter)
- Normalization of spectra (Norm-L1)
- Range of analysis: 3733 to 501 cm^{-1}

Exploratory study (without knowledge)

- Ascending hierarchical classification (AHC)
  - ➢ Soil typology (classes)
- Principal component analysis (PCA)
  - ➢ Discrimination of soil classes

Exploratory study (with knowledge)

- Projection of soil classes based on land uses and parent materials on the PCA

Calculations were made using eigenvectors toolbox under MATLAB.

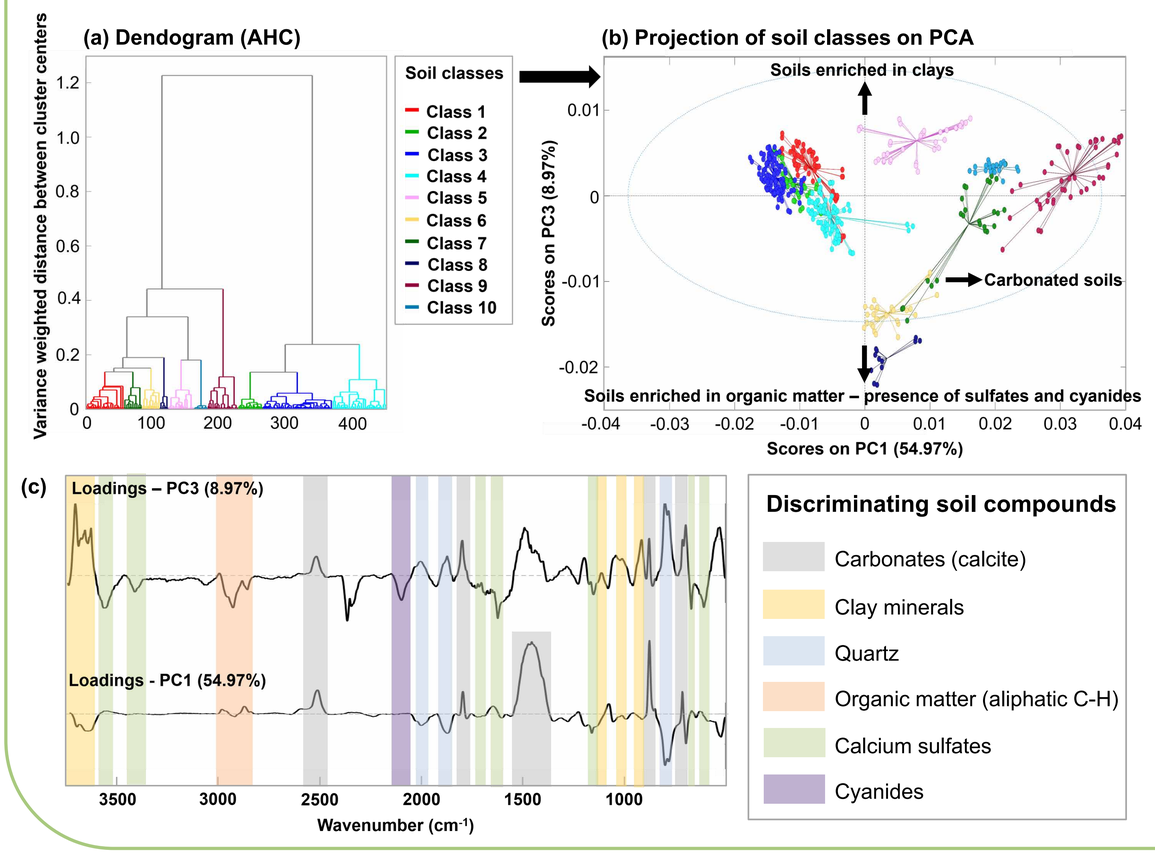
Raw mid-IR spectra

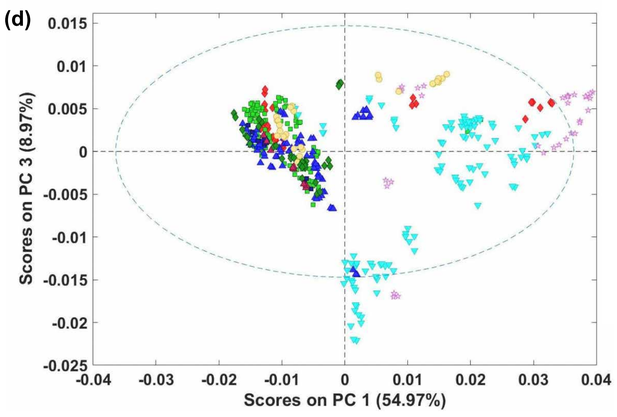
Preprocessed spectral data

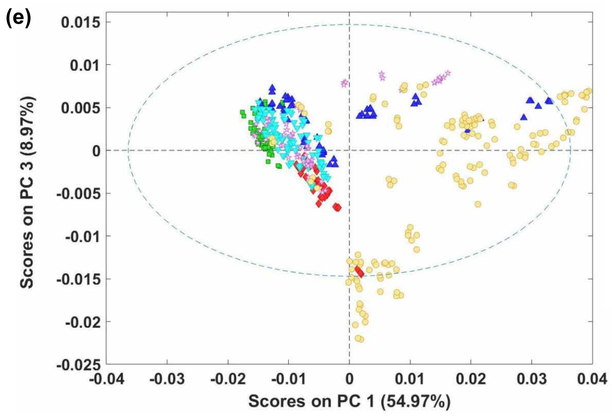
Exploratory study of the spectral data

Ten soil classes were defined based on the similarity of the spectra (AHC)(a). Some classes can be discriminated based on soil compounds (PCA) (b and c).

Soil classes defined on the land uses (d) and the parent materials (e) were projected on the PC1-PC3 plan of the PCA to see how the soils can be discriminated based on these criteria.







Conclusions and perspectives

Mid-IR spectroscopy shows a potential for:

- **separating soil classes** based on their mineralogy (carbonates, clays, quartz) and, to a lesser extent, the presence of organic compounds (aliphatics, aromatics);
- **discriminating some forms of impacts of human activities**, such as those related to industry. However, changes related to old settlements, mining or charcoal production are more difficult to distinguish based on mid-IR fingerprints.
  Markers of industrial activities include sulfates, cyanides or aromatic compounds.

The **discrimination of artificialized soils** could be improved:

- by improving the spectra analysis and having references of soil compounds and products produced by human activities;
- by coupling several spectroscopic analyses providing complementary information of the soil samples (*e.g.* elemental analyses by XRF);
- by taking into account soil samples collected at different depths.

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