



## **Characterisation and quantitative estimation of the hydrophobic, transphilic and hydrophilic fractions of DOC in soil using direct UV spectroscopy**

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Dissolved Organic Carbon (DOC) represents a small fraction, ranging from 0,1 to 0,01%, of the total Soil Organic Matter (SOM) and is the most mobile form of carbon in soil. It is considered as the most important vector of organic and mineral micro-contaminants and could represent, in itself, a source of contamination of groundwater. DOC characterization is essential for the comprehension of its origins, evolution and functioning in the environment. In complement of accurate conventional analytical procedures, understanding DOC dynamic in soils needs the development of simpler, faster and suitable alternative procedures for on site analysis. The interest of this approach is to obtain a greater number of spatiotemporal data and hence a more reliable interpretation of results. In the present work, a combined approach of characterization is used based both on conventional method of chemical fractionation on XAD-resins and on the study of UV absorbance spectrum. Several works have already used UV exploitation, frequently using mono wavelength, for qualitative and quantitative estimation of total DOC (Deflandre and Gagné, 2001), but few works deal with direct UV fractionation of DOC (Novak et al, 1992, Dilling and Kaiser, 2002). For this purpose, a robust spectral deconvolution method, commonly used for on line analysis of water samples, is used (Suryani et al., 1995).

In order to understand spatiotemporal evolution of DOC, including the influence of depth, ageing and environmental conditions, soil samples were collected from an open-air field cultivated with maize, during a period of 6 months at 3 different depths: 0.00-0.30, 0.30-0.60 and 0.60-0.90 m. They were used as source of DOC or Water Extractable Organic Carbon (WEOC). Running classical fractionation on macrop-

orous XAD resins (Martin-Mousset et al, 1996) DOC was divided into hydrophobic ( $C_{XAD-8}$ ), transphilic ( $C_{XAD-4}$ ) and hydrophilic ( $C_{not-ret}$ ) compound groups. The acquisition of the UV absorbance spectra of raw samples and fractions is realised in the range 230-400 nm. Results of fractionation allow the determination of the Humification Index (HIX) defined as  $C_{XAD-8}/TOC$ . Qualitative exploitation of spectra is based on calculation of specific absorption at two wavelengths : 254 nm and 280 nm. Quantitative exploitation by spectrum deconvolution needs the selection of well defined spectra allowing the restitution of sample UV spectra. The choice of these spectra depends on the final objectives of the work i.e. direct quantification of hydrophobic, transphilic and hydrophilic fractions.

The values of HIX and specific absorption of raw samples and hydrophobic fractions are significantly higher in the 0.0-0.30 m soil depth range than in the 0.30-0.90 m one. This indicates that the most humified and highest molecular weight compounds are more abundant near the surface, and this remains true despite modifications of the environmental conditions. This indicate a low migration of these compounds in the soil profile. Nevertheless, variations with time of these parameters, the amplitude of which decreases with depth, makes it evident that the composition of the hydrophobic fraction is affected by climatic conditions. The specific absorption of the transphilic and hydrophilic compounds show high variations, even in the depths greater than 0.30 m, which indicates large variations in their nature and probably high mobility.

Selection of reference spectra for the deconvolution procedure is realized manually or automatically with a specific mathematical programme (UV pro, S1000PC Secomam). They are extracted from the spectrum data base previously established. Constitution of parameter file for hydrophobic, transphilic and hydrophilic DOC estimation is realised by multiple regression using measured values of carbon concentration of raw samples and of the different fractions. Results of the deconvolution show a good restitution of raw sample spectra and regression lines established by comparison of measured and estimated values of parameters show satisfactory results with slopes close to 1 and intercepts close to 0. Correlation coefficients are of 96% for total DOC and higher than 80% for fractions.

The obtained results prove the possibility of UV spectrum exploitation to obtain elements of DOC characterization such as specific absorption and to directly quantify total DOC, hydrophobic, transphilic and hydrophilic fractions. These results and the development of new technologies such as optic fibres and automation open the way to the development of cheap and practical analytical tools for on site measurements with portable or automatic devices.

## **References:**

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