EGU23-1389, updated on 01 Apr 2023
https://doi.org/10.5194/egusphere-egu23-1389
EGU General Assembly 2023

Complete thermodynamic characterization of the soil organic matter from forest ecosystems.

Nieves Barros[1], Marko Popovic[2], and César Pérez-Cruzado[3]
[1]University of Santiago de Compostela, Facultyof Physics, Applied Physics, Spain (nieves.barros@usc.es)
[2]School of Life Sciences, Technical University of Munich, 85354 Freising, Germany.
[3]PROEPLA. Higher Polytechnic School of Engineering. Campus Terra (Lugo). University of Santiago de Compostela (Spain).

Thermodynamic characterization of soils is a developing field that involves the calculation of the enthalpies, Gibbs energy, and entropy of the soil organic matter, SOM. Its achievement would contribute to the development of the bioenergetics of soil systems beyond the existing theoretical models.

This work shows different experimental procedures and theoretical models for the complete thermodynamic characterization of SOM. It was applied to a total of 31 samples representing different soil horizons from different locations.

Thermodynamic characterization of SOM was achieved through the calculation of empirical formulae for SOM from the SOM elemental composition, application of Patel-Erickson, Sandler-Orbey, and Battley methods, as well as direct measurements of the energy content by simultaneous TG-DSC.

The used computational methods belong to a group of approaches modeling thermodynamic properties of SOM as a sum of contributions from its constituent elements. The first computational approaches were those from the Patel-Erickson and Battley equations. Patel-Erickson equation was used to find the standard enthalpy of combustion, $\Delta_C H^0_{PE}$, of SOM based on its elemental composition:

$$\Delta_C H^0_{PE}(SOM) = -111.14 \text{ kJ/mol} \cdot (4n_C + n_H - 2n_O - 0n_N + 5n_P + 6n_S)$$

where n_J is the number of atoms of element J in the empirical formula of SOM. The Battley equation gives the standard molar entropy, S^0_m, of SOM:

$$S^0_m(SOM) = 0.187 \sum_J [\, S^0_m(J) / a_J \,] \, n_J$$

where $S^0_m(J)$ and a_J are standard molar entropy and the number of atoms of element J in its standard state elemental form. The enthalpy from the Patel-Erickson equation is combined with entropy from the Battley equation, to find the Gibbs energy of SOM.

The second computational approach handled equations proposed by Sandler and Orbey that

allow finding standard enthalpy of combustion $\Delta_C H^0_{SO}$ and standard Gibbs energy of combustion, $\Delta_C G^0$, of SOM:

$\Delta_C H^0_{SO}(SOM)$ = –109.04 kJ/C-mol □ $(4n_C + n_H - 2n_O - 0n_N + 5n_P + 6n_S)$

$\Delta_C G^0(SOM)$ = –110.23 kJ/C-mol □ $(4n_C + n_H - 2n_O - 0n_N + 5n_P + 6n_S)$

The enthalpy and Gibbs energy obtained using the Sandler-Orbey method were combined to find entropy.

Results obtained by the application of Patel-Erickson and Sandler-Orbey methods to calculate the enthalpy of SOM combustion did not significantly differ when comparing data given by the TG-DSC with those obtained from the SOM empirical formulation. The same results were obtained when comparing the Gibbs energy. These results enabled the calculation of the entropy of SOM and the comparison of those values among different soil layers and sampling sites.