AI-based simulation of hydrochars production from Lignocellulosic Residues for Green Electronics, Environmental Remediation and Agricultural Applications

Required background : Any Master, MSc or Engineering degree with solid skills in artificial intelligence and Machine Learning (Deep learning knowledge will be appreciated). Some basic understanding of biochemistry would be a bonus, but is not required.

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Place(s) of work : ISEP campus in Issy-Les-Moulineaux (Subway line 12, Corentin Celton). A mobility in Equator is also very likely.

Project Description

Hydrothermal carbonization (HTC) of lignocellulosic residues (e.g.: peels, husks, hulls) has become an attractive method for the production of hydrochars from which valuable materials can be obtained for diverse applications. HTC is a lower energy consumption process compared to other conventional thermal treatments with other advantages such as a higher conversion rate and preparation of heteroatom-doped materials (Yang et al., 2023). However, predicting the outcome of HTC is a difficult task and a costly process due to the high number of parameters, as well as the time and energy consumption that would be required to test all possible cases. For this reason, HTC is a good candidate to be simulated using artificial intelligence and predictive Machine Learning methods. Indeed, hydrochar materials are easy to characterize and large amounts of data are already available on existing experiments, waiting to be exploited by AI methods.

Hydrochars can be characterized physically, chemically and electrically to gain understanding of their crystallographic structure, composition, morphology, surface area, vibrational modes, chemical state and dielectric/conductive properties. HTC temperature, HTC processing times and activation methods can influence the suitability of hydrochars for a potential application.

Hydrochars are being used for pollutant removal from water (Garcia & Perez, 2019)(Omran & Baek, 2022), for CO_2 capture and soil conditioning (Pacheco & Vilela, 2017) without the use of toxic reagents (Muñoz et al., n.d.). In addition, applications of these materials are found within nanoelectronics, semiconductors and consumer electronics industry and energy storage (Laverde et al., 2019).

To understand the influence, evolution of these materials and even predict the HTC process itself; proximate analyses in native samples, FTIR, TGA, BET, XPS, Raman and XRD data from the experimental HTC treatments are acquired as input for AI algorithms. These data are compiled for each lignocellulosic residue (e.g.: mango endocarp, moringa husk, ripe banana peel, cocoa husk, blackberry residues, rice husk) available in Ecuador.

With this in mind, our goal is to leverage the potential of AI methods such as deep neural networks to simulate the HTC process in a way that would make it possible to predict the properties of output materials based on which materials were used as inputs and the parameters for the HTC process. Doing so should be possible using a large enough training database of HTC experiences in known conditions, and could be used to avoid having to test all possible combinations of materials and conditions (which is both costly and ineffective).

Properties that we will try to predict cover several purposes: i. energy purposes (as dielectric materials or semiconductive ones), ii. soil amendments due to the amount of nutrients present in hydrochars and, iii. water treatment applications. HTC gives greater added value to these agroindustrial residues to develop the Circular Bioeconomy in the country and find new industrial applications with a sustainable approach (Landázuri et al., 2023).

Main challenges

The main challenge for our problem would be to have an Artificial Intelligence system good enough to efficiently simulate the HTC process (which is quite complex), based on a limited and incomplete amount of data. This could be achieved by leveraging the following key elements:

- The use of expert knowledge to curate the data as much as possible to essential properties of source materials (while knowing in advance the most likely to be relevant), and by focussing on a small number of desirable output properties
- The use of AI methods capable of coping with uncertainty (as some data may be incomplete), bias (specific materials and conditions will have a lot more available training exemple than other), and few shots learning to produce a neural network capable of good quality results based on a somewhat low number of examples (relative to the problem complexity)
- Designing AI blocks or neural network blocks closely matching the known physical processes of HTC (at least in terms of complexity) based on expert knowledge.

From the literature, we know that similar works exist using neural networks to simulate hydrochars and that they have been somewhat successful (Kapetanakis et al, 2021;Zhang et al., 2023).

Input Data

Examples of characterization data (from experimental procedures) for each biomass (native and hydrochars) involve the following (Table 1):

Table 1. Main input data

Process	**Input**
Hidrothermal Carbonization	HTC temperature
	HTC processing time
Chemical Characterization of Native Materials and Hydrochars	Lignin content
	Cellulose content
	Hemicellulose content
	Carbon content
	Nitrogen content
	Oxygen content
	Sodium content
	Potassium content
	Metal & metalloid content
XRD Analyses	Absolute intensity as a function of angle of diffraction
	Intermolecular distance as a function of angle of diffraction
	Other parameters
BET Analyses	Mean particle diameter
	Particle surface area

Process	Input
	Pore volume
XPS Analyses	Intensity as a function of binding energy
	C, N, O, Na, K and other elemental content
Electrical analyses	Relative permittivity as a function of frequency
	Loss tangent as a function of frequency
FTIR analyses	Absorbance of infrared radiation as a function of absorbance or frequency.

In parallel, several criteria can be assigned depending on the ranges of results. For example: the position of binding energy relates to the elemental and chemical composition at the surface of the material, high relative permittivity values indicate their usefulness of the materials to be used in supercapacitors or batteries, high particle surface areas mean that more sites are active and materials can be used as pollutant adsorbents, among others.

References

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