OFFRE D'ALLOCATION DE THESE / PhD GRANT

ÉCOLE DOCTORALE SCIENCES EXACTES ET LEURS APPLICATIONS - ED 211 / NATURAL SCIENCES DOCTORAL SCHOOL

Avenue de l'université BP 1155 64 013 PAU Cedex – France

PhD SUBJECT

TITLE: Development Bio Oil characterization by ICP MS and FT IRC MS

As a major environmental and economic issue, the valorization of corn is now a priority for both industrial and academic players. Supported by the funding of three doctoral theses at the Université de Pau et des Pays de l'Adour (UPPA), this interdisciplinary project aims to develop a new pyrolysis and characterization technology, and to study the economic impact of agricultural waste recovery, particularly with a view to accelerating the integration of the circular economy into the practices of economic players in the Nouvelle-Aquitaine region. To achieve this, it relies on the close collaboration of several regional research laboratories in a complex and ambitious study, situated at the interface between physico-chemical and economic fields. Corn waste has been widely used for agronomic purposes (soil fertility/quality) and for animal feed (pasture/hay). In view of the region's high corn production, which accounts for 30% of national output, the region has significant potential for this residue compared with other parts of the country. However, the region has not yet exploited the potential of agricultural waste for energy purposes or the production of valuable goods.

Through three interconnected lines of research (PhDs), this project will benefit from the expertise developed in UPPA laboratories to improve the characterization process to understand the physico-chemical properties of corn, and the pyrolysis process to simultaneously obtain silica particles and a bio-oil with improved quality.

This PhD will be foccued on the development of some characterization methodology of the produces BioOil by hyphenated technique with ICP MS and by FT ICR MS.

Keywords: Speciation, ICP MS, FT ICR MS, BioOil

WORKING CONDITIONS

Laboratoire : UMR 5254 CNRS-UPPA, Institut des Sciences Analytiques et de Physico-Chimie pour l'Environnement et les Matériaux (IPREM)

Site web : www.iprem.univ-pau.fr

PhD Director: Pierre Giusti / Brice Bouyssiere

PhD co-supervisor: Sadia Rajdi

In Collaboration with:

Place: IPREM. Hélioparc, 2 Avenue du Président Angot 64053 Pau cedex 09

Start: October 2024	**Duration:** 3 years

Employeur (employer): Université de Pau et des Pays de l'Adour (UPPA)

Salaire mensuel brut (monthly salary before taxes): 2100 €

(Si enseignement : salaire mensuel brut pour 32h d'enseignement par année universitaire : 110 €)

HOST LABORATORY PROFILE

The PhD will principally work at IPREM, specifically, he/she will be member of the Analytical Chemistry, Physical and Theoretical (CAPT) Cluster. He will be part of the iC2MC Pau group that has a vast experience on analytical chemistry, trace metal speciation in complexes matrices. To reach the outlined objectives, the project will be supported by the unique instrumental facilities of the host laboratory. This platform possesses, among others, the state of the art instruments required for these project (ICP-MS, ICP HR MS, HPLC/GC/LA ICP MS, FT ICR MS

(ESI and MALDI)).

This PhD will be also link with TotalEnergies iC2MC part and some stay at the TRTG Research center (Gonfreville) or at the Florida State University will be possible.

See details at https://iprem.univ-pau.fr/fr/activites-scientifiques/poles-scientifiques/chimie-analytique-physique-et-theorique/capt-membres.html

MISSION - ACTIVITES PRINCIPALES / MISSION – PRINCIPAL ACTIVITIES

I. *Scientific Context*

Thermochemical conversion appears to be the most promising method for producing bio-oils and other compounds, such as silica particles. Pyrolysis has proved to be an excellent technique for increasing the value of biomass, and can be carried out on virtually any biomass source. The process involves heating biomass polymers in the absence of oxygen, enabling their depolymerization while inhibiting their combustion. From the biomass pyrolysis process, 3 phases of material can be obtained: ash (solid), bio-oil containing a mixture of water and organic matter (liquid) and non-condensable gases (gas). Then, by calcining the ash at 700°C, it is possible to obtain, when the initial material contains a significant proportion of it, silicon particles. The aim of this research is to improve the prospects for using biomass from corn production waste as a raw material for the production of bio-oil (subsequently refinable into SAF (Sustainable Aviation Fuel / Carburant d'Aviations Durable) and silica particles.

When silica particles reach the nanoscale, they begin to exhibit new characteristics, such as photoluminescence, antibacterial capacity and a size-dependent electrical band gap, which are not observed in bulk silicon. The high surface area of nano-silica makes it ideal for various applications, such as filler reinforcement in the rubber industry (tire manufacture), improving the properties of concrete, the insecticide industry, paint, the food industry, medicine [H. El-Didamonyet al 2020], adsorption for water decontamination and adsorption of contaminants in pyrolisis oils, are other possible applications. Biomass-derived nano-silica is also being investigated for various biological and biotechnological uses, such as cancer treatment, DNA transfection, drug delivery, enzyme immobilization and environmental bioremediation. Characterizing silica with regard to their properties is essential for their effective application.

Corn biomass pyrolysis oils are a complex mixture of organic compounds containing a mass of highly oxygenated compounds, including phenols, ketones, carboxylic acids, etc., which can be determined by techniques such as Gas Chromatography coupled to Mass Spectrometry (GG MS). On the other hand, FTIR spectra indicate the presence of functional groups in bio-oils. The liquid product can be valorized or used directly in boilers, diesel engines or turbines. This liquid form is much easier to transport and store than the biomass itself. Pyrolysis optimization (pretreatment, temperature, gas flow, etc.) can produce a product that can then be refined into a sustainable aviation fuel (SAF), notably through systematic monitoring by Fourier Transform Very High Resolution Mass Spectrometry (FT ICR MS).

II. *Objectives*

This thesis proposes the characterization of products derived from the pyrolysis of corn parts. The research project is structured around three main axes, each of which aims to optimize analytical parameters and develop a characterization of bio-oils and silicas derived from corn biomass, in order to understand and valorize these pyrolysis products according to their possible applications.

1. First phase: Bibliographical review and training in characterization instruments, in particular in conjunction with the new FT ICR MS acquired at LCABIE. In this first phase, the emphasis will be on a literature review, with the aim of establishing a solid base of existing knowledge in the field of

characterization of pyrolysis products from different parts of maize (leaf, stalk, hulls, etc.). In addition, the necessary training will be provided on characterization instruments, such as GC MS, ICP MS, AFM, SEM, FT ICR MS, etc., to ensure complete mastery of analytical methodologies for specific developments in the characterization of pyrolysis products.

2. Second axis: Optimization of experimental and analytical parameters. This stage of the project will focus on the optimization of experimental and analytical parameters specific to the characterization of bio-oils and silicas recovered from corn pyrolysis. The aim is to optimize analytical methods to obtain accurate and reproducible results.
3. Third axis: link with pyrolysis processes in order to optimize them to obtain the best oil allowing, in an optimal way, an upgrade towards a sustainable aviation fuel and optimum silica particles for local use.
4.

Through these three axes, this thesis aims to make a significant contribution to the characterization of pyrolysis products from corn production waste, which will enable these products to be valorized for future applications, in a more environmentally-friendly circular economy approach.

REQUIRED COMPETENCES

The candidate should have a Master (or BAC+5 homologated) on Analytical/Bioanalytical/Environmental Chemistry

Previous experience on hyphenated chromatographic techniques, mass spectrometry would be appreciated.

CRITERIA USED TO SELECT CANDIDATE

Selection process steps:
- Establishment of the selection committee.
- Evaluation of the applicants Cv's
- Interview with the selected candidates and ranking.

Criteria used in selection of the candidate:
- The candidate's motivation, scientific maturity and curiosity.
- Previous experience on hyphenated chromatographic techniques, mass spectrometry or stable isotopes would be appreciated
- Candidate's marks and rankings in M1 and M2.
- English proficiency

REQUIRED DOSSIER, DATE

Send an e-mail with your candidature containing (with "PhD Candidate in the object of the message"):

- CV
- Cover letter detailing candidate's motivations
- Candidate's MSc marks and ranking
- Minimum two contact details for 2 referees

Limiting date:	**4/07/2024**

CONTACTS

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