Plan Overview

A Data Management Plan created using DMPonline

Title: Systematic investigation of pyrolysis process and products for sustainable biochar production

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Project abstract:

The pyrolysis of raw biomass typically requires high operating temperatures and extended residence times to achieve the desired degree of C conversion. However, the optimal operating window for such conditions is narrow, as excessive temperature or duration can result in uncontrolled volatilization and significant tar formation, resulting in C losses to the gaseous and liquid fractions and thereby reducing the overall char yield. Consequently, the introduction of mineral additives has gained increasing attention as a strategy to mitigate these limitations and enhance the efficiency of the pyrolytic process. Understanding the impact of mineral additives on the balance between volatilization, condensation, and gasification reactions is thus essential for developing pyrolysis systems that are both efficient and tunable. Although previous studies have reported apparent changes in kinetic parameters and provided macroscopic insights into the effects of additives on the pyrolysis process, a significant gap remains in identifying the underlying mechanisms, i.e., why and how these additives alter reaction behavior. Thus, the present study seeks to establish a detailed mechanistic framework through a time-resolved investigation of biomass evolution in both doped and undoped systems, integrating spectroscopic, compositional, and kinetic analyses. Rather than treating pyrolysis as a single, unified process, this approach divides it into distinct reaction windows to evaluate how dopants modulate the transition from carbon accumulation to carbon consumption. Moreover, the derived mechanistic and kinetic insights will form the basis for evaluating the influence of mineral additives and the corresponding shifts in reaction windows within a bench-scale pyrolysis system. This approach will account for the effects of heat and mass transfer limitations, thus facilitating the identification of

optimal reactions windows viable for commercial additive-assisted biomass pyrolysis

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Systematic investigation of pyrolysis process and products for sustainable biochar production

Data Collection

What data will you collect or create?

In the current work, spectroscopic, kinetic, compositional and product characterisation data will be collected. The kinetic data will be used to create kinetic triplet models and reaction pathways.

How will the data be collected or created?

All data in the present study will be obtained through traditional and custome designed experimental procedures. Thermal degradation behavior will be characterized through thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC), providing the data for determining kinetic triplets and identifying reaction mechanisms using established computational models implemented in Python. Spectroscopic analyses, including in-situ Raman spectroscopy, in-situ Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis-mass spectrometry (TGA-MS) and Pyrolysis-Gas Chromatography-Mass Spectrometry (Py-GC-MS), will be used to monitor the real-time evolution of chemical species and structural transformations during pyrolysis. For the bench-scale experiments, comprehensive compositional characterization of raw biomass and resulting biochar will be performed through proximate and ultimate analyses, as well as lignocellulosic composition determination. Additionally, high-performance liquid chromatography (HPLC) and gas chromatography with flame ionization detection (GC-FID) will be used to analyze the composition of bio-oil and biogas products, respectively. Moreover, FTIR and Powder X-ray Difraction (P-XRD) would be used for identifying the structural and chemical features of the derived char.

Documentation and Metadata

What documentation and metadata will accompany the data?

- All the files would be named in the format "yyyymmdd" followed by "exp_name" and "trial number"
- The TGA datafiles would be imported in the .txt format and converted to .csv formats for applcaition in kinetic modelling as "yyyymmdd" followed by "sample name", "heating rate value" and "trial number"
- The python files would be stored in .py format as "yyyymmdd" followed by "computationla method", and "iteration"
- The files from XRD, Raman spectroscopy, HPLC, GC-FID and Mass spectroscopy would be stored in their respective file formats and would be named as "yyyymmdd" followed by "sample_name", "characterisation technique" and "trial number"

Ethics and Legal Compliance

How will you manage any ethical issues?

The current study does not have any ethical issues and the clearence of the same has been obtained.

How will you manage copyright and Intellectual Property Rights (IPR) issues?

The copyright and Intellectual Property Rights (IPR) will be managed through the University policy, UKRI and ESPRC policies and as per the norms detailed in the agreement with the industrial partner.

Storage and Backup

How will the data be stored and backed up during the research?

Shared file store provided by Newcastle University. Also, the data would be stored in a personal hard drive, google drive and university sharepoint to prevent failure of one source

How will you manage access and security?

University (NUIT) cybersecurity

Selection and Preservation

Which data are of long-term value and should be retained, shared, and/or preserved?

None

What is the long-term preservation plan for the dataset?

Newcastle University has a contractual agreement with Microsoft to abide by Principle 7 of the Data Protection Act 1998.

Data Sharing

How will you share the data?

The data will be shared alongside the publciations in the supplimentry section of open-access journals and we would ensure that additional data can be obtained by contacting the investigators, unless restricted by the industrial contract.

Are any restrictions on data sharing required?

The restrictions will depend on the terms enlisted by the industrial partner in the contract which is being drafted at the moment.

Responsibilities and Resources

Who will be responsible for data management?

Project PI

What resources will you require to deliver your plan?

Standard shared file store