Plan Overview

A Data Management Plan created using DMPonline

Title: Kinetic and mechanistic analysis of mineral added pyrolytic process for enchanced biochar production

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Project abstract:

Understanding how mineral dopants influence the balance between volatilization, condensation, and gasification reactions is key to designing pyrolysis systems that are both efficient and tunable. While existing studies have reported apparent changes in kinetic parameters and macroscopic improvements in biochar yield upon dopant addition, they often overlook the mechanistic role of dopants or how these additives alter the balance between the competing post-devolatilization reactions that ultimately determine product selectivity and distribution. Thus, the present study aims to bridge this gap by developing a mechanistic framework through a time-resolved analysis of biomass evolution in both doped and undoped systems, linking spectroscopic, compositional, and kinetic analysis. This approach is intended to uncover how specific dopants modify the transition between secondary charring and gasification, and whether a distinct tipping region exists within the pyrolytic process where the reaction balance shifts from carbon accumulation to carbon consumption. Beyond advancing the fundamental understanding of post-devolatilization reactions, this mechanistic method offers a systematic way to correlate behavior of the additives with the lignocellulosic composition of biomass rather than the type of biomass. By emphasizing reaction window dynamics instead of relying on extensive experimental combinations across temperatures, this approach provides a more predictive basis for developing the working range for pyrolysis based on the requirement for the promotion of char or gas. Consequently, it can present a suitable alternative to the conventional trial and error strategies currently employed in industrial settings to improve process control.

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Copyright information:

Kinetic and mechanistic analysis of mineral added pyrolytic process for enchanced 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 experimental procedures and analyzed using custom-developed Python modules. 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, Fourier-transform infrared spectroscopy (FTIR), and thermogravimetric analysis-mass spectrometry (TGA-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 X-ray Photoelectron Spectroscopy (XPS) would be used for identifying the chemical composition of the biochar matrix.

Documentation and Metadata

What documentation and metadata will accompany the data?

In the current study, following instances of metadata will be used:

- Feedstock characteristics (ultimate/proximate analysis, lignin-cellulose-hemicellulose ratio, ash content, particle size)
- Dopant identity and preparation method (type, loading %, mixing technique, pre-treatment, purity, manufacturer)
- TGA operational details (heating rate, gas flow rate, sample mass, crucible type, atmosphere)
- Derived kinetic parameters (Ea(α), lnA, model function, conversion range)
- Instrument calibration data (baseline correction, buoyancy effects if corrected)
- Environmental or batch information (moisture content, sample conditioning, replicate consistency)
- Data processing: Baseline correction, smoothing/filtering applied
- Kinetic modelling: Methods (Friedman, KAS, Vyazovkin, Master Plot, etc.) and any numerical

approximations

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