Data Article

Data on FTIR, TGA – DTG, DSC of invasive *Pennisetum purpureum* grass

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**Abstract**

The aim of this research is to characterize the invasive grass, *Pennisetum purpureum*, to evaluate the potentiality of the bioenergy production. Fourier transform infrared (FTIR) spectra are measured in order to understand the functional groups and their structure in the biomass. The thermogravimetric analysis (TGA) and the derivative thermogravimetric analysis (DTG) data are provided under Pyrolysis (N\(_2\)) and combustion (O\(_2\)) conditions to reveal the degradation pattern of the biomass. Differential scanning calorimetry (DSC) is the thermochemical process to measure the enthalpy changes pattern of the biomass. The original data presented in this work can be found in a research paper titled “Evaluation of the bioenergy potential of invasive *Pennisetum purpureum* through pyrolysis and thermogravimetric analysis”, by Md Sumon Reza, Shafi Noor Islam, Shammya Afroze, Muhammad S. Abu Bakar, Rahayu S. Sukri, Saidur Rahman, and Abul K. Azad [1].

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Specifications table

| Subject                  | Chemical Engineering, Energy   |
|--------------------------|--------------------------------|
| Specific subject area    | Biomass and Bioenergy, Renewable Energy |
| Specific type of data    | Graph, Figure                  |
| How data were acquired   | The FTIR data were collected on an FTIR Two-Spectrum PerkinElmer with the integrated detector of MIR TGS (15,000–370 cm⁻¹) and the TGA-DTG data were obtained on a PerkinElmer thermogravimetric analyzer of TGA7 series. Differential scanning calorimetry (DSC) analysis was done by the SETARAM thermogravimetric analyzer. |
| Data format              | Raw                            |
| Parameters for data collection | FTIR was obtained for the wavenumber from 4000 to 500 cm⁻¹ with a 1 cm⁻¹ step size. Thermogravimetric analysis (TGA-DTG) was performed under a flow of pure N₂ gas and pure O₂ gas from 40 °C to 900 °C temperature with a constant heating rate of 10 °C/min. DSC was done for 25 °C to 780 °C temperature at a 10 °C/min heating rate with 50 ml/min Nitrogen (N₂) gas flow. |
| Description of data collection | FTIR values were obtained for the transmittance percentages on different wavenumbers. Thermogravimetric analysis (TGA-DTG) data were collected for weight loss and the degradation rate for temperature. Differential scanning calorimetry has been provided the values of heat flow for different temperatures. |
| Data source location     | FTIR data were collected at the Research centre for Nano-Materials and Energy Technology, Sunway University, Bandar Sunway, 47500 Selangor Darul Ehsan, Malaysia. The Thermogravimetric and Derivative thermogravimetric analysis data were collected at the Scientific and Testing equipment center, Prince of Songkla University, Hat Yai District, Songkhla 90110, Thailand. DSC experiment was performed in the Physics Laboratory of the Faculty of Science at Universiti Brunei Darussalam, Jalan Tungku Link, BE1410 Brunei Darussalam. |
| Data accessibility       | With the article               |
| Related research article | Md Sumon Reza, Shafi Noor Islam, Shammya Afroze, Muhammad S. Abu Bakar, Rahayu S. Sukri, Saidur Rahman, Abul K. Azad, Evaluation of the bioenergy potential of invasive Pennisetum purpureum through pyrolysis and thermogravimetric analysis, Energy, Ecology and Environment, DOI: 10.1007/s40974-019-00139-0 [1] |

Value of the data

- The data provides detailed information on the chemical structures, chemical composition, thermal degradation behavior, and enthalpy change characteristics of the invasive grass biomass sample.
- Information on this data article will be helpful for the researcher to determine the functional groups of the biomass sample to know the structure and bondage between carbon, hydrogen, and oxygen in this sample.
- The data show essential calculation on the decomposition of the biomass particles occurring in the first phase as the elimination of moisture content, in the second phase as the removal of major volatile matter by the degradation of hemicellulose and cellulose and in the third stage as the decomposition of lignin.
- The data show the endothermic reaction started from 25 to 217 °C for moisture removal and 564 °C to 780 °C for lignin breakdown whereas the exothermic reaction happened from 217 °C to 564 °C temperature for the decomposition of hemicellulose and cellulose mainly.
- This data set will be beneficial for researchers who want to understand the functional groups, chemical structure, proximate analysis, and the thermal degradation behavior with the change in heat flow for the temperature of this biomass.

1. Data description

Pennisetum purpureum grass contains very low moisture content, moderate ash content and fixed carbon with a high amount of volatile matter. As it has a negative impact on biodiver-
sity for invasiveness, it can be used to produce bioenergy to meet the shortfall of fossil fuel and also can reduce greenhouse CO\textsubscript{2} gas emission in the environment. The thermochemical processes like pyrolysis and gasification are the most suitable procedure for converting this invasive biomass into effective bioenergy [2]. The FTIR, TGA, DTG, and DSC data were presented in Fig. 1, Fig. 2(a), and (b), and Fig. 3 respectively. FTIR measurements were performed over a range of wave numbers from 4000–5000 cm\textsuperscript{-1}. TGA and DTG were carried out under pyrolysis (N\textsubscript{2}) and combustion (O\textsubscript{2}) conditions from 40 °C to 900 °C with 10 °C/min heating rate. For the differential scanning calorimetry (DSC), the data were collected from 25 °C to 780 °C with a heating rate of 10 °C/min under 50 ml/min N\textsubscript{2} gas flow.

In FTIR, it is found that this invasive grass has a similar structure to the other biomass. It has the O–H, C–H and C=O groups in the formation of cellulose, hemicellulose, and lignin. Peaks found for the structure of C=O bond, O–H bond, C–O bond manly in the lignin and the xylan. The significant peak of this sample found for the C–O bond mainly in the cellulose and hemicellulose for the wavenumber of 1045 cm\textsuperscript{-1} [3]. It also showed the presence of aromatic rings in the biomass sample [4].

In TGA, the initial decomposition of the biomass occurred around 5% at the temperature of 40 °C-192 °C to eliminate the moisture content and light volatile matter present in the biomass. The major degradation (59.61% in pyrolysis and 50.75% in combustion) happened at the second stage in the temperature of 192 °C - 441 °C, due to the breakdown of the cellulose and hemicellulose. The highest decomposition has occurred at the rate of 6.56 (wt%/min) for the temperature at 334 °C in the pyrolysis condition and 7.66 (wt%/min) for the temperature at 312 °C in the combustion condition due to the cracking of the major cellulose and hemicellulose. In the last stage, for the temperature of 441 °C-900 °C the weight loss of 11.58% (N\textsubscript{2}) and 15.88 (O\textsubscript{2}) due to the slow and constant decomposition of the complex compound lignin. After 900 °C, the residue 23.56% was considered as biochar for pyrolysis condition and 8.12% ash for combustion condition [3].

Differential scanning calorimetry (DSC) is a thermochemical technique to determine the heat flow property of biomass on the basis of temperature change. In this data, the DSC curve indicates the reaction pathway of the biomass. The curve started with endothermic reaction from room temperature to 317 °C where the first peak appeared at 89 °C due to the evaporation of water molecules, which is the signifies of an endothermic reaction. The curve went to the exothermic region from endothermic at the temperature of 217 °C and continues up to 564 °C with the peak occurred at 315 °C temperature was due to the degradation of hemicellulose and cellulose.
Fig. 2. (a) TGA and (b) DTG curves for *Pennisetum purpureum* biomass sample under pyrolysis and combustion condition.

Fig. 3. DSC curve for *Pennisetum purpureum* biomass sample.
components. After 564 °C to 780 °C, it started with an endothermic area mainly for the decomposition of lignin [5].

2. Experimental design, materials, and methods

2.1. Materials and methods

The invasive Pennisetum Purpureum grass was collected from the forest near the Universiti Brunei Darussalam (UBD) area. After washing by water thoroughly, the grasses were kept in sunlight for one week. Then the dried feedstock was crushed into small pieces by a lab blender. After that, the samples were sieved by standard 60 no sieve to get the particle size <0.25 mm. Finally, the biomass samples were stored in the airtight bags to avoid air contraction.

2.2. FTIR

FTIR data were collected on PerkinElmer of Spectrum Two series. The scanning speed used to detect the Fourier Transform Infrared Spectrum (FTIR) of the sample was maintained at a constant 1 cm⁻¹ step size with a scan range of 4000–500 cm⁻¹.

2.3. TGA-DTG

Thermogravimetric analysis was performed for a sample of invasive biomass species. Measurement was carried out on sample loaded in small alumina pans, using a PerkinElmer thermogravimetric analyzer of the TGA7 series thermal analyzer. The temperature was set from 40 °C to 900 °C, with a constant heating rate of 10 °C/min, under a flow of nitrogen gas in pyrolysis condition and oxygen gas in combustion condition.

2.4. DSC

Differential scanning calorimetry (DSC) analysis was done for this invasive grass. A small amount of biomass powder was measured in a ceramic crucible by a micro-balance pan. The crucible with the sample was set in the SETARAM thermogravimetric analyzer. The experiment was done for the temperature of 25–780 °C with a heating rate of 10 °C/min under the Nitrogen Gas flow rate of 50 ml/min.

Declaration of Competing Interest

The authors declare that they have no known competing for financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

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