Bioresource Technology 232 (2017) 87–92

Contents lists available at ScienceDirect

Bioresource Technology

journal homepage: www.elsevier.com/locate/biortech

Uncertainty estimation by Bayesian approach in thermochemical conversion of walnut hull and lignite coal blends

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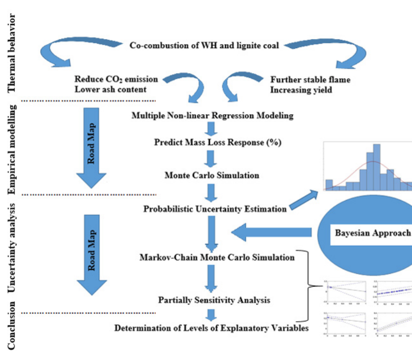
HIGHLIGHTS

- Walnut hull was utilized in (co-) combustion with lignite coal.
- Thermal behaviors of (co-) combustion process was investigated.
- MNLR technique was used to predict the mass loss percentage.
- Bayesian approach was found quite effective in identification of uncertainties.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 5 January 2017
Received in revised form 2 February 2017
Accepted 4 February 2017
Available online 8 February 2017

Keywords:
Walnut hull
Co-combustion
Non-linear regression
Uncertainty analysis
Monte Carlo simulation
Bayesian approach

ABSTRACT

The main purpose of the present study was to incorporate the uncertainties in the thermal behavior of walnut hull (WH), lignite coal, and their various blends using Bayesian approach. First of all, thermal behavior of related materials were investigated under different temperatures, blend ratios, and heating rates. Results of ultimate and proximate analyses showed the main steps of oxidation mechanism of (co-)combustion process. Thermal degradation started with the (hemi-)cellulosic compounds and finished with lignin. Finally, a partial sensitivity analysis based on Bayesian approach (Markov Chain Monte Carlo simulations) were applied to data driven regression model (the best fit). The main purpose of uncertainty analysis was to point out the importance of operating conditions (explanatory variables). The other important aspect of the present work was the first performance evaluation study on various uncertainty estimation techniques in (co-)combustion literature.

1. Introduction

Fossil fuels were the most common used materials in thermal-based electricity production plants. One of these fossil fuels, lignite coal, could be stated as an important primary energy source in the world and it has been generally used in these plants. Although the abundant reserve in the world, lignite coal has been also stated as one of the most important reasons of global warming based on CO_2 emissions, and also air pollution. There exist many studies that point out this situation in related literature (e.g. Yildiz et al., 2016; Kurekci, 2016; Cepeliogullar and Putun, 2014; Kayahan and Ozdogan, 2016). Considering these hazardous effects, decreasing CO_2 emission based on combustion of fossil fuels has become a necessity to be addressed.

Many researchers have suggested usage of fossil fuels especially lignite coal with biomass in co-combustion process. So that, many advantages can be gained such as reducing CO_2, protecting the air pollution, and also decreasing both of greenhouse gas emissions and fossil fuel consumption. Co-combustion provides these advantages with a cost-effective way as many researchers have already stated (e.g. Hu et al., 2015; Mi et al., 2016). The main goal of co-

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http://dx.doi.org/10.1016/j.biortech.2017.02.021
0960-8524/

combustion of fossil fuels and biomass underlies the phenomena that providing a further stable flame and also a better handle of the burning process depending on increasing the volatile matter content while increasing the mass loss percentage and decreasing the ash content (e.g. Yildiz et al., 2016; Iegorov et al., 2017).

Turkey places in quite important geography in the world. As a result of this situation, Turkey has important underground and aboveground resources such as lignite coal, copper, alumina, hazelnut, walnut, peanut, ant etc. (e.g. Ozer et al., 2007; Tanyildizi, 2011; Uzuner and Cekmecelioglu, 2015; Buyukada, 2016; Ozkal and Yener, 2016; Yildiz et al., 2016). These materials have been used in several types of industries for related purposes for example energy and electricity production. Huge amount of hull as biomass sources have been produced as a result of industrial food production. These hull have no alternative uses except for production of domestic animal feed and storage of them causes a disposal problem because of the large volumes. Unfortunately, there are a few studies on utilization and also recovery of this biomass although this potential. Thus, investigation of WH as one of important agricultural waste of Turkey in co-combustion process with lignite coal as one of the most important fossil fuel of Turkey using a thermogravimetric method has been on demand considering this issue.

Nowadays, probabilistic uncertainty analyses have also gained an importance in statistical modeling studies. It can be considered a simple and partial sensitivity analysis. There are a lot of techniques to incorporate the uncertainties in proposed model such as likelihood (e.g. Chaudhary and Hantush, 2017), maximum a posterior (e.g. Pan and Pandey, 2016), Monte Carlo (e.g. Evrendilek et al., 2016), Bayesian approach (e.g. Pan and Pandey, 2016; Zhang et al., 2016), and etc. The effect of each explanatory variable on response variable is saved while the explanatory variables keeping constant. This may generally help in identifying the uncertainty in a linear model but it is not applicable for non-linear models because of the larger deviation. The solution is just possible to apply a suitable framework for identification of the uncertainties in model predictors (Evrendilek et al., 2016; Pan and Pandey, 2016). It is certainly clear that there are very few studies on this subject in the related literature.

There are a lot of studies on co-combustion of biomass and coal but approximately none of them use WH and lignite coal. Thermochemical conversion of WH and its co-combustion with lignite coal can cotribute to enhancing air quality in Turkey. Additionally, statistical approaches based on uncertainty estimation can be useful for the improvement of design parameters and also researchers. Therefore, the main objectives of the present study is to investigate effects of blend ratio, temperature and heating rate on mass loss percentage (MLP) of (co-) combustion of WH and lignite coal (1), to guide the researchers by stating the importance of uncertainty estimation in determination of the levels of operating conditions using MC simulation in the absence and presence of Bayesian approach (MCMC) (2).

2. Materials and methods

2.1. Samples

Lignite coal samples were provided from Chemical Engineering Department of Fırat University, Elazig, Turkey. Walnut hull samples were provided from a local domestic feed production plant, Giresun, Turkey. A similar pretreatment procedure was applied to samples that Buyukada (2017) had performed.

2.2. Co-combustion process

Co-combustion experiments were performed by the lignite coal (C), walnut hull (WH), and their various blend ratios of C60WH40, C70WH30, C80WH20, and C90WH10 (%, wt to wt). After the temperature arrangement to 25 °C had been done with a heating rate of 20 °C min^{-1} in the atmosphere, the temperature was raised to 1000 °C with various heating rates of 10, 20 and 30 °C min^{-1} (10.00 ± 0.5 mg of samples). The air flow was determined as 20 mL min^{-1} and it was kept constant. The mass loss percentage (MLP, %) and the mass loss rate (MLR, % min^{-1}) of the samples were analyzed under non-isothermal conditions. All the runs were performed with three replicates to determine the standard deviation and to prevent the experimental errors.

2.3. Uncertainty estimation

Mass loss percentage (MLP, %, response to co-combustion process) as a function of three explanatory variables of (1) blend ratio (wt%), (2) heating rate (°C min^{-1}), and (3) temperature (°C) was investigated by MNLR modeling technique considering the adjusted regression coefficient (R^2_{adj}) and predictive regression coefficient (R^2_{pred}). Predictors in the best-fit MNLR model were chosen by following the best-subset procedure. The main goal of the best-subset procedure was to choose the proposed MNLR model which having the maximum values of adjusted and predicted R^2 values with the lowest number of predictors (except for intercept), the lowest multicollinearity (considering variation inflation factor, VIF), and the lowest autocorrelation (considering Durbin Watson factor, D-W). Monte Carlo (MC) and its modified form based on Bayesian approach (Markov Chain Monte Carlo, MCMC) simulations were used to analyze the uncertainties in predictors of proposed MNLR model. Thereby, a comparison study and also a partial sensitivity analysis were performed on estimation of uncertainty. Minitab 17 (Minitab PA), Matlab 2012b (Matlab, USA), and Microsoft Excel-based Model Risk (trial version, Vose Software) were used for MNLR, MC, and MCMC analyses, respectively.

3. Results and discussion

3.1. Proximate analyses

Volatile content, harmful gas emissions (SO_x and NO_x), and ash amount (including fixed carbon) of pure lignite coal, pure WH, and their various blend ratios were investigated by proximate analyses and related results were given in Table 1. The first result of proximate analyses showed that volatile content of coal and WH were 28% and 56%, respectively. This finding showed that WH can be removed at a lower temperature than lignite coal. The second finding was about reduction of harmful gas release. Utilization of WH with lignite coal in a co-combustion process can be resulted as a reduction in SO_x and NO_x production according to combustion of the pure lignite coal. This claim was justified by the following third finding that was about ash contents. When considering the ash contents of WH and coal (as 4% and 48%, respectively on dry basis), these data supports significantly the expectation that the blends of WH and lignite coal may be beneficial for reduction of waste combustion. Furthermore, higher ash amounts may also decrease the efficiency of the combustion process considering the formation of aggregates and decrease of the coefficients of mass and heat transfer. All the findings in this part were in good accordance with the results of similar studies (Buyukada, 2016; Kayahan and Ozdogan, 2016; Yildiz et al., 2016; Atimtay et al., 2017; Chen et al., 2017; Yao et al., 2017).

3.2. Ultimate analyses

Results of elemental findings were obtained by ultimate analyses and given in Table 1. As a result of ultimate analyses, 58% and