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Parametric study and global sensitivity analysis for co-pyrolysis of rape straw and waste tire via variance-based decomposition

Li Xu, Yong Jiang[*], Rong Qiu

State Key Laboratory of Fire Science, University of Science and Technology of China, Heifei 230027, China

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ABSTRACT

In present study, co-pyrolysis behavior of rape straw, waste tire and their various blends were investigated. TG-FTIR indicated that co-pyrolysis was characterized by a four-step reaction, and H_2O, C−H, O−H, CO_2 and C=O groups were the main products evolved during the process. Additionally, using BBD-based experimental results, best-fit multiple regression models with high R^2-*pred* values (94.10% for mass loss and 95.37% for reaction heat), which correlated explanatory variables with the responses, were presented. The derived models were analyzed by ANOVA at 95% confidence interval, *F*-test, lack-of-fit test and residues normal probability plots implied the models described well the experimental data. Finally, the model uncertainties as well as the interactive effect of these parameters were studied, the total-, first- and second-order sensitivity indices of operating factors were proposed using Sobol' variance decomposition. To the authors' knowledge, this is the first time global parameter sensitivity analysis has been performed in (co-)pyrolysis literature.

1. Introduction

New technologies, means and resources are currently attracted tremendous attention as the world is confronted with energy shortage and environment deterioration. The consumption of traditional fossil fuels has led to its depletion as well as emissions of toxic and harmful pollutants such as NO_x, SO_2, chlorides. Parallel to this, there also exists a worldwide problem of solid wastes treatment. Waste tire (WT) is a kind of renewable resource, with the booming global economy, especially the rapid development of the automobile industry in recent decades, approximately 1.4 billion units (about 17 million tons) of waste tires have been generated all over the world annually (Sienkiewicz et al., 2012). The incineration management of waste tire will cause the emissions of dioxins, PAHs, VOCs, particulate matter, etc. to the atmosphere thus leading to a serious air pollution (Lahijani et al., 2013). The composition of scrap tires are 60–65 wt% rubber, 25–35 wt% carbon black (CB) and some other accelerators and fillers (Leung and Wang, 1998). Since the contained rubber has a higher calorific value, from the perspectives of both economy and ecology, it is meaningful to recycle and utilize scrap tires to take advantage of their high energetic and energy conversion potential as raw material (Haydary et al., 2012).

Various conventional means are adopted in waste tire treatment such as incineration and stockpiled in open landfills. Such improper disposal management caused severe "black pollution" to the environment and fire hazards (Kebritchi et al., 2013). Among the multiple techniques, one of the widely applicable ways for solving such kind of problems is pyrolysis (Kah et al., 2016). However, single pyrolysis of WT could barely produce high quality fuels because of the high ash content and fixed carbon. Besides, the considerable percentage of CO_2 generated in the pyrolysis gas greatly decreases the heating value (Laresgoiti et al., 2004). On the other way around, analysis of the pyrolysis process of biomass liquid composition shows that the pyrolysis liquid is mainly a series of oxygen containing higher organic compounds such as phenol, cresol, ethers, and so on (Lu et al., 2009). Although these oxygen-containing compounds are likely to become the fuel in the future. However, there are still many problems to be solved, such as high oxygen content, low heating value, ignition delay, and serious corrosion, etc.

Considering these issues, simultaneous co-pyrolysis of WT and biomass, especially agricultural residues, could be an effective approach as WT addition enhances the biomass energy utilization and improves the heating value of bio-oil from co-pyrolysis (Martínez et al., 2014). Meanwhile, the liquid generated by the pyrolysis of WT is a complex mixture consisting the sulfur- and nitrogen-containing compounds. If used as fuel, it may lead to SO_2 and NO_x emission problems. These problems would also be relieved if waste tires were co-pyrolyzed with biomass (Hassan et al., 2016).

China is considered as the biggest producer of rape worldwide, with the huge planting area, approximately 1.96×10^7 tons of rape straw is generated as byproduct in the harvest season every year (Xu et al.,

2017). While the huge amount of rape straw in China are mainly disposed by extensive combustion, which is of low efficiency and causes heavy environmental pollution. Therefore, thermogravimetric investigation of rape straw as an important agricultural residue in co-pyrolysis process with waste tire as a high energetic and energy conversion potential raw material has been on demand.

Over the years, various statistical modelling approaches have been developed with increasing interest in biomass (co-)pyrolysis. As a matter of fact, these modelling methods are only mathematical and the different parameter values present a large discrepancy as a function of the authors (Pan and Pandey, 2016). Besides, the influences of these sundry techniques adopted for the mathematical descriptions on the qualitative and quantitative characterization of the modelling are usually not clearly defined. Hence, more research is needed, especially with respect to the impact of these parameters and their consequences on the model adequacy to quantitatively describe all variables with low uncertainties. For incorporating uncertainties in these models, many approaches have been employed in previous literatures, for example Monte Carlo approach (e.g. Samsudin and Mat, 2015; Batan et al., 2016), Bayesian method (e.g. Pan and Pandey, 2016; Buyukada, 2017a,b), likelihood (e.g. Fachet et al., 2014), etc. However, global sensitivity analysis of operating factors effect on (co-)pyrolysis is still missing, as all the mentioned studies only use the one-factor-at-a-time (OFAT) approach, or performing a partial sensitivity analysis. Such kind of approach does not illustrate the combined influences of the input parameters, and cannot be applied to non-linear models due to the larger deviation. Obviously, there exists no studies with a global sensitivity analysis considering the interactions of each parameters, what is nevertheless of great importance, for uncertainty identification in model predictors in related literature.

Therefore, the main aim of present work is to: (i) investigate the influences of temperature, heating rate and mixing ratio, especially the interactive effects on mass loss and reaction heat during RS and WT co-pyrolysis; (ii) to organize in a hierarchy the importance of various operating factors as well as their interactions on proposed models via a global sensitivity analysis for the first time.

2. Materials and methods

2.1. Samples

Steel free waste tire samples tested in this study were collected from a tire recycling plant in Shijiazhuang City, Hebei Province, China. A typical agricultural residue biomass, rape straw, was obtained from a biomass production workshop around Zhengzhou in Henan Province, China. The materials were firstly cleaned, then crushed and passed through 150 mesh sieve to achieve < 125 μm particle size according to Tyler Standard Screen Scale. The samples were dried in 101A-4 electric forced air dry oven (Shanghai, China) at 105 °C until their mass stabilized. Dried waste tire and rape straw materials were then well mixed together and sealed in Ziploc bags for following experiments. The ultimate and proximate analysis of RS and WT used in this study were presented in Table 1. The high heating value (HHV) was calculated by Dulong equation (Fang et al., 2017) based on ultimate analyses:

$$HHV = 338.2C + 1442.8(H-O/8) \tag{1}$$

in which C, H, and O stand for the mass fractions of carbon, hydrogen and oxygen.

2.2. Experimental procedure

2.2.1. TGA

Co-pyrolysis experiments were conducted with rape straw (RS), waste tire (WT), and their various blends with mixing ratios (RS to WT, wt%) of RS40WT60, RS60WT40 and RS80WT20, using a NETZSCH STA 449 F3 Jupiter (NETZSCH, Germany) thermogravimetric analyzer. Tested samples with initial weight about 5 ± 0.5 mg were heated from room temperature to 850 °C at heating rates of 10, 20, and 30 °C/min in pure nitrogen with a flow rate of 60 ml/min. The thermogravimetric TG, DTG and DSC profiles were recorded by NETZSCH Proteus software. All tests were repeated at least twice.

2.2.2. FTIR analysis

The gaseous products evolved from co-pyrolysis of RS and WT were characterized using Fourier transform infrared (FTIR) spectrometer (PerkinElmer Frontier, USA), with pure nitrogen at 60 ml/min flow rate. TG analyzer and FTIR were connected by a heated transfer line which was heated and maintained at 200 °C for preventing the condensation of gaseous products during co-pyrolysis process. FTIR spectra record regions is from 4000 to 450 cm^{-1}.

2.3. Data-driven modelling and parametric study

2.3.1. Reaction heat calculation from DSC profiles

The data from differential scanning calorimetry (DSC) profiles has been used to measure the reaction heat. According to previous researches, the heat from DSC curves mainly consists of the heat heating the sample and the heat required for the reaction (Fang et al., 2006, 2009), which can be calculated using Eq. (2), in which Q (kJ) is the reaction heat of sample pyrolysis, Q_p (kJ kg^{-1} s^{-1}) is the heat flow from the DSC data, T (K) and t (s) denote the reaction temperature and time, respectively. $m_{s,0}$ (kg) is the initial sample mass, m_s (kg) is the sample mass at time t, and the heat capacity of the sample is represented by $c_{p,s}$ (kJ kg^{-1} K^{-1}).

$$\frac{dQ/dt}{m_{s,0}} = \frac{m_s c_{p,s} dT/dt}{m_{s,0}} + \frac{Q_p}{m_{s,0}} \tag{2}$$

In fact on the right part of Eq. (2),

$$\frac{Q_p}{m_{s,0}} \gg \frac{m_s c_{p,s} dT/dt}{m_{s,0}} \tag{3}$$

Based on Eq. (3), the reaction heat in Eq. (2) can be calculated by:

$$\frac{dQ/dt}{m_{s,0}} = \frac{Q_p}{m_{s,0}} \tag{4}$$

Therefore, the reaction heat of the sample pyrolysis can be obtained by integrating the DSC profiles using the following equation:

Table 1
Proximate and ultimate analysis of materials used in this study.

Sample	Proximate analysis (wt%)				Ultimate analysis (wt%)					HHV (kJ/kg) Q
	M	A	VM	FC	C	H	O[a]	N	S	
RS	10.46	5.63	80.20	3.71	42.90	5.75	49.90	0.87	0.58	14840.07
WT	1.19	10.17	63.24	25.40	80.67	7.47	9.51	0.59	1.76	34179.53

Abbreviations: M, Moisture; A, Ash; VM, Volatile matter; FC, Fixed carbon; HHV, high heating value.
Note: [a]Calculated by difference.