Fuel 212 (2018) 431–436

Contents lists available at ScienceDirect

Fuel

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

Full Length Article

Design of simplified models for the estimation of higher heating value of refused derived fuels

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ARTICLE INFO

Keywords:
HHV
RDF
Estimation
Low errors
Ultimate analysis

ABSTRACT

In this paper we disclose two new models for the estimation of the higher heating value of refused derived fuels as an answer to the question – "Are the available models to predict the HHV of biomasses suitable to be applied with an acceptable accuracy to RDFs?". Based on the carbon and hydrogen content the newly developed equations were used to predict, accurately, the higher heating value of 25 samples available from open database sources and then compared with other 35 equations already introduced by other authors. The models herein presented have demonstrated, within the test group used to lead to very low average absolute and bias errors. The models were then validated with samples obtained locally, showing that the results were in line with that obtained for the test group.

1. Introduction

Nowadays, one of the most prized assets of a research group, in addition to the human and time resources, is the budget available to carry out your research and studies. The funds available to produce knowledge should be used wisely only whenever is strictly necessary. In this sense, for instance, the analysis and characterization of raw materials and products must be streamlined and carried out when they are strictly necessary.

During the course of our studies based on the use of biomass to produce energy in alternative to the petroleum-based ones, a parameter that is often screened is the higher heating value. Although, such analysis can be rather expensive and time-consuming.

The calorific value of the biomass depends mainly on its chemical composition, moisture content, ashes amounts and its heating value [1]. The heat capacity of a fuel is usually measured regarding the higher heating value (HHV) or lower heating value (LHV). HHV evaluates the heat that is released during combustion with the original and generated water in a condensed state. On the other hand, LHV consider water as a product of the combustion reaction. These parameters can be determined experimentally employing an adiabatic bomb calorimeter while measuring the enthalpy change [2]. Despite being accurate measurement processes, the HHV and LHV, sometimes, such technique is not available to all researchers [1]. The outsourcing is most of the times the solution to access it although such analysis can be quite expensive. Alternatively, the elemental analysis is an economical and easily accessible technique, disclosing the chemical composition of a sample, i.e. the carbon, hydrogen, sulfur, nitrogen content.

With the information provided by elemental analysis numerous empirical models have been described and developed over the years, offering an easy and simple alternative to evaluate, approximately, the LHV and HHV [2–6]. The first studies conducted towards the establishment of such estimation models dates back to 1880 and are known as Dulong's formula [1,4].

The basis of the of HHV predicting correlations is the use of statistical analysis of a reference test group. Although those correlations are limited to the type of materials used as references and often cannot be extrapolated to a different kind of matter [6].

Regarding what has been mentioned above, there are many correlations based only in the ultimate analysis established for various types of materials [4], but very few [7], especially related to refused derived fuels (RDFs).

RDFs contains mainly high quantities of biodegradable material but also a small fraction of plastics. More particularly, RDFs are composed mainly of paper, cardboard, non-recyclable plastics, and other uneven materials. This waste is shredded, dried and hard-pressed before its use. The use of this materials as fuel is a solution for the valorization of a particular non-recyclable waste fraction resulting from solid municipal, industrial or commercial wastes. The usage of such waste to generate energy begun during the last quarter of the

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http://dx.doi.org/10.1016/j.fuel.2017.10.062
Received 17 March 2017; Received in revised form 3 May 2017; Accepted 11 October 2017

nineteenth century [9]. RDFs are often envisaged as a direct substitute for primary fossil fuels[8].

The aim of the study was to obtain a model that can be used to estimate the HHV of RDFs as accurate as possible. The nuts and the bolts of the methodology applied was based on statistic tools usually used within this context, the multivariable correlation, and linear regressions.

This paper aims to reply to the query – "Are the available models to predict the HHV of biomasses suitable to be applied with an acceptable accuracy to RDFs?". The models developed were then compared with other equations already disclosed and published using the chemical analysis of a test group of 25 samples of RDFs. The average absolute errors and average bias errors were determined to all models for comparison purposes. Later on, the models developed in this study were validated with two different samples of RDFs obtained locally.

2. Methodology

2.1. Test database

A database composed by 25 the samples of RDFs comprising the ultimate analysis (on a dry and ash free basis) and higher heating value were randomly selected from ECN Phyllis2 – Database for biomass and waste [10]. The samples used are presented in Table 1. For all 25 samples, the HHV ranged from 18.74 to 32.59 MJ/kg. The chemical composition is presented in Table 1.

2.2. Models used for comparison

For comparison purposes 35 already established models for predicting HHV based on the ultimate analysis of biomass were selected from the literature. Table 4 presents the equations of those models.

2.3. Estimation method

The evaluation method was developed using statistic software IBM® SPSS® version 24. Based on the data retrieved from the chemical analyses of the samples used as references, correlations between the variables and the HHV were obtained as well as their influence and relevance to the model.

The Pearson coefficient (R) in addition of *p*-values were used to identify the variables that were more prone to affect the HHV value. Each *p*-value shows the probability of obtaining the observed correlation; such value should be lower than 0.05. Linear regressions were studied using the factors that revealed to have greater statistical significance.

2.4. Statistical analysis

The errors used for comparison between the established models with that developed within our studies were the average absolute error (AAE), and average bias error (ABE). These two criteria have been widely employed by other authors within the same context [5,11,6,1–3] ABE and AAE are defined by the following equations:

$$AAE(\%) = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{HHV_{est}-HHV_{exp}}{HHV_{exp}}\right| \times 100 \quad (1)$$

$$ABE(\%) = \sum_{i=1}^{n}\left(\frac{HHV_{est}-HHV_{exp}}{HHV_{exp}}\right) \times 100 \quad (2)$$

where HHV_{est} and HHV_{exp} are, respectively, the estimated and experimental values for HHV and whereas n is the number of samples.

Generally speaking, the statistical parameters used, AAE and ABE were calculated to evaluate the estimated results. AAE estimates (based on the average of the data set) the accuracy of the estimated HHVs in relation to the experimental ones; small values indicate higher accuracy. While for ABE a positive value reveals an overall over-estimation while under-estimated values are identified by the negative values. Smaller absolute values of ABE demonstrate the smaller bias of the correlation between both data sets, estimated vs. experimental.

Table 1
Chemical composition and higher heat value for the test group.

Sample	Chemical composition (%) [10]					HHV (MJ/kg)
	C	H	N	S	O	
1	47.62	7.44	0.69	0.00	42.77	20.90
2	46.17	8.58	0.31	0.61	43.73	22.92
3	53.13	7.76	1.49	0.30	36.86	26.57
4	56.67	7.59	0.40	0.00	33.91	25.04
5	52.54	7.33	0.00	0.29	39.01	23.42
6	52.21	7.25	0.68	0.43	38.87	23.18
7	51.45	6.99	1.04	0.35	39.49	23.26
8	53.53	7.76	0.97	0.98	36.01	24.44
9	52.43	7.33	0.64	0.50	38.57	23.56
10	53.91	7.17	0.86	0.40	37.16	21.55
11	51.56	6.82	0.84	0.12	40.55	21.64
12	53.56	7.07	1.46	0.63	36.46	23.43
13	51.20	6.70	1.00	0.60	40.50	22.47
14	68.72	15.16	0.36	0.00	15.75	32.59
15	63.89	6.88	0.66	0.17	28.17	28.45
16	55.19	7.16	0.9	0.08	36.11	24.33
17	50.92	7.22	1.96	0.00	39.47	24.00
18	62.43	6.83	2.37	0.35	27.45	29.75
19	60.63	13.4	0.25	0.02	25.69	28.74
20	60.03	12.38	0.33	0.01	26.78	29.95
21	55.44	11.49	0.22	0.00	32.05	24.91
22	66.93	11.25	1.19	0.16	20.57	28.04
23	48.70	7.69	1.79	0.51	40.54	23.68
24	55.57	7.39	0.88	0.35	35.58	24.63
25	45.18	5.75	1.47	0.73	46.6	18.74

Table 2
Correlation between the chemical composition and HHV of the test group.

	Independent variables				
	C	H	N	S	O
Pearson's r	0.894	0.713	−0.085	−0.442	−0.923
p-value	0.000	0.000	0.685	0.027	0.000

Table 3
Equation of models A and B obtained by linear regression and their respective errors.

Model	Equation	R	R^2	*p*-value	Error (%)	
					AAE	ABE
A	0.404207C + 0.318857H	0.9987	0.9974	0.000	3.90	0.28
B	0.45309C	0.9984	0.9968	0.000	4.65	0.44