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MODELING AND ANALYSIS

Estimating the specific chemical exergy of municipal solid waste

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Abstract

A new model for predicting the specific chemical exergy of municipal solid waste (MSW) is presented; the model is based on the content of carbon, hydrogen, oxygen, nitrogen, sulfur, and chlorine on a dry ash-free basis (daf). The proposed model was obtained from estimations of the higher heating value (HHV) and standard entropy of MSW using statistical analysis. The ultimate analysis of 56 different parts of MSW was used for the derivation of the HHV expression. In addition, 30 extra parts were used for validation. One hundred and seventeen relevant organic substances that represented the main constituents in MSW were used for derivation of the standard entropy of solid waste. The substances were divided into different waste fractions, and the standard entropies of each waste fraction and for the complete mixture were calculated. The specific chemical exergy of inorganic matter in the waste was also investigated by considering the inorganic compounds in the ash. However, as a result of the extremely low value calculated, the exergy of inorganic matter was ignored. The results obtained from the HHV model show a good correlation with the measured values and are comparable with other recent and previous models. The correlation of the standard entropy of the complete waste mixture is less accurate than the correlations of each individual waste fraction. However, the correlations give similar results for the specific chemical exergy, indicating that HHV has a greater impact when estimating the specific exergy of solid waste than entropy.

Introduction

The quantities of solid wastes increase as the population continues to grow throughout the world, whereas the available space for disposal decreases. If this waste is not properly treated and handled, it will pollute the air, land, ground water, and soil as well as has a negative impact on the hygienic conditions of the people [1]. A waste-to-energy (WTE) plant is one of the most robust and effective posttreatment options to decrease the volume of produced waste, reduce greenhouse gas emissions, and utilize the energy content in nonrecyclable waste for the production of electricity and heat, thereby reducing the dependence on fossil fuel.

For the efficient design of energy conversion processes, the chemical exergy and energy content of the fuel are basic properties to be considered to estimate the maximum available energy entering the system for performance analysis and optimization of the entire process. This can be done by detecting and evaluating quantitatively the thermodynamic imperfection (exergy loss) of the process under consideration, its main sources of loss and possible ways of improving such process can be indicated [2]. Estimating the chemical exergy of fuel is an important step when performing exergy analysis [3] in waste-to-energy plants. Exergy analysis is a method that uses the conservation of mass and energy together with the second law of thermodynamics. This analysis method is useful to achieve a more efficient energy-resource use because it enables the locations, types, and magnitudes of losses to be identified and to determine meaningful efficiencies [4].

However, because many solid fuels have unknown structures and chemical compositions, their exergy values cannot be calculated directly because of the lack of standard

absolute entropy values [5]. Many models for the prediction and estimation of the chemical exergy of carbon-based fuels with complex bond interactions and unknown thermodynamics properties have been proposed based on the characteristics of the known homogeneous organic substances in the fuel. The first attempt was performed by Rant [6], involving the formulation of a semiempirical model to evaluate the availability (exergy) content of a structurally complicated material species. In that model, the chemical exergy of a fuel is evaluated from the computation of pure organic substances of known absolute entropies. Rant evaluated the ratios of the estimated chemical exergies and the higher heating values for seven gases and 12 liquid organic substances. Szargut and Styrylska [7] improved Rant's correlation by considering the chemical composition of the fuels. They obtained correlation formulas to express the dependence between the ratio of the standard chemical exergy to the lower heating value using mass ratios of hydrogen, oxygen, nitrogen and sulfur to carbon that describe the chemical composition of the fuel. Due to lack of thermodynamic data, sulfur was not considered in their model for solid fuels, and their correlations were theoretically limited to Szargut's reference environmental (R.E) model.

Using a model for estimating the thermodynamic properties of coal, char, tar, and ash, Eisermann et al. [8] approximated the standard entropy of coal by comparing the behavior of the standard entropies of a number of aliphatic and aromatic hydrocarbons as a function of several elemental ratios: H/(C + N), O/(C + N), N/(C + N) and S/(C + N). Shieh and Fan [9] estimated the specific chemical exergy of a structurally complicated material by adopting the concepts of the dead (or reference) state and the properties of the constituents in the material based on the first and second laws of thermodynamics. It was assumed that the entropy of a fuel is equal to the entropies of its constituent elements. This assumption is not accurate in many cases. Ikumi et al. [10] developed a method for estimating the entropies of coals based on the mole ratios of hydrogen, oxygen, nitrogen, and sulfur elements to the carbon element. Bilgen and Kaygusuz [11] used the entropy correlation proposed by Eisermann et al. [8] to improve the Shieh and Fan [9] model for the calculation of the chemical exergy of coals, and Stepanov [5] applied the entropy model developed by Ikumi et al. [10] to modify Shieh and Fan [9] to calculate the exergies of coke-oven gases of different metallurgical mills. These models are limited to coal fuels only because their constituent organic compounds have been derived from the standard entropies of the relevant organic substances of coals.

Song et al. [3] developed a model based on Shieh and Fan [9] to estimate the specific entropy of the organic matter in biomass used for the exergy calculations. Although their model showed a high accuracy and was simpler than the Szagut and Styrylska's correlation, it has a limited application, as it is only applicable to biomass. Song et al. [12] also proposed a model for estimating the entropy of solid fuels and then extended the Shieh and Fan [9] model using the major organic constituents of solid fuel for the prediction of the specific chemical exergy of solid fuels. However, they combined the higher heating value derived on a dry basis (db) with values of the standard entropy obtained based on a dry ash-free basis (daf) for the estimation of the chemical exergy. Furthermore, their model cannot be used for estimating the chemical exergy of substances containing elements other than C, H, O, N, and S and for combustible materials, such as certain categories of leather, plastic, and rubber, that are part of municipal solid waste. To the author's knowledge, no model has been found in the literature that is derived for predicting the chemical exergy of MSW.

The objective of this work is to propose a model for calculating the specific chemical exergy of MSW containing the C, H, O, N, S, and Cl from its elemental compositions on a dry ash-free basis.

Derivation of the Estimated Model

Municipal Solid Waste consists of a complex, heterogeneous mixture of organic and inorganic substances. The organic elements in MSW are mainly C, H, O, N, S, and Cl, which can be obtained from ultimate analysis, whereas the inorganics are commonly Si, Ca, K, P, Al, Mg, Fe, S, Na, Zn, Cu, Mn, and Cr, from which their oxides can be obtained from ash analysis data. Previous reports have shown that the influence of inorganic matters on the exergy value can be neglected in solid fuel as a result of their relatively small value [3, 12].

The standard chemical exergy of a substance that is not present in the environment can be evaluated by considering a reaction of the substance with other substances for which the chemical exergies are known [13]. The exact calculation of the chemical exergy of a material with complicated structures is difficult [14]; as a result, the standard chemical exergy of the substance in the environment is not readily available.

Standard chemical exergy of a substance

The chemical exergy of a substance is equal to the maximum amount of work that can be obtained from the substance by taking it to chemical equilibrium with the reference environment [15]. The standard exergy of a substance can be evaluated by considering an idealized reaction of the substance with other substances (generally

Table 1. Standard chemical exergy and standard entropies of various compounds.

Substance	e^0 (kJ/mol)	s^0 (kJ/mol K)
CO_2	19.87	0.214
H_2O_l	0.95	0.070
O_2	3.97	0.205
N_2	0.72	0.192
SO_2	310.93	0.248
SiO_2	1.636	0.041
HCl	85.5	0.187
CaO	129.881	0.038
K_2O	412.544	0.102
P_2O_5	377.155	0.117
Al_2O_5	4.479	0.051
MgO	62.417	0.027
Fe_2O_3	17.656	0.087
SO_3	242.003	0.257
Na_2O	296.32	0.075
MnO	122.390	0.060
ZnO	37.080	0.042
Cr	538.610	0.024
Pb	226.940	0.065
As	477.040	0.035
Cd	290.920	0.052
Cl	163.940	0.166

l, liquid phase.
Source: [3, 17, 18].

reference substances) of known chemical exergies [16]. The known chemical exergies can be obtain from the table of standard chemical exergy based on Szargut's R.E model (Model II), as shown in Table 1. With consideration of the reversible reaction for chemical formation of a compound, Szargut et al. [2] expressed the standard chemical exergy of elements or compounds as

$$b^o_{\text{ch}} = \Delta G^o_f + \sum_i n_i b^o_{\text{ch}i}\,(\text{kJ/mol}) \tag{1}$$

where ΔG^o_f, n_i, and $b^o_{\text{ch}i}$ represent the standard Gibbs energy of formation, the mole fraction of component i in the mixture, and the standard chemical exergy of the constituent element i, respectively.

Calculation of the specific chemical exergy of municipal solid waste

For simplicity, suppose 1 kg of MSW (daf), expressed as $C_mH_nN_pO_qC_rS_t$, undergoes complete combustion at a standard state for the steady condition to produce carbon dioxide, water, nitrogen, hydrogen chloride, and sulfur dioxide as follows:

$$\begin{aligned} &C_mH_nN_pO_qCl_rS_t + \left(m + t - \frac{q}{2} + \frac{n-r}{4}\right) O_2 \\ &\rightarrow \text{mCO}_2 + \left(\frac{n-r}{2}\right) H_2O + \frac{P}{2}N_2 + r\text{HCl} + \text{tSO}_2 \end{aligned} \tag{2}$$

All substances are assumed to enter and exit at the reference temperature, T_0 = 298.15 K, and reference pressure, P_0 = 101.325 kPa. The subscripts m, n, p, q, r, and t are the numbers of atoms of C, H, N, O, Cl, and S, respectively, in kmol/kg MSW or the molal compositions per kg of MSW expressed as:

$$m = \frac{0.01\text{C}}{12.011}\,\text{kmol/kg} \quad \text{or} \quad \frac{10\text{C}}{12.011}\,\text{mol/kg} \tag{3}$$

$$n = \frac{0.01\text{H}}{1.008}\,\text{kmol/kg} \quad \text{or} \quad \frac{10\text{H}}{1.008}\,\text{mol/kg} \tag{4}$$

$$p = \frac{0.01\text{N}}{14.007}\,\text{kmol/kg} \quad \text{or} \quad \frac{10\text{N}}{14.007}\,\text{mol/kg} \tag{5}$$

$$q = \frac{0.01\text{O}}{15.999}\,\text{kmol/kg} \quad \text{or} \quad \frac{10\text{O}}{15.999}\,\text{mol/kg} \tag{6}$$

$$r = \frac{0.01\text{Cl}}{35.45}\,\text{kmol/kg} \quad \text{or} \quad \frac{10\text{Cl}}{35.45}\,\text{mol/kg} \tag{7}$$

$$t = \frac{0.01\text{S}}{32.066}\,\text{kmol/kg} \quad \text{or} \quad \frac{10\text{S}}{32.066}\,\text{mol/kg} \tag{8}$$

where the elements in Equations (3–8) are expressed in wt% (daf). For the steady state, under the standard condition, the energy balance of the reaction in Equation (2) is given by

$$\begin{aligned} W = Q + h^0_{\text{MSW}} + \left(m + t - \frac{q}{2} + \frac{n-r}{4}\right) h^0_{O_2} - mh^0_{CO_2} \\ - \left(\frac{n-r}{2}\right) h^0_{H_2O} - \frac{p}{2} h^0_{N_2} - rh^0_{\text{HCl}} - th^0_{SO_2} \end{aligned} \tag{9}$$

The entropy balance is expressed as

$$\begin{aligned} 0 = \frac{Q}{T_o} + s^0_{\text{MSW}} + \left(m + t - \frac{q}{2} + \frac{n-r}{4}\right) s^0_{O_2} - ms^0_{CO_2} \\ - \left(\frac{n-r}{2}\right) s^0_{H_2O} - \frac{p}{2} s^0_{N_2} - rs^0_{\text{HCl}} - ts^0_{SO_2} + S_{gen} \end{aligned} \tag{10}$$

where W and Q are the work and heat transfer, respectively. S_{gen} is the entropy generated by the irreversibility in the reaction, and s^0 and h^0 represent the standard entropy and enthalpy, respectively.

Eliminating the heat transfer Q between Equation (9) and (10) gives the following:

$$W = \left[h^0_{MSW} + \left(m + t - \frac{q}{2} + \frac{n-r}{4}\right) h^0_{O_2} - hs^0_{CO_2} - \left(\frac{n-r}{2}\right) h^0_{H_2O} - \frac{p}{2} h^0_{N_2} - rh^0_{HCl} - th^0_{SO_2}\right] - T_o\left[s^0_{MSW} + \left(m + t - \frac{q}{2} + \frac{n-r}{4}\right) s^0_{O_2} - hs^0_{CO_2} - \left(\frac{n-r}{2}\right) s^0_{H_2O} - \frac{p}{2} s^0_{N_2} - rs^0_{HCl} - ts^0_{SO_2}\right] - T_o S_{gen} \quad (11)$$

The maximum work, W_{max}, will occur when there is no irreversibility in the system. Hence, Equation (11) can be expressed as

$$W_{max} = \left[h^0_{MSW} + \left(m + t - \frac{q}{2} + \frac{n-r}{4}\right) h^0_{O_2} - mh^0_{CO_2} - \left(\frac{n-r}{2}\right) h^0_{H_2O} - \frac{p}{2} h^0_{N_2} - rh^0_{HCl} - th^0_{SO_2}\right] - T_o\left[s^0_{MSW} + \left(m + t - \frac{q}{2} + \frac{n-r}{4}\right) s^0_{O_2} - ms^0_{CO_2} - \left(\frac{n-r}{2}\right) s^0_{H_2O} - \frac{p}{2} s^0_{N_2} - rs^0_{HCl} - ts^0_{SO_2}\right] \quad (12)$$

or

$$W_{max} = -\Delta H^o_r - T_o\left[s^0_{MSW} + \left(m + t - \frac{q}{2} + \frac{n-r}{4}\right) s^0_{O_2} - ms^0_{CO_2} - \left(\frac{n-r}{2}\right) s^0_{H_2O} - \frac{p}{2} s^0_{N_2} - rs^0_{HCl} - ts^0_{SO_2}\right] \quad (13)$$

where ΔH^o_r represents the heat of reaction of the combustion process, which is equal to the negative higher heating value [9], that is

$$\Delta H^o_r = -\text{HHV} \quad (14)$$

then

$$W_{max} = \text{HHV} - T_o\left[s_{msw} + \left(m + t - \frac{q}{2} + \frac{n-r}{4}\right) s^0_{O_2} - ms^0_{CO_2} - \left(\frac{n-r}{2}\right) s^0_{H_2O} - \frac{p}{2} s^0_{N_2} - rs^0_{HCl} - ts^0_{SO_2}\right] \quad (15)$$

Assume that the reaction in Equation (2) at 298.15 K and 101.325 kPa is an adiabatic process with no irreversibility. The exergy balance equation, in absence of changes in the kinetic and potential energy for reacting systems, is given by

$$0 = -W_{max} + e_{MSW} + \left(m + t - \frac{q}{2} + \frac{n-r}{4}\right) e^0_{O_2} - me^0_{CO_2} - \left(\frac{n-r}{2}\right) e^0_{H_2O} - \frac{p}{2} e^0_{N_2} - re^0_{HCl} - te^0_{SO_2} \quad (16)$$

where e represents the specific chemical exergy. Substituting Equation (15) into Equation (16), the specific chemical exergy of MSW (daf), e_{MSW}, is presented as

$$e_{MSW} = \text{HHV} - T_o\left[s^0_{MSW} + \left(m + t - \frac{q}{2} + \frac{n-r}{4}\right) s^0_{O_2} - ms^0_{CO_2} - \left(\frac{n-r}{2}\right) s^0_{H_2O} - \frac{p}{2} s^0_{N_2} - rs^0_{HCl} - ts^0_{SO_2}\right] + me^0_{CO_2} + \left(\frac{n-r}{2}\right) e^0_{H_2O} + \frac{p}{2} e^0_{N_2} + re^0_{HCl} + e^0_{SO_2} - \left(m + t - \frac{q}{2} + \frac{n-r}{4}\right) e^0_{O_2} \quad (17)$$

or

$$e_{MSW} = m\left[\left(e^0_{CO_2} + T_o s^0_{CO_2}\right) - \left(e^0_{O_2} + T_o s^0_{O_2}\right)\right] + \frac{n}{2}\left[\left(e^0_{H_2O} + T_o s^0_{H_2O}\right) - \frac{1}{2}\left(e^0_{O_2} + T_o s^0_{O_2}\right)\right] + \frac{q}{2}\left(e^0_{O_2} + T_o s^0_{O_2}\right) + \frac{p}{2}\left(e^0_{N_2} + T_o s^0_{N_2}\right) + t\left[\left(e^0_{SO_2} + T_o s^0_{SO_2}\right) - \left(e^0_{O_2} + T_o s^0_{O_2}\right)\right] - \frac{r}{2}\left[\left(e^0_{H_2O} + T_o s^0_{H_2O}\right) - \frac{1}{2}\left(e^0_{O_2} + T_o s^0_{O_2}\right) - 2\left(e^0_{HCl} + T_o s^0_{HCl}\right)\right] + \text{HHV}_{MSW} - T_o s^0_{MSW}\ (\text{kJ/kg}) \quad (18)$$

where e^0 is the standard exergy in kJ/mol and s^0 is the standard entropy in kJ/mol K, as tabulated in Table 1. s^0_{MSW} is the standard entropy of municipal solid waste, in kJ/K kg (daf), and HHV_{MSW} is the higher heating value (HHV) of MSW, in kJ/kg (daf). The specific chemical exergy of MSW can be calculated once the standard chemical exergies of CO_2, $H_2O(l)$, N_2, O_2, SO_2, and HCl; the higher heating value; and the absolute entropies are known.

Estimating the higher heating value of municipal solid waste

In the absence of a measured value, the HHV of fuel can be estimated from their elemental composition [19, 20]. In this study, the HHV estimate was performed by considering 56 data points and 30 data points of MSW samples for the derivation and validation of the

Table 2. Assumed correlations used for the selection of the proposed model for HHV (daf).

S. No.	Assumed expression	Criteria for selection	Reference
1.	HHV = aC + bH + cO + dN + eS + fCl	Assuming fuel HHV to be a linear function of it constituents.	Current model
2.	HHV = aC + bH + cO + dN + eS	Based on Gumz's criteria	[19]
3.	HHV = a^0 + bH + cO + dN + eS + fCl	Based on Chang's criteria	[23]
4.	HHV = aC + b (H – O/8) + eS	Based on Dulong's criteria	[19]
5.	HHV = aC + bH + cO + eS	Based on modified version of Dulong's criteria	[19]
6.	HHV = a^0 + aC + bH + cO^2	Based on Seyler's criteria	[19]
7.	HHV = a (C – (3/8) O) + b (3/8) O) + c (H – (1/6) O) + eS	Based on Steuer's criteria	[19]
8.	HHV = a (C – 0.75 (O/2)) + b (H – 0.125 (O/2)) + eS	Based Sumegi's criteria	[19]
9.	HHV = aC + bH + c ((N + O – 1)/8) + eS	Dulong-Berthelot's criteria	[19]

where C, H, O, N, S, and Cl represents carbon, hydrogen, oxygen, nitrogen, sulfur, and chlorine, respectively, in % by mass on a dry ash free basis. a^0, a, b, c, d, e, and f are constants of correlation.

correlation, respectively; in addition, the chemical composition and HHV of each sample was collected from the published literature and presented in Tables A1 and A2 (Appendix 1). These data cover six categories of combustible MSW fractions, namely, food, wood, paper, textiles, plastics, and rubber waste [21, 22]. For the selection of a suitable model, 9 assumed algebraic expressions from previous work based on the correlation of the HHV and ultimate analysis of solid fuel (daf) were used, as shown in Table 2. Using regression analysis based on the generalized method of least squares [19] on the 56 data points, the constant terms of these algebraic expressions were evaluated. The correlation that has the least error and highest coefficient of determination, as described in Selection of the best correlation, was selected. The newly estimated correlation was compared with the experimental values of HHV and the results of previous models collected from the open literature, for further validation.

Estimating the standard entropy of municipal solid waste

Municipal solid waste (MSW) contains mainly organic polymers in plastics, wood, paper, textile, rubber, and food waste. The entropies of these polymers in the organic waste are estimated or evaluated by the entropies of their organic monomers structures as there is no significant difference between the entropies of the solid organic monomers and their polymers [24]. The difference ranges from 0.1 to 12.5% (Table 3).

The standard entropy of MSW was derived from organic substances with known standard entropies. In this work, 117 samples of organic compounds relevant to MSW were collected from the published literature [3, 8, 10, 12, 17, 24] and tabulated in Table A3 (Appendix 1). The data points where selected based on the molecular structures of the organic substances that are associated or linked with the formation of larger molecular structure network of municipal solid waste. The organic compounds were grouped into the six categories of waste fractions, as previously used for the higher heating value, namely: food, plastic, textile, rubber, wood, and paper. This was accomplished by considering the molecular structures of the organic substances that can be found in each of the molecular structures of the waste fractions. For wood, it contains three major chemical components: cellulose, hemicelluloses, and lignin [25]. Each of the chemical structure of the wood constituents [26, 27] was studied and organic compounds (monomers) that can be made or found from these structures are selected. In the food, the main structural elements identified are proteins, carbohydrate and lipids [28]. The molecular structures of these food components [29, 30] were also investigated and organic monomers that are linked with the structure are selected. The same method was carried on chemical structures of plastic [31], textile [32, 33], and rubber [34] materials with identifications of biologically important molecules which form the building structure of their polymers. Based on the absolute entropies and elemental compositions of the selected organic substances, a first-order polynomial correlation

Table 3. Standard entropies of some solid organic polymers and monomers at 298.15 K.

S. No.	Substance	S^0 (J/mol K)
1.	$C_6H_{11}NO$	173.21
	$(C_6H_{11}NO)_n$	173.0
2	$C_4H_4O_4$	157.2
	$(C_4H_4O_4)_n$	151.4
3	$C_{15}H_{10}N_2O_2$	332.5
	$(C_{15}H_{10}N_2O_2)_n$	294
4	$C_{13}H_{24}O_2$	401.9
	$(C_{13}H_{24}O_2)_n$	351.6

Source: [24].

was derived statistically for the standard entropy of the waste fractions and the mixture.

Selection of the best correlation

Three statistical parameters were used as evaluating parameters for both HHV and the standard entropy of MSW, which are computed as follows:

$$\text{Average absolute error (AAE)} = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{Z_{\text{est}}-Z_{\text{exp}}}{Z_{\text{exp}}}\right|\times 100\% \quad (19)$$

$$\text{Average bias error (ABE)} = \frac{1}{n}\sum_{i=1}^{n}\frac{Z_{\text{est}}-Z_{\text{exp}}}{Z_{\text{exp}}}\times 100\% \quad (20)$$

$$\text{Coefficient of determination } (R^2) = 1-\sum_{i=1}^{n}\frac{\left(Z_{\text{est}}-Z_{\text{exp}}\right)^2}{\left(Z_{\text{exp}}-\overline{Z}_{\text{exp}}\right)^2} \quad (21)$$

where Z_{est} and Z_{exp} denote the estimated and experimental values, respectively. $\overline{Z}_{exp}$ is the experimental average value. AAE is the average error of a correlation. A smaller error of correlation will occur when AAE is low, which indicates higher accuracy. ABE denotes the average bias error of correlation. A positive value of ABE indicates an overall overestimation, whereas a negative value implies an overall underestimation. The smaller the absolute value of ABE, the smaller the bias of correlation. R^2 is used as a comprehensive parameter to measure the accuracy of the model. A higher R^2 value means a better estimation and fitting [20]. These three parameters are the important statistical criteria and are primarily employed to assess correlations [3, 12, 19].

Specific chemical exergy of inorganic matter in municipal solid waste

Inorganic substances of waste materials are contained in the ash and obtained from complete combustion of solid fuel; ash is mainly contained in various metallic oxides and has a high thermal stability [35, 36]. The specific chemical exergy of inorganic matter in kJ/kg MSW was calculated from the major ash compositions data in Table 4 from a stoker-type incinerator [37] as follows [3, 12, 36]:

$$e_{\text{ioc}} = 0.01A\left(\sum n_i x_i e^0_{\text{ioc}} + \text{R}T_o\sum n_i x_i \ln x_i\right)\ (\text{kJ/kg}) \quad (22)$$

where n_i represents number of moles of the component in inorganic matter, in mol/kg. e^0_{ioc} and x_i are the standard chemical exergy and mole fraction of components i in inorganic matter, respectively. R is the universal gas constant, 0.0083145 kJ/mol K, and A is the ash content of MSW in wt%.

Table 4. Chemical composition of MSW ashes.

Component	Bottom ash, BA (wt%)	Fly ash, FA (wt%)
SiO_2	37.8	2.47
CaO	20.79	44.5
K_2O	0.85	3.01
P_2O_5	3.63	0.26
Al_2O_3	13.4	0.55
MgO	2.91	0.57
Fe_2O_3	7.46	0.32
SO_3	1.01	1.61
Na_2O	5.38	4.39
ZnO	0.52	2.25
CuO	0.51	0.096
MnO	0.17	0.04
Cr	0.63	0.008
Pb	0.22	0.51
As	0.021	0.062
Cd	0.0003	0.003
Cl	3.51	35.15

Source: [37].

Results and Discussion

Correlation based on the higher heating value

For the higher heating value of MSW, the correlation derived that showed the minimum error with a higher accuracy among the nine assumed correlations used in Table 2 was expressed as

$$\begin{aligned}\text{HHV} &= 0.364\text{C} + 0.863\text{H} - 0.075\text{O} \\ &\quad + 0.028\text{N} - 1.633\text{S} + 0.062\text{Cl}\ (\text{MJ/kg})\end{aligned} \quad (23)$$

$$\begin{aligned}35.8\% \le \text{C} \le 86.1\%, 4.1\% \le \text{H} \le 13.9\%, 0.0\% \\ \le \text{O} \le 54.9\%, 0.0\% \le \text{N} \le 20.3\%, 0.0\% \\ \le \text{S} \le 2.7\%, 0.0\% \le \text{Cl} \le 56.4\%, \\ 13.0\ \text{MJ/kg} \le \text{HHV} \le 43.2\ \text{MJ/kg}.\end{aligned}$$

The results of the validation of the derived model and the comparison with published correlations using the experimental values of 30 samples of MSW in the different categories of food, wood, plastic, textile, rubber, and paper waste are shown in Table 5 and represented in Figures 1–5. Figures 1, 2, and 4 show the best correlation with experimental data (highest coefficient of determination), representing the model developed in this work, model by Channiwala and Parikh [19] and Dulong's correlation. However, the proposed model shows significantly better estimations when considering the errors (AAE and ABE) compared to the other models. This is not surprising, as these models have been derived from mixed solid fuel and coal. Figure 3 shows a correlation proposed by Sheng and Azevedo [20]. Although the correlation has a good coefficient of determination (R^2 = 0.92), it has a higher error and

Table 5. Derived correlation compared with previous models.

S No.	Name	Correlation (MJ/kg)	Application	AAE (%)	ABE (%)	R^2	Reference
1.	Proposed Model	HHV = 0.364C + 0.863H – 0.075O + 0.028N – 1.633S + 0.062Cl	MSW	5.738	0.032	0.95	Current model
2.	Channiwala and Parikh	HHV* = 0.3491C* + 1.1783H* + 0.1005S* – 0.1034O* – 0.0151N* – 0.0211A*	Mixed waste	6.456	2.254	0.95	[19]
3.	Sheng and Azevedo	HHV* = –1.3675 + 0.3137C* + 0.7009H* + 0.0318 (100 – C* – H* – A*)	Biomass	9.657	–3.650	0.92	[20]
4.	Dulong	HHV = 0.3383C + 1.443 (H – (O/8)) + 0.0942S	Coal	11.822	–4.832	0.95	[19]
5.	Chang	HHV = 35.8368 + 0.7523H – 0.2674S – 0.4654O – 0.3814Cl – 0.2802N	MSW	7.234	3.067	0.93	[19]

(*) shows the correlations obtained in % by mass on a dry basis, whereas the others are on dry ash-free basis.

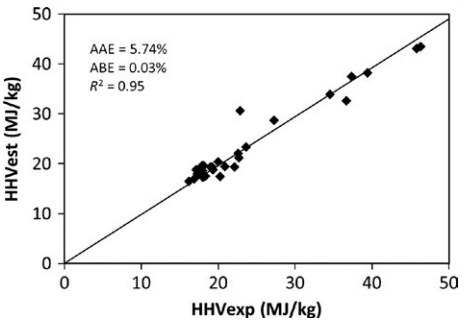

Figure 1. Comparison between the experimental and the estimated HHV by the developed correlation.

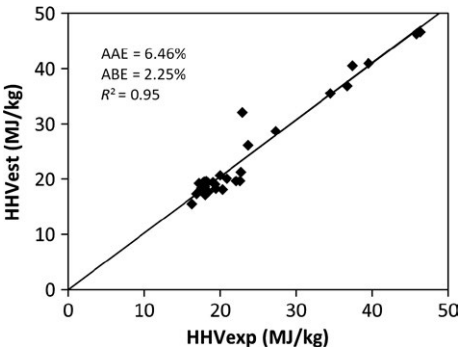

Figure 2. Comparison between the experimental and the estimated HHV by the Channiwala and Parikh [19] correlation.

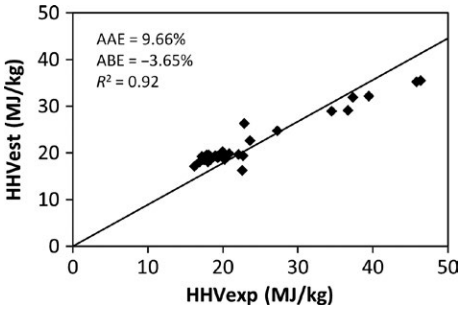

Figure 3. Comparison between the experimental and the estimated HHV by the Sheng and Azevedo [20] correlation.

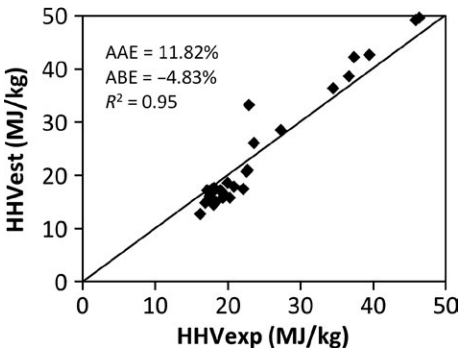

Figure 4. Comparison between the experimental and the estimated HHV by Dulong's correlation.

underestimated the HHV. In addition, the correlation is limited to biomass. The correlation proposed by Chang (Table 5 and Fig. 5) has a considerable accuracy, with a coefficient of determination of $R^2 = 0.93$. Although this correlation was derived from MSW, it overestimated the correlation and has a higher error value when compared with the present model.

Standard entropy of municipal solid fuel

For the prediction of the standard entropy of the organic substance in MSW, a correlation in the form of the first-order polynomial was used. The five correlations derived for estimating the standard entropy of waste fractions and the mixture of waste were expressed as follows:

For Plastic waste

$$s^0_{pl} = 0.0087\mathrm{C} + 0.0753\mathrm{H} + 0.0134\mathrm{O} + 0.0077\mathrm{N} + 0.0084\mathrm{Cl}\ (\mathrm{kJ/K\,kg}) \quad (24)$$

$$10.3\% \le \mathrm{C} \le 94.7\%, 0.0\% \le \mathrm{H} \le 14.3\%, 0.0\% \le \mathrm{O} \le 54.2\%, 0.0\% \le \mathrm{N} \le 66.7\%.$$

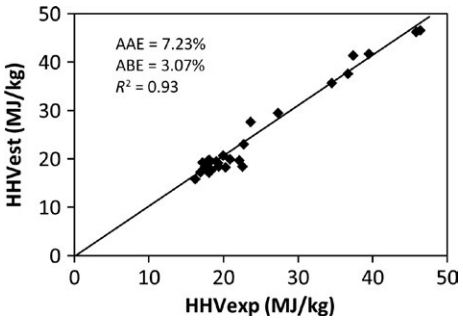

Figure 5. Comparison between the experimental and the estimated HHV by Chang's correlation.

With ABE, AAE, and R^2 of 0.722, 7.314, and 0.7674, respectively.

For Textile/Rubber waste

$$s^0_{tr} = 0.0097C + 0.0635H + 0.0128O + 0.0136N + 0.0165S\ (kJ/K\,kg) \quad (25)$$

$$15.8\% \le C \le 95.1\%, 3.0\% \le H \le 9.7\%, 0.0\% \le O \le 55.2\%, 0.0\% \le N \le 66.7\%, 0.0\% \le S \le 42.1\%$$

With ABE, AAE, and R^2 of 0.714, 6.476, and 0.5457, respectively.

For Wood/Paper waste

$$s^0_{wp} = 0.0162C + 0.0116H + 0.0081O + 0.00691Cl\ (kJ/K\,kg) \quad (26)$$

$$26.7\% \le C \le 77.8\%, 0.4\% \le H \le 7.7\%, 5.1\% \le O \le 71.1\%, 0.0\% \le Cl \le 66.3\%$$

With ABE, AAE, and R^2 of 0.329, 5.215, and 0.728, respectively.

For Food waste

$$s^0_{fo} = 0.0065C + 0.0808H + 0.0127O + 0.0101N + 0.0100S\ (kJ/K\,kg) \quad (27)$$

$$19.2\% \le C \le 92.3\%, 1.4\% \le H \le 14.1\%, 0.0\% \le O \le 59.7\%, 0.0\% \le N \le 51.9\%, 0.0\% \le S \le 34.0\%$$

With ABE, AAE, and R^2 of 0.414, 5.886, and 0.6922, respectively.

For Mixed waste

$$s^0_{msw} = 0.0101C + 0.0630H + 0.0106O + 0.0108N + 0.0155S + 0.0084Cl\ (kJ/K\,kg) \quad (28)$$

$$10.3\% \le C \le 95.1\%, 0.00\% \le H \le 14.3\%, 0.0\% \le O \le 71.1\%, 0.0\% \le N \le 66.7\%, 0.0\% \le S \le 42.1\%, 0.0\% \le Cl \le 89.7\%,$$

with ABE, AAE, and R^2 of 1.118, 8.293, and 0.5414, respectively.

Comparing the five equations obtained, the results show that the standard entropy correlations for each waste fraction in MSW are more accurate than the standard entropy correlation for the waste mixture. This is as a result of complicated mixture, heterogeneous molecule structure and variation in municipal solid waste chemical compositions and properties. Nevertheless, because the standard entropy of plastic, textile/Rubber, wood/paper, food, and waste mixture gave similar average values for the specific exergy of the MSW estimation of 24,359, 24,364, 24,426, 24,393, and 24,387 (kJ/kg), respectively, the correlation of the standard entropy of the waste mixture can be used for the derivation of exergy.

Specific chemical exergy of municipal solid fuel (daf) and specific chemical exergy of ash

By substituting Equation (3)–(8), (23), and (24)–(28) into Equation (18), along with the standard chemical exergy data from Table 1, the specific chemical exergy of solid waste on a dry ash-free basis can be expressed as follows:

For Plastic waste:

$$e_P = 376.879C + 787.351H - 58.654O + 46.398N - 1533.261S + 100.981Cl\ (kJ/kg) \quad (29)$$

For Textile/Rubber waste:

$$e_{TR} = 376.580C + 790.869H - 58.475O + 44.639N - 1538.180S + 98.566Cl\ (kJ/kg) \quad (30)$$

For Wood/Paper waste

$$e_{WP} = 374.642C + 806.343H - 57.074O + 48.693N - 1533.261S + 101.425Cl\ (kJ/kg) \quad (31)$$

For Food waste

$$\text{Food } e_F = 377.535C + 785.711H - 58.446O + 45.682N - 1536.242S + 103.486Cl\ (kJ/kg) \quad (32)$$

For mixed waste

$$e_{msw} = 376.461C + 791.018H - 57.819O + 45.473N - 1536.242S + 100.981Cl\ (kJ/kg) \quad (33)$$

The minimum, maximum, and average specific exergy values of municipal solid waste calculated were 17,602, 43,396, and 24,387 in (kJ/kg), respectively. Although Equation (33) slightly underestimated the specific chemical exergy calculated by Equations (29) and (30), that is, an ABE of −0.139 and −0.113, respectively, and slightly

overestimated the exergy estimated by Equations (31) and (32), that is, an ABE of 0.179 and 0.009, respectively, when compared, the coefficient of determination shows that Equations (29–32) are similar to Equation (33) (i.e., a value of 1 was achieved in all cases). This result indicates that Equation (33) can be used to estimate the specific exergy of municipal solid waste, that is, the HHV has more impact on the exergy.

The overall average ratio of the specific exergy of MSW developed with the higher heating value was obtained as 1.036, showing that the value of exergy is slightly higher than the HHV. The ratio of exergies to heating values obtained in this work is similarly when compared with Szargut and Styrylska [7] model with ratio of 1.047. As their methods were commonly used for evaluating the chemical exergy of solid fuels. This result indicates that the present model is reliable and accurate. However, the slight variation in the ratios is due to different types of fuel used.

The specific exergies of inorganic matter in MSW calculated from Equation (22) using the chemical ash composition data in Table 4 are 0.86 and 1.79 kJ/kg for bottom ash and fly ash, respectively. These values are very small when compared with the average specific chemical exergy values, 24,387 kJ/kg of MSW (daf) estimated, demonstrating that the specific chemical exergy of inorganic matter can be neglected.

Conclusions

Following the evaluations of the previous equations for estimating the specific chemical exergy of solid fuels, the present proposed models in this study were found to be more accurate when using municipal solid waste as a fuel. All other methods have either ignored the inclusion of chlorine from the elemental compositions of waste or have used other solid fuels with a limited amount of MSW. In this work, a simple method for estimating the specific exergy of municipal solid waste on (daf) from their ultimate analysis based on HHV, standard entropy, and exergy equation of reaction was proposed.

The higher heating values of the estimated MSW showed a good correlation and a higher accuracy compared with previous models. It is calculated as

$$\mathrm{HHV} = 0.364\mathrm{C} + 0.863\mathrm{H} - 0.075\mathrm{O} + 0.028\mathrm{N} - 1.633\mathrm{S} + 0.062\mathrm{Cl}\ (\mathrm{MJ/kg})$$

The standard entropy of the estimated waste mixture has a rather low accuracy when compared with the waste fractions. However, the standard entropy can be used for the estimation of the specific chemical exergy of a solid, as it showed a similar result with the standard entropy of waste fractions; the standard entropy is expressed as

$$s^0_{\mathrm{msw}} = 0.0101\mathrm{C} + 0.0630\mathrm{H} + 0.0106\mathrm{O} + 0.0108\mathrm{N} + 0.0155\mathrm{S} + 0.0084\mathrm{Cl}\ (\mathrm{kJ/K\,kg}).$$

This result indicates that a higher heating value has more impact on the derivation of the specific chemical exergy of solid waste than entropy. In other words, the specific exergy of MSW mainly depends on the values of HHV.

Due to very low calculated values of specific chemical exergy of inorganic matter in MSW, the specific chemical exergy developed in this work is equal to the specific chemical exergy of the organic matter in MSW and is presented as

$$E_{\mathrm{msw}} = 376.461\mathrm{C} + 791.018\mathrm{H} - 57.819\mathrm{O} + 45.473\mathrm{N} - 1536.242\mathrm{S} + 100.981\mathrm{Cl}\ (\mathrm{kJ/kg}).$$

The results obtained demonstrate that the specific chemical exergy is always slightly higher than the highest heating value, indicating the validity and accuracy of the model.

The present correlation can be accepted for estimating the specific chemical exergy of MSW using the elemental compositions of the fuel within the range specified based on a dry ash-free basis. The model is applicable for the efficient modeling of a combustion system in a waste-to-energy plant.

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Conflict of Interest

None declared.

Nomenclature

AAE	average absolute error
A	ash content in the waste (%)
ABE	average bias error
E	chemical exergy (kJ)
e	specific chemical exergy (kJ/kg) or (kJ/mol)
FC	fixed carbon (%)
G	Gibbs energy (kJ/kg) or (kJ/mol)
H	enthalpy (kJ/kg)
HHV	higher heating value (kJ/kg)
MSW	municipal solid waste
P	pressure (kpa)
R^2	coefficient of determination

S	entropy (kJ/K)
S_{gen}	entropy generated
s	specific entropy (kJ/kg K) or (kJ/mol K)
T	Temperature (K)
V	volatile matter (%)

Subscripts

ba	bottom ash
daf	dry ash-free basis
est	estimate
exp	experiment
fa	fly ash
f	formation
fo	food
ioc	inorganic compound
max	maximum
msw	municipal solid waste or mixed solid waste
o	standard state
pl	plastic
R	reaction
tr	textile/rubber
wp	wood/paper

Superscripts

0	reference state

Greek Symbols

Δ	change
$\sum$	summation

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Appendix

Table A1. Chemical characteristics of MSW (daf) used for derivation.

MSW groups, Subgroup and variety	Proximate analysis (wt %)			Ultimate analysis (wt %)						HHV (MJ/kg)	Reference
	A	V	FC	C	H	O	N	S	Cl		
Food waste											
1. Flour	–	–	–	42.78	6.19	48.39	2.48	0.15	–	18.157	[21]
2. Rice	0.40	84.42	15.18	45.97	6.35	45.74	1.67	0.25	–	18.213	[22]
3. Peanut shell	–	–	–	53.6	6.70	38.3	1.20	0.20	–	20.598	[21]
4. Pea	–	–	–	42.13	5.88	48.62	3.14	0.22	–	16.533	[21]
5. Scallion	–	–	–	48.12	6.27	41.74	3.09	0.78	–	18.042	[21]
6. Potato	3.15	79.52	17.33	44.41	5.33	47.82	1.81	0.64	–	17.656	[22]
7. Spinach	15.97	65.26	18.77	47.58	6.48	43.93	1.57	0.43	–	20.326	[22]
8. Celery	14.58	65.36	20.06	38.46	6.16	54.52	0.21	0.65	–	15.886	[22]
9. Pakchoi	18.44	63.97	17.59	43.37	5.93	48.64	1.25	0.81	–	23.173	[22]
10. Tangerine peel	2.91	76.49	20.6	48.74	5.92	43.83	1.43	0.08	–	19.024	[22]
11. Banana peel	10.85	64.38	24.77	35.8	4.79	54.93	4.37	0.10	–	18.385	[22]
12. Orange peel	2.44	76.27	21.29	43.93	5.64	48.93	1.34	0.07	0.08	18.550	[21]
13. Rib	–	–	–	52.92	8.83	25.63	2.29	0.32	–	17.277	[21]
14. Fish bone	39.82	56.25	3.93	63.87	8.01	19.08	8.39	0.64	–	26.245	[21]
15. Food waste	6.1	82.11	18.00	51.54	7.14	37.06	3.13	0.21	0.92	21.619	[38]
Wood waste											
16. Poplar wood	7.54	73.85	18.61	51.36	5.86	41.00	1.52	0.22	–	20.009	[22]
17. Poplar leaf	15.69	68.74	15.57	49.54	5.24	43.30	1.32	0.59	–	19.986	[22]
18. Chinar leaf	9.23	69.74	21.03	52.95	4.88	40.51	1.01	0.65	–	21.064	[22]
19. Gingko leaf	11.62	73.19	15.19	41.35	5.54	50.88	1.36	0.87	–	17.289	[22]
20. Pine wood	0.95	83.5	15.54	50.51	5.95	43.39	0.11	0.03	–	19.834	[21]
21. Sawdust	0.42	81	18.58	49.42	7.26	42.92	0.39	0.01	–	21.267	[21]
22. Wood	1.00	81.62	18.38	50.10	6.16	43.47	0.17	0.02	0.07	19.697	[38]
23. Wood chips	1.95	82.66	15.4	49.54	6.21	44.06	0.12	0.04	0.03	19.544	[21]
24. Bamboo	0.69	81.03	18.27	50.46	6.32	42.73	0.22	0.1	0.16	19.716	[21]
25. Leaves	8.92	73.7	17.38	47.25	5.57	46.26	0.19	0.73	–	18.882	[21]
26. Pine needles	–	–	–	52.57	6.3	40.44	0.54	0.16	–	20.843	[21]
27. King grass	7.44	74.12	18.43	46.91	5.89	46.3	0.7	0.21	–	19.428	[21]
Paper waste											
28. Blank printing paper	10.69	79.33	9.98	45.12	5.31	48.91	0.38	0.28	–	15.127	[22]
29. Tissue paper	0.52	90.47	9.01	45.18	6.13	48.32	0.25	0.11	–	17.340	[22]
30. Newspaper	8.07	79.54	12.39	48.01	5.71	45.86	0.33	0.09	–	18.666	[22]
31. Magazine	29.49	62.44	8.07	41.04	8.99	49.15	0.42	0.4	–	16.771	[21]
32. Writing paper	–	–	–	43.66	5.84	50.16	0.16	0.18	–	13.69	[21]
33. Cardboard	5.27	81.75	12.97	46.09	5.36	48.02	0.32	0.21	–	18.239	[21]
34. Carton	7.22	83.95	8.82	48.97	6.14	44.52	0.21	0.16	–	18.430	[21]
35. Printing paper	9.70	82.83	17.17	47.51	5.98	46.25	0.14	0.03	0.09	18.051	[38]
36. Packaging paper	12.2	85.88	14.12	46.92	5.92	46.74	0.22	0.09	0.10	17.654	[38]
Textile											
37. Absorbent cotton gauze	0.14	94.85	5.01	46.74	5.69	47.23	0.27	0.08	–	14.664	[22]
38. Cotton cloth	3.09	78.71	18.21	56.49	5.87	33.3	3.52	0.18	0.65	14.664	[21]
39. Wool	1.24	84.76	14.00	60.07	4.24	31.48	2.65	1.55	–	21.183	[21]
40. Acrylic fiber	0.14	75.25	24.61	66.78	5.2	7.31	20.26	0.45	–	29.812	[21]
41. Chemical fiber	–	–	–	48.09	7.16	34.06	9.43	1.26	–	21.959	[21]
42. Polyester taffeta	0.44	90.63	8.93	60.1	4.5	35.11	0.28	0.01	–	22.178	[21]
43. Terylene	0.49	88.6	10.91	62.16	4.14	33.12	0.29	0.28	–	20.963	[22]
44. Textiles	1.40	82.86	17.14	52.54	6.19	39.26	1.76	0.20	1.42	21.197	[38]
Plastics waste											
45. PS	0.04	99.57	0.39	86.06	6.27	1.93	5.73	–	–	38.946	[22]
46. LDPE	–	99.98	0.02	85.98	11.20	2.61	0.21	–	–	46.480	[22]
47. HDPE	0.18	99.57	0.25	85.35	12.70	1.90	0.05	0.14	–	46.444	[22]

Table A1. Continued.

MSW groups, Subgroup and variety	Proximate analysis (wt %)			Ultimate analysis (wt %)						HHV (MJ/kg)	Reference
	A	V	FC	C	H	O	N	S	Cl		
48. PVC	–	94.93	5.07	38.34	4.47	–	0.23	0.61	56.35	20.830	[22]
49. PET	0.09	90.44	9.47	63.01	4.27	32.69	0.04	–	–	23.111	[22]
50. PE	0.15	99.85	–	85.45	14.32	–	0.16	0.07	–	46.388	[21]
51. PP	0.02	99.97	0.01	85.41	12.51	1.85	0.23	–	–	46.248	[21]
52. Packaging plastic	3.90	95.21	4.79	75.75	9.78	12.00	0.35	0.03	2.08	26.951	[38]
53. Other plastic	1.30	99.09	0.91	84.90	9.63	0.97	3.35	0.03	1.11	41.135	[38]
Rubber waste											
54. Rubber	8.36	84.77	6.86	77.72	10.12	7.42	0	2.66	2.08	25.474	[21]
55. Tire	25.70	68.05	6.25	79.19	8.45	11.38	0.69	0.28	–	35.654	[21]
Other combustibles											
56. Other combustibles	20.40	90.83	9.17	70.48	8.79	17.53	1.63	0.83	0.74	32.161	[38]

All the proximate, ultimate analysis data and HHV on dry basis are converted to dry ash-free basis. Also all HHV are converted to MJ/kg.

Table A2. Chemical characteristics of MSW (daf) used for validation.

MSW groups, Subgroup and variety	Proximate analysis (wt %)			Ultimate analysis (wt %)						HHV (MJ/kg)	Reference
	A	V	FC	C	H	O	N	S	Cl		
Food waste											
1. Rice	0.42	87.74	11.84	44.2	5.73	48.75	1.20	0.1	0.02	18.048	[21]
2. Potato	–	–	–	42.09	6.5	49.06	2.12	0.23	–	16.912	[21]
3. Orange peel	2.91	76.49	20.6	48.74	5.92	43.72	1.43	0.19	–	19.024	[21]
4. Rib	38.22	61.56	0.23	51.61	6.38	31.91	9.48	0.69	–	22.716	[21]
Wood waste											
5. Wood	0.82	81.64	17.54	48.35	6.62	44.7	0.04	0.29	–	20.868	[21]
6. Wood chips	3.45	81.5	15.05	49.03	5.69	44.98	0.22	0.07	–	19.255	[21]
7. Wooden chopsticks	2.18	83.45	14.37	48.79	5.16	45.7	0.3	0.04	–	19.355	[39]
8. Bamboo	1.79	81.36	16.84	51.42	6.01	41.92	0.36	0.29	–	19.974	[40]
9. Leaves	9.43	74.32	16.25	47.18	5.61	46.35	0.18	0.68	–	20.278	[21]
10. King grass	–	–	–	48.37	6.30	44.58	0.49	0.25	–	22.127	[21]
Paper waste											
11. Newspaper	5.43	85.04	9.53	45.24	7.17	47.1	0.25	0.23	–	17.204	[21]
12. Printing paper	12.3	87.65	0.04	44.93	4.55	50.43	0.09	–	–	16.233	[21]
13. Cardboard	–	–	–	46.71	5.31	47.35	0.32	0.32	–	18.367	[21]
14. Toilet paper	0.52	90.47	9.01	45.18	6.13	48.32	0.25	0.11	–	17.337	[21]
15. Paper food cartons	6.93	–	–	48.07	6.55	45.04	0.16	0.17	–	18.137	[41]
16. Magazine stock	29.26	–	–	46.55	6.56	46.44	0.16	0.30	–	17.967	[41]
17. Plastic-coated paper	2.77	–	–	44.53	6.35	46.80	0.19	0.08	–	17.556	[41]
Textile											
18. Cotton cloth	1.52	84.53	13.95	46.51	5.8	46.98	0.43	0.28	–	17.699	[22]
19. Cotton	1.45	86.7	11.85	46.19	6.12	47.07	0.54	0.08	–	17.500	[21]
20. Wool	–	–	–	58.53	6.48	18.23	15.12	1.65	–	23.632	[22]
21. Shoe heel and sole	30.09	–	–	76.13	10.14	11.10	0.72	1.92	–	36.676	[41]
22. leather	10.1	–	–	66.74	8.90	12.79	11.12	0.44	–	22.892	[41]
23. Upholstery	2.80	–	–	48.46	6.28	44.86	0.31	0.10	–	17.891	[41]
Plastics waste											
24. PE	0.15	99.85	–	85.45	14.32	–	0.16	0.07	–	46.388	[42]
25. PP	0.16	99.84	–	84.3	14.44	1.05	0.18	0.03	–	45.842	[21]
26. PVC	0.04	95.16	4.8	38.75	5.21	–	0.22	–	55.82	22.575	[21]
27. Polyurethane	4.38	87.29	8.32	66.17	6.55	18.46	6.26	0.02	2.53	27.300	[41]
28. Plastic film	6.72	–	–	72.05	10.42	16.96	0.49	0.08	–	34.519	[41]
Rubber waste											
29. Rubber	15.38	65.26	19.36	89.18	8.54	–	1.23	1.05	–	39.473	[21]
30. Tire	19.27	63.11	17.61	88.56	8.52	0.88	0.75	1.29	–	37.364	[21]

All the proximate, ultimate analysis data and HHV on dry basis are converted to dry ash-free basis. Also all HHV are converted to MJ/kg.

Table A3. Standard entropies at 298.15K of organic compounds relevant to MSW.

Name	Formula	S^0 (kJ/kg K)
Food		
1. Allantoin	$C_4H_6N_4O_3$	1.233
2. Alloxan	$C_4H_2N_2O_4$	1.314
3. Arginine	$C_6H_{14}N_4O_2$	1.439
4. Asparagine	$C_4H_8N_2O_3$	1.322
5. Aspartic acid	$C_4H_7NO_4$	1.279
6. Citric acid	$C_6H_8O_7$	1.312
7. Creatine	$C_4H_9N_3O_2$	1.445
8. Cystine	$C_6H_{12}N_2O_4S_2$	1.347
9. D-Glutamic acid	$C_5H_9NO_4$	1.230
10. L-Lactic acid	$C_3H_6O_3$	1.579
11. L-Phenylalanine	$C_9H_{11}NO_2$	1.293
12. L-Proline	$C_5H_9NO_2$	1.425
13. Maleic acid	$C_4H_4O_4$	1.373
14. Malic acid	$C_4H_6O_5$	1.199
15. Methionine	$C_5H_{11}NO_2S$	1.552
16. Phenanthrene	$C_{14}H_{14}$	1.207
17. Trytophan	$C_{11}H_{12}N_2O_2$	1.229
18. Tyrosine	$C_9H_{11}NO_3$	1.181
19. Uric acid	$C_5H_4N_4O_3$	1.030
20. Valine	$C_5H_{11}NO_2$	1.527
21. Xanthine	$C_5H_4N_4O_2$	1.059
22. Stearic acid	$C_{18}H_{36}O_2$	1.531
23. Taurine	$C_2H_7NO_3S$	1.231
24. Urea	CH_4N_2O	1.742
25. Hexadecanoic acid	$C_{16}H_{32}O_2$	1.764
26. Adenine	$C_5H_5N_5$	1.118
27. Creatinine	$C_4H_7ON_3$	1.483
28. L-Serine	$C_3H_7O_3N$	1.419
29. L-Glutamine	$C_5H_{10}O_3N_2$	1.335
30. DL-Alanyl glycine	$C_5H_{10}O_3N_2$	1.460
31. Glycylglycine	$C_4H_8N_2O_3$	1.438
32. Alanine	$C_3H_7NO_2$	1.450
33. Cysteine	$C_3H_7NO_2S$	1.402
34. Dimethyl sulfone	$C_2H_6O_2S$	1.509
35. D-Lactic acid	$C_3H_6O_3$	1.593
36. Fumaric acid	$C_4H_4O_4$	1.447
37. Guanine	$C_5H_5N_5O$	1.061
38. Gycine	$C_2H_5NO_2$	1.379
39. Isoleucine	$C_6H_{13}NO_2$	1.586
40. Leucine	$C_6H_{13}NO_2$	1.586
41. L-Glutamic acid	$C_5H_9NO_4$	1.279
42. 1-Hexadecanol	$C_{16}H_{34}O$	1.864
43. Hypoxanthine	$C_5H_4ON_4$	1.070
44. Glycolide	$C_4H_4O_4$	1.354
Plastic		
45. 1,3,5-Trioxane	$C_3H_6O_3$	1.476
46. Benzophenone	$C_{13}H_{10}O$	1.346
47. Biphenyl	$C_{12}H_{10}$	1.358
48. Hexachloroethane	C_2Cl_6	1.002
49. Diphenyl carbonate	$C_{13}H_{10}O_3$	1.300
50. Diphenyl ether	$C_{12}H_{10}O$	1.372
51. Diphenylcarbinol	$C_{13}H_{12}O$	1.330
52. Polypropylene, isotatic	$(C_3H_6)_n$	1.662
53. Polypropylene, syndiotic	$(C_3H_6)_n$	1.798
54. Pyromellitic dianhydride	$C_{10}H_2O_6$	1.087
55. Naphthalene	$C_{10}H_8$	1.306
56. Succinic acidic	$C_4H_6O_4$	1.417
57. Cyanuric acid	$C_3H_3N_3O_3$	1.947
58. Acetamide	C_2H_5NO	1.840
59. Durene	$C_{10}H_{14}$	1.166
60. Hexamethlenetetramine	$C_6H_{12}N_4$	1.116
61. Triphenylene	$C_{18}H_{12}$	1.273
62. Hydroquinone	$C_6H_60_2$	1.182
63. Melamine	$C_3H_6N_6$	1.251
64. Phthalic acid	$C_8H_6O_4$	1.215
65. Phathalic anhydide	$C_8H_4O_3$	1.405
66. Triethylenediamine	$C_6H_{12}N_2$	1.947
67. 4,4′-diphenylmethane diisocyanate	$C_{15}H_{10}N_2O_2$	1.329
68. Polyisocyanurate	$(C_{15}H_{10}N_2O_2)_n$	1.175
69. Tridecanolactone	$C_{13}H_{24}O_2$	1.893
70. Polytridecanolactone	$(C_{13}H_{24}O_2)_n$	1.656
71. Polyvinylidene chloride	$(C_2H_2Cl_2)_n$	0.894
72. Polyvinyl chloride	$(C_2H_3Cl)_n$	1.042
73. poly(1-butene), isotactic	$(C_4H_8)_n$	1.836
74. Polystyrene	$(C_8H_8)_n$	1.294
Textile		
75. 3-Nitrobenzoic acid	$C_7H_5NO_4$	1.227
76. 1,2-Diphenylethene	$C_{14}H_{12}$	1.39
77. Adipic acid	$C_6H_{10}O_4$	1.504
78. 2-Methlnaphthalene	$C_{11}H_{10}$	1.547
79. Acenaphthene	$C_{12}H_{10}$	1.225
80. Anthracene	$C_{14}H_{10}$	1.164
81. 1,4-Benzoquinone	$C_6H_4O_2$	1.506
82. Diphenylamine	$C_{12}H_{11}N$	1.666
83. Pyrene	$C_{16}H_{10}$	1.112
84. Thiourea	CH_4N_2S	1.523
85. Ammonium thiocyanate	CH_4N_2S	1.842
86. 3-Nitroaniline	$C_6H_6N_2O_2$	1.276
87. Resorcinol	$C_6H_6O_2$	1.341
88. Triphenylmethane	$C_{19}H_{16}$	1.277
89. Triphenylmethanol	$C_{19}H_{16}O$	1.265
90. Isoquinoline	C_9H_7N	1.324
91. Acridine	$C_{13}H_9N$	1.161
92. 2-Nitrobenzoic acid	$C_7H_5O_4N$	1.247
93. 1,3-Phenylenediamine	$C_6H_8N_2$	1.429
94. Dicyanodiamide	$C_2H_4N_4$	1.538
95. ε-Caprolactam	$C_6H_{11}NO$	1.531
96. Poly-ε-Caprolactam	$(C_6H_{11}NO)_n$	1.529
97. Polyglycolide	$(C_4H_4O_4)_n$	1.304
Wood		
98. L-Sorbose	$C_6H_{12}O_6$	1.226
99. *o*-Cresol	C_7H_8O	1.530
100. Oxalic acid	$C_2H_2O_4$	1.220
101. *p*-Cresol	C_7H_8O	1.547
102. Sucrose	$C_{12}H_{22}O_{11}$	1.052
103. D-Mannitol	$C_6H_{14}O_6$	1.309
104. Pentachlorophenol	C_6HCl_5O	0.946
105. Galactose	$C_6H_{12}O_6$	1.14
106. Phenol	C_6H_6O	1.53
107. 2-Hydroxybenzoic acid	$C_7H_6O_3$	1.29
108. Glucose	$C_6H_{12}O_6$	1.161

Table A3. Continued,

Name	Formula	S^0 (kJ/kg K)
109. Xylose	$C_5H_{10}O_5$	0.956
110. 3-Hydroxybenzoic acid	$C_7H_6O_3$	1.281
111. 4-Hydroxybenzoic acid	$C_7H_6O_3$	1.272
112. Benzoic acid	$C_7H_6O_2$	1.372
113. Catechol	$C_6H_6O_2$	1.364
114. Lactose	$C_{12}H_{22}O_{11}$	1.128
115. *o*-Hydroxybenzoic acid	$C_7H_6O_3$	1.29
116. *o*-Hydroxybenzoic acid	$C_7H_6O_3$	1.281
117. *o*-Hydroxybenzoic acid	$C_7H_6O_3$	1.272

Source: [3, 8, 10, 12, 17, 24].