Carbon-relative molar mass for the prediction of RDF torrefaction and calorific value of the carbonized solid fuel

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Numerous regressive and machine-learning models describing the performance of pyrolysis and torrefaction were developed. Typically, these models were based on 13-16 independent variables describing the feedstock parameters and thermal treatment conditions. Due to that, we propose a new parameter, the carbon-relative molar mass (CRMM) of the feedstock, as a parameter unifying all feedstock parameters like moisture content, volatile matter, ash content, content of C, H, N, S, and O. In this paper, we validated CRMM applicability for the Refuse-Derived Fuel (RDF) torrefaction performance and calorific value of carbonized RDF modeling. Based on this approach, the experiment with nine RDF components and their 1:1 mixtures (e.g., polyethylene, polypropylene, paper, and textiles, …) and real RDF samples were torrefied for 60 minutes under the highest treatment temperature (HTT) ranging from 200 to 300°C with the interval of 20°C. For the RDF torrefaction performance and calorific value of the carbonized solid fuel modeling, the CRMM and HTT independent variables were used.

Based on the elemental composition (CHNSO) and ash content, the CRMM was calculated based on the following equations. Using the elemental composition and ash content of the RDF sample, the ash-free content of individual elements (%Cont.(C; H; N; S; O)$_{(DAF)}$) was determined according to Equation 1. This calculation method has been recently presented by Białowiec and Syguła (2024).

$$\%\mathrm{Cont.\,(C;\,H;\,N;\,S;\,O)_{(DAF)}} = \frac{\%\mathrm{Cont.\,(C;\,H;\,N;\,S;\,O)} \cdot 100\%}{(100\% - \mathrm{Ash}\%)} \quad (1)$$

where: %Cont.(C; H; N; S; O)$_{(DAF)}$ – ash-free elemental content, %dm, C – carbon content, % dm, H – hydrogen content, % dm, N – nitrogen content, % dm, S – sulfur content, % dm, O – oxygen content, % dm, Ash% – ash content as a percentage of dry residue, % dm.

The obtained ash-free elemental contents were converted to mass (g), assuming a total ash-free sample weight of 1,000 grams. This allowed for the calculation of the mass (g) of each element in 1,000 grams of the ash-free sample, denoted as gM(C;H;N;S;O)$_{(DAF)}$. The elemental masses were then divided by their atomic masses to calculate the number of moles for each element in the ash-free 1,000 g biomass sample, Lmol(C;H;N;S;O)$_{(DAF)}$, as described in Equation 2.

$$\mathrm{Lmol(C;\,H;\,N;\,S;\,O)_{(DAF)}} = \frac{\mathrm{gM(C;\,H;\,N;\,S;\,O)}}{(12;\,1;\,14;\,32;\,16)} \quad (2)$$

where: Lmol(C; H; N; S; O)$_{(DAF)}$ – ash-free number of moles of elements in 1000 g of RDF, mol, gM(C; H; N; S; O)$_{(DAF)}$ – ash-free mass of elements in 1000 g of RDF, g, 12 – atomic mass of carbon, u, 1 – atomic mass of hydrogen, u, 14 – atomic mass of nitrogen, u, 32 – atomic mass of sulfur, u, 16 – atomic mass of oxygen, u.

The number of moles for each element was then normalized to the number of carbon moles, treating carbon as the reference element. This allowed for the determination of the relative number of moles for each element (L/C)mol(C;H;N;S;O)$_{(DAF)}$, as shown in Equation 3.

$$\mathrm{(L/C)mol(C;\,H;\,N;\,S;\,O)_{(DAF)}} = \frac{\mathrm{Lmol(C;\,H;\,N;\,S;\,O)_{(DAF)}}}{\mathrm{Lmol(C)_{(DAF)}}} \quad (3)$$

where: (L/C)mol(C; H; N; S; O)$_{(DAF)}$ – ash-free relative number of moles of elements, mol, Lmol(C; H; N; S; O)$_{(DAF)}$ – ash-free number of moles of elements in 1000 g of RDF, mol, Lmol(C)(DAF) – ash-free number of carbon moles, mol.

To determine the CRMM, the number of moles for each element (relative to 1 mole of carbon) was multiplied by their respective atomic masses Mdaf(C;H;N;S;O), and the resulting masses were summed, as shown in Equation 4.

$$\mathrm{CRMM} = \sum \Big(\big((\mathrm{L/C)mol(C)_{(DAF)}} \cdot 12 \big); \big((\mathrm{L/C)mol(H)_{(DAF)}} \cdot 1 \big); \big((\mathrm{L/C)mol(N)_{(DAF)}} \cdot 14 \big); \big((\mathrm{L/C)mol(S)_{(DAF)}} \cdot 32 \big); \big((\mathrm{L/C)mol(O)_{(DAF)}} \cdot 16 \big) \Big) \quad (4)$$

where: Mdaf – ash-free molar mass of RDF, g·mol^{-1}, (L/C)mol(C)$_{(DAF)}$ – ash-free relative number of carbon moles, mol, (L/C)mol(H)$_{(DAF)}$ – ash-free relative number of hydrogen moles, mol, (L/C)mol(N)$_{(DAF)}$ – ash-free relative number of nitrogen moles, mol, (L/C)mol(S)$_{(DAF)}$ – ash-free relative number of sulfur moles, mol, (L/C)mol(O)$_{(DAF)}$ – ash-free relative number of oxygen moles, mol.

Based on CRMM and HTT, the polynomial model describing the influence of CRMM and HTT influence on the mass yield (MY) and higher heating value (HHT) of carbonized solid fuel was determined. This model was validated for the real RDF samples. Predicted and measured MY and HHV were compared.

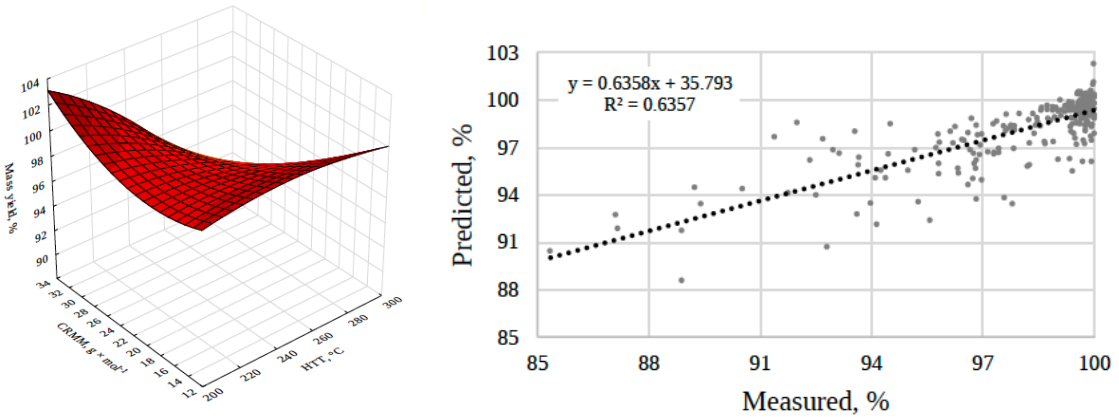

Figure 1. Left: The 3D graph showing the influence of the CRMM and HTT on the MY of the carbonized solid fuel from RDF components torrefaction. Right: the comparison of the measured and predicted MY values from real RDF torrefaction.

The determined model of CRMM and HTT influence on MY of RDF components torrefaction showed that with the increase of the temperature and increase of CRMM, the MY of RDF components torrefaction decreases (Figure 1, left). The influence of the temperature is relatively obvious, as with the increase of the temperature, a higher degree of thermal degradation of organic compounds occurs. High values of CRMM are related to the high content of oxygen in the organic molecules. Therefore, the decrease of MY with the increase of CRMM may be related to the high volatilization of organic compounds with high oxygen content. The validation of the model shows relatively good fitness of the predicted to measured data (R^2=0.636), however, the model tends to underestimate the prediction (regression coefficient below 1) (Figure 1, right).

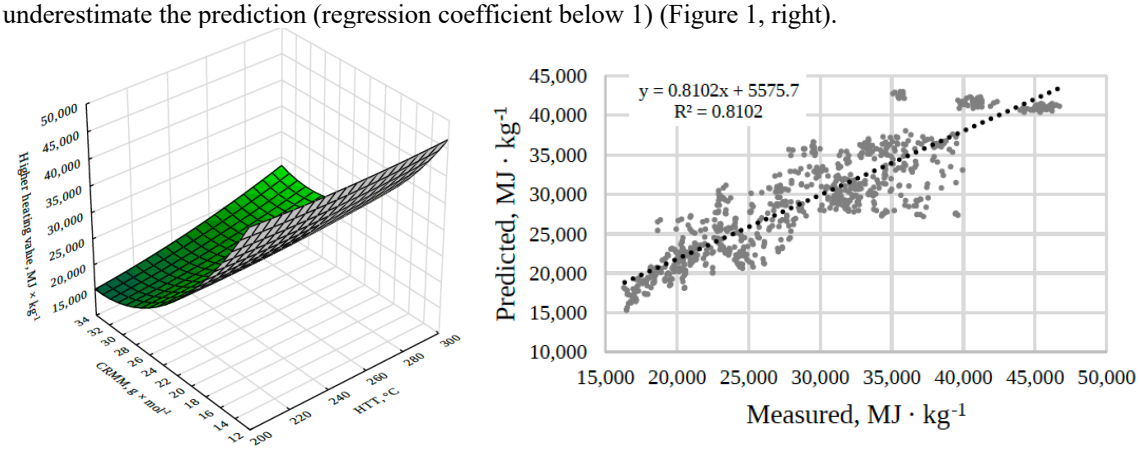

Figure 2. Left: The 3D graph showing the influence of the CRMM and HTT on the HHV of the carbonized solid fuel from RDF components torrefaction. Right: the comparison of the measured and predicted HHV values from real RDF torrefaction.

In the case of HHV, the model shows that with the increase of the temperature, the HHV slightly increases. However, the decrease of the CRMM causes a very strong increase in HHV, caused mostly by the presence of low-oxygen compounds in RDF-like plastics (Figure 2, left). The validation of the model on real RDF samples showed a high overlapping of the predicted and measured data (R^2=0.810). The model slightly underestimated the predicted values (Figure 2, right).
The presented results show that CRMM may be a good estimator for the modeling of the organic feedstock (RDF, biomass) thermal treatment performance and fuel properties of produced solid fuels.

A. Bialowiec, E. Syguła, Carbon-relative molar mass is a new parameter for experimentation with different biomasses. Prediction of higher heating value case study (December 23, 2024). Available at SSRN: http://dx.doi.org/10.2139/ssrn.5097575.