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Exploring Sustainable Energy Solutions: Gasification, Thermogravimetric Analysis, and AI in Bioenergy Systems

Report

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OVERVIEW

ABSTRACT

This paper delves into waste-to-energy technologies, emphasizing AI applications in bioenergy systems and gasification processes. It examines fixed bed gasification procedures, thermogravimetric analysis, and modeling powered by artificial intelligence in relation to municipal solid waste. The review emphasizes how gasification might be optimized, drawing attention to differences across financial contexts and comparisons with other incineration options. Additionally, it emphasizes the value of operational parameter analysis and the use of AI to bioenergy systems.

INTRODUCTION

Investigation of waste-to-energy technology has become an important path in the search for sustainable energy solutions. Gasification techniques and the use of artificial intelligence (AI) into bioenergy systems are two of these technologies that show great promise. This thorough review explores the most recent developments in these fields, concentrating on four main areas: simulation of fixed bed gasification processes, modeling and comparative evaluation of municipal solid waste (MSW) gasification, a thorough examination of thermogravimetric analysis in biomass gasification, and applications of AI-based modeling in bioenergy systems. This review aims to provide valuable insights into optimizing waste-to-energy conversion processes and leveraging AI for enhanced efficiency and sustainability in bioenergy production.

OBJECTIVE

This work encompasses several objectives aimed at advancing the understanding and application of gasification processes for waste-to-energy systems. It seeks to develop a numerical simulation model for the integrated production of synthesis gas from municipal solid waste (MSW), agricultural, and forestry waste. Specifically, the focus is on modeling the gasification reactor, employing a one-dimensional approach to simulate agro-industrial waste gasification in a fixed bed configuration. Additionally, the aim is to create a library of mathematical models tailored for simulating processes involving particulate solids. The study further aims to evaluate gasification as a waste-to-energy technology, comparing it to incineration for energy recovery from MSW. Moreover, this intends to review existing literature, emphasizing the benefits of employing thermogravimetry in biomass gasification, outlining the current state-of-the-art, and discussing future prospects in the field.

METHODOLOGY

1. Modeling and comparative assessment of municipal solid waste gasification for energy production

To understand MSW and its gasification potential, conduct proximate and ultimate tests. Proximate analysis determines moisture, fixed organic matter, volatile organic matter, and ash content. Ultimate analysis reveals chemical composition and formula. These tests inform gasification modeling, impacting energy and waste conversion. Ultimate analysis data for various waste streams are summarized in Table.

Table 1

Ultimate analysis of MSW streams as mass percentage of carbon (C), hydrogen (H), oxygen (O), nitrogen (N) and ash and the resulting chemical formula (Niessen, 2010; Themelis et al., 2002).

Category	%C	%H	%O	%N	%Ash	Chemical formula
Paper	43.41	5.82	44.32	0.25	6.0	$C_{3.6}H_{5.8}O_{2.8}N_{0.02}$
Plastics	60.0	7.2	22.8	0	10.0	$C_{5.0}H_{7.1}O_{1.4}$
Textiles	55.0	6.6	31.2	4.6	2.4	$CH_{1.7}O_{0.7}N_{0.04}$
Wood	49.4	6.1	43.7	0.1	0.6	$C_{4.1}H_{6.1}O_{2.7}N_{0.007}$
Food wastes	44.99	6.43	28.76	3.3	16.0	$C_{3.7}H_{6.4}O_{1.8}N_{0.2}$
Yard wastes	40.31	5.64	39.0	2.0	13.0	$C_{3.4}H_{5.6}O_{2.4}N_{0.1}$

Table 2

Proximate analysis of the as-received MSW streams reported as percentages by weight (Niessen, 2010; Themelis et al., 2002).

Category	Moisture	Volatile organic matter	Fixed organic matter	Ash
Paper	10.24	75.94	8.44	5.38
Plastics	2.00	95.80	2.00	0.20
Textiles	10.00	66.00	6.50	17.50
Wood	12.00	75.05	12.41	0.54
Food wastes	72.00	20.26	3.26	4.48
Yard wastes	62.00	26.74	6.32	4.94

In the next step, the chemical formulas were input into Gasify, a MATLAB-based solver with a built-in gasification model. Gasify computes molar concentrations of main gasifier products: CO, CO_2, H_2, H_2O, CH_4, C, N_2, NH_3, and HCN. Users input MSW components, their properties, reactor conditions (temperature, air flow rate), and select equilibrium equations. Familiarity with gasification nuances, required inputs for convergence, relevant equations, and equation characteristics (linear/nonlinear, divergent/convergent) is essential.

The following general chemical equation sums up the reactants and products involved in the gasification process using air (air = $1O_2 + 3.76N_2$):

$$\text{Feedstock}\ (C_nH_xO_yN_z) + m(O_2 + 3.76N_2) \rightarrow x_1H2 + x_2CO + x_3CO_2 + x_4H_2O + x_5CH_4 + x_6C + (z/2 + 3.76m)N_2 \quad \text{Eq. (1)}$$

In Eq. (1), m, x1, x2, x3, x4, x5, and x6 represent stoichiometric amounts, while n, x, y, and z denote atomic ratios of C, H, O, and N in the feedstock. These seven unknowns require solving. Temperature and m are interrelated, needing seven independent equations: three mass balances (C, H, O), three from chemical equilibrium, and one from overall energy balance.

Three equilibrium reactions are mainly dominant in the gasification process.
The Boudouard reaction : $C + CO_2 \longleftrightarrow 2CO$
The water—gas reaction : $C + H_2O \longleftrightarrow CO + H_2$
The Methanation reaction : $C + 2H_2 \longleftrightarrow CH_4$
The total moles of gaseous products, xTotal, is defined as:
$x_{Total} = x_1+x_2+x_3+x_4+x_5+(z/2 + 3.76m)$

2.Modeling and simulation of a fixed bed gasification process for thermal treatment of municipal solid waste and agricultural residues.

The combined gasification and combustion system, depicted in Fig. 1, was simulated using a computational model. Operational parameters, limited to steady-state and primary airflow (102.4 Nm³/h), corresponded to $\varphi = 0.33$ based on oxygen consumption for biomass combustion.

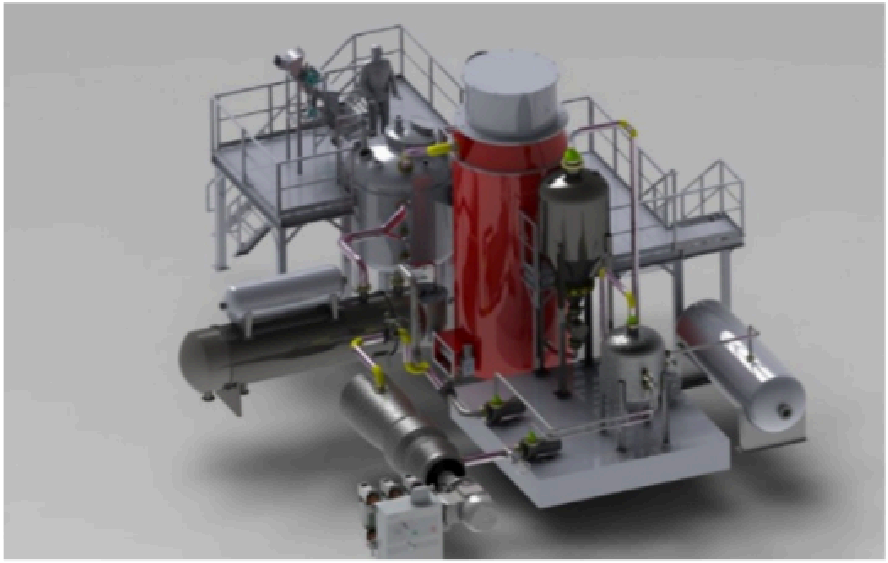
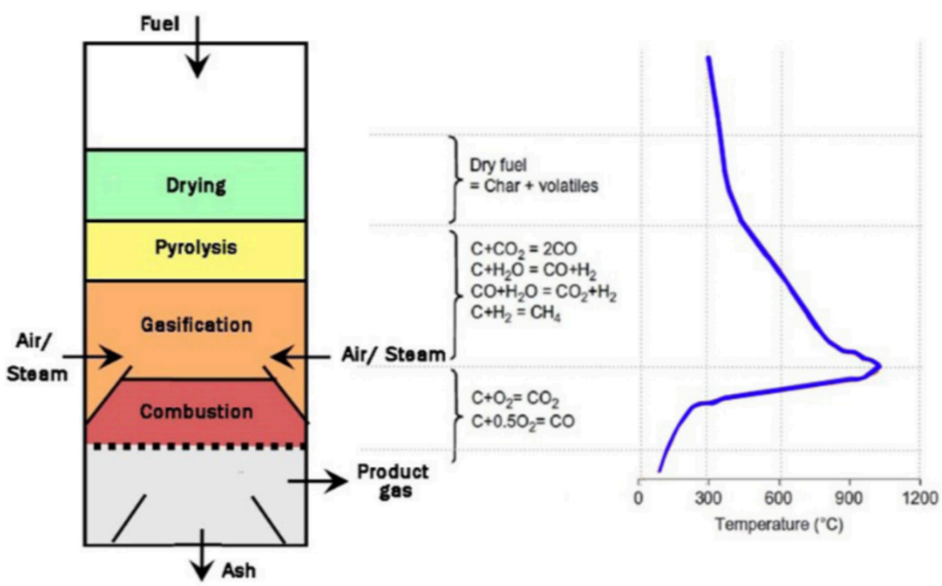


Fig. 1. 3D modeling of the waste processing plant.

The reactor, a fixed-bed gas cylinder with a kinetic (1-D) model, was divided into four sections for process study (Fig. 2), following classic phases: drying (>150°C), pyrolysis (150–700°C), oxidation (700–1500°C), and reduction (800–1100°C). The drying zone decreases residual moisture, assumed to evaporate at 120°C. Pyrolysis occurs from 200 to 500°C, transitioning primary tar to gas and secondary tar beyond 500°C. Gasification decomposes biomass, producing H2O and O2. The reactor features high temperature (HTZ) and low temperature (LTR) regions, operating around 800–1200°C for complete gasification and syngas production.



3.

Fig. 2. Process diagram and temperature variation.
Source: Adapted from [20].

3.Comprehensive Analysis Using Thermogravimetric Analysis (TGA) and Fourier Transform Infrared Spectroscopy (FTIR)

This review focuses on the benefits of utilizing thermogravimetry for the biomass gasification process,with particular attention paid to the determination of kinetic parameters such as the pre-exponential coefficient and activation energies, resulting from model-fitting and model-free approaches.

Thermograms depict distinct sections which correspond to the sequential reaction phases of mass decomposition of a particular sample and provide information regarding the weight loss and weight loss rates with respect to either time or temperature. Biomass gasification consists of several phases, including dewatering, devolatilization, and carbonization, which occur at increasing temperature ranges, as depicted in Fig.

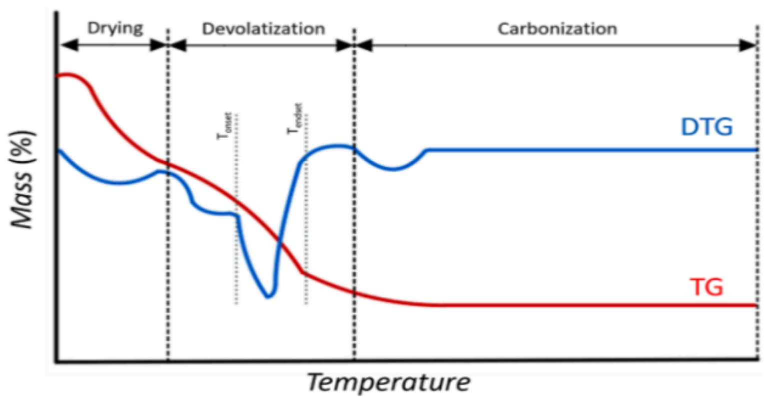


Fig. 5. Different phases of global gasification process as depicted in a thermogram of non-isothermal gasification.

Coupling of TGA with FTIR

The coupling of TG and FTIR (TG-FTIR) technology provided unique features including simultaneous and continuous real-time analysis to obtain the transient mass loss and the evaluation of the functional groups of volatiles produced, which cannot be obtained by the TG and FTIR individually.

Fourier Transform Infrared Spectroscopy (FTIR) complements TGA by rapidly providing infrared spectra, aiding in the identification of molecular structures and chemical bonds in biomass thermochemical process byproducts. FTIR offers qualitative and quantitative data on molecular systems, with detailed information on surface and bulk chemical structures. By selecting individual peaks or taking peak ratios in FTIR spectra, concentrations of thermal decomposition products can be determined. FTIR has also been integrated with fast pyrolysis reactors for quantitative analysis of volatile species, expanding its application in characterizing gas evolution during thermochemical conversion. Combining TGA and FTIR enables comprehensive analysis of evolved gasses, facilitating the identification of gas species released at different temperature ranges during biomass thermochemical processes.

4.Applications of artificial intelligence-based modeling for bioenergy systems:

Data Collection: Gather biomass feedstock properties via proximate and ultimate analysis, including moisture, volatile matter, fixed carbon, ash content, carbon, hydrogen, oxygen, nitrogen, sulfur content, and higher heating value (HHV).

Data Preprocessing: Clean, normalize, standardize, and split the dataset into training, validation, and testing sets to ensure data quality and compatibility with AI algorithms.

Feature Selection/Extraction: Select or extract relevant features using techniques like PCA or domain knowledge-driven selection to improve model performance by reducing dimensionality.
Model Selection: Choose an appropriate AI model such as artificial neural networks (ANN), support vector machines (SVM), decision trees, random forests, or ensemble methods based on problem nature and data availability.

Model Training: Train the selected AI model using the training dataset, allowing it to learn the relationship between input features and the target variable through iterative parameter adjustments to minimize prediction errors.

Model Evaluation: Assess the model's performance using metrics like MSE, RMSE, R-squared, or accuracy on the validation dataset to gauge generalization to unseen data.

Hyperparameter Tuning: Optimize the model's performance by adjusting hyperparameters using techniques such as grid search or randomized search.

Model Testing and Deployment: Test the trained model on the testing dataset to confirm performance on unseen data. If satisfactory, deploy the model for real-world biomass feedstock property prediction.

Continuous Iteration: Iterate and refine the model based on feedback and new data to enhance accuracy and reliability in predicting biomass properties.

RESULTS & DISCUSSION

METHOD 1

1.MSW gasification products:

- Gasify software analyzed gasification products from six MSW categories across temperatures of 800 to 1800°C.
- Trends showed reduced combustible gas yield at higher temperatures.
- Equilibrium reactions, like Boudouard and water gas, indicated shifts in product yields with temperature changes.
- Validation through experiments confirmed the model's accuracy, particularly at higher temperatures.
- Application to bulk MSW compositions highlighted regional variations, with the USA exhibiting the highest gasification product yields influenced by waste composition.
- Combining results from different waste streams provides insights into potential gasification outcomes for diverse mixtures, aiding in waste-to-energy process optimization.

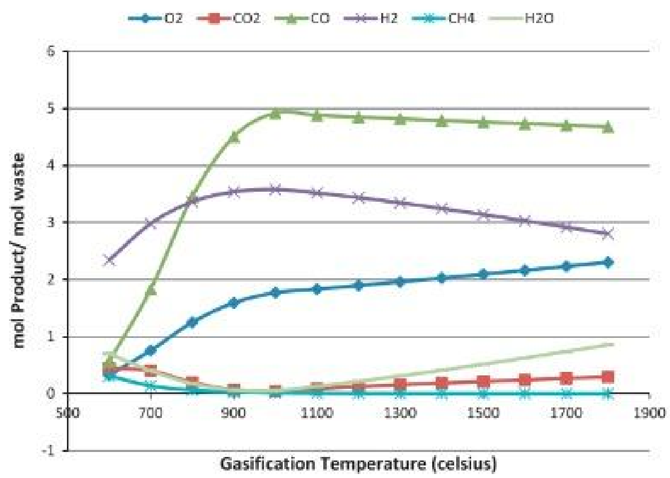


Fig. 4. Molar concentration of gasification products for plastic waste.

2.Energy and efficiency analysis:

- Energy efficiency trends show fluctuating energy yields, highlighting the importance of a narrow temperature range.
- Cold Gas Efficiency (CGE) analysis indicates plastic waste as the most efficient in converting to combustible gasses.
- Plastic waste demonstrates the highest CGE due to efficient conversion, while food waste shows the lowest efficiency.
- Efficiency varies across energy cycles (steam, ignition engines, gas turbines) influenced by pretreatment requirements.
- Gasification of bulk MSW exhibits significant energy differences between countries, with the USA leading due to its higher plastic fraction.
- Waste composition influences gasification energy outputs, emphasizing the need for process optimization through waste stream analysis.

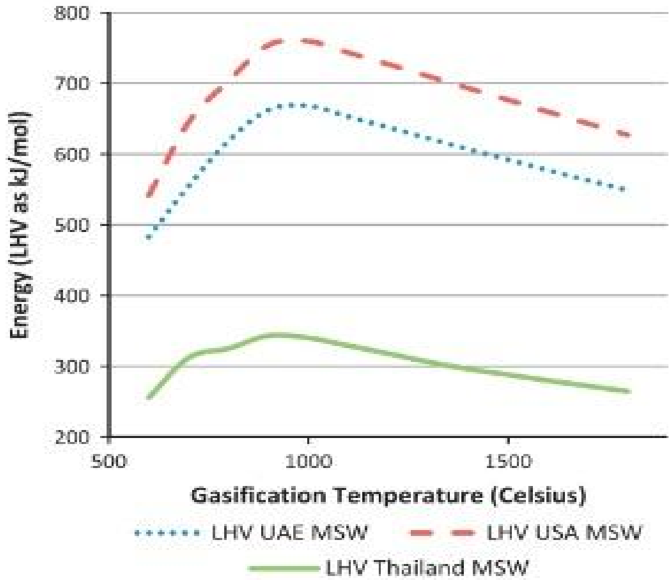


Fig. 8. Lower heating value (LHV) from combusting the products of waste gasification of MSW from UAE, USA, and Thailand.

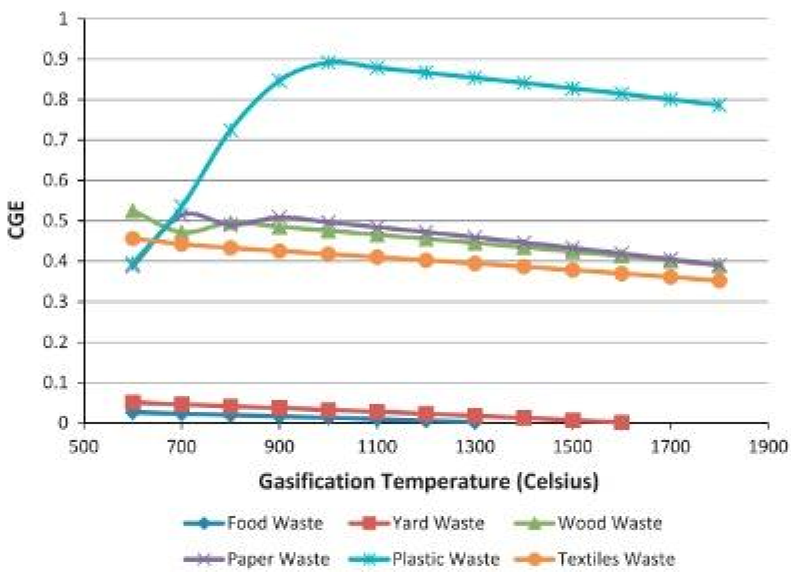


Fig. 9. Cold gas efficiency (CGE) of the six gasifiable streams in MSW.

METHOD 2

1.Equivalence Ratio Effect:

- Syngas composition analysis reveals the impact of Equivalence Ratio (ER) and temperature on gasification.
- ER, ranging from 0.1 to 1.0, influences air–fuel ratios and thus the concentration of CO2 and CO in syngas.
- Fig. illustrates that higher ER values lead to increased CO2 concentration while decreasing CO and H2 levels.

Variations in ER affect gasification efficiency, with low ratios risking incomplete gasification and high ratios promoting excess combustion.

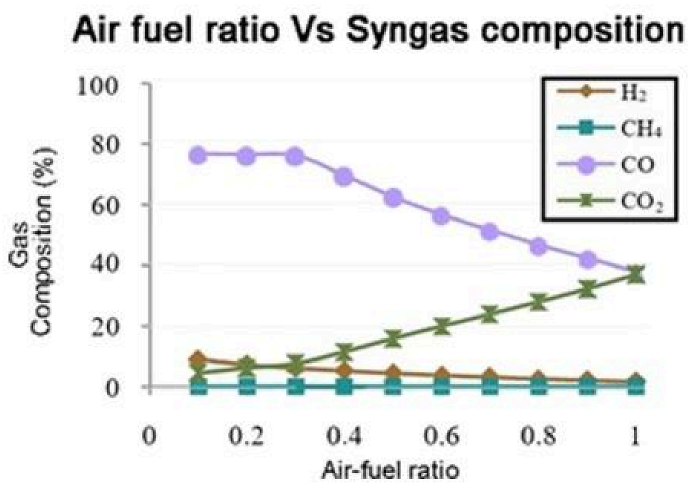


Fig. 5. Effect of air–fuel ratio (gasifier temperature: 700 °C).

2.Temperature Effect:

- Gasification temperature, a critical variable, affects the composition of final gas products due to competing reactions.
- Fig.demonstrates the effect of temperature variation (500 ◦C to 850 ◦C) on CO, CO2, and H2 concentrations in the gasifier.
- Increased temperature leads to higher CO concentrations and reduced CO2 levels due to the Boudouard and water-gas shift reactions.
- The constant CH4 concentrations suggest minimal temperature influence on methane production.

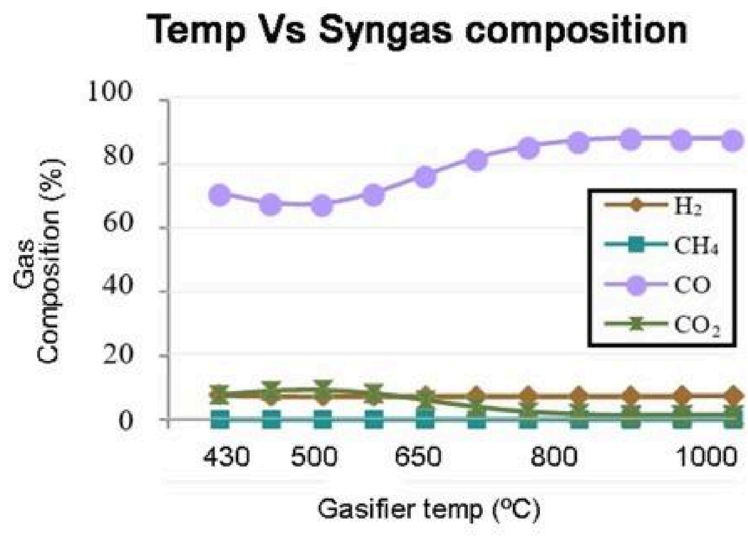


Fig. 6. Effect of gasifier temperature (air–fuel ratio: 0.2).

METHOD 3
1.Comprehensive Analysis:

- TG-FTIR allows for a more comprehensive analysis by combining the thermal behavior information from TG with the chemical composition information from FTIR .
- This integration provides a more detailed understanding of the evolved volatile products during the thermochemical processes of biomass, which is crucial for optimizing gasification processes.

2.Identification of Evolved Gasses:

- FTIR in TG-FTIR can identify and quantify the evolved gasses during the gasification process, providing valuable information on the gas composition and reaction pathways .
- This is essential for understanding the gasification kinetics and mechanisms.

3.Synergistic Interaction Studies:

- TG-FTIR is particularly useful for studying the synergistic interactions between different biomass or coal blends during co-gasification processes .
- By analyzing the evolved gasses using FTIR, researchers can determine the optimal blending ratios for maximizing the synergetic effects in gasification.

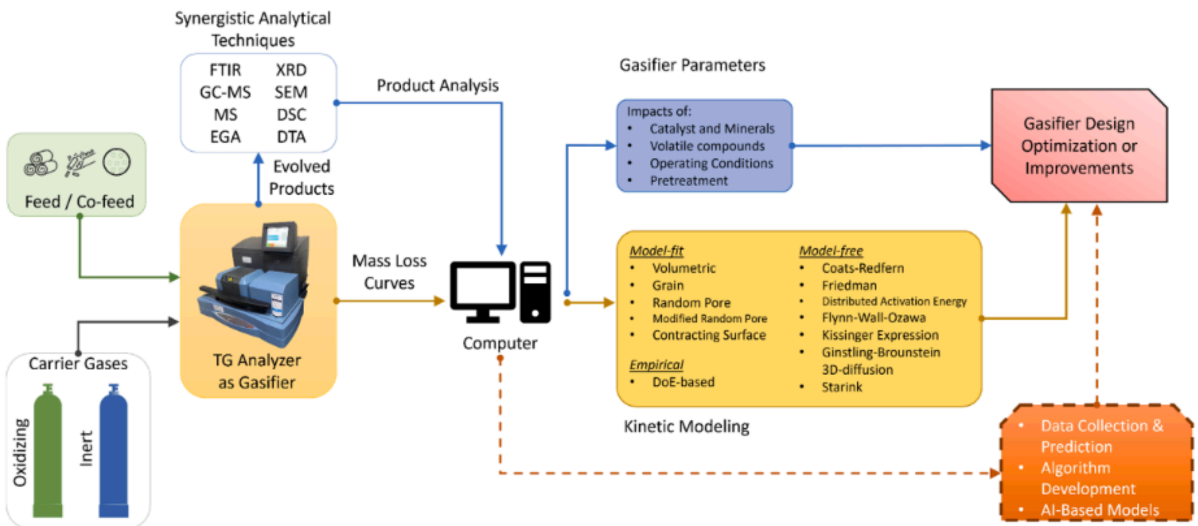


Fig. 4. Framework of gasification process using thermogravimetric analysis.

METHOD 4

- AI models outperform traditional empirical correlations in terms of R-squared values. Some studies explore predicting ultimate analysis data from proximate analysis, showing promising results. However, model accuracies vary based on AI techniques, training algorithms, and statistical analysis methods.

- The number of output (e.g.,HHV) and input (e.g Fixed carbon, volatile matters, and ash content) are similar, and most of them achieved high accuracy (e.g., R2> 0.9, root mean squared error <1.5).

- One study indicated that using ultimate analysis data to predict HHV is likely to be more accurate than using proximate analysis data.

CONCLUSION

In this study, we compared gasification and incineration for municipal solid waste (MSW) recovery, finding that gasification offers potential advantages, especially in affluent countries with higher plastic and textile waste fractions. Thermogravimetric analysis (TGA) emerged as a crucial tool for understanding biomass gasification kinetics, despite limitations in detecting phase transitions independently of mass changes. However, the integration of TGA with complementary analytical techniques shows promise for advancing biomass thermochemical conversion. Moreover, artificial intelligence (AI) applications have significantly contributed to bioenergy research, particularly in predicting biomass properties and process performance. Future efforts should focus on standardizing AI procedures, enhancing data collection and sharing, and exploring AI's role in promoting sustainable bioenergy systems.

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