

PROCESS SIMULATION AND MACHINE LEARNING MODELING OF BIOMASS
WASTES CO-GASIFICATION FOR SYNGAS AND BIOCHAR PRODUCTION

BY

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Industrial and Textile Engineering, in Partial Fulfilment of the Requirements for the
Award of the Degree of Doctor of Philosophy in Industrial Engineering

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2025

DECLARATION

DECLARATION BY STUDENT:

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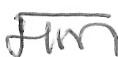
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DEDICATION

To

My loving wife,

My dear daughter,

My parents,

My brothers,

My sisters,

My uncle,

&

My friends and colleagues,

*Whose unwavering support, love, and guidance have been the fountain of inspiration
throughout this journey.*

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ABSTRACT

The urgency of climate change has accelerated research into renewable energy, including biomass co-gasification. While biomass waste offers a sustainable resource for producing syngas and biochar, the conversion process remains complex due to variability in feedstock properties, reactor design, and operating conditions. Additionally, traditional experimental and mechanistic modeling approaches are often time-consuming, costly, and limited in generalizability. This study addresses this gap by integrating experimental characterization, process simulation (PS), and machine learning (ML) to enhance understanding and prediction of autothermal biomass co-gasification outcomes. The primary objective of this research is to develop predictive models to optimize syngas and biochar production. Specifically, the study characterizes the physico-chemical and thermo-kinetic properties of five biomass feedstocks (coffee husks, groundnut shells, macadamia nutshells, rice husks, and tea wastes); develops a PS model to represent biomass co-gasification dynamics; develops and validates ML models to predict co-gasification outcomes; assess model robustness using new biomass blends; and evaluates the impact of model interpretability techniques on feature importance rankings. Proximate analysis method followed ASTM E1131-08, while ultimate analysis was conducted using a Carbon-Hydrogen-Nitrogen-Sulfur (CHNS) analyzer. Thermogravimetric analysis under a nitrogen atmosphere was employed to study thermal degradation, and kinetic parameters were estimated using the Coats-Redfern method. Aspen plus PS method was used to simulate a pilot-scale downdraft gasifier. ML models (Random Forest, Artificial Neural Networks, Gradient Boosting Regression, Support Vector Regression, and SuperLearner ensembles (SLE)) were developed and validated in MATLAB. Robustness was tested by validating the models with new feedstock blends. Interpretability was evaluated using permutation importance, Gini importance, and partial dependence plots. Proximate and ultimate analysis results revealed variability among feedstocks. Volatile matter ($63.96\% \pm 3.57\%$) indicated high syngas and tar potential, fixed carbon ($19.62\% \pm 2.69\%$) contributed to char formation, and carbon content ($47.69\% \pm 4.80\%$) suggested high energy conversion efficiency. Thermo-kinetic analysis showed peak devolatilization temperatures between 345°C and 380°C , activation energies ranging from 39 to 46 kJ/mol, and Gibbs free energy values between 151 and 162 kJ/mol, indicating favorable decomposition behavior. PS model achieved high accuracy with temperature deviations of 2°C (pyrolysis), 4°C (combustion), and 7°C (reduction), and syngas yield deviations of $0.21 \text{ Nm}^3/\text{kg}$ (Equivalence Ratio (ER) 0.17) and $0.34 \text{ Nm}^3/\text{kg}$ (ER 0.29). Sensitivity analysis showed that increasing ER enhanced hydrogen concentration by 10–15% and reduced carbon dioxide by 20–25%. All ML models performed well with Coefficient of Determination (R^2) > 0.90 and Root Mean Square Error (RMSE) $< 5\%$, confirming their effectiveness. Robust analysis showed that SLE maintained superior generalizability ($R^2 > 0.75$, RMSE $< 5\%$) for predicting char and syngas yields. However, hydrogen and cold gas efficiency predictions were less robust, indicating needs for more diverse datasets to improve generalization. Interpretability analysis identified ER and steam-to-biomass ratio as key predictors, with macadamia nutshells playing a critical role in enhancing char yield. In conclusion, this study demonstrates biomass waste co-gasification using integrated experiments, simulation, and ML, providing insights for sustainable energy. The findings recommend applying the developed ML models in academic research and practical gasification systems to support reliable process prediction and decision-making.

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ACRONYMS, ABBREVIATIONS, AND SYMBOLS**List of Acronyms**

AI	Artificial Intelligence
ANN	Artificial Neural Network
ASTM	American Society for Testing and Materials
CC	Corn Cobs
CS	Coconut Shells
CCE	Carbon Conversion Efficiency
CCD	Central Composite Design
CGE	Cold Gas Efficiency
CH	Coffee Husk
CHNS	Carbon, Hydrogen, Nitrogen, Sulfur
CFD	Computational Fluid Dynamics
COG	Co-Gasification
CR	Coats Redfern
DTG	Derivative Thermogravimetric
DTR	Decision Tree Regression
ER	Equivalence Ratio
GBR	Gradient Boosting Regression
GHG	Greenhouse Gas
GPR	Gaussian Process Regression
GS	Groundnut Shell
HHV	Higher Heating Value
LHV	Lower Heating Value
LR	Linear Regression

MAE	Mean Absolute Error
MIMO	Multiple Input Multiple Output
MISO	Multiple Input Single Output
ML	Machine Learning
MS	Macadamia Nutshell
MSE	Mean Squared Error
PDP	Partial Dependence Plot
PS	Process Simulation
RF	Random Forest
RH	Rice Husk
RMSD	Root Mean Square Deviation
RMSE	Root Mean Square Error
SB	Sugarcane Bagasse
SHAP	Shapley Additive exPlanations
SLE	SuperLearner Ensemble
SVR	Support Vector Regression
SVM	Support Vector Machine
TGA	Thermogravimetric Analysis
TW	Tea Waste
WC	Wood Chips

List of Abbreviations

Eqn.	Equation
kJ/mol	Kilo Joules per Mole
kJ/mol.K	Kilo Joules per Mole Kelvin
MJ/kg	Mega Joules per Kilogram

Nm^3/kg	Normal Cubic Meter per Kilogram

List of Symbols

α	Conversion Fraction
&	And
%	Percentage
$^{\circ}\text{C}$	Degree Celsius
E_a	Activation Energy
A	Pre-exponential Factor
ΔG	Gibbs-Free Energy
ΔH	Enthalpy Change
ΔS	Entropy Change
H	Hydrogen atom
H_2	Hydrogen molecules
H_2O	Water/steam
C	Carbon
CH_4	Methane
CO	Carbon monoxide
CO_2	Carbon dioxide
N	Nitrogen
NO_x	Nitrogen oxides
O	Oxygen
S	Sulfur
SO_x	Sulfur oxides
$k(T)$	Reaction Rate Constant
R_p	Maximum Reaction Rate

R^2	Coefficient of Determination
T_p	Peak Temperature
vol. %	Volume percentage
wt. %	Weight percentage

CHAPTER ONE: INTRODUCTION

1.1 Background and Motivation

The urgent need to mitigate climate change and reduce greenhouse gas (GHG) emissions has accelerated the global transition toward renewable energy (Bongomin & Nziu, 2022). Among renewable resources, biomass is a versatile and abundant feedstock that can be converted into energy carriers such as biofuels, biochemicals, syngas, and biochar (Alper et al., 2020; Reddy et al., 2023). Biomass waste, in particular, presents a sustainable alternative to fossil fuels by repurposing organic residues that would otherwise contribute to environmental degradation through decay or open burning (Abdel-Shafy & Mansour, 2018; Abubakar et al., 2022; Ferronato & Torretta, 2019).

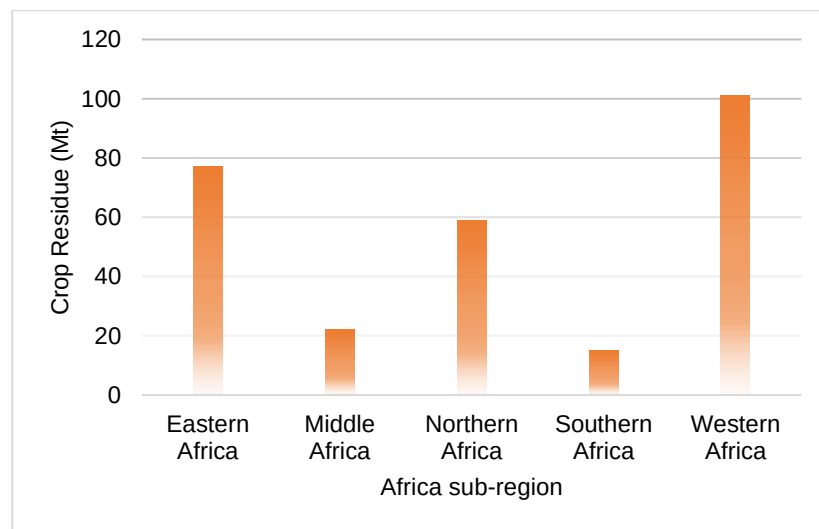


Figure 1.1: Estimated annual crop residue in Africa by regions
Legend: data source (Kazawadi et al., 2022).

Africa possesses vast amounts of agricultural residues, as illustrated in *Figure 1.1*, highlighting the continent's significant potential for biomass-based gasification (Kazawadi et al., 2022). However, despite the availability of feedstock, several project evaluations and case studies in Sub-Saharan Africa (*Figure 1.2*) (NIRAS-LTS, E4tech, AIGUASOL, & Aston University., 2021), have documented biomass gasification systems

that became non-operational after installation due to challenges such as inadequate technical expertise, insufficient maintenance capacity, frequent equipment breakdowns, limited access to spare parts, and weak policy and institutional support (Barry et al., 2021; Giwa & Taziwa, 2024). Addressing these barriers is critical for unlocking Africa's biomass resources to enhance sustainable energy generation.

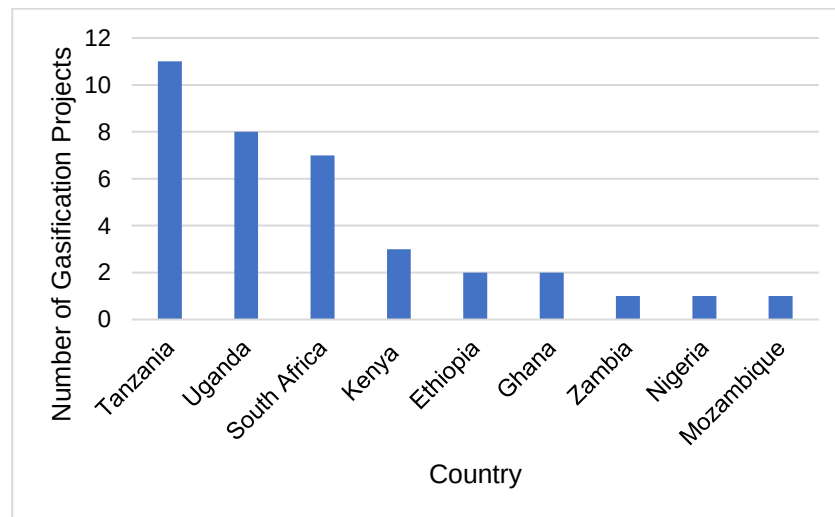


Figure 1.2: Installed gasification systems in Sub-Sahara Africa
 Legend: data source (NIRAS-LTS, E4tech, AIGUASOL, & Aston University., 2021)

Co-gasification (COG), a thermochemical process, has emerged as a promising technology for converting biomass into valuable energy products (Ögren et al., 2024; Song et al., 2022). The process involves the simultaneous gasification of biomass and/or other wastes to produce syngas, a mixture rich in hydrogen (H_2), carbon monoxide (CO), and methane (CH_4) (Singh et al., 2023). Syngas is a versatile energy carrier, widely used for hydrogen production, power generation, and chemical synthesis. Additionally, COG produces biochar, which holds potential for carbon sequestration, soil enhancement, and environmental remediation (Fang et al., 2022).

Despite its advantages, COG is a highly complex process influenced by various factors, including feedstock composition, moisture content, particle size, reactor type, temperature, pressure, and equivalence ratio (ER). These parameters significantly affect

syngas quality, process efficiency, and biochar yield (Bahadar et al., 2022; Shahbaz et al., 2020). Variations in these factors can lead to substantial differences in product composition and process performance, posing challenges to process optimization (Kumar et al., 2022; Lestander et al., 2022; Rosyadi et al., 2022; Santos et al., 2022). Additionally, challenges such as tar formation, ash deposition, and feedstock variability further complicate efforts to achieve consistent and efficient COG (Bahadar et al., 2022; Shahbaz et al., 2020).

To address these complexities, advanced computational tools such as process simulation (PS) and machine learning (ML) offer robust solutions. PS software, such as Aspen Plus, enables the detailed modeling of gasification processes by integrating thermodynamic, kinetic, and reactor-specific parameters to simulate and optimize system performance (Fernando & Naser, 2024; Pandey et al., 2020; Stanger et al., 2024; Zhang et al., 2024). PS facilitates the exploration of a wide range of operating conditions without the need for costly experimental studies while providing valuable insights into the interactions between process variables and their impact on efficiency and product yields (Ayub et al., 2023; Rabea et al., 2023; Tuntiwongwat et al., 2025).

ML complements PS by leveraging data-driven predictive modeling to analyze large datasets from experiments and simulations. Algorithms such as Artificial Neural Networks (ANN), Random Forest (RF), Gradient Boosting Regression (GBR), and Gaussian Process Regression (GPR) have been successfully applied to predict syngas composition, optimize process parameters, and enhance system control (Adeleke et al., 2024; Devasahayam & Albijanic, 2024; Nguyen et al., 2024; Sison et al., 2023; Zhang et al., 2024). ML is particularly effective in capturing nonlinear relationships between input

variables and process outcomes, enabling high-accuracy predictions and continuous model refinement as new data becomes available.

The integration of PS and ML not only enhances the accuracy and efficiency of COG but also aligns with the broader objectives of Industry 4.0, which emphasizes digitalization, automation, and intelligent decision-making in industrial processes (Bongomin, Gilibrays Ocen, et al., 2020; Bongomin, Nganyi, et al., 2020; Bongomin, Yemane, et al., 2020; Sarker, 2022). This convergence has the potential to revolutionize biomass valorization, enabling optimized energy production while minimizing environmental impact (Bastos et al., 2024).

COG is recognized as a transformative approach to biomass valorization, addressing key challenges in waste management and renewable energy production (Ciliberti et al., 2020; Inayat & Sulaiman, 2018; A. Kumar, 2023; Mariyam et al., 2022; Pati et al., 2021; Umar & Sulaiman, 2022; Yang et al., 2021). It provides a dual benefit, reducing reliance on fossil fuels while utilizing diverse feedstocks, including agricultural residues, municipal solid waste (MSW), and industrial by-products (AlNouss et al., 2020; Baruah & Baruah, 2021; Ciliberti et al., 2020). This technology is particularly relevant for regions with abundant biomass resources and growing energy demands, such as rural electrification projects, which use gasification to meet local energy needs (Fang et al., 2023, 2024).

However, due to its complexity, COG demands innovative approaches to process optimization. Traditional modeling methods, such as kinetic and thermodynamic equilibrium models, while valuable, struggle to capture dynamic and nonlinear interactions among process variables (Fernando & Naser, 2024; Pandey et al., 2020; Stanger et al., 2024). ML, with its superior pattern recognition and predictive analytics,

provides a compelling alternative, particularly when combined with PS to form hybrid approaches that maximize predictive accuracy and operational insights.

Recent studies have demonstrated the potential of PS-ML hybrid models in gasification optimization (Akinpelu et al., 2023; Carvalho et al., 2024; Coşgun et al., 2023; Fang et al., 2024; George et al., 2023; Hai et al., 2023; Khurram et al., 2024; Lee et al., 2024; Li et al., 2024; Li et al., 2023; Ögren et al., 2024; Peng et al., 2024; Rodgers et al., 2024; Shahzad et al., 2024; Tomasek et al., 2024; Wang et al., 2024). However, most of these studies focus on single biomass types or simple binary mixtures, use simplified simulation models, and rarely evaluate the robustness or interpretability of the machine learning predictions. Additionally, there is limited work applying PS–ML frameworks to diverse agricultural residues common in East Africa. These gaps highlight the need for a more comprehensive and rigorously validated PS–ML hybrid approach, one that integrates detailed process simulation, multiple biomass blends, and robust machine learning evaluation. This study addresses these gaps.

1.2 Problem Statement

Despite the potential benefits of COG, optimizing the process for maximum syngas yield and efficiency remains challenging. The complexity arises from the inherent variability in biomass feedstocks, the intricate interactions between different feedstock components during gasification, and the sensitivity of the process to various operational parameters such as ER, pressure, and feedstock blend ratio.

Traditional experimental approaches to study and optimize COG are time-consuming and costly. Experimental setups require precise control over numerous variables, and multiple trials are needed to capture the effects of feedstock variability and process conditions, further increasing costs. In addition, the scalability of experimental findings is often

limited, making it difficult to directly translate laboratory results into industrial applications.

Given these challenges, there is a need for alternative approaches that can provide deeper insight into the COG process while being cost-effective, flexible, and scalable. Advanced process simulation tools and data-driven modeling techniques have the potential to address this gap by enabling the systematic exploration of process behavior and parameter interactions without the constraints of physical experimentation.

1.3 Justification of the Study

There was a pressing need to overcome the limitations of traditional experimental approaches to COG and to develop more efficient and scalable methods for optimizing syngas and biochar production from biomass waste. The high costs and complexities associated with experimental studies necessitated the exploration of alternative approaches that could provide similar insights at a fraction of the cost and time.

In this study, PS provided a powerful tool for modeling and analyzing the COG process under various conditions. By simulating different feedstock combinations and operating parameters, the study generated valuable insights into the factors influencing gasifier performance. These insights were used to guide the design and optimization of gasification processes, significantly reducing the need for extensive physical experimentation.

ML added another layer of sophistication by enabling the development of predictive models that accurately forecasted the outcomes of the COG process. These models were trained on simulated data, allowing them to capture the complex relationships between feedstock properties, process parameters, and syngas composition. Once validated, the models were employed to predict the performance of new feedstock combinations.

The integration of PS and ML in this study was justified not only by the need to reduce costs and improve efficiency but also by the potential to advance the field of biomass gasification. By providing a deeper understanding of the COG process and developing reliable predictive tools, this research made a significant contribution to the development of sustainable energy technologies.

1.4 Research Aim and Objectives

1.4.1 Primary Aim

The aim of this study was to develop an integrated process simulation and machine learning framework for the co-gasification of diverse biomass waste to enhance syngas and biochar yields prediction and optimization.

1.4.2 Overall Objective

The overall objective was to develop and implement predictive models through experimental characterization, process simulation using Aspen Plus, and machine learning techniques in order to evaluate and optimize the performance of biomass co-gasification systems.

1.4.3 Specific Objectives

The specific objectives were:

1. To characterize and evaluate the physicochemical properties, thermal decomposition behaviors and reactivity kinetics of rice husks, groundnut shells, coffee husks, macadamia nut shells, and tea waste feedstocks.
2. To develop and validate a process simulation model for the co-gasification of biomass waste using Aspen Plus.

3. To develop and validate machine learning models (Random forest, gradient boosting regression, support vector regression, artificial neuron network, and superlearner ensemble) for biomass waste co-gasification.
4. To investigate the robustness of machine learning models to new feedstock blends.
5. To evaluate the influence of various model interpretability techniques on feature importance rankings in predicting co-gasification performance

1.5 Research Questions

The fundamental research questions that guided this study include:

- a) What are the physicochemical properties, thermal decomposition behaviors, and reactivity kinetics of selected biomass feedstocks (rice husk, groundnut shell, coffee husk, macadamia nut shell, and tea waste)?
- b) How can a comprehensive process simulation model be developed using Aspen Plus to accurately represent the co-gasification of biomass waste, and what are the key factors influencing its accuracy?
- c) How can machine learning models be developed and validated to predict the outcomes of the co-gasification process, and what levels of accuracy and generalizability can these models achieve on test data?
- d) How do variations in input data and model parameters affect the robustness of machine learning models in predicting biomass co-gasification performance, and what strategies can be applied to enhance model reliability?
- e) What is the impact of different model interpretability techniques on feature importance rankings in predicting real-world co-gasification performance?

1.6 Scope of the Study

This study focused on the following key areas:

The research specifically investigated the gasification of rice husk, groundnut shell, coffee husk, macadamia nutshell, and tea waste, both individually and in their binary blends. These feedstocks were selected based on their availability, energy content, and potential for syngas and biochar production. Their thermal decomposition behavior and reactivity kinetics were characterized and analyzed through experimental techniques.

Aspen Plus software was employed to simulate the co-gasification process. The simulation included modeling an autothermal pilot-scale downdraft reactor and operating parameters such as ER, pressure, and feedstock blending ratios. The simulation was limited to steady-state conditions and did not extend to dynamic modeling or scale-up for industrial applications.

Machine learning models were developed and validated to predict co-gasification outcomes, with a specific focus on syngas composition (CO and H₂), gas yield, char yield, cold gas efficiency (CGE), and lower heating value (LHV). These models were trained using data generated from the process simulation. The machine learning techniques employed included linear regression (LR), ANN, support vector regression (SVR), and ensemble methods.

A sensitivity analysis was conducted to examine the influence of ER on reactor zone temperatures, gas and char yields, and syngas composition. This analysis, based on simulation results, was used to guide optimization of the co-gasification process.

The study was primarily limited to feedstocks readily available in regions such as Uganda and Kenya. Although the findings may be relevant in other contexts, the study did not explicitly account for geographical variations in biomass availability or quality.

1.7 Significance of the Study

This study is significant because it addresses the high cost, complexity, and limited scalability of experimental co-gasification research. By integrating PS with ML, it demonstrates a modern, data-driven approach capable of improving the efficiency, accuracy, and flexibility of biomass co-gasification analysis. This integrated methodology offers an alternative pathway for optimizing syngas and biochar production without relying solely on expensive and time-consuming laboratory experiments.

The research is particularly important for regions such as Uganda and Kenya, where biomass waste is abundant but advanced testing facilities are limited. By promoting the utilization of agricultural residues for clean energy production, the study directly supports global efforts toward sustainable energy development, waste valorization, and greenhouse gas reduction.

Furthermore, the application of PS and ML in this context exemplifies the practical value of Industry 4.0 technologies in the renewable energy sector. The study provides a foundation for researchers, engineers, and policymakers seeking scalable tools and approaches for designing, analyzing, and improving co-gasification systems. Its significance lies in advancing more accessible, intelligent, and sustainable methods for biomass-based energy production.

1.8 Thesis Structure

This thesis is organized into six chapters. Chapter 1 introduces the study by presenting the research background, problem statement, objectives, research questions, justification, scope, and significance. Chapter 2 provides an extensive literature review covering biomass characterization techniques, gasification processes, process simulation methodologies, machine learning methods and applications, robustness and

interpretability analysis approaches, and relevant conceptual frameworks. The chapter concludes by identifying the existing research gaps that the study seeks to address.

Chapter 3 outlines the materials and methods, including the research design, biomass feedstocks, experimental procedures for physicochemical and thermokinetic characterization, the Aspen Plus simulation setup, machine learning model development and validation, robustness and interpretability analysis techniques, and the tools, assumptions, challenges, and limitations associated with the study.

Chapter 4 presents and discusses the results obtained from the physicochemical characterization, TGA analysis, process simulation and validation, sensitivity analysis, machine learning model performance evaluation, robustness assessment, and interpretability analysis. Chapter 5 summarizes the key findings, draws conclusions in relation to the research objectives, and offers recommendations for future research and potential applications. REFERENCES provide a list of all sources cited in accordance with APA formatting guidelines, while the APPENDICES contain supplementary materials, including extended datasets, detailed tables, model codes, and other supporting information.

CHAPTER TWO: LITERATURE REVIEW

2.1 Introduction

Gasification and co-gasification (COG) are promising thermochemical technologies for converting biomass wastes into hydrogen-rich syngas, a cleaner alternative to fossil fuels with broad industrial applications. The increasing demand for renewable energy has driven interest in utilizing biomass feedstocks, with COG offering benefits such as enhanced syngas quality, efficiency, and resource utilization. However, variations in feedstock properties and operating conditions introduce complexities that require robust modeling and optimization strategies.

This chapter reviews key factors influencing gasification and COG, including physicochemical properties, thermo-kinetics, feedstock blending, process simulation (PS), and machine learning (ML) applications. It highlights advancements in Aspen Plus modeling, explores AI-driven process optimization, and examines the synergies of COG. Despite progress, challenges remain in integrating experimental and computational approaches, refining predictive models, and improving interpretability. Part of this review has been published in our previous study (Bongomin et al., 2024), which explored ensemble ML techniques in gasification research, emphasizing the importance of model interpretability.

2.2 Physicochemical and Thermo-kinetic Analysis

2.2.1 Biomass feedstocks

Biomass feedstocks play a pivotal role in thermochemical conversion processes such as pyrolysis, gasification, and COG, offering a sustainable and renewable energy source (Joshi et al., 2024). These processes convert biomass into valuable products such as syngas, biochar, and bio-oils, which can be utilized for energy generation, carbon

sequestration, and industrial applications (Jha et al., 2022). The selection of feedstocks is critical, as their physical and chemical properties significantly influence the efficiency, product yields, and environmental impact of thermochemical processes (Begum et al., 2024; Ivanovski et al., 2023; Iwuozor et al., 2022; Rout et al., 2023; Vanisree et al., 2024). Figure 2.1 illustrates the main biomass feedstock sources for thermochemical conversion, highlighting the diversity of raw materials available for processes such as gasification and pyrolysis (Tursi, 2019).

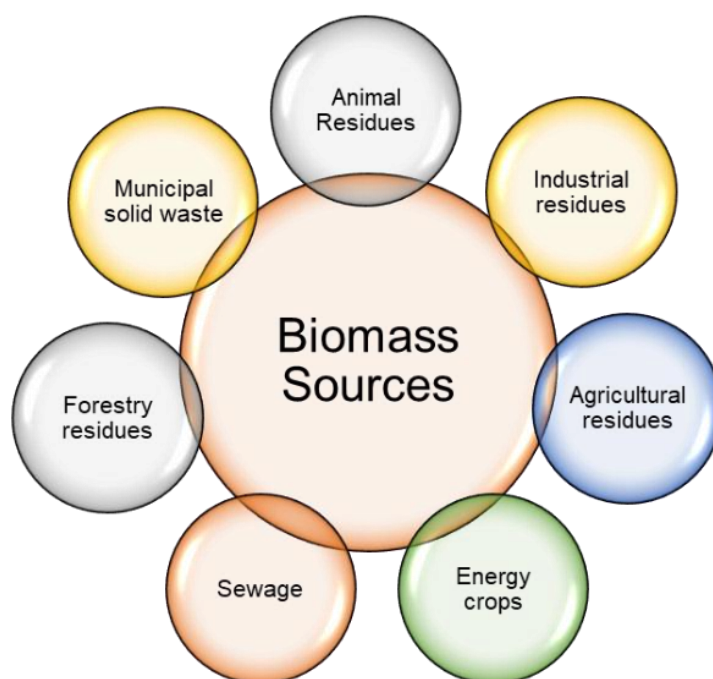


Figure 2.1: Main biomass feedstock sources for thermochemical conversion

2.2.2 Physicochemical analysis

Physicochemical characterization of biomass is essential for evaluating its suitability for thermochemical conversion processes like gasification and pyrolysis. Key parameters include proximate analysis, ultimate analysis, calorific value, and lignocellulosic composition, all of which influence energy yield and conversion efficiency (Abdallah et al., 2023; Fajobi et al., 2022; Tomczyk, 2020). Proximate analysis determines moisture content, volatile matter, fixed carbon, and ash. High moisture reduces energy efficiency, while volatile matter enhances syngas production. Fixed carbon contributes to char

formation, and ash content affects slagging and fouling in reactors (Chaiklangmuang et al., 2015; Nam et al., 2021).

Ultimate analysis identifies the elemental composition (C, H, O, N, S), influencing combustion efficiency and emissions. A higher C/H ratio improves energy content, while oxygen content affects oxidation reactions. Nitrogen and sulfur must be minimized to reduce NO_x and SO_x emissions (Nimmanterdwong et al., 2021; Xing et al., 2019). Calorific value indicates biomass energy potential, with higher heating value (HHV) being crucial for gasification. HHV is influenced by carbon and hydrogen content, while moisture and ash lower effective energy yield (Bhattarai et al., 2023).

Lignocellulosic composition (cellulose, hemicellulose, and lignin) dictates decomposition behavior (Nimmanterdwong et al., 2021; Onokwai et al., 2022). Cellulose and hemicellulose degrade at lower temperatures, favoring syngas production, while lignin decomposes slowly, contributing to char yield and process stability (Kamruzzaman et al., 2024; Kumar et al., 2020). Understanding these properties allows for optimized biomass selection and conversion process design, ensuring efficient and sustainable bioenergy production.

2.2.3 Thermogravimetric analysis

Thermogravimetric analysis (TGA) is a key technique for assessing the thermal decomposition behavior of biomass, providing insights into mass loss patterns, thermal stability, and reaction kinetics (Kumar et al., 2020). It is essential for optimizing pyrolysis and gasification processes by evaluating how biomass components degrade under controlled heating conditions. In a typical TGA experiment, biomass samples are heated from room temperature at 10–30°C/min heating rates up to 800–1,000°C under an inert (e.g., nitrogen) or oxidative (e.g., air) atmosphere. The thermogravimetric analyzer records weight loss, while the differential thermogravimetric (DTG) curve identifies

decomposition phases. Coupling TGA with Fourier-transform infrared spectroscopy (FTIR) or mass spectrometry enables real-time gas analysis (Afessa et al., 2023; Pan et al., 2023).

TGA results show three primary decomposition stages (Xavier et al., 2016): moisture loss (50–150°C), hemicellulose and cellulose decomposition (200–400°C), and lignin degradation with char formation (250–600°C). Higher lignin content leads to greater char yield, affecting biochar quality and gasification efficiency (Balsora et al., 2023). The remaining residue consists of fixed carbon and ash, influencing reactor performance and syngas composition. TGA also estimates activation energy using kinetic methods, providing insights into reaction kinetics (Kumar et al., 2021; Lei et al., 2024; Linh et al., 2021; Nam et al., 2021). By understanding biomass thermal behavior, TGA aids in selecting suitable feedstocks and optimizing thermochemical conversion systems for efficient bioenergy production.

2.2.4 Kinetic and thermodynamic analysis

Various kinetic models and reaction mechanisms have been developed to describe the thermal decomposition behavior of biomass including model-free and model-fitting methods (Fischer et al., 2024; Najafi et al., 2024; Steven et al., 2024). The model-free methods include the Flynn-Wall-Ozawa (FWO), Friedman, Starlink and Kissinger-Akahira-Sunose (KAS) methods (Arumugam & Ganesan, 2024; Wang et al., 2024). The model-fitting methods include direct Arrhenius (Kumar Shrivastava & Prasad Chakraborty, 2024), Coats-Redfern (CR) (Ferfari et al., 2024), Kennedy-Clark (Li et al., 2024), Criado master plot (Choudhary et al., 2024; Li et al., 2023), and Distributed Activation Energy Model (DAEM) methods (Escalante et al., 2022; Fatmawati et al., 2023). Model-free methods provide an advantage by not assuming a specific reaction model, allowing for a more flexible analysis across different temperature ranges and

heating rates. However, they often require extensive experimental data and can be computationally intensive.

The CR method, a model-fitting approach, is widely used due to its simplicity and effectiveness in estimating kinetic parameters such as activation energy and pre-exponential factor (Ferfari et al., 2024; Tariq et al., 2023). This method assumes a first-order reaction model and linearizes the Arrhenius equation, facilitating straightforward calculations from TGA data (Kumar & Prasad, 2024). By applying the CR method, researchers can obtain reliable kinetic parameters with fewer data points compared to model-free methods, making it an efficient choice for preliminary analysis of biomass pyrolysis (Coats and Redfern, 1964; Ebrahimi-Kahrizsangi & Abbasi, 2008). The method's ability to provide accurate and consistent results with limited data enhances its applicability in studies aiming to optimize pyrolysis conditions for various biomass materials.

Understanding the kinetic and thermodynamic parameters associated with biomass pyrolysis is crucial for the successful industrialization of this process (Guo et al., 2022; Sivaraman et al., 2023; Wang et al., 2023). These parameters provide fundamental insights into the reaction mechanisms, energy requirements, and product distribution, enabling the optimization of reactor design, operating conditions, and product recovery (Quintero-Naucil et al., 2024; Wang et al., 2024). Kinetic parameters, such as activation energy (E_a), pre-exponential factor (A), and reaction order (n), quantify the rate at which biomass undergoes pyrolysis (Najafi et al., 2024; Okot et al., 2023; Parthasarathy et al., 2023; Zhang et al., 2023).

This information is essential for several reasons. Firstly, it aids in reactor design by allowing for the accurate modeling and simulation of pyrolysis reactors, leading to optimized reactor configurations and operating conditions (Aboelela et al., 2023; Ascher

et al., 2022; Balsora et al., 2022; Clemente-Castro et al., 2023; Huang et al., 2024; Nasfi et al., 2022). Secondly, understanding the reaction kinetics is vital for process control, enabling precise regulation of process variables like temperature and residence time to achieve desired product yields and qualities (Gupta et al., 2024; Lei et al., 2023). Thirdly, accurate kinetic models help predict energy consumption and identify potential energy-saving strategies, enhancing overall energy efficiency (Chinenye et al., 2024; Liu et al., 2024; Osman et al., 2024; Zhang et al., 2024).

Thermodynamic parameters, including enthalpy (ΔH), entropy (ΔS), and Gibbs free energy (ΔG), provide insights into the energy balance and spontaneity of the pyrolysis process (Sánchez-Ávila et al., 2024). This information is crucial for predicting product yields, as thermodynamic data can estimate the equilibrium yields of different products, aiding in process optimization (Amoloye et al., 2023; Choudhary et al., 2024). Additionally, understanding the energy requirements of the pyrolysis process facilitates the integration of heat recovery systems and energy-efficient process design (Chen et al., 2020). Thermodynamic analysis also helps assess the feasibility of different biomass feedstocks and identify suitable pyrolysis conditions, ensuring process viability (Osman et al., 2024; Vanisree et al., 2024).

The dynamics between kinetic and thermodynamic parameters is essential for a comprehensive understanding of the pyrolysis and biomass valorization processes (Kumar et al., 2024; Rashd et al., 2024). By combining these parameters, researchers and engineers can develop predictive models, optimize reactor performance, and assess the economic feasibility of biomass pyrolysis (Lingamdinne et al., 2024). This knowledge is critical for the successful commercialization of pyrolysis technologies and the production of high-value products from biomass waste (Dai et al., 2024). Ultimately, the accurate determination of kinetic and thermodynamic parameters contributes to the development

of sustainable and efficient biomass conversion processes (Temireyeva et al., 2024; Bongomin, Elagroudy, et al., 2025). This promotes a circular economy and reduces reliance on fossil fuels, paving the way for a more sustainable future (Nath, 2024; Olugbenga et al., 2024).

2.3 Biomass Wastes Gasification

2.3.1 Overview of gasification

Gasification is a thermochemical process that converts carbonaceous materials into hydrogen-rich syngas, offering advantages over pyrolysis and direct combustion (Mpungu et al., 2024; Zahra et al., 2024; X. Ma et al., 2025). Unlike pyrolysis, which primarily produces bio-oil and char, gasification operates under partial oxidation, yielding a versatile gas mixture suitable for hydrogen production and synthetic fuel generation (Kuttin et al., 2024; Gan et al., 2025; T. Ma et al., 2025). This process enhances thermal efficiency, feedstock flexibility, and resource recovery, making it a key technology for sustainable energy and waste management (Aguado et al., 2023; Allesina et al., 2018; He et al., 2021; Wang et al., 2023). Table 2.1 provides a comparison of gasification, pyrolysis, and combustion, highlighting their distinct advantages and applications.

Gasification occurs in four main stages: drying, pyrolysis, combustion, and reduction, where carbonaceous materials decompose into H_2 , CO , CH_4 , and CO_2 in the presence of air, oxygen, or steam (Bongomin et al., 2024; Prajapati & Tirkey, 2025). Various gasifier designs, including fixed-bed, fluidized-bed, entrained-flow, plasma, and rotary kiln systems, influence syngas composition and process efficiency (Indrawan et al., 2020; Kittivech & Fukuda, 2020; Mallick et al., 2020). Figure 2.2 illustrates the classification of gasifiers based on physical structure, showcasing their design variations. The choice of gasification agent including air, CO_2 , oxygen, or steam, affects reaction pathways, product composition, and hydrogen yield (Erdiwansyah et al., 2023; Sikarwar et al.,

2020). Effective syngas cleanup ensures environmental sustainability and its suitability for power generation, fuel synthesis, and chemical production (Bongomin & Nziu, 2022; Eghtedaei et al., 2017).

COG, an innovative approach, enhances process efficiency by gasifying multiple feedstocks simultaneously, leveraging synergistic interactions to improve tar conversion and gas quality (Ramos et al., 2018; Thengane et al., 2019). This method optimizes resource utilization, reduces emissions, and contributes to circular economy goals, addressing waste management challenges while advancing sustainable energy solutions (Esmaeili et al., 2020; Salavati et al., 2019).

Table 2.1: Ranking of biomass thermochemical conversion processes

Rank	Thermochemical process	Key importance	Clean factor	Applications
1	Gasification	Produces syngas for electricity, hydrogen, synthetic fuels, biochar as byproduct	High energy efficiency; syngas purification reduces harmful emissions.	Energy generation, chemical synthesis, hydrogen production, biochar production
2	Hydrothermal Gasification	Converts wet biomass into syngas without pre-drying, hydrochar as byproduct	Efficient with reduced greenhouse gas emissions; ideal for wet biomass.	Wet biomass and sludge conversion to hydrogen and methane, hydrochar production
3	Pyrolysis	Produces bio-oil, biochar, and syngas; supports carbon sequestration.	Captures carbon in biochar; reduces waste and mitigates emissions.	Biochar production, liquid fuels, syngas for energy and heat.
4	Hydrothermal Liquefaction	Produces bio-crude with high energy density.	Avoids drying energy loss; bio-crude can be refined into cleaner fuels.	Advanced fuel production, waste management for wet feedstocks.
5	Combustion	Simple, widely used for direct heat and power production.	Higher emissions; less clean but mitigated by modern scrubbers and filters.	Industrial and residential energy production.
6	Torrefaction	Enhances biomass quality for efficient energy conversion.	Reduces transport emissions; not a standalone energy production method.	Pre-treatment for combustion, gasification, and pyrolysis.
7	Hydrothermal Carbonization	Converts wet biomass into hydrochar for fuel or soil amendments.	Clean but less energy-intensive; suitable for waste valorization.	Fuel production, waste-to-resource strategies, carbon sequestration through hydrochar.

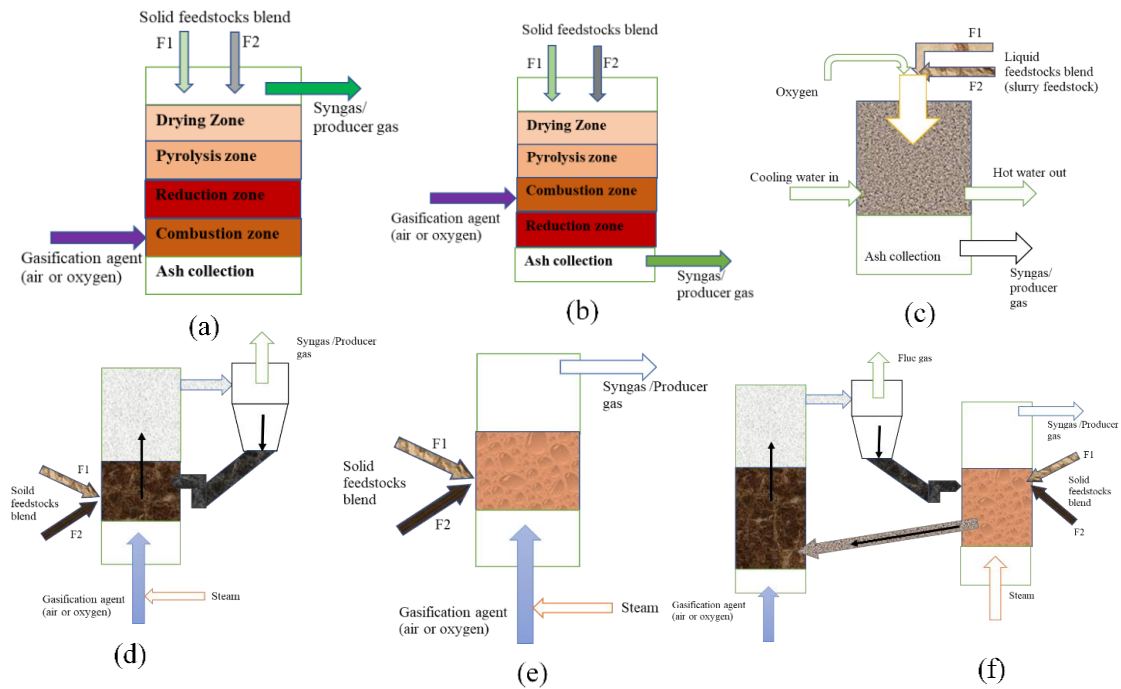


Figure 2.2: Schematic representation of the different gasifier systems

Legend: (a) Updraft gasifier, (b) downdraft gasifier, (c) entranced-flow gasifier, (d) circulating fluidized-bed gasifier, (e) bubbling fluidized-bed gasifier, (f) dual fluidized-bed gasifier, F1 and F2- feedstocks in the blend. The figure redrawn based on Indrawan et al. (2020).

2.3.2 Gasification technologies

Innovative gasification technologies are advancing biomass waste conversion, enhancing efficiency and sustainability. Chemical looping gasification utilizes metal oxide carriers for oxygen separation, improving process efficiency while reducing emissions (Lu et al., 2021; Peng et al., 2017; Song et al., 2022). Catalytic gasification accelerates reaction rates, enhancing syngas yield and operational flexibility. Supercritical water gasification (SCWG), also known as hydrothermal gasification, operates at high temperatures and pressures, converting wet biomass into syngas without external gasifying agents (Hantoko et al., 2018; Heeley et al., 2024; Seçer et al., 2020; Xiao et al., 2020). SCWG is particularly suitable for high-moisture feedstocks and offers a cost-effective, environmentally friendly approach to hydrogen production (Ghavami et al., 2021; Huang et al., 2019; Nanda et al., 2021). Figure 2.3 highlights these innovative gasification pathways, showcasing their potential for low-emission, high-efficiency energy conversion.

Further advancements include multi-stage gasification, where two-stage processes involve an initial pyrolysis or partial oxidation step followed by a secondary conversion phase, optimizing syngas composition (Haydary, 2017; Jeong et al., 2021; Kargbo et al., 2021; Kosov & Zaichenko, 2016; Pei et al., 2018; Yazdanpanah Jahromi et al., 2019). Three-stage gasification introduces an additional step for enhanced control over reaction pathways and product quality (Chao et al., 2014; Hu et al., 2017; Hu et al., 2021). These evolving technologies offer diverse solutions to meet energy and environmental goals, driving sustainable hydrogen-rich syngas production from biomass waste (Makwana et al., 2023; Ögren et al., 2024; Song, Yang, Xue, et al., 2022).

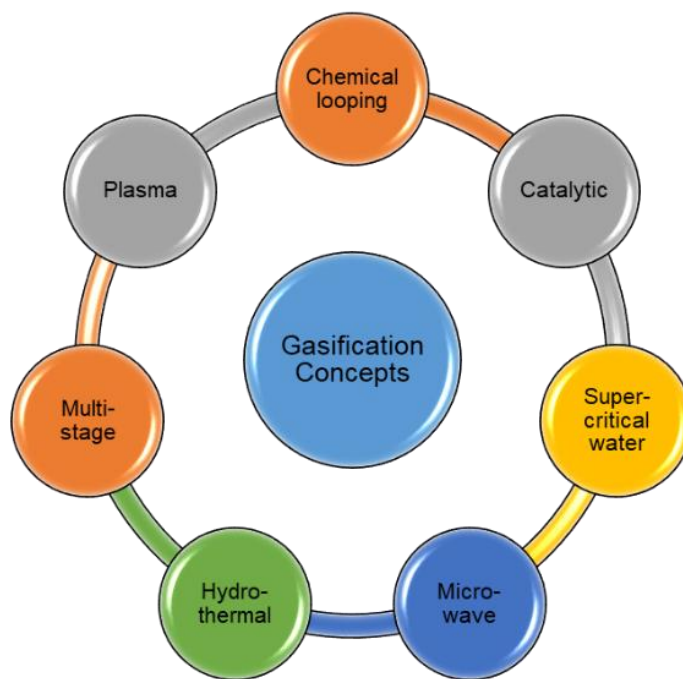


Figure 2.3: Innovative technologies of gasification systems

2.3.3 Co-gasification

COG addresses challenges in syngas quality and feedstock availability, ensuring continuous operation and improved gasification efficiency (AlNouss et al., 2020; Baruah & Baruah, 2021; Ciliberti et al., 2020). By blending different feedstocks, it optimizes resource utilization while reducing tar formation and pollutant emissions, particularly in coal-biomass COG (Ciliberti et al., 2020; Inayat & Sulaiman, 2018; Yang et al., 2021).

However, process control remains complex, as syngas composition and heating value depend on feedstock properties, reactor types, gasification agents, and operating conditions (Kumar, 2023; Mariyam et al., 2022; Pati et al., 2021; Umar & Sulaiman, 2022).

A review of 184 studies (2017–2022) highlights growing research interest in COG. Keyword analysis (Figure 2.4) showed "co-gasification" as the most dominant term, with related themes including hydrogen production, Aspen Plus simulation, synergistic effects, kinetics, and reactivity, demonstrating the focus on optimizing process efficiency and fuel flexibility.

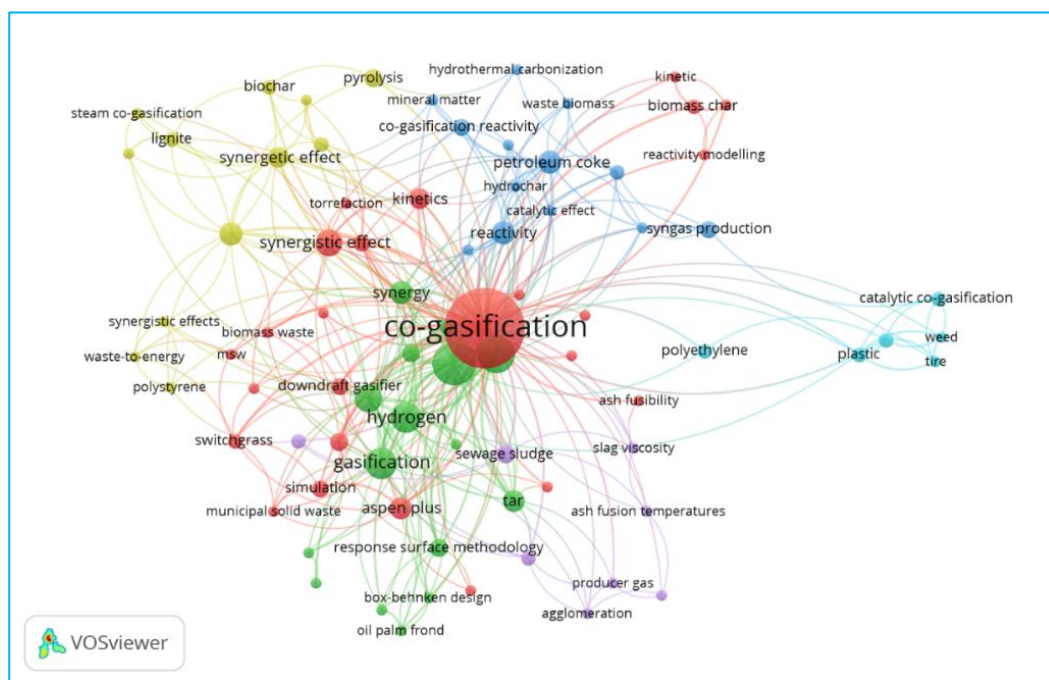


Figure 2.4: Network visualization of keywords from the published articles on COG

2.3.4 Biomass-biomass blend feedstock

Biomass-biomass COG combines different biomass types to enhance syngas yield, gas composition, and process efficiency (Monir et al., 2018). The most common feedstock combinations include binary, ternary, and quaternary blends, with binary blends being the most widely studied. Biomass blends are generally classified by the number of feedstocks used: binary blends consist of two biomass types, ternary blends incorporate three, and

quaternary blends include four different materials. Many studies favour binary blends because they provide a clearer and more controlled platform for examining interaction effects between specific feedstock pairs (Zahra et al., 2024; Gan et al., 2025). Compared to higher-order mixtures, binary blends reduce compositional complexity and enable more accurate interpretation of thermal behaviour, reaction pathways, and gasification performance, making them the preferred choice in much of the existing literature (Anniwaer et al., 2021; Kittivech & Fukuda, 2019).

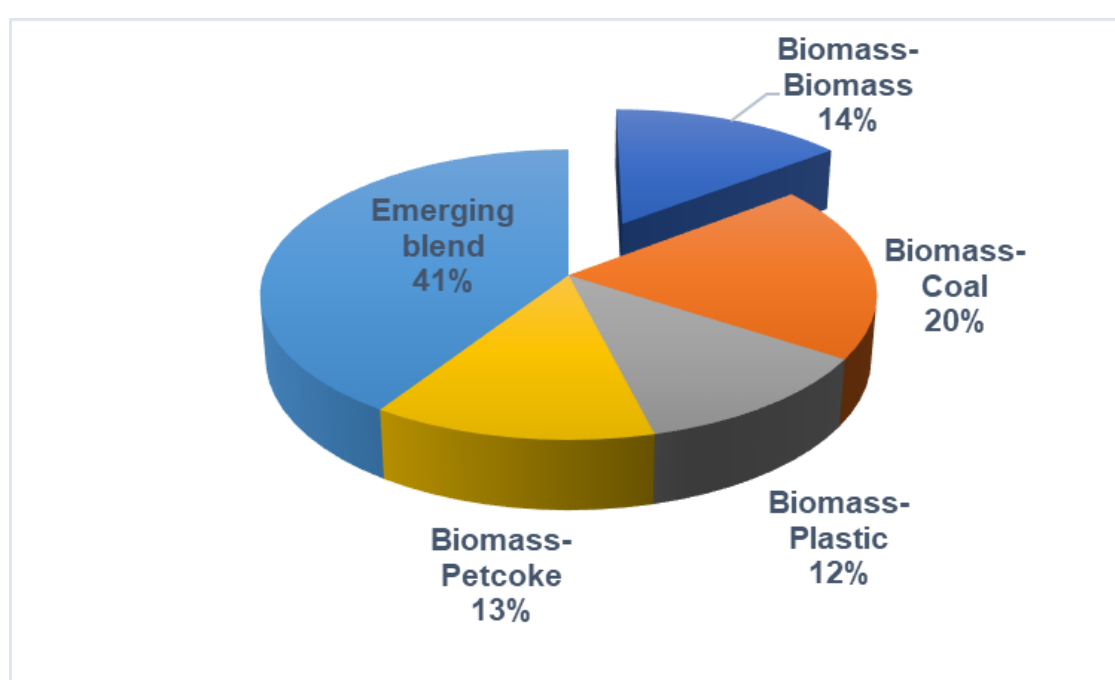


Figure 2.5: Feedstock blend categories for co-gasification

Figure 2.5 illustrates the classification of feedstock blends, including biomass-biomass blend, biomass-coal blend, biomass-plastic blend, biomass-petroleum coke (PC), biomass-coal blend and other blends (emerging feedstock blends). Pretreatment methods such as pelletization, briquetting, torrefaction, and carbonization improve fuel properties, increasing density, calorific value, and gasification reactivity (Chun et al., 2022; Wiyono et al., 2021). Biochar-based blends also show potential for reducing NO_x emissions and enhancing reaction stability (Zhao et al., 2022). Studies highlight the catalytic role of

alkali and alkaline earth metals (AAEMs) in improving char oxidation and reactivity (Jiao et al., 2022).

Blending biomass mitigates feedstock limitations, such as high-ash content or low calorific value, and improves resource availability, reducing dependence on a single biomass type (Awais et al., 2022). Gasifier performance can also be enhanced through biomass blending. For instance, COG of rice husk, banana peel, and cedarwood improved syngas production at lower temperatures due to the catalytic effects of potassium and calcium (Anniwaer et al., 2021). A unique example is the crude glycerol-animal fat blend, demonstrating the versatility of biomass combinations (Almeida et al., 2022).

Despite these advantages, not all performance metrics (e.g., LHV, CGE, gas yield) improve with biomass-only blends. Incorporating non-biomass materials into blends can help optimize syngas quality and overall efficiency (Lv et al., 2022). A summary of previous biomass-biomass blend COG studies is presented in Table 2.2.

Table 2.2: A summary of studies on co-gasification of biomass-biomass blends

S/N	Biomass-biomass blend	Blending ratio (%)	Reactor type	Operating conditions	Performance measures	Reference
1	Banana peel and Japanese cedarwood; Banana peel and Rice husk	-	Fixed-bed gasifier	Temperature; Water injection rate	Gas yield; CCE	Anniwaer et al. (2021)
2	Coffee husk and sawdust	-	In-house bubbling fluidised bed gasifier	Particle size, Temperature, ER, Biomass feed rate, Air supply rate	Gas composition, LHV, Gas yield, CCE, CGE	George et al. (2019)
3	Palm empty fruit bunches and rubber wood sawdust	25/75, 50/50, 75/25	fluidized beds with silica sand as bed material	ER	De-Fluidization Time, Bed temperature; CGE; CCE; LHV; Gas composition	Kittivech & Fukuda (2019)
4	digestate and almond shells	60/40	Pilot-scale rotary kiln plant	ER, BFR, Heating rate, pressure: 1–5 hPa	CGE: 55% LHV: 4-5 MJ/Nm ³	Freda et al. (2019)

S/N	Biomass-biomass blend	Blending ratio (%)	Reactor type	Operating conditions	Performance measures	Reference
5	Spent mushroom substrate and Erianthus, Japanese cedar	75/25, 50/50, 25/75	Fixed-bed downdraft	Temperature, steam flow rate: 0.45-0.65 mL/min	CCE; gas yield, tar yield, char yield and ash	Koido et al. (2021)
6	Forest residue and wood charcoal	90/10, 80/20, 70/30, 60/40	Pilot-scale 50 kWth downdraft	Particle size: 20–25 mm; Pressure (bar): (1, 5, 15, 25, 35, 45) Temperature; Air flow rate: 0 to 60 m ³ /h	Syngas ratio; gas yield; LHV and HHV); syngas composition; exergy efficiency; feedstock consumption rate	Monir et al. (2020)
7	Rice husk and sugarcane bagasse; wheat husk and sugarcane bagasse; rice straw and wheat straw	50/50	Fixed-bed downdraft	Feed rate: 100 kg/hr; Temperature: 750 °C; ER: 0.35; steam to biomass ratio: 0.5.	LHV, Gas yields Energy efficiency, exergy efficiency	Pati & De (2021)
8	Rice straw and sugarcane bagasse pellet	80/20, 50/50, 20/80	Pilot-scale 50 kWth downdraft	ER: 0.2 to 0.5 Temperature: 600 to 900 °C	LHV Gas yields energy efficiency; exergy efficiency	Pati et al. (2021)
9	Japanese cedar wood and Japanese cedar biochar	50/50, 1:2, 2:1,	Lab-scale fixed-bed downdraft	heating rate: 10 °C/min Temperature: 650-850 °C	Gas yield	Anniwaer et al. (2021)
10	Wood-coconut fiber pellets and rice husk pellets	75/25, 50/50, 25/75	open-top downdraft gasifier	ER: 0 to 0.32 Fuel flowrate	LHV; Tar content	Wiyono et al. (2021)

2.3.5 Benefits, challenges and opportunities

Gasification offers sustainable energy solutions while reducing reliance on fossil fuels (Singh et al., 2023). The produced syngas serves as a valuable fuel for power generation (gas engines, turbines, and Combined Heat and Power (CHP) systems), direct heating, and synthetic fuel production (Ding et al., 2022; He et al., 2021). Additionally, gasification contributes to waste valorization, transforming municipal solid waste and agricultural residues into energy and high-value byproducts like biofuels, biochemicals, and biochar (He et al., 2021; Omol et al., 2020; Sikarwar et al., 2016). Figure 2.6 highlights these diverse applications, emphasizing gasification's role in renewable energy and waste management.

Despite its advantages, feedstock variability, economic constraints, and environmental concerns pose challenges (Filho et al., 2022). Variability in moisture content, composition, and contaminants (e.g., sulfur, chlorine, alkali metals) affects efficiency and reactor performance, causing issues like slagging, fouling, and corrosion (Hussain et al., 2023). Tar formation is another major issue, requiring effective removal strategies to prevent equipment failure (Sharma & Kaushal, 2020; Sikarwar et al., 2016). Scaling up gasification processes introduces complexities in heat transfer, process optimization, and syngas cleanup, increasing operational costs (Schmid et al., 2021). Additionally, compliance with environmental regulations necessitates rigorous emissions monitoring and mitigation strategies (Kamaruzaman et al., 2023).

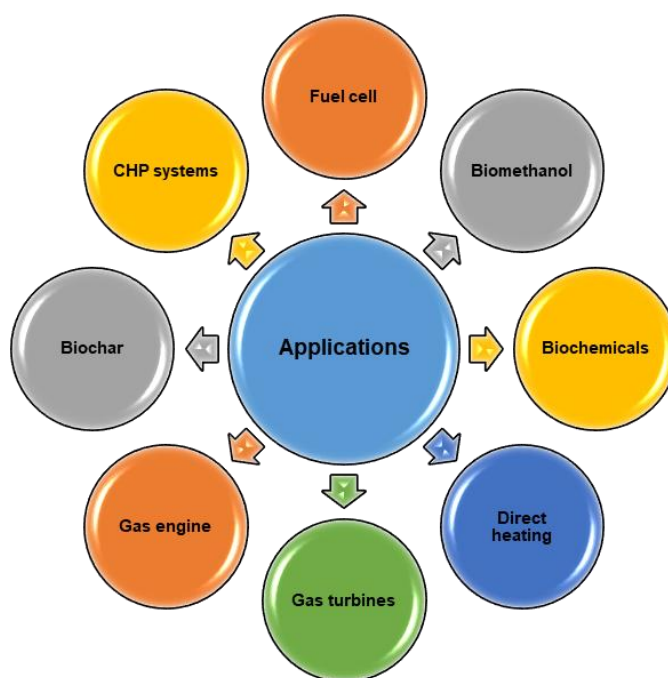


Figure 2.6: Applications of syngas and byproducts from gasification process.

Advancements in machine learning (ML), computational modeling, and process optimization are addressing these challenges (Puig-Gamero et al., 2020; Wang et al., 2024). Computational Fluid Dynamics (CFD) and kinetic modeling enhance understanding of thermochemical reactions, guiding process improvements (Al-Qadasi & Ozkan, 2021; Rabea et al., 2022). Data-driven modeling integrates ML to optimize

operating conditions, improve efficiency, and minimize environmental impact (Arumugasamy et al., 2020; Cerinski et al., 2020; George et al., 2023). Life cycle assessment (LCA), techno-economic analysis (TEA), and risk mitigation (RM) further support sustainable gasification deployment (Fang et al., 2023, 2024; Rodgers et al., 2024; Sapariya et al., 2021).

Despite challenges, ongoing research and technological advancements demonstrate gasification's potential in the renewable energy transition, offering scalable solutions for clean energy production, waste reduction, and resource efficiency (Kargbo et al., 2023).

2.3.6 Biochar production and application

Biochar is a carbon-rich material produced through the thermochemical conversion of biomass under oxygen-limited conditions, typically via pyrolysis, gasification, or hydrothermal carbonization (Yadav & Khalid, 2025). The interplay between feedstock properties and process parameters (such as temperature, heating rate, and residence time), determines the resulting biochar's physicochemical characteristics, including surface area, porosity, elemental composition, and functional groups (Makowska et al., 2025; Yang & Ergas, 2025). These intrinsic properties influence the performance of biochar across diverse environmental, industrial, and technological applications (Figure 2.7).

In agriculture and environmental management, biochar is widely used as a soil amendment due to its ability to enhance nutrient retention, water-holding capacity, aeration, and microbial activity (Li et al., 2025). Its strong adsorption capacity also supports applications in soil remediation, immobilization of heavy metals, and reduction of greenhouse gas emissions (Frene et al., 2025). Furthermore, the recalcitrant carbon structure of biochar contributes to long-term carbon sequestration, making it a valuable tool in climate mitigation and circular economy strategies (Lin et al., 2025).

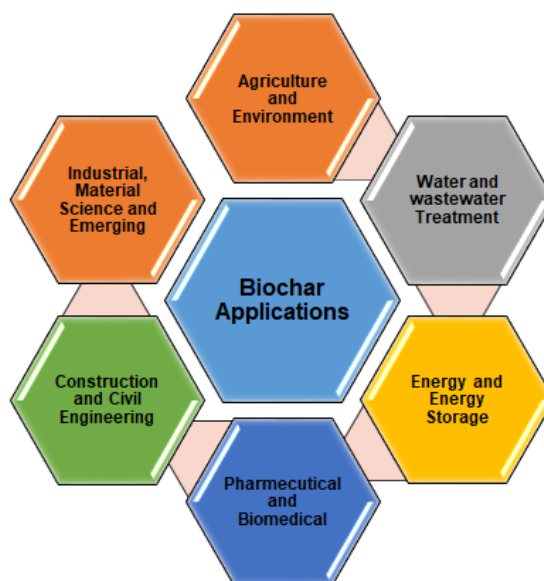


Figure 2.7: Major application areas of biochar

Biochar has gained traction in water and wastewater treatment, where its high surface area and modifiable surface chemistry enable efficient removal of heavy metals, dyes, organic pollutants, micro-plastics and emerging contaminants (Chu et al., 2025; Taskin et al., 2025, 2025). Modified biochars (such as activated, magnetized, or metal-doped forms) offer enhanced adsorption performance and easier recovery, extending their usefulness in decentralized water purification systems and effluent treatment (Tigalana et al., 2025).

In the energy sector, biochar is applied as a solid biofuel, co-fired with coal or biomass to improve combustion efficiency and reduce emissions (Peters et al., 2015). When upgraded or activated, it serves as a precursor for high-performance carbon materials used in supercapacitors, lithium-ion and sodium-ion battery anodes, fuel cells, and hydrogen storage systems (Mehdi et al., 2022). Its porous structure, conductivity, and surface tunability make biochar a promising component for next-generation energy storage technologies (Ganesapillai et al., 2023).

Biochar and its derivatives also find application in pharmaceutical and biomedical fields. Their biocompatibility and high adsorption capacity support uses in drug delivery systems, toxin adsorption, removal of pharmaceutical residues from wastewater, and

development of antimicrobial materials. Research continues to explore biochar's role in wound dressings, biosensors, and controlled-release platforms (Speksnijder et al., 2025).

In construction and civil engineering, biochar is incorporated into cement, bricks, mortar, and asphalt to improve mechanical strength, durability, and thermal insulation while reducing material density (Gimbun et al., 2025). Its ability to enhance moisture regulation and mitigate cracking makes it useful in sustainable building materials (Yao et al., 2025). Additionally, biochar-reinforced composites are increasingly explored in lightweight panels, insulation boards, and geotechnical engineering applications (Khitab et al., 2021).

In industrial, material science and emerging applications, Biochar is used as a reinforcing filler in polymers, rubbers, and composite materials, improving tensile strength, thermal stability, and biodegradability. Functionalized biochar supports heterogeneous catalysts in biodiesel production, biomass upgrading, and chemical synthesis (Bipin et al., 2022; Osman et al., 2023). In metallurgy, biochar serves as a reducing agent to partially replace coke in iron production, reducing carbon emissions. It is also explored in electronics for developing conductive inks and electromagnetic interference (EMI) shielding materials. Biochar is also being explored for applications in animal husbandry (as a feed additive and bedding material). These innovations reflect biochar's versatility and its growing role in supporting sustainability, resource efficiency, and low-carbon industrial systems (Zhang et al., 2024).

2.4 Process Simulation Modeling

2.4.1 Simulation methods

PS models are essential computational tools for analyzing, designing, and optimizing industrial systems by integrating thermodynamics, reaction kinetics, and fluid dynamics (Parathesi et al., 2025; Meraz et al., 2025). These models provide a virtual representation

of real-world chemical and physical processes, enabling researchers to predict system behavior and optimize operational parameters (Akbari et al., 2018; Bahadar et al., 2022).

Gasification and COG of biomass blends involve complex chemical reactions, heat and mass transfer phenomena, and multi-feedstock interactions, making process control challenging (Gao et al., 2018; Xiang et al., 2018). To address these challenges, various simulation techniques are employed, including thermodynamic equilibrium models, kinetic models, mathematical models, and CFD (Amani & Akhlaghian, 2022; Smith et al., 2020). Table 2.3 presents a comparison of these modeling techniques.

Table 2.3 Types of process simulation models

Type	Focus	Advantages	Limitation	Examples	Reference
Thermodynamic Models	Use equilibrium calculations to predict the composition of gasification products.	Fast and computationally efficient	Assumes the system reaches equilibrium, which may not reflect real-time behavior.	Minimization of Gibbs free energy in Aspen Plus	Gao et al. (2018) and Xiang et al. (2018)
Kinetic Models	Incorporate reaction kinetics to predict the rates of chemical reactions.	Captures dynamic behavior and intermediate species.	Requires detailed kinetic data, making them more complex to implement.	Time-dependent pyrolysis and combustion reactions using Arrhenius equations	Ding et al. (2021) and Gabbrielli et al. (2022)
CFD-Based Models	Focus on fluid flow, heat, and mass transfer within the gasifier.	Provides detailed spatial and temporal insights.	Computationally expensive.	ANSYS Fluent simulations for downdraft or fluidized bed gasifiers.	Deraman et al. (2019) and Elmaz et al. (2020)
Combined Models	Integrate thermodynamic, kinetic, and fluid dynamics principles	Offers a more comprehensive and realistic simulation	Computationally expensive	Aspen Plus with custom kinetic parameters coded in Fortran	Liang et al. (2021)

Among these methods, thermodynamic equilibrium models which are often implemented using Aspen Plus, are widely used due to their computational efficiency and ability to model complex systems (Gao et al., 2018; Shahabuddin & Bhattacharya, 2021; Naderi et

al., 2025). These models assume that all reactions reach equilibrium, eliminating the need for detailed kinetic parameters, making them highly suitable for multi-feedstock COG studies (Liang et al., 2021; Chen & Hsu, 2025; Shi et al., 2025). Their flexibility across various feedstocks and operational conditions allows for optimization of ER, blending ratios, and syngas composition (Elmaz et al., 2020; Niu et al., 2025; Hantoko et al., 2025; Alam et al., 2025).

While kinetic and CFD models offer detailed insights into reaction mechanisms and spatial variations, they require extensive experimental data and high computational resources (Ali et al., 2017). Thermodynamic models, on the other hand, provide reliable steady-state predictions of syngas composition, energy efficiency, and process performance, making them a preferred choice for biomass COG studies (Gao et al., 2018; Xiang et al., 2018; De et al., 2025; Gao et al., 2025).

2.4.2 Process simulation tools

Various PS tools support the analysis and optimization of gasification and COG, each with unique strengths and limitations. Aspen Plus is widely preferred for process flowsheet simulation, thermodynamic and kinetic modeling, and reactor scalability, making it ideal for equilibrium (Gibbs) and non-equilibrium modeling (Emad & Vahid, 2019; Shahabuddin & Bhattacharya, 2021). However, it relies on accurate input data and lacks inherent spatial or dynamic modeling.

CFD tools such as ANSYS Fluent provide detailed fluid flow, heat transfer, and reaction dynamics, making them suitable for reactor-level analysis but computationally demanding (Amani & Akhlaghian, 2022). CHEMKIN specializes in detailed gas-phase reaction kinetics but lacks process flowsheet integration. Chemical Equilibrium with Applications (CEA) is effective for equilibrium-based combustion analysis but is limited in broader system modeling (Das et al., 2018).

For customized modeling, MATLAB and Python offer high flexibility, enabling thermodynamic and kinetic modeling as well as ML integration, though they require advanced coding skills. HYSYS and UniSim Design are user-friendly for hydrocarbon and gas processing, but their biomass modeling capabilities are limited (Arnaiz et al., 2021; Deraman et al., 2019). General Algebraic Modeling System (GAMS) is suited for optimization applications, while COMSOL Multiphysics captures coupled heat transfer and fluid flow phenomena, albeit with high computational costs.

Among these, Aspen Plus remains the most comprehensive tool for biomass COG simulation, while MATLAB, Python, and CFD tools offer deeper customization for kinetic analysis and reactor-level modeling.

2.4.3 Thermodynamic models in Aspen Plus

Thermodynamic equilibrium modeling in Aspen Plus is a widely used approach for optimizing biomass-biomass COG, leveraging Gibbs free energy minimization or stoichiometric models to evaluate syngas composition, hydrogen yield, CGE, and HHV (Ferreira et al., 2019; Mutlu & Zeng, 2020; Niu et al., 2025). Its computational efficiency and adaptability make it a preferred tool for academic and industrial applications (Parthesi et al., 2025; Meraz et al., 2025). Aspen Plus has been instrumental in modeling feedstock blending effects and operational parameter optimization (Table 2.4). Studies on rice husk and woody biomass blends in a circulating fluidized bed (CFB) gasifier reported improved gas yield ($1.75 \text{ Nm}^3/\text{kg}$) and HHV (5.39 MJ/Nm^3) due to complementary feedstock properties (Cao et al., 2022). Similarly, COG of wheat straw and sugarcane bagasse in a downdraft gasifier increased energetic efficiency from 50.7% to 64.8%, demonstrating the benefits of blending (Pati et al., 2021).

Operational parameters such as temperature, ER, and blending ratio significantly impact performance. For example, optimized conditions for rice straw and sugarcane bagasse

pellets resulted in maximum exergy efficiency of 40.25% with minimized tar yields (Pati et al., 2021). The synergistic effects of feedstock blending, such as improved gas yield, CGE, and hydrogen production, further highlight the importance of Aspen Plus modeling in optimizing COG processes (Tuntiwongwat et al., 2025; Escalante et al., 2025). Aspen Plus excels in simulating diverse reactor configurations (e.g., downdraft, fluidized bed) and predicting equilibrium gas compositions and system efficiencies across varying conditions. Its role in advancing biomass COG research continues to drive innovation in renewable energy and waste-to-energy technologies (Cao et al., 2022; Pati & De, 2021).

Table 2.4: A summary studies on thermodynamic equilibrium modeling of biomass COG

Feedstock blend	Gasifiers/ agent	Input Parameters	Computational tool/method	Key findings	References
Forest residue and wood charcoal	50 kW downdraft fixed bed	Mixture ratio FR:WC; 100:0, 90:10, 80:20, 70:30 and 60:40.	Aspen plus; Stoichiometric reactor	LHV: 3.98 to 4.71 MJ/kg HHV: 4.22 to 5.02 MJ/kg H ₂ yield: 19.76 % to 26.13% Exergy efficiency: 46.6 to 69.04%	Monir et al. (2020)
Wheat straw and sugarcane bagasse, rice straw and sugarcane bagasse, wheat straw and sugarcane bagasse	Downdraft	Blend ratio, feedstock type, temperature	Aspen plus; Gibbs free energy minimization	Energetic efficiency: 50.7% to 64.8%	Pati & De (2021)
Rice husk and sawdust/ bamboo dust	CFB	ER; temperature; Feedstock blend ratio	Aspen plus	Gas yield: 1.75 Nm ³ /kg HHV: 5.39 MJ/Nm ³	Cao et al. (2022)
Rice straw and sugarcane bagasse pellets	Downdraft	Biomass ratio; ER; temperature	Gibbs free energy minimization	Tar yield: 5.67% Highest exergy efficiency of 40.25% and lowest 21.83%	Pati et al. (2021)

2.5 Machine Learning Models and Applications

ML has become an indispensable tool in predictive modeling, particularly for complex processes like biomass and waste gasification, where nonlinear relationships and diverse datasets pose significant challenges. By learning patterns and dependencies in data, ML

algorithms provide accurate predictions and support process optimization. Among these, ensemble ML methods have gained prominence due to their ability to combine multiple models, utilizing their strengths while minimizing individual weaknesses. This section focuses on ensemble ML, a powerful approach that enhances predictive performance and robustness in gasification studies.

For a detailed discussion of various ML algorithms, including their theoretical underpinnings and applications, readers can refer to the following published studies on ML techniques and applications (Alfarra et al., 2024; Ascher et al., 2022; Bin et al., 2024; Khan et al., 2023; Kushwah et al., 2022; Liao & Yao, 2021; Sakheta et al., 2023; Sedej et al., 2022; Umenweke et al., 2022; Zhang et al., 2023; Zhang et al., 2021). Furthermore, we acknowledge that part or all of this section has already been published in our study (Bongomin et al., 2024), emphasizing its relevance and contribution to advancing ML applications in biomass waste gasification.

2.5.1 Ensemble ML models

Ensemble ML models combine predictions from multiple base learners to enhance accuracy, robustness, and generalization (Sun et al., 2021; Azadvar & Tavakoli, 2024). By leveraging model diversity, ensembles mitigate individual model weaknesses and improve predictive stability, making them widely used in classification, regression, and anomaly detection (Mahajan et al., 2023). However, ensemble methods pose interpretability challenges, as aggregating multiple models makes it difficult to trace individual decision-making processes, which can be a limitation in regulatory or trust-sensitive applications (Ali et al., 2023; Hassija et al., 2023).

Ensemble techniques enhance predictive performance by ensuring diversity among base models, with each contributing unique insight (Feng et al., 2023; Zizaan & Idri, 2024). While ensembles generally improve accuracy, they do not always outperform the best-

performing base learner (Sharafati et al., 2020). In regression problems, ensemble accuracy is often an average of base model performances, and combining outputs can enhance prediction quality, particularly for small datasets (Minaei-Bidgoli et al., 2014; Sagi & Rokach, 2018).

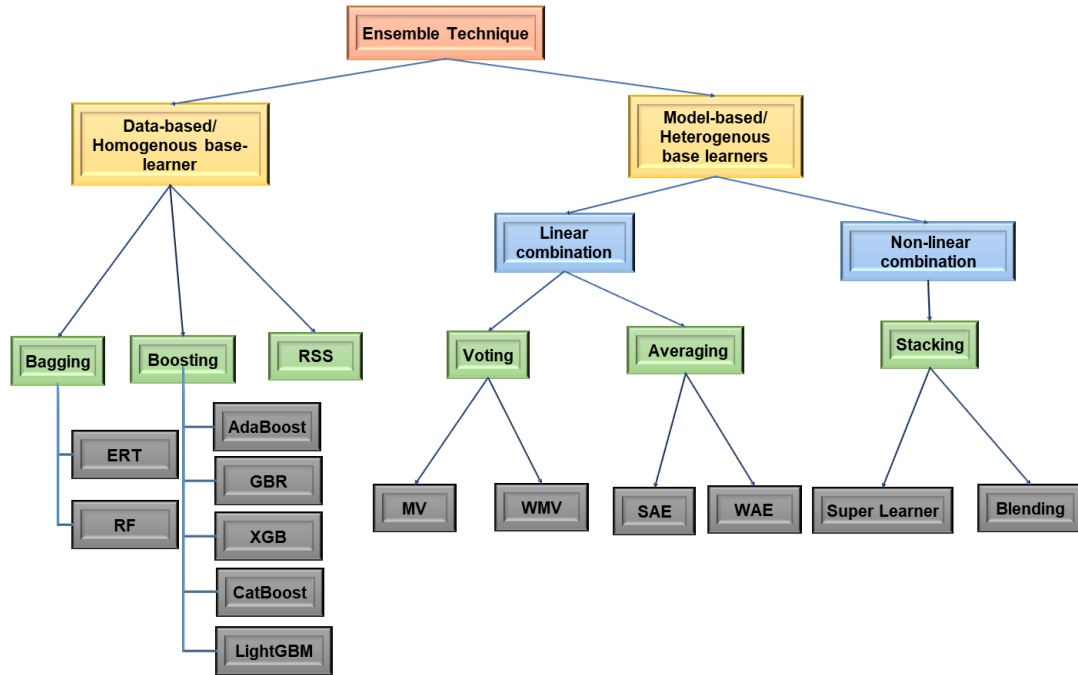


Figure 2.8: Classification of ensemble machine learning methods

Legend: MV-majority voting, SAE-simple averaging ensemble, WAE-weighted average ensemble, RSS-random subspace, WMV-weighted majority voting, RF- Random Forest, ERT- extremely randomized trees, GBR- gradient boosting regression.

Ensemble methods are classified into bagging, boosting, voting, averaging, and stacking, as illustrated in Figure 2.8 (Lee et al., 2022; Mienye & Sun, 2022; Sharafati et al., 2020). Other advanced techniques include cascade generalization, stochastic gradient boosting, and meta-decision trees (Erdal, 2013; Giraud-Carrier, 2022). Tree-based approaches such as bagging and boosting are well-developed, but other methods like stacking and voting continue to gain traction (Yang, 2017). A summary of the advantages and limitations of each ensemble technique is presented in Table 2.5.

2.5.1.1 Bagging ensemble

Bagging (Bootstrap aggregating) is an ensemble learning technique that reduces variance errors by training multiple base learners on bootstrap-resampled subsets of data and

aggregating their predictions via averaging (for regression) or voting (for classification) (Lee et al., 2022). This method enhances stability and generalization, particularly when base models exhibit different local minima (De Clercq et al., 2020).

Table 2.5: Advantages and limitations of ensemble methods

Ensemble method	Advantages	Limitations
Bagging ensemble	Reduces variance error. Works well when base learners have different local minima. Suitable for both regression and classification tasks.	May not significantly improve base model accuracy. Limited interpretability.
Boosting ensemble	Combines weak learners into a highly accurate model. Strong interpretability. Works well for both regression and classification.	Sensitive to noisy data. Computationally intensive. Require careful tuning of hyperparameters.
Random subspace	Decreases the likelihood of overfitting to specific features or noise in the data. Captures various aspects of the data, leading to better performance on unseen data. Each base learner focuses on different feature subsets, enhancing overall model diversity. Enables efficient exploration of the feature space, especially beneficial in high-dimensional datasets.	Interpreting the overall model becomes more complex due to diverse base learners Managing multiple models and their predictions adds complexity to the modeling process. Noisy or irrelevant features in random subsets may degrade individual base learner performance. Training multiple models on different feature subsets can increase computational requirements.
Voting ensemble	Simple and easy to implement. Typically used for classification tasks. Reduce bias towards individual base learners.	Loss of information may occur in majority voting. Weighted majority voting may be challenging to implement.
Averaging ensemble	Provides an unweighted average of base learner outputs. Suitable for both regression and classification tasks. Weighted averaging can improve predictions.	Vulnerable to weaker base learners. Sensitive to over-confident base learners.
Stacking ensemble	Combines base learners in a hierarchical, non-linear way. Maximizes prediction accuracy by leveraging strengths of diverse models. Optimizes weights through cross-validation.	Requires a large number of base learners for optimal results. More complex to implement than other ensemble models. Overfitting can be a concern with smaller datasets.

Decision trees (DTs) are commonly used as base models due to their ability to capture complex data interactions. Random Forest (RF) and Extremely Randomized Trees (ExtraTrees) are popular bagging-based methods, valued for their simplicity, robustness,

and effectiveness (Chen et al., 2020; Dodo et al., 2022). In RF, each tree is trained on randomly sampled feature subsets, with predictions made using independent decision trees (Breiman, 2001). This meta-algorithm combines the flexibility of DTs with improved accuracy in both classification and regression tasks (Sharafati et al., 2020; Xing et al., 2019).

Performance optimization in bagging ensembles depends on hyperparameters such as the number of predictors, splitting rules, and minimal node size. Techniques like k-fold cross-validation, grid search, or trial-and-error testing help fine-tune these parameters for optimal results (Tang et al., 2020; Xing et al., 2019).

2.5.1.2 Boosting ensemble

Unlike bagging, boosting employs a sequential learning approach, where weak models are iteratively trained and refined to form a highly accurate ensemble (Ribeiro & Santos, 2020; Zhou, 2012). Boosting algorithms adjust model weights at each step, focusing on misclassified instances to improve overall performance. Common boosting techniques include Gradient Boosting for Regression (GBR), Adaptive Boosting (AdaBoost), Gradient Boosting Machine (GBM), Extreme Gradient Boosting (XGB), Light Gradient Boosting Machine (LightGBM), and Categorical Gradient Boosting (CatGBM) (Aslam et al., 2022; Cakiroglu et al., 2022; Mienye & Sun, 2022; Zheng et al., 2023). Gradient boosting models are particularly effective in gasification process modeling, outperforming other ensemble techniques (Leng et al., 2022). Table 2.6 summarizes the strengths and weaknesses of different boosting algorithms.

GBM and GBR are widely used for classification and regression, respectively (Sharafati et al., 2020). GBR builds trees based on the errors (pseudo-residuals) of previous trees, iterating until additional trees no longer improve predictions (Kardani et al., 2021). Key

advantages of GBR include strong interpretability, robust generalization, fast convergence, and adaptability to multi-feature datasets (Leng et al., 2022).

Table 2.6: Advantages and disadvantages of boosting ensemble algorithms

Boosting ensemble	Advantages	Disadvantages
Gradient boosting regression (GBR)	Builds strong predictive models by iteratively improving weak models. Handles heterogeneous data types well. Provides flexibility in defining loss functions. Less prone to overfitting compared to Adaboost.	Susceptible to overfitting if not properly tuned. More complex to implement compared to simpler algorithms. Requires careful tuning of hyperparameters.
Adaptive boosting (Adaboost)	Can combine weak learners into a strong learner. Less susceptible to overfitting. Works well with a variety of base classifiers. Handles high-dimensional data effectively.	Sensitive to noisy data and outliers. Training can be time-consuming. May not perform well with complex datasets.
Extreme gradient boosting (XGB)	Fast and scalable implementation. Handles missing data well. Provides regularization to prevent overfitting. Often achieves state-of-the-art performance.	Requires careful tuning of hyperparameters. Can be memory-intensive for large datasets. Prone to overfitting if not properly tuned.
Light Gradient Boosting (LightGBM)	Extremely fast training speed, making it suitable for large datasets. Efficient handling of high-dimensional data. Reduced memory usage compared to other gradient boosting implementations. Supports categorical features without requiring one-hot encoding.	Prone to overfitting if not properly tuned. Requires careful tuning of hyperparameters. Less interpretability compared to simpler models.
Categorical gradient boosting (CatBoost)	Automatically handles categorical features without preprocessing. Robust to overfitting, thanks to built-in regularization techniques. Handles missing data internally. Provides strong performance with minimal hyperparameter tuning	Slower training compared to some other gradient boosting implementations. May require more memory for large datasets. Limited interpretability due to its complex nature.

2.5.1.3 Random subspace ensemble

The random subspace method is an ensemble learning technique where multiple models are trained on randomly selected feature subsets, reducing overfitting and improving prediction robustness (Boot & Nibbering, 2019; Shin, 2020). Predictions are then aggregated, typically through averaging, to enhance overall accuracy. By focusing on

different feature combinations, this method minimizes the influence of irrelevant or noisy features, making it particularly useful for high-dimensional datasets.

While random subspace ensembles have not been directly applied in gasification modeling, they hold significant potential. Gasification involves numerous variables, including feedstock properties, operating conditions, and syngas composition, making feature selection critical for model performance. This technique could enhance prediction accuracy, handle complex input variables, and mitigate overfitting in gasification models (Yaman et al., 2018). Future research should explore its applicability to gasification process optimization and modeling.

2.5.1.4 Voting ensemble

Voting is a straightforward ensemble method that aggregates predictions from multiple classifiers to enhance model performance (Ballabio et al., 2019). It operates through two primary approaches: majority voting (MV) and weighted majority voting (WMV). Majority voting (MV) is widely used in classification tasks, where each base model predicts a class label, and the final prediction is determined by the most frequent vote among the models (Ganaie et al., 2022; Ju et al., 2018). Weighted majority voting (WMV), in contrast, assigns different weights to classifiers based on their validation set performance, selecting the class with the highest weighted probability (Dogan & Birant, 2019; Satapathy et al., 2017).

Unlike MV, where all models have equal influence, WMV prioritizes higher-performing models (Kardani et al., 2021). Despite its advantages, WMV faces challenges in determining optimal voting weights for different classifiers, which can limit its effectiveness (Zhang et al., 2014). Nonetheless, voting ensembles remain a reliable method for improving prediction stability and generalization in ML applications (Ganaie et al., 2022; Osamor & Okezie, 2021).

2.5.1.5 Averaging Ensemble

Averaging, also known as voting regression, is an ensemble method that combines predictions from multiple base learners through a linear combination (Erdebilli & Devrim-İçtenbaş, 2022; Nourani et al., 2018). This technique is commonly used in neural networks and regression models and operates through two main approaches: simple averaging (SAE) and weighted averaging (WAE). SAE, or unweighted averaging, calculates the mean of all base learners' predictions, treating each model equally (Ganaie et al., 2022; Ju et al., 2018; Nourani et al., 2018). While SAE is widely applied in both regression and classification, it can be sensitive to weaker base learners and over-confident predictions, reducing its reliability (Nti et al., 2020).

WAE improves upon SAE by assigning different weights to each model based on its relative contribution to prediction accuracy (Nti et al., 2020). WAE typically provides better calibration and validation performance than SAE, enhancing model robustness (Abba et al., 2020). Currently, SAE and WAE have not been explored in gasification modeling, though their ability to improve prediction accuracy and reduce variability suggests potential applications in this field. Further research could assess their effectiveness in predictive modeling for gasification processes.

2.5.1.6 Stacking

Stacking, or stacked generalization, is a hierarchical ensemble learning method that combines base learners using a meta-learning model to enhance prediction accuracy (Massaoudi et al., 2021; Nourani et al., 2018). Unlike other ensemble techniques, stacking leverages heterogeneous base models, such as ANN, naive Bayesian, and logistic regression, to create a more powerful ensemble (Shafieian & Zulkernine, 2022). Stacking can be structured into multiple layers, with the meta-learner often being a generalized linear model (Lee et al., 2022).

Stacking is implemented using two primary approaches: super learner and blending. The super learner approach applies cross-validation (CV) to train the meta-model on out-of-fold predictions, optimizing model selection (Valdes et al., 2021; Van Der Laan et al., 2007; Wu et al., 2021; Yao et al., 2022). While effective for large datasets, it can be computationally expensive. A single split cross-validation can be used instead to reduce the costs (Ju et al., 2019). Blending, on the other hand, uses a holdout validation set rather than full cross-validation, making it simpler and faster but potentially prone to overfitting on small datasets (Ganaie et al., 2022; Wu et al., 2021; Yao et al., 2022).

Although stacking holds promise for gasification modeling, research in this area remains limited. Ascher et al. (2022) developed an ensemble using a SLE approach with six base learners (ANN, RF, GBR, XGB, AdaBoost, and SVR), but the specific meta-model details were not provided. This highlights the need for further research to assess the effectiveness of stacking in gasification modeling and whether a true super learner or a simpler averaging method was employed.

2.5.2 ML applications in gasification

Gasification performance is influenced by multiple factors, including feedstock properties, operational conditions, and process efficiency (Dhrioua et al., 2022; Hamad et al., 2016; Jenkins, 2020). Key performance indicators (KPIs) such as heating values, gas yield, carbon conversion efficiency (CCE), gasification efficiency (GE), cold gas efficiency (CGE), and tar yield assess the economic viability and quality of gasification systems (Henao et al., 2022; Shahbaz et al., 2020; Wang et al., 2025; Alrbai et al., 2025). KPIs can be categorized into gas composition, product yields and quality, heating values, and process efficiency.

ML has been widely applied in regression and classification tasks in gasification modeling, with a stronger focus on single-feedstock gasification than COG (Mutlu &

Yücel, 2018; Kiriş & Yaşar, 2025; Salisu et al., 2025). Expanding ML models to include heterogeneous datasets with multiple feedstock blends is essential for improving predictive accuracy and applicability (Khandelwal et al., 2025; Haq et al., 2025; Abdelrahim & Yücel, 2025). Multiple Input Multiple Output (MIMO) modeling in gasification often leads to varying prediction accuracies across target variables, making overall model performance an insufficient metric. Evaluating individual target variables provides deeper insights into model strengths and weaknesses (Xing et al., 2019; Zhao et al., 2021; Kafle et al., 2025; Cihan et al., 2025).

ANNs remain the most widely used ML technique for gasification modeling (Li & Song, 2022; Mikulandrić et al., 2014; Pandey et al., 2016), as illustrated in Figure 2.9a. Other explored ML techniques include SVR, Decision Tree Regression (DTR), Linear Regression (LR), Polynomial Regression (PR), Gaussian Process Regression (GPR), K-Nearest Neighbor (KNN), and ensemble methods such as Random Forest, GBR, XGBoost (XGB), AdaBoost, Optimized Ensemble Models (OEM), and Super Learner Ensemble (SLE) (Umenweke et al., 2022; Yang et al., 2025; Q. Chen et al., 2025; Uregen Guler et al., 2025).

Heating value (LHV and HHV) has been the most common target variable in gasification modeling (Figure 2.9b), along with other metrics such as gas composition (CO, CO₂, H₂, CH₄), product yields (total gas yield, H₂ yield, char yield, tar yield), and process efficiency (CCE, CGE).

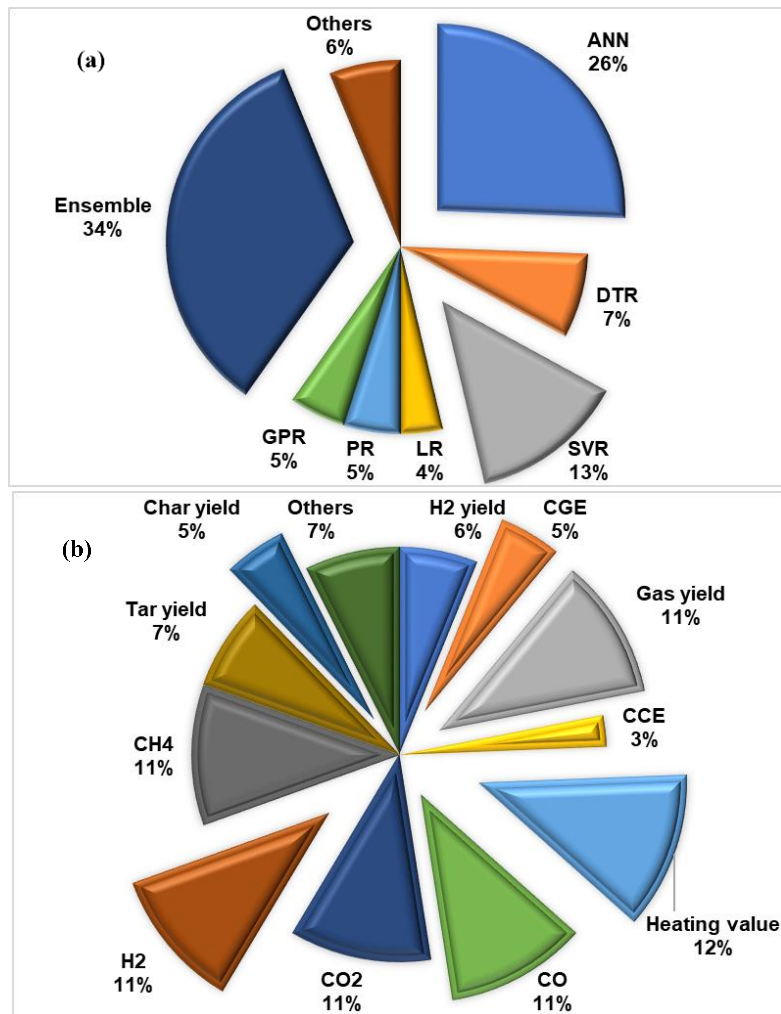


Figure 2.9: Comparative analysis of ML applications in literature.
 Legend: (a) ML methodologies and (b) gasification performance metrics.

2.5.2.1 Syngas composition prediction

Syngas composition is a key indicator of gasification performance, primarily consisting of CO, CO₂, H₂, CH₄, and H₂O, with additional components like tar (C₁₀H₈), H₂S, N₂, and unconverted carbon (char) (Dhrioua et al., 2022; Khonde et al., 2021; Molino & Braccio, 2015; Shahbaz et al., 2017, 2020; Valin et al., 2020). ML models predict syngas composition using two approaches: Multiple Input Single Output (MISO), where each gas species is predicted separately, and Multiple Input Multiple Output (MIMO), where all gas species are predicted collectively (Ascher et al., 2022).

Studies have demonstrated high predictive accuracy for syngas composition using models such as ANNs, SVR, DTR, and GBR (Ascher et al., 2022; Elmaz et al., 2020; Gil et al.,

2023; Wen et al., 2021). ANNs, in particular, have consistently shown strong performance, achieving coefficient of determination (R^2) values above 0.7 and up to 0.92 for key gas components (Ascher et al., 2022; Elmaz et al., 2020).

While some studies focus on comparing multiple ML models to determine the best-performing approach (Ascher et al., 2022; Elmaz et al., 2020), others prioritize optimizing a single model, particularly ANNs, for enhanced accuracy (Wen et al., 2021). Regardless of the method, ML enables deeper insights into the relationships between process parameters and syngas composition, facilitating gasification system optimization for improved efficiency and performance.

2.5.2.2 Product yields and quality prediction

Optimizing gasification, particularly COG, requires a thorough understanding of product yields, including gas yield, hydrogen yield, tar, and char formation (Hu et al., 2017). Gas yield, a critical parameter, excludes inert gases and focuses on the usable gas produced per unit of dry feedstock, directly influencing hydrogen-rich syngas production (Anniwaer et al., 2021; Hamad et al., 2016). The addition of steam and steam-related reaction kinetics significantly impact hydrogen yield (m^3/kg) (Zhang & Pang, 2017).

ML has proven highly effective in predicting gas yield. Mutlu et al. (2019) applied various ML models (SVR, DTR, PR, ANN, LR, and PLR) and achieved R^2 values above 0.85, with ANN (0.92), LR (0.91), and PR (0.89) performing exceptionally well. Kardani et al. (2021) further improved gas yield predictions using XGB (0.996), OEM (0.99), RF (0.979), and ANN (0.93) in a fluidized bed reactor.

While gas yield prediction has been extensively studied, research on hydrogen yield (H_2) is less common. Ozbas et al. (2019) applied SVR, DTR, KNN, and LR to a fixed bed reactor, achieving R^2 values above 0.9. Zhao et al. (2021) explored SCWG systems using

SVR, ANN, GPR, and RF, all exceeding R^2 of 0.9. However, limited input features in these studies may restrict their broader applicability. Devasahayam & Albijanic (2024) utilized DTR, AdaBoost, GBR, and RF for biomass-plastic COG, with GBR achieving the highest R^2 (0.99).

Char is a beneficial byproduct often optimized alongside syngas, whereas tar, a mixture of aromatic hydrocarbons, is undesirable and must be minimized to maintain gas quality (Asadullah, 2014). Tar formation is complex, influenced by feedstock properties and operating conditions (Chan & Tanksale, 2014; Serrano & Castelló, 2020). Tar yield is calculated as the total tar concentration in syngas multiplied by the gas yield per unit dry ash-free feedstock (Serrano & Castelló, 2020).

ML-based tar yield prediction has received limited attention, with only a few studies available. Ascher et al. (2022) developed an ANN model achieving $R^2 > 0.9$ for universal gasification systems, aligning with Serrano & Castelló (2020) whose lab-scale ANN model reached $R^2 = 0.977$. However, in a broader study, Ascher et al. (2022) tested seven ML models (SVR, ANN, RF, GBR, XGB, AdaBoost, and SLE), where XGB (0.85) and GBR (0.76) outperformed ANN (0.62) and RF (0.59). SVR performed the worst ($R^2 = 0.09$), highlighting dataset and model configuration influences on prediction accuracy.

ML models enable accurate predictions of syngas yield, hydrogen yield, and tar formation, contributing to gasification process optimization. Continued research and refinement of these models will enhance process control and efficiency for improved gasification performance.

2.5.2.3 Heating values prediction

Heating value, also known as calorific value, quantifies the energy released during fuel combustion (MJ/Nm^3 or MJ/kg) (Kardani et al., 2021; Pandey et al., 2016). It is classified

into Higher Heating Value (HHV) and Lower Heating Value (LHV). HHV accounts for energy released when water vapor condenses, while LHV assumes water vapor remains gaseous, making LHV the preferred metric for gasification assessments (Jenkins, 2020).

ML models have been widely applied for HHV and LHV prediction. Elmaz et al. (2020) used SVR, DTR, PR, and ANN to predict HHV in downdraft gasification, with ANN achieving the highest R^2 (0.931), followed by DTR (0.921), SVR (0.886), and PR (0.858). Mutlu et al. (2019) applied SVR, DTR, PR, ANN, LR, and GPR, where GPR performed best ($R^2 = 0.78$), though their smaller dataset (56 samples) may have limited accuracy compared to Elmaz et al. (2020), who used 4826 samples.

For LHV prediction, Kardani et al. (2021) tested SVR, DTR, ANN, XGB, RF, and OEM in fluidized bed gasification, with OEM performing best ($R^2 = 0.973$). Similarly, Ascher et al. (2022) evaluated seven ML models, where ANN ($R^2 = 0.88$) underperformed compared to other models like SVR, XGB, and RF, possibly due to differences in dataset size and feature selection. Hasanzadeh & Azdast (2023) demonstrated that PR achieved an $R^2 > 0.99$, showcasing its potential for highly accurate heating value prediction.

In general, ANNs, SVR, and PR models have demonstrated strong predictive capabilities for HHV and LHV, with performance heavily influenced by dataset size, feature selection, and hyperparameter tuning. Larger, diverse datasets and optimized model configurations enhance accuracy and generalization for gasification heating value predictions.

2.5.2.4 Process efficiency prediction

Carbon Conversion Efficiency (CCE), Cold Gas Efficiency (CGE), and Gasification Efficiency (GE) are key metrics for assessing gasification performance, measuring how effectively feedstock is converted into usable gaseous products (Shahbaz et al., 2020). CCE represents the fraction of carbon in the feedstock converted into CO, CO₂, and CH₄

(Khan et al., 2014), while CGE compares the heating value of the produced gas to the heating value of the feedstock, reflecting energy conversion efficiency (Alamia et al., 2017; Jenkins, 2020). GE quantifies the total gas yield per unit of feedstock, though it is less commonly reported (Khan et al., 2014; Shahbaz et al., 2017).

While ML applications in gas yield and heating value prediction are well established, CCE and CGE prediction remains underexplored. Ascher et al. (2022) suggested estimating CCE and CGE based on other predicted parameters, but direct ML predictions offer potential benefits. Mutlu et al. (2019) tested SVR, ANN, LR, GPR, DTR, and PR for CCE and CGE prediction, with GPR performing best for CGE ($R^2 = 0.71$) and SVR leading for CCE ($R^2 = 0.79$). However, dataset size and feature selection significantly impacted results.

Ozonoh et al. (2020) applied ANN models, achieving higher R^2 values (0.9 for CGE, 0.84 for CCE), highlighting ANNs' predictive potential. Hasanzadeh & Azdast (2023) demonstrated that PR achieved $R^2 > 0.99$ for CGE prediction, suggesting its effectiveness for efficiency modeling. Despite promising results, ML-based CCE and CGE prediction remains limited, necessitating further research to refine models and validate findings across different gasification scenarios. The availability of high-quality datasets and improving model interpretability is crucial for enhancing predictive accuracy and optimizing gasification efficiency.

2.5.3 Effect of Feedstock and Inputs on ML Gasification

Feedstock properties and input variables significantly affect the performance of machine learning models in gasification. This subsection reviews studies using various models, feedstock types, and reactor designs. It highlights how inputs such as elemental composition, proximate analysis, and process conditions influence prediction accuracy.

The findings emphasize the importance of selecting relevant features to enhance model reliability and generalizability.

Table 2.7: A summary of literature on the predictive modeling of gasification

S/N	Reactor type	Predictive methods	Data size / feedstock	Variables	Key finding/ validation	Reference
1.	Downdraft	ANN	1032 (from 86 biomass feedstocks)	Input: MC, VM, FC, ash, C, O, H, N, S, Output: T and AFR.	MSE =1.497, $R^2 = 0.9976$.	Ayub et al. (2022)
2.	CFB	Deep learning model	1 million samples (from 56 biomasses)	Input: C, H, O, T, FR, SR, Output: LHV	$R^2 > 0.99$.	Kartal & Özveren (2020)
3.	Downdraft	ANN	1800 (50 feedstocks)	Input: M, VM, FC, Ash, C, O, H, N, S, T, AFR, SBR Output: SMFR of Hydrogen	$R^2 > 0.999$ RMSE < 0.25.	Safarian et al. (2021)
4.	CLG	SVM, RF, GBR	236, several feedstocks	Input: C, H, O, N, S, FC, VM, Ash, T, OC, SBR Output: H ₂ yield, Char yield	GBR has the highest R^2 score of 0.9453 for both H ₂ and char yield.	Sison et al. (2023)
5.	Water-gas shift reactor	RF, ANN, GBR, CART, SVR, KNN	9000, Plastic (polystyrene and PE)	Input: T, pressure Output: CGE, mass flow rate, GC (CH ₄ , H ₂ , CO, CO ₂)	RF model excels with $R^2 > 0.99$.	Lahafdoozian et al. (2024)

SVR- support vector regression, VM-volatile matter, FC-Fixed carbon, ER- Equivalence ratio, FR- fuel flow/feed rate, T- temperature, AFR- air/fuel ratio, SFR-steam/fuel (biomass) ratio, SBR- steam biomass ratio, MC- moisture content, BFR-biomass feed rate, GC- gas composition, RMSE- root mean square error, MSE- mean square error.

Table 2.7 presents a summary of key studies applying machine learning to predict gasification outcomes across various reactor types and feedstocks. The models consistently achieved high predictive accuracy, with R^2 values often exceeding 0.99, particularly for ANN and ensemble methods like RF and GBR. In downdraft reactors, ANN models trained on large and diverse biomass datasets demonstrated excellent performance in predicting temperature and air–fuel ratio (Ayub et al., 2022) as well as hydrogen production rates (Safarian et al., 2021). In circulating fluidized bed (CFB) systems, deep learning (ANN) models also achieved R^2 values above 0.99 for predicting the LHV (Kartal & Özveren, 2020), showcasing their scalability with large datasets.

Sison et al. (2023) applied support vector machines, RF, and GBR for chemical looping gasification (CLG) using multiple feedstocks. GBR achieved the highest R^2 (0.9453) for both hydrogen and char yield predictions, highlighting the advantages of ensemble methods for complex feedstock interactions. Similarly, in a water-gas shift reactor, Lahafdoozian et al. (2024) found that RF outperformed other models in predicting cold gas efficiency and gas concentrations, with R^2 values above 0.99.

In general, these studies confirm that model accuracy is strongly influenced by the quality and diversity of input variables, the type of reactor system, and the chosen algorithm. Models incorporating proximate and ultimate analysis, temperature, and process-specific parameters consistently showed better generalization and reliability.

2.6 Model Evaluation and Robustness Analysis

The evaluation of ML models is a critical step in determining their reliability and applicability. Model performance evaluation focuses on the use of statistical metrics to assess predictive accuracy, while robustness analysis aims at finding insights on the resilience of models under varying conditions such as unseen data, noise, and perturbations. Together, these analyses ensure the models are both accurate and adaptable for practical applications.

2.6.1 Model performance evaluation

Model performance evaluation is essential for assessing a ML model's generalization ability, primarily relying on data splitting techniques and resampling methods. Data splitting techniques divide the dataset into training and testing subsets using approaches such as random sampling (simple or stratified), dissimilarity sampling (maximizing differences between subsets), and rational splitting (domain-specific criteria). Resampling methods, such as cross-validation (K-fold, leave-one-out, repeated, Monte

Carlo, leave-group-out) and bootstrap techniques (standard or modified), improve the reliability of performance metrics (Ascher et al., 2022; Elmaz et al., 2020).

The choice of method depends on dataset size, computational resources, and evaluation objectives. Repeated 10-fold cross-validation is recommended for small datasets, while bootstrap methods are useful for low-variance comparisons between models. For large datasets, computational efficiency becomes a priority, making differences between methods less significant. Resampling techniques ensure reliable performance estimates on unseen data (Ascher et al., 2022; Elmaz et al., 2020).

A range of performance metrics is available for assessing ML model accuracy. The most widely used include Mean Absolute Error (MAE), Coefficient of Determination (R^2), Mean Squared Error (MSE), and Root Mean Squared Error (RMSE), as they effectively measure predictive performance (Baashar et al., 2022). However, with many available metrics, presenting multiple measures is recommended for comprehensive interpretation (Hodson, 2022).

Additional metrics such as Mean Absolute Percentage Error (MAPE), Normalized Mean Bias Error (NMBE), Coefficient of Variation of RMSE (CV(RMSE)), and Mean Bias Error (MBE) provide further insights into model accuracy and bias (Chicco et al., 2021; Du et al., 2022).

2.6.2 Model robustness analysis

Robustness in ML refers to a model's ability to maintain high predictive accuracy across varying datasets, noise levels, and operational conditions (Cardoso et al., 2019; Villegas-Ch et al., 2024). In COG studies, a robust model should accurately predict key outputs such as syngas composition, CGE, hydrogen yield, and process efficiencies, even when feedstock properties or process conditions deviate from the training data. Given the

inherent variability in biomass proximate properties such as moisture content, robust ML models are crucial for ensuring reliable, interpretable, and scalable predictions.

Several methods assess the robustness of ML models in gasification and COG processes (Freiesleben & Grote, 2023). Stress testing evaluates model performance under extreme or unusual conditions (Sekmen & Bilgin, 2024). For COG, this could include testing the model on unseen feedstocks, introducing outliers, or varying key parameters such as equivalence ratio and temperature to assess the model's adaptability to diverse scenarios. Cross-validation, particularly K-fold and stratified approaches, ensures comprehensive evaluation by dividing the dataset into multiple training and validation subsets (Li et al., 2023). This method minimizes overfitting and improves generalizability, validating model performance across diverse feedstocks and operational settings. Unseen data testing further evaluates the applicability of ML models by training on specific biomass blends (e.g., coffee husk and macadamia nutshell) and testing on different feedstock combinations (e.g., sugarcane bagasse and coconut shell) to assess generalization ability.

Another critical approach is perturbation analysis, which introduces noise or variations in input features, such as measurement errors in feedstock composition, to evaluate the model's stability (Lambert et al., 2023). This technique ensures that models can handle uncertainties in real-world gasification scenarios without significant accuracy degradation. Ensemble techniques, including RF and GBR, enhance robustness by aggregating predictions from multiple learners (Lin et al., 2022). These methods reduce the impact of outliers, minimize prediction variance, and improve stability, making them highly suitable for handling noisy and diverse gasification datasets.

Lastly, uncertainty quantification methods, such as GPR and Monte Carlo Dropout, provide confidence intervals for predictions, helping identify outputs with higher uncertainty (Ganthavee et al., 2024). This approach is particularly useful for safety-

critical applications and when working with incomplete datasets, ensuring reliable decision-making in gasification modeling.

2.7 Model Interpretability Analysis

Understanding the decision-making process of ML models is crucial for building trust, ensuring transparency, and improving usability in practical applications. This section provides insights into the significance of interpretability, the methodologies and tools used to explain model behavior, with a specific emphasis on their application in biomass gasification studies.

2.7.1 Overview of interpretability analysis

Interpretability techniques are essential for understanding and optimizing gasification processes, particularly in the thermochemical conversion of biomass into syngas. These techniques provide insights into complex system mechanisms, enabling improvements in efficiency, environmental impact mitigation, and system reliability (Sapariya et al., 2021).

In ML and AI, interpretability refers to the ability to explain a model's decisions in a clear and human-understandable manner (Erasmus et al., 2021). While models like linear regression (LR) offer straightforward interpretability, deep neural networks and ensemble models pose challenges due to their complexity. Striking a balance between model accuracy and transparency remains a key research focus.

Interpretability analysis, also known as feature importance assessment, aims to extract relationships between input features and predictions, enhancing trust and usability in ML models (Doshi-Velez & Kim, 2017; Lipton, 2018). Highly interpretable models allow humans to easily predict and understand outputs, whereas complex models require additional tools to uncover decision-making patterns (Ascher et al., 2022; Doshi-Velez &

Kim, 2017; Molnar, 2019). These techniques play a crucial role in advancing data-driven gasification optimization by ensuring models are both accurate and explainable.

2.7.2 Importance of understanding models

In biomass gasification, understanding ML models is crucial for stakeholders, including operators, researchers, and policymakers. Clear model interpretation enhances process optimization and decision-making, particularly in fields where model-driven insights have significant consequences, such as healthcare, finance, and law (Ale & Slater, 2023).

Interpretability and explainability empower practitioners to comprehend model predictions, troubleshoot issues, and fine-tune parameters for improved performance (Ahmed et al., 2023; Ráz & Beisbart, 2022). A clear understanding of model applicability prevents misuse and helps select the most suitable approach for a given problem. Additionally, feature engineering benefits from interpretability, allowing for better data selection and model accuracy improvement (Sarker, 2021; Kandpal et al., 2025).

Beyond technical aspects, model comprehension facilitates effective communication of results to non-technical audiences, enabling clearer decision-making (Taye, 2023). It also helps identify and mitigate biases, ensuring responsible and ethically sound model usage (Varsha, 2023). Given that ML models evolve, ongoing understanding is essential for continuous improvement and adaptation to new data and requirements (Aldoseri et al., 2023; W. Tian et al., 2025). Ultimately, model interpretability enhances trust, reliability, and ethical considerations, making it indispensable for sustainable and data-driven advancements in gasification research and beyond.

2.7.3 Interpretability methods

Interpretability techniques are essential for understanding gasification ML models, optimizing performance, diagnosing faults, and making informed decisions. These

methods are broadly categorized into model-agnostic and model-specific approaches (Figure 2.10), each providing valuable insights into gasification system behavior (Table 2.8) (Chen et al., 2023).

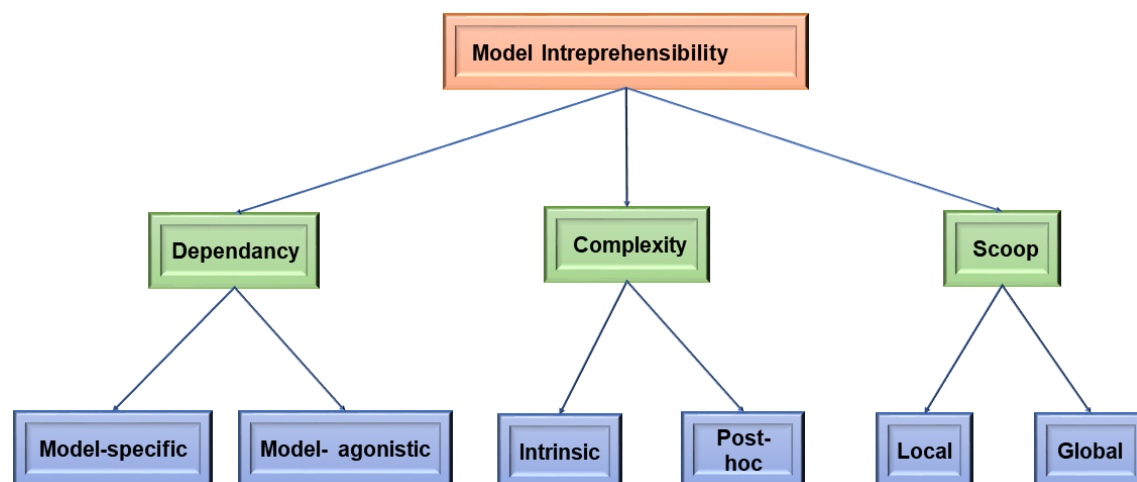


Figure 2.10: Classification of model interpretability analysis method

Model-agnostic methods can be applied to various gasification models without altering their structure. Sensitivity analysis quantifies the impact of individual input variables on model outputs (Muschalik et al., 2022). Feature importance analysis identifies key variables driving predictions, while partial dependence plots (PDPs) visually illustrate relationships between input features and model predictions (Laugel et al., 2018).

Model-specific methods provide deeper insights tailored to specific gasification models. Rule extraction reveals decision rules in rule-based models, feature interaction analysis explores variable dependencies, and counterfactual explanations illustrate cause-and-effect relationships (Adadi & Berrada, 2018; Greenwell et al., 2018). These techniques enhance transparency, ensuring gasification models remain interpretable and actionable for stakeholders.

Despite their importance, interpretability remains an underdeveloped area in gasification research. Many studies prioritize model accuracy over transparency, particularly in complex models like ensembles and ANNs (Li et al., 2023). However, recent research

highlights five key methods for feature importance assessment: permutation importance, Gini importance, Shapley additive exPlanations (SHAP), sensitivity analysis, and partial derivative plots. Among these, sensitivity analysis is the most widely used, particularly for ANN interpretation (Figure 2.11).

Table 2.8: Advantages and limitations of interpretability methods

Technique	Dependency	Scoop	Advantages	Limitations
Permutation importance	Model-agnostic	Global	Intuitive and highly compressed global interpretation. Considers interactions between features. Easy to implement for any model type.	Unclear whether training dataset or testing dataset can be used. Causes unrealistic data instances to be created during shuffling which limit interpretability.
Partial dependence plot	Model-agnostic	Global	Provides intuitive and clear interpretation. Very effective and straight forward for illustrating input/output relationship	Makes assumption of independence between features Becomes infeasible for MIMO models Cannot capture confounding factors
SHAP	Model-agnostic	Local/ Global	Gives explanation based on strong game theory Not only informs about the importance of features but also their relationship with the output Predictions are fairly distributed among feature values	High computational cost
Gini impurity	Model-specific	Global	Provides a straightforward measure to interpret tree-based methods such as RF and GBR.	Not applicable to other model types Biased towards inputs with more categories.
Sensitivity analysis	Model-specific/ model-agnostic	Global/ Local	Effective and powerful algorithm to understand the stability of black box models.	High computational cost. Mainly used for ANN models

Note: SHAP- Shapley additive exPlanations

Ensemble models, while highly accurate, often lack interpretability. Techniques such as SHAP and Gini importance can bridge this gap, improving transparency, trust, and feature selection in ensemble learning (Parr et al., 2024; J. Tian et al., 2025). However, challenges remain, including scalability, standardization, and balancing accuracy with interpretability (Saadallah & Rouissi, 2023; He et al., 2025).

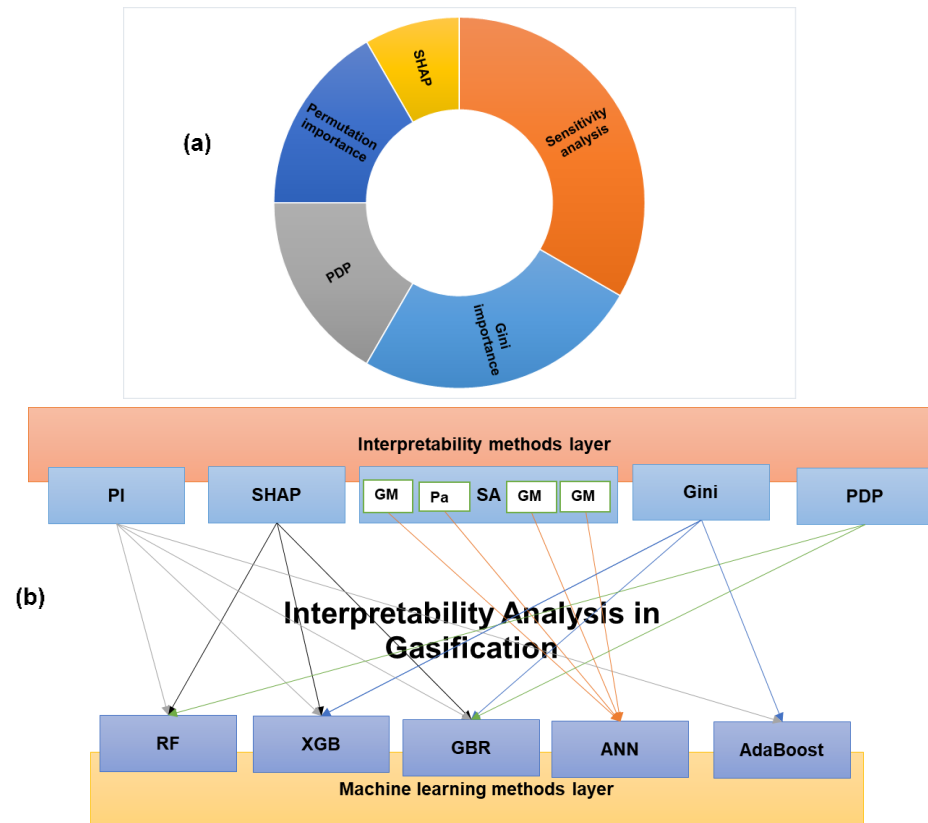


Figure 2.11 Interpretability methods in gasification studies.

Legend: extent of use among studies, (b) linking with ML models. Note. SHAP-Shapley additive exPlanations, PDP- partial dependence plot, GM- Garson method, SA- sensitivity analysis, PI-permutation importance, PaD- partial derivatives.

Further research is needed to develop robust interpretability techniques for gasification models, ensuring greater trust, accountability, and optimization. Table 2.9 summarizes existing studies on interpretability in gasification, identifying gaps and inconsistencies, such as the misuse of "Gini importance" as a form of sensitivity analysis (Kardani et al., 2021). Addressing these challenges will be critical for advancing transparent and explainable ML models in gasification research.

2.7.3.1 Permutation importance

Permutation importance, also known as permutation feature importance, permutation accuracy importance, or mean decrease accuracy, is a widely used technique for assessing the significance of input features in a ML model (Breiman, 2001; Muschalik et al., 2022). It provides a global measure of feature importance by quantifying the impact of permuting

each input variable on model performance (Fisher et al., 2019). This method is effective in identifying which features contribute most to a model's predictions and how sensitive the model is to variations in those features (Gregorutti et al., 2017).

The principle behind permutation importance is straightforward: a feature is considered highly important if randomly shuffling its values results in a significant increase in model prediction error (Zhao et al., 2021). This technique is advantageous because it automatically accounts for feature interactions and performs well even with correlated variables (Molnar, 2019; Rodríguez-Pérez & Bajorath, 2020). The importance score of each feature can be calculated using Eq. (2.1) (Laugel et al., 2018).

$$PFI_j(\hat{f}) = E \left(L(\hat{f}(X_{[j]}), Y) \right) - E \left(L(\hat{f}(X), Y) \right) \quad (2.1)$$

Where, $X_{[j]}$ is the p-dimensional random variable vector of features, the idea behind this method is to break the association between the j -th feature and the target variable by permutating its feature values. If a feature is not useful for predicting an outcome, changing its values by permutation will not increase the expected loss.

Studies have demonstrated the effectiveness of permutation importance in gasification modeling. Ascher et al. (2022) applied permutation importance to four ensemble models (RF, XGB, GBR, and AdaBoost) and found strong agreement in feature rankings, with temperature consistently identified as the most influential variable. However, slight variations in rankings were observed across ensemble sub-models for different output variables. Zhao et al. (2021) further applied permutation importance to a random forest model for SCWG, analyzing H_2 yield prediction. Their results showed that biomass concentration was the most influential process parameter, while hydrogen and oxygen content played key roles among biomass properties. These findings emphasize the distinct

nature of SCWG, where high moisture content necessitates careful optimization of parameters like biomass concentration, temperature, and pressure.

Table 2.9: A summary of literature on feature importance analysis for gasification

Reference	Method	Feedstock	ML model	Feature	Target	Key findings
Kardani et al. (2021)	Gini importance or MDA	MSW	XGB	C, H, S, O, MC, Ash, ER and T	LHV, LHVp and gas yield	T is the most influential for LHV, LHVp, gas yield
Ascher et al. (2022)	SHAP, Gini and Permutation importance	biomass and waste	GBR, RF, XGB, AdaBoost	24 input variables including particle size, gasifying agents, moisture, reactor types, T, etc.	Gas compositions, tar, gas yield, LHV, char yield	Feedstock's particle size and choice of gasifying agent are key for all the models, with particle size being the top for GBR, RF, and AdaBoost.
Zhao et al. (2021)	Permutation importance and PDP	Agricultural waste and MSW	RF	C, H, O and ash, BC, T (P) and residence time (t)	H ₂ yield	For biomass properties: H > O > C > ash order of importance, For process parameter: BC > T > P > t Overall BC is the key input for H ₂ yield
Li et al. (2023)	Gini importance and PDP	Food waste, sludge, and mixed biomass waste	GBR	C, H, S, N, O, ash, SBR, ER, T	char, tar, gas, H ₂ , CH ₄ , CO ₂ , and CO	Ash, N, and temperature were the most important to H ₂ yield
Haq et al. (2022)	SHAP	Sewage sludge	GPR	H, N, O, C, MC, VM, Ash, T, P, time	H ₂ yield	Features impacts trends are T > MC > P > time
Sison et al. (2023)	SHAP, PDP	Agricultural residues, energy crops, municipal waste, algae biomass, and poultry waste.	GBR	SBR, OC, C, H, N, S, O, T, FC, VM, Ash, MC	H ₂ yield, char yield	T > SBR > OC, FC > C > Ash > VM > S > H > moisture (for H ₂ yield) Ash > VM > S > C > H > FC (for char yield)

Legend: ML-machine learning, T- temperature, P-pressure, GPR- process gaussian regression, GBR-gradient boosting regression, RF-random forest, ANN- artificial neural network, XGB- Extreme gradient boosting, AdaBoost-Adaptive boosting, MDA- mean decrease accuracy, MSW-municipal solid waste, LHVp-product gas lower heating value, LHV-lower heating value, C-carbon, H-Hydrogen, N-nitrogen, S-Sulphur, O-oxygen, PDP- partial dependence plots, ER-equivalence ratio, BC- biomass concentration, MC-moisture content, SBR-steam/biomass ratio, VM- volatile matter.

2.7.3.2 Sensitivity analysis

Sensitivity analysis (SA), also known as uncertainty analysis, is a crucial technique for understanding how input variables influence model outputs, particularly in complex, black-box models like ANNs (Ozonoh et al., 2020; Rasheed et al., 2022). SA provides insights into model robustness, feature significance, and decision-making processes, making it valuable for non-linear and non-monotonic gasification models (Ankenbrand et al., 2021; Ritsema, 2021).

SA methods are classified into local and global approaches. Common techniques include one-at-a-time analysis, Morris's method, Sobol indices, perturb-and-profile methods, and ANN-based methods (de Oña & Garrido, 2014; Iooss & Lemaître, 2015; Link et al., 2018; Olden & Jackson, 2002). For ANN models, SA methods fall into two categories: pure SA (e.g., perturb-and-profile) and network-based SA (e.g., connection weights and Garson's algorithm) (Cao et al., 2016; Gevrey et al., 2003; Shojaeefard et al., 2013). Among these, partial derivative (Pad) methods have been recognized as more reliable than connection weights or step-wise perturbation methods (Ozonoh et al., 2020). Using Pad, Ozonoh et al. (2020) found that carbon content was the most influential feature for CGE, gas yield, and LHV, followed by volatile matter and temperature.

Several studies have applied SA to ANN-based gasification models. Serrano & Castelló (2020) used Garson's algorithm to analyze the effect of input features on tar yield, concluding that biomass elemental composition (C, H, O) contributed over 45%, while gasification conditions (ER, temperature) influenced over 30%. Similarly, Yucel et al. (2019) found that temperature was the dominant feature in one case, while air-fuel ratio (AF) and air ratio (AR) were more important in another, highlighting how input selection affects gasification predictions. Baruah et al. (2017) discovered that reduction zone

temperature was the most critical factor for predicting CO and H₂, with input features contributing between 8% and 31% to model outputs.

These studies demonstrate that sensitivity analysis is a powerful tool for interpreting ANN models in gasification research, offering a deeper understanding of feature importance and process optimization.

2.7.3.3 Partial Dependence Plot

PDPs provide a global visualization of how individual input features influence a ML model's output, offering insights into feature-response relationships within a reduced feature space (Rasheed et al., 2022). However, PDPs have limitations, particularly when dealing with strongly correlated predictors, as they assume independence among input variables. This assumption can lead to misleading interpretations, especially when the model extrapolates responses for predictor values outside the observed training data range (Apley & Zhu, 2020). The computation of PDPs is often achieved using Eq. (2.2).

$$\hat{f}_s(x_s) = \frac{1}{n} \sum_{i=1}^n f(x_s, x_c^{(i)}) \quad (2.2)$$

Where, i is a generic observation, x_s represent the features(s) of interest, and $x_c^{(i)}$ the other features included in the model, n is the number of instances which the dataset consists of.

While PDPs share similarities with regression models, they are less effective for MIMO models and may not account for confounding factors affecting predictions (Ascher et al., 2022). Despite these limitations, PDPs remain useful when combined with other interpretability techniques, such as permutation feature importance, which identifies the most influential variables, while PDPs visualize their specific impact (Rzychoń et al., 2020).

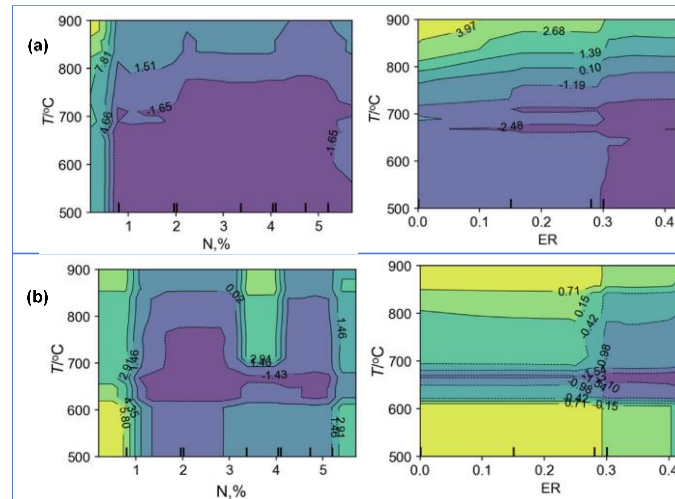


Figure 2.12: PDP plot on impacts of the interaction of temperature with other factors
 Legend: (a) on H₂ yield, (b) on CO₂ yield in syngas. Source: adapted from Li et al. (Li et al., 2023). ER- equivalent ratio, N- nitrogen atom. Copyright © Elsevier 2023

PDPs can be generated in one-dimension (1D) or two-dimension (2D) formats. 1D PDPs illustrate how a single feature affects model predictions, whereas 2D PDPs are valuable for examining feature interactions, showing how two variables jointly influence an output (Li et al., 2023). Zhao et al. (2021) used PDPs in a RF model to illustrate how biomass concentration and temperature synergistically impacted H₂ yield. Similarly, Li et al. (2023) applied PDPs in a GBR model to visualize the correlation between input features and predicted targets (Figure 2.12).

Therefore, PDPs are a powerful visualization tool for enhancing interpretability in ML-based gasification models, particularly when used in conjunction with other methods to provide a more comprehensive understanding of model behavior.

2.7.3.4 Shapley Additive exPlanations

SHAP is a powerful and widely used interpretability technique for machine learning models, offering a more robust and theoretically grounded approach than Local Interpretable Model-Agnostic Explanations (LIME) (Vishwarupe et al., 2022). Unlike LIME, which provides local explanations for individual predictions, SHAP offers both

local and global insights by quantifying the contribution of each feature to the model's overall prediction (Omobolaji et al., 2022).

SHAP is based on coalitional game theory, assigning Shapley values to features, which represent the fair distribution of feature contributions to the model's output (Rasheed et al., 2022). These values determine how much each feature influences predictions, considering all possible feature combinations. The Shapley value formula shown in Eq. (2.3), ensures that feature attributions are fairly distributed:

$$g(z') = \phi_0 + \sum_{j=1}^M \phi_j z'_j \quad (2.3)$$

Where g equals the model and z' is the coalition vector. The z'_j stands for a coalition vector where if a specific feature value is included, it is represented by a 1 and a 0 if it is not included. M is the maximum size of the coalition and j is the feature attribution for a feature j , i.e. Shapley values ϕ_0 indicating a constant value when all inputs are missing. The generic ϕ_j is the weight against the feature contribution summation for the output of the model for overall feature combinations.

One of SHAP's key strengths is its ability to provide both feature importance rankings and insights into feature relationships with the target output (Li et al., 2021; Molnar, 2019). Unlike traditional methods that only evaluate feature importance in isolation, SHAP captures interactions between features, leading to more reliable and interpretable results (Li et al., 2021; Molnar, 2019).

SHAP is often combined with other interpretability techniques, such as PDPs, to enhance interpretability and uncover deeper patterns (Cakiroglu et al., 2022). For instance (Figure 2.13), Ascher et al. (2022) used SHAP to explain predictions across ten output variables in three different ensemble models.

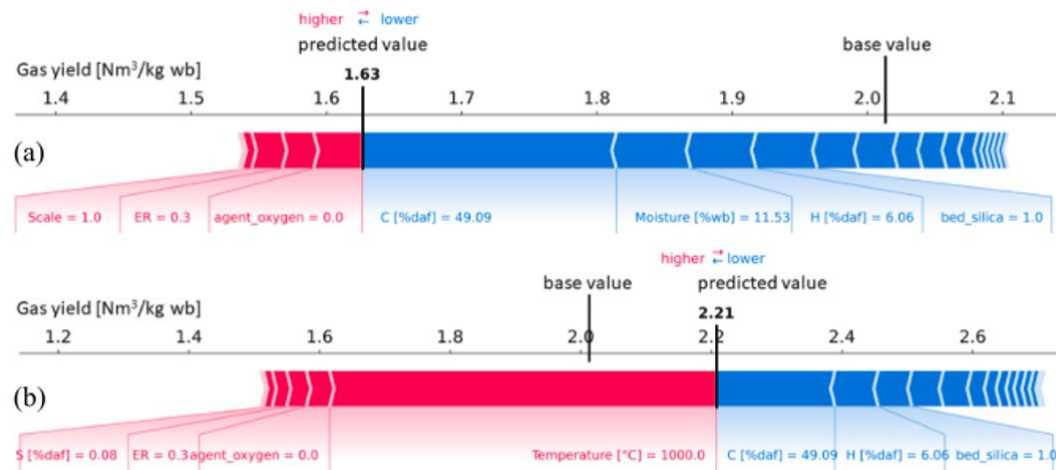


Figure 2.13: SHAP explanations of some selected individual predictions

Legend: The syngas yield from barley straw gasification is shown for (a) a base case at 800 °C, and (b) a high temperature case at 1,000 °C. Source: extracted from Ascher, Wang, et al. (2022). Copyright © Elsevier 2022

In their gas yield prediction model, which utilized 24 input features, SHAP identified carbon content, ER, and temperature as the most influential features. They also demonstrated how SHAP visualizations can effectively communicate machine learning model predictions to stakeholders and policymakers, highlighting its potential for transparent and explainable AI in gasification research (Ascher et al., 2022).

From these findings, SHAP's fairness, consistency, and ability to reveal both individual and collective feature contributions make it an indispensable tool for gasification modeling and process optimization.

2.7.3.5 Gini importance

Gini importance, also known as impurity importance or mean decrease impurity, is a widely used method for evaluating feature significance in decision tree-based models (Li et al., 2023; Yaman et al., 2018). Introduced by Breiman (2001), it quantifies how much a feature contributes to reducing impurity in a decision tree. Impurity refers to how mixed the data is within a node; features that frequently split data into purer subsets are assigned higher importance. While typically applied in classification problems, a similar approach using sum of squares as the impurity measure is employed for regression tasks (Ishwaran,

2015; Nembrini et al., 2018). Gini importance is computationally efficient and easy to interpret, making it a popular choice for feature selection. This can be estimated using Eq. (2.4) (Nembrini et al., 2018).

$$\hat{I}(t) = \sum_{j=1}^J \hat{\phi}_j(t) (1 - \hat{\phi}_j(t)) \quad (2.4)$$

Where; $\hat{\phi}_j(t)$ is the class frequency for class j in the node t

Despite its advantages, Gini importance has limitations. It tends to favor categorical features with many unique values and can be biased toward continuous features that have little correlation with each other (Breiman, 2001). Additionally, it is exclusive to tree-based models, limiting its versatility compared to model-agnostic techniques like SHAP or permutation importance (Wei et al., 2015). However, studies have found that Gini importance can provide comparable feature rankings to permutation importance for ensemble models like GBR and RF (Ascher et al., 2022).

Several studies have applied Gini importance to biomass gasification modeling. Kardani et al. (2021) used Gini importance to interpret an XGB model predicting LHV and gas yield. Their findings showed that temperature was the most influential factor, with importance scores ranging from 35% to 40.8%. Similarly, Ascher et al. (2022) analyzed feature importance across GBR, RF, XGB, and AdaBoost models, identifying particle size and gasification agent as consistently critical predictors (Figure 2.14). They also observed variation in feature rankings across different models, highlighting the need to consider model-specific behaviors when interpreting feature importance.

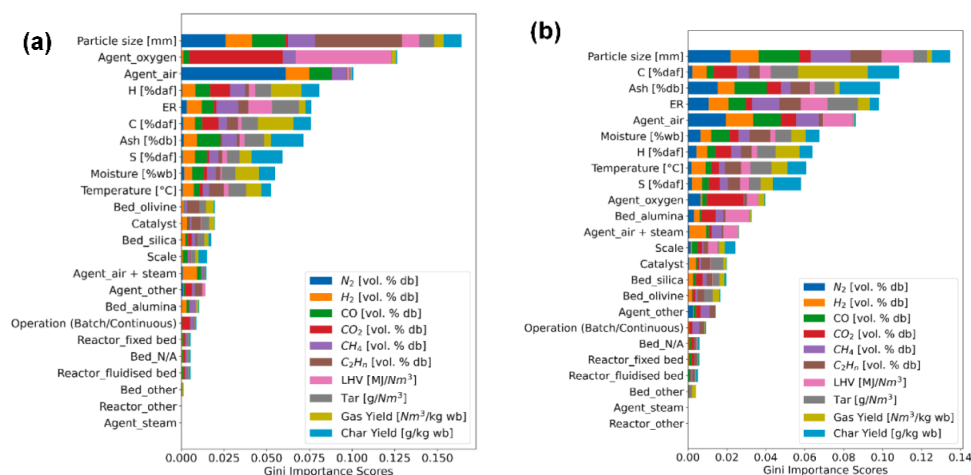


Figure 2.14: Comparison of Gini importance ranking of features

Legend: (a) gradient boosting models and (b) random forest models. Source: adapted from Ascher et al. (2022). Copyright © Elsevier 2022

In another study, Li et al. (2023) applied Gini importance to a GBR model predicting syngas composition, tar, char, and gas yields. Their results indicated that ash content, nitrogen content, and temperature were the most influential features for H_2 yield, alongside factors like hydrogen and sulfur content, oxygen content, steam-to-biomass ratio, and equivalence ratio. Interestingly, temperature emerged as a key feature in both Li et al. (2023) and Kardani et al. (2021). However, Kardani et al. (2021) included proximate analysis features (e.g., moisture content), which were not considered in Li et al. (2023). Since both studies employed GBR and XGB models, their interpretations are comparable, reinforcing the importance of temperature in gasification modeling.

From these examples, it is conformed that Gini importance remains a valuable interpretability tool, particularly for tree-based ensemble models, despite its biases. It provides a quick and effective way to rank feature significance but should be complemented with other interpretability techniques, such as SHAP or permutation importance, for a more comprehensive analysis.

2.8 Challenges and Opportunities in ML

ML holds great promise for optimizing gasification, yet several challenges and opportunities remain. A major challenge is data limitations, as ML models often rely on small datasets from literature or experiments, restricting prediction accuracy (Mutlu & Yücel, 2018). While cross-validation helps, inconsistent implementation and limited data augmentation hinder scalability (Mutlu et al., 2019). Improved feature selection, preprocessing, and key variable identification are crucial for enhancing model accuracy.

Hyperparameter optimization is another critical factor. Traditional trial-and-error tuning, especially for ANNs, is time-consuming. Alternative methods like grid search, particle swarm optimization, genetic algorithms, and Bayesian optimization offer more efficient tuning (Ayodele et al., 2021; Yahya et al., 2021). While tree-based models (e.g., Random Forest, XGB) are less sensitive to hyperparameter tuning (Ascher et al., 2022), comparative studies are needed to identify the best approaches.

Beyond accuracy, model generalizability is essential for handling real-world complexity. Few studies have explored universal models that manage high-dimensional and heterogeneous data (Elmaz & Yücel, 2020). More research is needed on encoding categorical variables and developing ML models that adapt to diverse feedstock blends. For COG, models should capture synergistic effects across binary, ternary, and quaternary blends, as well as emerging technologies like chemical looping and catalytic gasification.

Model interpretability remains a challenge, particularly for complex gasification systems. While methods like SHAP and permutation importance aid in explainability, their suitability varies across ML models. For instance, SHAP may not be compatible with AdaBoost models (Ascher et al., 2022). Establishing benchmark datasets and standardized evaluation frameworks would improve interpretability comparisons.

Integrating multiple interpretability techniques could provide a more holistic understanding of model decision-making.

Reproducibility is another key issue. Standardized frameworks and open-access benchmark datasets are needed for model validation and comparison. Finally, real-world deployment should be prioritized. Developing graphical user interfaces (GUIs) and software applications would enable engineers to apply ML for real-time gasification optimization. Bridging the gap between research and practical implementation accelerates the adoption of ML-driven gasification technologies, enhancing efficiency and sustainability (Haq et al., 2022).

2.9 Industry 4.0 in Energy and Waste Management

Industry 4.0 represents a paradigm shift in manufacturing and industrial processes, integrating IoT, AI, ML, big data analytics, and cyber-physical systems (Kumar, 2024; Kurniawan et al., 2023; Mohammadi et al., 2023). These advancements significantly impact energy production and waste management, driving efficiency, optimization, and sustainability (Hassoun et al., 2023).

In biomass waste COG, Industry 4.0 enhances syngas production efficiency through real-time process monitoring and predictive modeling (Bongomin, Nzila, et al., 2025). IoT sensors track operational parameters, enabling immediate adjustments for optimized hydrogen yield. ML algorithms analyze historical and live data to predict trends, minimize downtime, and maximize process efficiency (Mohammadi et al., 2023).

Industry 4.0 offers several benefits, including improved efficiency, lower costs, enhanced resource management, and reduced emissions. Predictive maintenance ensures system reliability by identifying potential failures in advance, minimizing operational disruptions (Kurniawan et al., 2022; Zhang et al., 2023). However, challenges remain. Infrastructure

investments are needed for IoT and digital twin implementation, while robust cybersecurity measures are essential to safeguard data. Additionally, the complexity of ML models requires expertise in data science and algorithm development, posing adoption barriers for some organizations (Hasan et al., 2025).

Looking ahead, the continued evolution of Industry 4.0 and Industry 5.0 technologies will play a crucial role in optimizing biomass gasification and broader renewable energy systems (Masoomi et al., 2025; Li et al., 2025; Erdiwansyah et al., 2025). The integration of process simulation, digital twins, and ML models in COG enhances syngas production and waste management, aligning with global sustainability goals (Chauhan et al., 2021; Kanojia & Visvanathan, 2021; Zhou, 2025; Khan et al., 2025).

2.10 Key Gaps in the Literature

Despite significant advancements in gasification and COG research, several key gaps remain, particularly in integrating innovative approaches and ensuring practical applicability. Addressing these gaps requires a multi-disciplinary approach, combining robust experimental validation, advanced process simulation, and ML techniques to enhance predictive accuracy and real-world relevance.

2.10.1 Feedstock characterization and synergistic effects

Gasification research has primarily focused on widely available feedstocks such as rice husk and sugarcane bagasse, while underutilized biomass like coffee husks, macadamia nutshells, and tea wastes remain poorly studied (Abdallah et al., 2023; Fajobi et al., 2022; Sivaraman et al., 2023). Most investigations analyze feedstocks individually, missing the synergistic effects that arise from blending, which can significantly enhance reactivity, syngas yield, and gasification efficiency (Guo et al., 2022; Balsora et al., 2023; Wang et al., 2023; Zahra et al., 2024). This gap is linked to Objective 1 and Objective 2.

Addressing this gap is significant because it expands the scientific understanding of underexplored feedstocks and their potential in co-gasification. In this study, detailed physicochemical characterization and kinetic analysis of selected feedstocks and binary blends were performed using TGA and the Coats–Redfern method, providing new insights into thermal behavior and reaction pathways.

2.10.2 Thermodynamic modeling and experimental validation

Existing thermodynamic models often assume equilibrium and ignore kinetic, heat, and mass transfer limitations, causing discrepancies between predicted and experimental outcomes (Cao et al., 2022; Pati & De, 2021). Many studies also fix biomass blend ratios, limiting understanding of performance under variable operational conditions (Ferreira et al., 2019; Mutlu & Zeng, 2020; De et al., 2025; Niu et al., 2025). This gap relates to Objective 2, which involves developing and validating a comprehensive Aspen Plus co-gasification model. Addressing this gap is significant because validated models improve predictive accuracy and enable practical process optimization. In this study, experimental TGA and proximate analysis data were integrated into the Aspen Plus model, and model predictions were validated against laboratory observations.

2.10.3 Co-gasification and reactor modeling

Current co-gasification models inadequately account for varying biomass blend compositions, reducing applicability to real-world systems (Pati et al., 2021; Cao et al., 2022; Alam et al., 2025). Industrial-scale systems such as circulating fluidized beds or autothermal downdraft gasifiers remain underexplored, and modeling of heat and mass transfer, temperature distribution, and gas exit pathways is limited (Ding et al., 2021; Gabbrielli et al., 2022; Elmaz et al., 2020; Liang et al., 2021). This gap is linked to Objectives 2, focusing on blend interactions and autothermal gasifier modeling. Addressing this gap is significant because improved reactor modeling enables better

process efficiency, syngas quality, and scale-up feasibility. This study simulates an autothermal downdraft gasifier, capturing temperature profiles, airflow, and exit gas effects, providing insights into optimizing reactor performance.

2.10.4 ML challenges in gasification

ML applications in gasification are typically limited to ANN, RF, or GBR models and evaluated using simple metrics such as MSE, RMSE, or R^2 , without stress-testing or robustness analysis (Ayub et al., 2022; Kartal & Özveren, 2020; Khandelwal et al., 2025; Haq et al., 2025). Real-time adaptation for dynamic industrial conditions is rarely explored, and ensemble or hybrid methods remain largely untapped (Sison et al., 2023; Lahafdoozian et al., 2024; Yang et al., 2025; Q. Chen et al., 2025). This gap aligns with Objective 3, which aims to develop predictive, and Objective 4 which focus testing the robustness of ML models for co-gasification. Addressing this gap is significant because it improves predictive reliability, generalizability, and industrial applicability. In this study, hybrid ML models were trained, tested under perturbed inputs, and stress-tested to ensure resilience against noise, outliers, and unseen feedstocks.

2.10.5 Interpretability and decision-making in ML models

While ML models can achieve high predictive accuracy, interpretability is often limited, reducing actionable insights for process optimization (Kardani et al., 2021; Ascher et al., 2022; Kandpal et al., 2025; W. Tian et al., 2025). Most studies focus on syngas yield, neglecting other key performance indicators like char yield, syngas composition, and cold gas efficiency (Zhao et al., 2021; Serrano & Castelló, 2020; Li et al., 2023; He et al., 2025). This gap is linked to Objective 5, which involves interpretability analysis of ML models. Addressing this gap is significant because transparent ML models support informed decision-making and process improvement. In this study, interpretability

techniques were applied to identify key process parameters affecting outputs, enabling data-driven optimization of co-gasification operations.

2.10.6 Summary of gap addressing

By addressing these gaps, this study makes several key contributions: characterizing underutilized biomass feedstocks (Objectives 1), developing validated Aspen Plus co-gasification models (Objective 2), implementing robust and interpretable ML models (Objectives 3, 4, and 5), and simulating autothermal downdraft gasifiers to improve understanding of reactor temperature and gas dynamics. These efforts advance predictive modeling, process understanding, and practical applicability, supporting sustainable energy production and integration of Industry 4.0 technologies in biomass gasification.

2.11 Theoretical Framework

2.11.1 ML-Process Simulation Integration

The framework utilizes Aspen Plus for detailed PS, generating datasets on biomass behavior under varying conditions (e.g., biomass type, temperature, pressure, and syngas composition). ML algorithms analyze these datasets, identifying complex patterns and correlations beyond traditional analysis. By training ML models on simulated data, the system can forecast COG outcomes, optimize operational parameters, and enable real-time process adjustments, enhancing both prediction accuracy and industrial applicability.

2.11.2 Conceptual Model

This conceptual model (Figure 2.15) outlines the dynamic interactions between biomass properties, process parameters, and output parameters, incorporating a ML feedback loop to optimize COG. The framework enhances process prediction, optimization, and adaptability through continuous learning and data-driven adjustments.

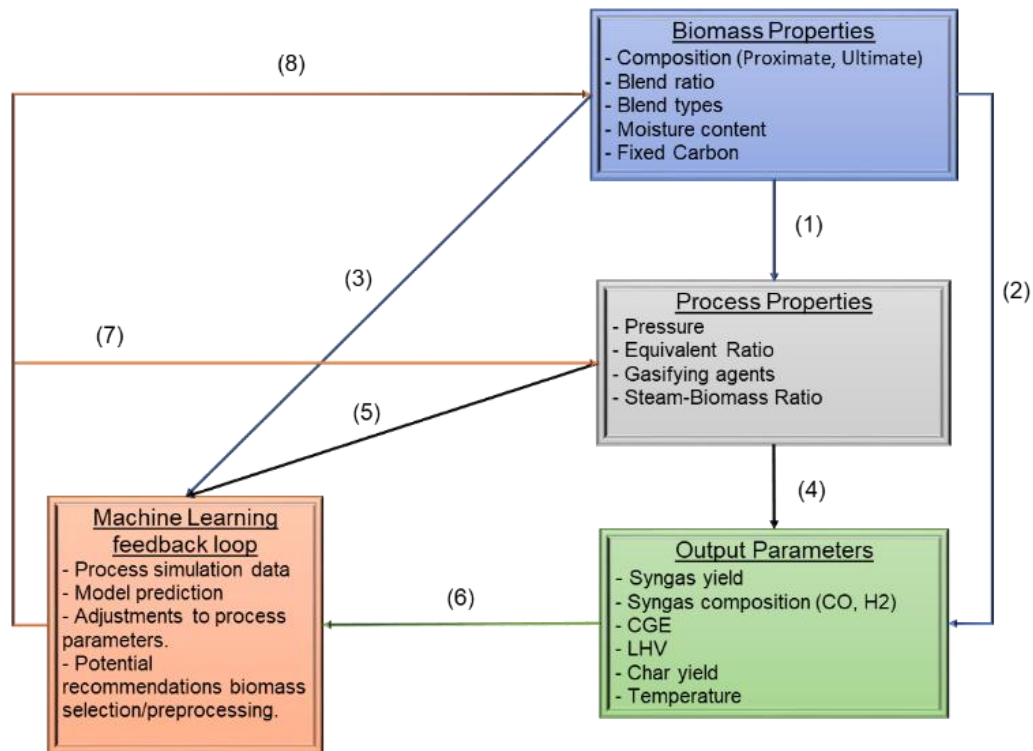


Figure 2.15: Conceptual model guiding this Research

Key Relationships in the Model include:

- Biomass properties → Process parameters (1): Biomass characteristics (e.g., composition, moisture, particle size) influence gasification settings. Feedstocks with high moisture content require higher temperatures, while carbon-hydrogen ratios dictate the optimal ER, pressure, and gasifying agents for efficiency.
- Biomass properties → Output parameters (2): Biomass composition directly affects syngas yield and quality. High-carbon biomass increases CO production, while hydrogen-rich biomass enhances gas yield.
- Biomass properties → ML feedback loop (3): ML models use biomass data to predict COG outcomes, improving accuracy and enabling real-time process adjustments. The loop adapts to feedstock variability, refining recommendations over time.
- Process parameters → Output parameters (4): Settings like ER, pressure, and gasifying agents control gasification efficiency and syngas composition. Optimized parameters maximize gas yield and minimize unwanted byproducts.

- e) Process parameters → ML feedback loop (5): ML models analyze historical and real-time process conditions to refine predictions. Patterns in operational data inform future parameter adjustments, improving process control.
- f) Output parameters → ML feedback loop (6): Gasifier performance data (syngas composition, yield, and efficiency) is fed into ML models for ongoing improvement. The loop enhances predictive accuracy and refines process recommendations.
- g) ML feedback loop → Process parameters (7): ML suggests process adjustments for optimal syngas production, ensuring dynamic, real-time optimization. This improves system adaptability to feedstock and operational variations.
- h) ML feedback loop → Biomass properties (8): ML-driven insights guide biomass selection and preprocessing, aligning feedstock properties with gasification goals.

CHAPTER THREE: RESEARCH METHODOLOGY

3.1 Introduction

This chapter outlines the research design and methodologies used to achieve the study's objectives. It details biomass physicochemical characterization, thermo-kinetic analysis, process simulation (PS), and machine learning (ML) model development and validation. The chapter also covers model evaluation, robustness, and interpretability analysis to ensure reliability and transparency. Key challenges, assumptions, and methodological constraints in PS and ML modeling are discussed. Additionally, it presents the software, equipment, computational resources, ethical considerations, and quality assurance measures to ensure systematic and replicable outcomes.

3.2 Research Design

This research integrated experimental analysis, PS, and ML techniques to comprehensively understand and predict biomass co-gasification (COG) processes. The methodology followed a sequential approach, illustrated in Figure 3.1, with five key phases:

- a) **Physicochemical characterization:** The composition (proximate and ultimate analysis) and energy potential of selected feedstocks were assessed to understand their fundamental properties.
- b) **Thermo-kinetic analysis:** Thermogravimetric analysis (TGA) was employed to study the thermal degradation behavior of the feedstocks. TGA data were used to determine kinetic and thermodynamic parameters critical for optimizing COG conditions.
- c) **Process simulation:** Aspen Plus was used to model the COG process, refine operational parameters, and predict reactor zone temperatures, syngas

composition, and char output under varied conditions and feedstock combinations.

- d) **Machine learning modeling:** ML models were developed to predict syngas yield and quality. These models supported real-time process optimization and enhanced decision-making efficiency.
- e) **Model robustness and interpretability:** The models were evaluated using cross-validation and stress-testing to ensure reliability. Interpretability techniques, such as permutation importance and Gini importance, were applied to validate the scientific soundness of the models and to reveal causal relationships in the co-gasification process.

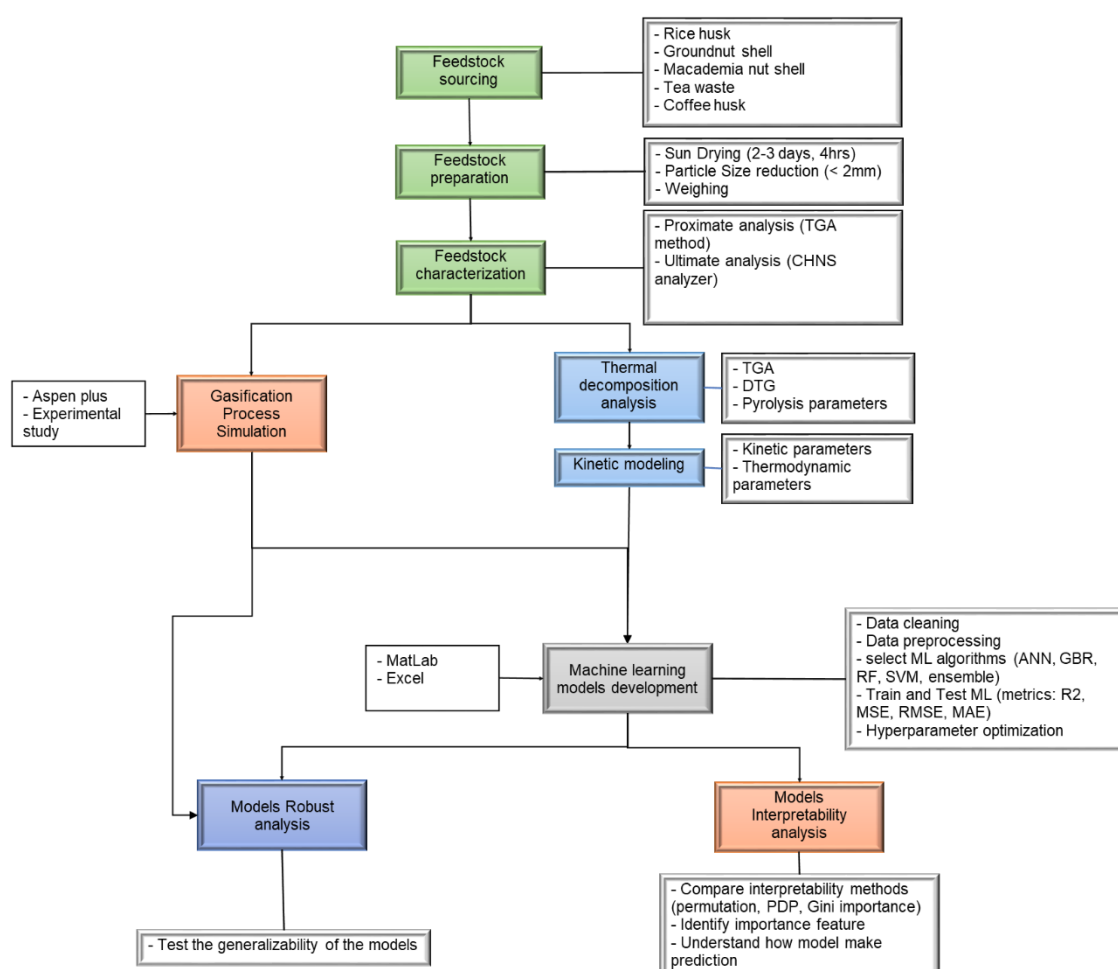


Figure 3.1: Overall research methodology approach for this study

This integrated approach enhanced the efficiency, sustainability, and scalability of COG research. By combining detailed feedstock characterization, PS, and ML-driven predictions, the study advanced the development of robust and interpretable models that support the real-world implementation of biomass-to-energy solutions.

3.3 Physicochemical and Thermo-kinetic Characterization

This section focuses on the proximate and ultimate characterization of biomass feedstock, along with its thermal degradation behavior, kinetic, and thermodynamic properties which are key aspects for optimizing the COG process. Much of the research presented here, including methodologies and figures, has been previously published (Bongomin et al., 2024), providing a strong foundation for the experimental approaches in this thesis. This acknowledgment reinforces the reliability and validity of the experimental data and analytical techniques employed.

3.3.1 Biomass waste feedstocks

The biomass wastes used in this study included coffee husks (CH), groundnut shells (GS), macadamia nutshells (MS), rice husks (RH), and tea wastes (TW) (Figure 3.2).



Figure 3.2: Biomass waste feedstocks

Legend: (a) Coffee husk, (b) groundnut shell, (c) macadamia nutshell, (d) rice husk, (e) tea waste.

Each biomass feedstock was sourced directly from its primary industrial processor to ensure material consistency, traceability, and relevance to real-world thermochemical applications. MS were obtained from the Kenya Nut Company in Thika, Kenya; RH and GS were collected from local millers in Amuru District, Uganda; TW was sourced from Litein Tea Factory in Litein, Kenya; and CH was acquired from Grainpulse Limited in

Mukono District, Uganda. The selection of these sources was purposive, based on their reliability, sustainability, and continuous feedstock availability, making them representative of typical industrial residues in East Africa.

For each material, approximately 10 kg of biomass was collected from multiple batches at the processing facility. These subsamples were composited into a single representative bulk sample and homogenized through drying, grinding, and sieving to minimize intra-source variability. This compositing approach, widely used in biomass characterization studies, ensured that the samples captured the inherent variability of each feedstock while remaining practical given the study's objectives and laboratory constraints. The resulting representative samples were suitable for proximate analysis, ultimate analysis, and thermogravimetric experiments, providing a robust foundation for subsequent simulation and machine-learning modelling.

3.3.2 Samples preparation

The biomass samples were initially sun-dried for 2–3 days, approximately 4 hours per day, to remove surface moisture. They were then ground using a small laboratory benchtop grinder (labeled 'Electrical Powder Grinder'), commonly used for milling dry biomass, grains, herbs, and minerals. The ground material was subsequently sieved to obtain a uniform particle size of <1 mm, ensuring homogeneity. Prepared samples were stored in airtight containers to prevent moisture uptake prior to analysis. All sample preparation procedures were conducted at the Textile Laboratory of Moi University, Kenya.

3.3.3 Physicochemical characterization

The proximate properties (moisture, volatile matter, fixed carbon, and ash content) of the biomass feedstocks were determined using a macro-thermogravimetric analyzer (ELTRA THERMOSTEP) from Makerere University, Uganda, following the ASTM E1131-08

standard (Lubwama & Yiga, 2017). Elemental composition (carbon, hydrogen, nitrogen, and sulfur) was analyzed using a CHNS Automatic Analyzer (Elementar-Vario EL III, Germany) from Cairo University, Egypt. The lower heating value (LHV) and higher heating value (HHV) were estimated from ultimate analysis using correlation models proposed in the previous studies (Hosokai et al., 2016; Channiwala & Parikh, 2002; Huang & Lo, 2020).

3.3.4 Thermogravimetric analysis

A thermochemical conversion study was conducted to evaluate resource recovery potential of five biomass waste samples by analyzing their thermal decomposition behavior using TGA. The analysis was performed with a STA 6000 (PerkinElmer, USA) at a constant heating rate of 20°C/min in an inert N₂ atmosphere, with a purge gas flow of 50 mL/min from 25°C to 950°C (Figure 3.3). The TGA experiment was done from Busitema University, Uganda.

Previous studies have shown that a 20°C/min heating rate ensures complete material degradation in less time while maintaining high data quality with minimal outliers (Vyas et al., 2024). Approximately 10 ± 1 mg of each biomass sample was placed in a platinum crucible and heated under the specified conditions. The TGA instrument continuously recorded weight loss as a function of temperature and time, generating TG and DTG curves for each sample.

The TGA in this thesis report mass changes using the expression “weight loss as %”. This notation is fully equivalent to “percentage weight loss”, as both represent the proportion of mass lost during heating normalized to the initial sample mass. Since all TGA computations, plots, and interpretations were based on this normalized metric, the original unit has been retained for consistency across all figures and sections. Readers should therefore interpret “weight loss as %” and “percentage weight loss” interchangeably.

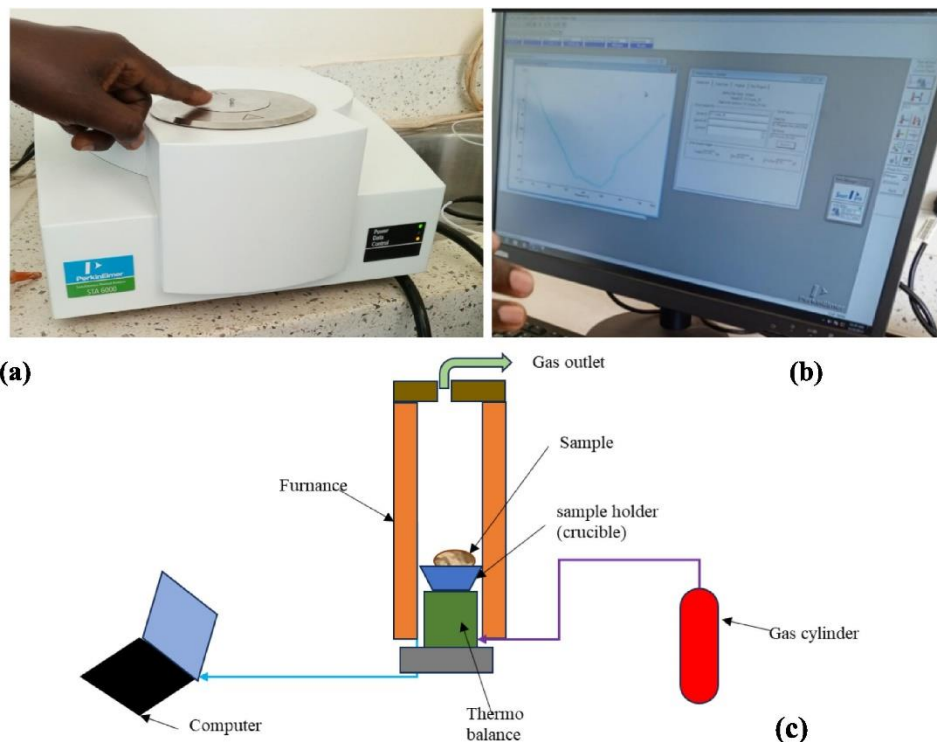


Figure 3.3: Experimental setup for thermogravimetric analysis
 Legend: (a) STA 6000, (b) computer monitor (c) schematic of TGA working principle

3.3.5 Coat-Redfern kinetic method

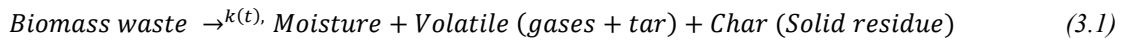
The Coats-Redfern (CR) method, a widely used technique for determining kinetic parameters from TGA data, was chosen for this study due to its robustness, simplicity, and effectiveness under non-isothermal conditions typical of biomass pyrolysis (Ebrahimi-Kahrizsangi & Abbasi, 2008; Li et al., 2023). Unlike advanced isoconversional methods such as Flynn-Wall-Ozawa (FWO) and Kissinger-Akahira-Sunose (KAS), which require multiple heating rates for detailed insights, the CR efficiently estimates the activation energy (E_a , from the slope) and pre-exponential factor (A , from the intercept) by linearizing the Arrhenius equation. This approach aligns with our study's experimental design, which employs a single heating rate.

While Vyazovkin & Muravyev (2024) highlight the limitations of single heating rate methods, such as potential inaccuracies in determining kinetic triplets due to the complex nature of biomass decomposition, the CR remains suitable for preliminary studies. It

allows for meaningful comparisons across biomass samples under consistent conditions and reflects real-world pyrolysis applications, where constant heating rates are often used. Moreover, conducting experiments at multiple heating rates demands substantial time, resources, and equipment, which may not always be feasible. Despite its constraints, the CR has demonstrated reliability in numerous studies when applied with an awareness of its limitations (Uddin Monir et al., 2024).

3.3.5.1 Fundamental equations

Biomass waste consists of a complex matrix of biopolymers, with numerous reactions occurring simultaneously during pyrolysis within a given timeframe (Mishra & Vinu, 2024). This complexity makes predicting the specific reaction mechanisms formed during pyrolysis challenging. To address this, a generalized decomposition reaction is proposed, as shown in Eq. (3.1).



Where; k is rate constant, the volatile mean sum of condensable (tar) and non-condensable gasses. The rate constant (k) is dependent on absolute temperature (T), which is expressed by the Arrhenius equation:

The kinetic equation for such heterogeneous system can be written as in Eq. (3.2).

$$\frac{d\alpha}{dt} = k(t)f(\alpha) \quad (3.2)$$

Where; da/dt represents rate of degradation. It is a linear function of temperature dependent rate constant, and $f(\alpha)$ is the temperature independent function of conversion, which depends on reaction mechanism.

The normalized conversion (α) is given by Eq. (3.3).

$$\alpha = \frac{m_0 - m_t}{m_0 - m_\infty} \quad (3.3)$$

where, m_0 is initial mass of the material, m_t is mass of the material at time t , and m_∞ is the final mass or residue weight of the material after degradation.

Weight loss percentage is given by Eq. (3.4);

$$\text{Weight Loss (\%)} = \frac{m_i - m_t}{m_i} \times 100\% \quad (3.4)$$

Where, m_i is the initial mass of the samples, and m_t is the mass at time t .

The $k(T)$ is rate constant and is expressed by the Arrhenius equation using Eq. (3.5), substituting into Eq. (3.2), gives Eq. (3.6) (Gajera et al., 2020).

$$k(T) = A \exp\left(-\frac{E_a}{RT}\right) \quad (3.5)$$

$$d\alpha/dt = A \exp\left(-\frac{E_a}{RT}\right) \cdot f(\alpha) \quad (3.6)$$

The following integral form of Eq. (3.6) is given by Eq. (3.7).

$$g(\alpha) = \int_0^\alpha \left(\frac{d\alpha}{f(\alpha)} \right) = A/\beta \int_{T_0}^T \exp\left(-\frac{E_a}{RT}\right) dT \quad (3.7)$$

where, A is pre-exponential factor (min^{-1}), E_a is activation energy (kJ/mol), $k(T)$ is the rate constant, R universal gas constant (0.008314 kJ/mol K), T is the temperature of reaction (K), α is the conversion rate (mass loss) and $f(\alpha)$ is the kinetic model, $g(\alpha)$ is the integral form of the kinetic model, β is the heating rate ($^{\circ}\text{C/min}$).

Coats-Redfern method was employed to find out pre-exponential factor and activation energy by fitting the TGA experimental data using Eq. (3.8);

$$\ln\left(g(\alpha)/T^2\right) = \ln\left[AR/\beta E_a \left(1 - 2RT/E_a\right)\right] - E_a/RT \quad (3.8)$$

3.3.5.2 Multiple reaction mechanism functions

To enhance the accuracy and comprehensiveness of the kinetic analysis, this study employed nine different reaction mechanism functions ($g(\alpha)$), representing various kinetic models such as order-based chemical reaction, diffusion-controlled, and

contracting sphere models, as summarized in Table 3.1 (Balasundram et al., 2017; Khawam & Flanagan, 2006; Yu et al., 2013).

Biomass pyrolysis involves multiple overlapping reactions due to the distinct thermal degradation characteristics of cellulose, hemicellulose, and lignin. By incorporating multiple reaction models, a more precise fit to the TGA data was achieved, leading to accurate kinetic parameter estimation (Najafi et al., 2024). This approach provides a comprehensive understanding of thermal degradation kinetics, facilitating the optimization of pyrolysis conditions to maximize energy recovery and improve the efficiency of biomass conversion processes (Raza & Abu-Jdayil, 2023).

Table 3.1: The common reaction model for determining the mechanism of biomass degradation

Reaction model	Reaction mechanism	Code	$f(\alpha)$	$g(\alpha)$
Diffusion	1D diffusion (parabolic rule)	D1	$(2\alpha)^{-1}$	α^2
	2D diffusion (Va lensi equation)	D2	$[-\ln(1 - \alpha)]^{-1}$	$(1 - \alpha) \ln(1 - \alpha) + \alpha$
	3D diffusion (Jander)	D3	$3/2(1 - \alpha)^{2/3}[1 - (1 - \alpha)^{1/3}]^{-1}$	$[1 - (1 - \alpha)^{1/3}]^2$
	3D diffusion (Ginstling-Brounshtein)	D4	$3/2[(1 - \alpha)^{-1/3} - 1]^{-1}$	$1 - \frac{2}{3}\alpha - (1 - \alpha)^{\frac{2}{3}}$
Geometrical contraction models/ Shape contraction model	Contracting area of sphere	G5	$2(1 - \alpha)^{1/2}$	$1 - (1 - \alpha)^{1/2}$
	Contracting volume of cylinder	G6	$3(1 - \alpha)^{2/3}$	$1 - (1 - \alpha)^{\frac{1}{3}}$
Order-based chemical reaction	1 st order reaction	R7	$1 - \alpha$	$\ln(1 - \alpha)$
	2 nd order reaction	R8	$(1 - \alpha)^2$	$(1 - \alpha)^{-1} - 1$
	3 rd order reaction	R9	$(1 - \alpha)^3$	$1/2[(1 - \alpha)^{-2} - 1]$

3.3.5.3 Kinetic parameters

Activation Energy (E_a) is a key kinetic parameter that quantifies the minimum energy required to initiate biomass decomposition during thermal degradation (Almusafir & Smith, 2024). It represents the energy barrier that reactant molecules must overcome for bond breakage and product formation. In pyrolysis, E_a provides insights into the thermal stability of biomass components, with cellulose, hemicellulose, and lignin exhibiting

distinct activation energies due to their varying resistance to thermal decomposition (El-Sayed et al., 2024; Silva et al., 2023; Sribala et al., 2022). E_a was estimated using the slope of the linearized Coats–Redfern plot (Eq. (3.9)), where the slope of the plot of $\ln[g(\alpha)/T^2]$ versus $1/T$ corresponds to $-E_a/R$, $g(\alpha)$ is a integral form of arrhenius equation and computed using the coessing reaction mechanisms in Table 3.1.

$$\text{Slope} = -E_a/R \quad (3.9)$$

The pre-exponential factor (A), also known as the frequency factor, is a critical kinetic parameter in the Arrhenius equation. It represents the frequency of successful molecular collisions leading to decomposition (Sbirrazzuoli, 2020). The A value provides insight into the number of productive reactant interactions per unit time, influencing the reaction rate (Sribala et al., 2022). It was estimated from the intercept of the linearized Coats–Redfern plot using Eq. (3.10), where the intercept corresponds to $\ln(AR/\beta E_a)$.

$$\text{Intercept} = \ln(AR/\beta E_a) \quad (3.10)$$

3.3.5.4 Kinetic modeling approaches

The multi-step segmented approach models each pyrolysis stage as a single-step reaction with distinct kinetic parameters, capturing dominant reaction pathways at different temperature ranges for greater accuracy (Mishra & Vinu, 2024). The overall kinetic parameters were determined by combining segmented values using a weighted average approach (Eqs. (3.11) - (3.13)).

$$w_i = \frac{\Delta m_i}{\Delta m_{total}} \quad (3.11)$$

$$E_{a,overall} = \sum_i w_i E_{a,i} \quad (3.12)$$

$$A_{overall} = \exp(\sum_i w_i \ln A_i) \quad (3.13)$$

Where; A_i is the pre-exponential factor for stage i . Overall Pre-Exponential Factor ($A_{overall}$), $E_{a,i}$ is the activation energy for stage i , overall activation energy ($E_{a,overall}$): fractional weight (w_i), Δm_i mass loss at stage i , Δm_{total} mass loss at the entire temperature range.

The global single-step approach models the entire pyrolysis process as a single reaction with uniform kinetic parameters across the temperature range. It simplifies the process by assuming a dominant reaction pathway, characterized by a global activation energy ($E_{a,global}$) and a pre-exponential factor (A_{global}). This method provides a generalized kinetic model, useful for preliminary process design and scaling up applications where a simplified representation is sufficient (Alashmawy et al., 2023; Shahdan et al., 2022).

3.3.6 Thermodynamic analysis

The thermodynamic parameters including enthalpy change (ΔH), Gibbs free energy change (ΔG), and entropy change (ΔS), offer a comprehensive understanding of the energy dynamics, spontaneity, and disorder associated with the pyrolysis process. Analyzing these parameters helps optimize pyrolysis conditions, improve energy efficiency, and enhance the performance and yield of desired products. There were calculated using Eqs. (3.14) - (3.16) (Ali et al., 2021; Balogun et al., 2021; Gajera et al., 2022; Hai et al., 2021).

$$\Delta H = E_a - RT_p \quad (3.14)$$

$$\Delta G = E_a + R.T_p \ln \left(\frac{K_B T_p}{h A} \right) \quad (3.15)$$

$$\Delta S = \left(\frac{\Delta H - \Delta G}{T_p} \right) \quad (3.16)$$

Where; Gas constant (R): 0.08314 kJ/mol.K, peak temperature (T_p , in Kevin), Boltzmann constant (K_B): 1.381×10^{-23} J/K, Plank's constant (h): 6.626×10^{-34} Js)

3.4 Process Simulation Model Development

A systematic approach was used to develop the Aspen Plus simulation model for biomass gasification, incorporating feedstock properties and gasification operating conditions. The model was calibrated with experimental data and refined through sensitivity analysis to ensure accuracy in pyrolysis, combustion, and reduction zones. The stepwise development process, including model configuration, dynamic computation, and validation, is illustrated in Figure 3.4.

3.4.1 Aspen plus model configuration

Aspen Plus is a widely used process simulation software for designing, optimizing, and analyzing industrial processes, including biomass gasification (Pati & De, 2021). Its robust thermodynamic models, such as the Peng-Robinson equation of state with Boston-Mathias modifications (PR-BM), enable accurate modeling of gas mixtures under high-temperature and pressure conditions typical of gasification (Ranjan et al., 2023).

The software supports non-conventional components, allowing precise modeling of biomass properties using proximate and ultimate analysis data (Kappagantula et al., 2024). It features reaction engineering blocks like RStoic, RGibbs, and REquil, which simulate different gasifier zones (drying, pyrolysis, combustion, and reduction) under both equilibrium and kinetic conditions (Zhu et al., 2022). This flexibility is essential for downdraft gasification studies.

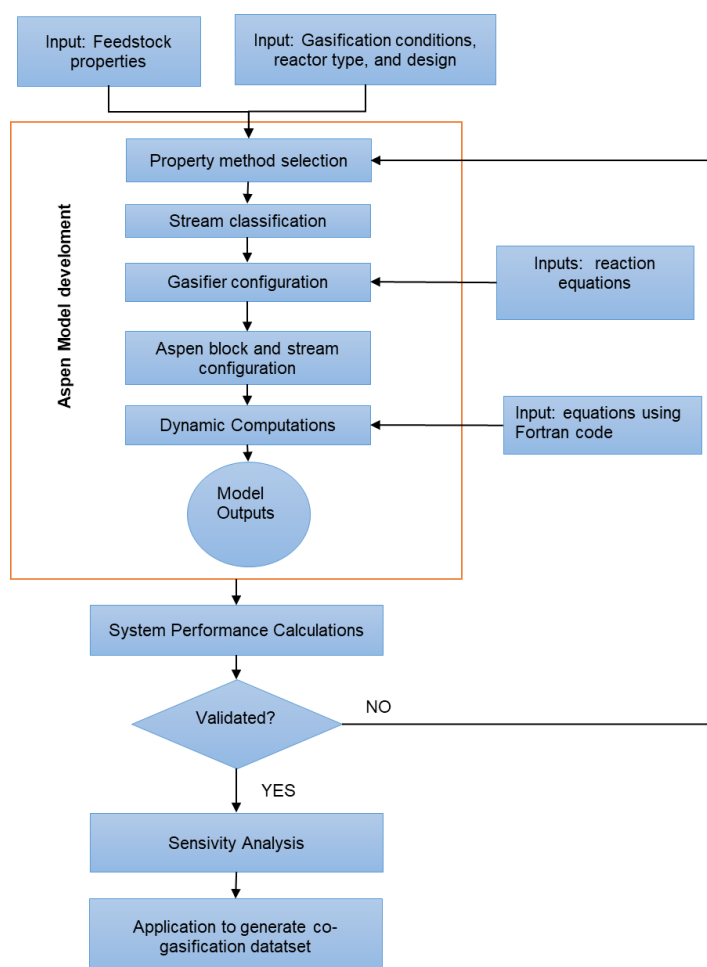


Figure 3.4: Flowchart of the process simulation model development

Aspen Plus also excels in stream and energy integration, managing complex stream splits, mixtures, and energy balances within a gasifier (Li et al., 2024). Its data handling and analysis tools enhance process optimization and scalability by leveraging comprehensive datasets on feedstock properties, operational parameters, and outputs (Ranjan et al., 2024).

3.4.1.1 Property method selection

The PR-BM was selected for the gasification model due to its suitability for high-temperature processes and ability to handle the non-ideal behavior of gas mixtures under extreme conditions. Additionally, the model incorporates the DCOALIGT property model for density calculations and HCOALGEN for enthalpy calculations, utilizing proximate, ultimate, and sulfate analysis data to enhance accuracy.

3.4.1.2 Stream classification

The Aspen model classified streams into material and heat streams to represent various system components and energy flows. In this study, material streams were divided into:

- a) Non-conventional streams (e.g., FEED1, FEED2 for biomass feedstocks and ASH for solid residues), which required specialized handling due to their complex composition.
- b) Conventional streams, which included well-defined gases (CO, CO₂, CH₄, N₂, O₂, H₂S, NH₃, H₂O), and followed standard thermodynamic and chemical definitions.
- c) Solid streams (carbon, C and sulfur, S) were treated as pure components representing elemental phases, enabling accurate tracking of their transformations during pyrolysis, gas–solid reactions, and char formation.

This classification ensured an accurate representation of biomass gasification processes, and enhanced the simulation's ability to model diverse materials and reactions effectively.

3.4.1.3 Downdraft gasifier configuration

The gasification model used in this study was based on a pilot-scale downdraft gasifier, as illustrated in Figure 3.5. This design was adopted from the study by Awais et al. (2022), which was fabricated and optimized at the Department of Energy Systems Engineering, University of Agriculture Faisalabad, Pakistan.

The gasifier features a unique configuration that enhances tar cracking by directing syngas through the hot zone surrounding the combustion chamber. This innovative design reduces tar content, improves syngas quality, and simplifies gas cleaning and utilization. It also improves thermal management, as syngas passing through the high-temperature region undergoes additional tar breakdown, resulting in a cleaner gas output.

This configuration supports autothermal operation, whereby partial combustion of the biomass generates the thermal energy required for gasification. As a result, the process eliminates the need for external heat sources, improving energy efficiency and system integration (Awais et al., 2018, 2021, 2022; Omar et al., 2018).

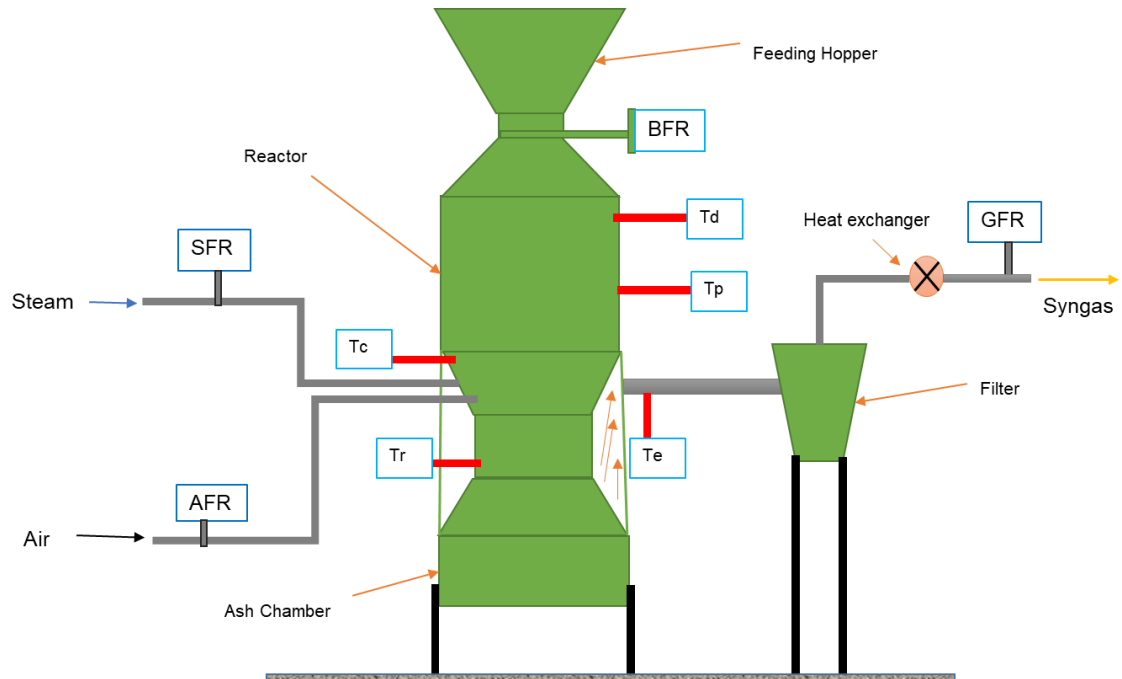


Figure 3.5: Schematic of a pilot-scale downdraft gasifier system

Legend: AFR: air flowrate, SFR: steam flowrate, BFR: biomass flowrate, GFR: gas flowrate meter; T_d , T_p , T_c , T_r , T_e are the drying, pyrolysis, combustion, reduction and exit temperature measuring points

In this study, each reaction zone, namely drying, pyrolysis, combustion, and reduction, was modeled independently (Table 3.2) to capture the specific chemical dynamics occurring at each stage. This detailed modeling provided insights into the performance and operational challenges of the novel gasifier design, supporting its further development and optimization. By systematically analyzing the interactions among the zones and evaluating process efficiency, the model contributed to the advancement of downdraft gasification technology and promoted cleaner and more sustainable biomass conversion solutions.

Table 3.2: Key chemical reactions in the downdraft biomass gasification system

Reactor Zone	Chemical Equation	Reaction heat energy(kJ/mol)	Reaction name	Reaction ID
Drying	<i>Wet biomass</i> → <i>Dried biomass</i> + <i>moisture</i>	NA	Drying	R ₁
Pyrolysis	<i>Dried Biomass</i> → <i>volatiles</i> ($CO_2, CH_4, H_2, CO, H_2O$) + <i>Char</i>	NA	Pyrolysis	R ₂
Combustion	$C + O_2 \rightarrow CO_2$	-393.77	Full oxidation	R3
	$C + 0.5 O_2 \rightarrow CO$	-110.4	Partial oxidation	R4
Reduction	$H_2 + 0.5O_2 \rightarrow H_2O$	-241.8	H ₂ oxidation	R5
	$CO + 0.5O_2 \rightarrow CO_2$	-282	CO oxidation	R6
	$CH_4 + 2O_2 \rightarrow CO_2 + H_2O$	-802.3	CH ₄ oxidation	R7
	$CO + H_2O \rightarrow H_2 + CO_2$	-42	Water Gas Shift	R8
	$CH_4 + H_2O \rightarrow H_2 + CO$	232.8	Steam Methane Reforming	R9
	$C + H_2O \rightarrow H_2 + CO$	138.3	Water Gas	R10
	$C + CO_2 \rightarrow 2CO$	170.45	Boudouard	R11
	$C + H_2 \rightarrow CH_4$	-93.8	Methanation	R12
	$H_2 + S \rightarrow H_2S$	NA	H ₂ S formation	R13
	$0.5N_2 + 1.5H_2 \rightarrow NH_3$	NA	NH ₃ formation	R14
Hot Exit	$CO + H_2O \rightarrow H_2 + CO_2$	-42	Water Gas Shift (High temperature)	R15

3.4.1.4 Aspen block and stream configuration

The Aspen Plus simulation was structured using distinct block configurations to accurately model each stage of the biomass gasification process (Figure 3.6). This approach ensured that the specific characteristics of each feedstock were effectively represented. The block types were configured to handle various physical and chemical transformations, as detailed below:

- RStoic Blocks were used to model feedstock drying at 150°C, with separate blocks assigned to each feedstock type to account for differences in moisture content before further processing.
- Flash2 and Sep Blocks facilitated the separation of moisture (SEP-F1, SEP-F2) and impurities from syngas (SEP-WAT).

- c) FSplit and SSplit Blocks managed the distribution of steam and air across the drying, pyrolysis, and combustion zones. Steam distribution (SPLIT-AS) was configured to enhance gasification reactions, while air distribution (SPLIT-AIR) ensured adequate combustion.
- d) Heater and REquil Blocks were used to cool the syngas to room temperature (SR-COL block), while the COM-ZON block simulated combustion under equilibrium conditions to generate heat within the gasifier.
- e) Mixer and RYield Blocks enabled the combination of various feed streams and facilitated the decomposition of unconventional components into conventional elements to improve accuracy in process representation.
- f) RGibbs Blocks were applied to simulate the pyrolysis (PYRO-ZON) and reduction (RED-ZON) zones under equilibrium conditions, ensuring precise modeling of gas-phase reactions.

3.4.1.5 Dynamic computations

Calculator blocks were employed in the Aspen Plus simulation (Figure 3.6) to enable dynamic computations, ensuring precise modeling of feedstock blending and process conditions. These blocks allowed for real-time adjustments to key variables, aligning with the specific requirements of the gasification process. Their functions included:

- a) CAL1-F1 and MAS-F2: Determined the percentage of each feedstock in the blend based on total feed flow rates.
- b) CAL5: Computed the exit temperature of the gasifier.
- c) ER: Calculated the total airflow rate required based on the ER input.
- d) SBR: Determined the steam flow rate relative to biomass input.

3.4.1.6 Measurable output parameters

The measurable output parameters of the simulation included temperature distribution metrics such as pyrolysis temperature (T_p), combustion temperature (T_c), reduction temperature (T_r), and exit temperature (T_e), all recorded in degrees Celsius. Additionally, the model quantified the airflow rate, gas flow rate, and char flow rate, measured in kilograms per hour. These parameters provided essential insights into the operational dynamics of the gasifier, enabling accurate performance assessment and process optimization.

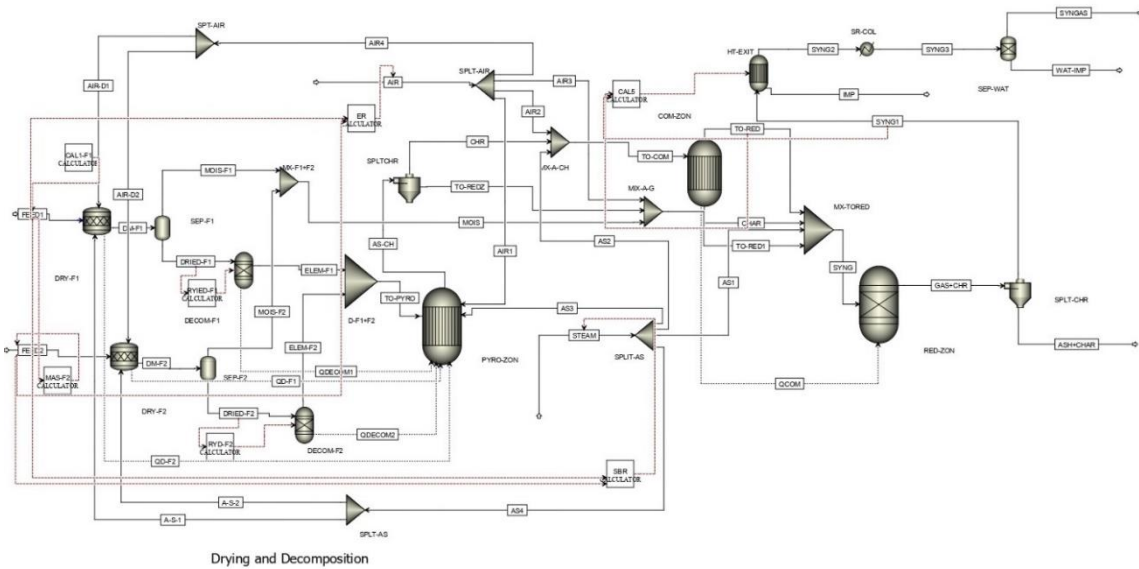


Figure 3.6: Flowsheet of the Aspen plus simulation model for co-gasification process. APPENDIX A and B provide detailed description and enlarged flowsheet of the diagram, respectively.

3.4.2 Performance metric calculation

The evaluation of the biomass co-gasification process relied on various performance metrics to assess the system's effectiveness and efficiency. These metrics were derived from simulation output parameters, such as syngas flow rate and char flow rate. Key calculated parameters included syngas composition, gas yield, char yield, lower heating value (LHV) of syngas, cold gas efficiency (CGE), and carbon conversion efficiency (CCE).

3.4.2.1 Syngas composition

The syngas composition (vol.%), representing the volumetric percentages of H₂, CO, CO₂, and CH₄, was analyzed to assess syngas quality and suitability for various applications. Accurate determination of syngas composition enabled the optimization of gasification conditions for improved energy recovery and tailored syngas utilization in power generation, hydrogen production, and chemical synthesis (Mutlu & Yucel, 2018; Lestander et al., 2022). The composition was calculated using Eqs. (3.17) - (3.19), which quantifies the contributions of individual gases to the total syngas yield.

$$\text{Moles of component} = \frac{\text{Mass flow rate of component}}{\text{Molecular weight}} \quad (3.17)$$

$$\text{Total moles of syngas} = \sum \text{moles of gas component} \quad (3.18)$$

$$\text{Gas component (vol\%)} = \frac{\text{Moles of Component}}{\text{Total Moles of Gas}} \times 100 \quad (3.19)$$

Where; total moles of syngas (mol/h) is the sum of molar flow rates of all syngas components. Mass flow rate (kg/h) is the mass of syngas or its components processed per hour. Molecular weight (kg/mol) is the molar mass of each gas, converting mass to moles. Moles of component (mol/h) is the molar flow rate of individual gas components like H₂, CO, or CO₂.

3.4.2.2 Syngas yield

Syngas yield, expressed in standard cubic meters per kilogram of biomass (Nm³/kg), quantifies the volume of syngas produced per unit mass of feedstock under standard temperature and pressure (STP) conditions. It was calculated using the total molar flow of gaseous components and the molar volume at STP, relative to the biomass feed rate, as shown in Eq. (3.20):

$$\text{Gas yield (Nm}^3\text{/kg)} = \frac{n_{\text{gas}} \times V_m}{\text{BFR}} \quad (3.20)$$

Where n_{gas} is the total moles of syngas produced (mol), V_m is molar volume at standard conditions ($22.414 \times 10^{-3} \text{ m}^3/\text{mol}$), BFR is biomass feed rate (kg/h).

This calculation allows the conversion of the total moles of syngas into a volumetric yield per unit mass of biomass. Syngas yield is an essential metric for evaluating gasification efficiency, comparing feedstock performance, and optimizing process parameters (Ma et al., 2024).

3.4.2.3 Char yield

Char yield, expressed in kg of char per kg of biomass feedstock (kg/kg), was calculated to determine the solid residue remaining after gasification. Using Eq. (3.21), the mass of generated char was evaluated relative to the total feedstock mass:

$$\text{Char yield (kg/kg)} = \frac{CFR}{BFR} \quad (3.21)$$

Where CFR is the char is flow rate (kg/h), and BFR is the biomass feed rate (kg/h).

Char yield provides an important measure of biomass conversion efficiency and helps understand the distribution of products among gaseous, liquid, and solid phases. Additionally, it plays a key role in optimizing reactor design and operational parameters for achieving the desired product balance (Sison et al., 2023; X. Zhu et al., 2019).

3.4.2.4 Lower heating value of syngas

The LHV of syngas represents the energy released per kilogram of syngas during combustion, excluding the latent heat of water vapor. It was calculated using Eq. (3.22), which accounts for the volumetric composition and heating values of individual gas components. This parameter is essential for evaluating the energy potential of syngas, optimizing gasification for maximum energy recovery and efficiency (Kartal & Özveren,

2020). Understanding the LHV also facilitates the assessment of syngas suitability for various energy applications (Hossain et al., 2024).

$$LHV (MJ/Nm^3) = [30 \times CO (\%) + 25.7 \times H_2 (\%) + 85.4 \times CH_4 (\%)] \times 4.2 \quad (3.22)$$

Where: CO (%), H₂ (%), and CH₄ (%) are the volume percentages of each component in the syngas.

3.4.2.5 Cold gas efficiency

The Cold Gas Efficiency (CGE) measures the efficiency of converting the chemical energy in biomass into the chemical energy of the produced syngas. It was calculated using Eq. (3.23), which considers the lower heating values (LHV) of both the syngas and the biomass feedstock:

$$CGE (\%) = \left(\frac{LHV_g \times GFR}{LHV_b \times BFR} \right) \times 100 \quad (3.23)$$

Where LHV_g is the lower heating value of syngas (MJ/Nm³), GFR is volumetric flow rate of syngas (Nm³/h), LHV_b is the lower heating value of biomass (MJ/kg), BFR is biomass feed rate (kg/h).

CGE, expressed as a percentage, provides a key performance indicator of energy transfer efficiency from biomass to syngas and helps evaluate the effectiveness of the gasification process (Awais et al., 2021). Higher CGE values indicate optimized process conditions and improved energy utilization, making it a crucial metric for assessing the economic and environmental feasibility of gasification systems (Hossain et al., 2024).

3.4.2.6 Carbon conversion efficiency

The carbon conversion efficiency (CCE) quantifies the percentage of carbon in biomass that is converted into gaseous products during gasification. It was calculated using Eq. (2.4), incorporating the carbon content in both the feedstock and gaseous products. CCE

serves as a key indicator of carbon utilization efficiency, with higher values reflecting effective carbon conversion, reduced char formation, and maximized gaseous product yield (Awais et al., 2021).

$$CCE (\%) = \left(\frac{TC_g}{TC_b} \right) \times 100 \quad (3.24)$$

Where: TC_g is the total carbon in syngas which refers to the mass of carbon in syngas components such as CO, CO₂, CH₄, and other hydrocarbons. TC_b is the total carbon in biomass which accounts for the total carbon content in the biomass feed material.

3.4.3 Model validation

The model was operated under standard conditions, maintaining a reactor pressure of 1 bar and a feed temperature of 25°C, with a biomass feed rate of 30 kg/h. The drying zone was set at 150°C, aligning with steam temperature to enhance moisture removal before gasification. For validation, experimental data from Awais et al. (2022), were analyzed, focusing on a 24 kWe downdraft biomass gasifier (Figure 3.7). The study investigated two biomass blends: 50/50% wood chips (WC) and corn cobs (CC) (WC&CC), and 50/50% sugarcane bagasse (SB) and coconut shells (CS) (SB&CS). The proximate, ultimate, and calorific properties of these feedstocks are presented in Table 3.3, with HHV and LHV calculated using Eqs. (3.25) and (3.26).

The experimental trials evaluated gasification efficiency, reactor thermal profiles, and the impact of ER on syngas yield and tar content. Trials were conducted over a temperature range of 650–950°C for combustion zone, with equivalence ratios from 0.15 to 0.30, providing a basis for comparing model predictions with real-world gasification performance. During validation, reactor zone temperatures (pyrolysis, combustion, and reduction) were compared for SB&CS and WC&CC blends at ER 0.17, while gas yield was assessed at ERs 0.17 and 0.29 for SB&CS.

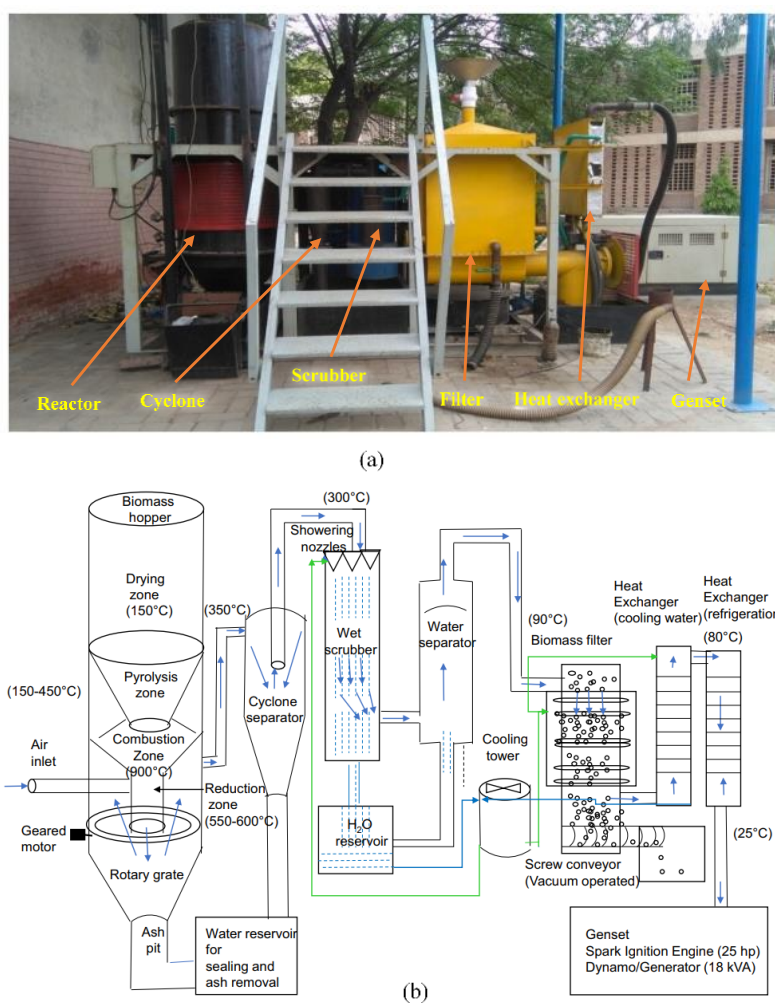


Figure 3.7: Pilot-scale downdraft gasification system
 Legend: (a) Pictorial view and (b) schematic diagram; source (Awais et al., 2021).

Table 3.3 Proximate, ultimate and calorific value of the feedstock (Awais et al., 2022)

Biomass	Coconut shell (CS)	Sugarcane bagasse (SB)	Wood Chip (WC)	Corn Cob (CC)
Proximate analysis (wt.%)				
Moisture	3.0	7.90	7.50	12.00
Volatile	77.94	81.56	74.50	68.50
Fixed carbon	18.06	10.98	14.50	17.00
Ash	0.65	5.33	3.50	2.50
Ultimate analysis (wt.%)				
C	54.68	45.52	48.12	44.00
H	7.15	5.69	6.12	6.90
O	39.12	43.58	42.18	44.71
N	0.58	0.35	0.08	1.80
S	0.06	0.15	0.00	0.09
Ash	0.65	5.33	3.50	2.50
Calorific value (MJ/kg)				
HHV	23.38	17.75	19.42	18.56
LHV	21.76	16.33	17.92	16.78

Root Mean Square Deviation (RMSD), calculated using Eq. (3.27), was used to validate the model due to its sensitivity to large errors and reliability in measuring discrepancies (Ranjan et al., 2024). By emphasizing significant deviations, RMSD ensured precise evaluation of temperature distribution and gas yield predictions. It served as a robust metric for assessing model accuracy and guiding further improvements.

$$HHV = 0.3417C + 1.3221H + 0.1232S - 0.1198(O + N) - 0.0153A \quad (3.25)$$

$$LHV_{biomass} = HHV_{biomass} - hf_g \left(\frac{9H+M}{100} \right) \quad (3.26)$$

$$RMSD = \sqrt{\frac{\sum_{i=1}^n (y_{model,i} - y_{exp,i})^2}{n}} \quad (3.27)$$

Where; $y_{model,i}$ represents the value predicted by the model, $y_{exp,i}$ denotes the value obtained from experiments, n is the number of observations or data points., M is the moisture of biomass, hf_g is a specific heat (2.4MJ/kg), and H is a weight percentage of hydrogen in the fuel.

3.4.4 Sensitivity analysis

Sensitivity analysis was conducted to optimize and understand the dynamics of biomass co-gasification, with a focus on the effect of ER on temperature distribution, gas composition, and gas and char yields. The ER was varied across 0.17, 0.22, 0.27, 0.28, and 0.29 for SB&CS and WC&CC feedstock blends, while all other parameters were held constant to isolate its impact.

The blend ratio was maintained at 50%, ensuring equal mass contributions from both biomass types. The Steam-to-Biomass Ratio (SBR) was set at 0.5, and the biomass feed rate remained 30 kg/h. This systematic approach allowed for a precise evaluation of changes in thermal behavior, syngas composition, and conversion efficiency induced by

variations in the ER. Such analyses were essential for identifying optimal operating conditions and for improving the efficiency and robustness of the gasification system.

3.4.5 Aspen plus simulation challenges

Developing and validating the biomass gasification simulation model involved overcoming several challenges. The following challenges were encountered during model development:

- a) Ensuring balanced air and steam flow across reactor zones was critical for maintaining appropriate temperature profiles throughout the system.
- b) Both excessively high and low temperatures in the combustion zone led to convergence failures during simulation. These unstable thermal conditions hindered the generation of reliable results and affected the accurate prediction of gasification efficiency and syngas quality.
- c) The combustion zone involved complex reactions with multiple reactants under varying conditions, increasing the difficulty of accurate modeling.
- d) Selecting the appropriate reaction models and kinetic parameters was essential to achieving realistic biomass-to-syngas conversion.
- e) Managing heat transfer between zones required precise calculations to prevent localized temperature imbalances that could affect gas composition and system efficiency.
- f) Each reaction zone including drying, pyrolysis, combustion, and reduction, exhibited distinct thermal and chemical behaviors, which made accurate representation of their interactions particularly challenging.
- g) Aligning the simulation results with real-world gasification performance data required iterative testing and parameter adjustments.

Addressing these challenges required careful use of experimental data, and refining control strategies, to enhance model accuracy and practical applicability.

3.5 ML Development and Application

This section outlines the methodological approach used to develop and evaluate machine learning (ML) models for optimizing biomass waste co-gasification. The methodology consists of six main stages: data generation, data preprocessing, data splitting, model training, model validation, and hyperparameter optimization, as illustrated in Figure 3.8.

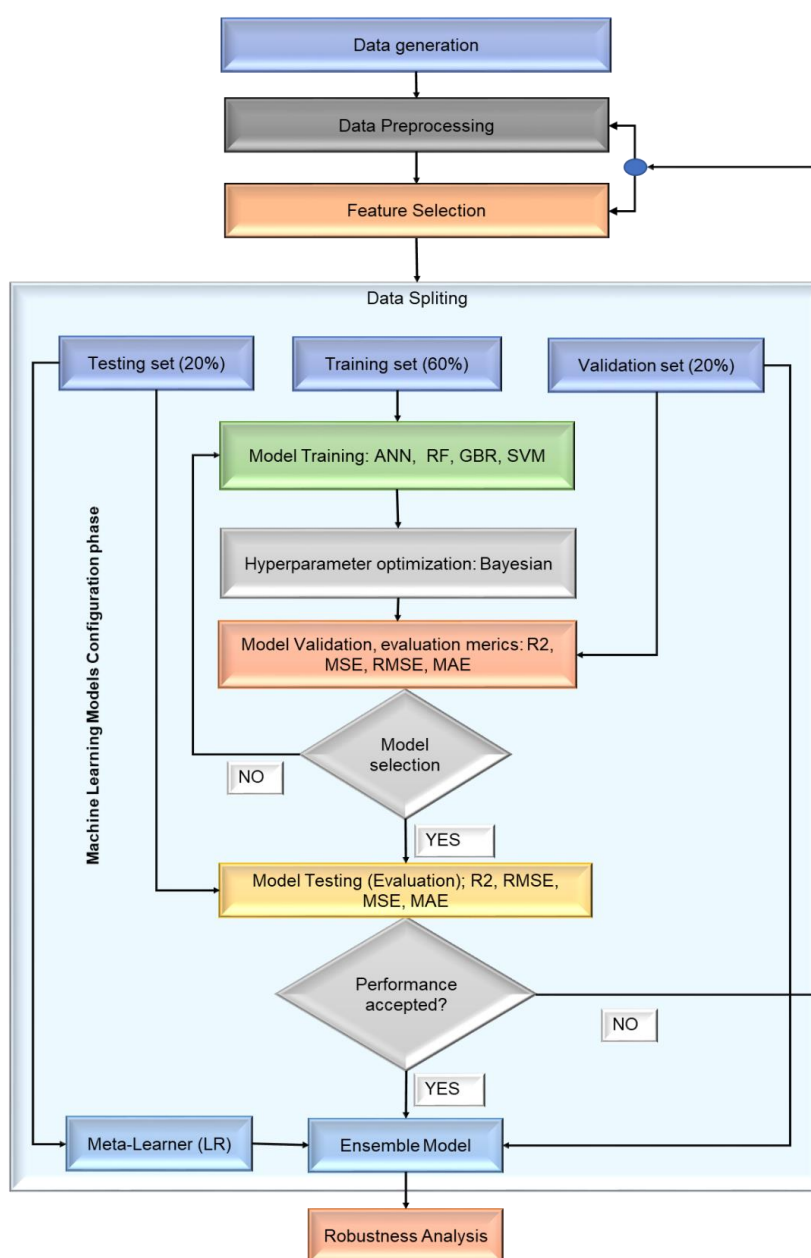


Figure 3.8: Flowchart illustrating the ML model development process

The process began with data generation, ensuring that high-quality experimental data serve as reliable inputs. Next, data preprocessing techniques, including cleaning, normalization, and feature selection, were applied to prepare the data for effective modeling. The dataset was then splitted into training, validation, and test sets to facilitate model learning and performance assessment. Various ML algorithms were trained and optimized to enhance predictive accuracy. Finally, model evaluation metrics were used to assess performance in terms of accuracy and generalizability, ensuring that the models were suitable for real-world biomass COG optimization.

3.5.1 Data generation

Data were generated through simulation experiments using the validated co-gasification model, ensuring a systematic and structured approach to capturing process dynamics. The Central Composite Design (CCD) framework was employed to organize the experiments efficiently, but the intent was not statistical optimization (Response surface methodology, RSM). Instead, CCD facilitated comprehensive data collection across a well-defined experimental space, which enhanced the model's predictive capabilities.

The simulations involved binary blends of five biomass feedstocks (coffee husk, groundnut shell, macadamia nutshell, rice husk, and tea waste) and considered two gasifying agents: air and air-steam mixture. The study examined four key process variables under air gasification: pressure (0.5 to 2.5 bar), ER (1.5 to 3.5), blend percentage (0 to 100%), biomass feed rate (25 to 45 kg/h). For air-steam mixture, the same experimental design was adopted, except that pressure was kept constant while the steam-to-biomass ratio (SBR) was varied from 0.5 to 2.5. These ranges were selected based on values commonly reported in literature for pilot-scale downdraft gasifiers, as well as their relevance to practical operating conditions in biomass-rich regions. The chosen ranges ensured adequate coverage of both under- and over-gasification conditions.

Each variable was tested at five levels (-2, -1, 0, 1, 2) to systematically explore their effects (Table 3.4). The rotatable CCD design ensured uniform variance across the experimental space, enabling detailed analysis of interactions without bias. This structured data generation approach provided a comprehensive dataset for ML model training, while preserving realism and enhancing generalizability in biomass co-gasification simulations.

Table 3.4: Experimental factors and their levels used in the CCD for this study

Factor	Unit	$\alpha = -2$	-1	0	1	$\alpha = 2$
Pressure	Bar	0.5	1.0	1.5	2.0	2.5
Equivalence Ratio	(-)	1.5	2.0	2.5	3.0	3.5
Blend percentage	%	0	25	50	75	100
Biomass feed rate	kg/h	25	30	35	40	45

Building on the structured data generation setup, the approach ensured a comprehensive representation of various gasification conditions. A total of 500 data points were collected, equally divided between air and air-steam mixture experiments. This extensive dataset allowed for an in-depth analysis of how different gasifying agents interacted with various feedstock blends, capturing critical process dynamics.

The size and diversity of the dataset were essential in developing a robust and generalizable model. By encompassing a wide range of conditions and feedstock combinations, the dataset facilitated the application of ML techniques, enhancing model accuracy and predictive power. This structured data generation laid a strong foundation for advancing biomass co-gasification technology, which provided valuable insights for future research and practical applications.

3.5.2 Data preprocessing

Data preprocessing was essential for ensuring accuracy, reliability, and optimal performance of the ML models. A multi-step approach was employed, including feature

engineering, data encoding, normalization, and shuffling to enhance the dataset's usability.

3.5.2.1 Feature engineering

Feature engineering was conducted to enhance the representational capacity of the dataset, particularly by incorporating blend ratios of different biomass types. Engineered features included: CoffeeHusk_Ratio (percentage of coffee husks in the blend), GroundnutShell_Ratio (percentage of groundnut shells), MacadamiaNutshell_Ratio (percentage of macadamia nutshells), RiceHusk_Ratio (percentage of rice husks), and TeaWaste_Ratio (percentage of tea wastes). These ratios provided a quantitative basis for analyzing the impact of each biomass type on gasification performance.

To further refine the dataset and improve predictive accuracy, proximate and ultimate analysis values were adjusted to reflect the blend composition of each data point. This involved recalculating: Proximate analysis (Moisture content, ash content, volatile matter, and fixed carbon) and Ultimate analysis (Carbon, hydrogen, nitrogen, sulfur, and oxygen content).

For the blends, these properties were calculated using the weighted average method, which considers the proportional contributions of each biomass component in the mixture. The weighted average ensures that the blend's overall properties accurately reflect the mass fraction of each biomass type, as described by Eq. (3.28):

$$P_{blend} = \sum_i^n (P_i \times W_i) \quad (3.28)$$

Where: P_{blend} is property value of the blend, P_i is property value of individual biomass component, W_i is mass fraction of the biomass component in the blend, and n is total number of biomass components in the blend.

This method allowed the ML models to capture variations in biomass composition and their influence on gasification efficiency. The calculations were performed using Microsoft Excel, leveraging its efficient computation tools for adjusting input parameters based on biomass composition.

3.5.2.2 Encoding of categorical variables

For categorical variables, one-hot encoding was implemented to convert categorical data into a binary format, ensuring that the model could process these variables without introducing artificial relationships. This method was preferred over label encoding or ordinal encoding, as it prevents the model from misinterpreting categorical values as having a ranked or numerical relationship.

One-hot encoding transformed each categorical variable into multiple binary columns, with each column representing a distinct category. This approach was particularly beneficial for nominal data, such as biomass types and operational settings, which do not follow an inherent order. The encoding process was conducted using MATLAB, facilitating its functionality to segment categorical inputs into multiple columns, ensuring seamless integration into the ML modeling workflow.

3.5.2.3 Normalization of numerical variables

Normalization of numerical variables was conducted using the Min-Max scaling method, which scales features to a $[0,1]$ range. This approach was chosen because it preserves the original distribution of variables while ensuring that features are on a consistent scale, which is particularly beneficial for scale-sensitive models such as neural networks and distance-based algorithms. By standardizing numeric features, Min-Max scaling prevents issues related to model convergence and performance degradation caused by features with varying scales.

The normalization process was performed in MATLAB, utilizing its robust capabilities for efficiently handling large datasets and applying mathematical operations. The Min-Max normalization equation (Eq. (3.29)) used for scaling is:

$$\hat{x} = \frac{x - \min(x)}{\max(x) - \min(x)} \quad (3.29)$$

Where; $\hat{x}$ is the normalized value of the feature, x is original value of the feature, $\min(x)$ is the minimum value of the feature in the dataset, $\max(x)$ is the maximum value of the feature in the dataset.

It is important to note that all output variables used for ML model training, validation, and testing were normalized prior to modeling. Normalization transforms the data into a unitless scale, allowing fair comparison across variables with different measurement units and preventing model bias toward high-magnitude features. Consequently, performance visualizations such as Predicted vs. True scatter plots display normalized values, which do not carry physical units.

3.5.2.4 Data shuffling

To enhance the integrity and robustness of data analysis, data shuffling was implemented after the structured collection of 500 data points across different gasification conditions. Since the data was generated in sets corresponding to specific experimental conditions, there was a risk of order-specific biases influencing model training. These biases could stem from sequential data collection, potentially introducing artificial patterns unrelated to the underlying gasification process.

To mitigate this, the dataset was randomized before model training using MATLAB's *randperm* function, which efficiently generates random permutations of dataset indices. This ensured a thorough and unbiased mixing of data points, preventing the model from learning spurious time-based or sequence-based dependencies. By shuffling the data, the

study eliminated potential biases, reduced overfitting risks, and improved model generalizability, ensuring that predictions were based on a representative and diverse sample of the gasification process.

3.5.3 Feature and response selection

To optimize the dataset and enhance model accuracy, a strategic feature and response selection process was implemented. This approach focused on reducing redundancy, improving model stability, and ensuring the inclusion of key variables that influence gasification performance.

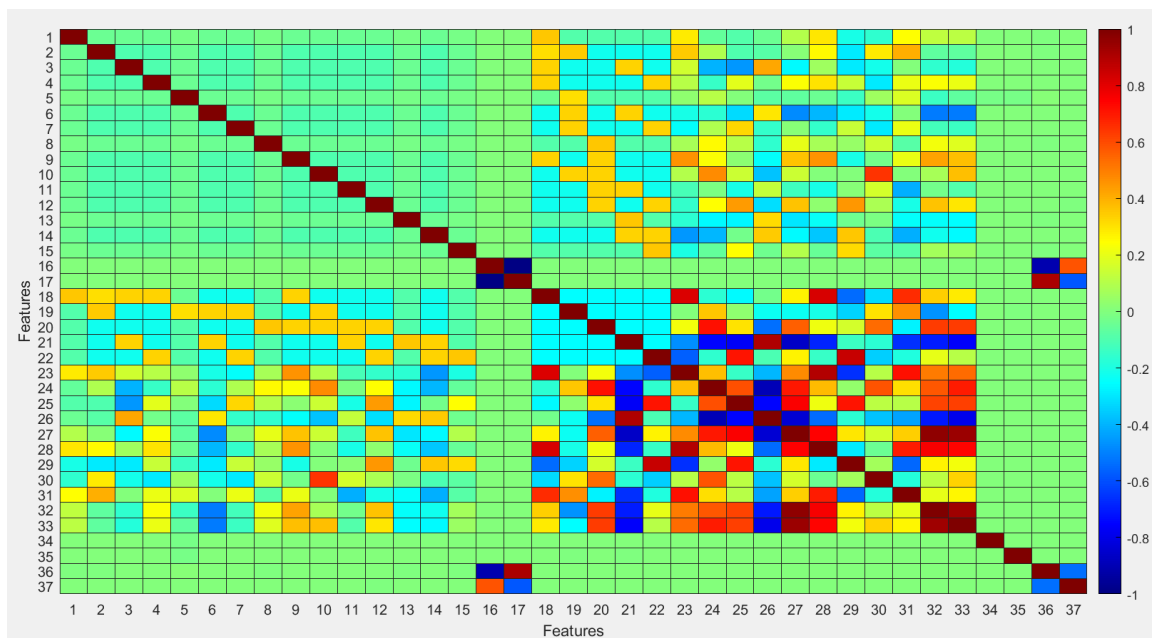


Figure 3.9: Correlation matrix of original features in the dataset

Legend: The number 1-37 are the feature label as appeared in the dataset [see APPENDIX C]

3.5.3.1 Feature selection

Feature selection was performed using correlation coefficient analysis to identify and eliminate highly correlated features, mitigating multicollinearity that could affect model interpretability. Variables such as biomass HHV and LHV were excluded due to their strong correlation with other predictors (Figure 3.9). However, Air and AirSteam

gasifying agents and the SBR were retained despite potential correlations, as they directly impact syngas composition, calorific value, and key thermochemical reactions.

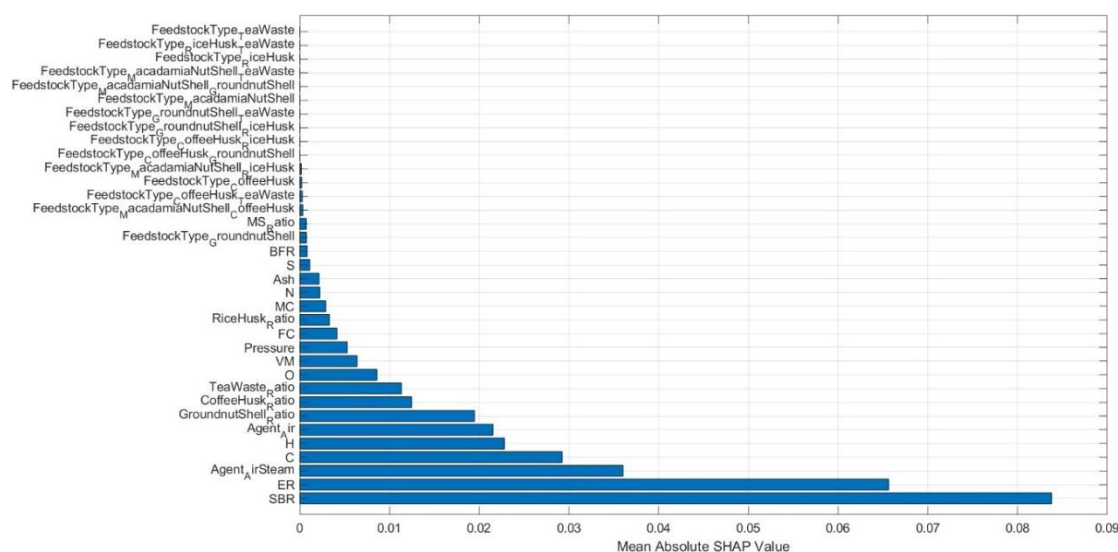


Figure 3.10: Preliminary feature importance analysis using global SHAP method

Table 3.5: Descriptive statistics of selected feature/predictor/input variables

Variable	N	Unit	Mean	StDev	Min	Max	Norm
Agent	500		Air (encoded), air and steam (encoded)				[1,0]
Feedstock1_Ratio	500	-	0	0	0	0	0...0
Feedstock2_Ratio	500	-	0	0	0	0	0...0
CoffeeHusk_Ratio	500	-	0.2	0.290118	0	1	0...1
GroundnutShell_Ratio	500	-	0.2	0.290118	0	1	0...1
MacadamiaNutshell_Ratio	500	-	0.2	0.290118	0	1	0...1
RiceHusk_Ratio	500	-	0.2	0.290118	0	1	0...1
TeaWaste_Ratio	500	-	0.2	0.290118	0	1	0...1
MC	500	wt%	6.914	0.783622	5.69	8.67	0...1
VM	500	wt%	63.96	2.31387	59.19	68.52	0...1
FC	500	wt%	19.62	1.74632	15.9	23.01	0...1
Ash	500	wt%	9.506	3.83506	3.03	19.01	0...1
C	500	wt%	47.692	3.11327	40.31	52.49	0...1
H	500	wt%	5.198	0.499209	4.26	6.33	0...1
N	500	wt%	1.636	0.419861	0.96	2.68	0...1
O	500	wt%	35.056	1.93678	32.58	40.76	0...1
S	500	wt%	0.04	0.0155591	0.01	0.07	0...1
BFR	500	kg/h	35.2506	5.63995	0.3	50	0...1
ER	500	-	0.2528	0.0539257	0.15	0.4	0...1
SBR	500	-	0.162	0.189282	0	0.8	0...1
Pressure	500	Bar	1.265	0.466594	0.5	3	0...1

To further refine the dataset, SHAP analysis was applied (Figure 3.10). This technique identified low-impact categorical features, such as feedstock types, which were excluded due to their minimal influence on model predictions. However, Macadamia Nutshell_ratio

was retained despite its relatively low SHAP value, as it contributed uniquely to feedstock interactions, improving the model's predictive accuracy.

The final selected features are presented in Table 3.5, which also includes their descriptive statistics. Additionally, new variables (Feedstock1_Ratio and Feedstock2_Ratio) were introduced and initially set to zero. These placeholders allow the model to adapt to potential new feedstocks in future iterations, enhancing its versatility and responsiveness to varying input conditions.

3.5.3.2 Response selection

For model responses, six key performance metrics relevant to electricity generation and biochar production were selected. These include:

- a) H₂ and CO (major syngas components)
- b) CGE (Cold Gas Efficiency) (energy conversion efficiency)
- c) LHV (Lower Heating Value) (energy content of syngas)
- d) Gas yield (syngas production efficiency)
- e) Char yield (biochar production assessment)

These responses were chosen for their critical roles in evaluating syngas quality, energy efficiency and by-product utility, and their descriptive statistics are depicted in Table 3.6.

Table 3.6: Descriptive statistics of selected response/target/output variables

Variable	N	Unit	Mean	StDev	Min	Max	Norm
H2	500	Vol%	39.4856	3.32999	29.1372	49.6467	0...1
CO	500	Vol%	38.6343	9.78959	14.1867	56.6949	0...1
GasYield	500	Nm ³ /kg	1.22166	0.194308	0.743858	1.74443	0...1
CharYield	500	Kg/kg	0.0555569	0.0558805	0	0.224954	0...1
CGE	500	%	65.1635	8.36718	42.3284	79.3130	0...1
LHV	500	MJ/m ³	10.0625	0.551852	7.48435	11.0847	0...1

3.5.4 ML models configuration

To ensure optimal performance and reliability, ML models were configured with a structured approach involving data splitting, algorithm selection, hyperparameter tuning,

and validation strategies. These configurations aimed to maximize predictive accuracy and enhance generalization capabilities.

3.5.4.1 Data splitting strategy

A total of 500 simulated data points were compiled for machine-learning model development. This sample size is adequate for supervised regression tasks involving medium-complexity models and a moderate number of input features. Several studies have demonstrated that datasets in the range of 300–500 observations provide sufficient statistical power for training non-linear ML models (e.g., Random Forest, Gradient Boosting, ANN) while still allowing reliable generalization to unseen data. In this study, the dataset size was also justified by the nature of the gasification process: generating a significantly larger dataset experimentally or through simulations would require substantial time and computational cost, whereas 500 well-distributed data points allow for efficient model learning without redundancy or overfitting (Ozonoh et al., 2020; Rasheed et al., 2022).

To optimize model training and ensure rigorous performance evaluation, the dataset was partitioned into three subsets using a 60-20-20 split:

- a) Training set (60%) – 300 data points
- b) Validation set (20%) – 100 data points
- c) Testing set (20%) – 100 data points

The 60% training portion provides a sufficiently large subset for the model to learn underlying relationships between input features and target variables, which is essential given the heterogeneity of biomass properties and operating conditions. The validation set (20%) enables effective hyperparameter tuning and early-stopping decisions, helping prevent overfitting and optimizing model complexity. The test set (20%), kept completely independent from model development, ensures an unbiased estimate of the model's

predictive performance and real-world applicability (Ozonoh et al., 2020; Rasheed et al., 2022).

The 60-20-20 partition is one of the most widely accepted strategies in ML research because it balances three competing needs: (i) enough data to train complex models, (ii) sufficient validation samples for model tuning, and (iii) a completely independent dataset for final performance assessment (Ozonoh et al., 2020; Rasheed et al., 2022). This structure enhances the robustness, reliability, and reproducibility of the resulting models, ensuring that conclusions drawn from the ML analysis are statistically sound and applicable across a wide range of operational scenarios in biomass co-gasification.

3.5.4.2 Algorithm selection

To develop robust predictive models for gasification performance, a combination of ensemble and non-ensemble models was integrated into a SLE framework, optimizing predictive accuracy. Each algorithm was selected for its ability to handle nonlinear relationships and high-dimensional data effectively.

- a) Ensemble Models: Random Forest (RF); Chosen for its robustness and ability to reduce overfitting by averaging multiple decision trees. Gradient Boosting Regression (GBR); Selected for its strength in capturing complex patterns through sequential learning.
- b) Non-Ensemble Models: Support Vector Regression (SVR); Effective in handling high-dimensional data and capturing nonlinear dependencies. Artificial Neural Networks (ANN); Ideal for modeling complex relationships, particularly in thermochemical processes.
- c) SuperLearner Framework: Aggregates predictions from all models; Assigns weights to individual models based on performance; Train meta-learner based on

the prediction of the individual models; Enhances overall predictive accuracy and generalization capability.

3.5.4.3 Cross-validation training technique

A 10-fold cross-validation technique was employed, alongside a 10% independent test set, to ensure robust model evaluation and generalization capability. This approach was preferred over simpler methods, such as the hold-out validation, due to its ability to minimize bias and maximize data utilization, particularly in scenarios with limited data availability.

In 10-fold cross-validation, the dataset was divided into ten equal parts, with each part alternately used as a validation set while the remaining data served as the training set. This method ensured that every data point was used for both training and validation, reducing variance and providing a more stable accuracy estimate across multiple subsets.

Additionally, a 10% independent test set was reserved for final evaluation, providing an unbiased assessment of model performance on truly unseen data. This step was crucial for verifying the model's ability to generalize beyond the training phase and detecting potential overfitting.

By combining 10-fold cross-validation with an independent test set, the study ensured that the models were comprehensively trained and rigorously evaluated, enhancing their reliability and applicability for gasification performance prediction.

3.5.4.4 Hyperparameters optimization

Bayesian optimization was used for efficient and effective hyperparameter tuning, reducing evaluations by selecting the most promising configurations rather than exhaustively searching (grid search) or randomly sampling (random search). This made it ideal for complex models and large datasets.

Each algorithm-specific hyperparameter was tuned to enhance performance:

- a) ANN: number of hidden layers and neurons per layer (determining network complexity); learning rate (influencing convergence speed and stability); activation functions (critical for capturing nonlinear patterns).
- b) GBR: number of trees (controls model complexity); learning rate (adjusts the weight of each tree in sequential learning); max tree depth (balances bias-variance tradeoff).
- c) RF: number of trees (determines overall model stability); maximum depth (prevents overfitting by limiting tree growth); minimum samples per split (controls how trees generalize).
- d) SVR: Kernel type (defines how data is transformed in high-dimensional space); C (penalty parameter) (adjusts the tradeoff between misclassification and margin maximization); Gamma (kernel coefficient) (influences decision boundary flexibility).

3.5.4.5 Multi-input single-output models

A Multi-Input Single-Output (MISO) approach was employed for its flexibility, simplicity, and computational efficiency over Multi-Input Multi-Output (MIMO) models. Each response (H_2 , CO, gas yield, char yield, CGE, and LHV) was modeled independently, allowing for precise tuning and optimized accuracy based on its unique distribution and predictor relationships. This approach enhanced control over optimization, improved interpretability, and ensured efficient resource utilization, making it ideal for gasification performance modeling.

3.5.4.6 SuperLearner framework

The SuperLearner model was developed using a refined retraining approach, where base models underwent 10-fold cross-validation on the validation dataset before final

evaluation on a separate test set. This method ensured comprehensive learning, reducing errors and enhancing generalization by exposing models to diverse data subsets.

LR was chosen as the meta-learner for its simplicity and effectiveness in combining predictions from ANN, GBR, RF, and SVR. By assigning optimal weights to each base model, it leveraged their strengths while compensating for weaknesses, maintaining computational efficiency and ensuring balanced, high-accuracy predictions for biomass co-gasification modeling.

3.1.1 Performance evaluation metrics

Selecting appropriate performance metrics is crucial for assessing model accuracy. While numerous statistical measures exist, their selection is guided by their effectiveness in related studies (Baashar et al., 2022). Presenting multiple metrics enhances interpretability (Ascher et al., 2022; Elmaz et al., 2020). This study employed four key evaluation metrics: R^2 , RMSE, MSE, and MAE.

3.1.1.1 Coefficient of determination

R^2 measures the proportion of variance in the dependent variable that can be explained by the independent variables in a regression model. It assesses the correlation between predicted and actual values, with values ranging from 0 to 1, where higher values indicate better model fit. R^2 is widely used to evaluate goodness-of-fit in regression models (Elmaz et al., 2020; Hasanipanah et al., 2016). It was calculated using Eq. (3.30).

$$R^2 = 1 - \left[\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \right] \quad (3.30)$$

Where R^2 is the coefficient of determination, y_i is the actual values of the dependent variable, $\hat{y}_i$ is the predicted values from the model, $\bar{y}$ is the mean of the actual values (y_i), n is the number of data points, i is an index used to denote each individual data point in a dataset (ranges from 1 to m).

3.5.4.7 Mean squared error

MSE is a widely used metric for evaluating regression models, calculated as the average squared difference between predicted and actual values. A lower MSE indicates better model performance, with a value of zero representing perfect accuracy. Due to the squaring of errors, MSE penalizes larger deviations more heavily, making it useful for detecting outliers (Chicco et al., 2021). MSE was computed using Eq. (3.31).

$$MSE = \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n} \quad (3.31)$$

Where; y_i is the actual values of the dependent variable, $\hat{y}_i$ is the predicted values from the model, n is the number of data points.

3.5.4.8 Root mean squared error

RMSE is the square root of the average squared differences between predicted and actual values, providing a measure of the average magnitude of prediction errors. A lower RMSE indicates better model accuracy. Due to the squaring process, RMSE is sensitive to outliers, as larger errors are amplified more than smaller ones (Hasanipanah et al., 2016; Olatunji et al., 2019; Yucel et al., 2019). RMSE was computed using Eq. (3.32).

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{n}} \quad (3.32)$$

Where; y_i is the actual values of the dependent variable, $\hat{y}_i$ is the predicted values from the model, n is the number of data points.

3.5.4.9 Mean absolute error

MAE measures the average magnitude of errors in predictions without considering their direction, making it suitable for datasets with uniformly distributed errors. Unlike MSE, MAE does not square errors, preventing the over-penalization of outliers, making it a

robust performance metric (Chai & Draxler, 2014; Goodfellow et al., 2019). MAE was computed using Eq. (3.33).

$$MAE = \frac{1}{n} \sum_{i=1}^n \left| \frac{y_i - \hat{y}_i}{y_i} \right| \quad (3.33)$$

Where; y_i is the actual values of the dependent variable, $\hat{y}_i$ is the predicted values from the model, n is the number of data points.

3.5.5 Challenges encountered during ML development

Developing ML models in MATLAB presented several challenges, affecting workflow efficiency and model implementation:

- a) MATLAB's *load* function sometimes returned structures that complicated direct variable access, which required additional steps for data extraction.
- b) Handling multiple models and datasets necessitated careful directory organization and naming conventions to avoid mismanagement.
- c) Issues like "Unable to use a value of type cell as an index" occurred, which required careful handling of data types and structures in tables and arrays.
- d) Different models required specific preprocessing steps, which added complexity when adapting techniques across models.
- e) Ensuring that functions were called correctly and in sequence, particularly for feature extraction and predictions, was critical.
- f) Merging different script components, such as model predictions and data denormalization, required careful coordination.
- g) MATLAB's error messages often indicated deeper data handling or function implementation issues, which necessitated a solid grasp of MATLAB structures and workflows.
- h) Implementing checks and balances was necessary to gracefully handle runtime errors and provide meaningful feedback for debugging and optimization.

These challenges required a structured approach to data processing, script management, and error handling to ensure smooth ML model development.

3.6 ML Model Robustness Analysis

A structured approach was employed to assess the robustness of SLE models, evaluating various combinations of base and meta-learners across multiple performance metrics. This analysis aimed to test the reliability and generalization of ML models developed for predicting key biomass gasification parameters, including CGE, char yield, gas yield, H₂, CO, and LHV, under diverse conditions.

The robustness analysis focused on evaluating model performance on unseen data, ensuring their practical applicability in real-world biomass gasification systems. This step was critical in validating the models' ability to maintain accuracy and stability across varying scenarios.

3.6.1 Unseen data generation and preparation

To rigorously test model robustness and generalization, an unseen dataset was generated using a simulation experiment in Aspen on a novel feedstock blend of sugarcane bagasse and coconut shell. This new feedstock challenged the model with previously unseen data, providing a stringent test of its predictive capabilities. The experimental setup and operating conditions mirrored those of the original dataset, ensuring that any performance differences were due to the new feedstock characteristics rather than variations in process conditions. Key features such as ER, SBR, and detailed feedstock composition were recorded, maintaining consistency with the original dataset.

3.6.2 SLE model configurations

Each Super Learner Ensemble (SLE) model was designed with a unique combination of base learners and a meta-learner to optimize predictions for different target variables

(CGE, char yield, CO, gas yield, H₂, and LHV). These configurations were tested under varied data conditions to evaluate model robustness and adaptability.

- a) SLE1: Base Learners (RF, GBR, ANN, SVR); Meta-Learner (LR); Configuration (Cross-validation on 400 data points to test stability across different subsets).
- b) SLE2: Base Learners (SVR, GBR, RF); Meta-Learner (LR, Eq. (3.34)); Configuration (Trained on 300 data points, validated on 100 data points, refining predictions using the best-performing base models);
- c) SLE3: Base Learners (SVR, GBR, RF); Meta-Learner (ANN); Configuration (Trained on 300 data points, validated on 100 data points, assessing ANN's impact compared to LR).

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n + \varepsilon \quad (3.34)$$

Where, β_0 is the intercept of the model. $\beta_1, \beta_2 \dots \beta_n$ are the coefficients of predictors (here x represents the predictions from base models) $x_1, x_2, \dots, x_n$, respectively.

For SLE3, the ANN meta-learner (Figure 3.11) processes base model predictions as inputs ($x_1, x_2, \dots, x_n$) through hidden layer or node (Σ , neuron) before generating final predictions (Y_m). The ANN structure, including the number of hidden layers and nodes, is optimized via backpropagation, adjusting weights (w_j, w_l) and biases (B_j, B_l) for improved accuracy (Ozonoh et al., 2020; Rasheed et al., 2022). Non-linearity is introduced through activation functions ($f^2(net)$), enabling the model to learn complex patterns (Ankenbrand et al., 2021; Ritsema, 2021).

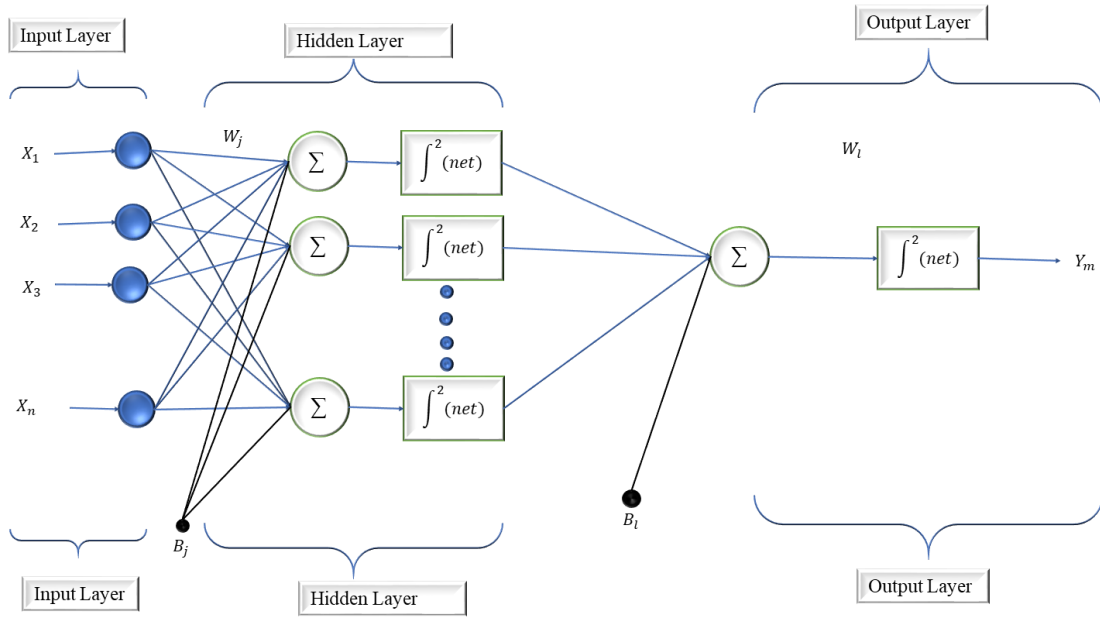


Figure 3.11: ANN meta-learner architecture

By using different meta-learners, the study assessed the effectiveness of a simple linear model (LR) versus a complex ANN-based approach. The combination of cross-validation and split-training with validation ensured that each SLE was rigorously tested, confirming its consistency and performance across different datasets. The varied base learner configurations leveraged RF's ability to handle large feature spaces and SVR's efficiency in high-dimensional settings, providing a balanced and comprehensive analysis of gasification modeling performance.

3.6.3 Model stress testing and evaluation

The stress testing phase evaluated the robustness of ML models by testing them on unseen feedstocks, biomass types not included in the training dataset. This approach simulated real-world conditions, where models must generalize to biomass with different properties than those they were trained on. Testing on unseen feedstocks assessed the model's ability to adapt predictions without prior exposure, ensuring applicability across diverse biomass sources. This process provided critical insights into potential biases or overfitting issues, helping verify model reliability beyond controlled training conditions.

3.6.4 Evaluation of model prediction

A comprehensive evaluation of model robustness was conducted by analyzing SuperLearner performance, variability in metrics, and error distribution.

- a) Comparison across SLE variants: SLE1, SLE2, and SLE3 were assessed under identical conditions to determine the most consistent and accurate configuration.
- b) Performance variability analysis: R^2 and RMSE fluctuations were examined across different datasets and operating conditions, providing insights into model adaptability and reliability.
- c) Error distribution analysis: Prediction errors were visualized to detect systematic biases, such as overfitting, underfitting, or data handling issues.

Because the robustness assessment required comparing the model predictions directly with the experimental (real-world) values, all predicted outputs were de-normalized before analysis. This ensured that the model predictions and experimental measurements were evaluated on the same physical scale. Consequently, the robustness plots and statistical metrics (R^2 and RMSE) were computed using the de-normalized data, allowing for accurate, meaningful, and interpretable comparison between model outputs and experimental results.

3.7 ML Model Interpretability Analysis

Interpretability analysis was essential for validating ML models, ensuring transparency, and understanding feature influence on predictions. This enhanced trust in model decisions, particularly in applications with significant operational impacts. A structured approach was employed to identify influential features, assess their effects, and detect potential biases using: permutation importance (PI) (evaluates feature contributions across model architectures) and Gini importance (GI) (assesses feature relevance in tree-based models) (Ascher et al., 2022; Zhao et al., 2021). This analysis focused on two key

gasification performance parameters (gas yield and char yield) due to their high prediction accuracy within robust models. By analyzing feature influence on these parameters, insights were gained to optimize process conditions, improving overall system efficiency and reliability.

3.7.1 Feature importance methods

To evaluate the influence of input features on model predictions, two global interpretability techniques were employed including PI and GI.

PI assesses feature relevance by randomly shuffling the values of each feature and measuring the resulting change in MSE. This disruption of the feature-target relationship allows for a direct quantification of the feature's contribution to model performance. PI is particularly effective at capturing nonlinear dependencies and interaction effects, making it suitable for a wide range of model types (Zhao et al., 2021).

GI was applied specifically to tree-based models, including RF and GBR. GI evaluates how much each feature contributes to reducing impurity within decision trees. The importance scores are computed by aggregating the reduction in impurity across all splits involving a given feature, thereby highlighting features most frequently used in the decision-making process. GI provides model-specific interpretability insights tailored to tree-based algorithms (Li et al., 2023; Yaman et al., 2018).

By integrating PI, which offers model-agnostic evaluation, with GI, which delivers tree-specific interpretability, this study achieved a comprehensive understanding of feature significance. This dual approach enhanced model transparency and provided valuable guidance for feature selection and engineering in future model development.

3.7.2 Feature effect visualization

PDPs were used to analyze how key features influence model predictions, focusing on both main and interaction effects. These visualizations provided critical insights for interpretation and decision-making in biomass gasification modeling.

Main factor effect: PDPs illustrated the marginal impact of features such as ER, SBR, and feedstock properties on predicted outcomes. By isolating individual feature effects while averaging others, PDPs revealed the direction and magnitude of relationships, aiding in process parameter tuning.

Interaction effects: Pairwise PDPs examined how simultaneous variations in two features influenced gas yield and char yield predictions. This helped identify synergistic or antagonistic interactions, informing process optimization and control strategies

3.7.3 Dataset and model selection

The testing dataset was utilized for interpretability analysis, incorporating key features such as ER, SBR, Carbon Content, and Ash Content, alongside documented process conditions to ensure a robust dataset for meaningful insights.

For model selection, a combination of tree-based models (RF, GBR) and non-tree ML models (ANN, SVR) was employed. These models were chosen for their effectiveness in predicting gas yield and char yield, ensuring a diverse analytical approach.

By applying interpretability methods across these varied architectures, the study provided a comprehensive evaluation of feature importance.

3.7.4 Evaluation of feature importance

A comparative analysis of PI and GI was conducted to assess feature rankings, identifying consistent patterns and methodological discrepancies. This evaluation provided insights into the strengths and limitations of each interpretability approach, ensuring a nuanced understanding of feature influence on model predictions.

Key features, which consistently ranked high across both methods were further analyzed for their operational and compositional relevance in biomass gasification. Additionally, PDPs were used to cross-reference findings, validating the actual impact of these features on model predictions.

3.8 Software Tools and Equipment

A comprehensive suite of software tools and experimental equipment was utilized to support data analysis, PS, ML model training, and experimental investigations.

Software tools: (i) MATLAB 2022b was used for ML model training (RF, GBR, ANN, and SVM), SuperLearner development, and interpretability analyses (PDPs, Permutation, and Gini Importance). (ii) Minitab 22 was used to design experiments to guide dataset generation. (iii) Microsoft Excel assisted with feature engineering, performance metric calculations, and data management. (iv) OriginPro 2022b was used for visualization of TGA and DTG Curves and kinetic modeling. (v) Aspen Plus V11 was used to Model the gasification process, integrating FORTRAN code for custom simulations, and generated simulated datasets for ML model training.

Experimental equipment: (i) Macro TGA & Micro TGA (STA 6000) were used to conducted proximate analysis and detailed thermal decomposition studies, respectively. (ii) CHNS Elemental Analyzer was used to perform ultimate analysis of biomass samples.

Computational setup: (i) HP ProBook 430 G4 Laptop with 12 GB RAM, 500 GB SSD, Core i7 (2.7 GHz) was used to handle data processing, ML modeling, and gasification simulations efficiently. (ii) Microsoft OneDrive was used as cloud storage system for data backup and security, ensuring protection against data loss.

3.9 Ethical Considerations

This research upheld ethical standards by ensuring data integrity, transparency, and environmental responsibility throughout the study.

- a) Maintained rigorous documentation of data collection, analysis methods, and model development to ensure reproducibility and reliability. Provided clear traceability and verification for other researchers, reinforcing scientific credibility.
- b) Simulated gasification processes were designed to minimize emissions and energy consumption, aligning with sustainable development goals.

3.10 Quality Assurance Measures

To ensure the accuracy and reliability of findings, quality assurance measures were rigorously implemented throughout the study.

- a) Thermogravimetric analyzers were regularly calibrated per manufacturer guidelines to maintain measurement precision.
- b) Tools like MATLAB, Aspen Plus, and OriginPro were verified against established standards and previous research to ensure data processing and simulation accuracy.
- c) Error checks and outlier analysis, maintained data consistency and accuracy. Experiments and simulations were repeated under consistent conditions to confirm stability and reliability of results.
- d) All procedures, analyses, and decision-making processes were thoroughly recorded to ensure traceability and future replication.

3.11 Research Assumptions

This study relied on several assumptions across biomass characterization, process simulation, and machine learning modeling to ensure feasibility, reproducibility, and interpretability of results. Clearly stating these assumptions is essential for understanding the scope and limitations of the study.

3.11.1 Biomass characterization assumptions

- a) Biomass samples are representative of the broader feedstock population, ensuring generalizability of results.
- b) Laboratory conditions adequately replicate relevant field conditions for thermal and chemical analysis.
- c) Measurement instruments, including TGA and proximate/ultimate analyzers, are properly calibrated and functioning according to manufacturer specifications.
- d) Seasonal or geographic variations in biomass properties are negligible within the scope of this study.
- e) Sample preparation procedures, including drying, grinding, and sieving, do not alter the intrinsic physicochemical properties of the feedstock.

3.11.2 Aspen plus simulation Assumptions

To streamline computations while maintaining predictive capability, the following assumptions were adopted:

- a) Gases behave as ideal gases, simplifying calculations under varying airflow, steam flow, and pressure conditions.
- b) All chemical reactions are assumed to reach equilibrium, eliminating the need for detailed kinetic modeling.
- c) Biomass is uniform in physical and chemical properties, neglecting compositional variability to maintain model consistency.
- d) The system is treated as adiabatic (no heat loss) or with uniform heat transfer, reducing computational complexity.
- e) Tar production is not modeled, avoiding syngas cleanup challenges but limiting real-world accuracy.
- f) The system operates under steady-state conditions, avoiding transient simulations.

- g) Ash is non-reactive, simplifying mass and energy balances.
- h) Heat and mass transfer limitations within the reactor are considered negligible, focusing on bulk behavior.

These assumptions facilitated the development of a manageable and efficient process simulation model. However, they introduce limitations in representing certain real-world dynamics, and results should be interpreted within this context (Ranjan et al., 2023, 2024).

3.11.3 ML Model Development Assumptions

- a) Training datasets are representative of the operational space and cover the relevant range of process conditions.
- b) Feature-target relationships remain stationary over time, allowing reliable learning from historical data.
- c) Missing data patterns are random (MCAR), and data imputation does not introduce bias.
- d) Models can generalize to unseen data beyond the training set.
- e) Prediction errors are assumed to be normally distributed, facilitating statistical evaluation.
- f) Features are not highly multicollinear, avoiding instability in model parameter estimation.
- g) Sufficient high-quality data are available to ensure robust model training and evaluation.

3.11.4 Model Robustness and Interpretability analysis

- a) Model performance metrics (e.g., RMSE, R^2 , MAE) accurately reflect predictive reliability under experimental and simulated conditions.
- b) Perturbation or stress-testing of input features adequately represents real-world operational variability.

- c) Interpretability methods, such as permutation importance, Gini importance, and partial dependence analysis, can meaningfully capture feature importance and interactions.
- d) The ML models' outputs are assumed to be actionable for guiding co-gasification process optimization.

3.12 Study Limitations

Although this study provides important contributions across thermal degradation analysis, process simulation, machine learning modeling, robustness assessment, and interpretability analysis, several limitations were encountered. These limitations should be considered when interpreting the results and when designing future research.

3.12.1 Scope Limitations

The scope of the study was intentionally focused but inherently restrictive.

- a) Only five biomass types (RH, GS, CH, MS, TW) were analyzed. While these are locally abundant feedstocks, the findings may not generalize to other biomass types with different physicochemical properties.
- b) Gasification operating conditions were explored within a limited parameter window. Extreme pressures > 2.5 bars, very low or high equivalence ratios, and wider steam–air ratios were not investigated.
- c) The study focused exclusively on binary blends. More complex ternary or quaternary mixtures, which may behave differently due to synergistic or antagonistic interactions, were not examined.
- d) Experimental conditions, including TGA and batch reactors, cannot fully replicate industrial-scale gasification characterized by continuous feed, heterogeneous biomass, and non-uniform heating profiles.

These scope-related constraints limit the degree to which the results may be extrapolated beyond the conditions and feedstocks studied.

3.12.2 Methodological Limitations

Several methodological constraints influenced the precision and representativeness of the findings.

- a) Kinetic parameters were derived using the Coats–Redfern method at a single heating rate. This limited the ability to capture the dynamic decomposition behavior across different thermal environments. Isoconversional multi-rate methods could provide more robust and heating-rate-independent results.
- b) TGA heating rates (20°C/min) differ significantly from those in real gasifiers, where heating occurs more rapidly and non-linearly. This discrepancy limits transferability of TGA-based decomposition insights to practical systems.
- c) The simulation relied on equilibrium assumptions, uniform temperature distributions, ideal gas behavior, and steady-state operation. These simplifications overlook important real-world phenomena such as reaction kinetics, tar formation, localized turbulence, and transient changes.
- d) The PS model was calibrated using only two blend types (SB&CS and WC&CC), restricting its ability to represent a wider range of biomass mixtures.
- e) Experimental setups were batch-based, whereas commercial gasifiers operate continuously, introducing differences in mass flow, heat transfer, and reaction progression.
- f) Limited diversity in the training dataset constrained the ML models' ability to generalize to unseen feedstocks and operational conditions.
- g) Normalization and preprocessing of data, while necessary for training, may have masked subtle relationships in the input variables, affecting predictive accuracy.

These methodological assumptions and constraints introduce uncertainties and highlight opportunities for improved experimental and modeling approaches.

3.12.3 Data Limitations

Data availability and quality influenced both model development and interpretability.

- a) Time, cost, and equipment availability constrained the number of experimental runs of the case of proximate and thermal degradation analyses, reducing statistical robustness.
- b) Some relevant parameters (e.g., tar content, particle size distributions, ash fusion temperatures) were not included in the gasification model due to laboratory and simulation limitations.
- c) The ML dataset contained approximately 500 samples and limited diversity, which restricted the ability to capture highly nonlinear relationships, especially for complex targets such as H_2 , LHV, and CGE.
- d) Gasification is a dynamic process, but the study relied on static datasets, limiting the ML models' ability to represent temporal or transient behavior.
- e) Data derived from specific sources and single batches may not represent all industrial conditions, which could affect ML model performance in broader applications.

These data-related limitations affected prediction accuracy and model generalizability.

3.12.4 Resource Limitations

Resource constraints influenced several aspects of the research design.

- a) TGA equipment had a limited temperature range and lacked advanced control for variable heating rates.
- b) Long-duration experiments (e.g., multi-rate kinetics or continuous gasification trials) were not feasible within the project timeline.

- c) Funding limitations reduced sample replications, restricted the number of heating rates tested, and limited the scope of large-scale validation experiments.
- d) High-complexity simulation models (e.g., CFD-coupled gasification models) could not be developed due to computational and licensing constraints.

These limitations shaped the methodological choices and the depth of analyses conducted.

3.12.5 Generalizability Limitations

Several factors limit the broader application of the results.

- a) The biomass samples originated from Uganda and Kenya. Variations in climate, soil composition, harvesting methods, and storage conditions may influence properties of the same biomass types in other regions.
- b) Findings are based on downdraft gasification conditions. Performance may differ significantly in fluidized bed, entrained-flow, or updraft gasifiers.
- c) Both the Aspen Plus and ML models were developed and validated under a narrow set of operating conditions and feedstock ranges. Extrapolation beyond these domains may reduce accuracy.
- d) The feature importance results depend heavily on the dataset. Under different operating conditions, the ranking of influential parameters may change.

As a result, caution is required when applying the models or conclusions beyond the defined experimental and simulation boundaries.

CHAPTER FOUR: RESULTS AND DISCUSSION

4.1 Introduction

This chapter presents the research findings, covering physicochemical characterization, thermo-kinetic analysis, process simulation (PS) in Aspen Plus, machine learning (ML) model development and validation, robustness analysis, and interpretability assessment. The results are discussed in relation to the research objectives, with insights into their implications for the co-gasification (COG) process.

4.2 Physicochemical and Thermo-Kinetic Analysis

This section presents the results of biomass physicochemical characterization alongside thermal, kinetic, and thermodynamic analyses. Using TGA and CR methodologies, the study examines the pyrolysis behavior of selected biomass feedstocks, providing insights into decomposition pathways, reaction kinetics, and thermodynamic properties. These findings serve as a foundation for optimizing biomass conversion processes. Notably, most of the results and discussions here have been published in Bongomin et al. (2024).

4.2.1 Physicochemical characterization

The physicochemical characterization of biomass feedstocks: coffee husk (CH), groundnut shell (GS), macadamia nutshell (MS), rice husk (RH), and tea waste (TW), offers essential insights into their suitability for gasification. This discussion integrates key findings from proximate and ultimate analyses, as well as heating value measurements, to evaluate their impact on thermal degradation, gasification optimization, and syngas production.

The physicochemical characterization results are presented graphically in this section, with detailed data tables provided in APPENDIX D. Graphs are used to clearly illustrate

trends and comparative differences among feedstocks, while the appendix provides the full numerical values for reference

4.2.1.1 Proximate analysis

The proximate analysis revealed significant variations in moisture content, volatile matter, fixed carbon, and ash content among the feedstocks, each influencing their performance during gasification (Figure 4.1). Low moisture content in TW (5.69%) and MS (5.73%) enhances their suitability for gasification by minimizing the energy required for drying. Conversely, higher moisture levels in CH (8.67%) and GS (7.92%) could reduce overall process efficiency without pre-treatment. The volatile matter, which drives syngas production, was highest in MS (68.52%) and lowest in RH (59.19%). This suggests that MS has greater potential to produce volatile gases essential for syngas generation (Vu et al., 2023), whereas RH may require optimization strategies to improve reactivity (Bandara et al., 2020).

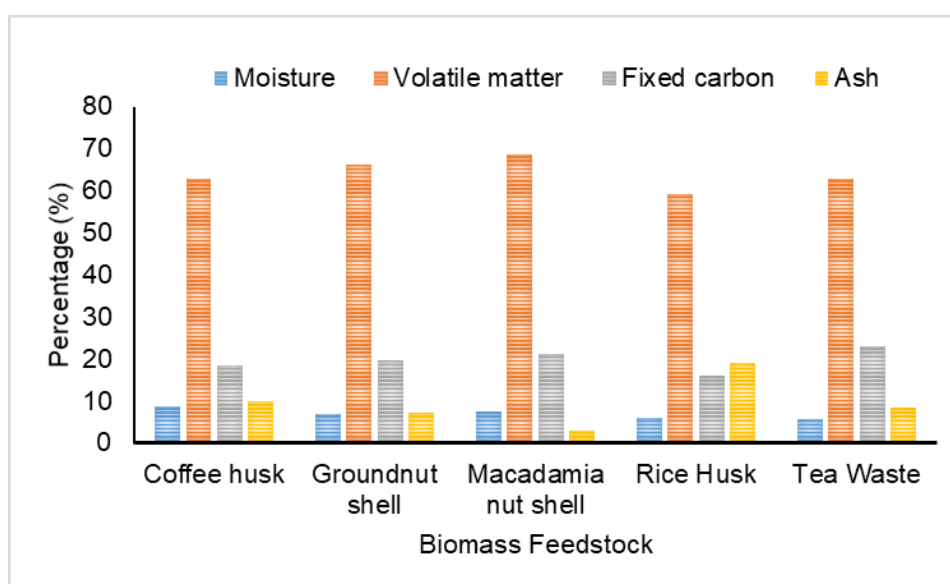


Figure 4.1: Comparison of proximate analysis of biomass feedstock

The fixed carbon content, crucial for char formation and subsequent reduction reactions (Chaiklangmuang et al., 2015; Nam et al., 2021), was highest in TW (23.01%) and lowest in RH (15.90%). This highlights the potential of TW for sustained char reactivity,

enhancing hydrogen and carbon monoxide production in the reduction zone. Ash content, a critical determinant of operational challenges, varied widely, with MS showing the lowest levels (3.03%) and RH exhibiting the highest (19.01%). High ash content in RH is likely to cause operational issues such as slagging and fouling (Chaiklangmuang et al., 2015; Nam et al., 2021), necessitating feedstock pre-treatment or blending to mitigate these challenges.

4.2.1.2 Ultimate analysis

The ultimate analysis revealed variations in elemental composition, particularly carbon (C), hydrogen (H), and oxygen (O), which directly affect syngas composition and energy density (Figure 4.2). MS exhibited the highest carbon content (52.49%), suggesting its superior calorific potential and suitability for high-quality syngas production. In contrast, RH, with the highest oxygen content (34.88%), is expected to have lower energy efficiency due to higher combustion byproducts such as CO₂ (Nimmanterdwong et al., 2021).

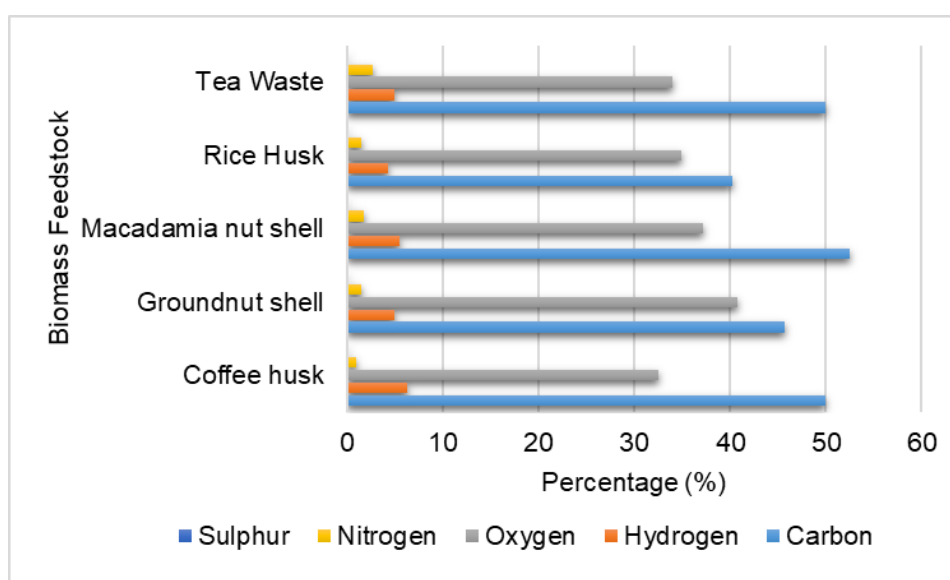


Figure 4.2: Comparison of ultimate analysis for different biomass feedstock

Hydrogen content, a critical factor for producing hydrogen-rich syngas (Xing et al., 2019), was highest in CH (6.33%), and followed by MS (5.49%) and lowest in RH

(4.26%). This positions CH and MS as a prime candidate for hydrogen production applications, such as fuel cells or chemical synthesis. Nitrogen and sulfur contents were consistently low across all feedstocks, minimizing the risks of harmful NO_x and SO_x emissions during gasification (Nimmanterdwong et al., 2021; Xing et al., 2019). RH's minimal sulfur content (0.009%) further enhances its environmental viability, despite its other limitations.

4.2.1.3 Heating values and energy potential

The HHV and LHV of biomass feedstocks provided a direct measure of their energy potential (Figure 4.3). MS had the highest HHV (21.5 MJ/kg) and LHV (20.8 MJ/kg), aligning with its high carbon and hydrogen content, making it ideal for high-calorific syngas applications. TW also showed strong potential with HHV (20.0 MJ/kg) and LHV (19.4 MJ/kg), suitable for energy-intensive applications. In contrast, RH exhibited the lowest HHV (16.8 MJ/kg) and LHV (16.6 MJ/kg), reflective of its higher oxygen and ash content, which dilute its energy potential. Pre-treatment strategies, such as torrefaction or blending with higher-HHV feedstocks like MS, could improve its performance (Bhattarai et al., 2023).

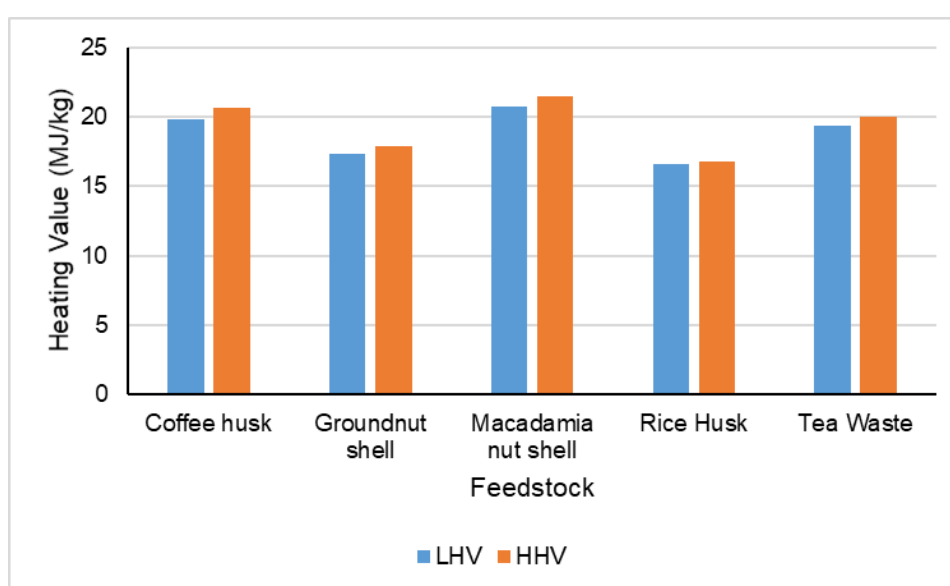


Figure 4.3: Comparison of heating value for different feedstocks

4.2.1.4 Comparative performance

The analysis revealed MS and TW as the most promising feedstocks for gasification. Both feedstocks showed high volatile matter and fixed carbon, combined with low ash content, which are widely recognized as favourable indicators for thermochemical conversion processes. These properties, supported by literature linking feedstock composition to gasification performance (Hasan et al., 2023), suggest that MS and TW possess desirable qualities for efficient thermal conversion in subsequent gasification stages. CH and GS, while moderate performers, can serve as complementary feedstocks, particularly in blended configurations. RH, despite its challenges, remains viable with pre-treatment strategies to mitigate high ash content and improve energy efficiency (Reddy et al., 2024).

4.2.1.5 Descriptive statistics and significance test

The descriptive statistics of proximate and ultimate analyses, along with the heating values, offered comprehensive insights into the physicochemical characteristics and energy potential of the selected biomass feedstocks. The mean moisture content of 6.91% ($\pm 1.21\%$) indicated relatively low water content across the feedstocks, which is favorable for energy recovery, as lower moisture levels reduce drying energy requirements (Abdallah et al., 2023). Volatile matter averaged 63.96% ($\pm 3.57\%$), dominating the feedstocks' composition and indicating strong potential for high syngas and tar yields (Fajobi et al., 2022). Fixed carbon with mean value of 19.62% ($\pm 2.69\%$), contributed significantly to char formation and sustained combustion. Meanwhile, the ash content showed the highest variability, averaging 9.50% ($\pm 5.91\%$), which may pose operational challenges such as slagging and fouling, and must be considered in reactor design and optimization (Abdallah et al., 2023; Fajobi et al., 2022; Tomczyk, 2020).

The ultimate analysis revealed that the carbon content averaged 47.69% ($\pm 4.80\%$), indicating the feedstocks' suitability for high energy conversion efficiency

(Nimmanterdwong et al., 2021). The hydrogen content was averaged 5.20% ($\pm 0.77\%$), supporting robust syngas production, particularly hydrogen-rich gas (Xing et al., 2019). The oxygen content was relatively high, with a mean of 35.87% ($\pm 3.21\%$), reflecting the inherent reactivity of biomass, although it may reduce the heating value due to its non-combustible nature (Nimmanterdwong et al., 2021). Nitrogen and sulfur contents were relatively low, averaging 1.69% ($\pm 0.63\%$) and 0.039% ($\pm 0.025\%$), respectively. These low levels are favorable for minimizing NO_x and SO_x emissions during gasification, thereby supporting cleaner energy production (Xing et al., 2019).

The heating values reinforced the compositional findings, with mean lower heating value (LHV) and higher heating value (HHV) recorded at 18.79 MJ/kg (± 1.76 MJ/kg) and 19.37 MJ/kg (± 1.95 MJ/kg), respectively. The observed range of values, from 16.6 to 20.77 MJ/kg for LHV and from 16.83 to 21.46 MJ/kg for HHV, reflected the diversity of the biomass feedstocks. This variation highlights the importance of careful feedstock selection and appropriate preprocessing to enhance energy recovery (Bhattarai et al., 2023). HHV values were positively correlated with carbon and hydrogen contents, while elevated ash and moisture contents were associated with reduced energy potential.

The Kruskal-Wallis (KW) test was conducted to assess whether there were statistically significant differences in the medians of the properties including moisture content, volatile matter, fixed carbon, ash, and ultimate analysis variables, among the five biomass feedstocks. The test produced an H-value of 4.00 and a p-value of 0.406, indicating that the null hypothesis (H_0 : all medians are equal) could not be rejected at a typical significance level of $\alpha = 0.05$. These results suggest that there were no statistically significant differences in the median values of the properties across the feedstocks, indicating a degree of compositional uniformity. However, the descriptive statistics revealed variability in specific attributes, such as ash content and fixed carbon content.

These variations may still influence gasification performance and should be taken into account during feedstock selection and process optimization.

4.2.2 Thermal degradation analysis

The thermal degradation behavior of different biomass waste feedstock was investigated using TGA (Figure 4.4) and derivative thermogravimetric (DTG) (Figure 4.5). The feedstock samples included CH, GS, MS, RH, and TW. The results are summarized in Table 4.1, highlighting the degradation stages, biomass component degradation temperature range, weight loss percentage, peak temperatures (T_p), and maximum degradation rate ($DTG_{\max}$ or $R_{p,\max}$), initial and final temperature for each stage.

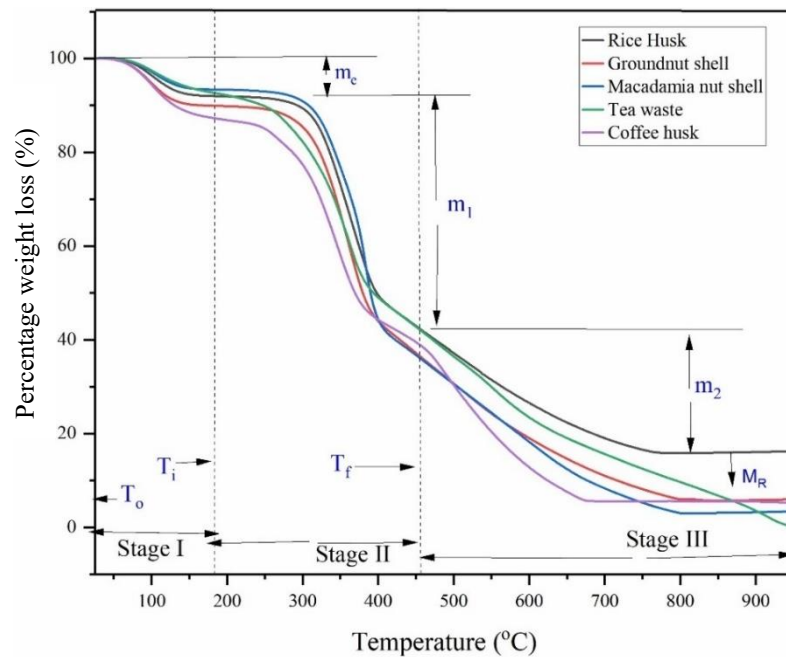


Figure 4.4: TGA curves for weight loss during thermal degradation of different biomass waste materials.

Legend: m_e : mass loss during drying stage, m_1 : mass loss during devolatilization stage, m_2 : mass loss during char formation stage, M_R : residue mass, T_o : starting or ambient temperature, T_i : initial devolatilization temperature, T_f : final devolatilization process temperature.

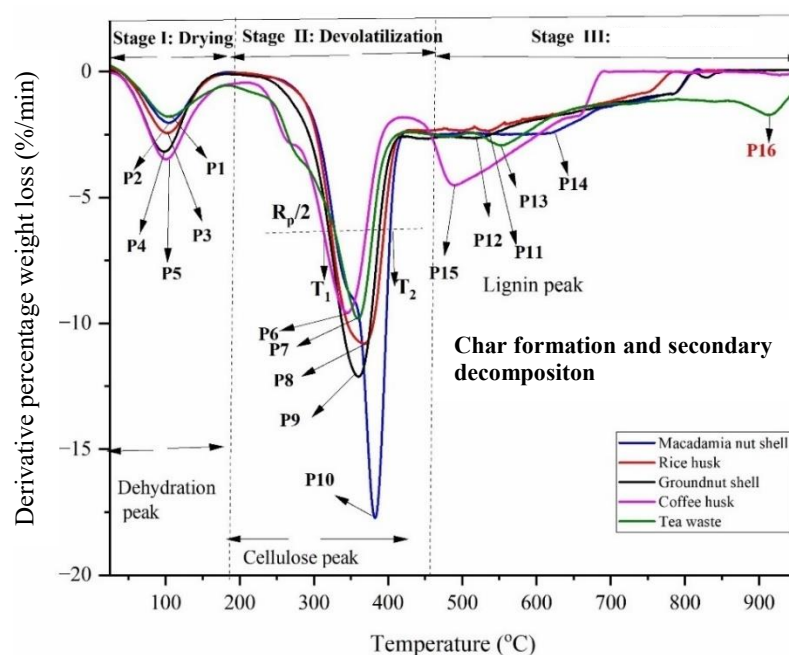


Figure 4.5: DTG curves of degradation rate for different biomass materials.

Legend: (P_1 - P_5): first peak at stage I, (P_6 - P_{10}): Second peak (hemicellulose, cellulose peak) at the stage II, (P_{11} - P_{15}): third peak (lignin peak) at stage II. P_{16} : fourth peak (oxidation peak) at the decomposition (stage III). R_p : maximum degradation rate at the main peak, $R_p/2$: half-width peak degradation rate. T_1 : lower end temperature at intersects of the half-width peak degradation rate, T_2 : upper end temperature at intersects of the half-width peak degradation rate.

Table 4.1: Changes in initial and final temperature during the three pyrolysis stages

Feedstock samples	Degradation Stages	Initial temp. (°C)	Final temp. (°C)	Weight loss (%)	Peak temp. (T_p), °C	DTGmax (%/min) (R_p)	Fractional weight (w)
CH	Stage 1: Drying	25	215	13.51	100	-3.475	0.142
	Stage 2: Devolatilization	215	425	44.87	345	-9.58	0.473
	Stage 3: Char formation	425	950	36.49	486	-4.483	0.385
GS	Stage 1: Drying	25	205	10.22	98	-3.182	0.109
	Stage 2: Devolatilization	205	415	48.79	361	-12.11	0.519
	Stage 3: Char formation	415	950	34.98	516	-2.628	0.372
MS	Stage 1: Drying	25	175	6.62	103	-2.024	0.069
	Stage 2: Devolatilization	175	440	55.56	382	-17.73	0.575
	Stage 3: Char formation	440	950	34.4	624	-2.404	0.356
RH	Stage 1: Drying	25	180	7.31	101	-2.430	0.087
	Stage 2: Devolatilization	180	435	48.14	369	-10.79	0.575
	Stage 3: Char formation	435	950	28.32	534	-2.360	0.338
TW	Stage 1: Drying	25	185	6.64	109	-1.770	0.067
	Stage 2: Devolatilization	185	430	48.2	358	-9.81	0.484
	Stage 3: Char formation	430	950	44.86	552 and 914	-2.918 and 1.714	0.450

4.2.2.1 Drying stage

The drying stage occurred between 25°C and 175–215°C, facilitating moisture removal (Cai et al., 2019; Huang et al., 2020; Petrovič et al., 2023). CH exhibited the highest weight loss (13.51%), followed by GS (10.22%) and RH (7.31%), while MS (6.62%) and TW (6.64%) had the lowest. CH also had the fastest drying rate (-3.475%/min), whereas MS and TW showed slower moisture removal (-2.024%/min and -1.770%/min, respectively). Comparisons with literature highlight variations in drying temperature ranges. For CH, the drying peak (< 215°C) at 100°C aligns with Nam et al. (2021), while MS dried at <175°C, lower than Linh et al. (2021) (<220°C). GS (205°C) had a broader range than reported by Mishra & Vinu (2024) (<150°C), and RH (180°C) was lower than Kumar et al. (2020), (<240°C). TW (185°C) also showed a slightly reduced range compared to Alashmawy et al. (2023) (<196.17°C). These findings highlight differences in moisture removal behavior, crucial for optimizing pyrolysis and gasification.

4.2.2.2 Devolatilization stage

The devolatilization stage, characterized by significant thermal degradation and volatile release, occurred between 175°C–215°C and 415°C–440°C. MS exhibited the highest weight loss (55.56%), indicating high volatile content and reactivity, followed by GS (48.79%), TW (48.2%), RH (48.14%), and CH (44.87%). The $T_{p,max}$ ranged from 345°C (CH) to 382°C (MS), with MS had the fastest decomposition rate (-17.73%/min), while CH and TW had slower rates (-9.58%/min and -9.81%/min, respectively).

Comparisons with previous studies reveal variations. CH devolatilization occurred between 215°C–425°C, with a DTG peak at 345°C, aligning with Nam et al. (2021) (238°C–400°C, peak at 310°C). GS (205°C–415°C) had a narrower range than Mishra & Vinu (2024) (150°C–600°C). MS showed $T_{p,max}$ at 382°C, higher than 295°C in Linh et al. (2021) (220°C–450°C). RH devolatilized between 180°C–435°C, lower than 240°C–

500°C in Kumar et al. (2020). TW had ($T_{p,max} = 358^{\circ}\text{C}$), slightly differing from Alashmawy et al. (2023) ($T_{p,max} = 340.47^{\circ}\text{C}$). These differences highlight the diverse thermal decomposition behaviors of biomass feedstocks, essential for optimizing gasification and pyrolysis processes.

4.2.2.3 Char formation and secondary decomposition stage

The char formation and secondary decomposition stage, occurred at higher temperatures between 415°C–440°C and extending up to 950°C, involved the conversion of the remaining solid residue into char. CH exhibited the highest weight loss (36.49% at $>486^{\circ}\text{C}$), followed by TW (44.86%), GS (34.98%), and MS (34.4%), while RH had the lowest weight loss (28.32%). The T_p varied significantly, with MS having the highest T_p at 624°C, indicating greater thermal resistance. GS, RH, and TW had T_p values of 516°C, 534°C, and 552°C, respectively, with TW showing an additional peak at 914°C, suggesting complex degradation behavior. The weight loss rate (R_p) was lower in this stage, indicating gradual char formation. GS and RH had the lowest R_p values (-2.628%/min and -2.360%/min, respectively), while TW exhibited multiple R_p values (-2.918%/min and -1.714%/min), further indicating prolonged char formation.

Comparison with previous studies revealed some variations. For CH, Nam et al. (2021) reported weight loss above 400°C, linked to lignin degradation, while this study observed it above 425°C, indicating a slight shift to higher temperatures. GS exhibited char formation above 415°C, lower than the 600°C reported by Mishra & Vinu (2024). RH showed char formation above 435°C, lower than 500°C in Kumar et al. (2020). MS had a char formation onset at 440°C, closely aligning with 450°C reported by Linh et al. (2021). TW started forming char beyond 430°C, lower than 558.15°C reported by Alashmawy et al. (2023).

These findings demonstrate a general consistency in thermal behavior across studies, although some discrepancies in temperature ranges and peak values were observed. These differences are attributed to variations in moisture content, sample preparation methods. Understanding such variations is essential for the effective optimization of biomass pyrolysis and gasification processes.

4.2.2.4 Proximate vs. TGA mass-loss interpretation

Although both proximate analysis and thermal decomposition results in this study were generated using TGA instruments, they represent fundamentally different measurements because each was conducted under distinct operating conditions, heating programs, and reaction atmospheres. Proximate analysis performed using a macro-TGA under controlled isothermal steps in both oxidizing and inert environments, quantified moisture content, volatile matter, ash, and fixed carbon following standard analytical procedures. In contrast, the thermal decomposition analysis (dynamic TGA) used a micro-TGA operated under a continuous heating rate in an inert atmosphere, producing a detailed mass-loss curve reflecting drying, devolatilization, char formation, and high-temperature secondary degradation.

Because proximate fixed-carbon content is determined indirectly from mass fractions after sequential heating steps, it cannot be numerically equated to the mass loss observed in the high-temperature region of a dynamic TGA run. The latter includes contributions from secondary char decomposition, cracking of heavy volatiles, and gradual mass reduction extending beyond the temperatures associated with fixed-carbon determination in proximate analysis. Therefore, the differences between the fixed-carbon values reported in the proximate analysis and the high-temperature mass-loss percentages obtained from thermal decomposition TGA reflect differences in methodology, purpose, and experimental conditions, rather than inconsistencies in the data.

4.2.3 Kinetic reaction mechanisms

Kinetic analysis was conducted over four temperature ranges: Stage I (drying: 25°C to T_f), Stage II (devolatilization: T_i to T_f), Stage III (char formation: T_f to 950°C), and the full temperature range (25°C to 950°C). To determine the best-fitted reaction mechanism for each stage and the overall pyrolysis process using a single-step approach, the CR method was applied. Various reaction models were assessed against the TGA data to identify the most representative mechanisms.

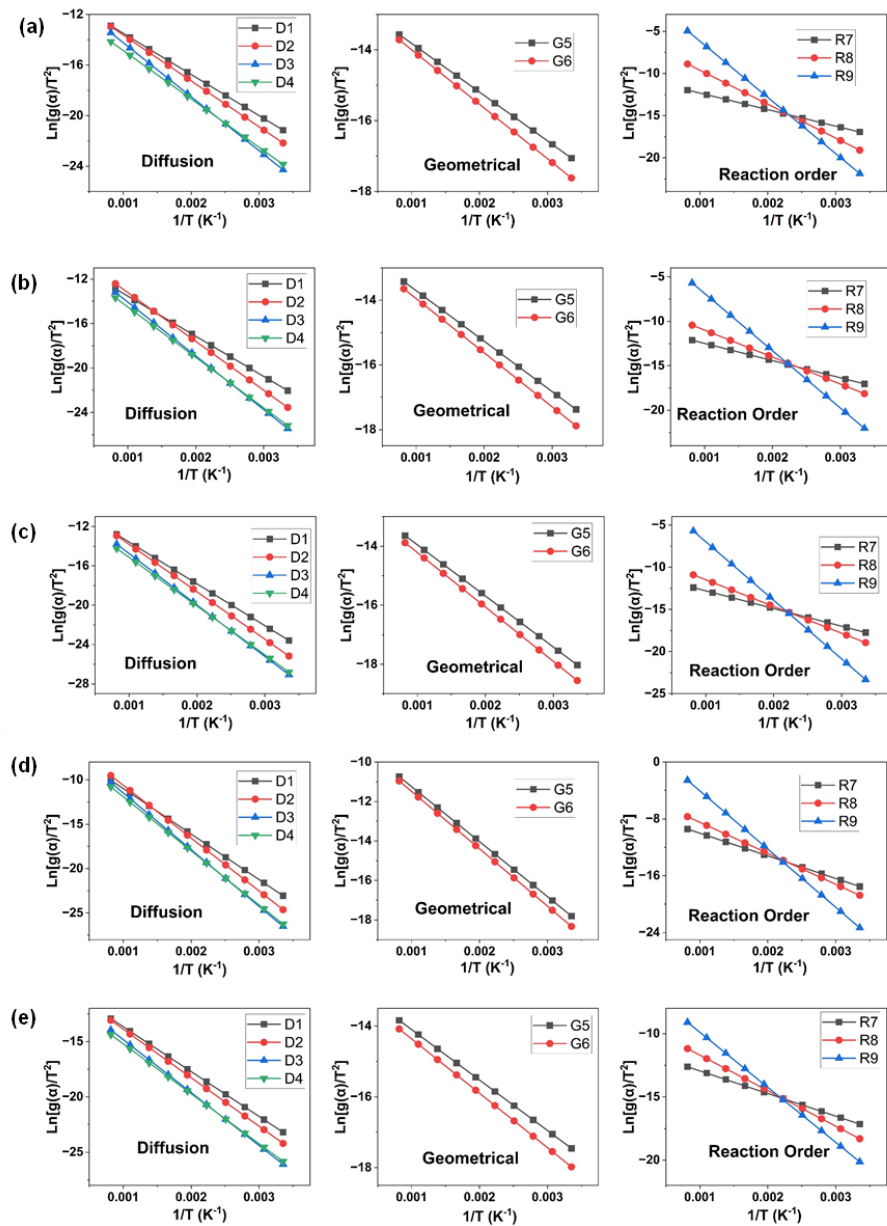


Figure 4.6: Fitting curves of the integral method for estimating the kinetic parameters. Legend: (a) CH, (b) GS, (c) MS, (d) RH, (e) TW.

The linear fitting curves for different models exhibited distinct patterns across degradation stages and the full temperature range. Figure 4.6 illustrates a comparison of linear fitting curves for the full temperature range (25°C to 950°C) across various integral models, highlighting differences in model performance. It shows the linear fitting of transformed TGA data for various integral reaction models. The y-axis represents $\ln[g(\alpha)/T^2]$, where $g(\alpha)$ is the integral form of the reaction model which was calculated using formula from Table 3.1, and α is the conversion fraction calculated from TGA mass loss using Eq. (3.3). The x-axis is $1/T$ (K^{-1}). The slope of each line provides the activation energy for the corresponding reaction mechanism.

For each degradation stage, the R^2 value was used to evaluate the goodness-of-fit, and residuals were analyzed to minimize discrepancies between experimental and predicted values. Given that biomass pyrolysis is a multi-step process with overlapping reactions of varying thermal stabilities, the optimal reaction model differed across stages, as detailed in APPENDIX E. The selection of models with the highest R^2 values and minimal residuals ensured that the derived kinetic parameters accurately represented the thermal decomposition behavior of the biomass (El-Sayed et al., 2024).

The pyrolysis behavior of the biomass feedstocks was best described by different reaction models at various stages, reflecting their distinct decomposition mechanisms. For CH, the D3 diffusion model was the best fit across the full temperature range ($R^2 = 0.8592$, $E_a = 35.52$ kJ/mol), indicating a three-dimensional diffusion mechanism. The D4 model governed drying, while D1 and R8 models best described devolatilization and char formation, respectively, highlighting stage-dependent reaction mechanisms. Similarly, GS followed a D3 diffusion model overall ($R^2 = 0.8097$, $E_a = 40.18$ kJ/mol), with D1 and D4 models governing devolatilization and char formation, suggesting a dominance of diffusion-driven processes throughout pyrolysis.

MS exhibited consistent three-dimensional diffusion across all stages ($R^2 = 0.8689$, $E_a = 45.76$ kJ/mol), with D3, D1, and D4 models capturing drying, devolatilization, and char formation, respectively, reinforcing its diffusion-controlled pyrolysis. RH, however, followed a first-order reaction model (R7) overall ($R^2 = 0.9138$, $E_a = 26.11$ kJ/mol), with diffusion models dominating drying and char formation, indicating a reaction-driven decomposition pathway. For tea waste, the D3 diffusion model was consistently the best fit ($R^2 = 0.8537$, $E_a = 39.78$ kJ/mol), suggesting a three-dimensional diffusion mechanism, with D3, D1, and D4 models capturing drying, devolatilization, and char formation stages, respectively. These findings highlight the multi-mechanistic nature of biomass pyrolysis, where diffusion mechanisms predominantly govern drying and char formation, while reaction models play a key role in overall decomposition for certain feedstocks like rice husk (Raza & Abu-Jdayil, 2023).

4.2.4 Kinetic parameters

Understanding the kinetic parameters of biomass pyrolysis is crucial for optimizing thermal conversion processes, predicting reaction rates, and improving gasification efficiency. This section analyzes the E_a and A , governing the drying, devolatilization, and char formation stages of pyrolysis. The findings provide insights into biomass reactivity, thermal stability, and energy requirements, essential for process optimization and feedstock selection.

4.2.4.1 Drying kinetics

The E_a and A for the drying stage vary significantly across biomass types, reflecting differences in moisture content and structural properties (Figure 4.7a). RH exhibits the highest E_a (100.03 kJ/mol) and A ($2.73 \times 10^{10} \text{ min}^{-1}$), indicating a high energy requirement for moisture removal due to its dense structure and high silica content, which impedes

moisture release. Similarly, MS shows a high E_a (98.86 kJ/mol) and A ($2.43\text{E}+09 \text{ min}^{-1}$), suggesting significant drying resistance due to its thick cell walls and complex structure.

In contrast, CH has the lowest E_a (71.88 kJ/mol) and A ($8.55\text{E}+05 \text{ min}^{-1}$), indicating easier moisture loss, likely due to its less dense structure. TW and GS exhibit moderate E_a and A values, suggesting intermediate drying behavior. These variations emphasize the role of biomass physical characteristics in determining drying kinetics, influencing overall thermal decomposition efficiency.

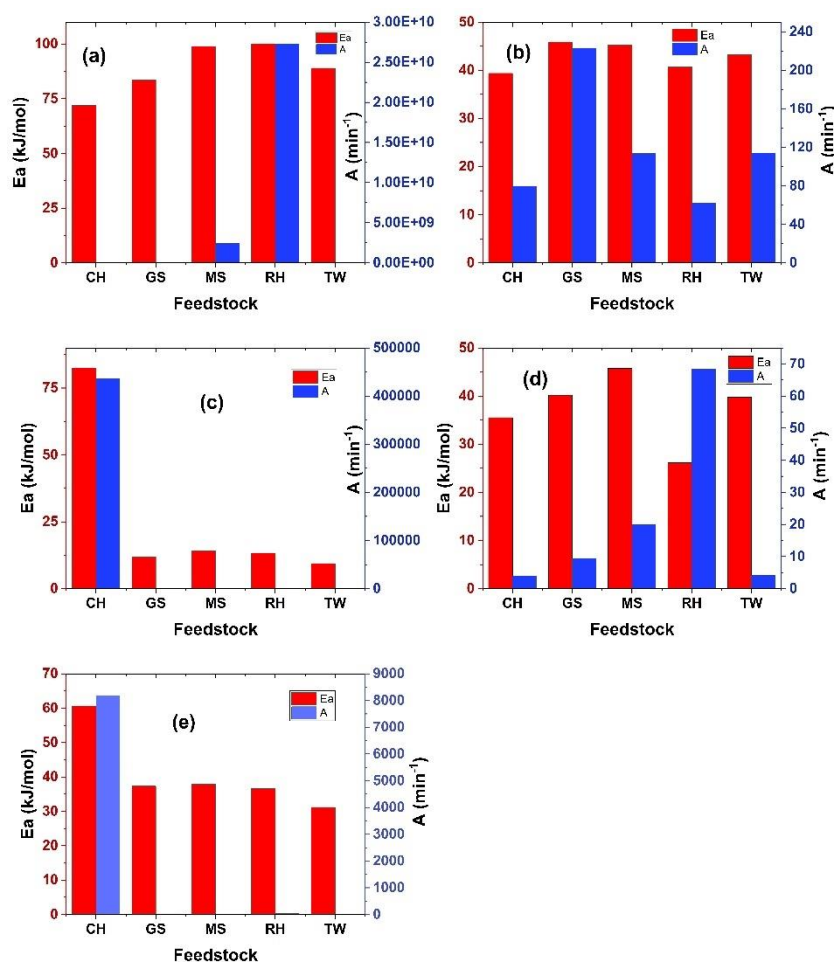


Figure 4.7: Comparison of the kinetic parameters of the different biomass wastes
 Legend: (a) Drying stage, (b) devolatilization stage, (c) char formation stage (d) global single-step approach, (e) overall multi-step approach

4.2.4.2 Devolatilization kinetics

The devolatilization stage exhibited distinct thermal decomposition behaviors among biomass types (Figure 4.7b). GS had the highest E_a (45.83 kJ/mol) and A (222.77 min^{-1}),

indicating a more energy-intensive devolatilization process due to its dense structure. MS showed a similar E_a (45.26 kJ/mol) but a lower A (113.49 min⁻¹), suggesting a slightly less complex decomposition pathway.

TW had a slightly lower E_a (43.26 kJ/mol) with a similar A (113.93 min⁻¹), implying comparable reaction kinetics but requiring less energy (Huang et al., 2020). In contrast, CH and RH exhibited the lowest E_a (39.35 and 40.66 kJ/mol, respectively) and A values (79.78 and 62.06 min⁻¹, respectively), indicating easier thermal breakdown due to their more accessible structures. These variations highlight the impact of biomass composition and structure on devolatilization kinetics.

4.2.4.3 Char formation and decomposition kinetics

During the char formation and secondary decomposition stage, CH exhibited the highest E_a (82.54 kJ/mol) and A (435,925.57 min⁻¹), indicating a more energy-intensive and kinetically complex thermal degradation process (Figure 4.7c). This significantly contrasts with the other biomass types, which required less energy for char formation (Huang et al., 2020). The high E_a of CH could be attributed to its higher lignin content, complex structural composition, and greater carbon matrix stability, making thermal degradation more resistant.

GS (11.87 kJ/mol), MS (14.15 kJ/mol), RH (13.26 kJ/mol), and TW (9.39 kJ/mol) all exhibited lower E_a values, suggesting that their char formation occurs more easily with less energy input. The very low A values for MS, RH, and TW further indicate simpler reaction pathways compared to CH.

Interestingly, TGA results showed that MS had a higher peak temperature (624°C) than CH (486 °C), suggesting greater thermal stability. This contradicts the higher E_a of CH, implying that its decomposition kinetics may be influenced by experimental factors such

as heating rate effects, sample composition, or reaction pathway complexities. Further validation through alternative kinetic models and structural analysis is necessary to determine whether this behavior is intrinsic or a result of methodological variations.

4.2.4.4 Overall and global kinetic parameters

Kinetic parameters (E_a and A) were determined using multi-step (overall) and global single-step approaches (Márquez et al., 2023; Uddin Monir et al., 2024), revealing distinct decomposition characteristics for each biomass type. The global approach (Figure 4.7d) generally yielded lower E_a values compared to the multi-step approach (Figure 4.7e), emphasizing the complexity of pyrolysis.

For example, CH exhibited a significantly higher E_a in the multi-step approach (60.59 kJ/mol) compared to the global model (35.52 kJ/mol), indicating multiple reaction pathways with varying energy demands. While GS and MS showed minor E_a differences, RH and TW exhibited notable variations, highlighting differences in kinetic behavior. The multi-step approach captured these variations more effectively, whereas the single-step model provided a more generalized overview (Uddin Monir et al., 2024).

The A value was generally higher in the multi-step approach, reflecting the complexity of reaction pathways. For instance, CH's overall A (8187.40 min⁻¹) was significantly higher than its global A (4.05 min⁻¹), reinforcing the necessity of a multi-step analysis for accurately capturing biomass degradation kinetics. Similar trends were observed for GS, MS, RH, and TW, further validating the effectiveness of the multi-step approach. These findings align with previous studies (Alashmawy et al., 2023; Collins & Ghodke, 2018).

These comparisons confirm that the multi-step approach provides a more detailed representation of biomass decomposition, while the single-step model offers a simplified but less accurate kinetic perspective (Fischer et al., 2024; Uddin Monir et al., 2024).

Since devolatilization is the most critical stage for syngas production, it was used as the primary criterion for biomass selection. This stage governs volatile release, energy output, and overall gasification efficiency, making it essential for assessing feedstock suitability. The kinetic parameters from devolatilization offer crucial insights into thermal decomposition behavior, reactivity, and process optimization, ensuring that the selected biomass feedstocks are ideal for high-yield syngas production.

4.2.5 Thermodynamic analysis

The thermodynamic parameters (ΔH , ΔG , and ΔS) were evaluated across different temperature ranges using kinetic parameters (E_a , A) and the peak temperature (T_p , in K) (Table 4.2). These parameters provide valuable insights into the thermal stability, energy requirements, and spontaneity of biomass pyrolysis (Gajera et al., 2022). Devolatilization was used as the primary criterion for biomass selection since it directly influences syngas production, determining energy efficiency and reactivity. Biomass with moderate ΔH , lower ΔG , and controlled ΔS changes ensures efficient volatile release and high gasification potential, making it the most relevant stage for evaluating biomass suitability.

4.2.5.1 Enthalpy change

ΔH determines whether pyrolysis is endothermic or exothermic, reflecting the energy required for biomass conversion (Najafi et al., 2024). During drying (Figure 4.8a), RH (96.92 kJ/mol) and MS (95.74 kJ/mol) showed the highest ΔH , indicating greater energy demand due to moisture retention (Kamruzzaman et al., 2024). CH (68.78 kJ/mol) showed the least, requiring less energy, while TW (85.72 kJ/mol) and GS (80.39 kJ/mol) was in between, indicating moderate energy requirement.

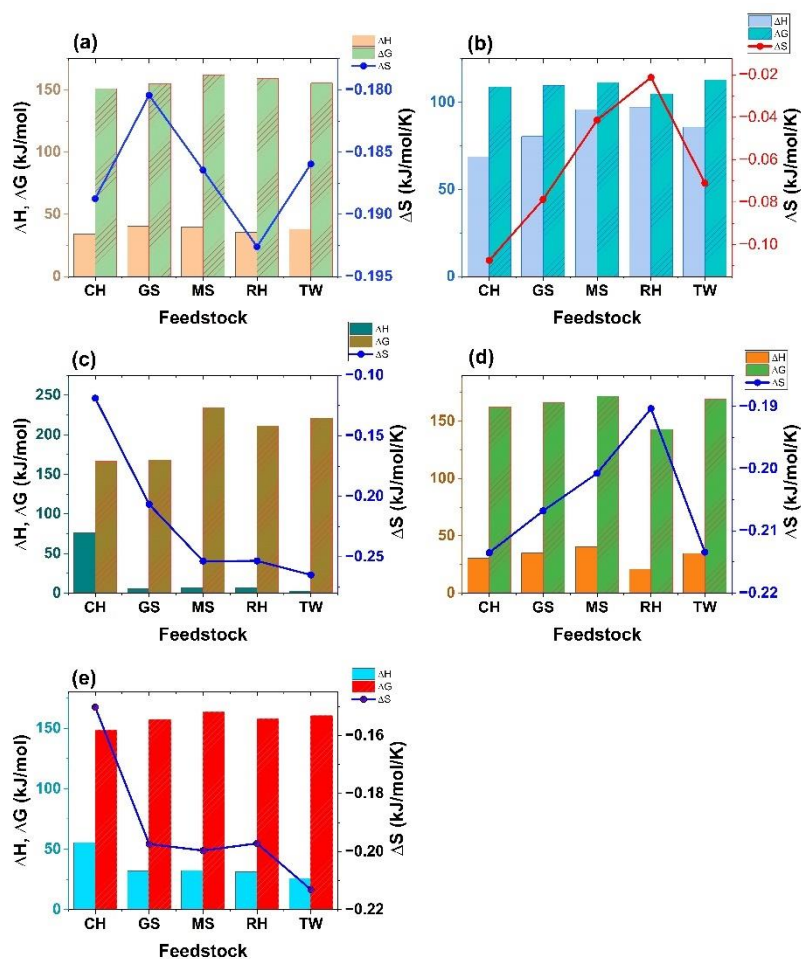


Figure 4.8: Comparison of thermodynamic parameters of the different biomass wastes. Legend: (a) drying stage, (b) devolatilization stage, (c) char formation stage, (d) full range temperature (single-step approach), (e) multi-step approach.

In devolatilization (Figure 4.8b), ΔH values decreased, reflecting lower energy needs. GS (40.56 kJ/mol) had the highest ΔH , indicating energy-intensive decomposition, whereas CH (34.20 kJ/mol) and RH (35.32 kJ/mol) had the least, require less energy, suggesting easier volatile release. MS (39.82 kJ/mol) and TW (38.02 kJ/mol) exhibited intermediate values. During char formation (Figure 4.8c), ΔH values were minimal, showing reduced energy demand. CH (76.23 kJ/mol) retained a relatively high ΔH , likely due to stable lignin components, while GS (5.31 kJ/mol), MS (6.69 kJ/mol), RH (6.55 kJ/mol), and TW (2.54 kJ/mol) had the least, necessitating significantly less energy during char formation.

For the full temperature range (Figure 4.8d), MS (40.31 kJ/mol) showed the highest ΔH , indicating consistent energy demand, while RH (20.77 kJ/mol) and CH (30.39 kJ/mol) exhibited lower values, suggesting a more gradual energy requirement (Choudhary et al., 2024). The multi-step approach (Figure 4.8e) provided a detailed stage-specific energy analysis, capturing variations more accurately. CH (55.46 kJ/mol), GS (32.03 kJ/mol), MS (32.44 kJ/mol), RH (31.22 kJ/mol), and TW (25.88 kJ/mol) exhibited distinct ΔH values, aligning with previous studies (Xu et al., 2020). These results confirmed that the multi-step approach better represented pyrolysis energy demands than the single-step model (Fischer et al., 2024).

Table 4.2: Thermodynamic parameters for different biomass feedstocks

Biomass waste	T_p (K)	A (s^{-1})	ΔH (kJ/mol)	ΔG (kJ/mol)	ΔS (kJ/mol.K)
Stage I (Drying)					
CH	373.15	5.13E+07	68.7832	108.8730	-0.1074
GS	371.15	1.61E+09	80.3940	109.6151	-0.0787
MS	376.15	1.46E+11	95.7367	111.3158	-0.0414
RH	374.15	1.64E+12	96.9222	104.8818	-0.0213
TW	382.15	4.19E+09	85.7152	112.8659	-0.0710
Stage II (Devolatilization)					
CH	618.15	4786.8	34.2032	150.8777	-0.1887
GS	634.5	13366.2	40.5573	155.0412	-0.1804
MS	655.15	6689.4	39.8157	161.9684	-0.1865
RH	642.15	3123.6	35.3237	159.0094	-0.1926
TW	631.15	6835.8	38.0151	155.3838	-0.1860
Stage III (Char formation and secondary decomposition)					
CH	759.15	2.62E+07	76.2271	166.5204	-0.1189
GS	789.15	712.0	5.3083	168.3569	-0.2066
MS	897.15	2.84	6.6913	234.1913	-0.2536
RH	807.15	2.62	6.5490	211.0638	-0.2534
TW	825.15	0.661	2.5361	221.2003	-0.2650
Full temperature range (25 to 950 °C)					
CH	618.15	243.2	30.3856	162.3671	-0.2135
GS	634.5	560.6	34.9065	166.1128	-0.2068
MS	655.15	1197.6	40.3129	171.8308	-0.2007
RH	642.15	4104.4	20.7696	142.9981	-0.1903
TW	631.15	250.9	34.5367	169.2384	-0.2134
Overall (based on multi-steps approach)					
CH	618.15	491244.0	55.4579	148.3434	-0.1503
GS	634.5	1736.4	32.0310	157.2042	-0.1974
MS	655.15	1367.1	32.4383	163.2355	-0.1996
RH	642.15	1808.4	31.2246	157.8268	-0.1972
TW	631.15	261.9	25.8762	160.3529	-0.2131

4.2.5.2 Gibbs free energy change

ΔG determined the spontaneity of pyrolysis, where lower ΔG values indicated a shift toward equilibrium and a more favorable decomposition process (Najafi et al., 2024). During the drying stage (Figure 4.8a), TW (112.87 kJ/mol) and MS (111.32 kJ/mol) exhibited the highest ΔG , indicating the least spontaneous drying, while RH (104.88 kJ/mol) showed the lowest, suggesting easier moisture removal. CH (108.87 kJ/mol) and GS (109.62 kJ/mol) displayed moderate spontaneity.

In the devolatilization stage (Figure 4.8b), MS (161.97 kJ/mol), RH (159.01 kJ/mol), and TW (155.38 kJ/mol) had the highest ΔG , requiring more energy for volatile release, while CH (150.88 kJ/mol) showed the lowest, indicating a more spontaneous process. During char formation (Figure 4.8c), MS (234.19 kJ/mol), TW (221.20 kJ/mol), and RH (211.06 kJ/mol) exhibited high ΔG , indicating non-spontaneous char stabilization, while CH (166.52 kJ/mol) and GS (168.36 kJ/mol) showed greater ease in char formation.

Across the full temperature range (Figure 4.8d), MS (171.83 kJ/mol) and TW (169.24 kJ/mol) resisted degradation, whereas RH (142.99 kJ/mol) showed the highest spontaneity. CH (162.37 kJ/mol) and GS (166.11 kJ/mol) showed intermediate values. The multi-step approach (Figure 4.8e) revealed generally lower ΔG values for all biomass types compared to the single-step method, indicating greater spontaneity and a shift toward equilibrium when pyrolysis is analyzed in stages. This confirmed that biomass decomposition is more thermodynamically favorable when assessed across individual reaction phases rather than as a single global process (Márquez et al., 2023; Uddin Monir et al., 2024).

4.2.5.3 Entropy change

ΔS measured the degree of disorder during pyrolysis, with negative ΔS values indicating increased order as biomass transforms into char and gas products (Mariyam et al., 2024).

During drying (Figure 4.8a), RH (-0.0213 kJ/mol·K) showed the least entropy reduction, while CH (-0.1074 kJ/mol·K), TW (-0.0710 kJ/mol·K), and GS (-0.0787 kJ/mol·K) exhibited more negative ΔS , indicating greater structural stabilization (Choudhary et al., 2024).

In devolatilization (Figure 4.8b), ΔS became more negative, reflecting ordered structure formation. GS (-0.1804 kJ/mol·K) and TW (-0.1860 kJ/mol·K) showed moderate entropy reduction, while CH (-0.1887 kJ/mol·K) and RH (-0.1926 kJ/mol·K) underwent more extensive reorganization (Zhang et al., 2019).

During char formation (Figure 4.8c), TW (-0.2650 kJ/mol·K), MS (-0.2536 kJ/mol·K), and RH (-0.2534 kJ/mol·K) exhibited the most negative ΔS , indicating extensive ordering. CH (-0.1189 kJ/mol·K) and GS (-0.2066 kJ/mol·K) showed less reduction, suggesting less ordered char formation (Yiga et al., 2023).

For the full temperature range (Figure 4.8d), TW (-0.2134 kJ/mol·K) and CH (-0.2135 kJ/mol·K) showed the greatest entropy reduction, followed by MS (-0.2007 kJ/mol·K), GS (-0.2068 kJ/mol·K), and RH (-0.1903 kJ/mol·K).

The multi-step approach (Figure 4.8e) provided a detailed assessment, with TW (-0.2131 kJ/mol·K) showing the most negative ΔS , followed by MS (-0.1996 kJ/mol·K) and RH (-0.1972 kJ/mol·K). CH (-0.1503 kJ/mol·K) and GS (-0.1974 kJ/mol·K) exhibited less entropy reduction, highlighting different decomposition pathways (Márquez et al., 2023).

The negative ΔS values suggest increased order during pyrolysis, aligning with char formation. However, the highly negative ΔS in devolatilization contradicts expectations, as volatile release typically increases randomness. This discrepancy likely stems from kinetic model limitations, particularly the CR method, which assumes a single dominant

reaction per stage, potentially oversimplifying competing pathways like volatilization and secondary reactions.

Compared to other studies, most reported positive ΔS in devolatilization, suggesting that the strongly negative values here may be model-induced rather than an actual pyrolysis characteristic (Alashmawy et al., 2023; Zhang et al., 2019). To validate these findings, alternative kinetic models (e.g., Friedman, Ozawa-Flynn-Wall) and experimental entropy analysis using calorimetry or spectroscopy should be explored for a more accurate thermodynamic interpretation.

4.3 Process Simulation Modeling

The process simulation model was fully described in the methodology Section 3.4, including the Aspen Plus flowsheet, feedstock properties, and operating parameters. Preliminary simulation outputs are reported there to illustrate model behavior. This section presents the results and discussion of the process simulation (PS) modeling conducted for biomass co-gasification (COG). The analysis included validation of the simulation model using experimental data, with a focus on reactor zone temperatures and gas yield, as well as a sensitivity analysis to evaluate the effect of the equivalence ratio (ER) on key gasification parameters.

The validation results confirmed the model's accuracy in replicating experimental trends, particularly in temperature distribution and gas yield prediction, thereby establishing confidence in its predictive capability. Furthermore, the sensitivity analysis examined the influence of ER on reactor zone temperatures, gas and char yields, and syngas composition. These findings provide valuable insights for optimizing biomass COG performance under varying operating conditions.

It is important to note that graphical results are presented in this section to validate the Aspen Plus simulation model, while the corresponding data tables are provided in APPENXIX F, for reference.

4.3.1 Simulation model validation

Simulation model validation was a critical step in ensuring the reliability and accuracy of predictions for biomass COG processes. This discussion focuses on the validation of the Aspen simulation model for temperature distribution and gas yield using experimental data, covering both strengths and limitations of the model, for two cases: sugarcane bagasse & coconut shell (SB&CS) and wood chip & corn cob (WC&CC), along with the RMSD.

4.3.1.1 Validation on temperature distribution

The validation of the Aspen simulation model for temperature distribution across the pyrolysis, combustion, and reduction zones demonstrated the ability of the model to replicate experimental results with high accuracy for two feedstock combinations (Figure 4.9): SB&CS and WC&CC. The RMSD values ranged between (2 to 6°C) in the pyrolysis zone and (7 to 8°C) in the reduction zone, highlighting the model's robust performance in the pyrolysis and combustion zones and its need for refinement in the reduction zone. These results underline the reliability of the Aspen model in simulating temperature profiles for biomass COG while also exposing areas for improvement.

In the pyrolysis zone, the model achieved excellent accuracy, with an RMSD of 2°C and 6°C for the two feedstock blends. It effectively captured the thermal decomposition of biomass into volatiles, tar, and char. These minimal deviations suggest that the assumptions regarding uniform heating rates and feedstock properties were appropriate for this zone. However, some limitations were identified. The model relied on uniform heating assumptions, which may not fully represent localized temperature gradients that

occur in practical systems. Additionally, it did not explicitly account for feedstock variability in volatile matter content. Despite these potential limitations, the strong agreement between the simulated and experimental results for both feedstocks highlight the robustness of the Aspen model in predicting pyrolysis behavior. Most of the observed constraints are attributed to the inherent assumptions in the Aspen simulation framework for this study, particularly its reliance on Gibbs free energy minimization for equilibrium prediction (Ferreira et al., 2019; Mutlu & Zeng, 2020).

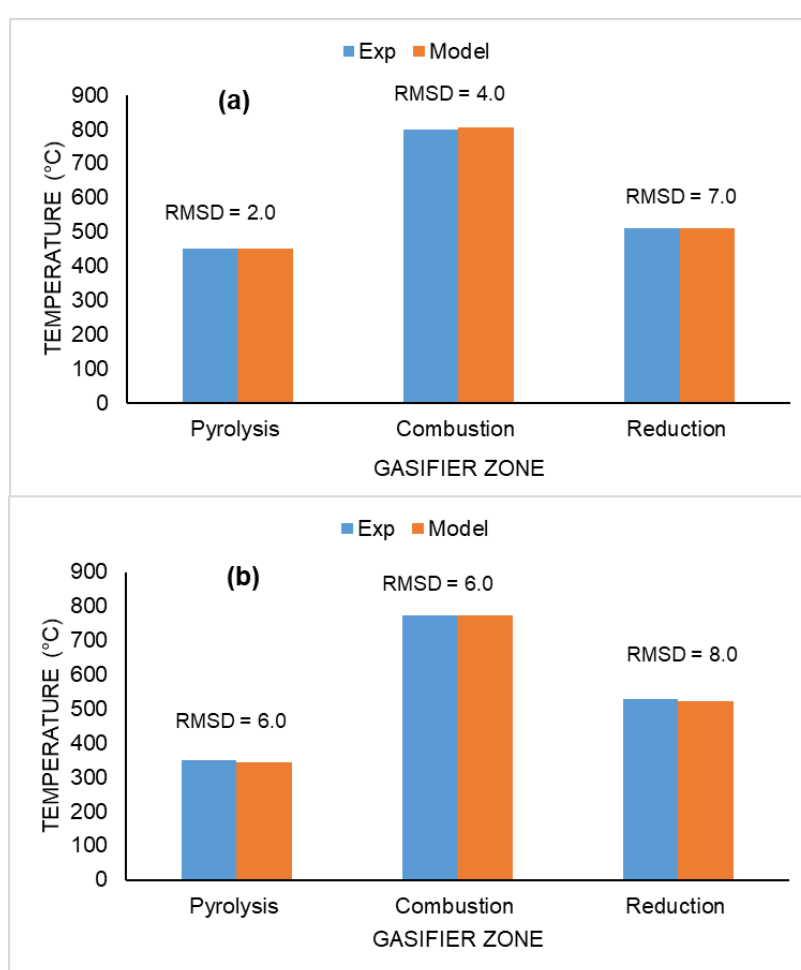


Figure 4.9: Process simulation model validation on reactor zone temperature.
Legend: (a) SB&CS (b) WC&CC.

The combustion zone also exhibited strong agreement, with an RMSD of 4°C and 6°C indicating reasonable accuracy in predicting exothermic oxidation reactions and heat transfer. The modeled temperatures slightly overestimated those observed for SB&CS and slightly underestimated them for WC&CC, likely due to differences in feedstock-

specific oxygen distribution and heat transfer characteristics (Awais et al., 2021). The model assumed complete oxygen availability and uniform heat generation, which may not accurately represent real-world turbulence and combustion dynamics. These simplifications likely contributed to the observed deviations and highlight the need for more advanced modeling approaches that incorporate oxygen diffusion effects and feedstock-specific combustion characteristics.

In contrast, the reduction zone presented larger deviations, with an RMSD of 7°C and 8°C, particularly for WC&CC. This discrepancy reflects the complexities of modeling solid-phase reactions, such as the Boudouard reaction and the water-gas shift, which dominate this zone (Gao et al., 2018; Xiang et al., 2018). Several factors likely contributed to the observed deviations. These include feedstock-specific properties such as char reactivity and ash behavior, as well as uneven temperature gradients and diffusion limitations within the reactor. The model's reliance on Gibbs free energy minimization assumed equilibrium conditions that may not accurately represent the kinetic constraints and incomplete reactions in real systems (Liang et al., 2021). Additionally, the underestimation of temperatures for WC&CC suggests that the model did not adequately capture the lower reactivity and catalytic effects of this feedstock (Jiao et al., 2022), indicating the need for more detailed kinetic modeling and feedstock-specific parameterization.

The modeling approach in this study relied heavily on several simplifying assumptions, including thermodynamic equilibrium, uniform feedstock properties, and idealized heat transfer. While these assumptions facilitated the simulation process, they introduced notable limitations, particularly in zones where kinetic effects play a dominant role. For instance, the use of Gibbs free energy minimization effectively predicted gas composition and heat release in the combustion and reduction zones. However, it failed to capture

incomplete char conversion and non-equilibrium dynamics that are often observed in practical systems. The assumption of uniform thermal and chemical properties for the SB&CS and WC&CC feedstock blends also overlooked critical variations in moisture content, ash levels, and volatile matter. These differences significantly influence gasification performance and reaction kinetics. Furthermore, the assumption of uniform temperature distribution ignored localized heat losses and temperature gradients within the reactor. This limitation was especially relevant in the reduction zone, where spatial variability in thermal conditions can substantially affect reaction pathways and product distribution (Awais et al., 2021).

Feedstock-specific behaviors provided additional insights. SB&CS consistently showed slightly higher modeled temperatures than experimental values, reflecting assumptions about its higher reactivity and thermal conductivity (Awais et al., 2021). Conversely, WC&CC exhibited slightly lower modeled temperatures, particularly in the reduction zone, suggesting that the model underestimated its char reactivity and failed to account for the moderating effects of ash content and other feedstock-specific properties (Awais et al., 2022). These observations indicate the need for refinement in feedstock-specific parameters to improve the model's predictive capabilities.

The findings demonstrate that the Aspen simulation model achieved high accuracy in predicting temperature distributions within the pyrolysis and combustion zones, with RMSD values of 2°C and 4°C, respectively. However, the higher RMSD of 7°C observed in the reduction zone, particularly for the WC&CC feedstock blend, revealed specific areas requiring improvement. The model's reliance on thermodynamic equilibrium and assumptions of uniform feedstock properties and ideal heat transfer simplified the simulation process. Nevertheless, these assumptions limited its ability to accurately represent kinetic processes and feedstock-specific effects, especially in the reduction zone

where solid-phase reactions and temperature gradients play a significant role (Ranjan et al., 2024). Addressing these limitations through the incorporation of kinetic models, refined feedstock properties, and enhanced heat transfer modeling could significantly improve the model's performance and reliability for biomass COG processes.

4.3.1.2 Validation on gas yield

The validation of gas yield predictions for the Aspen simulation model was conducted for SB&CS at two ER: 0.17 and 0.29 (Figure 4.10). The RMSD values were 0.21 Nm³/kg at an ER of 0.17 and 0.34 Nm³/kg at an ER of 0.29, demonstrating higher accuracy at lower ER. The validation highlighted the model's robustness in predicting gas yield under partial oxidation conditions, while exposed areas for improvement in handling dynamic effects at higher ER values.

At an ER of 0.17, the model exhibited good agreement with experimental results, achieving an RMSD of 0.21 Nm³/kg. The experimental gas yield was 1.1 Nm³/kg, while the modeled value was 1.31 Nm³/kg, indicating a slight over-prediction. This suggests that the model captured the primary reactions of partial oxidation and steam reforming effectively at lower oxygen availability (Cao et al., 2022). However, the minor over-prediction may reflect an overestimation of gas-phase reaction efficiency under these conditions (Pati et al., 2021). The model's reliability at lower ER makes it suitable for simulating processes where partial oxidation dominates.

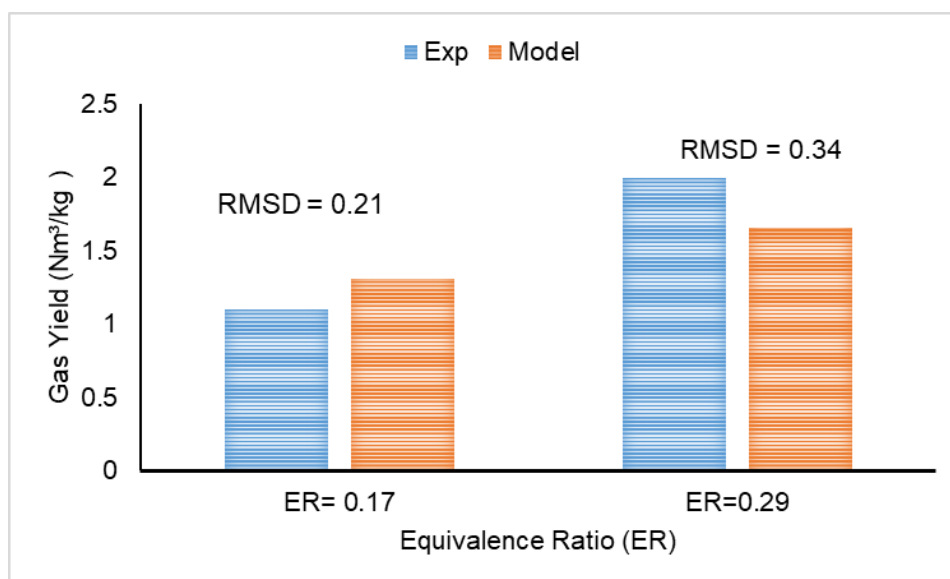


Figure 4.10 Process simulation model validation on gas yield

At an ER of 0.29, the model showed moderate accuracy, with an RMSD of 0.34 Nm³/kg. The experimental gas yield was 2.0 Nm³/kg, compared to a modeled value of 1.66 Nm³/kg, representing an under-prediction. This discrepancy likely stems from oversimplified assumptions about oxygen distribution and reaction kinetics at higher ER (Ding et al., 2021; Gabbrielli et al., 2022). Increased oxygen availability enhances secondary reactions, such as volatile reforming and tar cracking, driving syngas production. The model, however, relied on equilibrium assumptions that may not fully capture these dynamic effects, resulting in deviations (Ramos et al., 2019). Consequently, the model requires refinement to better predict gas yield under high ER conditions, where kinetic effects and non-equilibrium phenomena become significant.

The Aspen simulation model relied on Gibbs free energy minimization to predict equilibrium composition of syngas, particularly for gas-phase reactions. While this approach was effective in estimating thermodynamically favored products, it assumed ideal equilibrium conditions and complete oxygen utilization. These assumptions may not accurately capture kinetic limitations or mass transport constraints, especially under higher ER conditions, especially at higher ER (Sakheta et al., 2024). Additionally, the

model assumed uniform thermal and chemical properties for the SB and CS feedstock blend, which may have oversimplified real-world variability such as differences in ash content, moisture levels, and particle size. These limitations likely contributed to the observed under-prediction of gas yield at an ER of 0.29, where feedstock reactivity and volatile release played a significant role in influencing gasification outcomes (George et al., 2019; Anniwaer et al., 2021). The assumption of uniform heat and oxygen distribution also failed to account for localized temperature gradients and incomplete mixing, effects that become increasingly pronounced at elevated ER values. Furthermore, the model may not have adequately represented secondary reactions involving volatiles and tars, which are essential for syngas formation under high oxygen availability (Koido et al., 2021; Wiyono et al., 2021; Awais et al., 2018).

The validation results highlighted both the strengths and limitations of the Aspen simulation model. The model demonstrated strong performance in predicting temperature distribution within the pyrolysis and combustion zones and provided reliable gas yield estimates under lower ER conditions, indicating its robustness in partial oxidation scenarios. However, the greater deviations observed in the reduction zone and at an ER of 0.29 revealed limitations in accurately modeling solid-phase reactions, heat transfer dynamics, and the complex effects associated with elevated oxygen availability. These findings suggest that while the model is effective under certain conditions, further refinements are needed to improve its predictive accuracy under more reactive and non-equilibrium gasification environments.

To improve the predictive capability Aspen simulation model, several refinements are recommended. Incorporating detailed reaction kinetics would enable the model to capture non-equilibrium effects, particularly at higher ER values where increased oxygen availability significantly alters reaction rates (González-Vázquez et al., 2021). Enhancing

the representation of feedstock-specific parameters, such as volatile content, ash behavior, and moisture content, would improve model accuracy across diverse biomass types. In addition, incorporating more advanced heat and mass transfer modeling, including spatial variations in temperature and oxygen distribution, would enable more precise predictions of gas yield under varied operating conditions. Expanding model validation to include a broader range of ER values would also test its robustness and help address current limitations (Kuttin et al., 2024). Collectively, these refinements would strengthen the model's reliability and utility as a tool for optimizing biomass COG processes.

4.3.2 Simulation model sensitivity analysis

This section examines the sensitivity of the simulation model to variations in the ER, with a focus on its effects on temperature distribution, gas and char yields, and syngas composition for two feedstock combinations: SB&CS, and WC&CC. The analysis reveals feedstock-specific responses to ER adjustments and provides valuable insights into the role of ER in influencing gasification performance. These findings support the development of optimized operating strategies tailored to different biomass blends.

4.3.2.1 Effect of ER on temperature distribution

The sensitivity analysis of the ER on temperature distribution across the pyrolysis (T_p), combustion (T_c), reduction (T_r), and exit (T_e) zones revealed notable differences in thermal behavior between the WC&CC and SB&CS feedstock combinations (Figure 4.11). These variations reflect underlying differences in feedstock properties, reactivity, and overall gasification efficiency (Chun et al., 2022; Wiyono et al., 2021). The results provide valuable insights into how feedstock composition influences thermal profiles, offering practical guidance for optimizing gasification conditions to enhance performance and process stability.

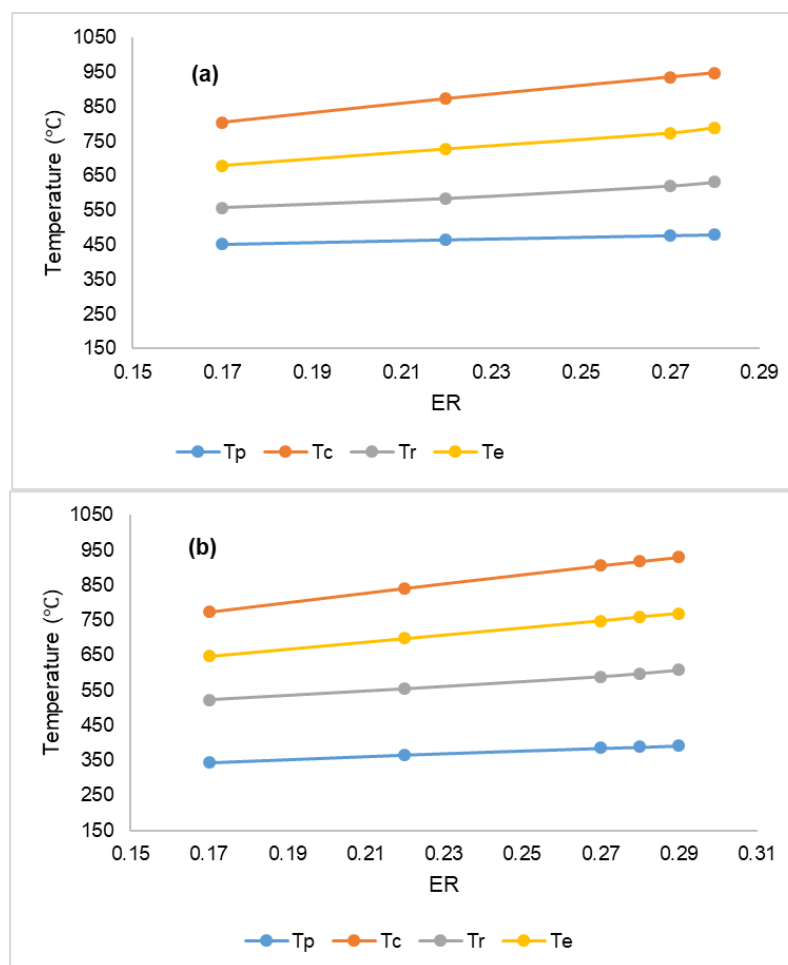


Figure 4.11. Effect of ER on gasifier reaction zone temperature.

Legend: (a) SB&CS, (b) WC&CC. T_p - pyrolysis temperature, T_c - combustion zone temperature, T_r - reduction zone temperature, T_e - exit zone temperature

For T_p , both feedstock combinations exhibited a steady increase with rising ER. The T_p for WC&CC increased from 344°C at an ER of 0.17 to 392°C at an ER of 0.29, while SB&CS showed an increase from 452°C to 481°C, over the same range. SB&CS consistently exhibited higher T_p values, which can be attributed to its superior thermal conductivity and higher volatile matter content (Awais et al., 2022). These properties facilitated more efficient heat absorption and transfer within the reactor. This trend indicates that SB&CS underwent more reactive and effective thermal decomposition compared to WC&CC. The enhanced thermal response suggests that SB&CS are more suitable for pyrolysis-dominated gasification systems, where rapid and efficient decomposition of biomass is essential for optimal performance (Awais et al., 2022).

In the combustion zone, T_c increased significantly with rising ER for both feedstocks. For WC&CC, T_c rose from 774°C at an ER of 0.17 to 931°C at an ER of 0.29. Similarly, SB&CS showed increase from 804°C to 959°C, over the same range. The consistently higher T_c values observed for SB&CS can be attributed to their greater fixed carbon content, which supports more intense exothermic reactions (Awais et al., 2022). This enhanced combustion contributed to improved heat transfer to the downstream zones, thereby enhancing overall gasification efficiency. The elevated T_c for SB&CS indicates its suitability for high-temperature combustion processes. However, this also underline the importance of careful thermal management to avoid exceeding reactor material limits and ensure safe, stable operation.

The T_r also exhibited a steady increase with rising ER. For WC&CC, T_r increased from 522°C at an ER of 0.17 to 608°C at an ER of 0.29. SB&CS showed a corresponding rise from 557°C to 646°C. The higher T_r values observed for SB&CS suggest more efficient heat transfer and endothermic reactions, such as the Boudouard reaction and water-gas shift (Awais et al., 2021). These reactions are critical for char conversion and the formation of carbon monoxide and hydrogen, both of which improve syngas quality (Monir et al., 2020). The results emphasize the importance of optimizing both heat transfer and reaction kinetics within the reduction zone. Inadequate heat supply or excessive energy loss in this zone can limit conversion efficiency and reduce the overall effectiveness of the gasification process.

For the T_e , both feedstocks displayed a linear increase with rising ER. The T_e for WC&CC increased from 648°C at an ER of 0.17 to 769°C at an ER of 0.29, while SB&CS rose from 680°C to 803°C, over the same range. SB&CS consistently demonstrated higher T_e values, indicating greater retention of thermal energy in the syngas and reflecting higher overall thermal efficiency (Awais et al., 2018; Omar et al., 2018). However, this elevated

T_e may necessitate the integration of advanced cooling systems to manage excess energy and prevent thermal stress on downstream components (Awais et al., 2022). Although a higher T_e is beneficial for syngas quality (Awais et al., 2018), it also highlights the importance of incorporating efficient heat recovery mechanisms to maximize energy utilization and maintain system stability within gasification operations.

Feedstock-specific observations further reinforced the performance differences between WC&CC and SB&CS. SB&CS consistently achieved higher temperatures across all zones, a trend attributed to their greater reactivity, higher volatile and fixed carbon content, and more efficient heat transfer characteristics (Awais et al., 2021). These properties support more vigorous thermal decomposition and enhanced conversion reactions during gasification (Pati et al., 2021). In contrast, WC&CC showed lower T_p and T_r , indicating slower thermal decomposition and char conversion. This may be due to lower intrinsic reactivity or higher ash content, which can inhibit heat transfer and reaction kinetics (Anniwaer et al., 2021). These findings suggest that SB&CS blend is more suitable for high-efficiency gasification systems, whereas WC&CC may require pre-treatment or operational optimization to reach comparable performance levels.

These findings demonstrate that increasing the ER significantly influences temperature distribution across all gasifier zones, with the SB&CS consistently achieving higher temperatures and superior performance compared to WC&CC. The optimal ER range was identified between 0.22 and 0.27, where heat transfer and reaction efficiency were balanced, resulting in improved syngas quality and reduced energy losses. This study concurs with the findings of Awais et al. (2018), who also reported that optimal gasification performance is achieved within a moderate ER range that avoids the inefficiencies of both under- and over-oxidation. These results highlight the importance

of both feedstock selection and precise ER control in optimizing biomass COG systems for maximum efficiency and product quality.

4.3.2.2 Effect of ER on gas and char yields

The sensitivity analysis of ER on gas yield and char yield revealed significant trends and differences between the feedstock blends of SB&CS and WC&CC (Figure 4.12). These trends highlight how increasing ER influences product distribution during gasification and provide insights into feedstock-specific behaviors that affect process efficiency.

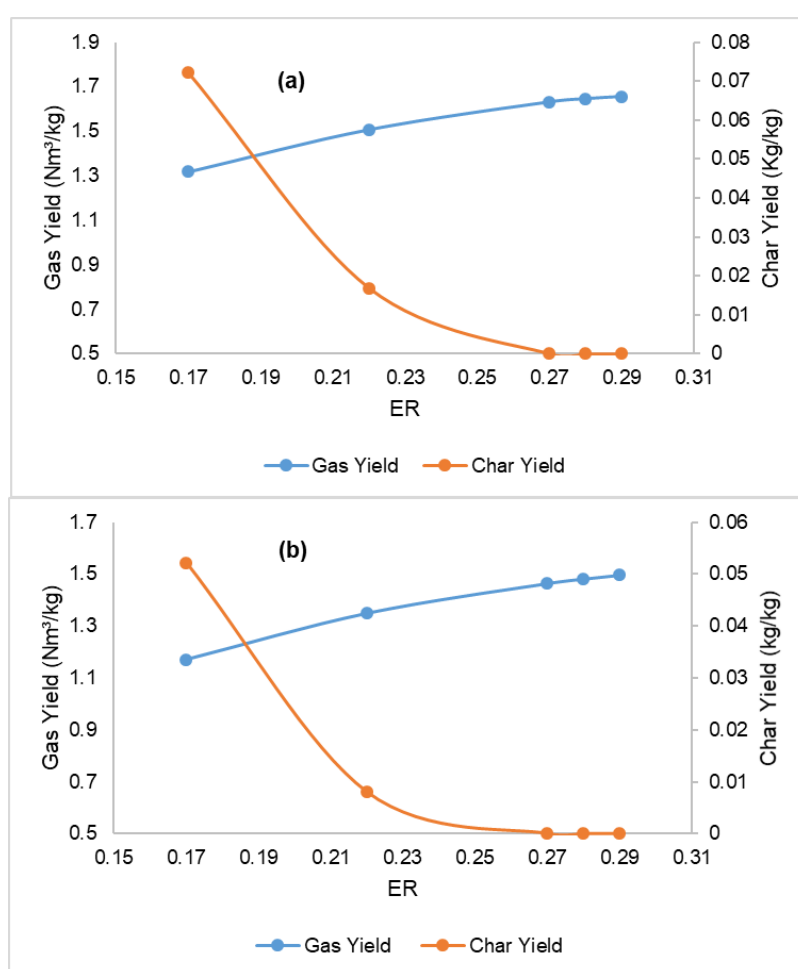


Figure 4.12: Effect of ER on gas and char yield.

Legend: (a) SB&CS (b) WC&CC.

Gas yield increased steadily with rising ER for both feedstocks, eventually stabilizing beyond an ER of 0.27. For SB&CS, gas yield rose from 1.3178 Nm³/kg at an ER of 0.17 to 1.6559 Nm³/kg at an ER of 0.29. This blend consistently outperformed the WC&CC,

which showed an increase from 1.1712 Nm³/kg to 1.4973 Nm³/kg over the same ER range. The superior performance of SB&CS is attributed to its higher reactivity and better heat transfer efficiency, which promote enhanced gas-phase reactions (Awais et al., 2022). At low ER (0.17), limited oxygen availability suppressed oxidation and reforming reactions, resulting in lower gas yield for both feedstocks. As ER increased to moderate levels (0.22 to 0.27), sufficient oxygen availability supported more complete gasification, leading to maximum gas yield. However, at higher ER values (0.28 to 0.29), gas yield stabilized as additional oxygen contributed diminishing returns due to near-complete conversion of the biomass.

Char yield decreased rapidly with increasing ER for both feedstocks, becoming negligible at $ER \geq 0.27$. For SB&CS, char yield declined from 0.0722 kg/kg at an ER of 0.17 to 0 at an ER of 0.27, while for WC&CC, it decreased from 0.0522 kg/kg to 0 over the same ER range. SB&CS consistently produced more char than WC&CC at lower ER, which can be attributed to their higher fixed carbon content and slower oxidation kinetics (Awais et al., 2022). At low ER (0.17), limited oxygen availability led to incomplete combustion, resulting in higher char residue. As ER increased to moderate levels (0.22 to 0.27), oxygen availability promoted char oxidation, leading to a significant reduction in char yield. At high ER values (0.28 to 0.29), the biomass was almost fully converted, and char was entirely consumed, indicating near-complete gasification.

The observed trends in gas yield and char yield are closely tied to the influence of ER on gasification reactions. As ER increased, oxygen availability was enhanced, thereby driving oxidation and reforming reactions that converted carbonaceous materials into syngas components such as H₂, CO, and CO₂. The higher temperatures in the combustion and reduction zones at higher ER values further accelerated char gasification reactions, resulting in increased gas yield (Awais et al., 2022). However, the stabilization of gas

yield beyond an ER of 0.27 suggests that the reactions had reached completion, limiting further increases despite the availability of additional oxygen. Conversely, the rapid decline in char yield with increasing ER reflect the enhanced promotion of oxidation and reforming reactions that consumed the remaining char. The complete disappearance of char at ER values equal to or greater than 0.27 indicates full conversion of the feedstock, leaving no solid residue.

Feedstock-specific observations revealed key differences in gasification performance between SB&CS and WC&CC. SB&CS exhibited higher gas yield across all ER values, attributed due to its superior reactivity, thermal stability, and volatile content, all of which promote efficient gas-phase reactions (Awais et al., 2021). Additionally, the higher fixed carbon content in SB&CS contributed to greater char formation at lower ER values and supported more complete gasification at higher ER. In contrast, WC&CC consistently produced lower gas yields, reflecting its lower reactivity and thermal stability (Awais et al., 2022). This feedstock blend also generated less char at low ER, likely due to its lower fixed carbon content (Koido et al., 2021; Awais et al., 2018), which limited char formation even when oxygen availability was restricted.

The results demonstrate that increasing ER had significant impact on gas yield and char yield for both feedstocks. Moderate ER values, particularly in the range of 0.22 to 0.27, provided optimal conditions for gasification by maximizing gas yield while minimizing char residue. Across all ER levels, SB&CS consistently outperformed WC&CC in terms of gasification efficiency and syngas production, indicating their greater suitability for high-yield gasification processes. These results also emphasize the importance of precise ER control and strategic feedstock selection in optimizing biomass COG performance.

4.3.2.3 Effect of ER on gas composition

This sensitivity analysis evaluated the impact of ER on the syngas composition (H_2 , CO_2 , CO , CH_4) for two feedstock combinations: SB&CS and WC&CC (Figure 4.13). The co-gasification process employed a mixture of air and steam as the gasifying agent. The findings revealed significant trends in gas composition as ER increases, reflecting the combined influence of oxygen availability and feedstock-specific reactivity.

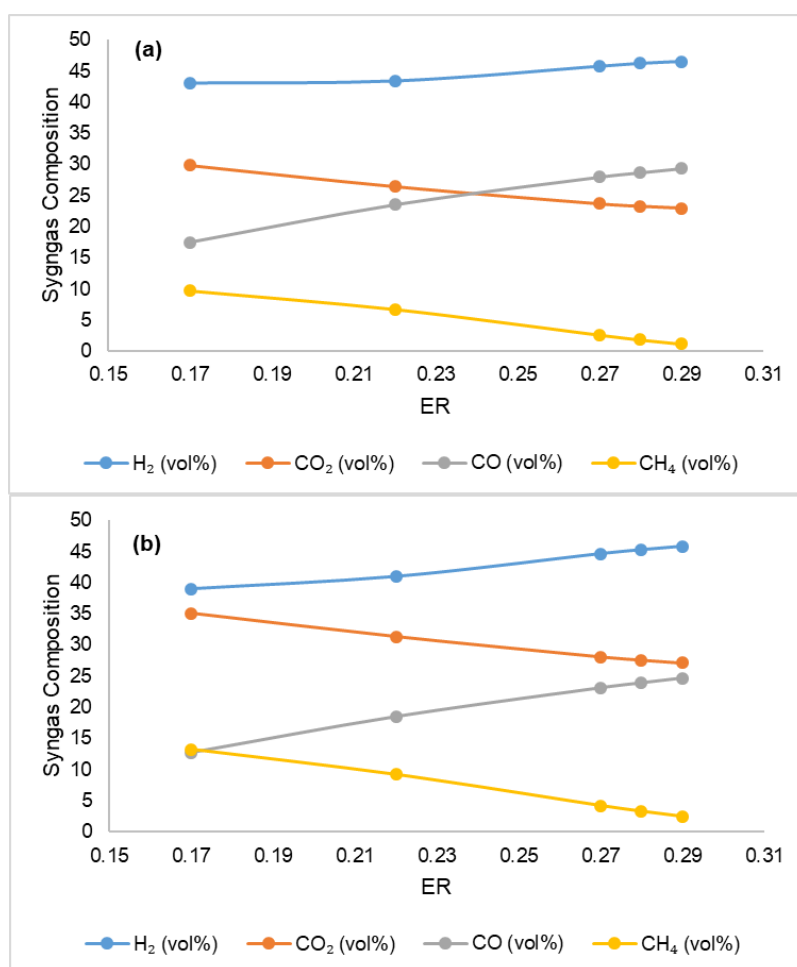


Figure 4.13: Effect of ER on syngas comp composition.
Legend: (a) SB&CS (b) WC&CC.

Hydrogen (H_2) content increased steadily with rising ER for both feedstocks, with SB&CS consistently producing higher H_2 levels than WC&CC. For instance, at an ER of 0.17, SB&CS produced 43.01 vol% H_2 , which increased to 46.52 vol% at ER of 0.29, representing percentage increase of 17.37. In comparison, WC&CC showed an increase

from 39.04 vol% to 45.82 vol% over the same range, corresponding to 8.16% increase. This increase in H₂ content is attributed to the promotion of steam reforming reactions at higher ER values, such as $\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$, which convert methane and steam into hydrogen (Monir et al., 2020; Kittivech & Fukuda, 2019). The higher volatile matter content in SB&CS provided more precursors for these reactions, resulting in superior hydrogen production (Awais et al., 2021, 2022). Enhanced H₂ levels at higher ER improve syngas quality, making it particularly suitable for hydrogen-rich applications such as fuel cells and chemical synthesis.

Carbondioxide (CO₂) content decreased with increasing ER for both feedstocks, with WC&CC consistently producing higher CO₂ levels than SB&CS. For example, at ER of 0.17, WC&CC produced 35.06 vol% CO₂, declined to 27.10 vol% at ER of 0.29, representing 22.7% decrease, while SB&CS exhibited a reduction from 29.86 vol% to 22.97 vol% over the same range, corresponding 23.07% decrease. This reduction in CO₂ content, is primarily attributed to the promotion of CO₂ reduction reactions at higher ER values, such as $\text{CO}_2 + \text{C} \rightarrow 2\text{CO}$ (Cao et al., 2022). These reactions convert carbon dioxide into carbon monoxide, enhancing syngas quality. The lower reactivity of WC&CC likely resulted in less efficient CO₂ reduction compared to SB&CS (Awais et al., 2022). Decreased CO₂ levels at higher ER values contribute to an increased calorific value of syngas (Pati et al., 2021), thereby improving energy efficiency for combustion and other downstream applications.

Carbonmonoxide (CO) content increased steadily with rising ER for both feedstocks, with SB&CS consistently achieving higher CO levels than WC&CC. At an ER of 0.17, SB&CS produced 17.47 vol% of CO, which increased to 29.34 vol% at an ER of 0.29. In comparison, WC&CC showed an increase from 12.67 vol% to 24.66 vol% over the same range. This upward trend is attributed to enhanced oxygen availability, at higher ER

values, which promotes both direct oxidation reactions ($C + O_2 \rightarrow CO$) and CO_2 reduction to CO (George et al., 2019). The higher reactivity of SB&CS enabled more efficient carbon conversion, resulting in superior CO production (Awais et al., 2022). Elevated CO content at higher ER values contributes to improved energy density of the syngas, enhancing its suitability for combustion and chemical synthesis applications.

Methane (CH_4) content decreased sharply with increasing ER, approaching negligible levels at $ER \geq 0.28$ for both feedstocks. WC&CC consistently retained higher CH_4 levels than SB&CS, reflecting its lower reactivity and less efficient reforming behaviors (Awais et al., 2022). At an ER of 0.17, WC&CC produced 13.23 vol% CH_4 , which dropped to 2.42 vol% at an ER of 0.29. In contrast, SB&CS exhibited a decrease from 9.67 vol% to 1.16 vol% over the same range. The reduction in CH_4 content is primarily attributed to reforming reactions ($CH_4 + H_2O \rightarrow CO + 3H_2$), which become more pronounced at higher ER values due to increased oxygen and steam availability (Awais et al., 2021). Lower CH_4 levels indicate improved syngas quality, as they respond with higher proportions of H_2 and CO, resulting in a more energy-rich and chemically favorable gas mixture.

Feedstock-specific observations revealed distinct differences between SB&CS and WC&CC in terms of syngas composition and quality. SB&CS consistently outperformed WC&CC, producing higher concentrations H_2 and CO levels, which can be attributed to their superior reactivity, thermal stability, and higher volatile matter content (Awais et al., 2022). Additionally, the lower concentrations of CO_2 and CH_4 levels observed in SB&CS further demonstrated their effectiveness in promoting reforming and reduction reactions (Awais et al., 2021). Conversely, WC&CC generated acceptable levels of H_2 and CO but exhibited lower overall syngas quality. The relatively higher residual CO_2 and CH_4 levels suggest reduced reactivity and less efficient conversion processes, likely due to their lower volatile and fixed carbon content (Awais et al., 2018; Omar et al., 2018).

The effect of ER on syngas quality was significant across different operating ranges. At low ER of 0.17, H₂ and CO levels were relatively low, while CO₂ and CH₄ concentration were high, implying incomplete gasification. WC&CC performed particularly poorly at this stage, exhibiting higher CO₂ and CH₄ contents compared to SB&CS. At moderate ER (0.22 to 0.27), H₂ and CO levels increased substantially, while CO₂ and CH₄ decreased, indicating optimal gasification conditions. SB&CS achieved higher levels of H₂ and CO than WC&CC, highlighting its superior performance. At higher ER (0.28 to 0.29), H₂ and CO levels stabilized, while CO₂ and CH₄ approached minimal levels, indicating near-complete gasification. Although SB&CS continued to outperform WC&CC in terms of syngas quality, the diminishing returns observed at these ER levels emphasizes the importance of precise ER optimization to avoid unnecessary input without corresponding performance gains.

This sensitivity analysis reveals that increasing ER enhanced syngas quality by increasing the concentrations H₂ and CO while simultaneously reducing CO₂ and CH₄. SB&CS consistently produced superior syngas due to its higher reactivity and efficient reforming reactions, making it the more favorable feedstock for hydrogen-rich applications and energy-intensive processes (Awais et al., 2022). While WC&CC generated syngas of acceptable quality, it requires additional optimization to achieve comparable performance to SB&CS. These findings highlight the importance of precise ER control and informed feedstock selection in maximizing syngas quality for air-steam COG systems.

4.4 Evaluation of ML Models

This section presents the evaluation of ML models for predicting key gasification performance indicators, including cold gas efficiency (CGE), char yield, carbon monoxide (CO) concentration in syngas, gas yield, hydrogen (H₂) concentration in syngas, and the lower heating value (LHV) of syngas. A comprehensive comparison was

conducted among several algorithms, namely Random Forest (RF), Gradient Boosting Regression (GBR), Artificial Neural Network (ANN), Support Vector Regression (SVR), and the SuperLearner Ensemble (SLE).

Model performance was assessed using both validation and test datasets. The evaluation metrics included root mean square error (RMSE), mean square error (MSE), coefficient of determination (R^2), and mean absolute error (MAE). The results offer valuable insights into the predictive accuracy, robustness, and generalizability of each model. It is important to note that plots comparing true and predicted values for each response were not included for the SLE models in this section (Figure 4.14-Figure 4.19), as these are specifically analyzed in the robustness evaluation presented in the subsequent section.

For reproducibility and transparency, the MATLAB code used to implement the SLE models for gas yield and char yield prediction is provided in APPENDIX G. The model performance is presented graphically in this section to clearly illustrate and compare the predictive behavior of the models on the test data, it is an approach that allows readers to visually assess trends, deviations, and overall accuracy. Detailed numerical evaluation results for both the validation and test datasets are included in APPENDIX H.

4.4.1 Evaluation for CGE prediction

For CGE prediction, ANN model demonstrated reasonable accuracy, achieving an R^2 of 0.9620 during validation and 0.9742 during testing. However, its error metrics, including RMSE (0.0433 for validation and 0.0373 for testing), were higher than those of the ensemble models. This suggests that while the ANN model effectively captures non-linear patterns, as shown in Figure 4.14a, it may be less robust than ensemble methods in predicting CGE. Similar findings were reported by Ozonoh et al. (2020), who applied ANN models and achieved higher R^2 of up to 0.90, highlighting the potential of ANN when properly optimized.

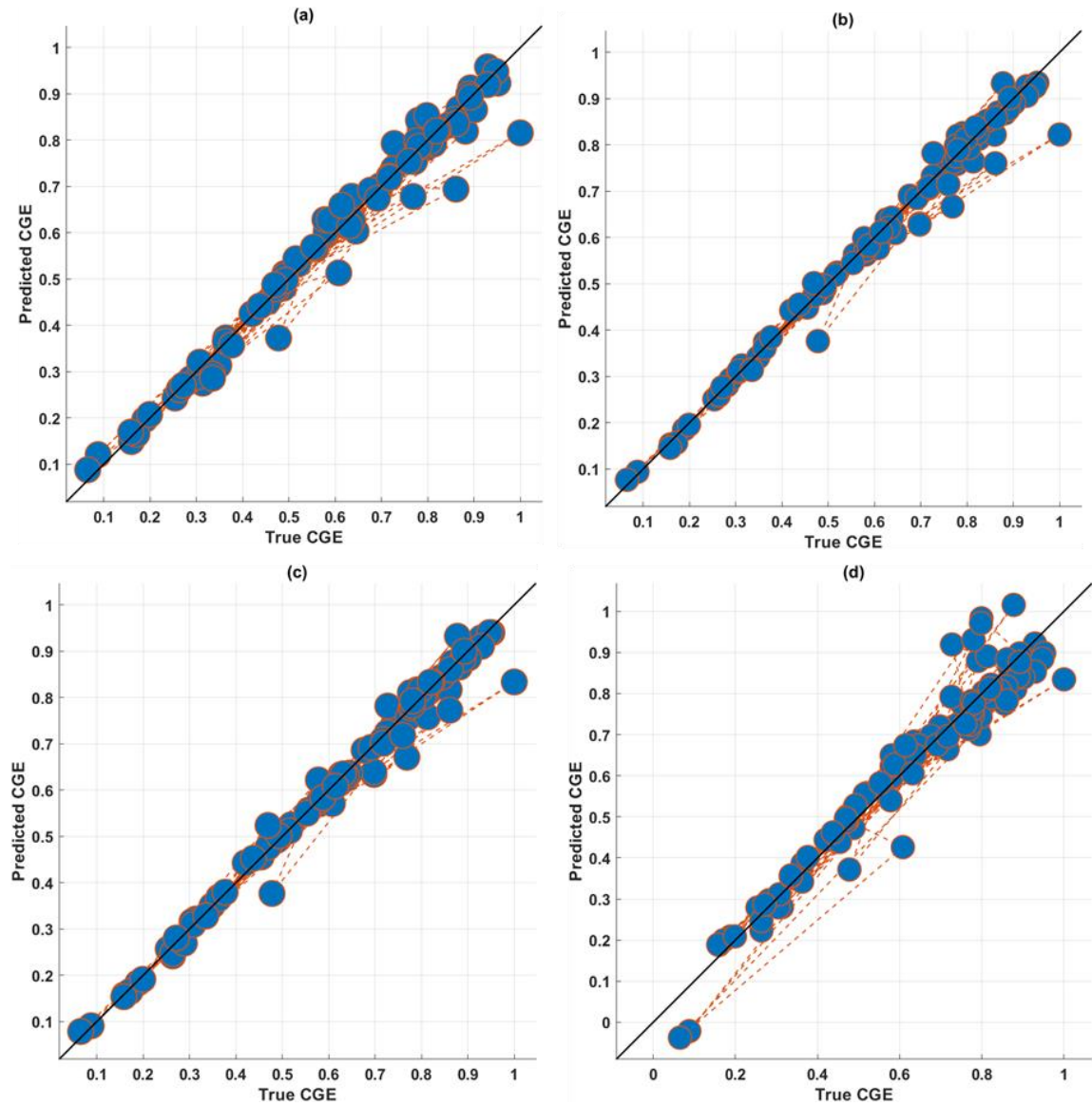


Figure 4.14: Predicted vs true values on normalized test data for CGE

Legend: (a) ANN, (b) GBR, (c) RF, (d) SVM. Note: Values are normalized; therefore, no units are shown.

The ensemble models demonstrated strong performance, with GBR slightly outperformed RF during validation (Figure 4.14b and Figure 4.14c), with an R^2 of 0.9802 and an RMSE of 0.0313. However, its test performance was marginally lower, achieving an R^2 of 0.9816. RF achieving an R^2 of 0.9783 on the validation set and 0.9833 on the test set, supported by low RMSE values of 0.0327 and 0.0301, respectively. These results confirm the effectiveness of ensemble methods, which improve predictive performance by averaging the outputs of multiple decision trees to reduce overfitting and enhance generalization. Lahafdoozian et al. (2024) similarly demonstrated the strong performance

of RF and GBR in modeling water-gas shift reactors to predict CGE and obtained accuracy of $R^2 > 0.90$.

The SVM model exhibited the weakest performance among all models, with the lowest R^2 values of 0.9228 during validation and 0.9325 during testing. It also had the highest RMSE values (0.0617 and 0.0605 for validation and testing, respectively) (Figure 4.14d). These results highlight the limitations of the SVR in capturing complex and non-linear relationships within the CGE dataset, rendering it less suitable for this application compared to other models. The suboptimal performance of SVR in predicting CGE was also reported by Mutlu et al. (2019), who achieved a relatively low R^2 of 0.70, further confirming its limited applicability in such contexts.

The SLE, which combines predictions from multiple base learners, achieved the best overall performance in predicting CGE. It obtained an R^2 of 0.9927 on the validation set and 0.9826 on the test set, accompanied by the lowest RMSE values of 0.0198 during validation and 0.0307 during testing. These results demonstrate the robustness of the SLE approach, as it effectively integrates the strengths of multiple algorithms to deliver accurate and reliable predictions (Massaoudi et al., 2021). While its MAE during testing (0.0176) was slightly higher than RF's (0.0165), this may reflect its broader generalization capability, making it well-suited for real-world applications where data variability is higher.

The results clearly demonstrate that ensemble models (RF and GBR) outperform individual learners such as ANN and SVM in both accuracy and error metrics, confirming the robustness of tree-based ensemble methods for this application. The superior predictive capability of the SLE model demonstrates the advantage of combining multiple base learners to capitalize on their complementary strengths. The high R^2 values and low error metrics achieved by the SLE demonstrate its reliability in capturing the complex

relationships governing CGE. These findings align with the study by Mutlu et al. (2019), which also highlighted the ability of ensemble models to outperform individual models in accurately predicting CGE.

4.4.2 Evaluation for char yield prediction

For char yield prediction, the ANN model showed exceptional performance during validation, achieving the highest R^2 of 0.9850 and the lowest RMSE of 0.0301 among the standalone models. However, its generalization capability slightly declined on the test set, with an R^2 of 0.9483 and an RMSE of 0.0571 (Figure 4.15a). This moderate drop in performance suggests potential overfitting during training, where the ANN model may have learned patterns that were overly specific to the training dataset, thus limiting its generalizability. A similar outcome was reported by Ascher et al. (2022), who applied an ANN model to predict char yield in a gasification process and achieved R^2 of 0.76, indicating moderate predictive capability.

The RF and GBR, performed significantly better than SVM (Figure 4.15b, Figure 4.15c, and Figure 4.15d). GBR demonstrated strong validation performance with an R^2 of 0.9746 and an RMSE of 0.0392, while its test performance yielded an R^2 of 0.9452 and an RMSE of 0.0588. Similarly, RF achieved an R^2 of 0.9807 during validation and 0.9490 on the test set, with RMSE values of 0.0342 and 0.0567, respectively.

Although both RF and GBR exhibited slight declines in performance on the test set, their capacity to model non-linear relationships and capture complex feature interactions rendered them reliable predictors of char yield. This finding aligns with the results of Ascher et al. (2022), who reported comparable performance of RF and GBR in predicting char yield during gasification, with an R^2 of 0.83. Additionally, the present study concurs with the findings of Sison et al. (2023), who demonstrated the superiority of GBR over RF for char yield prediction in a chemical looping gasification process.

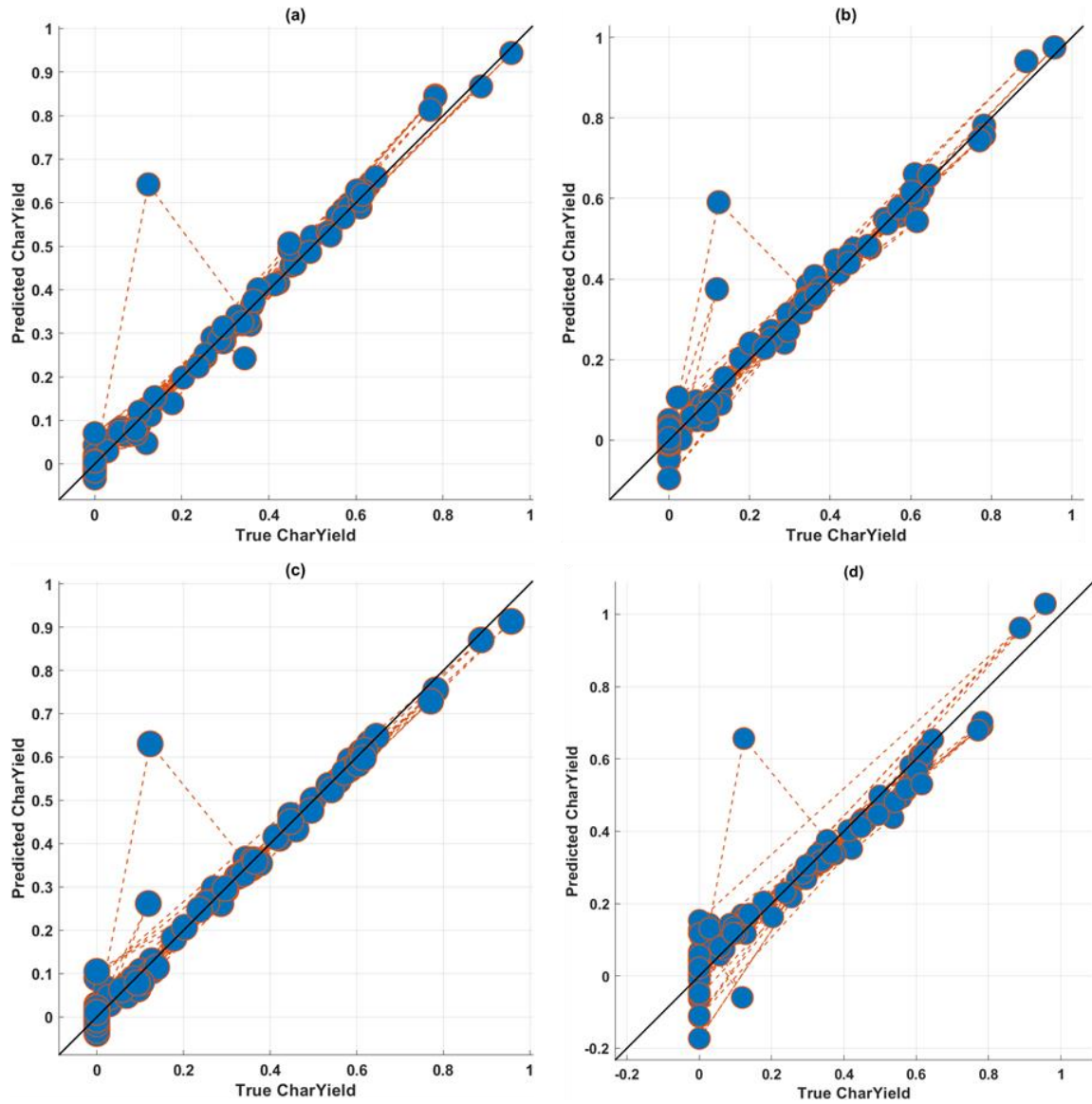


Figure 4.15: Predicted vs true values on test data for char yield.

Legend: (a) ANN, (b) GBR, (c) RF, (d) SVM. Note: Values are normalized; therefore, no units are shown.

The SVM model exhibited the weakest performance among all models, achieving an R^2 of 0.9292 during validation and 0.9017 on the test set. It also had the highest error metrics, with RMSE values of 0.0655 and 0.0788 for validation and test datasets, respectively. These results indicate that the SVM model struggled to capture the complex, non-linear relationships governing char yield, rendering it less suitable for this application. This observation is consistent with the findings of Ascher et al. (2022), who reported poor performance of SVM in char yield prediction, achieving a low R^2 of just 0.14.

The SLE model emerged as the most accurate approach. By combining predictions from multiple base learners, it achieved the highest R^2 values of 0.9951 during validation and 0.9531 on the test set. It also had the lowest RMSE values, with 0.0176 during validation and 0.0544 during testing. The ability of SLE model to integrate diverse prediction strategies effectively minimized errors, establishing it as the most reliable model for char yield predictions. Its lower MAE values further demonstrate its precision and robustness, making it the optimal choice for this application. This finding aligns with studies by Leng et al. (2022), Hai et al. (2023) and Hai et al. (2023), which also highlighted the superior performance of ensemble models in predicting char yield with high accuracy and reliability.

4.4.3 Evaluation of ML models for CO prediction

Similar to char yield prediction, the models' performance on validation and test datasets provided a comprehensive understanding of their predictive capabilities for CO concentration in the syngas (Figure 4.16). The ANN model demonstrated exceptional performance among the individual models. It achieved an R^2 of 0.9958 during validation and 0.9960 on the test set, recording the lowest RMSE values (0.0150 during validation and 0.0141 during testing) and MAE values (0.0100 for validation and 0.0101 for testing). These results highlight ability of ANN model to capture complex, non-linear relationships in the dataset (Figure 4.16a).

However, while the ANN exhibited high predictive accuracy, it demonstrated slightly lower robustness compared to the SLE in terms of generalization performance. This trend aligns with the findings of Ascher et al. (2022), who reported that although ANN achieved a high R^2 of 0.93 in predicting CO concentration, its accuracy was still lower than that of ensemble models, highlighting the superior generalization capability of ensemble approaches.

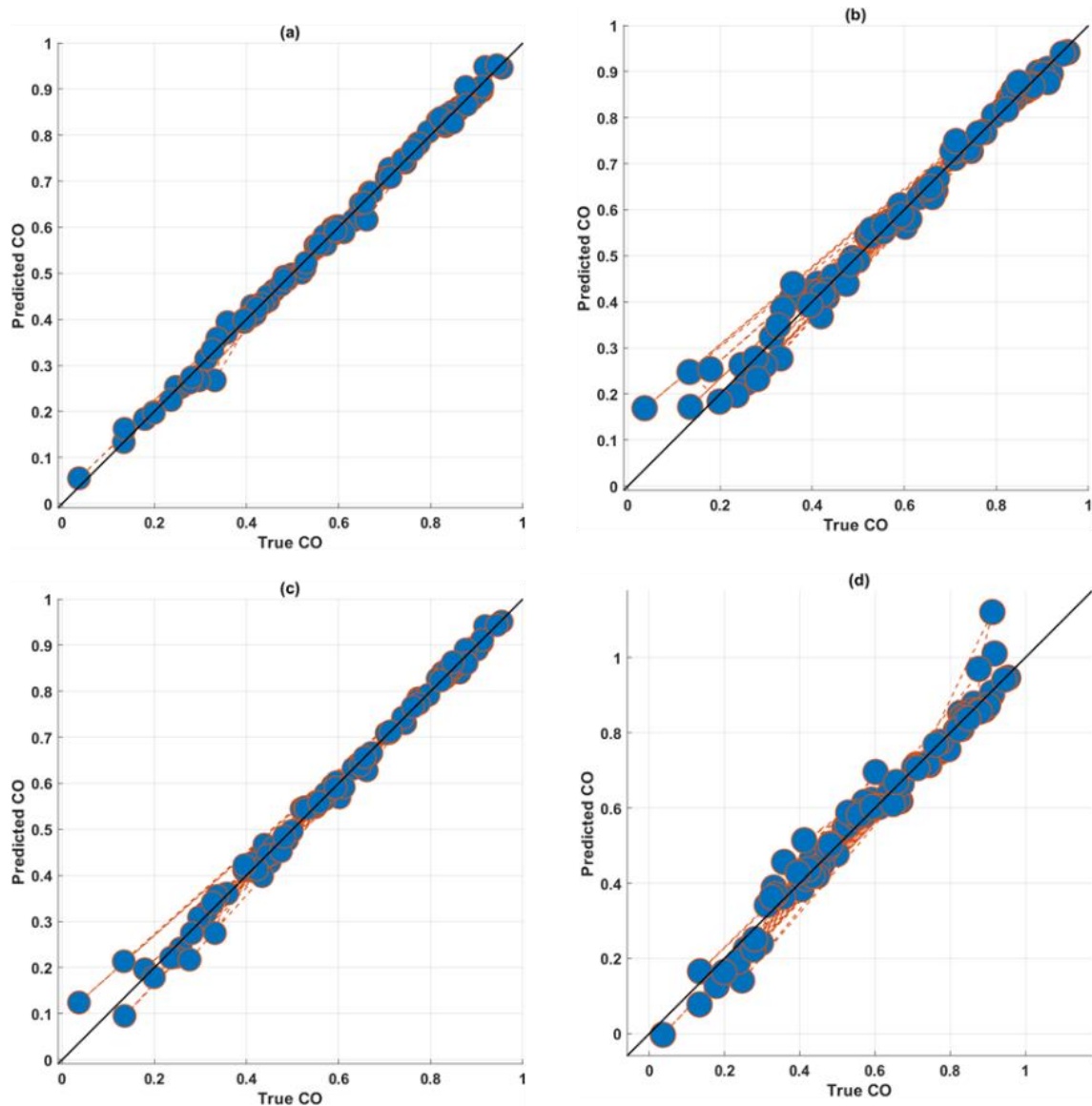


Figure 4.16: Predicted vs true values on test data for CO

Legend: (a) ANN, (b) GBR, (c) RF, (d) SVM. Note: Values are normalized; therefore, no units are shown.

The ensemble models, RF and GBR, exhibited strong predictive performance on CO concentration. GBR, while slightly less accurate than RF, still performed well, achieving an R^2 of 0.9854 during validation and 0.9834 on the test set (Figure 4.16b). Its RMSE values were slightly higher than RF (0.0279 for validation and 0.0285 for testing), reflecting its robustness but slightly limited precision compared to RF. The RF achieved an R^2 of 0.9920 during validation and 0.9922 on the test set, with low RMSE values of 0.0207 and 0.0196 for validation and test datasets, respectively. This indicates excellent accuracy in predicting CO (Figure 4.16c). However, RF slightly outperformed GBR in

this study. This observation is consistent with the findings of Ascher et al. (2022), who reported comparable performance between RF and GBR in predicting CO concentrations, with both models achieving a R^2 of 0.94.

The SVM model performed reasonably well, achieving an R^2 of 0.9754 during validation and 0.9666 on the test set. However, its RMSE values (0.0362 for validation and 0.0405 for testing) and MAE values (0.0237 for validation and 0.0277 for testing) were higher compared to other models, indicating relatively lower predictive accuracy (Figure 4.16d). While the SVM model demonstrated some capacity to capture patterns within the dataset, its performance lagged behind that of ensemble models and the ANN, particularly in minimizing prediction errors. This finding aligns with the study by Ascher et al. (2022), who reported that SVM showed the lowest performance among the models evaluated for predicting CO concentrations.

The SLE consistently outperformed all other models, achieving the highest R^2 values of 0.9983 during validation and 0.9966 on the test set. It also recorded the lowest RMSE values (0.0097 during validation and 0.0129 during testing) and MAE values (0.0074 for validation and 0.0093 for testing). These results highlight the exceptional ability of SLE to combine predictions from multiple base learners, effectively harnessing their strengths to deliver the most accurate and reliable predictions. Its marginally lower MAE compared to other models further validates its robustness for CO prediction on the test dataset. The superior performance of SLE and other ensemble models aligns with findings by previous studies (Ascher et al., 2022; Elmaz et al., 2020; Wen et al., 2021), which similarly highlighted their effectiveness in predicting CO with enhanced accuracy and reliability.

4.4.4 Evaluation for gas yield prediction

For gas yield prediction, The ANN model delivered exceptional performance, achieving an R^2 of 0.9887 for validation and 0.9866 for testing. It recorded RMSE values of 0.0206

during validation and 0.0238 during testing, with MAE values of 0.0140 and 0.0154, respectively, making it one of the most accurate standalone models (Figure 4.17a).

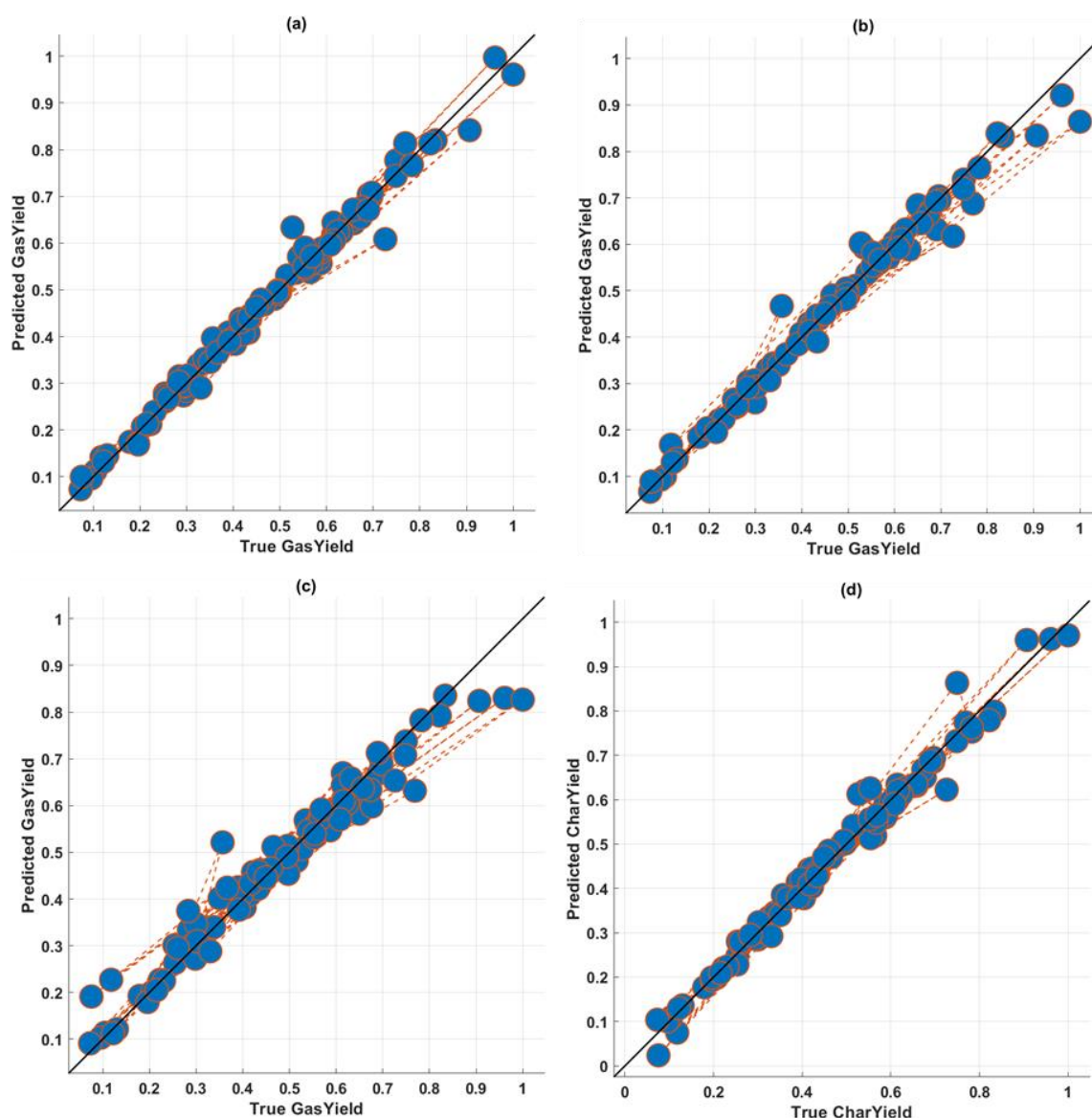


Figure 4.17: Predicted vs true values on test data for gas yield

Legend: (a) ANN, (b) GBR, (c) RF, (d) SVM. Note: Values are normalized; therefore, no units are shown.

These results highlight the ANN capability to effectively model the complex non-linear relationships involved in gas yield prediction. However, despite its strong performance, ANN was slightly outperformed by the SLE model, particularly in terms of generalization. This observation is consistent with the findings of Kardani et al. (2021), who compared the performance of ANN and ensemble models for gas yield prediction in a fluidized-bed reactor. Their study reported lower accuracy for ANN, with a R^2 of 0.93,

compared to higher values achieved by ensemble models. Similarly, Mutlu et al. (2019) applied ANN for gas yield prediction and achieved an R^2 of 0.92, further confirming ANN's strong, yet slightly inferior, performance relative to ensemble approaches.

On the other hand, GBR performed significantly better than RF (Figure 4.17b and Figure 4.17c), with R^2 values of 0.9807 for validation and 0.9796 for testing, and RMSE values of 0.0269 and 0.0293 for validation and testing, respectively. While GBR outperformed RF, its predictive accuracy remained slightly lower than ANN and SuperLearner. The RF achieved a prediction with an R^2 of 0.9603 during validation and 0.9512 on the test set. Its RMSE values were relatively high at 0.0386 for validation and 0.0454 for testing, indicating limited accuracy compared to the other approaches.

The findings are consistent with the study by Kardani et al. (2021), who reported similar performance of RF in predicting gas yield. They also align with the observations of Ascher et al. (2022), who compared RF and GBR for gas yield prediction and found that GBR outperformed RF in terms of predictive accuracy.

The SVM model showed strong predictive capabilities, achieving an R^2 of 0.9759 during validation and 0.9815 on the test dataset. It recorded RMSE values of 0.0301 and 0.0280 for validation and testing, respectively, alongside MAE values of 0.0204 and 0.0189. While the performance metrics demonstrate the SVM potential for gas yield prediction (Figure 4.17d), it was ultimately outperformed by other models, particularly the SLE, GBR, and ANN, in terms of predictive accuracy and error reduction. Similar observations were reported by Ascher et al. (2022), where SVM achieved a R^2 of 0.90, which was lower than that of other models used for gas yield prediction.

The SLE emerged as the most accurate and robust model for gas yield prediction. It achieved the highest R^2 values of 0.9938 during validation and 0.9884 during testing, with

the lowest RMSE values of 0.0145 for validation and 0.0221 for testing. Its MAE values were also the lowest among all models (0.0111 for validation and 0.0133 for testing). The findings demonstrate that the SLE approach provided a clear advantage over standalone models. By integrating predictions from multiple base learners, the SLE achieved better generalization and robustness, consistently delivering the most accurate gas yield predictions across both validation and test datasets. The strength of the SLE and other ensemble models, as highlighted in this study, is further supported by findings from the previous studies (Devasahayam & Albijanic, 2024; Kardani et al., 2021; Zhao et al., 2021), which also showcased their superior performance in predicting gas yield.

4.4.5 Evaluation of ML models for H₂ prediction

For H₂, the ANN model performed well during validation, achieving an R² of 0.9581 and an RMSE of 0.0335, with a validation MAE of 0.0191. However, its performance declined on the test dataset (Figure 4.18a), where it achieved an R² of 0.9204 and an RMSE of 0.0473, with an MAE of 0.0245. This decline in test performance suggests potential overfitting during training, which may have limited the model's ability to generalize effectively to unseen data. The performance of the ANN model in this study aligns with the findings of Wen et al. (2021) and Ascher et al. (2022), who reported similar ANN performance in predicting H₂ concentration.

The tree-based ensemble models delivered significantly better results (Figure 4.18b and Figure 4.18c). GBR showed slightly weaker performance, achieving R² values of 0.9567 during validation and 0.9416 on testing. Its RMSE values were higher (0.0341 for validation and 0.0405 for testing), as were its MAE values (0.0231 and 0.0262), suggesting less robust predictions compared to the RF. The RF achieved an R² of 0.9719 during validation and 0.9701 on the test set, with low RMSE values of 0.0274 and 0.0290 for validation and testing, respectively. Its MAE values were also among the lowest

(0.0170 for both datasets), indicating strong predictive accuracy and reliability. However, the weaker performance of GBR compared to RF in this study contrasts with the findings of Ascher et al. (2022), who reported superior H₂ prediction accuracy using GBR over RF. This discrepancy may be attributed to differences in dataset size, feature complexity, or model hyperparameter tuning. In particular, GBR is known to be more sensitive to parameter settings and overfitting in smaller or noisier datasets, which may have affected its performance in this case.

The SVM model showed the weakest performance among all evaluated models (Figure 4.18d), achieving an R² of 0.9037 during validation and 0.8943 on the test set. It recorded relatively high RMSE values (0.0508 for validation and 0.0545 for testing) and MAE values (0.0317 for validation and 0.0324 for testing), reflecting its inability to capture the complex, nonlinear relationships governing H₂ concentration. These results suggest that the SVM model is not well-suited for predicting H₂ output in COG processes. This finding is consistent with the study by Ascher et al. (2022), who reported relatively low H₂ prediction accuracy using the SVM model.

The SLE model outperformed all other models, achieving the highest R² values of 0.9774 for validation and 0.9640 for testing. It recorded the lowest RMSE values (0.0233 for validation and 0.0318 for testing) and MAE values (0.0119 for validation and 0.0174 for testing), reflecting its superior predictive accuracy and robustness. The results clearly demonstrate the advantages of ensemble approaches, particularly the SLE, in achieving superior predictive accuracy and robustness for H₂ concentration in syngas. The SLE capability to integrate predictions from diverse base learners enabled it to consistently outperform individual models, such as ANN, as well as standalone ensemble models like RF and GBR. These findings are consistent with previous studies (Ascher et al., 2022;

Elmaz et al., 2020; Wen et al., 2021), which also highlighted the superior performance of SLE and other ensemble models in predicting H_2 concentration.

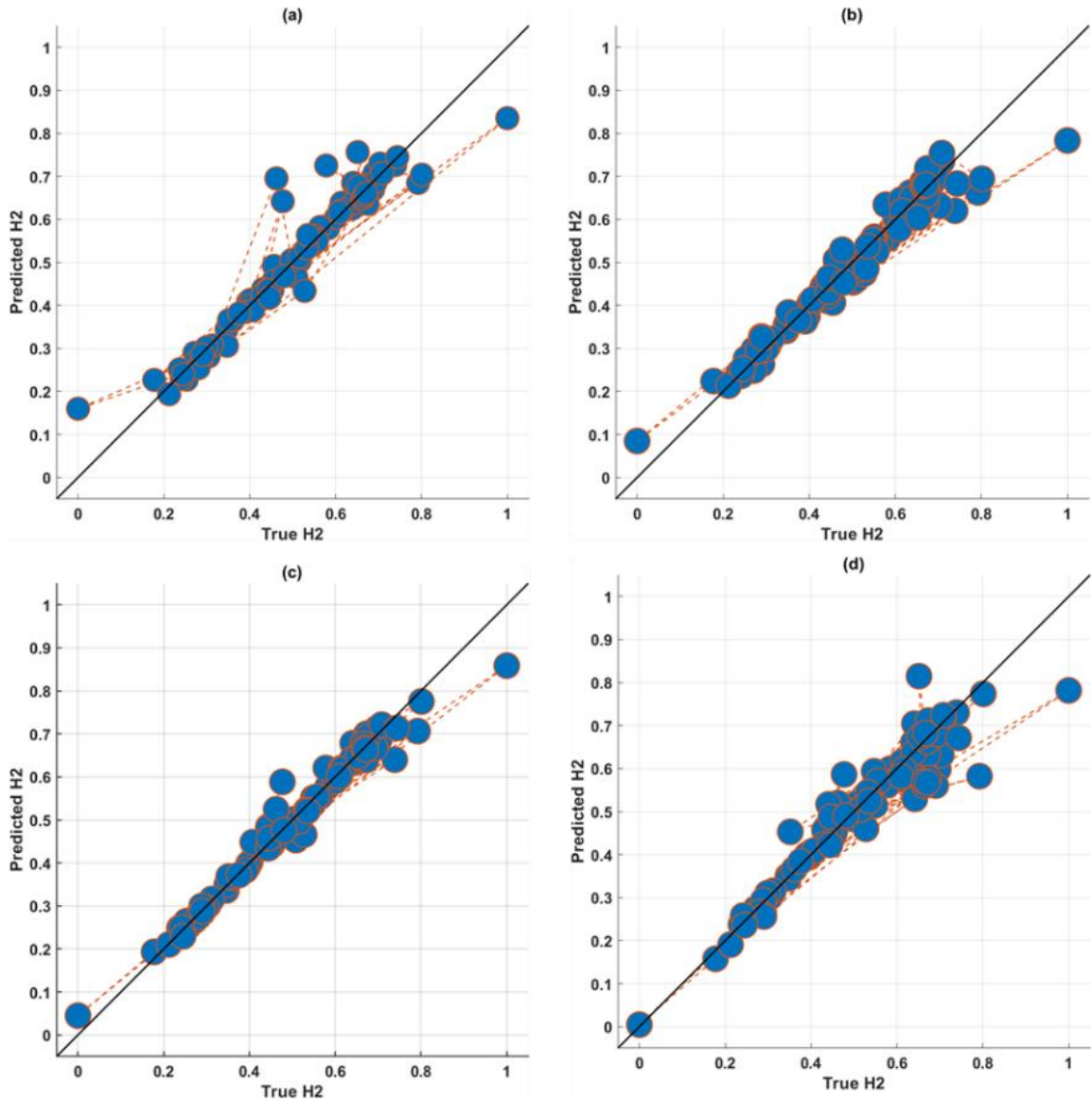


Figure 4.18: Predicted vs true normalized values on test data for H_2
 Legend: (a) ANN, (b) GBR, (c) RF, (d) SVM. Note: Values are normalized; therefore, no units are shown.

4.4.6 Evaluation of ML models for LHV prediction

For LHV, ANN model demonstrated exceptional performance, achieving R^2 values of 0.9754 for validation and 0.9840 on testing. It recorded low RMSE values (0.0245 for validation and 0.0200 for testing) and MAE values (0.0155 and 0.0123), highlighting its ability to capture complex, nonlinear relationships in LHV prediction accurately (Figure 4.19a). The ANN emerged as the best performer on the test dataset in this study,

demonstrating strong robustness and predictive accuracy. While not the top performer in previous studies, ANN achieved relatively high prediction accuracy for LHV in the work of Kardani et al. (2021) and Ascher et al. (2022), highlighting its competitive performance in similar gasification contexts.

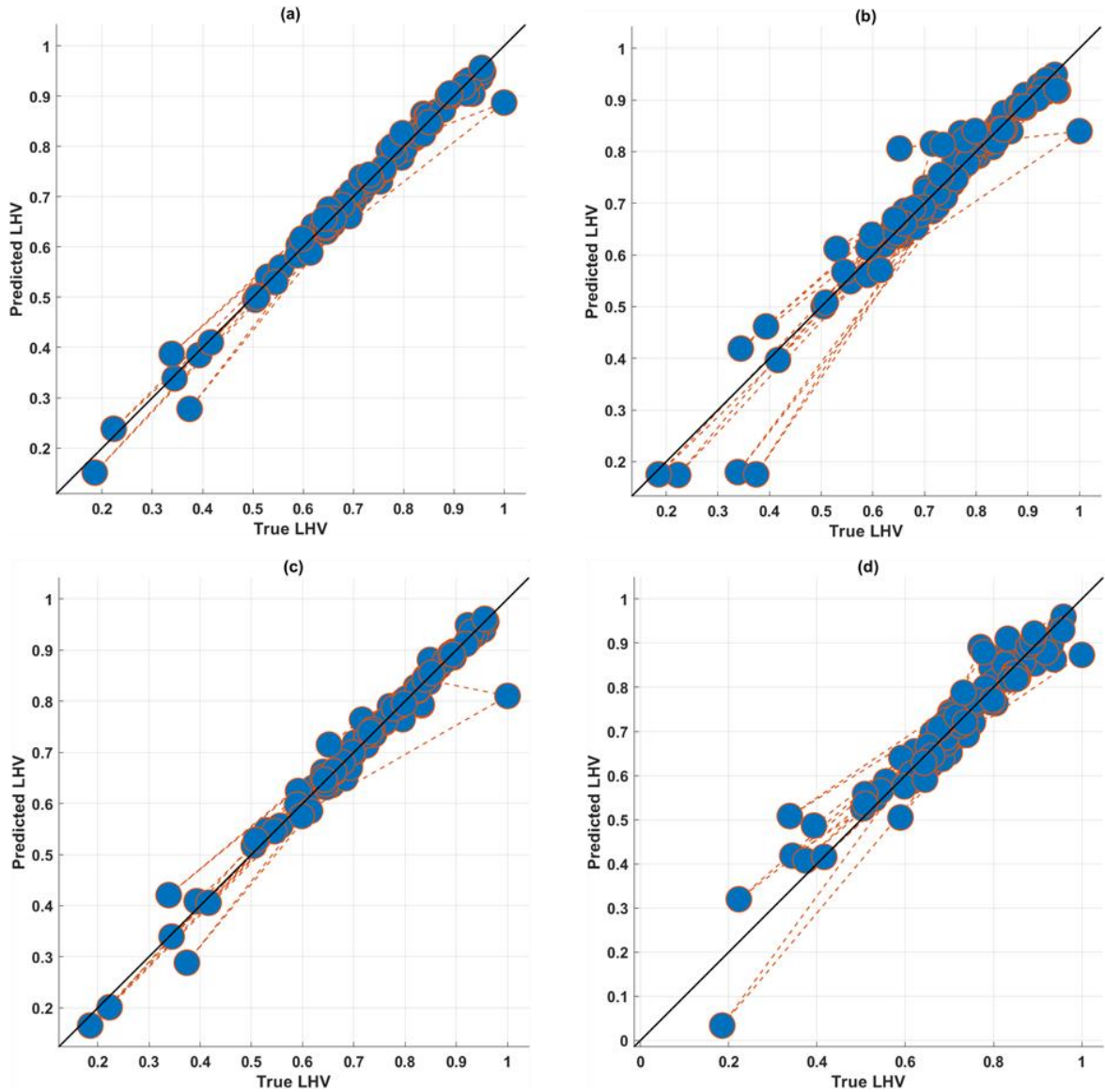


Figure 4.19: Predicted vs true normalized values on test data for LHV

Legend: (a) ANN, (b) GBR, (c) RF, (d) SVM. Note: Values are normalized; therefore, no units are shown.

Among the tree-based ensemble models, GBR model demonstrated moderate performance, achieving R^2 values of 0.9406 for validation and 0.9274 for testing (Figure 4.19b). Its RMSE values were higher (0.0380 for validation and 0.0426 for testing), as were its MAE values (0.0238 and 0.0240). While GBR delivered acceptable results, its

predictive accuracy was notably lower than RF. The RF model performed well, achieving R^2 values of 0.9708 during validation and 0.9707 on testing (Figure 4.19c). Its RMSE values were low (0.0266 for validation and 0.0270 for testing), as were its MAE values (0.0142 and 0.0136), indicating strong predictive accuracy and reliability. The relatively high prediction accuracy of ensemble models in predicting LHV in this study aligns with the findings of Kardani et al. (2021) and Ascher et al. (2022), who applied RF and GBR for LHV prediction and reported similarly strong performance.

The SVM model exhibited the weakest performance (Figure 4.19d), achieving R^2 values of 0.9051 during validation and 0.9178 on the test set. Its RMSE values were relatively high (0.0480 for validation and 0.0453 for testing), as were its MAE values (0.0337 and 0.0338). While SVM provided reasonable predictions, it was consistently outperformed by all other models. The results suggest that the SVM model struggles to capture the complex nonlinear relationships involved in LHV prediction. This finding is consistent with the studies by Kardani et al. (2021) and Ascher et al. (2022), both of which reported weaker performance for SVM compared to other models in predicting LHV.

The SLE consistently delivered the most robust and accurate predictions across both datasets. It achieved the highest R^2 values of 0.9906 during validation and 0.9810 on the test set. It also recorded the lowest RMSE values (0.0136 for validation and 0.0218 for testing) and MAE values (0.0086 and 0.0116), confirming its superior predictive capability than the standalone models. The SLE demonstrated a slight decline in performance on the test dataset compared to the validation dataset; however, it remained among the most reliable models for LHV prediction. This outcome aligns with studies by Kardani et al. (2021) and Ascher et al. (2022) which consistently found that SLE and other ensemble models outperformed individual models in predictive accuracy and robustness.

4.5 ML Model Robustness Analysis

The robustness and generalization of the SLE models were evaluated across multiple prediction targets, including CGE, char yield, CO, gas yield, H₂, and LHV. The assessment focused on key metrics such as R² and RMSE, along with the analysis of base learners and meta-learners employed in each model. The results highlighted significant variability in performance across targets, offering critical insights into the models' ability to handle unseen data and adapt to real-world scenarios.

4.5.1 SLE robustness on CGE prediction

The evaluation of SLE models for CGE prediction revealed significant challenges in achieving satisfactory performance (Table 4.3). While SLE2 and SLE3 demonstrated slight improvements in R² compared to SLE1, the overall results remained unsatisfactory. R² values across all models were below 0.2, and RMSE values were consistently high, indicating limited predictive accuracy and an inability to generalize beyond the training and validation datasets.

Table 4.3: Robustness evaluation results of CGE prediction by different SLE configurations

SLE variant	R ²	RMSE	Base learners	Meta-learner	Dataset information
SLE1	0.009	10.5829	RF, GBR, ANN, SVR	LR	Cross-validation with 400 data, 100 test data Trained on 300 data, 100 validation data, trained with the best models
SLE2	0.16	10.1178	SVR, GBR, RF	LR	Trained on 300 data, 100 validation data
SLE3	0.17	10.118	SVR, GBR, RF	ANN	

The poor performance of the models can be attributed to several reasons. For instance, high variability in CGE poses a substantial challenge. CGE is influenced by a complex interplay of factors, including equivalence ratio, feedstock composition, pressure, etc. (Freda et al. 2019; George et al., 2019). These interactions are highly nonlinear and may not have been adequately captured in the training data. Consequently, the models

struggled to accurately represent the combined effects of these variables, leading to suboptimal predictions.

Additionally, insufficient data diversity in the training dataset likely constrained the models' ability to generalize. If the dataset lacked representation of edge cases or outlier scenarios, such as extreme combinations of operating conditions or unusual feedstock properties, the models would have overfitted to the available data (Ishola et al., 2024). This limitation prevented them from effectively predicting CGE for unseen data, contributing to their poor performance.

4.5.2 SLE robustness on char yield prediction

The SLE models demonstrated notable robustness in predicting char yield (Table 4.4), with SLE3 outperforming all others. By utilizing an ANN as the meta-learner, SLE3 achieved the highest R^2 of 0.83 and the lowest RMSE of 0.0223, highlighting its superior predictive capability. Among the evaluated targets, char yield predictions showed the best performance, indicating that the models were able to generalize effectively for this parameter.

Table 4.4: Robustness evaluation results of char yield prediction by different SLE configurations

SLE Variant	R^2	RMSE	Base Model	Meta-learner	Dataset information
SLE1	0.53	0.037	RF, GBR, ANN, SVR	LR	Cross-validation on 400 data, 100 test data Trained on 300 data, 100 validation data trained with the best models
SLE2	0.8	0.0241	GBR, SVR	LR	Trained on 300 data, 100 validation data
SLE3	0.83	0.0223	GBR, RF, SVR	ANN	

The strong performance in char yield prediction can be attributed to several factors. For example, clear predictive patterns likely exist between char yield and critical features such as ER, SBR, feedstock composition, and pressure (Koido et al., 2021; Sison et al., 2023). These relationships are relatively well-defined and easier for the models to capture

compared to more complex targets like CGE. This predictability reduced the uncertainty and improved the model's accuracy.

In addition, the effective representation of features in the training dataset may have played a critical role (Ahmed et al., 2023). The training data likely captured sufficient variability in key parameters, such as equivalence ratio, feedstock properties, and thermal profiles, enabling the models to generalize well to unseen data. This comprehensive representation ensured that the models could learn the underlying relationships effectively, contributing to their success.

4.5.3 SLE robustness on CO prediction

The evaluation of SLE models for CO prediction revealed that SLE3 provided the best results among the models, achieving the highest R^2 of 0.61 and the lowest RMSE of 5.2448 (Table 4.5). The use of an ANN as the meta-learner in SLE3 offered a slight advantage, contributing to improved predictive performance. However, the results indicate only moderate capability in predicting CO, suggesting that the models still faced challenges in achieving high accuracy.

Table 4.5: Robustness evaluation results of CO prediction by different SLE configurations

SLE variant	R^2	RMSE	Base Models	Meta-learner	Dataset information
SLE1	0.58	5.4331	RF, GBR, ANN, SVR	LR	Cross-validation on 400 data, 100 test data Trained on 300 data, 100 validation data
SLE2	0.6	5.3148	RF, GBR, ANN, SVR	LR	trained with the best models Trained on 300 data, 100 validation data
SLE3	0.61	5.2448	GBR, RF, SVR	ANN	100 validation data

The moderate performance in CO prediction can be attributed to nonlinear dependencies which play a significant role in CO production. CO yield depends on complex, nonlinear interactions between factors such as equivalence ratio, feedstock type, and reaction temperature (Lahafdoozian et al., 2024; Monir et al., 2020). These interactions can be

difficult to model accurately, especially if the training data does not comprehensively represent the full range of possible conditions and their combined effects.

The performance may also be linked to the model architecture (Taye, 2023). While using ANN as the meta-learner provided some improvement in generalization, it still faced challenges in handling outliers or rare conditions present in unseen data. The ability of the model to capture and generalize from these edge cases is limited if the training data lacks sufficient representation of such scenarios (Ganaie et al., 2022; Wu et al., 2021; Yao et al., 2022). This limitation could have constrained the overall performance of the SLE models for CO prediction.

4.5.4 SLE robustness on gas yield prediction

The evaluation of SLE models for gas yield prediction revealed mixed performance, with SLE1 achieving the highest R^2 of 0.78 and the lowest RMSE of 0.0902 (Table 4.6). Conversely, SLE3 exhibited a significant drop in performance, with an R^2 of 0.53 and an RMSE of 0.1334, indicating challenges in generalization when using an ANN as the meta-learner. These results highlight varying levels of robustness and adaptability across the SLE models.

Table 4.6: Robustness evaluation results of gas yield prediction by different SLE configurations

SLE Variant	R^2	RMSE	Base Models	Meta-learner	Dataset information
SLE1	0.78	0.0902	RF, GBR, ANN, SVR	LR	Cross-validation on 400 data, 100 test data Trained on 300 data, 100 validation data trained with the best models
SLE2	0.75	0.0976	GBR, RF, SVR	LR	Trained on 300 data, 100 validation data
SLE3	0.53	0.1334	GBR, RF, SVR	ANN	

The mixed performance of the gas yield models presents a complex phenomenon in the prediction by the different model configurations. This can be attributed due to overfitting in SLE3 which likely contributed to its poorer generalization (Ying, 2019). While ANN

is effective at capturing complex, non-linear relationships, its high capacity can lead to overfitting, especially if the training data lacks sufficient variability or includes noise (Zhou et al., 2017). This could explain the significant decline in performance of SLE on gas yield prediction.

Furthermore, insufficient modeling of feature interactions may have affected the performance of simpler meta-learners, such as LR used in SLE1. Gas yield is influenced by intricate dependencies between feedstock composition and operating conditions (Sison et al., 2023; Cao et al., 2023; Anniwaer et al., 2021), which require sophisticated modeling to capture effectively. While LR might have missed some of these interactions, its simpler structure likely avoided overfitting (Charilaou & Battat, 2022), allowing SLE1 to achieve better generalization.

4.5.5 SLE robustness on H₂ prediction

The evaluation of SLE models for H₂ prediction revealed significant challenges, with all models demonstrating poor performance (Table 4.7). SLE1 achieved an R² of -0.05 and an RMSE of 2.6936, indicating limited predictive accuracy. SLE2, trained on a larger dataset, performed the worst, with an R² of -0.67 and an RMSE of 3.386, suggesting an inability to generalize effectively. SLE3, which utilized an ANN as the meta-learner, showed marginally better performance with an R² of -0.35 and an RMSE of 3.045, yet it still fell far short of satisfactory predictive capability. These negative R² values across all models indicate that the predictions were less accurate than a simple mean-based estimate.

Table 4.7: Robustness evaluation results of H₂ prediction by different SLE configurations

SLE variant	R ²	RMSE	Base Model	Meta-learner	Dataset information
SLE1	-0.05	2.6936	RF, GBR, ANN, SVR	LR	Cross-validation on 400 data, 100 test data Trained on 300 data,
SLE2	-0.67	3.386	GBR, SVR	LR	100 validation data Trained with the best models
SLE3	-0.35	3.045	GBR, RF, SVR	ANN	Trained on 300 data, 100 validation data

The poor performance can be attributed to several factors. Hydrogen concentration is influenced by complex and nonlinear interactions among ER, feedstock composition, SBR, and reactor pressure (George et al., 2019; Kittivech & Fukuda, 2019; Monir et al., 2020). The training data likely failed to capture the full variability of these critical factors, particularly outlier or edge cases, resulting in models that overfit to patterns in the limited dataset (Aldoseri et al., 2023). While SLE1 and SLE2 used linear LR as the meta-learner, which may have been too simplistic to capture nonlinear dependencies, SLE3 employed ANN, which, despite its potential for capturing complex relationships, likely overfit due to insufficient data diversity.

The inability of the models to generalize highlights the importance of addressing key issues such as dataset representation, feature engineering, and model architecture (Rather et al., 2024). Expanding and diversifying the training dataset to include a wider range of ER, feedstock properties, and operating conditions is critical to improving model learning. Advanced feature engineering to explicitly model interactions between critical parameters could also enhance predictive accuracy. Furthermore, optimizing meta-learners by employing more sophisticated approaches like gradient boosting or regularized neural networks can improve the balance between capturing complexity and maintaining generalization (Jui & Rivas, 2024). For ANN-based meta-learners, applying regularization techniques such as dropout or weight decay can mitigate overfitting.

4.5.6 SLE robustness on LHV prediction

The evaluation of SLE models for predicting the LHV of syngas revealed uniformly poor performance, with all models exhibiting negative R^2 values (Table 4.8), indicating predictions that were less accurate than a mean-based baseline. SLE1 and SLE2, both employing LR as the meta-learner, achieved R^2 values of -0.09 with RMSE values of 0.4858 and 0.4852, respectively, showing negligible differences despite the increased

dataset size in SLE2. SLE3, which used an ANN as the meta-learner, exhibited slightly worse performance, with an R^2 of -0.1 and an RMSE of 0.4878. These results highlight the models' inability to generalize and accurately predict LHV.

Table 4.8: Robustness evaluation results of LHV prediction by different SLE configurations.

SLE variant	R^2	RMSE	Base Models	Meta-learner	Dataset information
SLE1	-0.09	0.4858	RF, GBR, ANN, SVR	LR	Cross-validation on 400 data, 100 test data Trained on 300 data, 100 validation data
SLE2	-0.09	0.4852	ANN, SVR, RF	LR	trained the best models Trained on 300 data, 100 validation data
SLE3	-0.1	0.4878	GBR, RF, SVR	ANN	

The poor performance can be attributed to several factors. First, complex dependencies governing LHV were likely not adequately captured by the models. LHV depends on intricate interactions between feedstock composition, gas composition, ER, and thermal conditions, which are highly nonlinear (Pati & De 2021; Freda et al., 2019; Monir et al., 2020; Wiyono et al., 2021; Pati et al., 2021). The linear regression meta-learners in SLE1 and SLE2 were too simplistic to model these relationships, while the ANN meta-learner in SLE3 may have overfitted the training data due to its complexity and the lack of sufficient diversity in the dataset.

Second, insufficient data variability further exacerbated the models' limitations (Rather et al., 2024). The training dataset likely failed to represent edge cases or extreme operating conditions critical for capturing the full spectrum of LHV behavior. Without adequate diversity, the models struggled to generalize beyond the patterns present in the training data, resulting in negative R^2 values.

4.5.7 Suitability of ML models for deployment

The evaluation of SLE models for deployment in biomass COG applications revealed varying levels of readiness across target variables (Figure 4.20). Models for char yield,

gas yield, and CO demonstrated reasonable robustness and generalizability on unseen data, making them suitable for deployment in their current state. These models effectively captured the variability and complexity of real-world gasification processes, providing reliable tools for monitoring and optimization. The char yield model, in particular, achieved high accuracy due to well-defined relationships between key features and the target variable, while the gas yield and CO models, despite some limitations in modeling complex interactions, showed sufficient predictive capability for practical use (Sison et al. 2023; Lahafdoozian et al., 2024).

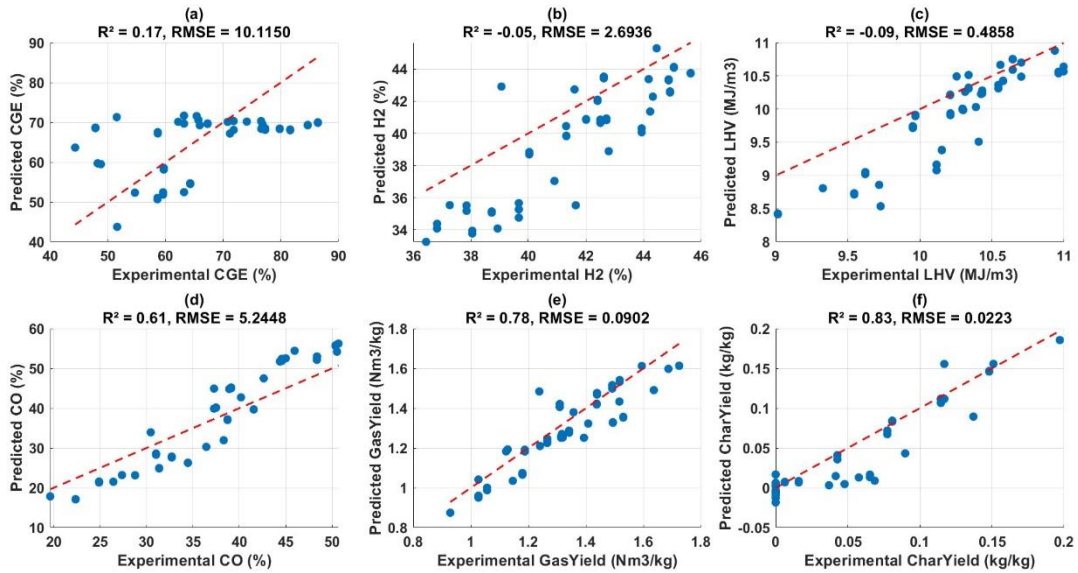


Figure 4.20: Robustness evaluation for SLE models on unseen dataset.

Legend: (a) CGE, (b) H₂, (c) LHV, (d) CO, (e) gas yield, (f) char yield

Conversely, the models for CGE, H₂, and LHV were found to be unsuitable for deployment due to poor generalization and accuracy on unseen data. These models exhibited negative or near-zero R^2 values and high RMSE, highlighting significant limitations in capturing the intricate, nonlinear dependencies governing these targets. Factors contributing to this poor performance include insufficient training data diversity, inadequate representation of key interactions, and overfitting in complex meta-learners like ANN (Aldoseri et al., 2023). These shortcomings indicate that these models lack the reliability necessary for real-world applications and require further development.

To enhance the deployment readiness of the underperforming models, several strategies are recommended. Expanding the training datasets to include a broader range of operating conditions and feedstock compositions would improve generalization and robustness. Feature engineering to explicitly model critical interactions, such as those between equivalence ratio, feedstock properties, and reaction conditions, can further refine model accuracy. Additionally, integrating domain knowledge through hybrid modeling approaches, such as combining ML with thermodynamic or kinetic constraints, would ensure physically realistic predictions and improve reliability.

4.6 ML Model Interpretability Analysis

This section presents an interpretability analysis of the ML models, employing techniques such as PI, GI, and PDP to identify the key features influencing model performance. These methods enhanced the transparency of otherwise black-box models, helping to build confidence in their predictions.

The analysis focused on the top ten features for each ML model (SVR, RF, GBR, and ANN) using the two global interpretability methods: PI and GI. The feature rankings generated by these approaches highlighted the most influential variables driving model outputs, offering valuable insights into the underlying relationships between input features and predicted responses. In addition, further analysis using PDP enabled a deeper examination of how individual features and their interactions affect model predictions. This approach facilitated a nuanced understanding of model behavior, particularly how changes in specific input variables impact key gasification outcomes.

4.6.1 Permutation feature importance for gas yield

The PI analysis provided a comprehensive evaluation of the features influencing gas yield prediction across ML models, as illustrated in Figure 4.21.

The analysis consistently identified ER and SBR as the two most influential features across all models (Table 4.9), indicating their critical role in gasification processes. ER directly governs the extent of gasification reactions, influencing syngas composition and gas yield, while SBR determines the steam available for reforming reactions, which enhance hydrogen and syngas production (Koido et al., 2021; Zhang & Pang, 2017).

Other important features include AirSteam, which balances the use of air and steam as gasifying agents, impacting reaction kinetics and gas yield (Pati & De, 2021). Its significance was particularly notable in RF and SVR. Carbon content (C), essential for driving the production of combustible gases (Monir et al., 2020), was a key factor for GBR and RF but less prioritized in ANN and SVR. Feedstock composition, represented by features like RH ratio and GS ratio, showed variable importance across models, reflecting their nuanced contributions to gasification outcomes (Wiyono et al., 2021; Anniwaer et al., 2021).

Table 4.9: Permutation importance across ML Models for Gas yield

Feature	ANN	GBR	RF	SVM	Comments
Equivalent ratio (ER)	1	1	1	1	The most critical feature across models' prediction
Steam-to-biomass ratio (SBR)	2	2	2	2	The second most importance across the model
Carbon content (C)	8	3	3	8	Ranked higher in GBR and RF, But low in ANN and SVM
Agent_AirSteam (AirSteam)	10	4	4	3	Ranked higher in SVM but lower in ANN, GBR and RF high rank order
RH Ratio	4	7	7	7	Feedstock specific, ranked higher in ANN, but influences both model
Pressure	-	5	8	6	Not Prioritized by ANN, but remains importance in other models
GS Ratio	5	-	9	9	Not captured by GBR but influence the other model prediction
Ash Content (Ash)	7	9	10	5	Consistently affect all the model prediction but ranked lower in RF and higher in SVM
Hydrogen Content (H)	-	6	6	-	It is ranked the same order in both ensemble models, but not captured by other models
Fixed Carbon (FC)	-	10	-	-	Uniquely captured by only GBR, showing in importance for gas yield

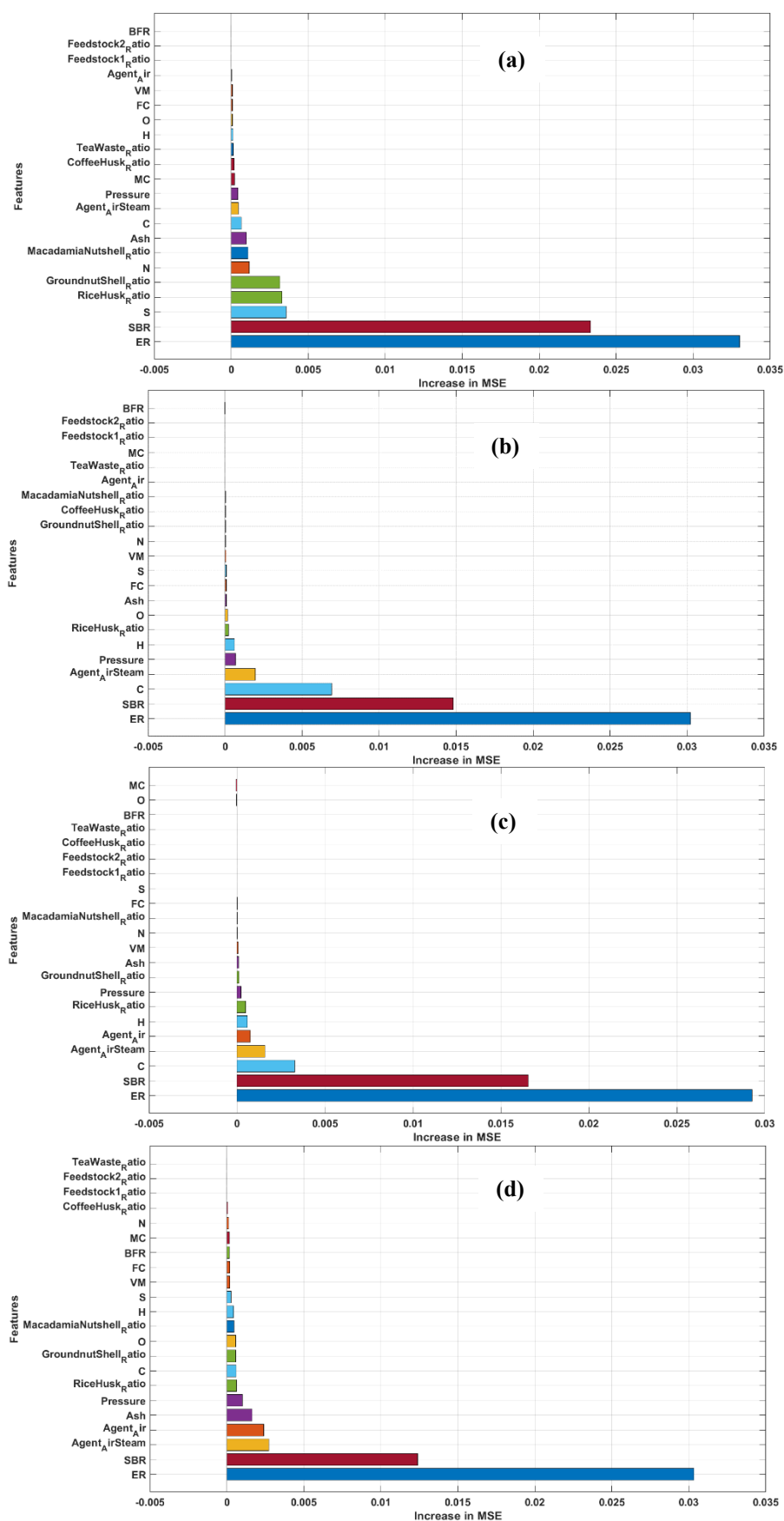


Figure 4.21: Permutation importance analysis of ML models on gas yield prediction
 Legend: (a) ANN, (b) GBR, (c) RF, (d) SVM

While ash content ranked lower in importance, its consistent relevance highlights its role in hindering reactions and reducing gas yield, especially in high-ash feedstocks (Kittivech & Fukuda, 2019; Cao et al., 2022). Pressure emerged as another influential feature in GBR, RF, and SVR, emphasizing its impact on gasification thermodynamics and reaction kinetics (Monir et al., 2020).

Model-specific behavior revealed variations in how features were prioritized. ANN focused heavily on ER and SBR, leveraging its ability to model nonlinear interactions directly affecting syngas generation (Serrano & Castelló, 2020). GBR and RF emphasized thermodynamic and reaction-related features, such as ER, SBR, and C, with RF showing a balanced focus and slight prioritization of Air and Ash. SVR highlighted ER, SBR, and AirSteam while efficiently handling interactions with features like pressure and ash through its kernel-based approach (Mutlu et al., 2019; Ozbas et al., 2019). These observations are consistent with the findings of Kardani et al. (2021) and Ascher et al. (2022), who also identified ER and SBR as pivotal factors influencing gas yield in biomass gasification models.

These findings reaffirm the dominance of ER and SBR as critical determinants in gas yield prediction, while also highlighting model-specific preferences for secondary features. Such insights enhance the interpretability of ML models and provide actionable guidance for refining feature selection and optimizing gasification processes. By understanding the nuanced contributions of key features, future modeling efforts can achieve greater predictive accuracy and robustness.

4.6.2 Permutation feature importance for char yield

The interpretability analysis of char yield prediction using the Permutation importance method revealed critical insights into the most influential features across ML models, as depicted in Figure 4.22. Consistently, ER and SBR emerged as the most important

features across all models, reflecting their dominant role in controlling the extent of gasification reactions and char decomposition (Table 4.10). Similarly, Ash ranked as a key feature, emphasizing its inhibitory impact on char reactivity by reducing the effective reactive surface area available for gasification reactions (Koido et al., 2021).

Each model exhibited unique feature prioritization, highlighting their specific strengths. ANN focused on feedstock-specific variables such as MS ratio and TW ratio, leveraging its ability to capture complex nonlinear relationships between feedstock composition and char yield (Ascher et al. 2022). While, GBR prioritized reaction-related variables, including FC, C, and N, reflecting its iterative optimization process that emphasizes variables contributing consistently to prediction accuracy (Kardani et al., 2021; Leng et al., 2022).

RF displayed a balanced approach, incorporating both reaction dynamics and feedstock properties, with significant importance given to pressure and MC, which influence char formation thermodynamics (Monir et al., 2020). SVM emphasized Ash and Air, reflecting its sensitivity to features that directly affect char formation, including those limiting or catalyzing gasification processes (Koido et al., 2021). The significance of Ash content for char yield prediction is corroborated by Sison et al. (2023), who also highlighted its critical role.

These findings emphasize the crucial roles of ER and SBR in determining gasification outcomes, while showing Ash content as a limiting factor for char yield. The model-specific feature prioritization indicates the varying abilities of ML algorithms to capture complex dependencies and interactions inherent in biomass gasification processes. These insights enhance model interpretability and provide a foundation for refining feature

engineering and modeling approaches, ensuring robust and accurate predictions for char yield in biomass COG systems.

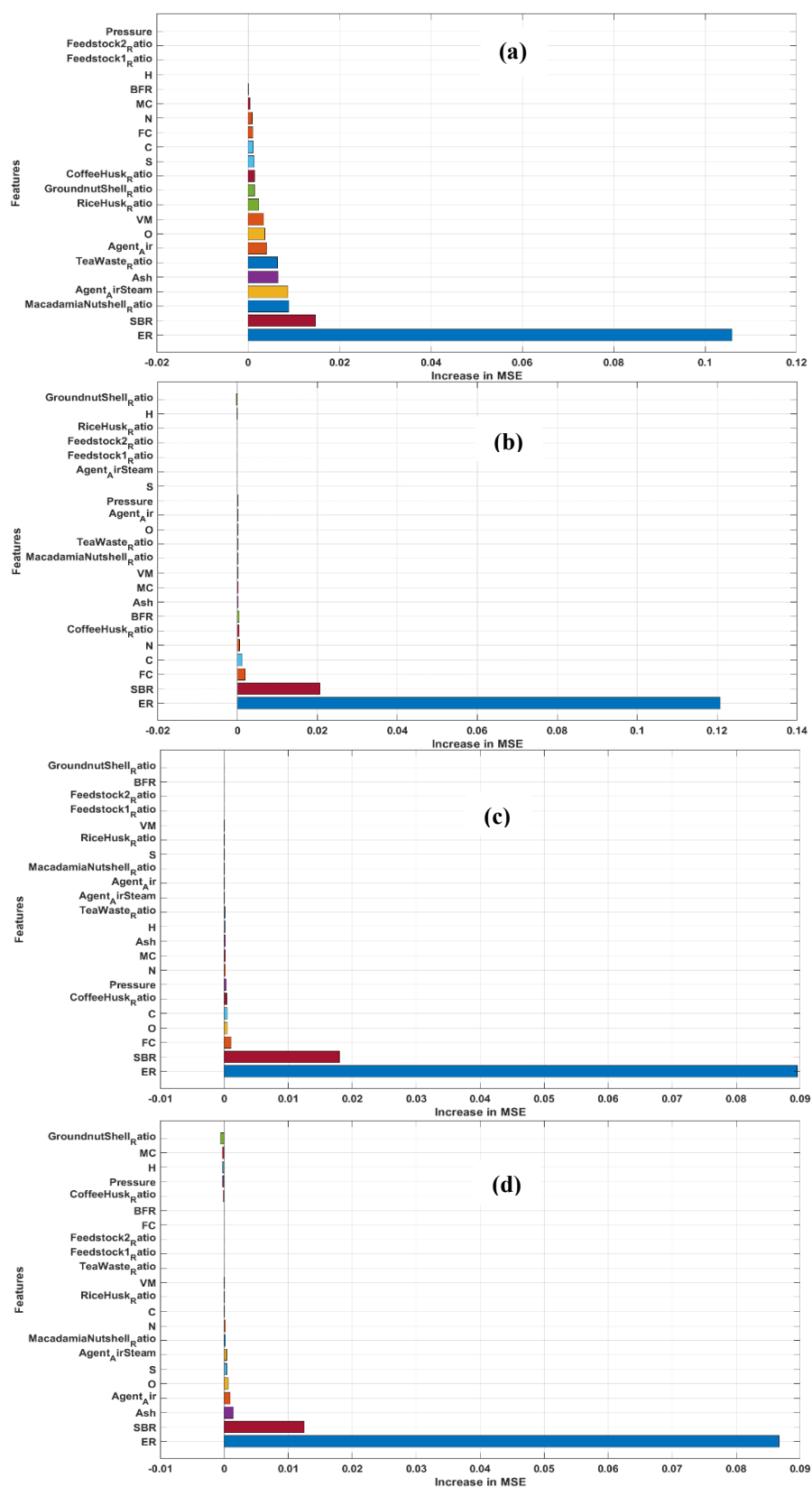


Figure 4.22: Permutation importance analysis for ML model on char yield prediction
Legend: (a) ANN, (b) GBR, (c) RF, (d) SVM

Table 4.10: Permutation feature importance rankings by ML models for char yield

Feature	ANN	GBR	RF	SVR	Comments
ER	1	1	1	1	Key factor regulating COG efficiency and yield.
SBR	2	2	2	2	Critical for controlling steam-driven reactions.
MS Ratio	3	-	-	8	Feedstock-specific contribution to char yield.
Agent_AirSteam	4	-	-	7	Balances air and steam for gasification reactions.
Ash content	5	8	10	3	Impacts char reactivity and formation.
TW Ratio	6	-	-	-	Feedstock-specific parameter influencing yield.
Agent_Air (Air)	7	-	-	4	Influences the oxygen availability for reactions.
Oxygen Content	8	-	4	5	Affects reaction pathways and char yield.
Volatile Matter (VM)	9	10	-	-	Determines the proportion of non-char components in feedstock.
RH Ratio	10	-	-	-	Feedstock-specific contribution to char yield.
FC	-	3	3	-	Directly influences the amount of char produced.
C	-	4	5	10	Contributes directly to char yield.
Nitrogen Content (N)	-	5	8	9	Impacts inert gas flow, indirectly affecting char yield
CH Ratio	-	6	6	-	Significant feedstock-specific variable.
Biomass Feed Rate (BFR)	-	7	-	-	Controls the rate of reactant input into the system.
Moisture Content (MC)	-	9	9	-	Reduces reaction temperatures, affecting char yield.
Pressure	-	-	7	-	Affects thermodynamics and reaction rates.
Sulfur Content (S)	-	-	-	6	Impacts char formation through its catalytic effects

4.6.3 Gini feature importance for gas yield

The GI method provided valuable insights into the contributions of features to gas yield prediction in tree-based models, specifically GBR and RF, as illustrated in Figure 4.23. This method assesses the reduction in impurity achieved by splitting on a given feature, thereby ranking features by their impact on predictive accuracy (Ascher et al., 2022; Li et al., 2023; Yaman et al., 2018). The analysis consistently identified ER and SBR as the top-ranked features in both models (Table 4.12), demonstrating their critical role in controlling gasification reactions. The ER influences the extent of oxidation and gasification (George et al., 2019; Freda et al., 2019), while SBR determines the availability of steam for reforming reactions (Pati & De, 2021). Together, these features directly affect syngas composition and gas yield, highlighting their importance in optimizing biomass COG outcomes.

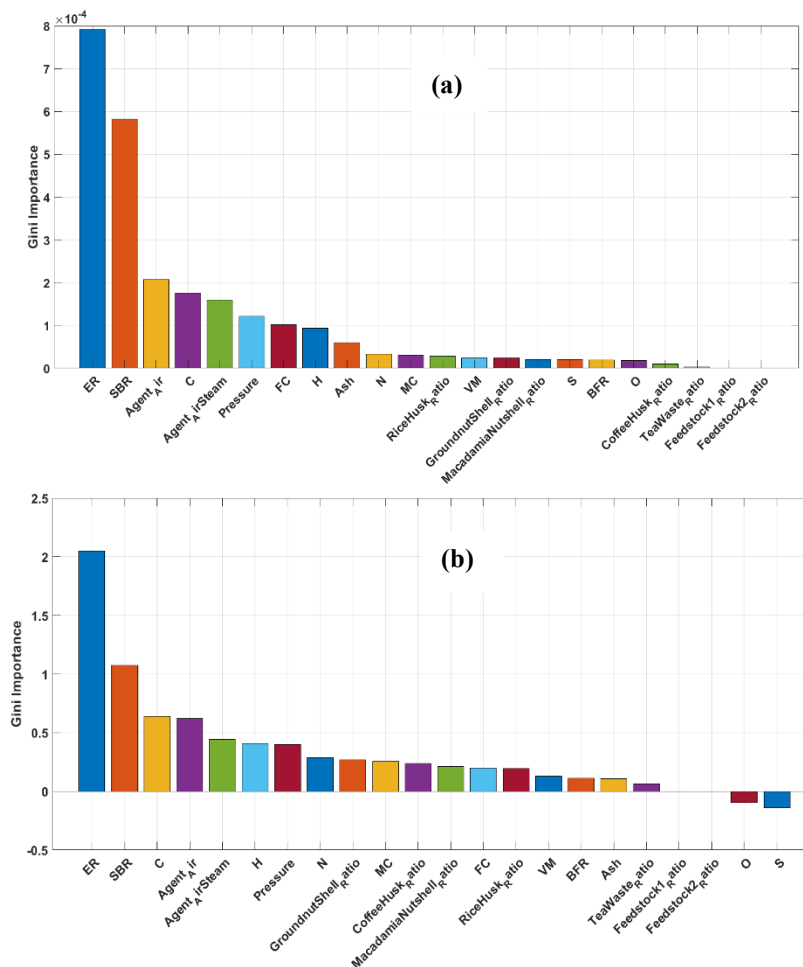


Figure 4.23: Gini feature importance analysis for tree-based ML on gas yield prediction
Legend: (a) GBR, (b) RF

Table 4.11: Gini importance feature ranking across ML models for gas yield prediction

Feature	GBR	RF	Comments
ER	1	1	Primary determinant of gas yield; affects reaction efficiency,
SBR	2	2	Regulates the availability of steam for reforming reactions and hydrogen production
Agent_Air (Air)	3	4	Balances the oxygen supply, influencing gasification reactions.
Carbon Content (C)	4	3	Directly impacts syngas generation through gasification reactions.
Agent_AirSteam (AirSteam)	5	5	Controls the balance between air and steam in the process.
Pressure	6	7	Affects thermodynamics and reaction kinetics.
Fixed Carbon (FC)	7	-	Represents unreacted carbon in feedstock; influences gas yield.
Hydrogen Content (H)	8	6	Contributes to syngas composition and reaction pathways.
Ash Content (Ash)	9	-	Reduces reaction efficiency due to inert residues.
Nitrogen Content (N)	10	8	Affects the inert gas balance, impacting gas yield indirectly.
GS Ratio	-	9	Feedstock-specific contribution to gas yield.
Moisture Content (MC)	-	10	Affects reaction efficiency by influencing heat balance.

Carbon Content (C) emerged as another key feature in both models, reflecting its central role in syngas generation through the gasification of carbon-rich feedstocks (Pati & De,

2021; Anniwaer et al., 2021). Despite these commonalities, the models exhibited notable differences in their sensitivity to secondary features. GBR ranked Air higher, indicating its greater responsiveness to variations in oxygen supply and its influence on reaction kinetics (Pati et al., 2021; Monir et al., 2020).

In contrast, RF emphasized feedstock-specific variables such as GS ratio and MC, reflecting its stronger focus on feedstock variability (Anniwaer et al., 2021). RF's inclusion of features like GS ratio highlights its ability to account for unique contributions from individual feedstocks, whereas GBR prioritized broader reaction conditions such as pressure and Ash.

Certain features emerged as uniquely significant for each model, offering additional insights into their predictive behavior. For example, FC was ranked seventh in the GBR model, underlining its role in solid-phase reactions and char conversion. In contrast, the RF model prioritized feedstock-specific variables such as the GS ratio, highlighting its strength in capturing nuanced variations in input characteristics. These findings align with the study by Li et al. (2023), which identified ash content, nitrogen, and temperature as the most influential variables for hydrogen yield prediction using GBR. Similarly, Ascher et al. (2022) reported that particle size and the choice of gasifying agent were critical across all models studied, with particle size being the top-ranked feature for both GBR and RF.

The findings confirmed ER and SBR as the most critical features of gas yield prediction, consistently ranked across both GBR and RF models. Notably, GBR emphasized global reaction conditions, while RF demonstrated greater sensitivity to feedstock-specific variability, reflecting the complementary strengths of these modeling approaches. These insights offer actionable guidance for refining COG modeling strategies. By leveraging

the distinct advantages of GBR and RF, it is possible to develop more accurate and adaptable predictive frameworks tailored to varying biomass COG scenarios.

4.6.4 Gini feature importance for char yield

The Gini importance analysis for char yield prediction using GBR and RF models identified critical features and revealed differences in the models' prioritization of reaction dynamics and feedstock properties (Figure 4.24). The ER and SBR consistently ranked as the two most influential features in both models, as shown in Table 4.12, reflecting their essential roles in controlling gasification reactions and char decomposition.

ER determines the extent of oxidation and reduction reactions, directly affecting the rate at which char is formed or consumed (Koido et al., 2021). SBR, on the other hand, regulates the availability of steam for reforming reactions, which also impacts char breakdown (Li et al., 2023; Sison et al., 2023). Together, these parameters served as critical levers for controlling char yield during biomass gasification.

Ash content also emerged as a key feature in both the GBR and RF models, emphasizing its negative influence on reaction efficiency. Elevated ash levels reduce the active surface area available for reactions and hinder gas–solid interactions, ultimately impairing gasification performance (Jiao et al., 2022). These findings are consistent with previous studies by Sison et al. (2023) and Li et al. (2023), who used GBR to predict char yield and similarly identified ash content as a critical variable influencing model accuracy and gasification outcomes.

Ash content also emerged as a key feature in both the GBR and RF models, highlighting its inhibitory effect on reaction efficiency. High ash levels reduce the active surface area available for reactions and hinder gas–solid interactions (Jiao et al., 2022). Thereby

impairing overall gasification performance. These observations are consistent with the studies by (Sison et al. (2023) and (Li et al. (2023) who used GBR for char yield prediction. The consistent ranking of ash across both models emphasizes the importance of managing ash content during feedstock preparation to improve process efficiency.

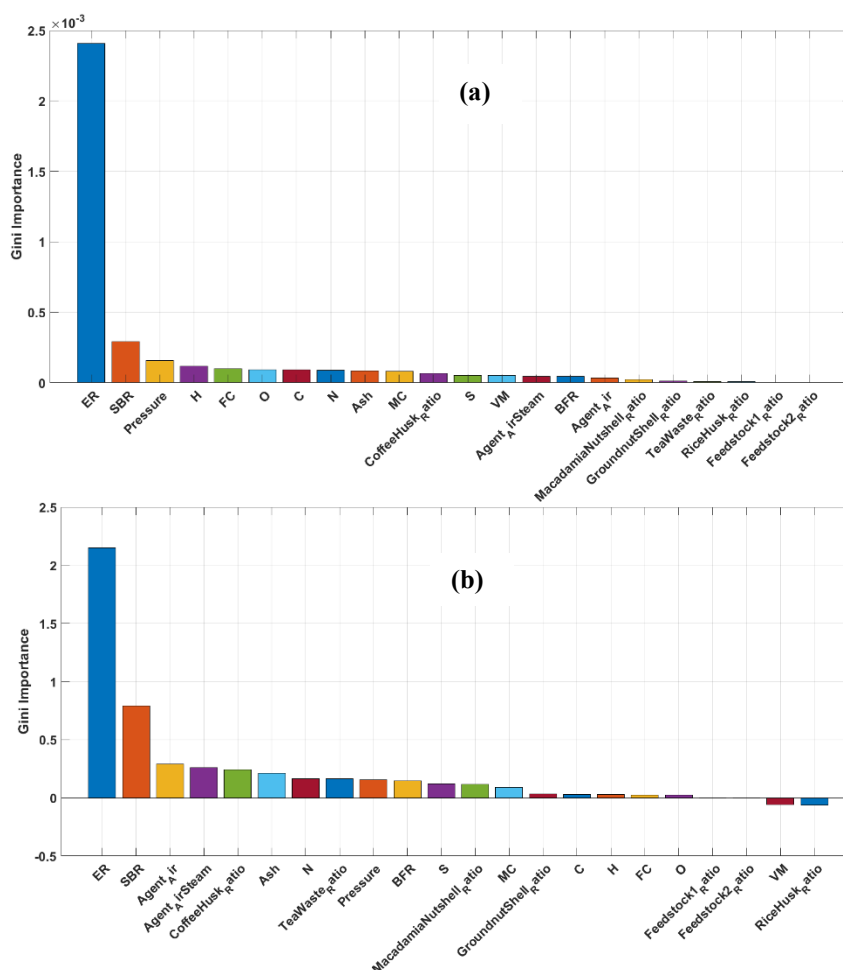


Figure 4.24: Gini feature importance analysis for tree-bases ML on char yield prediction
Legend: (a) GBR, (b) RF

Despite this agreement, notable differences were observed between the GBR and RF in their treatment of secondary features. These differences reflect each model's underlying structure and sensitivity to specific input parameters, offering complementary perspectives on the complex interactions governing char yield during gasification (Sharafati et al., 2020; Xing et al., 2019; Kardani et al., 2021).

Table 4.12: Gini importance ranking across tree-based ML for char yield prediction

Feature	GBR	RF	Comments
ER	1	1	The most significant feature for predicting char yield.
SBR	2	2	Key determinant for steam availability in reactions.
Pressure	3	9	Affects reaction kinetics and thermodynamics, it is ranked lower when RF is used, but remains importance in both models
Hydrogen Content (H)	4	-	Impacts syngas composition and reaction pathways. It only influences GBR prediction
Fixed Carbon (FC)	5	-	Key determinant of char formation in solid-phase reactions. However, not captured when RF is used
Oxygen Content (O)	6	-	Influences oxidation reactions critical to char yield. It is only present when GBR is used
Carbon Content (C)	7	-	Contributes directly to char formation, however, its importance not shown by RF
Nitrogen Content (N)	8	7	Affects inert gas flow and indirectly influences char yield. Both models recognized its importance
Ash Content (Ash)	9	6	Inhibits reactions, reducing char yield efficiency. Its impact all both models in prediction
Moisture Content (MC)	10	-	Impacts heat balance and reaction dynamics. It is only demonstrated by GBR model
Agent_Air	-	3	Regulates oxygen supply, influencing reaction efficiency.
Agent_AirSteam	-	4	Balances air and steam reactants during gasification.
CH Ratio	-	5	Feedstock-specific contribution to char formation.
TW Ratio	-	8	Another feedstock-specific parameter influencing char yield.
Biomass Feed Rate (BFR)	-	10	Controls the reactant flow rate, affecting char yield.

GBR prioritized global reaction conditions, such as pressure, H, and O, which influence thermodynamics and kinetics during gasification (Lv et al., 2022; Almeida et al., 2022) . It also assigned significant importance to intrinsic material properties like FC and MC, both of which are critical in determining feedstock reactivity and thermal decomposition characteristics (Awais et al., 2022). These feature priorities are consistent with iterative nature of GBR's optimization process, which systematically identifies and weights variables that contribute most to predictive accuracy across the entire dataset (Kardani et al., 2021; Sharafati et al., 2020; Leng et al., 2022).

In contrast, the RF model prioritized operational parameters such as Air and AirSteam, reflecting the specific reaction environments influencing char formation (Koido et al., 2021). It also assigned considerable importance to feedstock-specific variables, including the CH and TW ratios, underscoring its effectiveness in capturing subtle differences in biomass properties. This focus highlights RF's suitability for modeling diverse biomass

conditions, as it excels in recognizing localized patterns and variations in feedstock behavior. These findings are consistent with those of Ascher et al. (2022), who also reported that RF emphasizes feedstock-specific characteristics and gasifying agents as key factors in predicting char yield.

These results demonstrate the dominant roles of ER, SBR, and Ash in predicting char yield. While GBR excels at capturing global reaction dynamics and material properties, RF provides a detailed understanding of feedstock variability and operational influences. The complementary strengths of these models highlight their combined value in refining char yield predictions and optimizing COG processes across a range of biomass feedstocks and operating scenarios.

4.6.5 Comparison of interpretability methods for gas yield

The comparison of PI and GI methods for feature ranking in GBR and RF models offered valuable insights into the factors influencing gas yield prediction (Table 4.13). Both methods consistently identified ER and SBR as the most critical features, indicating their dominant role in governing gasification reactions and syngas production, as well as their overall impact on gasification efficiency (Pati et al., 2021; Pati & De, 2021). Additionally, features such as C, AirSteam, and Ash were consistently ranked among the top contributors. These variables are closely associated with the thermodynamic and kinetic behavior of the gasification system and reflect important aspects of feedstock composition and reactivity that significantly influence gas yield outcomes (Freda et al. 2019); George et al., 2019).

Despite these commonalities, the two methods diverged in their treatment of secondary features, largely due to differences in their underlying methodologies. PI was capable of capturing dynamic dependencies and nonlinear relationships within the dataset, making it particularly effective for identifying subtle yet significant variables (Zhao et al., 2021;

Fisher et al., 2019; Gregorutti et al., 2017). For example, it highlighted features like H and RH ratio, which may exert nuanced effects on gas yield that are not readily detected by tree-based decision models. However, a key limitation of the PI method was its sensitivity to multicollinearity. When features are highly correlated, PI may obscure their individual contributions, complicating the interpretation of overlapping effects and potentially diminishing model transparency (Laugel et al., 2018).

Table 4.13: Comparison of GBR permutation and Gini importance ranking for gas yield

Feature	PI	GI	Comments
Equivalence Ratio (ER)	1	1	Consistently ranked as the most important feature by both methods, indicating its critical role.
Steam-to-Biomass Ratio (SBR)	2	2	Both methods agree on SBR as the second most important feature.
Carbon Content (C)	3	4	Carbon Content is more prominent in Permutation but at higher rank in both
Agent_AirSteam	4	5	Permutation focuses more on Agent_AirSteam. It is favored by both
Pressure	5	6	Similar ranking, but Pressure is slightly prioritized in Permutation.
Hydrogen Content (H)	6	8	Permutation highlights H more, potentially reflecting dynamic dependencies in the data.
RH Ratio	7	-	Permutation focuses on RH Ratio.
Oxygen Content (O)	8	-	Hydrogen is consistently relevant but is ranked lower by Gini.
Ash Content (Ash)	9	9	Ash is consistently ranked but less influential overall.
Fixed Carbon (FC)	10	7	Permutation favors FC, while Gini does not
Agent_Air	-	3	Gini ranks Agent_Air higher, likely due to its consistent splitting in tree-based learning.
Nitrogen Content	-	10	Nitrogen is included in Gini due to its regular splits.

In contrast, GI reflects the splitting criteria used during tree construction, prioritizing features that consistently reduce impurity at each decision node (Li et al., 2023; Yaman et al., 2018). It ranked variables such as Air and FC higher, indicating their stable and direct contributions to gas yield predictions (Table 4.14). While GI was less sensitive to feature interactions and correlations, it excelled in highlighting variables that offer consistent and interpretable decision rules within the tree structure. This makes it particularly useful for identifying features that drive reliable and hierarchical decision-making (Kardani et al., 2021), thereby enhancing the transparency and performance understanding of tree-based models.

Table 4.14: Comparison of RF permutation and Gini importance ranking for gas yield

Feature	PI	GI	Comments
ER	1	1	Both methods agree on ER as the dominant feature for gas yield prediction.
SBR	2	2	Consistently ranked second, indicating its strong influence.
Carbon Content (C)	3	4	Gini ranks Agent_Air higher due to its splitting criteria in tree construction.
Agent_AirSteam	4	5	Agent_AirSteam ranks higher in Permutation, reflecting its direct impact on syngas composition.
Agent_Air	5	3	Slightly lower ranking for Agent_Air in Permutation, as it may interact with other features.
Hydrogen Content (H)	6	8	Hydrogen is ranked higher by Permutation, reflecting its importance in yield composition.
RH Ratio	7	-	Permutation focuses feedstock-specific properties.
Pressure	8	6	Pressure is more prominent in Permutation rankings.
GS Ratio	9	-	Permutation includes feedstock-specific properties.
Ash Content (Ash)	10	10	Ash is consistently less important but relevant to reaction efficiency.
Fixed Carbon (FC)	-	7	Gini emphasizes Fixed Carbon, which plays a significant role in solid-phase reactions.
Nitrogen Content	-	9	Gini highlights Nitrogen importance

This dual perspective aligns with the observations reported by Ascher et al. (2022), who also highlighted the combined utility of these methods for enhancing model interpretability in gas yield prediction. The findings demonstrate that PI and GI offer complementary insights into feature relevance for gas yield prediction. PI is well-suited for capturing broader, nonlinear dependencies among variables, while GI emphasizes features that provide stable and consistent contributions within the hierarchical structure of tree-based models. Utilizing both PI and GI enriches the understanding of key features, informs more effective feature selection strategies, and strengthens the overall robustness and reliability of gas yield prediction models in biomass COG systems.

4.6.6 Comparison of interpretability methods for char yield

The comparison of PI and GI methods for feature evaluation in GBR and RF models provided valuable insights into the key features of char yield prediction (Table 4.15). Both methods consistently ranked the ER and SBR as the most influential features, emphasizing their dominant roles in governing char formation. ER controls the extent of oxidation and reduction reactions, while SBR influences the availability of steam for

reforming reactions both of which are critical to char decomposition and gasification efficiency (Koido et al., 2021; Pati & De, 2021).

Table 4.15: Comparison of GBR permutation and Gini importance ranking for char yield

Feature	PI	GI	Comments
ER	1	1	Both methods agree on ER as the most important feature for Char Yield.
SBR	2	2	Consistently ranked second, highlighting its critical role.
Fixed Carbon (FC)	3	5	Permutation highlights FC as the third importance, while FC ranks lower in Gini but remains important across methods.
Carbon Content (C)	4	7	Carbon Content is more prominent in Permutation than in Gini
Nitrogen Content (N)	5	8	N ranks lower in Gini but remains important across methods.
CH Ratio	6	-	CH Ratio captures feedstock specificity in Permutation.
Biomass Feed Rate (BFR)	7	-	Permutation highlights BFR as one of the important feature while Gini does not.
Ash Content (Ash)	8	9	Both methods highlight Ash, albeit in different orders of importance
Moisture Content (MC)	9	10	Moisture ranks higher in Permutation, reflecting its dynamic process impact.
Volatile Matter (VM)	10	-	VM appears only in Permutation, reflecting its impact on char formation.
Pressure	-	3	Gini prioritizes Pressure for its global impact which is not captured by permutation
Hydrogen Content (H)	-	4	Gini focuses on H, while permutation does not
Oxygen Content (O)	-	6	Gini captures oxygen importance not captured by permutation

Additionally, features such as the CH ratio, ash content, pressure, and air agent were prominently ranked across models. Their consistent appearance highlights their importance in influencing the thermodynamic and kinetic conditions that shape char yield outcomes in biomass COG processes (Monir et al., 2020; George et al., 2019; (Awais et al., 2022)).

Key differences between the two methods arise from their distinct approaches to feature evaluation. PI captured dynamic and localized dependencies within the dataset (Molnar, 2019; Rodríguez-Pérez & Bajorath, 2020), which placed greater emphasis on variables such as FC, MC, and VM. These features often reflect nonlinear interactions and context-specific impacts that can significantly influence predictions under certain operating conditions (Sison et al., 2023). PI excelled at identifying subtle and nuanced influences that was overlooked by GI. This makes it particularly valuable for uncovering complex

relationships in biomass gasification, where feedstock variability and reaction dynamics interact in intricate ways.

Table 4.16: Comparison of RF permutation and Gini importance ranking for char yield

Feature	PI	GI	Comments
ER	1	1	Both methods agree on ER as the most significant feature.
SBR	2	2	Consistently ranked second, underscoring its importance.
FC	3	-	Permutation prioritizes FC, while Gini does not.
O	4	-	O is ranked higher in Permutation, reflecting its direct impact on reactions
C	5	-	C is only ranked higher in permutation, reflecting its direct impact on char formation
CH Ratio	6	5	Both methods highlight feedstock-specific features like CH Ratio.
Pressure	7	9	Pressure ranks lower in Gini but remains relevant across both methods.
N	8	7	N is ranked lower in PI but remains relevant across both methods.
MC	9	-	MC is only captured by PI, emphasizing its impact on char yield
Ash	10	6	Ash is ranked lower in PI but remains relevant across both methods.
Air	-	3	Gini focuses on Agent_Air, which not captured in permutation.
AirSteam	-	4	Gini also uniquely prioritizes Agent_AirSteam, while permutation does not.
TW Ratio	-	8	TW Ratio appears only in Gini, reflecting its feedstock specificity.
BFR	-	10	BFR is unique to Gini, capturing its role in controlling reactant flow rate.

On the other hand, GI focused on features that were consistently used for decision splits during tree construction, thereby emphasizing variables that contributed most to impurity reduction across the dataset (Li et al., 2023; Yaman et al., 2018). This method favored global contributors such as Air, AirSteam, and BFR, as shown in Table 4.16. It also highlighted feedstock-specific parameters such as TW ratio, which may play a critical role under particular conditions.

While GI was less responsive to dynamic interactions and nonlinear dependencies compared to PI, it provided a stable and interpretable perspective on overarching trends. Its strength lies in identifying robust, high-impact variables, making it a valuable tool for understanding the global drivers of model performance in biomass co-gasification systems. A similar interpretability analysis using GI and PI was conducted by Ascher et al. (2022), who reported comparable insights into the key features influencing char yield predictions. These findings demonstrate the complementary strengths of PI and GI methods in interpreting char yield predictions. These methods provide a comprehensive

understanding of feature relevance, offering guidance for improving model development and enhancing the robustness of char yield predictions in biomass COG processes.

4.6.7 Comparison of feature importance for gas and yield

The analysis of feature importance rankings for gas yield and char yield predictions revealed both critical overlaps and notable distinctions in the factors influencing these two key outcomes of biomass gasification, as shown in Table 4.17. Shared features reflected the fundamental parameters governing the gasification process, while target-specific features demonstrated the unique reaction dynamics that separately influence gas and char production.

Key features such as ER and SBR consistently ranked as the most critical variables for both gas yield and char yield predictions. ER, which was universally ranked the first, regulates the oxidation and reduction environment, directly influencing reaction pathways and product distributions (Pati et al., 2021; Pati & De, 2021; Cao et al., 2022). SBR, commonly ranked the second, controlled steam availability, which is essential for reforming reactions and char formation (Awais et al., 2022). Other shared features, including C, AirSteam, and Ash, further reflected their importance in driving reaction efficiency and feedstock conversion. The C serves as a primary reactant in gasification, while AirSteam helps maintain the balance of reactants needed for optimal gas-phase interactions. Ash negatively impacts reaction efficiency by obstructing gas–solid interactions, thereby reducing both gas and char yields (Koido et al., 2021; Monir et al., 2020; Anniwaer et al., 2021; Ascher et al., 2022).

Distinct features associated with gas yield prediction emphasized factors directly related to gas-phase reactions and syngas composition. Air plays a critical role in regulating oxygen availability, which is essential for sustaining oxidation reactions (Cao et al., 2022;

Pati et al., 2021). H-content influences the composition of syngas, particularly the production of H_2 , a key indicator of syngas quality (Zhao et al. (2021).

Table 4.17: Comparison of feature importance ranking for gas and char yield

Feature	Gas yield	Char yield	Reason for importance
ER	1	1	Dominates both Gas Yield and Char Yield prediction due to its influence on reaction efficiency.
SBR	2	2	Influences the partitioning of products between char and gas. Controls the availability of steam for reforming reactions
C	3	4	Key determinant of syngas composition and gas yield, Primary component contributing to char formation
AirSteam	4	8	Balances air and steam as reactants for gasification, affecting both gas production and char formation
Air	5	-	Regulates oxygen availability for partial oxidation reactions.
Pressure	6	-	Affects thermodynamics and reaction kinetics
H	7	-	Contributes to syngas composition, influencing gas yield.
Ash	8	3	High ash content reduces overall gas yield efficiency,
RH Ratio	9	-	Feedstock-specific contribution to gas yield.
GS Ratio	10	-	Feedstock-specific parameter influencing gas yield.
O	-	5	Affects reaction pathways that determine char yield.
N	-	6	Impacts inert gas balance and indirectly influences char yield.
CH Ratio	-	7	Feedstock-specific contribution to char yield
MS Ratio	-	9	Feedstock-specific parameter influencing char yield.
MC	-	10	Impacts heat balance and reaction dynamics.

Pressure significantly affects gas-phase thermodynamics and reaction kinetics (Monir et al., 2020; Freda et al., 2019), making it more relevant for gas yield prediction than for char yield (Sison et al. (2023). Feedstock-specific variables, such as the RH ratio and GS ratio, highlight the inherent variability in reactivity and composition among different biomass types (Ascher et al. 2022; Awais et al., 2022). These differences reflect their distinct contributions to syngas production and reinforce the importance of feedstock selection in optimizing gasification performance.

In contrast, features specific to char yield predictions were more closely associated with solid-phase reactions and thermal properties of the feedstocks. O-content influences the extent of oxidation and char retention (Koido et al., 2021), while N-content contributes to the inert gas balance (Awais et al., 2022), thereby affecting combustion and reduction processes. Feedstock-specific attributes such as the CH ratio and the MS ratio were particularly important for understanding char formation, as they reflect distinct biomass

characteristics including fixed carbon and ash content. MC also played a significant role in predicting char yield. By affecting the thermal balance within the reactor, MC influences both thermal decomposition and char retention, making it a critical factor in assessing the solid-phase dynamics of biomass gasification (Awais et al., 2021). These findings align with the studies by Sison et al. (2023) and Ascher et al. (2022), who also identified MC as a key factor in char yield prediction.

Based on these observations, it can be concluded that while shared features such as the ER, SBR, and C confirm the foundational importance of core gasification principles, the distinct feature rankings for gas yield and char yield show the unique processes governing each target variable. This dual perspective offers a comprehensive understanding of the factors influencing biomass COG and provides a basis for refining predictive models and optimizing process conditions to achieve specific performance outcomes.

4.6.8 Main and interactive feature effects on gas yield

The analysis of the main and interactive effects of features on gas yield, conducted using PDP) revealed critical insights into the roles of operational parameters and feedstock composition in shaping gasification performance (Figure 4.25). These findings offer actionable guidance for improving gas yield through targeted parameter optimization and informed feedstock selection, supporting the development of more efficient and adaptable biomass COG systems.

Key features, including the ER, SBR, and RH ratio, were found to significantly influence gas yield. ER emerged as the most critical parameter, with gas yield increasing consistently as ER increased (Figure 4.25a). This trend indicates the pivotal role of ER in promoting oxidation reactions, which are central to syngas production (Pati et al., 2021; Monir et al. 2020). SBR also exhibited a positive effect on gas yield, although with diminishing returns at higher values (Figure 4.25b). This suggests the existence of an

optimal range in which steam reforming reactions are maximized without incurring unnecessary energy input (Awais et al., 2022) . In contrast, the RH ratio negatively affected gas yield, with sharp declines observed as its proportion increased (Figure 4.25c). This reduction is likely attributable to the inhibitory effects of higher ash content or lower volatile matter in RH (Anniwaer et al., 2021; Pati & De, 2021; Wiyono et al., 2021), highlighting the importance of strategic feedstock blending to enhance gasification performance.

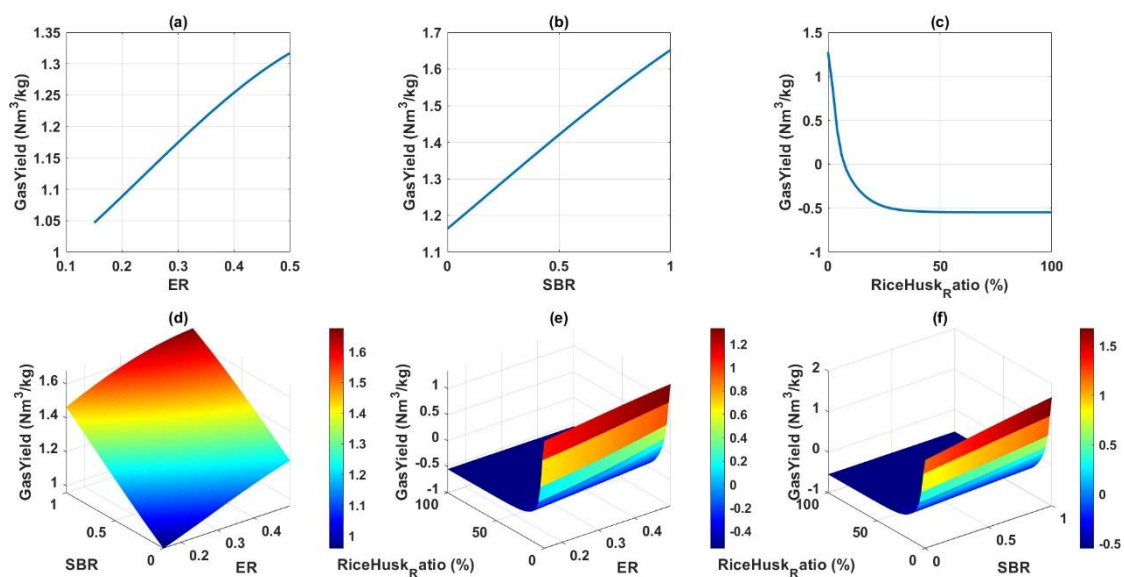


Figure 4.25: Main and interaction effects of features on syngas yield

Legend: (a) effect of ER on syngas yield, (b) effect of Steam-to-biomass ratio (SBR) syngas yield, (c) effect of rice husk percentage in blend, (d) interaction effect of ER and ER, (e) Interaction effect of ER and rice husk percentage, (f) interaction effect of rice husk percentage and SBR

Interactions between key features further clarified the underlying dynamics influencing gas yield. The interaction between the SBR and the ER was particularly significant, with gas yield increasing markedly when both parameters were simultaneously optimized, as shown in Figure 4.25d. This result highlights the importance of adjusting these operational variables in combination to maximize reaction efficiency and syngas output (Awais et al., 2021, 2022; Omar et al., 2018).

However, the negative impact of the RH ratio remained evident across all interaction scenarios. Even when combined with higher ER or SBR values, increased proportions of

RH continued to suppress gas yield, as illustrated in Figure 4.25e and Figure 4.25f. This suggests that the limiting effects associated with RH, likely due to higher ash content or lower volatile matter, can override the benefits of improved operating conditions (Koido et al., 2021; Anniwaer et al., 2021). The consistency of this reduction emphasizes the importance of careful feedstock management in order to minimize adverse impacts on COG performance.

4.6.9 Main and interactive feature effects on char yield

The main and interactive effects of features influencing char yield, as derived from PDP, provided critical insights into how operational parameters and feedstock composition impacted char production in biomass gasification (Figure 4.26). This analysis informs strategies for maximizing char yield through parameter optimization and feedstock management.

Key features such as ER, SBR, and MS ratio significantly influenced char yield. ER exhibited a linear decrease in char yield as its values increased (Figure 4.26a), indicating that higher ER levels favored oxidation reactions that reduce solid char formation (Awais et al., 2021, 2022). To maximize char yield, ER needs to be kept at lower levels. SBR also negatively affected char yield, with an initial decline followed by stabilization at higher levels (Figure 4.26b). This pattern reflects the enhanced steam reforming effects that consumed char, suggesting that optimizing SBR within a specific range was essential for balancing char formation and gas yield (Anniwaer et al., 2021; Awais et al., 2022). In contrast, the MS ratio had a positive effect, with char yield increasing sharply at higher proportions (Figure 4.26c). This trend highlights the role of the high fixed carbon content in MS in promoting char formation (Vu et al., 2023; Chaiklangmuang et al., 2015; Nam et al., 2021), making them a valuable feedstock for char-oriented gasification systems.

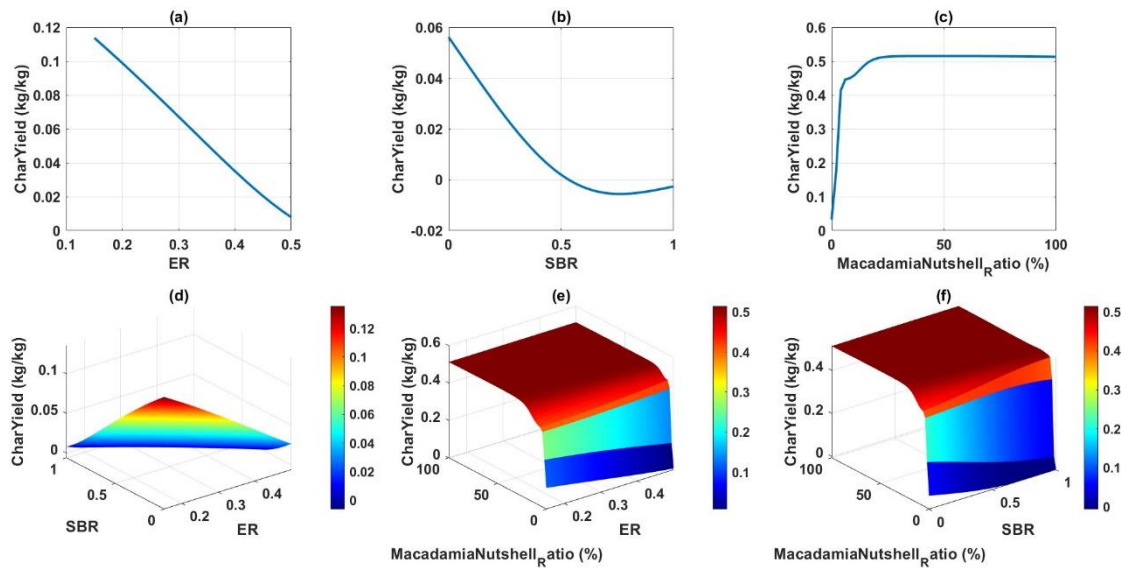


Figure 4.26: Main and interactive feature effects on char yield

Legend: (a) effect of ER, (b) effect of Steam-to-biomass ratio (SBR), (c) effect of rice husk percentage in blend, (d) interaction effect of ER and ER, (e) Interaction effect of ER and rice husk percentage, (f) interaction effect of rice husk percentage and SBR

The interactions between features further illustrate the dynamics influencing char yield.

The interaction between ER and SBR shows that the highest char yield occurred when both parameters were minimized, highlighting their synergistic effect in promoting char retention (Figure 4.26d). Similarly, the interaction between MS ratio and ER indicates that high proportions of MS mitigated the negative effects of increasing ER (Figure 4.26e), emphasizing the dominance of feedstock properties over operational parameters at higher MS ratios.

Furthermore, the interaction between the MS ratio and SBR demonstrates that char yield was maximized when high MS content was combined with low SBR (Figure 4.26f). Conversely, higher SBR values reduced char formation, particularly when MS content was low, likely due to the enhanced steam reforming and gasification reactions that actively consumed char in the presence of increased steam availability and lower fixed carbon input (Awais et al., 2021, 2022; Omar et al., 2018). These findings reinforce the importance of balancing both operational settings and feedstock composition to optimize char production in biomass COG.

The findings reveals that the MS ratio is the most critical factor for enhancing char yield, surpassing the influence of operational parameters such as the ER and the SBR. Feedstocks with high fixed carbon content, such as MS, not only increases char production but also reduces the sensitivity of char yield to variations in ER and SBR (Monir et al., 2018; Zhao et al., 2022; Jiao et al., 2022). The interaction between ER and SBR further demonstrates the importance of minimizing both parameters to achieve optimal char retention. However, feedstock composition plays a dominant role in mitigating the negative effects of operational conditions.

These results emphasize the value of implementing effective feedstock blending strategies alongside precise control of ER and SBR to maximize char yield while maintaining overall process efficiency. The insights gained from this analysis provide practical guidance for optimizing biomass COG systems to achieve targeted char production outcomes.

4.7 Practical Implications and Engineering Relevance.

The study offers actionable insights for enhancing the design and operation of biomass gasification systems. Detailed characterization of thermal decomposition and kinetic parameters enables engineers to fine-tune pyrolysis conditions for improved energy recovery and biofuel production. Activation energy and thermodynamic insights serve as critical inputs for optimizing reactor configurations, enhancing system efficiency, and improving output yields.

PS models proved effective in identifying temperature profiles and syngas production trends, particularly for varying ER levels. The range of 0.22 to 0.28 emerged as optimal for balancing heat transfer and syngas quality, guiding both process tuning and material

selection for reactors operating under high thermal stress. Moreover, simulation results support strategic decisions on feedstock blending to enhance gasification outcomes.

ML models added further value by offering accurate predictions of core performance indicators such as char yield, gas yield, and CO concentration. These tools enable real-time process monitoring and provide a foundation for intelligent control strategies. While lower accuracy in predicting CGE, H_2 , and LHV suggests the need for expanded datasets and more refined feature selection, the SLE models demonstrated strong generalization potential, making it suitable for integration into Supervised Control and Data Acquisition (SCADA)-based control systems.

Interpretability tools, including PI, GI, and PDP, revealed both dominant and interactive variables. Key process factors such as ER and SBR, along with feedstock properties like ash content and MS ratio, were consistently identified as influential. These insights offer engineers transparent and actionable guidance for refining gasification setups and feature selection strategies in ML pipelines.

Collectively, the findings validate the use of integrated PS and ML approaches as powerful tools for advancing COG system design, process optimization, and automation, with broader applicability in sustainable bioenergy production.

CHAPTER FIVE: CONCLUSION AND RECOMMENDATIONS

5.1 Conclusions

This study systematically investigated the co-gasification of selected biomass feedstocks using thermal characterization, process simulation (Aspen Plus), and machine learning (ML) techniques. The findings provide insights into feedstock properties, pyrolysis behavior, process modeling accuracy, ML predictive performance, and model interpretability, supporting the optimization of biomass-to-syngas conversion processes.

5.1.1 Objective 1: Characterization and Evaluation of Physicochemical Properties, Thermal Decomposition Behavior, and Reactivity Kinetics

Objective 1: To characterize and evaluate the physicochemical properties, thermal decomposition behaviors, and reactivity kinetics of rice husks (RH), groundnut shells (GS), coffee husks (CH), macadamia nut shells (MS), and tea waste (TW).

Based on the comprehensive physicochemical, thermogravimetric, kinetic, and thermodynamic analyses conducted on the five biomass feedstocks, the following conclusions were drawn:

- Physicochemical variability was observed across the feedstocks, especially in ash, fixed carbon, and volatile matter contents. This variability supports the feasibility of strategically blending feedstocks to enhance gasification performance and improve overall conversion efficiency.
- Nitrogen (<1.5%) and sulfur (<0.3%) contents were consistently low across all materials, indicating a low tendency for NO_x and SO_x formation during thermochemical conversion. This positions all five feedstocks as environmentally suitable for clean energy applications.

- MS demonstrated the most favorable fuel properties, including the highest elemental carbon content (52.49%) and calorific value (21.5 MJ/kg), making it the most energy-rich of the studied materials.
- TGA revealed three distinct decomposition stages: Drying (25°C – 215°C), Devolatilization (175°C – 440°C), Char formation and secondary cracking (415°C – 950°C). These temperature ranges illustrate the thermal complexity and varying devolatilization intensities among the feedstocks.
- Activation energies during devolatilization ranged from 39.35–45.83 kJ/mol, reflecting differences in thermal reactivity.
- GS (45.83 kJ/mol) and MS (45.26 kJ/mol) exhibited higher activation energies, indicating greater resistance to thermal degradation.
- CH (39.35 kJ/mol) and RH (40.66 kJ/mol) showed lower activation energies, implying higher reactivity and faster devolatilization.
- Thermodynamic parameters during devolatilization further clarified these reactivity differences: ΔH (34.20–40.56 kJ/mol), confirming that the reactions were endothermic and required external heat input to proceed, ΔG (50.88–161.97 kJ/mol) indicated that decomposition was non-spontaneous, requiring continuous energy supply, and ΔS (–0.18 to –0.19 kJ/mol·K) suggest increased molecular ordering during bond scission, which is characteristic of solid-phase pyrolysis reactions.
- MS had the highest devolatilization ΔG value (≈ 162 kJ/mol), indicating the least spontaneous decomposition, whereas CH had the lowest ΔG (≈ 151 kJ/mol), denoting a more energetically favorable degradation pathway.
- The D3 (Jander three-dimensional diffusion) model emerged as the dominant reaction mechanism across feedstocks and decomposition stages, implying that

diffusion-controlled transport of volatiles governs pyrolysis kinetics in these biomass types.

These findings establish a clear understanding of the chemical and thermal behavior of the selected feedstocks. The results provide a strong scientific basis for feedstock selection, blending strategies, and optimization of gasification operating parameters, ultimately supporting more efficient syngas and char production in thermochemical biomass conversion systems.

5.1.2 Objective 2: Development and Validation of a Process Simulation Model for Biomass Co-Gasification Using Aspen Plus

***Objective 2:** To develop and validate a process simulation model for the co-gasification of biomass waste using Aspen Plus.*

The development and validation of the Aspen Plus co-gasification model led to the following conclusions:

- The Aspen Plus model accurately predicted temperature distributions within key gasification zones, with low deviations observed in the pyrolysis (RMSD = 2°C) and combustion (RMSD = 4°C) zones. This high level of accuracy demonstrates the model's strong capability to replicate thermal behavior under controlled operating conditions.
- Larger deviations in the reduction zone (RMSD = 7°C), particularly at higher ER, indicate limitations in the current modelling assumptions. This suggests the need for improved incorporation of kinetic parameters, char–gas reaction mechanisms, and feedstock-specific thermochemical properties to enhance predictive accuracy.
- Sensitivity analysis identified ER as the most influential operational parameter affecting temperature profiles, gas yield, and syngas composition. This confirms

ER as a critical control variable for optimizing gasification performance in simulation and real-world systems.

The validated Aspen Plus model provides a reliable and practical tool for assessing biomass co-gasification performance and optimizing operating conditions. It enables systematic evaluation of gasification behavior without relying exclusively on resource-intensive experimental studies, thereby supporting process design, scale-up, and operational planning.

5.1.3 Objective 3: Development and Validation of Machine Learning Models for Biomass Co-Gasification

***Objective 3:** To develop and validate machine learning models using Random Forest (RF), Gradient Boosting Regression (GBR), Support Vector Regression (SVR), Artificial Neural Network (ANN), and SuperLearner Ensemble (SLE), for predicting biomass co-gasification performance.*

The development, training, and validation of the ML models led to the following conclusions:

- The SLE demonstrated the highest predictive accuracy among all models, achieving $R^2 > 0.92$ and low RMSE values for char yield, gas yield, and CO concentration. This confirms the effectiveness of ensemble learning in capturing nonlinearities and complex interactions inherent in biomass gasification processes.
- Model performance for CGE, H_2 , and LHV was comparatively lower ($R^2 < 0.85$), indicating challenges associated with limited dataset diversity, complex multi-variable interactions, and insufficient feature representation for these outputs. These findings highlight the need for expanded datasets, improved feature

engineering, and additional process descriptors to strengthen model generalizability.

The machine learning models, particularly the SLE, demonstrate strong potential for predicting key gasification performance indicators, thus reducing reliance on resource-intensive experiments. These models further support real-time process monitoring, optimization, and data-driven decision-making in thermochemical biomass conversion systems.

5.1.4 Objective 4: Robustness Assessment of Machine Learning Models for New Feedstock Blends

***Objective 4:** To investigate the robustness of machine learning models when applied to new and unseen feedstock blends.*

Based on the robustness assessment conducted using unseen experimental data, the following conclusions were drawn:

- The SLE demonstrated strong robustness, reliably predicting char yield ($R^2 = 0.83$, RMSE = 0.0223), gas yield ($R^2 = 0.78$, RMSE = 0.0902), and CO concentration ($R^2 = 0.61$, RMSE = 5.2448) for the new feedstock blend. This confirms that ensemble learning can generalize reasonably well beyond the training domain for selected variables.
- Predictions for CGE, H_2 , and LHV showed weak generalizability, characterized by low R^2 values and high errors. This indicates that the existing dataset lacked sufficient variability and representation for these outputs, and that more diverse training data or enhanced feature space is required for robust performance.
- The findings suggest that integrating time-series features, stress-testing techniques, and adaptive learning mechanisms (e.g., incremental learning, transfer

learning) could substantially improve model resilience under dynamic and industrially relevant gasification conditions.

The robustness analysis reveals the critical role of comprehensive and diverse datasets, together with adaptive modeling techniques, in ensuring reliable machine learning predictions for industrial-scale biomass co-gasification applications.

5.1.5 Objective 5: Evaluation of Model Interpretability Techniques for Feature Importance Analysis

***Objective 5:** To evaluate the influence of various model interpretability techniques on feature importance rankings in predicting co-gasification performance.*

Based on the interpretability analyses applied to the trained machine learning models, the following conclusions were drawn:

- ER and SBR consistently emerged as the most influential predictors across all models, confirming their dominant role in governing temperature distribution, gas yield, and char formation. Additionally, intrinsic feedstock properties, such as MS ratio and ash content, were found to significantly influence char yield and gasification reactivity.
- Comparative evaluations of Permutation importance and Gini importance demonstrated that each method captured different aspects of feature contribution. Their complementary nature provided a more holistic understanding of variable influence, strengthening confidence in the feature ranking outcomes.
- PDPs clarified both the main effects and interactive effects of key variables. These visual insights highlighted the synergistic impact of ER and SBR on syngas composition and char yield, illustrating the need for joint optimization of these parameters to enhance gasification performance.

The interpretability analysis improves transparency and trust in machine learning models, offering actionable insights for optimizing biomass co-gasification. These findings support data-driven decision-making in process design, feedstock selection, and operational control.

5.1.6 Overall conclusion

This study provides a comprehensive investigation into the co-gasification of underutilized biomass feedstocks through physicochemical characterization, thermal analysis, process simulation, and machine learning modeling. By integrating Aspen Plus simulations with ML techniques, the research advanced the understanding of feedstock behavior, synergistic effects, and process parameter influence on gasification performance. The findings demonstrate that the developed ML models offer reliable predictions for char yield, gas yield, and CO, supporting real-time process monitoring and optimization. Robustness and interpretability analyses further identified critical factors such as equivalence ratio and steam-biomass ratio, enabling actionable guidance for operational control. This work contributes valuable kinetic, thermodynamic, and modeling data for biomass co-gasification, promotes data-driven decision-making, and provides a framework for scaling up sustainable energy solutions using Industry 4.0 approaches.

5.2 Recommendations

5.2.1 Future research

This study provides a foundation for advancing biomass gasification research and technology. Future research should address identified limitations and explore innovative approaches to enhance thermal degradation analysis, PS, ML modeling, model robustness, and interpretability.

Expanding the range of biomass feedstocks will improve the generalizability of findings across diverse compositions. Advanced kinetic analysis methods, such as isoconversional techniques, should be used to better understand reaction mechanisms under varying heating rates. Experimental setups should replicate industrial-scale conditions, incorporating heterogeneous feedstocks and dynamic operating environments to bridge the gap between laboratory and real-world applications. Integrating thermogravimetric data with computational models can further refine thermal degradation predictions.

PS models should incorporate detailed reaction kinetics, feedstock-specific parameters (e.g., thermal conductivity, ash behavior, char reactivity), and spatial gradients to improve accuracy, particularly in the reduction zone. Validation should extend to broader feedstocks and operating conditions to enhance model robustness. Future models should integrate real-time monitoring data for adaptive process control and explore hybrid modeling approaches that merge data-driven and physics-based techniques for a more comprehensive understanding of gasification dynamics.

Advancing ML models requires expanding datasets to include diverse feedstocks, operating conditions, and transient states. Feature engineering should incorporate additional variables such as reaction kinetics and thermal gradients to enhance predictive accuracy. Integrating domain-specific knowledge (e.g., thermodynamic principles) into ML models could improve predictions for complex targets like CGE and H_2 . Future research should also focus on combining ML models with optimization tools (GA, PSO) to enhance process efficiency. Incorporating time-series data would enable dynamic predictions and better real-time monitoring of gasification processes.

To improve model robustness, future studies should focus on collecting representative datasets that include extreme operating conditions and edge-case scenarios. Exploring alternative meta-learners such as XGBoost, GBR, or deep neural networks could improve

performance for complex interactions. Developing adaptive models capable of real-time learning would enhance applicability in dynamic environments. Hybrid approaches integrating ML models with domain-based validation should be prioritized to ensure reliability in real-world applications.

For model interpretability, advanced techniques like SHAP and LIME should be incorporated to provide deeper insights into feature contributions and interactions. These methods could complement permutation and Gini importance by balancing global and local interpretability. Understanding the evolution of feature importance under varying operating conditions would further improve interpretability. Future research should aim to integrate interpretability techniques with optimization and control systems, ensuring that insights are actionable for real-time decision-making in biomass co-gasification.

5.2.2 Practice and Policy

Based on the findings of this study, the following recommendations are proposed to enhance biomass gasification processes, research methodologies, and industrial applications.

Optimize feedstock selection and pre-treatment for improved biofuel production: (i) Utilize thermal decomposition and kinetic parameter insights to develop optimized feedstock pre-treatment strategies (e.g., drying, torrefaction, and pelletization) to enhance gasification efficiency and energy recovery. (ii) Prioritize low-nitrogen and low-sulfur biomass feedstocks to minimize NO_x and SO_x emissions, promoting cleaner bioenergy production. (iii) Consider feedstock blending strategies based on proximate and ultimate analysis data to achieve desired syngas quality and operational efficiency.

Deploy process simulation models for real-time gasification optimization: (i) Integrate the Aspen simulation models into industrial gasification systems to enable real-time process monitoring and optimization. (ii) Utilize simulation models to refine ER

adjustments, predict zone-specific performance, and optimize reactor design. (iii) Expand validation efforts by applying models across varied biomass feedstocks to enhance their generalizability and real-world applicability. (iv) Implement ML models in industrial gasification for process monitoring and control. (v) Deploy SuperLearner ML models in gasification plants to improve process monitoring, feedstock selection, and optimize operational performance. (vi) Integrate ML-based gasification models into SCADA systems for automated real-time control and decision-making. (vii) Enhance ML model robustness by expanding training datasets to include diverse operating conditions and extreme case scenarios for better prediction accuracy.

Adopt ML models for research and virtual experimentation: (i) Research institutions should adopt these ML models for virtual experimentation, reducing reliance on expensive physical setups. (ii) Establish collaborative platforms for sharing gasification datasets and models, facilitating advancements in biomass research.

Enhance the accessibility and usability of ML models with intuitive user interfaces: (i) Develop user-friendly graphical interfaces to facilitate wider adoption of ML models in biomass gasification, even for non-expert users. (ii) Implement interactive dashboards for real-time data visualization, model predictions, and process adjustments. (iii) Provide customizable features for different biomass types, process conditions, and operational settings, ensuring broader applicability in industry and research.

Use interpretability insights to improve process control and feature engineering: (i) Use ML interpretability findings (Permutation Importance, Gini Importance, PDPs) to refine feature engineering and enhance model reliability. (ii) Identify and prioritize the most influential operational parameters (e.g., ER, SBR, ash content) to improve process control and syngas yield. (iii) Utilize interpretability dashboards in gasification plants to support

real-time decision-making, enhancing transparency and stakeholder trust in ML-driven gasification control systems.

5.3 Contributions of the study

5.3.1 Theoretical contributions

- Expanded understanding of thermochemical decomposition and reactivity behavior of multiple African biomass residues () using TG-derived kinetic and thermodynamic insights.
- Demonstrated synergistic and antagonistic interactions occurring during co-gasification, advancing theoretical knowledge of multi-feedstock conversion.
- Identified the influence of ER on syngas composition, gas yield and char yield, reinforcing existing gasification theory with new empirical evidence.
- Contributed theoretical clarity on the relationship between biomass physicochemical properties and gasification performance.
- Provided a theoretical framework integrating process simulation and machine learning for predicting biomass conversion outcomes.

5.3.2 Methodological contributions

- Developed a comprehensive Aspen Plus co-gasification model tailored to region-specific biomass feedstocks, incorporating kinetics and material properties.
- Designed machine learning models capable of predicting char yield, gas yield, and CO concentration, demonstrating a dual approach combining simulation outputs and experimental data.
- Implemented robustness testing (R^2 and RMSE after de-normalization) to evaluate model sensitivity to data variation, an approach not commonly applied in biomass co-gasification studies.

- Applied interpretability techniques to identify feature importance, introducing transparent AI methodologies into biomass conversion research.
- Established a workflow that integrates thermal analysis, PS, ML prediction, robustness evaluation, and interpretability into a single analytical framework.

5.3.3 Practical contributions

- Generated actionable insights for optimizing gasification operations, including appropriate ER ranges and blend ratios to enhance hydrogen-rich syngas.
- Delivered ML-based predictive tools that can support real-time monitoring and decision-making in biomass gasification processes.
- Produced data that can guide small-scale and industrial biomass energy systems towards improved efficiency and sustainability.
- Offered evidence-based recommendations that can support policymakers, project developers, and energy planners working on waste-to-energy initiatives.

5.3.4 Data contributions

- Compiled a unique dataset comprising proximate, ultimate, and TGA-derived kinetic data for five region-specific biomass feedstocks and their blends.
- Generated simulation-based performance data (syngas composition, char yield, process efficiencies) under systematically varied gasification conditions.
- Produced machine learning training and testing datasets derived from combined experimental and simulation results, enabling reproducibility.
- Provided denormalized ML performance metrics and predicted–actual value comparisons for robustness evaluation.
- Created a consolidated dataset that can serve as a reference for future research on African biomass resources and co-gasification modeling.

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APPENDICES

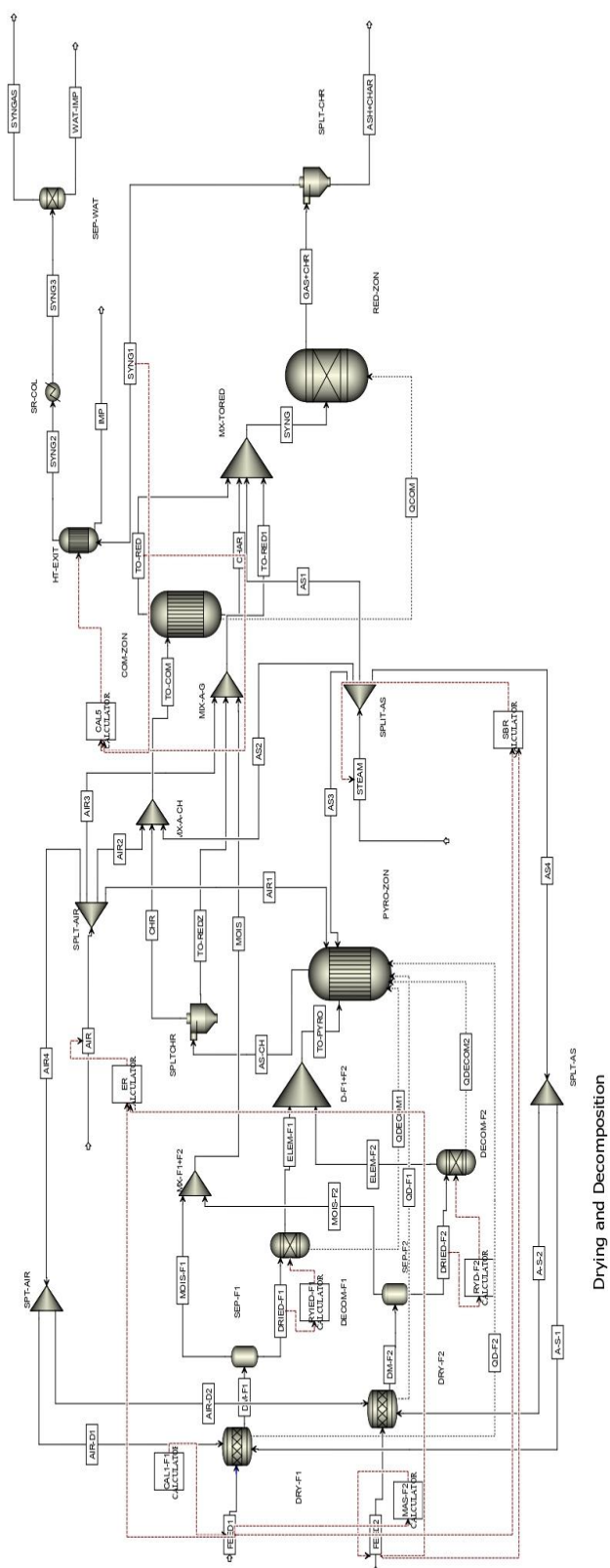
APPENDIX A: Aspen Process Model Details

Stream Type	Assigned ID	Description
MATERIAL	A-S-1	Model steam flow during drying feedstock 1
	A-S-2	Model steam flow during drying feedstock 2
	AIR	Model Air flow into the gasification system
	AIR-D1	Model air flow during drying feedstock 1
	AIR-D2	Model air flow during drying feedstock 2
	AIR1	Model air flow into the pyrolysis zone
	AIR2	Model air flow into the combustion zone
	AIR3	Model air flow into the reduction zone
	AIR4	Model air flow into the drying zone
	AS-CH	Products output of the pyrolysis zone
	AS1	Model steam flow into the reduction zone
	AS2	Model steam flow into the combustion zone
	AS3	Model steam flow into the pyrolysis zone
	AS4	Model steam flow into the drying zone
	ASH+CHAR	Model Ash and Char leaving the cyclone (solid product)
	CHAR	Solid product from combustion zone
	CHR	Char product from Pyrolysis zone fed to combustion zone
	DM-F1	Product from drying feedstock 1
	DM-F2	Product from drying feedstock 2
	DRIED-F1	Dried feedstock 1
	DRIED-F2	Dried feedstock 2
	ELEM-F1	Elements decomposed from feedstock 1
	ELEM-F2	Elements decomposed from feedstock 2
	FEED1	Feedstock 1 feeding into gasification system
	FEED2	Feedstock 2 feeding into gasification system
	GAS+CHR	Model gas and char products from reduction zone
	IMP	Model solid products falling at the Exit zone
	MOIS	Moisture removed from the two feedstock
	MOIS-F1	Moisture removed from feedstock 1
	MOSI-F2	Moisture removed from feedstock 2
	STEAM	Model steam feeding into the gasification system
	SYNG	Input materials (agent, gas, char) into the reduction zone
	SYNG1	Syngas from reduction zone
	SYNG2	Syngas exiting from the hot temperature exit zone
	SYNG3	Syngas after to cooling
	SYNGAS	Clean syngas (CO, H ₂ , CO ₂ , CH ₄) are removal of impurities and moisture,
	TO-COM	Input materials into the combustion zone
	TO-PYRO	Input materials into the pyrolysis zone
	TO-RED	Gaseous production from the combustion zone
	TO-RED1	Input material into the reduction zone (agent, solid, moisture)
	TO-RED2	Gaseous products from pyrolysis zone to the reduction zone
	WAT-IMP	Impurities removed from the syngas
HEAT	QCOM	Heat flow from the combustion to reduction zone
	QD-F1	Heat flow from drying feedstock 1 to pyrolysis zone
	QD-F2	Heat flow from drying feedstock 2 to pyrolysis zone
	QDECOM1	Heat flow from decomposition of feedstock 1 to pyrolysis zone
	QDECOM2	Heat flow from decomposition of feedstock 2 to pyrolysis zone

Block Type	Assigned ID	Description
Rstoic	DRY-1	Model drying of feedstock 1
	DRY-2	Model drying of feedstock 2
Flash2	SEP-F1	Model separation of moisture from dried feedstock1
	SEP-F2	Model separation of moisture from dried feedstock 2
Sep	SEP-WAT	Model separation of impurities and moisture from syngas
Fsplit	SPLIT-AS	Model distribution of steam to different reactor zone
	SPLT-AIR	Model distribution of air to different reactor zone
	SPLT-AS	Model distribution of steam for drying feedstock 1 and 2
	SPT-AIR	Model distribution of Air for drying feedstock 1 and 2
Ssplit	SPLT-CHR	Model separation solid from gas after pyrolysis zone
	SPLTCHR	Model separation of solid from gas after reduction zone
Heater	SR-COL	Model cooling of hot syngas to room temperature
REquil	COM-ZON	Model combustion reaction under equilibrium to generate heat inside the gasifier
	HT-EXIT	Model the high temperature Water-gas shift reaction under equilibrium at hot exit
Mixer	D-F1+F2	Combine elements from feedstock 1 and feedstock 2
	MIX-A-G	Combine moisture, air and gaseous product from pyrolysis
	MX-A-CH	Combine steam, air and char used in the combustion zone
	MX-F1+F2	Combine moisture from feedstock 1 and feedstock 2
	MX-TORED	Combine steam, mixed products, unburnt char feeding into reduction zone
RYield	DECOM-F1	Model conversion of unconventional component FEED1 (feedstock 1) into conventional elements
	DECOM-F2	Model conversion of unconventional component FEED2 (feedstock 2) into conventional elements
RGibbs	PYRO-ZON	Model pyrolysis zone for equilibrium modeling of gas-phase reactions.
	RED-ZON	Model Reduction zone for equilibrium modeling of gas-phase reactions.
Calculator	CAL1-F1	Calculate the percentage of Feedstock 1 into the feed mixture based on the blend ratio and total feed flow rate
	CAL5	Calculate the exit temperature at the exit zone
	ER	Calculate the Total air flowrate required for the gasifier based on the ER input
	MAS-F2	Calculate the percentage of feedstock 2 into the feed mixture based on the blend ratio and total feed flow rate
	RYD-F2	Calculate the product decomposition of feedstock 2
	RYIED-F1	Calculate the production decomposition of feedstock 1
	SBR	Calculate the steam flow rate based on the set steam-to-biomass ratio.

Component ID	Type	Component Name	Alias
FEED1	Nonconventional	-	-
FEED2	Nonconventional	-	-
ASH	Nonconventional		
C	Solid	CARBON-GRAPHITE	C
S	Solid	SULFUR	S
H2	Conventional	HYDROGEN	H2
O2	Conventional	OXYGEN	O2
N2	Conventional	NITROGEN	N2
H2O	Conventional	WATER	H2O
CO2	Conventional	CARBON-DIOXIDE	CO2
CO	Conventional	CARBON-MONOXIDE	CO
CH4	Conventional	METHANE	CH4
H2S	Conventional	HYDROGEN-SULFIDE	H2S
NH3	Conventional	AMMONIA	H3N

APPENDIX B: Gasification Model Flowsheet



APPENDIX C: Features

Code	Feature	Full name	Code	Feature	Full name
1	CH	Coffee Husks	20	MS_Ratio	Macadamia Nutshells Ratio/Proportion
2	GS	Groundnut Shells	21	RH_Ratio	Rice Husks Ratio/Proportion
3	MS	Macadamia Nutshells	22	TW_Ratio	Tea Wastes Ratio/Proportion
4	RH	Rice Husks	23	MC	Moisture Content
5	TW	Tea Wastes	24	VM	Volatile Matter
6	CH_GS	Coffee Husks and Groundnut Shells	25	FC	Fixed Carbon
7	CH_RH	Coffee Husks and Rice husks	26	Ash	Ash content
8	CH_TW	Coffee and Tea Wastes	27	C	Carbon
9	GS_RH	Groundnut Shells and Rice Husks	28	H	Hydrogen
10	GS_TW	Groundnut Shell and Tea Wastes	29	N	Nitrogen
11	MS_CH	Macadamia Nutshells and Coffee Husks	30	O	Oxygen
12	MS_GS	Macadamia Nutshells and Groundnut Shells	31	S	Sulfur
13	MS_RH	Macadamia Nutshells and Rice Husks	32	LHVb	Lower Heating Values Biomass
14	MS_TW	Macadamia Nutshell and Tea Wastes	33	HHVb	Higher Heating Values Biomass
15	RH_TW	Rice Husks and Tea Wastes	34	BFR	Biomass Feed Rate
16	Air	Air agent	35	ER	Equivalent Ratio
17	Air_Steam	Mixed Air and Steam agent	36	SBR	Steam-to-Biomass Ratio
18	CH_Ratio	Coffee Husks Ratio/proportion	37	Pressure	Low pressure gasification system
19	GS_Ratio	Groundnut Shells Ratio/Proportion	38		

APPENDIX D: Physiochemical Properties Data

Proximate Analysis

Proximate	Coffee husk	Groundnut shell	Macadamia nutshell	Rice Husk	Tea waste
Moisture (%)	8.67	6.92	7.39	5.9	5.69
Volatile matter (%)	62.9	66.24	68.52	59.19	62.95
Fixed carbon (%)	18.37	19.76	21.06	15.9	23.01
Ash (%)	10.06	7.07	3.03	19.01	8.35

Ultimate Analysis

Feedstock	Carbon (%)	Hydrogen (%)	Oxygen (%)	Nitrogen (%)	Sulphur (%)
Coffee husk	50.001	6.325	32.581	0.959	0.072
Groundnut shell	45.68	4.91	40.763	1.523	0.054
Macadamia nut shell	52.49	5.49	37.193	1.772	0.025
Rice Husk	40.31	4.26	34.88	1.53	0.009
Tea Waste	49.98	5.003	33.956	2.679	0.035

Calorific value

Feedstock	LHV	HHV
Coffee husk	19.85	20.68
Groundnut shell	17.32	17.89
Macadamia nut shell	20.77	21.46
Rice Husk	16.6	16.83
Tea Waste	19.41	20.01

Reaction Models	Coffee husk			Ground nutshell			Macadamia nutshell			Rice husk			Tea waste		
	A (min ⁻¹)	Ea (kJ/mol)	R ²	A (min ⁻¹)	Ea (kJ/mol)	R ²	A (min ⁻¹)	Ea (kJ/mol)	R ²	A (min ⁻¹)	Ea (kJ/mol)	R ²	A (min ⁻¹)	Ea (kJ/mol)	R ²
R7	7.55E-01	14.0168	0.7277	4.38E-01	12.1854	0.8048	7.18E-01	14.6753	0.8296	8.94E-01	15.2147	0.8114	8.19E-02	6.9604	0.6156
R8	4.36E+05	82.5356	0.8910	4.23E+03	56.6288	0.6574	9.74E+03	62.7875	0.7372	4.39E+04	70.5848	0.6296	7.25E+01	37.2491	0.6176
R9	2.51E+12	171.4493	0.8742	1.84E+12	174.5269	0.7896	8.26E+12	188.104	0.8113	5.36E+12	181.5557	0.8294	7.27E+05	89.1372	0.5831
Diffusion (Full range temperature; Start temperature (25 °C) to 950 °C); Global single step approach															
D1	2.3450	27.0652	0.7184	3.5749	30.0489	0.6968	7.5530	35.3534	0.7896	296.4180	42.6545	0.8349	5.4534	33.6915	0.7717
D2	3.3230	30.1831	0.7795	13.0306	36.5382	0.7644	29.2546	42.1962	0.8404	1138.1110	49.5072	0.8572	6.6336	36.4783	0.8111
D3	4.0529	35.5224	0.8592	9.3430	40.1792	0.8097	19.9607	45.7572	0.8689	787.4701	53.1097	0.8792	4.1821	39.7816	0.8537
D4	1.2510	31.8179	0.8080	4.2270	37.7075	0.7804	9.3430	43.3426	0.8507	364.8730	50.6654	0.8650	2.0625	37.5433	0.8264
Geometrical Contraction (Full range temperature; Start temperature (25 °C) to 950 °C); Global single step approach															
G5	0.1091	11.4478	0.6600	0.1661	12.9718	0.7025	0.2409	15.1402	0.7766	11.9440	23.2346	0.8946	0.0896	11.8556	0.6570
G6	0.1197	12.7906	0.7309	0.1558	13.9059	0.7400	0.2247	16.1159	0.8015	10.9902	24.2234	0.9055	0.0827	12.7696	0.7035
Order-based Reaction (Full range temperature; Start temperature (25 °C) to 950 °C); Global single step approach															
R7	1.2455	16.3180	0.8484	10.2037	161.2618	0.8026	1.4475	18.3888	0.8400	68.4073	26.1059	0.9138	0.5123	14.8741	0.7853
R8	3.04E02	33.4979	0.8306	21.4339	25.2569	0.7991	28.3939	27.7375	0.8209	1.44E03	36.3727	0.8450	7.7957	23.3694	0.8415
R9	2.22E05	55.4796	0.7304	8.62E04	53.6562	0.6578	1.35E05	57.7988	0.6748	1.04E07	68.2814	0.7398	341.4685	36.1779	0.7096
Overall (based on multi-step)	8187.4003	60.5947	-	28.9394	37.3008	-	22.7858	37.8826	-	30.1404	36.5609	-	4.3654	31.1210	-

APPENDIX F: Aspen Simulation Model Validation Data

A) Validation on Reactor zone temperature

Sugarcane bagasse and coconut shell blend

Reactor Zone	Experiment Temperature (°C)	Model Temperature (°C)	RMSD (°C)
Pyrolysis	450	452	2
Combustion	800	804	4
Reduction	550	557	7

Wood chip and corn cob blend

Reactor Zone	Experiment Temperature (°C)	Model Temperature (°C)	RMSD (°C)
Pyrolysis	350	344	6
Combustion	780	774	6
Reduction	530	522	8

B) Validation on Gas yield at two value of Equivalent Ratio

Sugarcane bagasse and coconut shell blend

ER	Experiment gas yield (Nm ³ /kg)	Model gas yield (Nm ³ /kg)	RMSD (Nm ³ /kg)
ER=0.17	1.1	1.31	0.21
ER=0.29	2	1.66	0.34

APPENDIX G: MATLAB Source Codes

SUPERLEARNER CODE FOR GAS YIELD

```
% Step 1: Save the base models
% Save base models to a .mat file
save('BaseModelsGasYield.mat', 'RFModelGasYield', 'ANNModelGasYield', 'GBRModelGasYield',
'SVMModelGasYield');
disp('Base models saved successfully!');

% Step 2: Build the SuperLearner
% Load base models
load('BaseModelsGasYield.mat', 'RFModelGasYield', 'ANNModelGasYield', 'GBRModelGasYield',
'SVMModelGasYield');

% Load Validation Data
valData = readtable('ValDataGasYield.xlsx'); % Ensure this file exists with predictors and
response
predictorNames = RFModelGasYield.RequiredVariables; % Ensure all models share the same
predictors
XVal = valData(:, predictorNames); % Extract predictors
YVal = valData.GasYield; % Extract response variable

% Initialize variables
k = 10; % Number of folds for cross-validation
cv = cvpartition(height(XVal), 'KFold', k);

% Initialize meta-features and target
metaFeatures = zeros(height(XVal), 4); % 4 base models
metaTarget = YVal;

% Generate meta-features using cross-validation
for fold = 1:k
    % Training and validation split for this fold
    trainIdx = training(cv, fold);
    testIdx = test(cv, fold);

    XTrainFold = XVal(trainIdx, :);
    YTrainFold = YVal(trainIdx);
    XTestFold = XVal(testIdx, :);

    % Predictions from base models on validation fold
    metaFeatures(testIdx, 1) = RFModelGasYield.predictFcn(XTestFold);
    metaFeatures(testIdx, 2) = ANNModelGasYield.predictFcn(XTestFold);
    metaFeatures(testIdx, 3) = GBRModelGasYield.predictFcn(XTestFold);
    metaFeatures(testIdx, 4) = SVMModelGasYield.predictFcn(XTestFold);
end

% Train the meta-learner (Linear Regression)
SuperLearnerModelGasYield = fitlm(metaFeatures, metaTarget);
disp('SuperLearner trained successfully!');

% Save the SuperLearner model
SuperLearner.metaModel = SuperLearnerModelGasYield;
SuperLearner.baseModels = {'RFModelGasYield', 'ANNModelGasYield', 'GBRModelGasYield',
'SVMModelGasYield'};
SuperLearner.predictors = predictorNames;

save('SuperLearnerModelGasYield.mat', 'SuperLearnerModelGasYield');
disp('SuperLearnerModel saved successfully!');

% Step 3: Evaluate the SuperLearner
% Load Test Data
testData = readtable('TestDataGasYield.xlsx'); % Ensure this file exists with predictors and
response
XTest = testData(:, predictorNames); % Extract predictors
YTest = testData.GasYield; % Extract response variable

% Generate meta-features for the test data
metaFeaturesTest = zeros(height(XTest), 4);
metaFeaturesTest(:, 1) = RFModelGasYield.predictFcn(XTest);
metaFeaturesTest(:, 2) = ANNModelGasYield.predictFcn(XTest);
metaFeaturesTest(:, 3) = GBRModelGasYield.predictFcn(XTest);
```

```

metaFeaturesTest(:, 4) = SVMModelGasYield.predictFcn(XTest);

% Predict using the SuperLearner
YValPred = predict(SuperLearnerModelGasYield, metaFeatures); % Meta-model predictions for
validation set
YTestPred = predict(SuperLearnerModelGasYield, metaFeaturesTest); % Meta-model predictions for
test set

% Calculate Validation Performance Metrics
valMSE = mean((YValPred - YVal).^2);
valMAE = mean(abs(YValPred - YVal));
valRMSE = sqrt(valMSE);
valR2 = 1 - sum((YVal - YValPred).^2) / sum((YVal - mean(YVal)).^2);

disp(['Validation MSE: ', num2str(valMSE)]);
disp(['Validation MAE: ', num2str(valMAE)]);
disp(['Validation RMSE: ', num2str(valRMSE)]);
disp(['Validation R^2: ', num2str(valR2)]);

% Calculate Test Performance Metrics
testMSE = mean((YTestPred - YTest).^2);
testMAE = mean(abs(YTestPred - YTest));
testRMSE = sqrt(testMSE);
testR2 = 1 - sum((YTest - YTestPred).^2) / sum((YTest - mean(YTest)).^2);

disp(['Test MSE: ', num2str(testMSE)]);
disp(['Test MAE: ', num2str(testMAE)]);
disp(['Test RMSE: ', num2str(testRMSE)]);
disp(['Test R^2: ', num2str(testR2)]);

% Plot Validation Predictions
figure;
scatter(YVal, YValPred, 'filled');
hold on;
plot([min(YVal), max(YVal)], [min(YVal), max(YVal)], 'r--');
xlabel('True GasYield (Validation)');
ylabel('Predicted GasYield (Validation)');
title('SuperLearner Predictions vs True Values (Validation)');
grid on;

% Plot Test Predictions
figure;
scatter(YTest, YTestPred, 'filled');
hold on;
plot([min(YTest), max(YTest)], [min(YTest), max(YTest)], 'r--');
xlabel('True GasYield (Test)');
ylabel('Predicted GasYield (Test)');
title('SuperLearner Predictions vs True Values (Test)');
grid on;

```

SUPERLEARNER CODE FOR CHAR YIELD

```

% Retrain SuperLearner for CharYield
disp('Retraining SuperLearner for CharYield...');

% Load necessary models and data
load('TrainDataCharYield.mat', 'TrainDataCharYield'); % Training data
load('ValDataCharYield.mat', 'ValDataCharYield'); % Validation data
load('TestDataCharYield.mat', 'TestDataCharYield'); % Test data
load('BaseModelsCharYield',
'ANNModelCharYield', 'GBRModelCharYield', 'RFModelCharYield', 'SVMModelCharYield'); % Best models

% Extract predictors and response
predictorNames = RFModelCharYield.RequiredVariables; % Update to your model's predictor
requirements
XTrain = TrainDataCharYield(:, predictorNames);
YTrain = TrainDataCharYield.CharYield;

XVal = ValDataCharYield(:, predictorNames); % Align validation predictors
YVal = ValDataCharYield.CharYield;

XTest = TestDataCharYield(:, predictorNames); % Align test predictors
YTest = TestDataCharYield.CharYield;

% Generate meta-features for training
disp('Generating meta-features...');
metaFeaturesTrain = zeros(height(XTrain), 3); % Adjust columns for the number of base models
metaFeaturesTrain(:, 1) = RFModelCharYield.predictFcn(XTrain);
metaFeaturesTrain(:, 2) = GBRModelCharYield.predictFcn(XTrain);
metaFeaturesTrain(:, 3) = SVMModelCharYield.predictFcn(XTrain);

% Generate meta-features for validation
metaFeaturesVal = zeros(height(XVal), 3); % Adjust columns for the number of base models
metaFeaturesVal(:, 1) = RFModelCharYield.predictFcn(XVal);
metaFeaturesVal(:, 2) = GBRModelCharYield.predictFcn(XVal);
metaFeaturesVal(:, 3) = SVMModelCharYield.predictFcn(XVal);

% Generate meta-features for Test
metaFeaturesTest = zeros(height(XTest), 3); % Adjust columns for the number of base models
metaFeaturesTest(:, 1) = RFModelCharYield.predictFcn(XTest);
metaFeaturesTest(:, 2) = GBRModelCharYield.predictFcn(XTest);
metaFeaturesTest(:, 3) = SVMModelCharYield.predictFcn(XTest);

% Train the SuperLearner
disp('Training SuperLearner...');

% Train a feedforward neural network as the SuperLearner
net = feedforwardnet(10);
net = train(net, metaFeaturesTrain', YTrain');
FinalSuperLearnerModelCharYield = net; % Store the trained network

% Save the trained network
save('FinalSuperLearnerModelCharYield.mat', 'FinalSuperLearnerModelCharYield');
disp('SuperLearner trained and saved successfully!');

% Test the SuperLearner on validation data
disp('Testing SuperLearner on validation data...');

metaPredictions = FinalSuperLearnerModelCharYield(metaFeaturesVal'); % Predict using the neural
network

% Evaluate performance
mse = mean((metaPredictions' - YVal).^2); % Transpose predictions to match YVal dimensions
mae = mean(abs(metaPredictions' - YVal));
r2 = 1 - sum((YVal - metaPredictions').^2) / sum((YVal - mean(YVal)).^2);

% Display metrics
fprintf('Validation Results: MSE = %.4f, MAE = %.4f, R^2 = %.4f\n', mse, mae, r2);

```

APPENDIX H: Machine Learning Evaluation Results

S/N	Model Type	Model Validation				Model Test			
		RMSE	MSE	R ²	MAE	MAE	MSE	RMSE	R ²
CCE									
1	RF	0.0327	0.0011	0.9783	0.0183	0.0165	0.0009	0.0301	0.9833
2	GBR	0.0313	0.0010	0.9802	0.0189	0.0180	0.0010	0.0315	0.9816
3	ANN	0.0433	0.0019	0.9620	0.0271	0.0223	0.0014	0.0373	0.9742
4	SVR	0.0617	0.0038	0.9228	0.0416	0.0432	0.0037	0.0605	0.9325
5	SLE	0.0198	0.0004	0.9927	0.0129	0.0176	0.0009	0.0307	0.9826
Char Yield									
1	SVR	0.0655	0.0043	0.9292	0.0452	0.0480	0.0062	0.0788	0.9017
2	RF	0.0342	0.0012	0.9807	0.0187	0.0202	0.0032	0.0567	0.9490
3	GBR	0.0392	0.0015	0.9746	0.0243	0.0243	0.0035	0.0588	0.9452
4	ANN	0.0301	0.0009	0.9850	0.0172	0.0215	0.0033	0.0571	0.9483
5	SLE	0.0176	0.0003	0.9951	0.0138	0.0193	0.0030	0.0544	0.9531
CO									
1	SVR	0.0362	0.0013	0.9754	0.0237	0.0277	0.0016	0.0405	0.9666
2	RF	0.0207	0.0004	0.9920	0.0133	0.0122	0.0004	0.0196	0.9922
3	GBR	0.0279	0.0008	0.9854	0.0174	0.0183	0.0008	0.0285	0.9834
4	ANN	0.0150	0.0002	0.9958	0.0100	0.0101	0.0002	0.0141	0.9960
5	SLE	0.0097	0.0001	0.9983	0.0074	0.0093	0.0002	0.0129	0.9966
Gas Yield									
1	SVR	0.0301	0.0009	0.9759	0.0204	0.0189	0.0008	0.0280	0.9815
2	RF	0.0386	0.0015	0.9603	0.0269	0.0299	0.0021	0.0454	0.9512
3	GBR	0.0269	0.0007	0.9807	0.0178	0.0164	0.0009	0.0293	0.9796
4	ANN	0.0206	0.0004	0.9887	0.0140	0.0154	0.0006	0.0238	0.9866
5	SLE	0.0145	0.0002	0.9938	0.0111	0.0133	0.0005	0.0221	0.9884
H2									
1	SVR	0.0508	0.0026	0.9037	0.0317	0.0324	0.0030	0.0545	0.8943
2	RF	0.0274	0.0008	0.9719	0.0170	0.0170	0.0008	0.0290	0.9701
3	GBR	0.0341	0.0012	0.9567	0.0231	0.0262	0.0016	0.0405	0.9416
4	ANN	0.0335	0.0011	0.9581	0.0191	0.0245	0.0022	0.0473	0.9204
5	SLE	0.0233	0.0005	0.9774	0.0119	0.0174	0.0010	0.0318	0.9640
LHV									
1	SVR	0.0480	0.0023	0.9051	0.0337	0.0338	0.0021	0.0453	0.9178
2	RF	0.0266	0.0007	0.9708	0.0142	0.0136	0.0007	0.0270	0.9707
3	GBR	0.0380	0.0014	0.9406	0.0238	0.0240	0.0018	0.0426	0.9274
4	ANN	0.0245	0.0006	0.9754	0.0155	0.0123	0.0004	0.0200	0.9840
5	SLE	0.0136	0.0002	0.9906	0.0086	0.0116	0.0005	0.0218	0.9810

APPENDIX I: Publication List and Expected Manuscript Titles

S/N	Title	Authors	Journals/ Publisher	Status/ link
1.	Exploring Insights in Biomass and Waste Gasification via Ensemble Machine Learning Models and Interpretability Techniques	Ocident Bongomin, Charles Nzila, Josphat Igadwa Mwasiagi, Obadiah Maube	International Journal of Energy Research, Wiley	Online: June 2024, Link
2.	Comprehensive thermal properties, kinetic, and thermodynamic analyses of biomass wastes pyrolysis via TGA and Coats-Redfern methodologies	Ocident Bongomin, Charles Nzila, Josphat Igadwa Mwasiagi, Obadiah Maube	Energy Conversion and Management: X, Elsevier	Online: Volume 24, October 2024, 100723. Link
3.	Machine Learning for Predictive Modeling of Co-Gasification: A Step towards Industry 4.0 in Biomass Waste Valorization	Author: Ocident Bongomin, Charles Nzila, Josphat Igadwa Mwasiagi, Obadiah Maube Editors: Marcel Odhiambo Ohanga, Puramanathan Naidoo	Book chapter: Measurement, Automation and Control in the Age of Artificial Intelligence (AI) and Machine Learning (ML)	Online: 16 November 2025, Link
4.	Synergistic and Antagonistic Interactions in the Co-Pyrolysis of Macadamia Nutshells and Coffee Husks: Thermogravimetric, Kinetic, and Thermodynamic Insights	Ocident Bongomin, Sherien Elagroudy, Josphat Igadwa Mwasiagi, Charles Nzila	Bioresource Technology Reports	Online: 7 July 2025 Volume 31, ID: 102207 Link
5.	Thermo-kinetic assessment of biomass wastes degradation behaviour using thermogravimetric and isoconversional methods	EXPECTED PUBLICATION TITLES		
6.	Modeling and Optimization of Biomass Co-Gasification Using Aspen Plus: Insights into Temperature Profiles and Syngas Yield at Varying Equivalence Ratios			
7.	Machine Learning for Predicting Syngas Composition and Char Yield in Biomass Co-Gasification: A Comparative Study of ANN, SVM, RF, GBR, and SuperLearner Ensemble			
8.	Evaluating Robustness and Generalization of SuperLearner Ensemble Models in Biomass Gasification Prediction Tasks			
9.	Interpreting Machine Learning Models for Biomass Gasification: Feature Importance and Interaction Insights from Gini, Permutation, and Partial Dependence Methods			
10.	Integrating Process Simulation and Machine Learning for Enhanced Prediction and Optimization of Biomass Co-Gasification Systems			

APPENIX J: Plagiarism Test Certificate



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PLAGIARISM AWARENESS CERTIFICATE

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In recognition for passing the University's plagiarism

Awareness test for Thesis entitled: **PROCESS SIMULATION AND MACHINE LEARNING MODELING OF BIOMASS WASTES CO-GASIFICATION FOR SYNGAS AND BIOCHAR PRODUCTION** with similarity index of 5% and striving to maintain academic integrity.

Word count:50327

Awarded by

Prof. Anne Syomwene Kisilu

CERM-ESA Project Leader Date: 07/04//2025