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Comparative Assessment of Aspen Plus Modeling Strategies for Biomass Steam Co-gasification

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ABSTRACT

The urgent need for sustainable energy drives the exploration of biomass and plastic waste co-gasification, a promising route for producing clean fuels and chemicals, reducing greenhouse gas emissions, and minimizing fossil fuel dependence. Modeling and simulation are vital for optimizing this process, particularly syngas yield, yet comparative studies on Aspen Plus modeling techniques for steam co-gasification are limited. This research addresses this gap by comparing three Aspen Plus strategies: thermodynamic equilibrium modeling (TEM), restricted thermodynamic modeling (RTM), and kinetic modeling (KM), for simulating the co-gasification of pine sawdust and polyethene (PE) with steam in bubbling fluidized bed gasifier (BFBG). The primary objective is to evaluate the effectiveness of each strategy in predicting the syngas composition under varying conditions. Three models were developed in Aspen Plus on the basis of each strategy, and their predicted syngas compositions were compared with published experimental data. A detailed sensitivity analysis was performed within the RTM framework to obtain optimized values of the approach temperatures to enhance predictive accuracy. The results showed that RTM provided the highest precision, with an average root mean square error (RMSE) of 0.0296, while TEM showed the lowest precision with RMSE of 0.1234. KM performed moderately with an RMSE of 0.0929. These findings demonstrate that RTM is superior for predicting the syngas composition for this co-gasification process, and its optimized solution presents a viable alternative when detailed kinetic data are lacking, thus reducing computational expense.

Keywords: Aspen Plus, Syngas prediction, Equilibrium modeling, Kinetic modeling

INTRODUCTION

The escalating global climate crisis, coupled with concerns regarding energy security and dependence on finite fossil fuel resources, has spurred a critical need for the development and implementation of sustainable energy alternatives [1]. In this context, steam co-gasification of biomass and plastic waste in BFBGs emerges as a promising technology, offering a dual benefit of renewable energy generation and waste valorization. This thermochemical conversion process effectively transforms these feedstocks into syngas, a valuable intermediate product for producing clean fuels, sustainable aviation fuels, and various chemicals such as methanol, ethanol, and dimethyl ether. By utilizing renewable biomass sources and mitigating the environmental impact of plastic waste, steam co-gasification holds the potential to significantly reduce greenhouse gas emissions and lessen reliance on fossil-based energy systems [2]. Therefore, the precise analysis and optimization of this process are vital for its widespread adoption and contribution to a sustainable energy future.

In this regard, some researchers have explored high-temperature steam gasification to enhance H_2 production. For instance, Chang et al. (2011) reported that steam gasification of agricultural waste in a fluidized bed reactor at 1000 °C and an equivalence ratio of 0.2 yielded a maximum bioH_2 of 29.5%, CO at 23.6%, and CO_2 at just 10.9% [3]. Ahmed et al. (2009) compared pyrolysis and steam gasification of paper, varying temperatures from 400 to 700 °C for pyrolysis and 600 to 1000 °C for gasification [4]. Numerous experimental studies have been

published in literature show that steam gasification has the ability to produce the medium heating value of up to 16 MJ/Nm^3 and H_2 concentration in syngas up to 60% [5-7].

However, accurate modeling and simulation of thermochemical processes are indispensable tools for gaining a fundamental understanding of their behavior and for optimizing gasification performance. Specifically, for gasification, modeling is crucial in predicting syngas yield, composition, and process efficiency under varying operating conditions. Syngas, as the primary product of gasification, serves as a versatile building block for numerous energy and chemical applications, making a reliable prediction of its composition very important. This requires the development and comparative analysis of different modeling strategies, each with its unique capabilities and limitations.

Although various modeling techniques have been proposed in the literature for gasification processes, there remains a noticeable gap in comprehensive comparative assessments, particularly concerning different Aspen Plus modeling approaches for steam co-gasification of biomass and plastic waste. This gap highlights the need for further investigation to identify the most effective and accurate modeling strategies for this specific process. Recognizing the limitations mentioned above in the existing literature, this study focuses on a comparative evaluation of three distinct Aspen Plus modeling strategies: thermodynamic equilibrium modeling (TEM), restricted thermodynamic modeling (RTM), and kinetic modeling (KM) for simulating steam co-gasification of pine sawdust and polyethene in a bubbling fluidized bed reactor.

METHODOLOGY

In this article experimental study was adopted from Pinto et al. (2002) for the pine and polyethylene (PE) co-gasification in BFBG by steam [5]. The reactor configuration is given in the article along with the ultimate and approximate analysis of the feedstocks. Modeling was carried out in 100% Pine, 10% PE and 90% pine mix, 40% PE and 60% pine, and 60% PE and 40% pine at varying temperature, while the steam-to-biomass ratio remains at 0.8kg/kg-feedstock. This study employed Aspen Plus V.14.0 to model the steam co-gasification process and predict syngas composition under various operating conditions, and both equilibrium and kinetic modeling strategies were implemented. In Aspen Plus platform all models began with the definition of biomass, PE, ash, and char as non-conventional components, using proximate and ultimate analyses from the ULTANAL and PROXANAL models, respectively. The built-in property database of Aspen Plus was utilized for the calculations, with the HCOALGEN and DCOALIGT models providing enthalpy and density data, respectively, based on biomass combustion and composition. Heat of combustion was derived from biomass combustion using the HCOALGEN model and elemental analysis, while density was determined using the DCOALIGT model, which is based on the IGT correlation and utilizes ultimate analysis data. The Peng-Robinson thermodynamic package with the Boston-Mathias function was chosen for its suitability in high-temperature gasification simulations.

Equilibrium Modeling

Thermodynamic Equilibrium Model (TEM) and Restricted Thermodynamic Model (RTM). TEM, a non-stoichiometric approach, determines the equilibrium composition by minimizing Gibbs free energy, requiring only the elemental composition derived from ultimate analysis. This makes it computationally efficient and useful for preliminary assessments. However, TEM does not incorporate reaction kinetics or stoichiometric constraints, leading to discrepancies in syngas predictions, particularly in underestimating syngas composition.

RTM, a stoichiometric approach, improves upon TEM by incorporating temperature-dependent constraints on chemical equilibria. Real-world gasification processes often do not reach complete equilibrium due to kinetic limitations, and RTM accounts for this by restricting selected reactions to better match experimental conditions. By restricting reaction equilibria to temperatures above or below the actual reactor temperature, accounting for stoichiometric constraints. This approach is designed to provide a more realistic representation of the gasification process, since the reactions in the reactor may not necessarily reach the true thermodynamic equilibrium. By incorporating temperature-based constraints, it improves the accuracy of syngas composition predictions and other performance metrics. A similar approach was previously applied to air gasification by Jadoon et al., (2025) this study implemented strategy for the steam gasification to improve the precision for optimizing operating conditions and improving the overall efficiency of predicting the syngas composition [6].

In this study the Aspen Plus model developed by Acar et al., (2019) for gasification, was adopted, using both TEM and RTM [7]. Biomass and plastic waste were first decomposed in the RYIELD reactor (DECOMP) into constituent elements based on its ultimate and proximate analyses. Ash was then separated from the other components using a separator (SEP1). The elemental components were mixed with steam and then fed to an RGIBBS reactor. The gasifier (EQIL) simulates the TEM approach, while another reactor (R-GASI) models RTM. Syngas is then separated from other byproducts in separators (SEP2 for R-GASI and SEP3 for EQIL) as shown in Figure 1.

Following Acar et al. (2019), four key reactions

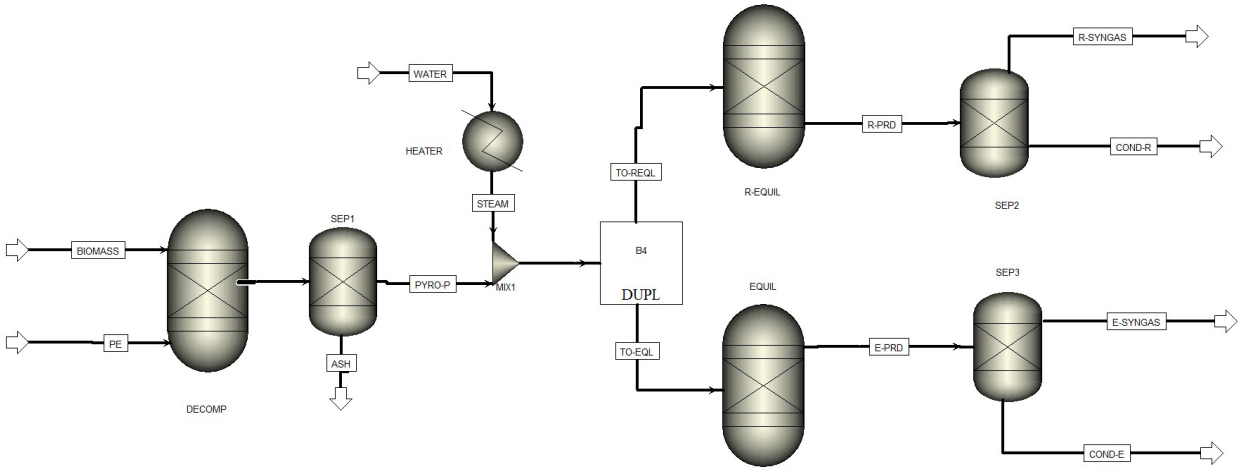

Figure 1: Process flowsheet of Equilibrium model

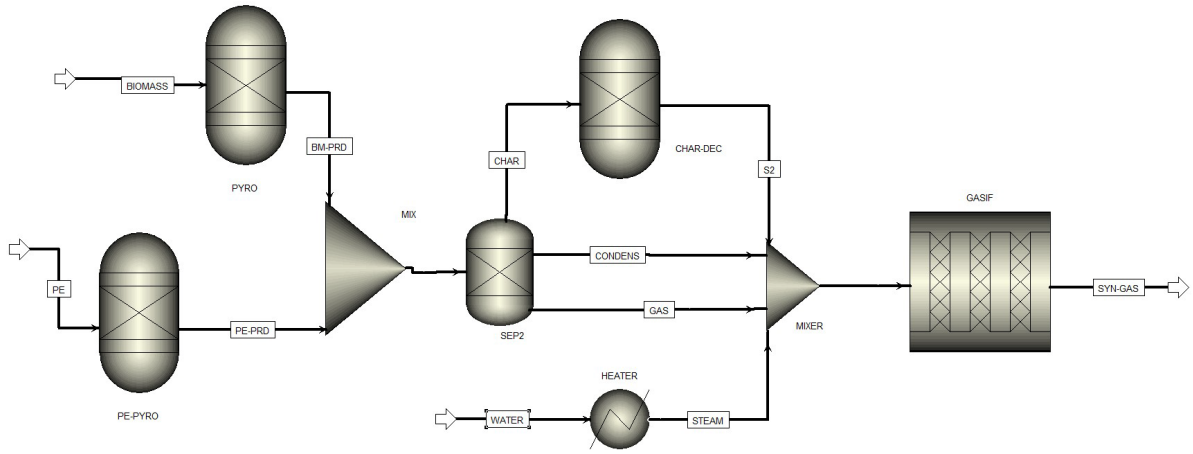

Figure 2: Process flowsheet of kinetic model

(listed in Table 1) were selected to constrain the chemical equilibrium within the RTM framework. A sensitivity analysis was performed for each of the 17 experimental instances by varying the approach temperature of individual reactions. Each sensitivity analysis consisted of 22,500 cases, and the case with the smallest absolute difference between experimental and predicted values was selected. The absolute difference between the molar fractions of the predicted and experimental syngas composition was calculated using Equation 1, where ME represents the minimum error, *e* is the experimental value, *p* is the predicted value, and *i* denotes the *i*-th case in the sensitivity analysis.

$$(ME)_i = |H_2^e - H_2^p|_i + |CO^e - CO^p|_i + |CO_2^e - CO_2^p|_i + |CH_4^e - CH_4^p|_i \quad (1)$$

Table 1: Reactions used in RTM

No.	Reaction	ΔHr (kJ/mol)
R1	C + H_2O → CO + H_2	131
R2	C + 0.5O_2 → CO	-111
R3	CO + H_2O → CO_2 + H_2	-41.2
R4	CH_4 + H_2O → CO + 3H_2	206

Kinetic Modeling

A KM was developed within the Aspen Plus environment to simulate the co-gasification feedstocks, explicitly representing the complex thermochemical reactions occurring within BFBG. The model's flowsheet, depicted in Figure 2, utilizes several interconnected unit operation blocks. Initial decomposition of biomass in the RYIELD reactor (PYRO) was modeled using empirical equations from Neves et al. (2011) [8]. In contrast, plastic waste decomposition (PE-PYRO) was based on its ultimate and proximate analyses, reflecting the primary and secondary depolymerization processes that occur at high temperatures. The resulting pyrolysis products were then separated by a separator (SEP2) into gaseous, condensable, and char fractions. The char fraction was further decomposed into elemental carbon, sulfur (if present), and ash

within another RYIELD reactor (CHAR-DEC). These decomposition products were then combined with the gasifying medium in a mixer (MIX2) before entering the gasification reactor. A plug flow reactor was opted for modeling the final gasification process to convert the pyrolysis products and gasifying medium into syngas. Kinetic models use rate equations to quantify the rates of various chemical reactions that occur during gasification. The reactions and kinetic data used in the gasification step are given in **Table 2** and **Table 3** [9].

Table 2: Chemical reactions and rate expressions

Reaction	Rate expression
$C + 0.5O_2 \rightarrow CO$	$r_1 = k_1 \cdot \exp\left(\frac{E}{RT}\right)[O_2]^{0.78}$
$H_2 + 0.5O_2 \rightarrow H_2O$	$r_2 = k_2 \cdot \exp\left(\frac{-E}{RT}\right)[H_2][O_2]$
$CO + 0.5O_2 \rightarrow CO_2$	$r_3 = k_3 \exp\left(\frac{-E}{RT}\right)[CO][O_2]^{0.5}[H_2O]^{0.}$
$C + H_2O \rightarrow CO + H_2$	$r_4 = k_4 \cdot \exp\left(\frac{-E}{RT}\right)[C][H_2O]$
$C + CO_2 \rightarrow 2CO$	$r_5 = k_5 \cdot \exp\left(\frac{-E}{RT}\right)[CO_2]$
$CH_4 + H_2O \rightarrow CO + 3H_2$	$r_6 = k_6 \cdot \exp\left(\frac{-E}{RT}\right)[CH_4][H_2O]$
$CO + H_2O \rightarrow CO_2 + H_2$	$r_7 = k_7 \cdot \exp\left(\frac{E}{RT}\right)[CO][H_2O]$
$C + 2H_2 \rightarrow CH_4$	$r_8 = k_8 \cdot \exp\left(\frac{-E}{RT}\right)[H_2]$
$C_{10}H_8 \rightarrow 7.38C + 0.275C_6H_6 + 0.94CH_4 + 1.235H_2$	$r_9 = k_9.\exp\left(\frac{-E}{RT}\right)[C_6H_6O]^{1.6}[H_2]^{-0.5}$
$C_6H_6 + 2H_2O \rightarrow 1.5C + 2.5CH_4 + 2CO$	$r_{10} = k_{10}.\exp\left(\frac{-E}{RT}\right)[C_6H_6]^{1.3}[H_2O]^{0.2}[$
$C_6H_6O + 3H_2O \rightarrow 4CO + 0.5C_2H_4 + CH_4 + 3H_2$	$r_{11} = k_{11}.\exp\left(\frac{-E}{RT}\right)[C_6H_6O]$

Table 3: Kinetic parameters

Reactions	k	E (J/mol)
r_1	$5.70 \cdot 10^{11}$	$5.50 \cdot 10^{4}$
r_2	$2.20 \cdot 10^{9}$	$1.08996 \cdot 10^{6}$
r_3	$1.00 \cdot 10^{10}$	$1.2599 \cdot 10^{5}$
r_4	200	$4.9887 \cdot 10^{4}$
r_5	4.364	$2.48123 \cdot 10^{5}$
r_6	$3.00 \cdot 10^{3}$	$1.2471 \cdot 10^{5}$
r_7	$2.20 \cdot 10^{-2}$	$3.473 \cdot 10^{4}$
r_8	$2.43 \cdot 10^{-4}$	$1.30 \cdot 10^{4}$
r_9	$1.70 \cdot 10^{14}$	$3.50 \cdot 10^{5}$
r_{10}	$2.00 \cdot 10^{16}$	$4.43 \cdot 10^{5}$
r_{11}	$1.00 \cdot 10^{7}$	$1.00 \cdot 10^{5}$

The syngas molar fraction predicted by each model is evaluated using RMSE, which measures the square root of the average squared differences between predicted and observed values. RMSE can be computed by equation 2.

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

RESULTS AND DISCUSSION

Aspen Plus models utilizing TEM, RTM, and KM were developed to simulate steam co-gasification in a BFBG. For RTM, a detailed sensitivity analysis was conducted to align the syngas composition as closely as possible with experimental values. This analysis, performed using Aspen Plus's built-in sensitivity tool by changing the temperature for each reaction given in Table 1. The temperature limit for the reactions R3 and R4 are zero to 1000 °C and -1 to -500 °C, respectively. A total of 22,500 sensitivity instances were computed for each sensitivity analysis, and this analysis was performed for all seventeen experimental cases. The absolute error was calculated for every instance, and then minimum absolute error was determined using equation 1. The syngas composition corresponding to this minimum error was selected as the final syngas composition in RTM framework.

Table 4: RMSE of different Aspen Plus models

	RTM	KM	TEM
H_2	0.0363	0.1705	0.2101
CO	0.0533	0.0953	0.1184
CO_2	0.0208	0.0374	0.0365
CH_4	0.0079	0.0682	0.1285
Average	0.0296	0.0929	0.1234

RMSE values for different modeling strategies—RTM, TEM, and KM—are presented in **Table 4**. These results highlight notable differences in the predictive performance of the models for co-gasification. RTM demonstrated the most favorable performance overall, achieving the lowest RMSE values across all outputs compared to the other models. The average RMSE for RTM is 0.0296, significantly outperforming TEM and KM, who's average RMSE values were 0.1234 and 0.0929, respectively.

Unlike the TEM model the RTM model accounts for kinetic constraints that influence reaction rates. This is particularly relevant in non-equilibrium conditions where factors such as heat and mass transfer limitations affect the reaction progress. Additionally, while the KM model includes kinetic mechanisms, its predictive capability is restricted by predefined reaction pathways and rate expressions that may not fully represent the complexities of co-gasification, especially for varying feedstock compositions. The RTM framework, by contrast, fine-tunes

reaction temperatures through sensitivity analysis, ensuring improved alignment with experimental data.

When examining individual syngas components, RTM consistently exhibited the lowest RMSE values. For CO, RTM achieved the lowest RMSE of 0.0533, followed by KM at 0.0953, while TEM performed poorly with RMSE values of 0.1184. A similar trend was observed for CO_2, where RTM had an RMSE of 0.0208, followed by KM at 0.0374 and TEM at 0.0365. For CH_4, RTM again excelled with the lowest RMSE of 0.0079 while KM and TEM have 0.0682 and 0.1285, respectively.

The predictions obtained from different models were analyzed and plotted to evaluate their performance. **Figure 3** illustrates the comparison between experimental and predicted H_2 values across various feedstock compositions. Among the models, the RTM demonstrates exceptional predictive accuracy, with blue data points closely aligning with the experimental values for all percentages of polyethylene (PE). The minimal error observed in RTM predictions underscores its reliability and effectiveness. In contrast, the KM model performs well for feedstocks containing 100% pine and mixtures with 80% pine + 20% PE, but its accuracy significantly deteriorates for feedstocks with 40% or 60% PE, where it tends to overpredict H_2 values. This decline in performance suggests that the KM model is less suitable for feedstocks with higher PE content. The TEM model, on the other hand, consistently overpredicts H_2 values across all feedstock compositions, likely due to limitations in Gibbs free energy estimations for syngas constituents, as highlighted by Ajorloo et al. (2022) [10].

Figure 4 illustrates the prediction of CO in Aspen Plus model's environment in comparison to the experimental values. The RTM model again demonstrates strong predictive accuracy, with blue data points aligning closely with experimental values across all percentages of PE, reaffirming its robustness in predicting CO concentrations. The KM model provides reasonable predictions for feedstocks with low PE content, such as 100% pine and 20% PE. However, as the PE content in the feedstock exceeds 40%, the KM model begins to underpredict CO concentrations, indicating its limited applicability for feedstocks with higher PE proportions. In contrast, the TEM model shows improved accuracy in predicting CO for feedstocks with 40% or more PE, suggesting that its performance improves with increasing PE content. As the PE content is increasing, 40% and above, in feedstock the TEM prediction tends to accurately predict it.

For CO_2 predictions, depicted in **Figure 5**, the RTM model once again delivers the most accurate results. However, predictions by the TEM and KM models exhibit similar trends and complement each other, as evidenced by their comparable RMSE values in **Table 4**. This alignment suggests that both models can provide reasonable CO_2 predictions under certain conditions, though they remain less accurate than the RTM model.

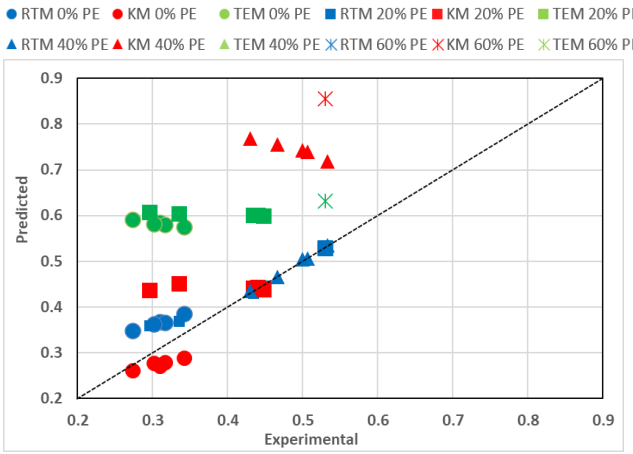

Figure 3: Experimental and Predicted mole fraction of H_2

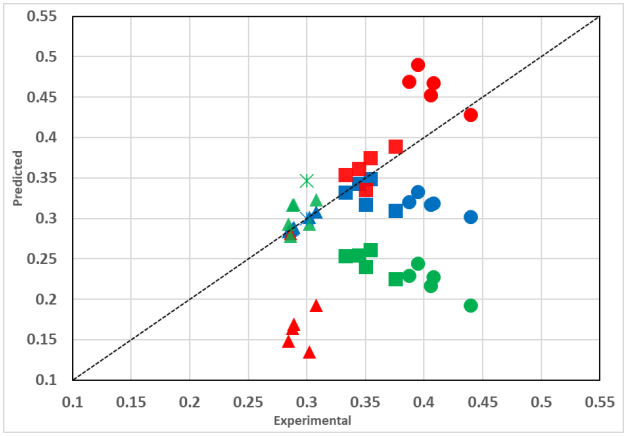

Figure 4: Experimental and predicted mole fraction of CO

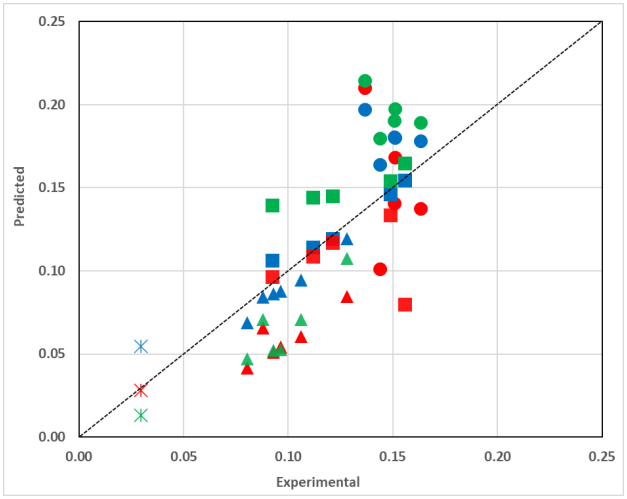

Figure 5: Experimental and Predicted mole fraction of CO_2

From the **Figure 6** CH_4 predictions further emphasize the superior performance of the RTM model, which consistently provides accurate results. In contrast, the

TEM model struggles significantly, often underpredicting CH_4 concentrations. The KM model performs adequately for feedstocks with low PE content, but its accuracy declines sharply as the PE proportion increases, resulting in poor predictions for higher PE feedstocks.

In this study the RTM model demonstrated exceptional predictive capabilities for molar concentration of H_2, CO, CO_2, and CH_4 across all feedstock compositions, making it the most reliable model overall. While the KM and TEM models exhibit some strengths in specific scenarios, their accuracy diminishes as the PE content in the feedstock increases, highlighting the importance of model selection based on feedstock composition.

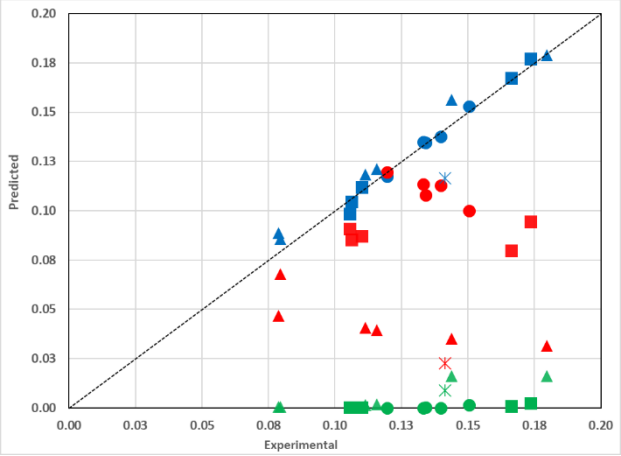

Figure 6: Experimental and Predicted mole fraction of CH_4

CONCLUSIONS

Pine and plastic steam co-gasification offers a promising route for renewable energy production; however, accurately predicting syngas composition remains a significant challenge. This study provides a comprehensive comparative analysis of three modeling approaches—TEM, RTM, and KM—in a BFBG. Among these models, RTM demonstrated the highest accuracy in predicting syngas composition, with an average RMSE of 0.0296. In contrast, the TEM model showed the lowest performance consistently overestimated or underestimated syngas composition, with an RMSE of 0.1234, while the KM model exhibited intermediate performance with an RMSE of 0.0929. The KM model's performance notably declined as the proportion of PE in the feedstock increased, further limiting its reliability for feedstocks with higher plastic content. In comparison, RTM proved to be the most robust and accurate, making it a strong candidate for future research on syngas composition across different technologies and fuel mixtures, including agricultural, forestry, and municipal solid wastes with steam or steam-O_2 gasification.

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