CHEMICAL ENGINEERING TRANSACTIONS
VOL. 120, 2025
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it
Guest Editors: Bing Shen How, Viknesh Andiappan, Denny K.S. Ng, Hon Loong Lam, Petar S. Varbanov

ISBN 979-12-81206-21-2; **ISSN** 2283-9216
DOI: 10.3303/CET25120048

Sustainable Valorization of Paper Industry Waste (Paper Dust) via Downdraft Air Gasification: A Comprehensive Aspen Plus® Process Model for Syngas Production

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The paper and paperboard industry generates substantial quantities of paper dust, an underutilized byproduct typically disposed of through incineration or landfilling, leading to environmental and economic inefficiencies. This study developed and validated a detailed Aspen Plus kinetic model to simulate the downdraft gasification of densified paper dust briquettes, aiming to valorize this waste stream for energy generation. The model incorporated both heterogeneous and homogeneous reaction kinetics across pyrolysis, combustion, and reduction zones and was validated using experimental data at equivalence ratios of 0.35, 0.37, and 0.39. The model accurately predicted syngas composition and syngas flow rates, achieving normalized root mean square error values below 16 % across all equivalence ratios conditions. Deviations for CO, CO_2, and N_2 were within 10 %, while H_2 and CH_4 showed higher deviations due to their sensitivity to reduction zone kinetics and thermodynamic equilibrium assumptions, consistent with prior literature. These results confirm the model's reliability for predicting gasification performance under realistic operational conditions. The validated framework provides a practical tool for process evaluation, optimization, and future integration with co-gasification strategies involving other waste streams. It also supports techno-economic and life cycle assessments to inform sustainable waste-to-energy applications. Overall, this research advances biomass valorization, promotes circular economy practices within the paper industry, and contributes to achieving Sustainable Development Goals (SDGs 7, 9, 12, and 13) by enabling low-carbon, resource-efficient energy solutions.

1. Introduction

The global paper and paperboard industry has maintained an annual production of over 400 × 10^6 t since 2010 (Del Rio et al., 2022), driven by the rising demand for sustainable packaging, growth in fast-moving consumer goods (FMCG), and the shift from plastic to paper-based alternatives. While countries such as China, the United States, and Japan lead global production, the industry's energy demands and emissions remain a concern. Depending on the grade and technology, energy consumption ranges from 7.3 to 35.2 GJ per t of paper (Moya and Pavel, 2018), with associated carbon emissions between 516 and 2,646 kg CO_2-equivalent per t of paper (Sun et al., 2018). In addition to its primary products, the pulp and paper industry generates several waste streams, including paper sludge, mill effluents, wastewater residues, pulper rejects, trimming scraps, and paper dust. Among these, paper dust remains one of the least utilized byproducts despite being consistently generated and comprising approximately 1–10 % of the total paper-based products by mass, depending on the production process and paper grade (Halba et al., 2025). It is typically generated during cutting and finishing operations and is often disposed of by landfills or incineration, although these methods are not always economically or environmentally viable.

Nonetheless, paper dust has considerable potential as a bioenergy resource, with a lower heating value (LHV) typically ranging between 12 and 16 MJ/kg (Tihin et al., 2023), depending on its composition and moisture content. Its chemical and physical characteristics make it a suitable feedstock for thermochemical conversion, particularly for gasification. Through gasification, paper dust can be directly converted into valuable products, such as syngas and biochar (Kumar and Arora, 2021). Compared to other thermochemical routes, such as

Paper Received: 15 May 2025; Revised: 7 September 2025; Accepted: 14 September 2025
Please cite this article as: Kumar S., Halba A., Arora P., 2025, Sustainable Valorization of Paper Industry Waste (Paper Dust) via Downdraft Air Gasification: A Comprehensive Aspen Plus® Process Model for Syngas Production, Chemical Engineering Transactions, 120, 283-288 DOI:10.3303/CET25120048

combustion or pyrolysis, gasification offers higher material and energy recovery efficiencies and a relatively lower environmental footprint, making it a favorable option for sustainable waste valorization (Halba et al., 2022a). Despite its potential, existing research seldom considers paper dust as the primary feedstock in gasification experiments or simulation models. It is often treated as a component of mixed municipal solid waste (MSW), leading to limited insight into its standalone thermochemical behavior. Although experimental studies are essential for evaluating the gasification characteristics of paper dust, they are often constrained by high costs, scalability challenges, and limited flexibility in exploring a wide range of process parameters (Halba et al., 2022b). Process simulation is a powerful tool for extending experimental findings and enabling broader system-level evaluations (Catalanotti et al., 2022). When integrated with experimental data for calibration and validation, simulation models can be effectively used for sensitivity analysis, design optimization, and scale-up planning (Vaccari et al., 2024). This combined approach is crucial for bridging current knowledge gaps and enhancing the predictive understanding of paper dust gasification under varied operational conditions.

Therefore, the present study builds upon prior experimental investigations conducted in our laboratory, wherein the gasification performance of briquette paper dust was systematically evaluated. A detailed kinetic model was developed in Aspen Plus, employing a plug flow reactor (RPlug) configuration to simulate both heterogeneous and homogeneous reaction kinetics. The model was validated against experimental results to ensure predictive accuracy across a range of operating conditions, specifically for equivalence ratio (ER) variations between 0.35 and 0.39. This ER range was selected based on the experimental data reported by Halba et al. (2025) for paper dust briquettes, which demonstrated stable gasification conditions, minimized tar formation, and maximum syngas yield. Moreover, this range falls within the typical ER window of 0.2–0.4 for effective biomass gasification (Susastriawan et al., 2017), consistent with operational ranges commonly adopted for such systems. This integrated experimental simulation framework provides valuable insights into syngas composition, reaction kinetics, and syngas flow rates. The outcomes of this study aim to advance sustainable waste-to-energy practices and offer meaningful contributions to both the scientific community and broader socioeconomic discourse.

2. Materials and methods

The experimental data used in this study were drawn from the work of Halba et al. (2025), conducted in our laboratory, where paper dust briquettes were gasified in a downdraft air gasifier under realistic operating conditions. An overview of the experimental data sources and simulation approaches used in this study is provided in Table 1. This study reported the detailed syngas composition, temperature profiles, and system performance parameters that were used for model development, calibration, and validation within Aspen Plus. The overall research methodology includes systematic steps, from literature review to model simulation, validation, and output analysis.

Table 1: Summary of experimental data sources and simulation methodology used in this study

Component	Approach	Description
Syngas composition data	Experimental (Halba et al., 2025)	Gasification experiments on paper dust briquettes in a downdraft gasifier at ER 0.35–0.39, providing detailed syngas composition and syngas flow rate data
Model development	Simulation	Aspen Plus kinetic modeling incorporating pyrolysis (RStoic), char decomposition (RYield), and combustion and reduction (RPlug) reactor blocks to simulate the downdraft gasification process.
Model validation	Simulation	Comparison of model-predicted syngas composition and syngas flow rate with experimental data at each ER condition

2.1 Model framework and development

The gasification process of paper dust was modeled using Aspen Plus to simulate the conversion of densified paper dust briquettes in a downdraft gasifier. Since paper dust was not available in the Aspen component database, it was defined as a non-conventional solid component using its proximate and ultimate analysis. Biochar and ash were similarly modeled as non-conventional solids. The RK-SOAVE property method was used for conventional gaseous species due to its robustness in predicting the thermodynamic behavior of non-polar and mildly polar gases at high temperatures typical of biomass gasification processes, as recommended by Catalanotti et al. (2022). For non-conventional solids such as paper dust, biochar, and ash, biomass components were input as non-conventional solids with their proximate and ultimate analyses, and the HCOALGEN and DCOALIGT models were used to estimate enthalpy and density, respectively, as also adopted

by HajiHashemi et al. (2023). This approach ensures accurate thermophysical property estimation and reliable simulation results. The thermodynamic models and assumptions used in the simulations are summarized in Table 2.

Table 2: Property methods and model assumptions

Component Type	Property Method	Enthalpy Model	Density Model	Notes
Conventional components	RK-SOAV	Built-in	Built-in	Includes H_2, CO, CO_2, CH_4, etc.
Non-conventional biomass	MIXCINC stream	HCOALGEN	DCOALIGT	Includes paper dust, biochar, and ash
Tar species	RK-SOAV	-	-	C_6H_6, C_6H_6O, $C_{10}H_8$

The moisture content in the feedstock was below 10 %; hence, a separate drying unit was excluded from the simulation. The gasification process was simulated through a sequence of thermochemical conversions representing the primary zones of a downdraft gasifier: pyrolysis, oxidation (combustion), and reduction (Arora et al., 2017). These zones were modeled using a combination of stoichiometric, yield-based, and kinetic reactor blocks, as described below and illustrated in Figure 1.

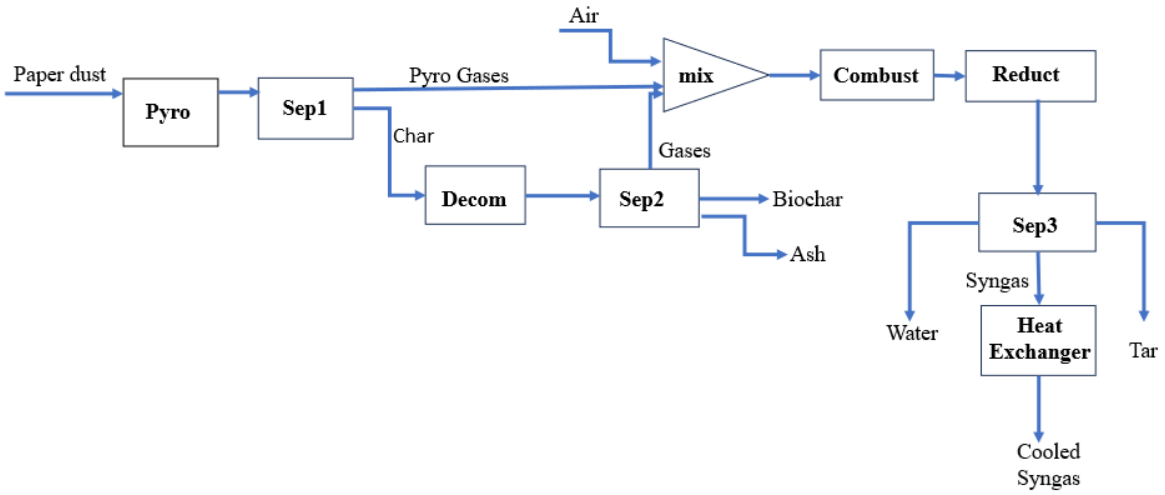

Figure 1: Aspen Plus flowsheet of the developed paper dust gasification model

The pyrolysis step was modeled using an RStoic reactor (Pyro), where paper dust undergoes thermal decomposition in the absence of oxygen. This produced volatile gases and solid residue (biochar). The output from this reactor was separated into a flash block (Sep1), which produced pyrogas and char. The char was further processed in an RYield reactor (Decomp), where it was decomposed into elemental gases, fixed carbon, and ash using its ultimate analysis data. This simulated the decomposition and gas release, typically observed during char conversion. The pyrolysis gas, along with gases from the char decomposition unit, was mixed with a controlled stream of air in a mixer (mix). Air input was calculated using a Fortran-based calculator to maintain the equivalence ratio between 0.35 and 0.39, which corresponds to typical downdraft air gasification conditions derived from experimental results. The resulting gas mixture entered the combustion zone, which was modeled using an RPlug reactor (Combust) operating under isothermal conditions. This zone simulated the partial oxidation of volatiles and tar, releasing the heat required to sustain downstream endothermic reactions. Tar is represented by three lumped species: benzene (C_6H_6), phenol (C_6H_6O), and naphthalene ($C_{10}H_8$), selected based on literature data as reported by Dhrioua et al. (2022) for biomass air gasification. Their study found that these dominant tar species are significantly influenced by gasification conditions, particularly oxidation temperatures between 800 and 1,000 °C. Selecting these three enables the model to capture tar behavior realistically while maintaining computational simplicity. After combustion, the gases flow into the reduction zone, modeled using another RPlug reactor (Reduct) operating adiabatically. This zone represents key endothermic reactions, including char gasification with CO_2 and H_2O, methane reforming, and the water-gas shift reaction (Arora et al., 2015). Different reactor blocks were selected based on the dominant reaction mechanisms and data availability for each zone of the downdraft gasifier. The pyrolysis zone was modeled using an RStoic reactor

block because pyrolysis involves thermal decomposition with yields derived from experimental proximate analysis and literature, allowing stoichiometric specification without detailed kinetic expressions (Vaccari et al., 2024). The char decomposition was modeled using an RYield reactor block to convert non-conventional char into conventional elemental components based on its ultimate analysis data, which is necessary as Aspen Plus does not support direct kinetic reactions for non-conventional solids (Puig-Gamero et al., 2021). The combustion and reduction zones were modeled using RPlug reactor blocks because these involve kinetically controlled reactions where temperature and concentration gradients along the reactor length significantly affect reaction rates. RPlug accurately simulates these plug flow behaviors with reaction kinetics, enabling realistic modeling of partial oxidation, char gasification, and reforming reactions typical in downdraft gasifiers (HajiHashemi et al., 2023). The kinetic parameters, including rate constants, activation energies, temperature dependencies, and concentration exponents used in this study, were adopted from Puig-Gamero et al. (2021) and are summarized in Table 3.

Table 3: Kinetic reactions used in the present study

Reactions	Rate expression (mol/m^3·s)
$1.25C + O_2 \rightarrow 0.5CO + 0.75CO_2$	$r = 3.7 \cdot 10^{10} \cdot T \cdot e^{\left(\frac{-150,000}{RT}\right)} \cdot [O_2]$
$CO + 0.5O_2 \rightarrow CO_2$	$r = 1.78 \cdot 10^{10} \cdot e^{\left(\frac{-180,000}{RT}\right)} [CO][O_2]^{0.25}[H_2O]^{0.5}$
$C_6H_6O + 4O_2 \rightarrow 6CO + 3H_2O$	$r = 655 \cdot e^{\left(\frac{-80,200}{RT}\right)} [O_2][C_6H_6O]^{0.5}$
$C_6H_6 + 4.5O_2 \rightarrow 6CO + 3H_2O$	$r = 2.4 \cdot 10^{11} \cdot e^{\left(\frac{-126,000}{RT}\right)} [O_2][C_6H_6]^{0.5}$
$C + H_2O \leftrightarrow CO + H_2$	$r = 0.008 \cdot e^{\left(\frac{-49,900}{RT}\right)} [C][H_2O]$
$CO + H_2O \leftrightarrow CO_2 + H_2$	$r = 278 \cdot e^{\left(\frac{-12,600}{RT}\right)} [CO][H_2O]$
$CH_4 + H_2O \leftrightarrow CO + 3H_2$	$r = 4.92 \cdot 10^{-11} \cdot e^{\left(\frac{-125,000}{RT}\right)} [H_2O][CH_4]^{0.5}$
$C + CO_2 \leftrightarrow 2CO$	$r = 1.05 \cdot 10^{13} \cdot e^{\left(\frac{-135,000}{RT}\right)} [C]$
$C_6H_6O \rightarrow CO + 0.1CH_4 + 0.75H_2 + 0.4C_{10}H_8 + 0.15C_6H_6$	$r = 10^7 \cdot e^{\left(\frac{-100,000}{RT}\right)} [C_6H_6O]$
$C_6H_6O + 3H_2O \rightarrow 4CO + CH_4 + 3H_2 + 0.5C_2H_4$	$r = 10^7 \cdot e^{\left(\frac{-100,000}{RT}\right)} [C_6H_6O]$
$C_{10}H_8 \rightarrow 6.5C + 0.5C_6H_6 + 0.5CH_4 + 1.5H_2$	$r = 1.7 \cdot 10^7 \cdot e^{\left(\frac{-350,000}{RT}\right)} [C_{10}H_8]^{1.6}[H_2]^{0.5}$

2.2 Model validation

The developed Aspen Plus model was validated by replicating the experimental conditions and comparing the simulated syngas composition and syngas flow rate with their corresponding experimental values at ER of 0.35, 0.37, and 0.39. To quantitatively assess the consistency and reliability of the model predictions, validation metrics included normalized root mean square error (nRMSE) and absolute percentage error, as defined in Eq(1) and Eq(2), respectively. Since the analysis includes syngas components expressed in volume fractions (v/v) and syngas flow rate in Nm^3/h, nRMSE was used to normalize errors across differing scales and units, enabling a balanced evaluation. Accordingly, the total number of evaluated parameters per equivalence ratio was m = 6, corresponding to five syngas components and one syngas flow rate. However, due to only one experimental value per syngas component and syngas flow rate at each ER, the coefficient of determination (R^2) could not be calculated individually. Therefore, absolute percentage errors were computed for each syngas component and syngas flow rate to provide an objective and detailed quantitative assessment.

$$nRMSE = \sqrt{\frac{1}{m}\sum_{k=1}^{m}\left(\frac{Z_k - \hat{Z}_k}{Z_k}\right)^2} \quad (1)$$

$$Absolute\ error\ (\%) = \left|\frac{Z_k - \hat{Z}_k}{Z_k}\right| \times 100 \quad (2)$$

where Z_k is the experimental value, $\hat{Z}_k$ is the corresponding model-predicted value, $\bar{Z}_k$ is the mean of all experimental values, and m is the total number of data points.

3. Results and discussion

This section presents the validation results of the developed Aspen Plus model for downdraft gasification of paper dust briquettes. Model predictions of syngas composition and syngas flow rates were compared with

experimental data across ER of 0.35, 0.37, and 0.39. A detailed summary of the results for all ER conditions, including the component-wise comparison between experimental and simulated values, is provided in Table 4. At ER = 0.35, the model predicted CO, CO_2, and N_2 concentrations with absolute errors below 7 %, suggesting good representation of oxidation and gasification reactions in the combustion and reduction zones. CH_4 showed a moderate deviation of 12.91 %, while H_2 was underpredicted by 33.01 %. Such discrepancies for H_2 have also been reported in previous gasification kinetic models due to its sensitivity to reduction zone kinetics, temperature distribution, and water-gas shift equilibrium assumptions (Puig-Gamero et al., 2021). The syngas flow rate prediction was within ~ 6 % of the experimental data. The overall nRMSE at this ER was 15.23 %, which is within the acceptable range (< 20 %) typically reported for gasification kinetic models (Vaccari et al., 2024). At ER = 0.37, the model's predictive accuracy improved. CO and CH_4 deviations were limited to 3.26 % and 8.68 %, respectively. CO_2 and N_2 errors were 10.22 % and 8.96 %, while H_2 deviation reduced slightly to 27.00 %. The syngas flow rate prediction had an error of 6.84 %. The nRMSE at this ER was 13.20 %, indicating reliable overall model performance. Similar improvements in predictive accuracy at intermediate ER levels have been reported in the literature, where optimal oxidation-reduction balance enhances syngas yield prediction (Dhrioua et al., 2022). At ER = 0.39, the model achieved its lowest nRMSE of 12.20 %, demonstrating consistent predictive capability. CO, CH_4, and N_2 predictions showed errors below 8 %, while CO_2 and H_2 deviations were 17.33 % and 14.94 %, respectively. The syngas flow rate prediction deviated by 6.21 % from experimental observations. This improved performance at higher ER may be attributed to enhanced reaction completeness and better char conversion, consistent with trends reported by HajiHashemi et al. (2023). Overall, the model showed good predictive capability across all ER conditions, with nRMSE values remaining below 16 %. These results demonstrate its suitability for simulating syngas composition and syngas flow rate in downdraft gasification of paper dust briquettes and establish a reliable framework for performance evaluation and future optimization studies.

Table 4: Comparison of experimental and model syngas composition (volume/volume), flow rate, and errors at different ER

ER	Component	Experimental value	Model value	Absolute error (%)
0.35	CO (v/v)	0.1535	0.1430	6.83
	CO_2 (v/v)	0.1347	0.1369	1.64
	H_2 (v/v)	0.1147	0.0768	33.01
	CH_4 (v/v)	0.0405	0.0457	12.91
	N_2 (v/v)	0.5566	0.5974	7.33
	Syngas flow rate (Nm^3/h)	15.73	14.84	5.99
	nRMSE (%)	15.23		
0.37	CO (v/v)	0.1502	0.1453	3.26
	CO_2 (v/v)	0.1398	0.1255	10.22
	H_2 (v/v)	0.1006	0.0734	27.00
	CH_4 (v/v)	0.0484	0.0442	8.68
	N_2 (v/v)	0.5610	0.6112	8.96
	Syngas flow rate (Nm^3/h)	18.87	17.58	6.84
	nRMSE (%)	13.20		
0.39	CO (v/v)	0.1487	0.1529	2.82
	CO_2 (v/v)	0.1478	0.1222	17.33
	H_2 (v/v)	0.0864	0.0735	14.94
	CH_4 (v/v)	0.0532	0.0446	16.17
	N_2 (v/v)	0.5639	0.6084	7.87
	Syngas flow rate (Nm^3/h)	22.00	20.63	6.21
	nRMSE (%)	12.20		

4. Conclusions

This study developed and validated a detailed Aspen Plus kinetic model for the downdraft gasification of paper dust briquettes, using experimental data at ER of 0.35, 0.37, and 0.39. The model accurately predicted syngas composition and syngas flow rates, with normalized root mean square error (nRMSE) values below 16 % across all ER conditions, demonstrating good overall predictive capability. Predictions for CO, CO_2, and N_2 showed deviations within 10 %, whereas H_2 and CH_4 exhibited higher deviations, consistent with trends reported in biomass gasification modeling due to their sensitivity to reduction zone kinetics and thermodynamic equilibrium assumptions. The validated model provides a reliable framework for evaluating paper dust gasification

performance under varying operational conditions. It can further support process optimization, integration with co-gasification strategies involving other waste streams, and coupling with techno-economic and environmental assessments to advance sustainable waste-to-energy solutions and promote circular economy practices in the paper industry. Future work should explore integration with co-gasification pathways, energy-emission trade-off analyses, and comprehensive economic and environmental assessments for informed decision-making.

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