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Simulation and Experimental Validation of Biomass Gasification in a Spouted Bed Reactor: Troubleshooting Using DWSIM

C. Moliner*, V. Carozzo, M. Curti, E. Arato

Dipartimento di Ingegneria Civile, Chimica e Ambientale (DICCA), Università degli Studi di Genova, Via Opera Pia 15, 16145 Genova (Italy)
* Corresponding Author: cristina.moliner@unige.it

ABSTRACT

Simulation plays a crucial role in the design and optimization of gasifiers by providing a detailed understanding of the involved physical processes and complex chemical reactions without the need for extensive trial-and-error experiments. It can also serve as a valuable tool for identifying potential technical issues in experimental devices that operate below expected performance. This study presents a comprehensive simulation of biomass gasification using the open-source software DWSIM. The simulated results were compared with experimental data from a pilot-scale spouted bed reactor, featuring a square-based design with a 20 kWth capacity, using pruning of apple tress as feedstock. Experimental results revealed that the reactor operated effectively at temperatures exceeding 850°C, maintaining stable conditions across a wide range of equivalence ratios. However, the distribution of products—particularly hydrogen (H_2)—did not match expected results based on both literature and simulations. A joint analysis of experimental data and expected behavior from simulation helped identify the observed inefficiencies and optimize the reactor's performance.

Keywords: Biomass, Syngas, Energy Efficiency, Gasification, Spouted Bed

INTRODUCTION

Simulation-based activities play a crucial role in assessing reactor performance by providing a deeper understanding of underlying processes without the need for costly and time-consuming experiments. Process simulation tools offer a structured approach to modeling chemical reactors, enabling engineers and researchers to analyze, optimize, and predict reactor behavior under various operating conditions, including gasifiers. Among the available simulation platforms, commercial software such as Aspen Plus has long been a standard in chemical engineering, particularly for thermochemical reactions [1], due to its extensive database and robust computational capabilities. However, its reliance on proprietary licenses and limited customization options presents challenges, especially for academic research and collaborative projects.

An alternative to commercial software is the use of open-source process simulators, such as COCO [2], which has been used to simulate the gasification of agricultural residues. Another example is DWSIM, developed by Daniel Medeiros [3], which provides a comprehensive suite of tools for modeling a wide range of chemical engineering processes, including reactors. DWSIM features a freely accessible database with over 1,500 compounds and more than 20 property methods [4].

In this study, a previously developed and validated DWSIM model [4] is used to simulate the gasification of pruning of apple tree in a spouted bed reactor. With an annual availability of 2.23 Mt in Italy [5], along with its renewable nature and favorable properties—such as low to moderate moisture content and high cellulose and lignin levels—apple tree prunings are an ideal feedstock for thermochemical conversion processes.

A 20 kWth spouted bed reactor (SBR) was used for the gasification reactions. An SBR differs from traditional fluidized bed reactors by replacing the perforated base

with a single central gas inlet. This design creates three distinct zones within the reactor: a central spout where the fluidizing agent flows, an annular region surrounding the spout, and a fountain-like region above the bed surface where solids circulate [6]. Due to this configuration, a systematic cyclic circulation of solids is established, enhancing mass and heat transfer rates [7]. SBRs have been successfully applied to the gasification of coal, biomass, and biomass-plastic mixtures [8].

In this study, a previously validated model was used to critically evaluate the experimental results from the spouted bed pilot plant. Specifically, discrepancies in the experimental H_2 content were observed, and comparison with the model outputs helped identify the source of the experimental error.

MATERIALS AND METHODS

Biomass properties

Pruning of apple trees (PAT) were gasified in a spouted bed reactor [9]. Table 1 summarises their proximate and ultimate analysis and its initial higher heating value (HHV). The moisture content was equal to 8.13 %wt.

Table 1: Proximate and ultimate analysis of biomass (% w/w on dry basis, besides for moisture) and HHV (MJ/kg)

Proximate Analysis		**Ultimate Analysis***	
Ash	2.87	C	48.88
Fixed carbon	19.95	H	5.71
Volatile matter	77.18	O	42.15
HHV	18.73	Ash	2.87

* 0.39%wt of N and S

Spouted bed reactor and testing conditions

The experimental unit is a pilot plant located in Biella, Italy, designed to operate with a biomass feed rate of 200 g/min, providing a thermal output of 20 kWth. The main components of the plant include a blower, a spouted bed reactor, a biomass feeding system, a gas preheater, and equipment for cleaning the gaseous product stream (filter, scrubber, and cyclone). To enhance mass and energy transfer within the reactor, an inert solid bed is used. This bed consists of 2 kg of silica sand, corresponding to an initial height of 17 cm.

Figure 1. Spouted bed reactor

PAT were evaluated under different equivalence ratios (ER). The ER represents the ratio of the actual oxygen supplied to the system to the oxygen needed for full stoichiometric combustion. The air inflow was maintained constant (17 Nm^3/h) and the biomass feed was varied to match the ER (Table 2).

Table 2: Experimental conditions

ER	**Biomass feed (g/min)**	**Temperature of the bed (°C)**
0.42	150	880
0.65	99	911

Details on the reactor design, operating procedure, and reaction steps—including preheating, stabilization, and product analysis—are available elsewhere [9].

Simulation set-up using DWSIM

DWSIM (V8.6.5) was used to simulate the gasification of PAT. A detailed description of the model and its validation using literature data can be found in [4]. In summary, steady-state simulations were performed under isothermal conditions using the Peng-Robinson property method at atmospheric pressure, with no pressure drops considered. The modeled gaseous components included H_2, H_2O, CO, CO_2, CH_4, and N_2, while char was represented by its main constituents (C(s), O, N, and H) based on experimental data [9].

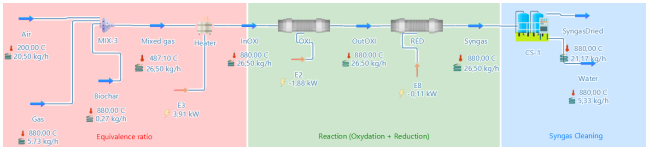


Figure 2. DWSIM flowsheet of the gasification plant.

Table 3: Kinetic reactions

	Rate (mol/m³·s)	k (sec⁻¹)	Ea (KJ/mol)
$1.25C(s) + O_2 \rightarrow 0.5CO + 0.75CO_2$	$r = k \cdot T \cdot e^{(-Ea/RT)} \cdot [O_2]$	$3.7 \cdot 10^{10}$	150
$CH_4 + 0.5O_2 \rightarrow CO + 2H_2$	$r = k \cdot e^{(-Ea/RT)} \cdot [O_2]^{0.8}[CH_4]^{0.7}$	$1.58 \cdot 10^{12}$	202
$CO + 0.5O_2 \rightarrow CO_2$	$r = k \cdot e^{(-Ea/RT)} \cdot [O_2]^{0.25}[CO][H_2O]^{0.5}$	$1.78 \cdot 10^{10}$	180
$H_2 + 0.5O_2 \rightarrow H_2O$	$r = k \cdot e^{(-Ea/RT)} \cdot [O_2]\ [H_2]$	$1.08 \cdot 10^{7}$	108
$C + H_2O \leftrightarrow CO + H_2$	$r = k \cdot T \cdot e^{(-Ea/RT)} \cdot [H_2O]\ [C]$	0.008	499
$CO + H_2O \leftrightarrow CO_2 + H_2$	$r = k \cdot e^{(-Ea/RT)} \cdot [CO]\ [H_2O]$	278	126
$CH_4 + H_2O \leftrightarrow CO + 3H_2$	$r = k \cdot e^{(-Ea/RT)} \cdot [H_2O]\ [CH_4]$	$4.92 \cdot 10^{-11}$	125
$C + CO_2 \leftrightarrow 2CO$	$r = k \cdot e^{(-Ea/RT)} \cdot [C]$	$1.05 \cdot 10^{13}$	135
$CO_2 + H_2 \leftrightarrow CO + H_2O$	$r = k \cdot e^{(-Ea/RT)} \cdot [CO_2]\ [H_2]^{0.5}$	258	126

The flowsheet is shown in Figure 2. The volatilization stage was modeled using an Excel file (embedded in the program) to calculate the mass balances (Gas and Biochar inlet streams), as described by Pio et al. [10]. The mass balance calculations (yields of pyrolysis products and composition of biochar) were specified, the temperature of decomposition was imported from the input data and the resulting compositions were exported to the corresponding input streams. Successively, the two inlet streams were mixed with the quantity of air (Air) ensuring autothermal conditions, as experimentally specified. Two Plug Flow Reactors (PFRs), with the geometries of the experimental device [9], were used to carry out the oxidation and reduction reactions. Both reactors were considered as isothermal at 880°C and their dimensions were set as 0.3 m of height for the oxidation reactor (corresponding to the bed of particles), 2 m for the reduction reactor (corresponding to the freeboard section) and 0.25 m of internal diameter in both cases. Kinetic reactions (Table 3) and parameters (Table 4) were set according to [11-13] to provide a more accurate representation of the reactor performance for reliable process predictions [14]. Lastly, the cleaning section, corresponding to the removal of moisture and tar before entering the analysing system, was simulated through a compound separator to obtain the final dry syngas stream.

RESULTS AND DISCUSSION

Table 4 presents the experimental and simulated results of the gasification of PAT under the described operational conditions. The balance term in the analyzer accounts for all products not measured, ensuring the total sums to 100%. In the simulations, this balance term corresponds to the N_2 concentration.

Table 4: Experimental and simulated results (%vol/vol) at ER=0.42 and ER=0.62

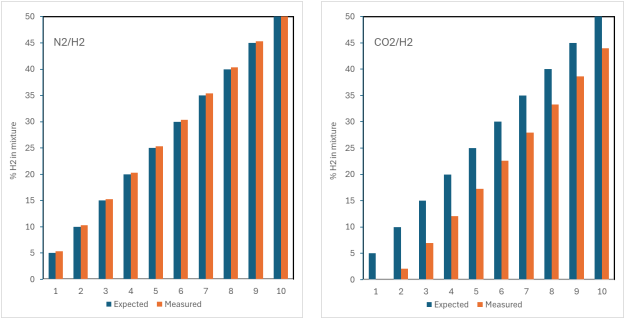
ER = 0.42	**CO**	**CO_2**	**H_2**	**CH_4**
Experimental	10.2	19.9	4.7	2.8
DWSIM	12.9	17.5	10	4.7
ER = 0.65	**CO**	**CO_2**	**H_2**	**CH_4**
Experimental	5.9	20.3	3.0	1.0
DWSIM	11.3	18.1	7.2	3.5

As expected, the CO and CO_2 concentrations were estimated with high accuracy, while CH_4, and especially H_2, were overestimated in the simulations. A consistent trend was observed when comparing the equivalence ratio (ER), with CO increasing and CO_2 decreasing as the ER decreased. Additionally, methane and hydrogen concentrations increased as ERs decreased, a trend that was effectively captured by the model. Energy balances were also examined in detail. The measured temperature at the bed of particles was used as the reaction temperature in isothermal conditions to ensure a fixed reaction temperature, as indicated by the experimental setup. According to the simulations, the exothermic contribution was insufficient to sustain the reduction reactions, and it was estimated that around 5 kW would need to be added to the system to achieve autothermal conditions. However, the experimental device performed well, and the gasification reactions occurred in a stable isothermal regime.

An evaluation was conducted to identify the potential experimental reasons for the large discrepancies observed in H_2 content and reaction temperature. Possible causes include:

- Unaccounted Heat Losses: Heat losses may reduce reaction efficiency, impacting syngas composition and temperature of reaction.
- Temperature Variations: If the actual operating temperature differs from the model's assumption, it can shift equilibrium reactions (such as the water-gas shift reaction, $CO + H_2O \rightleftharpoons CO_2 + H_2$), which can affect H_2 content.
- Unaccounted Side Reactions: Tar formation was not considered due to the lack of experimental data, though its contribution is likely to be significant under real operating conditions.
- Incomplete Mixing or Mass Transfer Limitations: mass transfer limitations, or localized temperature variations are not accounted for in the model.
- Calibration Issues: Gas chromatographs or other analytical instruments may not be properly calibrated, leading to inaccurate measurements.

To ensure consistency between input data, operating conditions, and gas composition measurements, the calibration of the gas analyzer (MCA100 Syn-P, ETG) was first checked. Two gas mixtures—CO_2/H_2 and N_2/H_2—with known compositions were used to test the instrument calibration. The calibration curve for N_2 (Figure 3a) showed perfect alignment between measured and applied compositions. However, the CO_2/H_2 calibration curve (Figure 3b) revealed underestimations of about 7%vol of H_2 (in average) between the measured and applied compositions, while the contribution from C-based compounds was accurately measured.



(a) (b)

Figure 3. Calibration of gas analyser

In summary, by simulating the experimental conditions and comparing the model's predictions with observed data, the study highlighted discrepancies that pointed to specific areas of concern, such as the H2 content in the product stream, led to the critical review of the experimental conditions, as measurement inaccuracies. Modeling is proven to be a powerful troubleshooting tool, enabling researchers to systematically isolate and address these issues, thereby improving the reliability and accuracy of the experimental results. This approach not only enhances the robustness of the current campaign but also provides a framework for optimizing future experimental designs.

CONCLUSIONS

This study demonstrated the effectiveness of using the open-source software DWSIM to simulate biomass gasification in a spouted bed reactor, providing valuable insights into the process and identifying potential sources of error in the experimental campaign. The simulation results were compared with experimental data from a pilot-scale reactor using pruning of apple tree as feedstock, revealing discrepancies in the hydrogen (H_2) content and other gas compositions. The model accurately predicted trends in CO and CO_2 concentrations but overestimated H_2 and CH_4 compositions. Key potential sources of error identified include unaccounted heat losses, temperature variations, side reactions such as tar formation, mass transfer limitations, and calibration issues with analytical instruments. By leveraging the model as a troubleshooting tool, the study successfully pinpointed these inefficiencies, enabling a critical review of experimental conditions and improving the reliability of the results. In successive steps, the other identified sources of error will be studied and analysed for their experimental assessment. This approach not only optimized the current gasification process but also established a robust framework for future experimental designs, emphasizing the importance of integrating simulation with experimental validation to enhance the accuracy and efficiency of biomass gasification systems.

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REFERENCES

1. Moliner, C., Bove, D., Bosio, B., Ribes, A., & Arato, E. Simulation activities for the pseudo-equilibrium modelling of the gasification of agricultural residues. 24th *European Biomass Conference and Exhibition Proceedings*, 934–940 (2016).
2. Moliner, C., Marchelli, F., Bosio, B., & Arato, E. Simulation of the gasification of agricultural residues using coco simulator. *26th European*

Biomass Conference and Exhibition Proceedings, 764–768 (2018).
3. Medeiros, D. *DWSIM simulator*. https://dwsim.org. Last access: 30/1/2025
4. Moliner, C., Carozzo, V., Arato, E. Modelling of biomass gasification: comparison between fre-licensed DWSIM and a commercial software. 32nd *European Biomass Conference and Exhibition Proceedings*, 764–768 (2025)
5. Cotana, F., Calavaglio, G., La valorizzazione energetica delle potature di olivo, Crbnet (2008)
6. K. B. Mathur, P. E. Gishler, J. Chem. Technol. Biot. 5, 624 (1955)
7. Moliner, C., Marchelli, F., Bosio, B., Arato, E. Modelling of Spouted and Spout-Fluid Beds: Key for Their Successful Scale Up. *Energies*, *10*(11), 1729 (2017)
8. Carozzo, V., Arato, E., Moliner, C. Review of Experimental Activities and Recent Developments of Spouted Bed Reactors at Different Operational Scales. *Energies*, *17*(5), 1046 (2024)
9. Bove, D., Moliner, C., Curti, M., Baratieri, M., Bosio, B., Rovero, G., Arato, E. Preliminary tests for the thermo-chemical conversion of biomass in a spouted bed pilot plant. *The Canadian Journal of Chemical Engineering*, *97*(1), 59–66 (2019)
10. Pio, D. T., Tarelho, L. A. C., Matos, M. A. A. Characteristics of the gas produced during biomass direct gasification in an autothermal pilot-scale bubbling fluidized bed reactor. *Energy*, *120*, 915–928 (2017)
11. Martínez González, A., Silva Lora, E. E., Escobar Palacio, J. C., Almazán del Olmo, O. A. Hydrogen production from oil sludge gasification/biomass mixtures and potential use in hydrotreatment processes. *International Journal of Hydrogen Energy*, *43*(16), 7808–7822 (2018)
12. Champion, W. M., Cooper, C. D., Mackie, K. R., Cairney, P. Development of a chemical kinetic model for a biosolids fluidized-bed gasifier and the effects of operating parameters on syngas quality. *Journal of the Air & Waste Management Association*, *64*(2), 160–174 (2014)
13. Puig-Gamero, M., Pio, D. T., Tarelho, L. A. C., Sánchez, P., Sanchez-Silva, L. Simulation of biomass gasification in bubbling fluidized bed reactor using aspen plus®. *Energy Conversion and Management*, *235*, 113981 (2021)
14. Marchelli, F., Moliner, C., Baratieri, M., Bosio, B., Arato, E. From equilibrium to kinetic modelling: The gasification of apple pruning residues in a spouted bed reactor. In Carvalho M.d.G., Scarlat N., Grassi A., & Helm P. (Eds.), 27th *European Biomass Conference and Exhibition Proceedings*, 813–820 (2019)