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Modelling of Hydrogen Generation from Woody Biomass in a Novel Modular Downdraft Gasifier–WGS–PSA System

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Abstract An advanced model was developed in Aspen Plus to simulate and optimize hydrogen-rich syngas production from a PP30-scale downdraft biomass gasifier integrated with Water-Gas-Shift (WGS) and pressure-swing adsorption (PSA). The adiabatic model combines equilibrium RGibbs blocks with corrective RStoic char–gas reactions and was validated against four independent experiments, predicting H_2 and CO within ± 1 % error. Sensitivity analysis identified an optimum "window" of T_pyrol at700 °C, T_gas at 900 °C, and equivalence ratio of 0.25, which double H_2 molar fraction to 40 wt % after a two-stage WGS system (S/C = 3, T_LT = 200 °C). Replacing air with pure O_2 as the gasifying agent effectively eliminates N_2 dilution, increasing H_2 concentration to 59 wt % raising the LHV from 4.5 to 6.7 MJ Nm^{-3}. A dual-column, four-step PSA (P_ads = 9.8 bar) delivers 98 % purity at 56 % recovery, while halving the purge stream improves recovery to 64 % with negligible purity loss. The combined interventions provide a realistic pathway for decentralized, biomass-derived clean hydrogen production, which competes with electrolysis on energy density and cleanup requirements. Future work will automate methane correction within Aspen and extend the flowsheet for full techno-economic assessment.

Keywords: Biomass gasification; Downdraft gasifier; Hydrogen production; Aspen Plus modelling; Water-Gas Shift

1. Introduction

The PP30 by All Power Labs is a commercial, prefabricated downdraft gasifier–power-generation unit (≈ 25–30 kWe and 60–75 kWth), designed to operate on dry woody chips and uses air as the oxidant. Although this study does not explicitly reference the PP30, the simulation results refer to a reactor of the same scale and architecture; they therefore offer a useful guide to the key operating conditions that must be maintained in the PP30 to produce clean syngas with a high hydrogen yield. The findings suggest that optimum performance is achieved when the pyrolysis zone is kept at about 700 °C and the reduction zone at 900 °C, with equivalence ratio (air/biomass) ER ≈ 0.25 and biomass moisture ≈ 12.5 %. Under optimal conditions, the gas exiting the gasifier is fed to a two-stage Water-Gas Shift (WGS) system;.When the second (low-temperature) reactor is set to 200 °C and the steam-to-carbon ratio is maintained at 3, the H_2 content almost doubles (from ≈ 26 % to ≈ 40 % wt) while CO falls below 0.2 %. The results confirm that the PP30 performs best when operated within a similar "window" of temperatures and air/steam ratios, offering a practical starting framework for tuning the reactor for electricity, heat, or even hydrogen-fuel production.

The study systematically examines how different operating conditions in the biomass gasifier and the WGS reactors affect the composition and lower heating value (LHV) of the product gas, with the ultimate goal of maximizing hydrogen production. In the gasification stage, a high pyrolysis temperature (T_pyrol ≈ 700 °C) enhance H_2 production, while a moderate gasification temperature (T_gas ≈ 900 °C) allows sufficient CO production for the next stage. At the same time, a low air excess (ER ≈ 0.25) and limited biomass moisture (≈ 12.5 %) keep the LHV high and avoid H_2 losses; excess moisture or air reduces both H_2 and LHV.

2. Description of the model

In this study, a comprehensive model was developed in Aspen Plus to simulate downdraft gasification of woody biomass. Adiabatic operation is assumed for the oxidation–reduction zones, tar is neglected, and char is treated as pure C, while all reactions between H_2, CO, CO_2, CH_4 and N_2 are assumed to reach thermodynamic equilibrium. Biomass is first decomposed using a RYield block, followed by an RGibbs rector to simulate pyrolysis. The resulting volatiles are then mixed with pre-heated air and enter an RGibbs block for the main gasification stage. Three corrective RStoic reactors—Boudouard (1500 °C), Water-Gas (1500 °C) and Methanation (400 °C)—receive split char streams (30 / 65 / 5 %) to fine-tune the final CO, H_2 and CH_4 ratios before the streams recombine. The model's reliability is tested against four independent experiments—carefully matching elemental analyses, temperature profiles and flow rates—giving a realistic range of reference conditions. In the WGS section, hydrogen yield is maximized when the second, low-temperature reactor operates near 200 °C and the steam-to-

carbon (S/C) ratio is maintained around 3, beyond which additional steam offers no practical benefit. Downstream of the gasifier, the model includes a Water-Gas-Shift Reactor and a PSA Unit for hydrogen purification. PSA system employs activated carbon in a dual-column configuration, following a four-step cycle of 70 s (adsorption) / 3 s (depressurisation) / 70 s (desorption) / 3 s (repressurisation).

3. Modelling Results

The comparison shows excellent prediction for H_2 and CO (error ≤ 1 %), but a systematic under-prediction of CH_4) and a corresponding over-prediction of N_2. By incorporating the empirical correlation of Mendiburu et al. (2014) to limit CH_4 formation, the absolute mean error (AME) was reduced, e.g. from 0.806 to 0.57, 1.77 to 1.03 and 1.39 to 0.82 in the three main datasets, bringing the methane accuracy close to experimental ranges. The next step proposed is to automate this correction via a MATLAB block in Aspen and to extend the flowsheet to include reforming and hydrogen separation for a techno-economic comparison with electrolysis.

The simulation of the Water-Gas -Shift reactor yields some very promising results. With the optimized parameters (T_pyrol 700 °C, T_gas 900 °C, ER 0.25, S/C 3, T_LT-WGS 200 °C), the final gas H_2 content doubles—from 26 % to 40 % wt—while CO is reduced to very low levels (around 0.2 %), resulting in a cleaner, hydrogen-rich fuel stream.

The most significant results of the present modelling are the two critical interventions for producing pure hydrogen from biomass gasification. First, replacing air (32.5 kg h^{-1}) with an equivalent mass of pure O_2 (7.475 kg h^{-1}) virtually eliminates N_2 in the product gas and boosts H_2 from 40 % to 59 % wt, while the LHV rises from 4.54 to 6.71 MJ Nm^{-3}—an improvement that greatly simplifies subsequent cleanup and compression. CO remains low (0.26 %), confirming that oxygen-blown operation yields a denser, more energy-rich syngas without needing more oxidant.

In the baseline setting (P_ads = 9.8 bar), the PSA system achieves a purity of 98.0 % and a recovery of 56 %. Reducing the purge stream by 50% increases the recovery to 64 % with minimal decrease in purity (97.7 %). However, tests with a double-bed material or changes in pressure and cycle times did not further improve the purity–recovery balance. For achieving purities above 99.9% H_2, an increase in process complexity, such as adding more steps or adsorption columns, is recommended. .

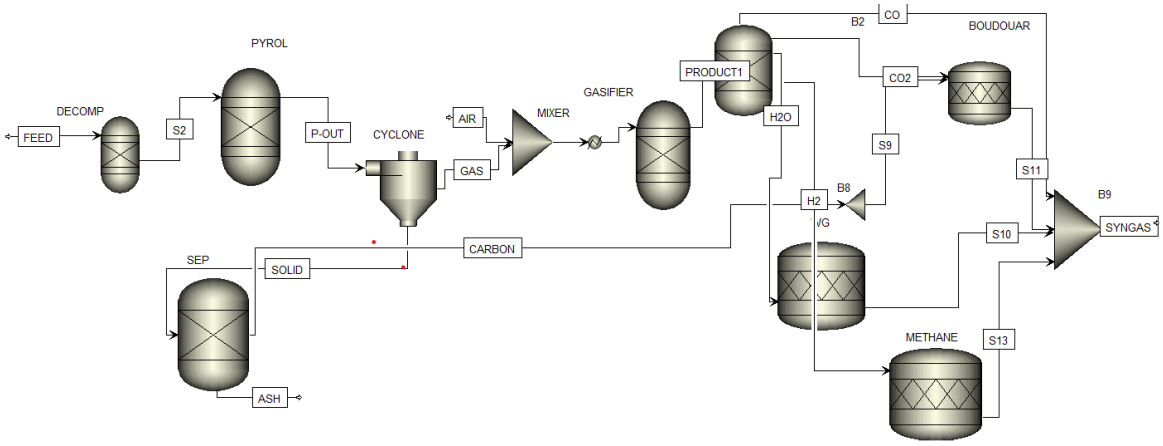

Figure 1. Advanced thermodynamic model with integrated char-gas reactions

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