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Research article

Techno-economic, energy, and exergy analyses of invasive weed gasification for hydrogen enriched producer gas production

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ABSTRACT

This research work deals with the examination of the techno-economic, exergy, and energy analyses of biomass gasification of the invasive weed *Parthenium hysterophorus* (PHP) using Steam - Carbon dioxide (CO_2) as a gasifying agent with the support of simulation modeling for sustainable energy conversion process. The aim of this work is to simulate the gasification process through consideration of the impacts of various operating factors on gasification. This study attains the gradual increase in hydrogen (H_2) concentration from 51% to 63% along with the rise in carbon monoxide (CO) from 14.5% to 19% using Aspen Plus simulation. CO_2 falls concurrently from 24% to 13.5%. The findings demonstrate significant advancements over earlier studies in terms of both gas composition and overall system performance. A computational model has been developed for the estimation of energy performance indicators such as total energy input, and energy consumed per mass of biomass gasified, which are used in the determination of the system's energy efficiency. The exergy analysis of the system is performed to assess the system's total losses in terms of efficiency gathered from the system's exergy ratios. The economic analysis evaluates the system's economies of scale by gas production at ₹.15/kg and long-term sustainability. The proposed system has been found with the potential to produce a high yield of alternative energy from PHP with increased economic efficiency and lower environmental impact.

1. Introduction

Modern life is highly reliant upon the fast depleting and scarce natural resource of non-renewable fossil fuels to meet its increasing energy needs [1]. There is a critical need for exploring alternative energy resources due to undesirable environmental changes, the limited and unequal distribution of rapidly diminishing natural fuels, and the imbalance in solid biomass resource trade for energy production [2,3]. The Intergovernmental Panel on Climate Change (IPCC) has proposed the use of bioenergy as a potential replacement for conventional fossil fuels [4,5]. The wild weed PHP was originally found in the riparian zones of tropical and subtropical regions, subsequently spreading globally to around 92 countries [6–8]. This species can grow up to a height of 2.5 m with a diameter of 8 mm –13 mm, it generally flowers about 35 days after germination, and a single plant is capable of producing 30,000 seeds over the course of its entire lifespan [6,7,9]. PHP infestation has a negative impact on the natural agroecosystem and detrimentally affects land productivity, crop yield and agricultural output [7,10,11]. Yields from pasture and crops decrease by as much as 80% due to the

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aggressive growth of PHP weeds [7]. The noxious weed can trigger allergic responses in individuals who come into contact with the plant or are exposed to the pollen, leading to ailments like contact dermatitis, hay fever, bronchitis, and influenza [11]. As the weed's invasion spread from less than 20 nations in the 1970s to over 40 countries in the early 2010s, these adverse effects have grown more obvious, rendering it a dangerous species and one of the most harmful plants in the world [11]. Following introduction to new regions, PHP quickly establishes and proliferates due to its potential to produce an abundant quantity of seeds and a rapid rate of germination [9,12]. Determination of the origin, distribution and population dynamics of the weed are crucial for devising efficient control and management tactics, such as selection and usage of biological barriers, in order to better regulate its invasive proliferation.

In India, this noxious species was first noticed in Pune, Maharashtra in 1955. It is now recognized as the "worst weed" in the nation. PHP was considered as an invasive species of stubble and desolation in the 1980's, but now it has spread to every crop field and into the forests [12]. Weed science experts and members of several weed eradication advocacy groups and weed control societies were forced to establish a space for those needing assistance with or impacted by PHP, due to the severity of the PHP infestation problem, which is now widespread across India [9,13,14]. A recent nationwide assessment revealed the widespread presence of this undesirable weed species in around 35 million hectares of land [9]. PHP thrives in India's diverse climatic conditions including adverse climate conditions, environments of various lands, and different types of soils. The abundance of this aggressive weed now poses a serious biological threat and its eradication therefore requires accordance with the highest priority. Employing PHP as plant biomass will help not only in eradication of the weed but also in obtaining useful producer gas for household use and other purposes. Conversion of PHP into producer gas is done through the use of the thermochemical conversion process. Thermochemical conversion of biomass involves the use of high temperatures and chemical equilibrium reactions R_1 to R_{11}, as shown in Table 1, for conversion of waste biomass into fuels and other useful products. Common thermochemical conversion processes include gasification, pyrolysis, and liquefaction. The process of gasification takes place with the use of a limited concentration of oxygen to facilitate incomplete combustion and thus produce a combustible gas. This conversion is the process by which biomass is broken down for the production of fuel products in the form of solids, liquids, and gases [15]. The thermochemical conversion process is most frequently used in the production of liquid (ethanol, biodiesel), gaseous (producer gas), and solid (char) fuels [16]. Biomass gasification is the process of converting organic matter into combustible gases such as carbon monoxide (CO), carbon dioxide (CO_2), hydrogen (H_2), and methane (CH_4). During gasification, the biomass raw material is heated to high temperatures in the absence of oxygen or air. This breaks down the organic matter into basic elements and produces a combustible gas mixture, which can be burned for generation of heat and power. Biomass gasification is an attractive renewable energy option as it offers the significant advantage of lesser greenhouse gas emissions and consequently a lower environmental impact than fossil fuels. This clean energy production technology from plant-derived biomass is also cost-effective and can be used for the generation of clean fuel for household cooking needs and other purposes. The decomposition reaction of biomass is highly influenced by material properties, time-dependent properties, operating conditions and thermal factors. The time and cost expended on lengthy practical experiments are substantially reduced by modeling and simulation investigations [17].

In this work, modeling of chemical and physical systems is carried out by using ASPEN Plus, a sophisticated system-oriented software adopted for process engineering [18,19]. In this research study, the gasification procedure is replicated in ASPEN Plus utilizing a unique model with a mixer zone for mixing the biomass material and the gasifying agent. An earlier study [20] used a kinetic reaction in ASPEN Plus for investigation of the impact of the feed, retention time, and temperatures on the yield and compositions of the producer gas obtained from the gasification. A thermodynamic model was simulated in ASPEN Plus for exploration of the biomass thermal decomposition. The findings showed a satisfactory consistency with the values reported in the literature [21]. The study examined the influence of the gasification temperature on the yields and the composition of the producer gas. The results showed an increase in the yield of quasi gases with an increase in gasification temperature. Additionally, the model showed good agreement with published values, indicating the feasibility of the effective development of ASPEN Plus in imitating the biomass gasification process.

To the best of the authors' knowledge, this study is the first to use a validated ASPEN Plus model for examination of the assessment of gasification using PHP feedstock and getting an understanding of the process involved in the determination of the quality of the producer gas fuel resulting from Steam - CO_2 gasification. Using the established model, Steam - CO_2 is supplied as a gasifying agent for enrichment of the yield of hydrogen by means of homogeneous and heterogeneous reactions. The results of this study have shown

Table 1
Chemical equilibrium reactions for the Thermo-chemical conversion process [28,36,39–41].

Reaction No	Reaction Type	Reaction	
Heterogeneous reactions			
R_1	Complete combustion	$C + O_2$	$\rightarrow CO_2$
R_2	Boudouard equilibrium reaction	$C + CO_2$	$\rightarrow 2CO$
R_3	Water-gas reaction	$C + H_2O$	$\rightarrow CO + H_2$
R_4	Methanation reaction	$C + 2H_2$	$\rightarrow CH_4$
Homogenous reactions			
R_5	CO partial combustion	$CO + 0.5O_2$	$\rightarrow CO_2$
R_6	H_2 combustion reaction	$H_2 + 0.5O_2$	$\rightarrow H_2O$
R_7	CO shift reaction	$CO + H_2O$	$\rightarrow CO_2 + H_2$
R_8	Steam- reforming reaction	$CH_4 + 2H_2O$	$\rightarrow CO_2 + 4H_2$
R_9	H_2S formation reaction	$2H_2 + S_2$	$\rightarrow 2H_2S$
R_{10}	Char reforming reaction	$C_xH_yO_z$	$\rightarrow$ Oxygenates + Hydrocarbons
R_{11}	Reversed reforming reaction	$CH_4 + CO_2$	$\rightarrow 2CO + 2H_2$

Steam - CO_2 gasification generating producer gas with a high hydrogen content. In addition to highlighting the environmental benefits of using PHP as biomass feedstock, this study establishes Steam - CO_2 gasification as a more efficient way to generate producer gas than air gasification. Optimum gasification process parameters have been identified based on the techno-economic assessments. Cost-benefit assessment using techno-economic, exergy, and energy analyses has been found to be useful in economic optimization of the gasification process while the predictions of the gas yields are primarily beneficial in selecting an appropriate biomass feedstock for the gasification.

2. Steam - CO_2 selection and source of CO_2 for biomass gasification

Traditional Steam - Oxygen (O_2) gasification is an older technology with lower operational costs incurred in the gasification process, the yield of producer gas and hydrogen is often found to be insufficient, whereas the tar content and nitrogen contents are found to be high compared with the Steam - CO_2 gasification. The use of Steam - CO_2 in gasification results in producer gas with a higher hydrogen content making it a more attractive fuel for applications such as fuel cells and hydrogen engines. Lower tar content makes it less harmful to the environment and easier to clean up, while lower nitrogen content and higher producer gas yield makes the process of obtaining producer gas from biomass through the gasification process more economically viable [22]. This makes Steam - CO_2 gasification a more attractive option for producing producer gas from biomass. However, there are still some challenges that need addressing, such as the cost of CO_2 and the development of more efficient gasifiers. The CO_2 source for biomass gasification with Steam - CO_2 as gasifying agents can be extracted from a variety of sources, including natural gas flue gas, industrial flue gas, air captured CO_2 and biomass-derived CO_2 [23]. The purity of the CO_2 plays a vital role in Steam - CO_2 gasification, as low purity has an adverse effect on the efficiency of the gasification process and the quality of the producer gas [24]. The CO_2 supplied for the production of producer gas of good quality should have a purity level of about 95% [24,25].

CO_2 for biomass gasification is captured from the gas emitted into the air after the burning of fossil fuels like coal, oil, natural gas, or wood. The captured CO_2 is already at high pressure and temperature, which can save energy in the gasification process. However, it is important to note that natural gas is a fossil fuel, so using it as a source of CO_2 for biomass gasification would not be considered a carbon neutral process.

Industrial flue gas is another good source of CO_2 for biomass gasification, due to its availability at a low cost. However, the CO_2 in industrial flue gas may contain impurities that could contaminate the producer gas produced.

Air captured CO_2 is a relatively new source of CO_2 for biomass gasification. This CO_2 is captured from the atmosphere using a variety of technologies, such as absorption, adsorption, and cryogenic separation. Air captured CO_2 is the most carbon neutral source of CO_2 for biomass gasification, but it is also the most expensive.

Biomass-derived CO_2 is typically at a lower pressure and temperature than CO_2 from other sources. It is a carbon neutral source of CO_2 for biomass gasification. The best source of CO_2 for biomass gasification depends on a number of factors, including cost, availability, and purity of the CO_2 source.

3. Simulation model development

ASPEN Plus V11 - software is used for the gasification process simulation, for the assessment of the influence of biomass components and process parameters on the varying yields of the elemental compounds produced by the gasification process [26–28]. ASPEN Plus simulations can manage interactions among the liquid, solid, and gaseous phase conversions of biomass using gasification. ASPEN Plus can be used for building a continuous process model, and its simulation for complicated systems like the manufacture of chemicals and evaluation production processes [29–31]. Chemical engineers can use the software for obtaining fully integrated solutions. There are substantial data banks of built-in properties that provide support for models, and FORTRAN subroutines can be used to perform elaborate operations of program units [18]. In this study, a kinetic-free equilibrium framework model has been employed for steady-state simulations using the ASPEN Plus simulator of steam - CO_2 biomass gasification. The characteristics of biomass elements have been considered for contemporary modeling investigations [18,32,33]. Simulation of the biomass gasification is carried out using zero-dimensional blocks. The simulation maintains an equal heat distribution, ignoring tar formation, pressure drop, and heat losses. The thermodynamic properties of modeling systems are based on zero-dimensional building components [34]. Ambient pressure, complete insulation, and reaction temperatures equivalent to exit steam temperatures are seen as the operating conditions for the modeling block. The remaining hypotheses are employed into practice for simplification of the thermodynamic equilibrium and kinetic-free simulation models of biomass gasification.

3.1. Process flow of biomass gasification

The gasification process produces a fuel gas commonly referred to as producer gas, which is rich in H_2, CO, CO_2, and CH_4 along with additional unwanted products, using gasifying agents at high temperatures ranging from 750 to 1000°C. The four stages of a common gasification method are drying (100–200°C), pyrolysis (200–500°C), combustion, and reduction [35]. Moisture is eliminated from the feedstock through the drying process, and then heated to high temperatures and then broken down using pyrolysis. Through the process of combustion and reduction, pyrolysis byproducts including tar, char, hydrocarbons, and combustible gases are mixing for the production of gasification end products like H_2, CO, CO_2, and CH_4 [35]. Implementation of an integrated arrangement of pyrolysis and gasification processes will result in the generation of valuable products from the reaction of pyrolysis products and gasification agents at higher temperatures considering the majority of pyrolysis products lack the requisite fuel characteristics. Table 1 provides a summary of the primary chemical reactions that occur throughout the gasification process, including the water-gas shift, boudouard, and methanation processes [35].

Fig. 1 shows the operational flow-sheet for the ASPEN Plus model. The gasification process begins with the use of dryer blocks working at 110°C for drying the biomass feed for the elimination of the 7.91% moisture content that is found in the invasive PHP biomass proximate analysis [36]. Separator (SEP1) blocks are fixed after the stoichiometric reactor (RSTOIC) eliminating the moisture content (H_2O) in the fuel (PHP) by raising the temperature inside the SEP1 up to 110°C by thermochemical conversion process of R_6. The dried stream reaches the decomposition block, which is modeled as a yield reactor and is used for the conversion of biomass into conventional elements using a calculator formulation unit [37,38]. By minimizing Gibb's free energy under a prescribed temperature and pressure, molecular compositions and phase equilibrium are estimated using the stream from the yield reactor (RYIELD) are estimated.

The RYIELD also functions as a two-phase separator, with solid particles (Ash) getting segregated at the reactor's base, and the gases exiting at the top and being diverted to the Gibb's reactor (RGIBSS). The RGIBSS brings about a vapor combination that is split into producer gas and lowers the temperature. In contrast, the solid particles in the RYIELD are directed to a solid separation area where the ash fractions are separated. The Peng-Robinson equations of state are chosen for replication of the actual and non-polar species included in the model. This research focuses on the evaluation of the production rates of producer gas, output producer gas yields, moisture content and ash effluents. More importantly, it also examines the viability of the gasification process in terms of profitability through the use of a techno-economic analysis for the determination of the extent of the impact of the gasification on the environment.

The following assumptions have been considered for the biomass gasification modeling:

1. Under equilibrium circumstances, the biomass gasification process is stable with a uniform distribution of temperature and pressure.
2. The ASPEN Plus process simulation technique uses a non-dimensional, kinetic-free model.
3. The drying and combustion operations occur instantly and are temperature-sensitive.
4. The phases of adiabatic and isothermal refrigeration are taken into account.
5. Gases like H_2, CO, CO_2, and CH_4 are not taken into consideration.
6. No other nitrogen oxide is created besides Ammonia (NH_3).
   a) Char is entirely composed of carbon.
   b) Ash and biomass are viewed as unconventional property sets.
   c) Both Nitrogen (N_2) and air have inert properties.
7. Heavier hydrocarbons including tar are considered as non-conventional byproducts, for the prevention of hydrodynamic complications.
8. At 110°C and 1 bar of pressure, the gasifying agent feed is regarded as superheated in the gasification process.

4. Assessment of ASPEN plus simulation of the biomass gasification process

4.1. Techno-economic assessment

Techno-Economic Assessment (TEA) was used in the evaluation of the economic feasibility of the gasification process using the ASPEN Plus process simulation tool. It involved estimation of the costs and revenues of the project, as well as the risks involved. TEA of biomass gasification with Steam - CO_2 as gasifying agents using ASPEN Plus simulation was conducted by considering various operating and selection parameters such as appropriate biomass feedstock selection, and the steam-to-biomass (S/B) ratio.

The results of the TEA helped determination of the economic feasibility of the gasification process. The next step taken was financial

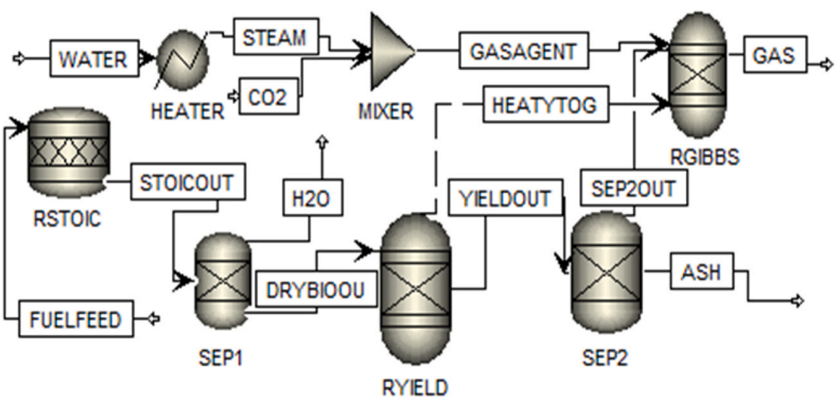

Fig. 1. Gasification of PHP with steam - CO_2 using ASPEN plus simulation.

analysis for determine of the profitability of the process. When the gasification process is found feasible, there are some the factors that can affect the Techno-Economic feasibility of biomass gasification with Steam - CO_2 used as the gasifying agents:

- The procurement cost of the biomass feedstock.
- The expenditure incurred with the use of Steam - CO_2 as gasifying agents.
- The investment in the gasification equipment.
- The revenue from the sale of the producer gas.
- The efficiency of the gasification process.
- The risks involved in the gasification process.

The Techno-Economic feasibility of biomass gasification with Steam - CO_2 as the gasifying agents can be improved by:

- Using a low-cost biomass feedstock.
- Adoption of efficient gasification equipment.
- Sale of the producer gas to a high-value market.
- Reduction in the risks involved in the project.

The Techno-Economic analysis of biomass gasification was conducted using the built-in tools of ASPEN Plus simulation software. The tools were used in the calculation of the costs associated with investments, operations, basic materials, commodity sales, utilities, equipment, and device installation. Assessment of the incurred costs and ecological impacts of the pollutants of the gasification process was done through a comparison with the findings of earlier studies [42].

The available guidelines comprised of the regulations and regulatory standards prescribed by the United States Environmental Protection Agency (U.S. EPA) in 1995, the IPCC's 2nd Annual Assessment Report on Climate Change in 1995 [43], and the IPCC's 4th Annual Assessment Report on Climate Change [44]. The past 100-years Global warming potential (GWP) has been provided by the prescribed guideline in the computation of the emissions as a balanced average of the total mass flow rate of the Greenhouse Gas (GHG) components. The IPCC 4th Assessment served as the standard for the net-stream CO_2 equivalent calculated with the use of the environmental emission equation. The 4th Assessment cycle presented numerous forecasts of the repercussions of several climate change scenarios. By 2030, the average global temperature is predicted to increase by more than 1.5°C [44]. As a result, many countries, notably India, have made immediate commitments for proactive enforcement of measures meant for a reduction in their carbon emissions for the achievement of net zero carbon emissions by 2030, in an attempt to tackle the increasing menace of climate change. Assessment of its main elements of invasive biomass as well as their effects on the production of producer gas are assessed, as shown in Table 2. The simulation also helped in the estimation of the cost and pollutants of the biomass decomposition procedure [42].

4.2. Energy analysis

Energy analysis of biomass gasification with Steam - CO_2 as gasifying agents using ASPEN Plus simulation was conducted considering various parameters such as selecting the biomass feedstock and the steam-to-biomass ratio (S/B), with calculation of the energy balance of the gasification process. The energy balance of the gasification process is expressed in equation (1).

$$\text{Energy}_{\text{in}}\,(\text{biomass} + \text{steam} + CO_2) = \text{Energy}_{\text{out}}\,(\text{producer gas} + \text{ash} + \text{heat losses}) \tag{1}$$

The energy in the biomass feedstock is the chemical energy that is released when the biomass is gasified. The energy released from

Table 2
Relative measures of economic analysis using ASPEN Plus simulator.

Economic expenditure analyses	Relative measures		
Initial investment cost	EC + IC + CC, EB & PC + AC + OC		
Unit Operation cost	O & LC + MC + OHC + AC		
Annual expenditure	II + OC + RMC		
Operating cost	25% of the shift operating LC/period		
Overhead cost	50% of LC and MC/period		
Initial working capital	5% of TIC		
Administrative expenditure	8% of total unit OC		
Salvage	PP – (TDC * TUL)		
Net stream	GWP* (PS – FS)		
Economic parameters	**Values**	**Parameters**	**Values**
No. of years (n)	5	Weeks per year	52
Hours per year	8760	Length of start-up	20 weeks
Duration of EPC	33 weeks	Duration of construction phase	20 weeks
Depreciation	Straight line	Interest rate	20%/year
Unit cost for supervisor	₹.25/h	Supervisors per shift	1
Unit cost for the operator	₹.15/h	Operators per shift	2
Cost of raw material	₹.3500/ton	Producer gas production price	₹.15/kg

the process is the heat energy that is carried away by the producer gas and the ash, and the heat losses that occur during the gasification process.

The results of the energy balance were used for determination of the following:

- The efficiency of the gasification process.
- The amount of heat that is required to gasify the biomass.
- The amount of heat that is lost during the gasification process.
- The amount of producer gas produced.

The energy analysis of biomass gasification with Steam - CO_2 as gasifying agents was used for improvement of the efficiency of the gasification process through the selection of a high-quality biomass feedstock, adoption of an efficient gasifier, and minimizing the heat losses during the gasification process. Calculations of the capital cost annualization factor are calculated using equations (2) and (3) respectively.

$$Capital\ cost\ annualization\ factor = \frac{\frac{ROR}{100} \times \left(1 + \frac{ROR}{100}\right)^{PL}}{\left(1 + \frac{ROR}{100}\right)^{PL-1}} \times 0.2638 \tag{2}$$

$$Capital\ cost = 10000 + \left(800 \times \left(\frac{Area}{N_s}\right)^{0.8} \times N_s\right) \tag{3}$$

The purpose of this research study is to use ASPEN Plus simulation for investigating the performance of biomass gasification with Steam - CO_2 as gasifying agents [45,46]. The biomass gasification process with Steam - CO_2 as a gasifying agents resulted in higher gasification efficiency than with air as the gasifying agent. The CO_2 gasification process produced a higher yield of CO, H_2, and a lower yield of CO_2 and CH_4 [47–49]. Energy analysis was done with the use of enthalpy values of the gaseous constituents using ASPEN Plus software. Calculation of the energy level of the solid constituents of the biomass is calculated by utilizing the lowest heating value. The energy performance of the gasification process showed the proportion of the output over the streams of input energy. For the energy analysis, the operating life of the gasifier was taken as five years although it has a maximum lifespan of around 15–20 years. Considering the capability of the newly installed gasifier in efficient functioning for five years without any problems like breakdown or failure, shown in Table 3.

4.3. Exergy analysis

Exergy analysis is a thermodynamic analysis used in the assessment of the efficiency of the gasification process. In the context of biomass gasification, exergy analysis can be used for identification of the sources of irreversibility in the process and determination of the exergetic efficiency of the gasifier. ASPEN Plus was used in the exergy analysis of biomass gasification by tracking the exergy of the different streams in the process. The following were the steps in the performance of exergy analysis of biomass gasification with Steam - CO_2 as gasifying agents using ASPEN Plus modeling:

- Creation of a model of the gasifier in ASPEN Plus.
- Definition of the properties of the biomass and the gasifying agents.
- Specification of the operating conditions of the gasifier.
- Tracking of the exergy of the different streams in the gasification process.
- Calculation of the exergetic efficiency of the gasifier.

Exergetic efficiency of the gasifier is the ratio of the useful exergy output to the total exergy input. The useful exergy output is the exergy of the producer gas produced by the gasifier. The total exergy input is the exergy of the biomass and the gasifying agents. The exergy analysis of biomass gasification with Steam - CO_2 as gasifying agents was conducted for the identification of the sources of irreversibility in the process. The main sources of irreversibility were the heat losses from the gasifier, the incomplete combustion of the biomass, and the tar formation. Improvement in the exergetic efficiency of the gasifier was seen through a reduction in the heat

Table 3
Relative measures of energy analysis using ASPEN Plus simulator.

Minimum LMTD correlation factor	0.8
Maximum area/shell	500 m^2
Exchanger minimum approach temperature	10°C
Rate of return	10%
Operating life of the plant	5 years
Operating hours	8760 h
Stream segment tolerance	0.90

losses from the gasifier, by increasing the combustion efficiency of the biomass, and a reduction in the tar formation. Exergy analysis for biomass gasification enabled the identification of irreversibility sources, calculation of exergetic efficiency, enhancement of gasifier design, and optimization of operational conditions.

Exergy analysis is a valuable tool for the design, optimization, and trouble-free operation of biomass gasification plants. It can be used for improvement of the efficiency of the gasifier and reduction in the environmental impact of the gasification process. Exergy analysis is utilized in the evaluation of the efficiency of a process and identification of areas and also for quantification of the energy required for the production of a desired product, the energy available in the feedstock, and the efficiency of the energy conversion process. By comparing these values, the process efficiency will be improved, and enhances the economic viability of the process. Additionally, exergy analysis can also be used in the diagnosis and troubleshooting of issues found within the process. When used in conjunction with other process modeling tools, such as ASPEN Plus, exergy analysis can help optimize a process for maximum efficiency and minimum energy consumption. Additionally, the analysis should consider the potential end uses of the products, which was done using the ASPEN Plus simulator and the results are tabulated below in Table 4 and Fig. 2.

Estimation of exergy of PHP gasification was done by considering the enthalpy of the reactants, products and energy losses. The enthalpy of the reactants and products was determined with the use of their chemical composition and the heat of the reaction, where the energy losses are calculated based on the heat transfer rate, temperature difference and the specific heat of the reactants and products.

Once the enthalpy of each component was determined, the change in exergy was calculated by considering the change in enthalpy and the change in entropy. The change in entropy is determined using the temperature difference between the reactants and products as well as the temperature of the environment. Finally, the overall exergy efficiency of the process was calculated by dividing the total exergy change by the total energy input. The highest amount of work that a system is capable of performing is its exergy which evaluates the caliber of energy. In contrast to the exergy efficiency which indicates the percentage of the total drop in exergy performance brought about by exergy loss, the conclusion provides an indicator of the proportion of each subsystem's exergy degradation to the change in exergy efficiency.

The calculation of exergy associated with the gasification of PHP feedstock using ASPEN Plus required an understanding of the thermochemical properties determined by the composition of the feedstock and the operating conditions of the gasification process. The following parameters must be known: the feedstock composition, the temperature, the pressure, and the reaction rate constants. Once the thermochemical properties of the gasification process are known, the exergy associated with the process can be calculated using equation (4). The enthalpy of the gasification reaction is determined by the heat of combustion of the feedstock and the reaction rate constants.

$$Exergy = Enthalpy - (Temperature \times Entropy) \tag{4}$$

5. Results and discussion

The results of the simulation of a gasifier using Steam - CO_2 as gasifying agents in ASPEN Plus indicate the production of H_2, CO, CO_2, and CH_4 in the gasification process. The results show that the yield of H_2 was the highest followed by CO, CO_2, and CH_4 in view of the homogeneous and heterogeneous reactions that played a major role in the conversion of biomass into H_2 and CO with the introduction of Steam and CO_2 into the gasifier as gasifying reaction agents. The yield of hydrogen was approximately 60.3% in view of the most prominent catalytic process R_3 (moderately exothermic reaction) which converts CO and steam into CO_2 and H_2. CO was removed from producer gas through the employment of R_3 to ensure the yield of high quality H_2. Considering that conversion involves an exothermic process, lower temperatures are selected for higher CO transformations. Higher temperatures, however, improve the

Table 4
Exergy result of biomass gasification using ASPEN Plus simulation.

Description	Units	GAS	YIELDOUT	Description	Units	GAS	YIELDOUT
From		RGIBBS	RYIELD	From		RGIBBS	RYIELD
Stream Class		MIXNC	MIXNC	Mass Enthalpy	J/kg	−4452025	115734
Temperature	K	925.42	673.15	Mass Density	kg/m^3	0.339	0.411
Pressure	N/m^2	100000	100000	Enthalpy Flow	Watt	−63658.89	884.21
Mass Vapor Fraction		0.77	0.46	Mass Flow	kg/s	0.0142	0.0076
Mass Solid Fraction		0.22	0.53	Volume Flow	m^3/s	0.0421	0.0185
Phase				Molar Entropy	J/kmol-K	49487.77	20194.3
Temperature	K	925.42	673.15	Mass Entropy	J/kg-K	2834.016	1791.29
Pressure	N/m^2	100000	100000	Molar Density	$kmol/m^3$	0.0194	0.0324
Molar Vapor Fraction		0.66	0.550	Mass Density	kg/m^3	0.339	0.3659
Molar Solid Fraction		0.33	0.449	Enthalpy Flow	Watt	−63658.89	4789.35
Mass Vapor Fraction		0.77	0.5193842	Average MW		17.46205	11.273
Mass Solid Fraction		0.2275	0.4806158	Mole Flow	kmol/s	0.00081	0.00030
Molar Enthalpy	J/kmol	−77741526	7941544.0	Volume Flow	m^3/s	0.042	0.018
Mass Enthalpy	J/kg	−4452025	704437.10	**Exergy flow**	**Watt**	**6425.4**	**1633.34**

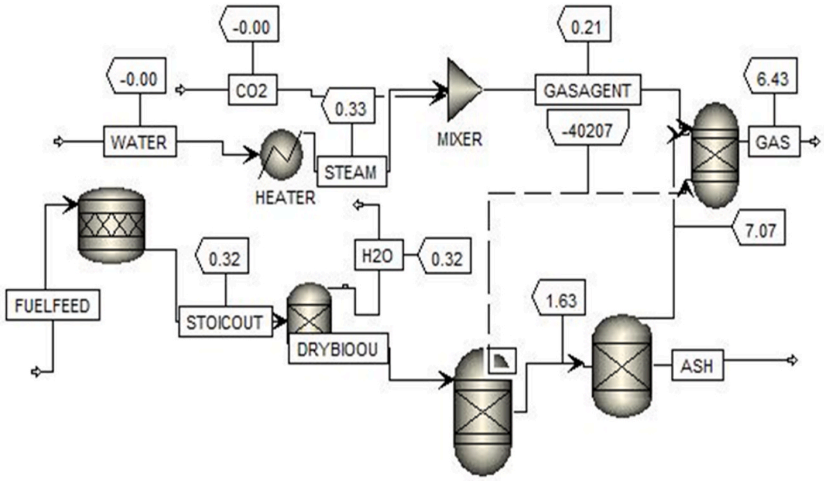

Fig. 2. Exergy analysis output of PHP gasification using ASPEN Plus simulation.

rate of reactions [50]. The yields of CO, CO_2, and CH_4 were approximately 20%, 16%, and 3.7%, respectively, at an optimal temperature of 800°C. The simulation results of the PHP biomass gasification obtained in the present study were in line with previous (PHP, *Lantana camara* (LC)) simulation and experimental studies [36,51], as shown in Table 5 and Fig. 6. The results of the present simulation showed gasification as an effective and affordable technology for production of H_2 and other products from biomass. Assessment of technology work made using a variety of analyses. The simulation results were used for further improvement of the design of the gasifier and optimize the gasification for higher producer gas yields and more efficient operation.

Figs. 3–5 illustrate the impact of rising temperatures on the composition of the simulated product gas and carbon conversion. An increase in temperature from 300°C to 1000°C in 50°C increments was seen while all other parameters were maintained constant, with equivalence ratio (ER) ranging from 0.2 to 0.4. Simulated predictions for H_2, CO, and CO_2 generation at higher gasification temperatures of 700°C–1000°C demonstrated good consistency. Results suggested, a gradual increase in the concentration of H_2 from 51% to 63% by temperature range of 700°C–1000°C, while CO slowly rises from 14.5% to 19%. In contrast, CO_2 volume percentage decreases from 24% to 13.5%. A study of these trends in H_2, CO and CO_2 in relation to rising temperatures was studied and validation was done with earlier research studies [36,51]. The results showed the equilibrium gas composition as established between 300°C and 1000°C with marked variations in the producer gas composition at the lower temperatures. With the increase in the temperature from 300°C to 1000°C, there was a change in the composition of the producer gas, the volume % of CO_2 with a significant reduction while that of CH_4 gradually increased from 2.7% to 7.56% by the thermochemical conversion of R_4. Figs. 3–5 show the presence of a close association between $H_{2,}$ and CO volume %, following analysis of the model results [36,51]. Therefore, the conclusions were that heterogeneous reactions contribute to the preferred reaction at higher temperatures. For temperatures between 300°C and 1000°C, simulation findings show as an increase in the composition of producer gas increases, as illustrated in Figs. 3–5. Improvement in the gasification process was done through a rise in the temperature to 800°C–1000°C, which was seen as advantageous for heterogeneous reactions. Conversely, at lower temperatures from 300°C to 500°C, there was a higher volume of unconverted char which caused a decrease in the rate of hydrogen, carbon, and oxygen within the volatile product which was reformed with the use of R_{10}, as reflected in the simulation findings.

5.1. *Effect of equivalence ratio*

The simulation of the biomass gasification process was carried out using ASPEN Plus software for the investigation of the performance of the gasifier with variation in temperature and equivalence ratio (ER). The results reveal that the composition of the gas by gasification is largely dependent on the equivalence ratio. The results of the simulation confirm that the gas composition is highly dependent on the equivalence ratio, and that a higher equivalence ratio results in more CO and H_2, and less CO_2 and CH_4, in view of variation of air flow rate while maintaining the other conditions as constant.

The temperature of the reactor was maintained at 800°C while variations were made in the equivalence ratio from 0.2 to 0.4 with

Table 5
Proximate analysis and ultimate analysis of published studies and the present study.

Fuel	C %	H %	N %	S %	O %	MC %	VM %	FC %	Ash %	CV MJ/kg	Reference
PHP	32.23	5.43	0.26	0	62.08	7.91	42.59	17.56	31.94	15.9	Present study & [36]
LC	24.01	9.81	0.91	0	65.2	7.9	53.2	14	24.7	23.2	[36]
LC	39.07	6.03	0.27	0.8	50.3	7.2	51.8	37.8	3.5	6.14	[51]

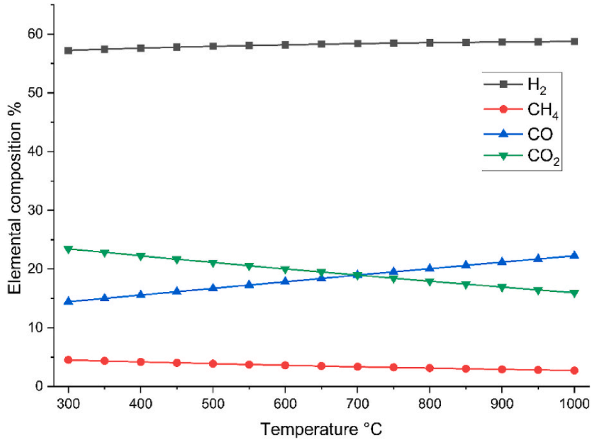

Fig. 3. Elemental composition of producer gas at ER 0.2 for steam - CO_2 gasification.

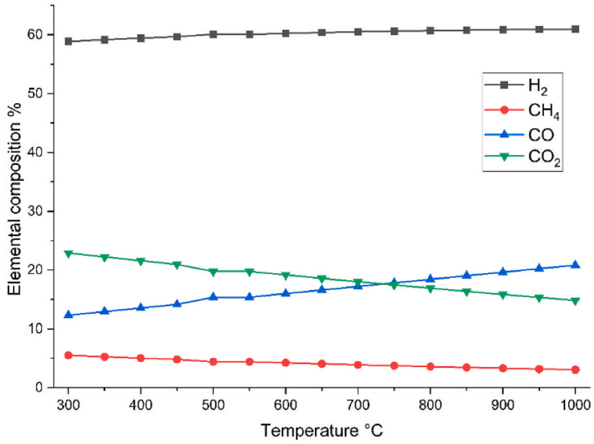

Fig. 4. Elemental composition of producer gas at ER 0.3 for steam - CO_2 gasification.

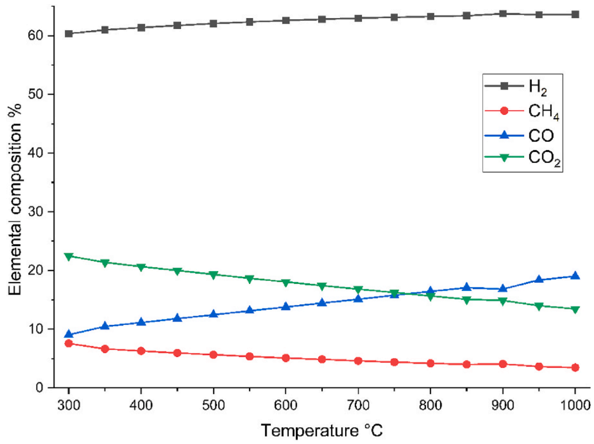

Fig. 5. Elemental composition of producer gas at ER 0.4 for steam - CO_2 gasification.

increments of 0.1. At an ER of 0.2, the hydrogen output was observed to be maximum (60.7% by volume). The CO content in the producer gas at the same ER of 0.2 is 19% (by volume). With a respective heating value (HV) of 11.25 MJ/Nm^3, CO and H_2 made a significant contribution to the producer gas heating value.

5.2. Techno-economic assessment

Evaluation of the specific economic profitability is crucial in investigating the impact on the overall sustainability of the gasification process. Table 2 displays the outcomes of the model's economic assessment. All four key economic indicators, namely product sales, capital expenditures, operational expenses, and raw material costs that the cost of raw materials is the major component of the total expenditure [52,53]. The simulation enables the prediction of producer gas composition, which is crucial for subsequent processing and selection of a product. The composition of the producer gas produced by this gasification of biomass is typically 15–19% CO, 51–63% H_2, 2.7–7.56% CH_4, and 13.5–24% CO_2. Optimization of the gasification process parameters can increase the yield of producer gas. The yield from biomass gasification is generally 2.3 to 2.6 Nm^3 producer gas/kg of dry biomass [54]. This techno-economic analysis of biomass gasification is carried out using ASPEN Plus simulation by simulating the process flowsheet and calculating the capital and operating expenses.

The analysis reveals about the composition, yield, capital expenditures, and operational costs of producer gas. This data was required for making well-informed decisions relating to the planning, construction, and operation of a gasification plant. The computation of feedstock costs, which might vary based on the type of biomass, location, and market conditions, is one of the major issues in the techno-economic analysis of gasification. The calculation of running costs presents a further challenge. The effectiveness of the facility, the type of producer gas cleaning equipment employed, and the type of gasification method selected are factors that affect operational expenses. Despite these difficulties, techno-economic evaluation is a useful technique for determining if gasification initiatives are feasible.

5.3. Validation of the developed ASPEN plus simulation model

A number of parameters need consideration for the validation of the ASPEN Plus simulation of biomass gasification using PHP as feedstock. These include the type and concentration of gasifying agents, the temperature and pressure, the feedstock type, the mass and energy balances, and the producer gas yields. The results of the model must be compared with existing experimental data obtained from lab-scale studies [36,51]. Modeling of the Steam - CO_2 biomass gasification in the present research is performed at several temperatures ranging from 300°C to 1000°C with intervals of 50°C for simulation of the gasification process. CO_2 and CH_4 production levels were seen at lower optimum temperatures whereas H_2 and CO concentrations were maximum at higher temperatures, as shown in Figs. 3–5. The present study results obtained a similar pattern to the existing studies [36,51]. R_2, R_3, and R_8 are examples of endothermic reactions that help to absorption of the heat. Le Chatelier's theory is similar in that an increase in the gasification temperature speeds up the formation of byproducts, especially for some endothermic reactions. Reactions that are comparable occur whenever CO and steam interact to generate CO_2 (R_7), and the CO_2 formed by the R_7 and R_8 reactions is subsequently processed further through the R_2 reaction resulting in CO. Additionally, the model should have the ability to do accurate prediction of the performance of the gasification process over different operating conditions, to ensure the behaviour of the system from the mathematical model used for invasive biomass. The created model is validated by comparing its outcome with previously conducted experiments [36,51]. Evaluation of the prediction accuracy of the model is performed by comparing the producer gas composition predicted by modelling results with available experimental data.

Table 5 provides an overview of the proximate and ultimate analyses of previously published studies and the present study. The elemental composition results of the PHP biomass gasification simulation have been validated through comparison with simulated data (PHP and LC) [36] and experimental data (LC) [51] from previous research studies. Through comparison of the present study with the existing studies [36,51], shows the superior performance of steam - CO_2 gasification performs better in the production of H_2 with a yield of 63% which is better than other gasification processes shown in Fig. 6. Once validated, the simulation model of steam - CO_2 has been used in the optimization of the process parameters for gaining a better understanding of the gasification process.

6. Conclusions

The techno-economic, energy, and exergy analyses of invasive weed gasification with Steam-CO_2 as gasifying agents for H_2 enriched producer gas production using the ASPEN Plus simulation model are presented in this research work. The technology can provide major economic, environmental, and energy efficiency benefits, as the process can be used for the production of high value bio-products, reduction in harmful emissions and creation of energy efficient fuels. The simulation has established that the gasification of PHP feedstock offers significant benefits by producer gas production at a cost of ₹.15/kg estimated by economic analysis. The exergy and energy analyses show high exergy efficiency and very low energy loss of 0.9% from the total energy supplied to the gasifier. The results of the simulation indicate that the gasification process is capable of producing high concentrations of H_2 with a maximum yield of 63%, 19% yield of CO, and low yields of 16% and 3.7% for CO_2 and CH_4 respectively, by volume. This shows that the proposed gasification process is an economically and environmentally viable option for producing fuels from biomass. The simulation results are encouraging with an indication of a gasifier with Steam - CO_2 as the gasifying agent as a promising strategy that can be deployed for the production of multiple gases from waste biomass which can be used as alternative fuels for household cooking and other applications.

6.1. Future scope

The future scope of this research aligns with current trends in biomass gasification, particularly using steam and CO_2 as gasifying agents, which hold promise as a sustainable and efficient energy production method. Additionally, the study recommends sensitivity

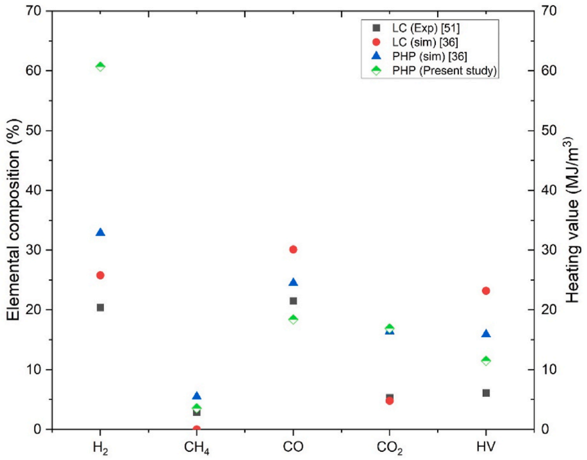

Fig. 6. Comparative analysis: validating the present study against published results [36,51].

analysis through the exploration of diverse gasifying agents and various invasive feedstocks, in line with present-day efforts to address pressing issues like climate change and the management of invasive species.

Data availability statement

- Data associated with our study has not been deposited into a publicly available repository.
- Data will be made available on request.

CRediT authorship contribution statement

Nivash V: Writing – original draft, Methodology, Conceptualization. **Sakthivadivel D:** Writing – review & editing, Validation, Supervision, Project administration, Investigation, Conceptualization. **A. Alaswad:** Writing – review & editing, Validation, Supervision. **Vigneshwaran V S:** Writing – review & editing, Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Nomenclature

₹	Indian Rupee
EC	Equipment Cost
IC	Installation Cost
CC	Construction Cost
EB & PC	Electrical and Plumbing Cost
AC	Administration Cost
OCC	Other Contingencies
OC & LC	Operating Cost & labour Cost
MC	Maintenance Cost
OHC	Overhead Cost
II	Initial Investment
OC	Operating Cost
RMC	Raw Material Cost
LC	Labour Cost

TIC	Total Investment Cost
PP	Purchase Price
TDC	Depreciation
TUL	Useful life
PS	Product Streams
FS	Feed Streams
EPC	Engineering, Procurement and Commissioning
N_s	Correlation factor
ROR	Rate of return
PL	Operating Life of plant
Area	Maximum area

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