

e-ISSN: 2319-8753 | p-ISSN: 2347-6710

DIA

International Journal of Innovative Research in SCIENCE | ENGINEERING | TECHNOLOGY

INTERNATIONAL JOURNAL OF INNOVATIVE RESEARCH

IN SCIENCE | ENGINEERING | TECHNOLOGY

Volume 13, Issue 3, March 2024

INTERNATIONAL STANDARD SERIAL NUMBER INDIA

Impact Factor: 8.423

9940 572 462

6381 907 438

 \bigcirc







|e-ISSN: 2319-8753, p-ISSN: 2347-6710| www.ijirset.com | Impact Factor: 8.423| A Monthly Peer Reviewed & Referred Journal |

|| Volume 13, Issue 3, March 2024 ||

| DOI:10.15680/IJIRSET.2024.1303122 |

Process Simulation of Allothermal Air-Steam Gasification of Biomass in Aspen Plus

Mohamed Rafi.M, Jovin.J, Mugesh Kumar.V, Mugesh Selvam.J, Muniya Samy.S

UG Scholar, Department of Mechanical Engineering, St. Mother Theresa Engineering College, Thoothukudi,

Tamil Nadu, India

ABSTRACT: A model based on reaction kinetics is essential to capture the underlying kinetic effects in biomass gasification. The gasification process can be described better by incorporating drying and devolatilisation stages in the kinetic model. For this, a model which simulates the various process stages separately is inevitable. A possible option for the process splitting is simulation of gasification in process simulator Aspen Plus[®]. The formulation and simulation of a kinetic model for allothermal air-steam gasification in Aspen Plus is presented. The sensitivity of the variables including gasification temperature, air equivalence ratio and steam to biomass ratio on performance of gasification is predicted. The performance measures are H_2 concentration in the syngas, heating value and process energy and exergy efficiencies. The model is validated with published experimental results and the optimum values of the operating conditions are suggested.

KEYWORDS: Biomass gasification, kinetic model, H₂ concentration

I. INTRODUCTION

Biomass gasification system is a thermo-chemical system exchanging heat and mass between the solid fuel and gasifying agent, and also among the intermediate products of gasification. Various chemical processes in biomass gasification are complicated and require the development of suitable mathematical models for its analysis. Models for biomass gasification can predict the mechanical and thermodynamic limits of energy conversion, and is beneficial for its design and scale up. Such models can evaluate the influence of the major input variables, such as sub-stoichiometric air supply rate, feed rate of biomass and its typology, rate of steam input and gasification temperature on the composition and heating value of the generated producer gas.

Aspen Plus models in biomass gasification

Aspen Plus (Aspen Technology Inc.) is a problem oriented input programme that is used to facilitate the simulation of physical, chemical and biological processes. Small sections of complex and integrated systems can be created and tested in Aspen Plus as separate modules before they are integrated. Many published on simulation of coal gasification models in Aspen Plus are available. Very few studies [1-5] are reported on Aspen Plus simulation of biomass gasification incorporating kinetic limitations of the individual chemical reactions involved. Some models were for specific gasifier designs such as bubbling fluidised bed [6], dual fluidised bed [7, 8] interconnected fluidised bed [8] and entrained flow bed. Majority of biomass gasification models [9-12] are based on thermodynamic equilibrium concept. The present model is unique in the sense that it incorporates the reaction kinetics and intermediate processes of biomass gasification by splitting the entire process into several sub-reactions accounting the respective rate costants.

II. MODELLING METHODOLOGY

The air-steam gasification process is divided into several sub-blocks performing specific operations such as drying, devolatilisation, partial combustion, char gasification and steam reforming. The model is formulated using wood sawdust as biomass material having chemical composition (wt.%) as Fixed Carbon: 11.7, Moisture: 7.7, Volatiles: 76.9, Ash: 3.7 and CHON: 46.9, 6.38, 46.5, 0.22. The pertinent chemical reactions involved in gasification [13, 14] are given in Tab. 1 along with the respective heat of reaction. The modelling framework is based on the following assumptions including (1) All the process blocks except the kinetic blocks are zero dimensional (2) The product gases considered are CO, CO₂, CH₄, H₂ and H₂O(g) neglecting higher order hydrocarbons being very small in concentration (3) Supply conditions of air and steam respectively are, 1 bar and 300 K, and 1 bar and 573 K (4) Pyrolytic tar is modelled as benzene (C₆H₆) neglecting other components such as naphthalene and phenols [15] and (5) All the streams obey RK real gas EOS.



|e-ISSN: 2319-8753, p-ISSN: 2347-6710| www.ijirset.com | Impact Factor: 8.423| A Monthly Peer Reviewed & Referred Journal |

|| Volume 13, Issue 3, March 2024 ||

| DOI:10.15680/IJIRSET.2024.1303122 |

Process description in Aspen Plus

Aspen Plus flow sheet developed is shown in Fig. 1. In general, biomass gasification consists of mainly the following processes. (1) Drying of the feedstock,

(2) Primary pyrolysis generating light gases, char and tar in liquid form, (3) Partial combustion of char and gases generated from pyrolysis (4) Heterogeneous gasification reactions (5) Reforming of the gases with steam. Biomass (7.7% moisture content) at a specific feed rate (1 kg/h on wet basis) is subjected to drying in the DRYREAC sub-block. DRYREAC simulates the drying process and the evaporated moisture is removed by DRYSEP, which is a FLASH SEPARATOR. The dried biomass is subjected to pyrolysis in DECOMP block which simulates its thermal decomposition. A RYIELD reactor which decomposes the biomass into char, gas and tar is introduced to simulate the actual process of pyrolysis. The yield of the pyrolysis products of wood sawdust is estimated as per the correlations suggested by Gomez-Barea et al. (2010). A calculator block based on FORTRAN subroutine is used for simulating the pyrolysis which will be executed before the RYIELD reactor. The pyrolysis products include char [16], tar (modelled as benzene) and gases (CO, CO₂, H_2 and CH₄). The char stream is assumed to be consisting of pure solid carbon and ash content of the dried biomass. The concentrations of the gas species is converted into mass fractions. The gases are separated from the output stream of the DECOMP block using PYSEP block. The solid yield (CANDASH) from the PYSEP contains the pyrolytic char. 25% the remaining char (CHAR) is removed as unconverted stream (UCCHAR), not participating in gasification which is achieved by a FSPLIT block. Remaining char is split into two streams to COMBUST block and to REFORM block, which is simulated using another calculation block defined in COMBSPLT. The gas mixture (VOLATILE) is fed into a chemical kinetic reactor, COMBUST (RPLUG reactor) which simulates the partial oxidation reactions R₁, R₇, R₈ and R₉. Tab. 1 provides the stoichiometry and rates of the reactions in terms of activation energy and pre-exponential factor. First order power law reaction scheme is employed for the estimation of the reaction rates. Products of partial combustion from COMBUST, tar (from PYSEP block), 70% of char, and steam are the inputs to another kinetic block, REFORM simulating the steam reforming, char gasification, boudouard and tar reforming reactions (R_3 - R_7 and R_{10}). Steam at 573 K and 1 bar is supplied to REFORM (RCSTR reactor) at predetermined feed rate maintaining the required Steam to Biomass Ratio (SBR). The model assumes the gas and liquid streams (tar) obey RK equation of state with Boston-Mathias modification. Twenty one material streams are used in the simulation.



FIGURE 1. ASPEN PROCESS FLOW SHEET



|e-ISSN: 2319-8753, p-ISSN: 2347-6710| www.ijirset.com | Impact Factor: 8.423| A Monthly Peer Reviewed & Referred Journal |

|| Volume 13, Issue 3, March 2024 ||

| DOI:10.15680/IJIRSET.2024.1303122 |

Simulation of the model

The objective of the simulation model is to predict the sensitivity of the operational variables on the performance of airsteam gasification. A parametric study is carried out with the help of data analysing tool 'sensitivity analysis' in Aspen Plus to achieve this. Equivalence Ratio (ER), SBR and Temperature (T) are varied in the range 0.15-0.45, 0.252.5 and 600-1300 K, respectively. The criteria for comparison of gasifiers include concentration of H₂ (biohydrogen) in the producer gas (on dry basis) and its Lower Heating Value (LHV) and process energy & exergy efficiencies.

III. RESULTS AND DISCUSSION

Variation of H_2 concentration, LHV and process energy & exergy efficiencies with respect to the aforementioned process operational variables are discussed in this section. Simulations are carried out for 1 kg/h feed of biomass (with 7.7% moisture) at a char conversion efficiency of 75%.

Effect of gasification temperature

The effect of allothermal gasification temperature on H_2 concentration is depicted in Fig. 2. In the analysed range (600-1300 K), H_2 concentration increases with temperature, reaches a peak value and decreases with further increase in temperature. The maximum H_2 concentration is predicted at about 900-950 K for all the SBR values. The temperature enhances the rate of endothermic reactions (R_2 , R_4 , R_5 and R_{12}), and slows down that of exothermic reactions (R_3 and R_6) in the reformation block. SMR (R_5) and reforming of benzene (R_{12}) are much higher temperature processes prominent above 1000 K. H_2 production is controlled by the endothermic char gasification and reverse Water Gas Shift (WGS) reactions. It is inferred that above a temperature of 900-950 K, reverse WGS reaction dominates the combined effect of char gasification, Steam Methane Reforming (SMR) and benzene reforming reactions resulting in the reduction in H_2 concentration beyond 950 K.

Effect of steam to biomass ratio (SBR)

SBR is simulated in the range of 0.25-2.5, by varying steam supply rate to the reformation block and keeping the biomass feed rate constant. The concentration of H_2 in the dry syngas (see Fig. 2) is improved with steam addition. More steam improves the rates of heterogeneous gasification of char (R_2), WGS (R_6), and reforming reactions of methane (R_5) and benzene (R_{12}). Higher rates of these reactions result in improved H_2 concentration. The highest H_2 concentration achieved in the simulation range is 34.6% at T=900 K, SBR=2.5 and ER=0.15.

Effect of equivalence ratio (ER)

Air input to the partial combustion block is increased to vary ER between 0.15 and 0.45, at constant steam input and constant biomass feed rate. Obviously, supply of more air shifts the whole reaction towards combustion yielding more CO_2 and H_2O (R_6 , R_7 and R_9). Consequently, the gas mixture entering the reformation block would contain more amounts of CO_2 , N_2 and H_2O than with lower ER values. The variation of the H_2 concentration is shown in Fig.3 for various SBR and ER values, keeping the temperature of the reformation block constant at 1000 K.

Reaction number	Reaction name	ers*	Reference	
		E _a (kJ/mol)	k (1/s)	
R ₁	Partial combustion	n 55.00	5.70E11	[17]
R ₂	Char gasification	129.60	3420.00	[18]
R ₃	Methane hydrogenation	129.60	3420.00	[18]
R_4	Boudouard	248.12	4364.00	[13]

TABLE 1: KINETIC CONSTANTS OF REACTIONSIN BIOMASIFICATION

e-ISSN: 2319-8753, p-ISSN: 2347-6710| www.ijirset.com | Impact Factor: 8.423| A Monthly Peer Reviewed & Referred Journal |



|| Volume 13, Issue 3, March 2024 ||

| DOI:10.15680/IJIRSET.2024.1303122 |



FIGURE 2. VARIATION OF H₂ CONCENTRATION WITH T AND SBR (ER=0.25)

LHV of dry gas mixture

The reduction in concentrations of the combustible gases with air addition results in poor heating value gas at higher ER (for example, above an ER value of 0.4, maximum LHV is 4.03 MJ/Nm³ only) values. As per the simulation results the two gases (CO and H₂) have comparable concentrations also. Moreover, maximum contribution of CH₄ to LHV is only 22% due to its low concentration in the dry gas mixture even though itsheating value is much higher. The favourable aspect of steam addition on H₂ and unfavourable aspect on CO concentrations result in subsided effect of SBR on LHV. The rate of increase in H₂ is much lower than the rate of decrease in CO while SBR is increased from 0.25 to 2.5. This is the reason for the slight reduction in LHV with steam addition for air-steam gasification process which is illustrated in Fig. 4.



FIGURE 3 VARIATION OF H₂ CONCENTRATION WITH ER AND SBR (T: 1000 K)



|e-ISSN: 2319-8753, p-ISSN: 2347-6710| www.ijirset.com | Impact Factor: 8.423| A Monthly Peer Reviewed & Referred Journal |

|| Volume 13, Issue 3, March 2024 ||

| DOI:10.15680/IJIRSET.2024.1303122 |

Process efficiencies

Energy efficiency is another performance benchmark for steam-assisted gasification. On an average, the system is thermally efficient by 54.5% (see Fig. 5). The reduction in LHV reduces the process efficiency at higher air feed rates and with higher steam supply rate also. The maximum energy efficiency predicted is 83.4% at ER=0.15 and SBR=0.25 for a gasification temperature of 900 K.



FIGURE 4 VARIATION OF LHV WITH ER AND SBR

(T: 1000 K)

The second law thermodynamic efficiency (exergy efficiency) is computed following the exergy modelling procedure. The destruction in chemical and physical exergies during gasification process makes exergy efficiency lower than the corresponding energy efficiency. The two thermodynamic efficiencies are given in Tab. 2 for different operating conditions.

Optimum operating conditions

Maximum H_2 concentration achieved is 34.6% for airsteam gasification of sawdust which corresponds to a much higher steam supply (SBR=2.5) rate. At this condition

(T=900 K, ER=0.15 and SBR=2.5, moisture content=7.7%) LHV and consequently process efficiencies are lower than their corresponding maximum achievable values.



FIGURE 5 VARIATION OF ENERGY EFFICIENCY WITH ER AND SBR (T: 1000 K)



|e-ISSN: 2319-8753, p-ISSN: 2347-6710| www.ijirset.com | Impact Factor: 8.423| A Monthly Peer Reviewed & Referred Journal |

|| Volume 13, Issue 3, March 2024 ||

| DOI:10.15680/IJIRSET.2024.1303122 |

TABLE 2: ENERGY AND EXERGY EFFICIENCIES OFAIR-STEAM GASIFICATION FROM ASPEN PLUSMODEL SIMULATION

ER	SBR	T(K)		Energy efficiency (%)		Exergy efficiency (%)	
0.25		0.5	10	00	71.6		47.3
0.45		0.5	10	00	54.4		29.8
0.25		1.5	10	00	66.2		39.7
0.45		0.5	90	00	56.6		31.3
0.15		2.5	90	00	69.4		42.1

Thus, with regard to the highest bio-hydrogen concentration in the syngas mixture, the operating conditions where airsteam gasification can generate syngas containing 34.6% bio-hydrogen holding 7.57 MJ/Nm³ heating value are suggested. The corresponding thermodynamic energy and exergy efficiencies are 69.4% and 42.1%, respectively. However, a SBR value above 1.5 is not recommended for steam-assisted gasification considering its energy efficiency. Thus, at ER=0.15 and SBR=1.5, the highest H₂ concentration predicted is 32.4% from this model.

EXPERIMENTAL VALIDATION OF THE SIMULATION RESULTS

The composition of the product gas is dependent on the type of the gasifier design. Thus, experimental results from BFB [21-23] as well as from fixed bed [24] gasifiers are utilised for the validation of the predicted results. The present model is developed for sawdust since the correlations for pyrolysis products are applicable to this biomass only. In short, in addition to the chemical composition, correlations deduced for pyrolytic yields are executed as FORTRAN subroutines before the DECOMP block to simulate the model for gasification of various feedstocks. The regression equations are developed from the experimental data for pyrolytic yield from the biomass compounds. Comparison of the simulation results with the corresponding experiments [21-24] for air-steam gasification is illustrated in Fig. 6. The deviation of the simulation results from the corresponding experimental results is quantified as Root

Mean Square Error (RMSE). The RMSE values estimated are 6.89, 4.62, 3.78, and 4.41, respectively for gasification of pine sawdust, pine bark, sewage sludge, and waste tire. The predicted results deviate slightly from the experimental results, however within satisfactory limits only.

Uniqueness of the model

The present model is based on the first order reaction scheme for all the major reactions involved in biomass gasification. Moreover, instead of the commonly discussed splitting of the biomass into its constitutive elements for simulating pyrolysis, this study simulates the actual pyrolysis process incorporating the yields of gas, steam, tar and char. The model can simulate the airsteam gasification with chemical composition and moisture of the feedstock, char conversion rate and the values of the operating conditions as inputs. The validation methodology is also unique since pyrolytic yields of the respective biomass compounds are incorporated based on the correlations deduced from experimental results.

IV. CONCLUSIONS

A reaction kinetic model for air-steam gasification of wood sawdust is formulated and simulated in Aspen Plus environment incorporating the necessary chemical reactions involved in air-steam gasification. The influence of the major process variables on performance indicators of gasification are discussed. The gasification system may operate at low ER, higher SBR and medium temperature for augmentation of H_2 in the gas mixture. Maximum biohydrogen concentration predicted is 34.6% at T=900 K, ER=0.15, SBR=2.5 and moisture content=7.7%. The model is validated for gasification of woody and nonwoody biomass materials. The results are found to be deviating slightly (RMSE ranging from 3.786.89), however within satisfactory limits only. The deviation of the results is attributed to the assumptions such as composition of tar and char, adiabatic condition of the process blocks and limitations of the correlations used for predicting pyrolytic products.

e-ISSN: 2319-8753, p-ISSN: 2347-6710| www.ijirset.com | Impact Factor: 8.423| A Monthly Peer Reviewed & Referred Journal |



|| Volume 13, Issue 3, March 2024 ||

| DOI:10.15680/IJIRSET.2024.1303122 |



FIGURE 6. COMPARISON OF SIMULATION RESULTS WITH EXPERIMENTAL RESULTS FROM (A)

[21]

(BIOMASS: PINE SAWDUST, ER: 0.19, SBR: 2.7, T: 1023 K, MOISTURE: 8.0 %, CARBON CONVERSION: 80.6 %) (B) [22] (BIOMASS: PINE BARK, ER: 0.4, SBR: 5.84, T: 1173 K, [24] (BIOMASS: WASTE TIRE, STEAM/AIR: 0.25, T: 973 K, MOISTURE: 0.68 %, CARBON CONVERSION: 80%) MOISTURE: 6.5 %, CARBON CONVERSION: 70.3 %) (D) [23] (BIOMASS: SLUDGE, (A) ER: 0.3, SBR: 0.5, T: 1123 K, MOISTURE: 7.0 %, CARBON CONVERSION: 86.7 %

REFERENCES

- Wallman, P. H., Thorsness, C. B., and Winter, J. D., 1998. "Hydrogen production from wastes". Energy, 23(4), pp. 271-278
- 2. Mathieu, P., and Dubuisson, R., 2002.



|e-ISSN: 2319-8753, p-ISSN: 2347-6710| www.ijirset.com | Impact Factor: 8.423| A Monthly Peer Reviewed & Referred Journal |

|| Volume 13, Issue 3, March 2024 ||

| DOI:10.15680/IJIRSET.2024.1303122 |

- "Performance analysis of a biomass gasifier". Energy conversion and management, 43(9), pp. 1291-1299 [3] Paviet, F., Chazarenc, F., and Tazerout, M., 2009. "Thermo-chemical equilibrium modelling of a biomass gasifying process using Aspen Plus". International Journal of Chemical Reactor Engineering, 7(1), A179 [4] Chen, C., Jin, Y., Yan, J. and Chi, Y., 2010. "Simulation of municipal solid waste gasification for syngas production in fixed bed reactors". Journal of Zhejiang University Science A, 11 (8), pp. 619-628
- Abdelouahed, L., Authier, O., Mauviel, G., Corriou, J. P., Verdier, G., and Dufour, A., 2012. "Detailed modeling of biomass gasification in dual fluidized bed reactors under Aspen Plus". Energy & Fuels, 26(6), pp. 3840-3855 [6] Nikoo, M. B., & Mahinpey, N. (2008). Simulation of biomass gasification in fluidized bed reactor using Aspen Plus. *Biomass and Bioenergy*, 32(12), pp. 1245-1254.
- 5. Murakami, T., Xu, G., Suda, T., Matsuzawa, Y., Tani, H., and Fujimori, T., 2007. "Some process fundamentals of biomass gasification in dual fluidized bed". Fuel, 86(1), pp. 244-255.
- 6. Shen, L., Gao, Y., and Xiao, J., 2008. "Simulation of hydrogen production from biomass gasification in interconnected fluidized beds". Biomass and Bioenergy, 32(2), pp. 120-127
- 7. Dong, C., Liang, H., Zhang, J., and Yang, Y., 2010. "Exergy evaluation of the biomass gasification system for varied fuel type". Proceedings of International Conference on Sustainable Power Generation and
- 8. Supply, 1-6 [10] Zhang, Y., Xiao, J., and Shen, L., 2009. "Simulation of methanol production from biomass gasification in interconnected fluidized beds". Industrial & Engineering
- 9. Chemistry Research, 48(11), pp. 5351-5359 [11] Atnaw, S. M., Sulaiman, S. A., and Yusup, S., 2011. "A simulation study of downdraft gasification of oil-palm fronds using ASPEN PLUS". Journal of Applied
- 10. Sciences, 11(11), pp. 1913-1920
- [12] Renganathan, T., Yadav, M. V., Pushpavanam, S., Voolapalli, R. K., and Cho, Y. S., 2012. "CO₂ utilization for gasification of carbonaceous feedstocks: A thermodynamic analysis". Chemical Engineering Science, 83, pp. 159-170.
- 12. Ji, P., Feng, W., and Chen, B. 2009. "Production of ultra pure hydrogen from biomass gasification with air". Chemical Engineering Science, 64, pp. 582-92
- 13. Inayat, A., Ahmad, M. M., Mutalib, M. I., and Yusup, S., 2012. Process modeling for parametric study on oil palm empty fruit bunch steam gasification for hydrogen production. Fuel Processing Technology, 93(1), pp. 26-34.
- 14. Göransson, K., Söderlind, U., He, J., and Zhang, W., 2011. "Review of syngas production via biomass DFBGs".
- 15. Renewable and Sustainable Energy Reviews, 15(1), pp. 482492
- 16. Mullen, C. A., Boateng, A. A., Goldberg, N. M., Lima, I. M., Laird, D. A., and Hicks, K. B., 2010. "Bio-oil and bio-char production from corn cobs and stover by fast pyrolysis". Biomass and Bioenergy, 34(1), pp. 67-74 [17] Sommariva, S., Grana, R., Maffei, T., Pierucci, S., and Ranzi, E., 2011. "A kinetic approach to the mathematical model of fixed bed gasifiers. Computers & Chemical Engineering, 35(5), pp. 928-935
- 17. Gerber, S., Behrendt, F., and Oevermann, M., 2010. "An Eulerian modeling approach of wood gasification in a bubbling fluidized bed reactor using char as bed material". Fuel, 89(10), pp. 2903-2917
- Lotrič, A., Sekavčnik, M., Kunze, C., and Spliethoff, H., 2011. "Simulation of water-gas shift membrane reactor for integrated gasification combined cycle plant with CO₂ capture". Strojniški vestnik-Journal of Mechanical Engineering, 57(12), pp. 911-926
- 19. Groppi, G., Tronconi, E., Forzatti, P., and Berg, M., 2000. "Mathematical modelling of catalytic combustors fuelled by gasified biomasses". Catalysis Today, 59(1), pp. 151-162
- Lv, P., Chang, J., Wang, T., Fu, Y., Chen, Y., and Zhu, J., 2004. "Hydrogen-rich gas production from biomass catalytic gasification". Energy & Fuels, 18(1), pp. 228-233 [22] Andres, D. J. M., Narros, A., and Rodríguez, M. E., 2011. "Behaviour of dolomite, olivine and alumina as primary catalysts in air-steam gasification of sewage sludge". Fuel, 90(2), pp. 521-527
- Karatas, H., Olgun, H., and Akgun, F., 2012. "Experimental results of gasification of waste tire with air&CO₂, air & steam and steam in a bubbling fluidized bed gasifier". Fuel Processing Technology, 102, pp. 166-174
- 22. Hanaoka, T., Inoue, S., Uno, S., Ogi, T., and Minowa, T., 2005. "Effect of woody biomass components on airsteam gasification". Biomass and bioenergy, 28(1), pp. 6976









INTERNATIONAL JOURNAL OF INNOVATIVE RESEARCH

IN SCIENCE | ENGINEERING | TECHNOLOGY





www.ijirset.com