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Simulation of a Circulating Fluidised Bed Biomass Gasifier Using ASPEN Plus – A Performance Analysis

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ABSTRACT: In the near future biomass gasification is likely to play an important role in energy production and conversion. Its application has great potential in the context of climate change mitigation, increasing efficiency and energy security. Atmospheric circulating fluidised bed (CFB) technology was selected for the current study. An original computer simulation model of a CFB biomass gasifier was developed using ASPEN Plus (Advanced System for Process ENgineering Plus). It is based on Gibbs free energy minimisation and the restricted equilibrium method was used to calibrate it against experimental data. This was achieved by specifying the temperature approach for the gasification reactions. The model predicts syn-gas composition, heating values and conversion efficiency in good agreement with published experimental data. Operating parameters such as equivalence ratio (ER), temperature, and air preheating were varied over a wide range. They were found to have great influence on syn-gas composition, heating value, and conversion efficiency. The results indicate an ER and temperature range over which hydrogen (H₂) and carbon monoxide (CO) production is maximised, which is desirable as it ensures a high heating value and cold gas efficiency (CGE). Gas heating value was found to decrease with increasing ER. Air preheating increases H₂ and CO production, which in turn increases gas heating value and gasifier CGE. The effectiveness of air preheating decreases with increasing ER. A critical air temperature exists after which additional preheating has little influence, this temperature is high for low ERs and low for high ERs.

Keywords: biomass gasification, circulating fluidised bed, simulation, ASPEN Plus

1. INTRODUCTION

Biomass is of major interest as a source of renewable energy. Currently energy is recovered from biomass through combustion. The efficiency of these plants is approximately 20 to 25%. For utilisation of coal, current plants achieve efficiencies of 30 to 35%. Coal gasification integrated with gas turbines and fuel cells offers much

higher efficiencies of up to 60%. Gasification is more energy efficient than conventional technology and it makes the utilisation of biomass for electricity generation a more feasible option.

Climate change is now recognised as perhaps the most significant policy issue internationally. Global warming, caused by the release of carbon dioxide (CO₂) and hydrocarbons into the atmosphere, is one of

the underlying reasons for the rising profile of biomass in world energy affairs. For gasification of fossil fuels, e.g. coal, emissions can be drastically reduced when compared to traditional power plants. This is due to increased efficiency and because the fuel input has been converted to gaseous form, making it possible to remove the contaminants that cause the emissions prior to combustion.

Energy security is of utmost importance and is vital for any country's continued economic growth. According to a recent study oil and gas prices are set to double by 2050 [1]. Also global energy demand is set to more than double by the middle of the century. Biomass gasification coupled with other renewable energy options would cut dependency on imported energy and would help to ensure energy security.

Gasification is a process for converting carbonaceous materials to a combustible or synthetic gas [2]. It occurs when oxygen (O₂) or air and steam or water is reacted at high temperatures with available carbon in biomass or other carbonaceous material within a gasifier. The syn-gas produced can be combusted in an engine or gas turbine or even utilised in a fuel cell to generate electricity and heat. Air gasification produces a poor quality gas with regard to the heating value, around 4-7 MJ/Nm³ higher heating value (HHV), while O₂ and steam blown processes result in a syn-gas with a heating value in the range of 10-18 MJ/Nm³ (HHV) [3]. Gasification with pure O₂ is not practical for biomass gasification due to prohibitively high costs for O₂ production using current commercial technology. Therefore, air gasification was modelled in this work.

The basis of gasification is to supply less oxidant than would be required for stoichiometric combustion of a solid fuel. The resulting chemical reactions produce a mixture of CO and H₂ (syn-gas), both of which are combustible. The energy value of this gaseous fuel is typically 75% of the chemical heating value of the original solid

fuel. In addition, the syn-gas temperature will be substantially higher than the original solid fuel due to the gasification process. The process of biomass gasification may be represented by the reactions given in Table I:

Table I: Gasification reactions.

Reaction	Reaction number
$C + 0.5O_2 = CO$	(R1)
$C + CO_2 \leftrightarrow 2CO$	(R2)
$C + H_2O \leftrightarrow CO + H_2$	(R3)
$C + 2H_2 \leftrightarrow CH_4$	(R4)
$CO + 0.5O_2 = CO_2$	(R5)
$H_2 + 0.5O_2 = H_2O$	(R6)
$CO + H_2O \leftrightarrow CO_2 + H_2$	(R7)
$CH_4 + H_2O \leftrightarrow CO + 3H_2$	(R8)
$H_2 + S = H_2S$	(R9)
$0.5N_2 + 1.5H_2 \leftrightarrow NH_3$	(R10)

The gasification process can be split into three linked processes; pyrolysis, gasification, and partial combustion. Partial combustion is necessary because it supplies the heat required by the endothermic gasification reactions. Pyrolysis occurs in a temperature range of 350-800°C and results in the production of char, CO, H₂, methane (CH₄), CO₂, H₂O, tars and hydrocarbons. These products are then used in the gasification and combustion reactions.

The objective of this research is to develop a computer simulation model of a CFB biomass gasifier that can accurately predict gasifier performance under various operating conditions. In this paper an original model of a biomass CFB gasifier developed using ASPEN Plus is presented. The model is based on Gibbs free energy minimisation. The approach assumes that only a limited number of chemical reactions (R1 to R10) are required to predict syn-gas composition, gas heating value and process efficiency. The influence of operating conditions on gasifier performance was investigated and the results and conclusions from these investigations are presented. This

work is part of a wider research on the integration of biomass gasification with high temperature fuel cells.

2. METHODOLOGY

2.1 Gasifier Classification and Selection

Gasifiers are classified in terms of the movement of the fuel through the vessel, the operating pressure and temperature and the size and condition of the entering fuel. The primary configurations are moving/fixed bed, fluidised bed and entrained flow.

Maniatis [4] found that atmospheric CFB technology is the most attractive in view of the market and technology strength. Maniatis [4] considered atmospheric and pressurised CFB and bubbling fluidised bed (BFB), updraft and downdraft fixed bed, and entrained flow technology.

Atmospheric CFB technology was selected for the current study as it is proven for biomass gasification, the most attractive in terms of technology strength and market attractiveness, has potential for scale-up (low MW to over 100 MW), and high fuel flexibility.

2.2 Simulation Software

ASPEN Plus was selected for modelling the gasifier. It is a steady state chemical process simulator, which was developed to evaluate synthetic fuel technologies. It uses unit operation blocks, which are models of specific process operations (reactors,

heaters, pumps etc.). The user places these blocks on a flowsheet, specifying material and energy streams. An extensive built in physical properties database is used for the simulation calculations. ASPEN Plus has the capability to incorporate Fortran code into the model. This feature is utilised for the definition of non-conventional fuels, e.g. biomass, specific coals and for ensuring the system operates within user defined limits and constraints. The development of a model in ASPEN Plus involves the following steps:

- (1) Stream class specification and property method selection.
- (2) System component specification (from databank).
- (3) Defining the process flowsheet (unit operation blocks and connecting material and energy streams).
- (4) Specifying feed streams (flow rate, composition, and thermodynamic condition).
- (5) Specifying unit operation blocks (thermodynamic condition, chemical reactions etc.).

3. MODELLING

3.1 ASPEN Plus Flowsheet

Fig. 1 displays the CFB biomass gasifier ASPEN Plus flowsheet.

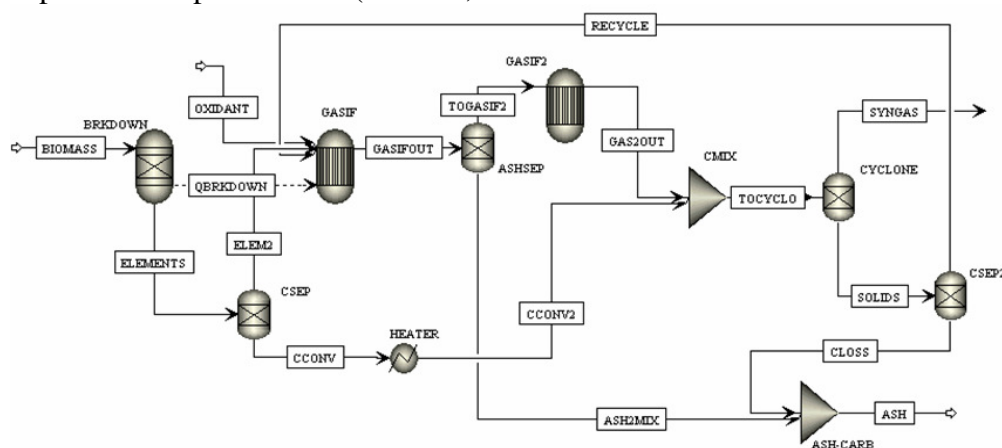


Figure 1: ASEPN Plus flowsheet of CFB biomass gasifier.

3.2 Model Description

Referring to Fig. 1, the stream 'BIOMASS' was specified as a non-conventional stream and the ultimate and proximate analyses were inputted as well as the thermodynamic condition and mass flow rate. The block 'BRKDOWN' yields are set by a calculator block, which in turn determines the mass flow of each component in the block outlet stream 'ELEMENTS'. The enthalpy of this stream will not equal the enthalpy of the feed stream 'BIOMASS', the heat stream 'QBRKDOWN' adds back the enthalpy loss to the system.

The function of the next block is to simulate carbon conversion by separating out a specified portion of the carbon from the fuel. The 'HEATER' block brings this carbon up to the gasifier temperature. The un-reacted carbon represents solids contained in the product gas that must be removed by the CFB gasifier cyclone.

The streams 'ELEM2', 'OXIDANT', and 'RECYCLE' enter the block 'GASIF', where pyrolysis, partial oxidation, and gasification reactions occur. The oxidant (air) mass flow is set using a user specified ER. ER is defined as the amount of air added relative to the amount of air required for stoichiometric combustion [5]. Most existing fluidised bed biomass gasifiers operate in the ER range 0.2-0.45 [6].

Ash removal is simulated using the block 'ASHSEP'. The material stream 'TOGASIF2' is fed to the block 'GASIF2', where the temperature approach is specified for reactions (R7), (R8) and (R10), which restricts equilibrium and means that the syn-gas composition is adjusted to match data reported in the literature.

The next block mixes the un-reacted carbon that was separated upstream with the gas from 'GASIF2' and its product stream is fed to a separator that simulates the CFB gasifier cyclone. The bottom outlet stream from 'CYCLONE' with the stream name 'SOLIDS' is composed of solid carbon only and is sent to a separator block 'CSEP2'.

The top outlet stream, which is called 'SYNGAS', is composed of all the gases from 'GASIF2' and a small amount of solid carbon and represents the final output from the gasifier.

'CSEP2' splits the 'SOLIDS' stream into a recycle stream 'RECYCLE', that is sent back through the gasifier, and another stream named 'CLOSS', which represents the carbon lost from the system in the ash. The stream 'CLOSS' is then mixed with the ash in the block 'ASH-CARB'.

The following is a list of all model assumptions:

- Steady state conditions.
- One-dimensional model.
- Isothermal (uniform bed temperature).
- Drying and pyrolysis instantaneous.
- Char is 100% carbon (graphite).
- All sulphur reacts to form H₂S [3].
- Only NH₃ formed no NO_x [3].
- Cyclone separation efficiency 85%.
- 2% carbon loss in ash [7].

3.3 Model Validation

The model was validated against the experiments of Li et al. [7]. The fuel used for model validation was hemlock wood with ultimate analysis: carbon 51.8, hydrogen 6.2, oxygen 40.6, nitrogen 0.6, sulphur 0.38, ash 0.4 and proximate analysis: volatile matter 84.8, fixed carbon 14.8, ash 0.4 (all dry wt. % basis) [7, 8]. Moisture content was 11.7 wt. % and the HHV was 20.3 MJ/kg dry basis [7].

The input data for the model are as follows [7]:

- Input fuel stream mass flow: 33.626 kg/hr
- Gasification temperature: 991 K
- Gasification pressure: 1.05 bar

Table II compares the experimental results as reported by Li et al. [7] to the model predictions using the input data presented above.

Table II: Experimental results versus model predictions

	Experimental	Model
Gas comp. (vol. %, dry)		
H ₂	5.5	5.53
N ₂	59.5	55.42
CO	16.6	16.79
CH ₄	3.4	7.65
CO ₂	15.0	14.62
HHV (MJ/Nm ³ , dry)	4.82	5.87
CGE (%)	71.4	62.61

The model predictions are in satisfactory agreement with the experimental data. For example H₂, CO and CO₂ are predicted within 2.5%. However the CH₄ is over-predicted, which causes an error in the calculation of the gas heating value and CGE. The under or over-prediction of CH₄ is a common problem for modellers; one example is the steady state model of a biomass downdraft gasifier done by Giltrap et al. [9], where CH₄ was over-predicted by a substantial amount, furthermore Prins et al. [10] stated that the product gas from fluidised bed gasifiers generally contains much more CH₄ than predicted. The low operating temperature (991 K) results in high CH₄ content, it will be seen in the next section that CH₄ content decreases rapidly with temperature (at ~870°C the model predicts virtually zero CH₄).

4. RESULTS AND DISCUSSION

Sensitivity analyses were performed to investigate the effects of varying ER, temperature, and level of air preheating on product gas composition, gas heating value, and CGE. During the sensitivity analyses the model input data was kept the same as for model validation with one parameter being varied at any given time. The CGE

(η_{CGE}) is a means of indicating a gasifier's performance and is defined as:

$$\eta_{CGE} = \frac{\dot{m}_{gas} \cdot LHV_{gas}}{\dot{m}_{fuel} \cdot LHV_{fuel}}$$

Where \dot{m}_{gas} and \dot{m}_{fuel} are the mass flow rate (in kg/s) of the gas and unconverted fuel respectively and LHV_{gas} and LHV_{fuel} are the lower heating value (in kJ/kg) of the gas and unconverted fuel respectively.

4.1 Effect of Gasification Temperature (T_g) and ER

The influence of T_g on product gas composition is illustrated in Fig. 2. T_g depends on the air flow, i.e. it is controlled by the ER. Therefore, varying ER or T_g will have the same effect on product gas composition, heating value, and CGE. The corresponding temperatures for ERs between 0.29 and 0.45 are given. In Fig. 2 H₂, H₂O, CO, CO₂, and CH₄ are plotted, with H₂S and NH₃ omitted. Nitrogen (N₂) content may be calculated by summing the other components and subtracting this from 100%. It varied between 53 and 61% over the T_g /ER range. The most interesting point from examination of Fig. 2 is that both H₂ and CO reach a maximum at a temperature of 874°C or at an ER of 0.35, after which their contents decrease steadily. H₂O increases over the whole range but experiences a small decrease close to the H₂ and CO peak. CO₂ decreases rapidly up to a temperature of 874°C and then increases slowly. CH₄ decreases and eventually reaches zero between a temperature of 1046 and 1195°C (ER of 0.4 and 0.45). These trends may be explained as follows:

- Reaction (R2) is endothermic; therefore, as temperature rises so to does the amount of CO₂ reacted with char to produce CO. For temperatures up to 874°C sufficient char is available for the reaction but not for higher temperatures

and as a result CO decreases and CO₂ increases.

- Reaction (R3) is endothermic, which means for increasing temperature and ER CO and H₂ production are increased and more char and H₂O are consumed.
- Reaction (R4) is exothermic, which means as T_g and ER increase the production of CH₄ decreases leaving more H₂ in the gas.
- CO is reacted with available O₂ (R5) producing CO₂.
- H₂ reacts with O₂ (R6) producing H₂O. Reaction (R6) produces more water than is consumed by reactions (R3) and (R8) because the H₂O content increases over the whole T_g/ER range. The slight H₂O drop occurs at a T_g of 837°C and ER of 0.34. One possible explanation is that at sufficient temperature reaction (R8) consumes more water than is produced by reaction (R6); however, this is short-lived because the other reactant, CH₄ is decreasing rapidly.
- Reaction (R7) being exothermic, produces less CO₂ and H₂ at higher temperatures, which means less CO and H₂O are consumed.
- CH₄ is reduced by reaction (R8). This reaction is endothermic meaning the forward reaction is favoured as temperature increases. Hence, CH₄ and H₂O decrease while H₂ and CO increase.

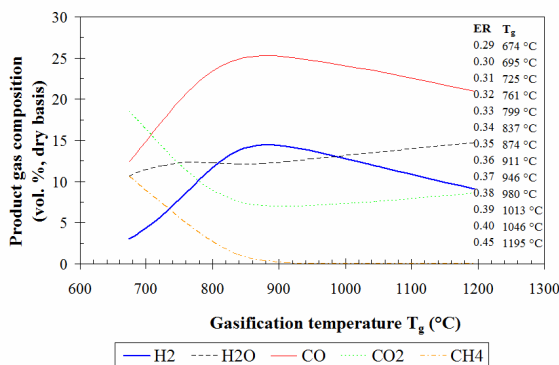


Figure 2: Effect of T_g on product gas composition.

The influence of ER on gas heating value and CGE is shown in Fig. 3. The gas LHV (mass basis) and the CGE (LHV basis) are plotted against ER. It is evident that the LHV decreases with increasing ER. The LHV is high for low ERs due to high CH₄ content. The CGE increases between ER = 0.29 to 0.34, reaches a maximum of 66.7% at ER = 0.34 and then decreases steadily. It is worth noting that the CGE peak corresponds to the point of maximum H₂ and CO content in Fig. 2. The CGE for ER = 0.31 as reported by Li et al. [7] is indicated. It is indicated for comparison with the model prediction at the same ER value.

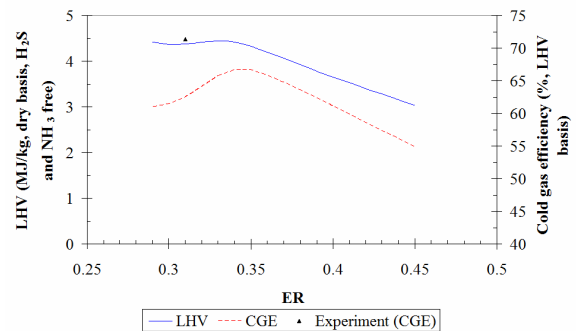


Figure 3: Effect of ER on gas LHV (mass basis) and CGE (LHV basis). ▲: indicates CGE as reported by Li et al. [7].

4.2 Effect of Air Preheating

Air preheating is a means of increasing the conversion efficiency of the gasification process. The sensible heat in the air causes a rise in the gasification temperature, which influences the gas composition, the gas LHV and hence the gasifier CGE. It's an alternate and more economical approach to O₂ blown systems and it achieves downsizing of the plant, which in turn reduces costs.

The influence of air preheating on T_g was investigated over the complete ER range. T_g increases almost linearly with air temperature (T_a). It was discovered that a limit on the level of air preheating exists for each ER. This level is limited by the effectiveness of the heat exchange equipment but is also limited by the

operating temperature constraint of fluidised beds. Fluidised bed biomass gasifiers should not be operated over 1000°C, so as to ensure that the ash melting temperature is not reached. For an ER of 0.37 a T_a no more than 114°C would be recommended because the corresponding T_g is 987°C whereas for ER = 0.29 the air could in theory be heated to 825°C as the T_g stays below the limit at 978°C.

The influence of T_a on gas composition is shown in Fig. 4. The gas composition for ER = 0.3 is plotted against T_a . The gas composition changes reflect the change in T_g . The rising temperature promotes the products of the endothermic reactions, (R2), (R3) and (R8), and simultaneously the reactants of the exothermic reactions (R4) and (R7). It was found that T_a has a greater influence on gas composition for low ERs. For ER = 0.3 CO and H₂ content increases 14.8 and 14 percentage points respectively whereas for ER = 0.34 CO and H₂ content increases by only 2.7 and 1.8 percentage points respectively over the same T_a range. It was also found that T_a has a significant influence on composition only up to a certain level, after which additional preheating has little effect. For ER = 0.3 this T_a is high at a value of ~560°C but for ER = 0.34 it is significantly lower at ~200°C. This finding agrees with published work [11, 12]. Yang et al. [12] refers to a critical T_a above which air preheating is no longer efficient if the purpose is to maximise the yield of gaseous products. This critical T_a was reported as 530°C. The results of this work indicate a critical temperature of ~560°C for an ER of 0.3.

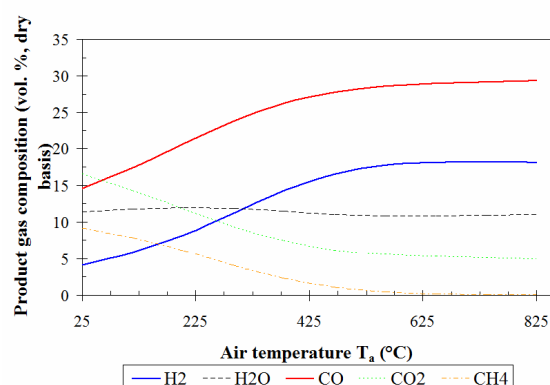


Figure 4: Effect of T_a on product gas composition for ER = 0.3.

The influence of air preheating on gas LHV and CGE was investigated. As expected, the gas LHV increases with T_a . The increase is in line with the gas composition change for each ER, i.e. the increase is greater for low ERs. The effect of T_a on CGE (LHV basis) is illustrated in Fig. 5. The CGE trends are in agreement with the changes in gas composition and LHV. T_a has a significant influence on CGE at low ER values. Its influence ceases for ERs greater than 0.35. As already seen for gas composition, T_a has a significant effect on CGE only up to a certain level, after which additional preheating has little influence. For ER = 0.29 this T_a is high at a value of ~650°C but for ER = 0.35 it is significantly lower at ~114°C.

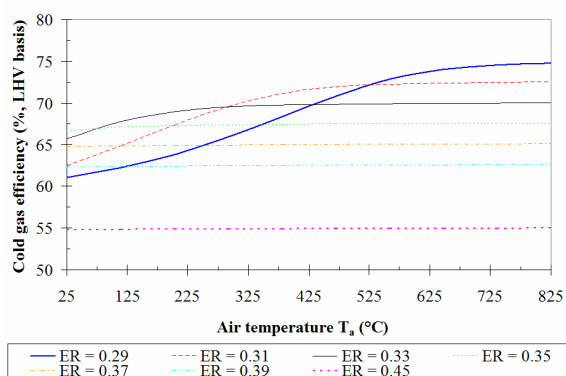


Figure 5: Effect of T_a on CGE (LHV basis) for complete ER range.

5. CONCLUSIONS

A CFB biomass gasifier model was developed using ASPEN Plus. The results obtained from the sensitivity analyses are in good agreement with published work. Therefore, the model is capable of predicting accurately gasifier performance over a wide range of operating conditions. The influence of ER, temperature, and level of air preheating on gas composition, heating value, and CGE were investigated, the results of which revealed the following:

- Without air preheating, optimum operating conditions are: ER = 0.34 to 0.35 and $T_g = 837$ to 874°C .
- Syn-gas LHV decreases with ER.
- Without air preheating, CGE reaches a peak of 66.7% at ER = 0.34.
- Air preheating increases production of H_2 and CO, which improves gas LHV and CGE.
- Air preheating is more effective at low ERs and should not be used for ERs greater than 0.35.
- A critical T_a exists after which additional preheating has little influence. This temperature is high for low ERs and low for high ERs.

In a future study, this CFB biomass gasifier model will be integrated with a high temperature fuel cell stack model and balance of plant models all developed in ASPEN Plus.

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