Aspen HYSYS simulation of biomass pyrolysis for the production of methanol

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Abstract. In terms of supplying energy carriers for the transport sector and storing electricity outflows from intermittent sources, the importance of renewable fuel production has become significant. In this work, the production of methanol fuel from biomass is simulated. Biomass is an excellent renewable resource for the production of methanol. It is of utmost importance to make effective use of biomass resources. There are different methods available for the production of methanol from biomass. One of the best methods is pyrolysis to convert biomass into methanol. This is due to the fact that pyrolysis is an efficient conversion method compared to other thermochemical conversion practices. Pyrolysis is the process of decomposing biomass in an inert atmosphere to convert it into worthwhile products. The production of methanol from sugarcane bagasse via pyrolysis was simulated using Aspen HYSYS because of its ability to solve chemical as well as energy problems. To simulate the microwave assisted pyrolysis reactor, an Aspen HYSYS model was developed. The model is based on Gibbs free energy and it has been calibrated using the restricted equilibrium method. The model was validated and foresees the percentage of methanol yield, the predicted values very well agreed with the available data. Important parameters of the pyrolysis process such as pyrolysis temperature, sweeping nitrogen gas flow rate, heating rate, biomass moisture content were varied. It was found that pyrolysis temperature, nitrogen flow rate, heating rate have a very profound influence on the pyrolysis process and methanol yield, while the moisture content of biomass had a lesser impact.

Key Word: Aspen HYSYS; Biomass; sugarcane bagasse; methanol; pyrolysis; simulation.

1. Introduction

Methanol is a promising renewable fuel that has very less carbon emissions contrasted with traditional fossil fuels [1]. Agricultural, municipal, and biowaste produced throughout the country could be used to produce methanol and the energy produced from this methanol could supply 9-23% of the electrical energy used up in four states of the country mentioned above. The utilization of methanol could decrease carbon outflows by engine vehicles by up to 79% just as up to 31% of carbon emanations, if methanol-enhanced fuel cells were utilized to produce power [2].

There are different methods available for the production of methanol from biomass. One of the best methods is pyrolysis to convert biomass into methanol [3]. This is due to the fact that pyrolysis is an efficient conversion method compared to other thermochemical conversion practices. Pyrolysis is...
the process of decomposing biomass in an inert atmosphere to convert it into worthwhile products. The creators showed that methanol was more profitable part in pyrolysis fluid and might be a conceivable substitution for traditional gas or diesel fuel. Methanol obtained as a result of pyrolysis, officially used as a fuel or part of fuel. [4]. The objective of this research was to simulate the production of methanol from sugarcane bagasse by microwave assisted pyrolysis process. This study also analyzed the effect of varying the parameters of the pyrolysis process such as pyrolysis temperature, sweeping nitrogen gas flow rate, heating rate, biomass moisture content on the yield of methanol.

Several researchers used Aspen HYSYS process simulator to simulate the pyrolysis reactor and gasifier [5,6]; Even so, the simulation made on the production of methanol from biomass pyrolysis is limited. An Aspen HYSYS model was used by Mansaray et al. [6] to predict the pyrolysis of biomass based on chemical equilibrium, energy equilibrium and equilibrium of components. Due to the presence of highly volatile material in biomass and the intricacy of kinetics in the biomass reaction rate in fluidized beds, they disregarded the formation of char and analyzed the process on the assumption of biomass pyrolysis tends to follow Gibbs equilibrium.

The ultimate purpose behind this research is to incorporate simulation to accurately predict the steady-state performance of a microwave assisted pyrolysis process by considering the reaction rate kinetics. Gibbs equilibrium defines the products of homogeneous reactions and kinetics are used to define exactly the pyrolysis products. This article illustrates the specifics of modelling strategies taken to acquire process computation for biomass pyrolysis in a microwave assisted pyrolysis reactor.

2. Modelling and simulation

The Aspen HYSYS flowsheet of the pyrolysis process for methanol production is portrayed in Fig. 1. The model is constructed based on the following key premises: Stable operation; zero-dimensional; ambient pressure; ideal gases; negligible drop of pressure; char is purely of carbon (C); pyrolysis process is prompt; the formation of tar is not taken into account; Pyrolysis reactor heat loss is neglected.

The state equation of Peng - Robinson was chosen as the property algorithm for the framework. Referring to Fig.1. non-traditional stream of sugarcane bagasse stated as ‘BIOMASS’ various properties of sugarcane bagasse were entered. Lower heating value of the chosen biomass was also quantified. Subsequently, the thermodynamic state of the stream (1 atm and 28 ° C) and the mass flow rate were inputted. The pressure was set to 1 atm for all the feed streams and unit operating blocks (i.e. There is no pressure drop). In this simulation R-Gibbs minimum energy reactor was used and named as ‘PYRO-RE’. The different yields of the pyrolysis reactor obtained from sugarcane bagasse were determined using a calculator block.

Fig 1. Pyrolysis process Aspen HYSYS flowsheet.
The outlet stream “VAP” from the pyrolysis reactor “PYRO-RE” is fed into a condenser “COND” whose purpose to condense the pyrolysis vapour into fuel oil and some non-condensable gas will also come out.

3. Results and Discussion

To analyze the susceptibility of the primary operating parameters with regard to pyrolysis reactor performance the evaluated model was used. Important parameters including pyrolysis temperature, nitrogen flow rate, heating rate, biomass moisture content. Sensitivity analysis was done by keeping input data same as used for the model validation and at any given time a single parameter was varied.

3.1. Sensitivity analysis; Pyrolysis temperature

Figure 2 shows the influence of pyrolysis temperature on the percentage of methanol yield. Pyrolysis temperature is varied from 300-590 °C and it shows that pyrolysis temperature has a very strong influence on pyrolysis yield. Fixed bed sugarcane bagasse pyrolysis reactor should be operated above 300 °C to ensure the yield formation. There is no yield formation below 300 °C as it can be seen from the simulation result and maximum yield is obtained at around 450°C even if pyrolysis temperature is increased beyond 450°C, there will be no change in yield percentage so we can conclude that optimum temperature for the methanol production from biomass is around 450°C.

![Fig.2. Variation of yield percentage with pyrolysis temperature (°C).](image)

3.2. Sensitivity analysis; Nitrogen flow rate

After pyrolysis temperature, flow rate of nitrogen supplied for purging the reactor vessel to create inert atmosphere and to drive out the pyrolysis vapour has a great influence on pyrolysis yield. When the nitrogen flow rate is low residence time of pyrolysis vapour inside the reactor vessel increases so the methanol oil yield will be less, on the other hand if the flow rate increased above optimum range then also oil yield will decrease because of less time available for the condensation. Maximum methanol yield was around 6.42 % at the nitrogen flow rate of 200 cc/min.
3.3 Sensitivity analysis; Heating rate
Simulation has been done for different heating rates (10 K/min, 20 K/min, 30 K/min) variation of methanol yield is shown in figure 4. Optimum heating rate was found to be 10 K/min and the corresponding methanol production was 6.36% on weight basis.

3.4 Sensitivity analysis; moisture content of biomass
Moisture content of the biomass has no significant effect on methanol yield as it can be seen in the figure 5 given below.
Fig. 5. Methanol yield for different percentage of moistures.

4. Conclusion
The objective of the research work was to develop a pyrolysis reactor model and to use the same for investigating the impact of main operating parameters on reactor performance. A pyrolysis reactor computer simulation model was developed using Aspen HYSYS and results were obtained varying operating parameters. The findings revealed the following: pyrolysis temperature, nitrogen flow rate, heating rate are the most important methanol yield variables; the pyrolysis process must be done in the temperature range of 400 – 500°C, nitrogen flow rate of 200 cc/min, and the heating rate of 10 K/min. The simulation showed that the maximum percentage of methanol yield from sugarcane bagasse is around 6.42 % on the weight basis.

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