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Research paper

A multicriteria comparison of utilizing sugar cane bagasse for methanol to gasoline and butanol production

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ABSTRACT

The present study makes a consistent and comparative assessment of the overall exergy, financial and environmental efficiencies of two biomass-to-fuels (utilised in internal combustion engines with spark ignition) conversion options and based on this result, gives a recommendation as to which of the options assessed is most desirable. These options are methanol to gasoline (MTG) and biochemical butanol, while as feedstock the solid residue of sugar cane, bagasse, was considered. For the work presented in this study, a base case scenario has first been developed for each pathway by employing either Aspen Plus or SuperPro Designer (as simulators) to perform mass and energy balance calculations while Matlab software has been used for modelling the reaction kinetics of each process. Based on the simulations, thermodynamic (exergy analysis), economic (financial and risk analysis) and environmental (CO_2 emissions) evaluations were carried out. Afterwards, sensitivity analyses have been performed in order to define the key parameters of each conversion route. Exergy and economic analysis favour the gasoline production while butanol produces less CO_2 emissions. The study concludes with multicriteria decision analysis (MCDA) where each process is issued a score according to the investigated criteria. This makes it possible for the investigated procedures to be compared on the same basis. According to this analysis, the production of gasoline achieves a higher overall score than butanol production, i.e. 97% and 90% respectively.

1. Introduction

In the last three decades, the pressing issue of energy security, fossil fuel price volatility, increasing awareness of global warming, and prevailing legislations confining the use of non-renewable energy sources have warranted a tremendous interest in, and growth of, the bioenergy industry. Additionally the manufacture of biofuels may contribute to the local economic growth [1]. In view of these and the related, inevitable, depletion of fossil reserves, the biorefinery concept has recently emerged. The focal aim of biorefineries is the integration of biomass conversion processes for the sustainable production of biofuels with the aim of substituting petroleum derived fuels such as gasoline, diesel and kerosene [2]. Resultant technologies producing first generation (1G) biofuels are already well-established; however exploitation of lignocellulosic biomass derived from forestry or agricultural residues, including bagasse, can positively contribute to the renewable production of biofuels and building block chemicals without competing for land [3]. Several studies have already raised the issue of waste utilization for developing a sustainable biofuel sector [4–6]. Sugar cane milling processes for ethanol or sugar production leave approximately 250 kg of solid residue bagasse for every tonne of raw sugar cane processed which can eventually be utilised as feedstock for biofuels production [7,8].

Traditionally, ethanol from sugarcane or corn has been recognised as the principal biofuel for the gasoline market. Nevertheless ethanol has some properties that make it somewhat incompatible with existing fuel distribution and motor vehicle infrastructure. The properties of butanol make it a more attractive fuel for blending with gasoline or for use directly in place of it. The advantages it has over ethanol include lower vapour pressure (thus safer to handle), higher flash point, decreased corrosiveness and decreased miscibility with water. It can be shipped and distributed through existing pipelines and filling stations and has a higher energy density (closer to that of gasoline) [9]. Thus, in this study, due to their high energy densities and compatibility with existing infrastructure,

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gasoline and butanol were chosen as the desired fuels to be produced in the bioenergy conversion routes evaluated. They are both advanced biofuels and as such they have been targeted to make a major contribution to the total amount of renewable fuels produced in the next 20 years [10].

Butanol is usually synthesised from fossil fuels. However, biomass can also be used as feedstock for butanol production. These feedstocks are the same as for ethanol and include corn, sugar beets, and lignocellulosic material [11]. The industry (for example DuPont, BP, or Cobalt Biofuels) has also shown interest in so-called 'biobutanol' generation and some facilities have already started operation [9]. The core stage of the process is the acetone-butanol-ethanol (ABE) fermentation of sugars catalysed by strains of Clostridium acetobutylicum In the case of lignocellulosic biomass processing, the addition of a pretreatment step to crack down the lignin structure is essential. During ABE fermentation, butanol, acetone, and ethanol are produced in a molar ratio of 6:3:1. This specification limits butanol productivity with researchers, nowadays, focusing on changing the metabolic pathway and selectively increase the butanol yields [12].

Methanol is one of the most significant platform chemicals, used as feedstock for the production of formaldehyde, propylene, dimethyl ether, plastics, acetic acid and other chemicals. Huge amounts of methanol are also used to produce gasoline additive methyl tert-butyl ether (MTBE). Currently, methanol is chiefly synthesised in low temperature (200–300 °C), high pressure (5–10 MPa) packed bed reactors, using a syngas feed. The main global producer is Lurgi [13]. Methanol can be used as fuel additive but can also be converted to gasoline in fluidized bed reactors over a zeolite based catalyst. The methanol to gasoline (MTG) process was first developed by Mobil Oil in the late 1970s. Nowadays, ExxonMobil produces 7000 barrels per day in 15 plants located in West Virginia, USA [14]. Syngas is principally derived from conventional sources such as coal and natural gas. In this framework, the design of alternative and based on renewable feedstocks MTG production processes is essential.

Recently, several studies conducted techoeconomic analysis on butanol production but they were limited to calculating the economic performance of the process without considering the energy efficiency and the environmental impact of the process [15–17]. The production cost for butanol is in the range of 0.59–0.75 $ kg^{-1}. Furthermore, butanol feasibility was mainly compared to ethanol. The main outcome from this comparison can be summarized as that butanol can be produced at higher energy efficiencies than ethanol but it provides lower profits [18,19]. Regarding the MTG process, the National Renewable Energy Laboratory (NREL) and the Pacific Northwest National Laboratory (PNLL) have conducted feasibility studies on gasoline production via the MTG pathway from biomass derived syngas. The main focus of these studies was to design comprehensive process models and subsequently to calculate the gasoline production cost which according to the NREL was equal to 16.73 $ GJ^{-1} and 17.46 $ GJ^{-1} based on the PNNL [20,21]. Kempegowda et al. [22] have also conducted a detailed technoeconomic analysis of biomethanol production which results in a positive net present value (NPV) of 600 $ t^{-1} but upgrade to gasoline was beyond the scope of that study.

As a result of a literature review, it was concluded that the assessment of biochemical butanol and MTG production process were carried out mainly based on economic criteria. Thus, the study presented here was focused on integrating exhaustive process simulations, thorough exergetic, economic and environmental calculations to evaluate and compare the sustainability of the investigated processes, and eventually suggest the best alternative. This methodology provides a robust mechanism and can be used as a reliable decision making tool.

2. Methodology

The scope of the study was to evaluate and compare two process scenarios for the exploitation of bagasse in a novel and sustainable manner with the aim of contributing to the development and establishment of a reliable biorefinery sector. Butanol and gasoline derived from biomass are direct biofuel competitors for the petrol gasoline market. These options were designed, evaluated and compared within an integrated framework. Sugarcane bagasse was selected as feedstock due to its availability and the fact that it is a waste and as such is readily accessible, provides no food or land competition (unlike first generation feedstocks) and reduce waste management problems. The synthesis of the study is illustrated in Fig. 1.

2.1. Process modelling

The Aspen Plus simulation package was used to model the thermochemical conversion route (MTG process) and SuperPro designer the production of biochemical butanol. The reactor models have been developed in the Matlab environment due to the insufficient kinetic options provided directly in the simulators. The outputs of the reactor kinetic analysis have been transferred as inputs to the simulators via a VBA Excel Macro by taking advantage of Microsoft's COM technology for software interaction. The inlet mass flow rate for all the cases was set equal to 100 t h^{-1}. User defined non-conventional solids were determined to symbolize bagasse and ash. Aimed at those modules, two Aspen models were allocated: one for the density (DCOALIGT) and the second one enthalpy (HCOALGEN) that necessitates awareness of proximate analysis and ultimate analysis of the bagasse [23].

2.2. Feedstock and non-conventional component properties

Lignocellulosic materials consist of complex polymers rather than easily accessible monosaccharides, thus they have to be hydrolysed so as to release the desired substances (sugars). The feedstock investigated in this research is the solid residue of the sugar cane milling process, bagasse. Typical ultimate and proximate analyses as well as the chemical composition of bagasse are illustrated in Table 1. Bagasse consists of cellulose, hemicellulose and lignin; it was assumed that cellulose and hemicellulose consist only of glucan and xylan respectively. For the thermochemical procedures, bagasse was defined in terms of the elements in the proximate and ultimate analysis, whereas for the biochemical process it was defined by its chemical composition.

The higher heating value (HHV) of bagasse is estimated from the following empirical equation [25]:

$$HHV = 0.349{*}C + 1.1783{*}H + 0.105{*}S - 0.1034{*}O - 0.0151{*}N \tag{1}$$

Where C, H, S, O, N represent the mass fractions of the respective elements. The lower heating value can be estimated as follows [25]:

$$LHV = HHV - h_g\left(\frac{9H}{100} + \frac{M}{100}\right) \tag{2}$$

Where H is the mass fraction of hydrogen (dry basis), M the moisture content and h_g stands for latent heat of steam (MJ kg^{-1}). Hence for this case HHV = 18.7 MJ kg^{-1} and LHV = 16.4 MJ kg^{-1}. The mass flow rate of dry bagasse is equal to 15.1 kg s^{-1}, so the LHV, in power units, is equivalent' to 247.6 MW. Subsequently the exergy content of sugar cane bagasse was calculated from the following empirical equation [26]:

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