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MATHEMATICAL MODELLING OF QUANTIFYING BIOETHANOL FUEL PRODUCTION FROM PINEAPPLE WASTE

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ABSTRACT

Wider-scale implementations of bioethanol production from different wastes are not happening mainly due to lack of confidence on potential production and net benefit. With the aim of accelerating real-life implementations of more bioenergy productions, this paper presents development of a simple mathematical model, which can be used to evaluate potential bioethanol production capacity from pineapple waste under different input conditions. Based on an earlier experimental study, the mathematical model was developed depending on three contributing factors; pH, temperature and substrate concentration as considered in the earlier experimental study. Results from the developed mathematical formulation were compared with the experimental data from the earlier study. It is found that the developed model is quite capable to estimate potential bioethanol productions from pineapple waste. Model estimated results are having a coefficient of correlation of 0.84 with the measured data. Standard errors of the model's estimations are also quite low; RMSE = 0.49, MAE = 0.39 and RAE = 0.06. To facilitate a wider industrial generation, a basic mathematical model framework for economic analysis is proposed involving evaluation of net present values of future yields, as well as costs (initial and maintenance). Such mathematical model of economic analysis will help stakeholders on selecting optimum input parameters through optimised energy consumption.

1. INTRODUCTION

In the process of combating imminent climate change impacts energy sector plays a significant role. Due to the excessive usage of fossil fuel, the increase of CO_2 level in the atmosphere causing to global warming (Rudolph et al., 2015). It is well-established that bioethanol is one of the significant alternatives in abating greenhouse gas emissions (Hossain and Fazliny, 2010; Hossain et al., 2010). Conversion of waste product, feedstock or lignocellulosic residues into biofuel is a crucial choice for global potential of bioenergy. Bioethanol was used as a fuel in vehicles, either in a neat form or in a mixture with gasoline (Demirbas, 2007; Rosenfeld et al., 2018). Biofuel is renewable, could reduce petroleum imports, improve national energy security and reduce the reliance on petroleum from unstable areas of the world (Arijana et al., 2018). It has been a growing interest for many years because of its alternative green energy sources, consequently minimizing greenhouse gas (GHG) emission and finally help alleviate the rise of fuel prices (Rudolph et al., 2015). Any feedstock containing sugar can be used to produce ethanol. The main feedstock, sugar cane or molasses in Brazil and starch crops was used to produce bioethanol (Arijana et al., 2018). However, in the future, the most promising could be from cellulosic materials. Basically, ethanol can be obtained from three main groups of raw materials (feedstock). These are sugars like sugar cane, molasses and fruits (pineapple, banana and rambutan) (Fazliny et al., 2010, Hadeel et al. 2011, Imteaz et al. 2022) which can be converted to ethanol through fermentation, starches like corn and cassava which hydrolysed into fermentable sugar, and cellulose like wood and straw which can be converted to sugar by the action of mineral acid (Rosillo-Calle and Walter, 2006).

Bioethanol production can be obtained from renewable resource and different kind of sources including household waste, lignocellulosic biomass, waste crop and fruit wastes. Sugar, starch and lignocellulosic components are potentially converted into ethanol. These components are from biomass resources such as agriculture residues, herbaceous crops, forestry wastes, wastepaper, food waste, fruits wastes and other wastes (Fazliny et al., 2010). The

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main potential feedstock for bioethanol yield was carbohydrate, which included starch sugar, cellulose and hemicellulose. A major potential feedstock for bioethanol was the waste crops (McAlloon et al., 2000). Much research has been done on the production of bioethanol from different sources including the main source, sugar cane, either in form of cane juice which is mostly produced in Brazil (Wilkie et al., 2000) or molasses in India (Ghosh and Ghose, 2003), fruit waste in Malaysia (Hossain, 2017).

Tiwari et al. (2014) studied the productions of ethanol from five different fruits (apple, berry, grapes, papaya and sapota) with inoculation of bacteria and reported that among the five fruits, rotten sapota (Manilkara Zapota) produced highest amount (9.4%) of bioethanol after 5th day of incubation. Productions of bioethanol including different forms of sugars from the peels of mango, papaya, pineapple and banana were studied by Jahid et al. (2018), who reported that although simple soaking of the peels in water and steaming can result the recovery of free sugars, however enzymatic hydrolysis using cellulase and xylanase enzymes resulted very good yields of different forms of sugars. They also reported that among the studied fruits, banana and pineapple are the potential ones to produce ethanol. Ingale et al. (2014) reported that pre-treated banana waste can be economically utilized as a cheaper substrate for ethanol production. They also reported that the maximum ethanol yield was 17.1 g/l after 72 h of incubation period of fermentation. Gosavi et al. (2017) studied productions of bioethanol from Indian water chestnut, sweet potato, jackfruit and pineapple through acid hydrolysis, which yielded fermentable sugar. They have reported that among the studied fruits, pineapple waste produced highest amount (0.90 mg/ml) of ethanol. Recently, Wandono et al. (2020) reported that pineapple peel waste containing carbohydrate and reducing sugar is a good feedstock for bioethanol production and one ton of pineapple produced 250 kg waste, and 2.5 kg of pineapple peel produced 1 liter of bioethanol with 27% content. They also reported that 4,125 tons of pineapple peel waste produced 4,125 kg of bioethanol.

In fact, potential production of bioethanol from different fruits vary, also for a particular fruit it depends on several different factors. Experimental studies on bioethanol productions are based on experiments with varying different factors, which were different for different studies. As such widespread implementations of such bioethanol production is not happening due to the absence any generalised relationship on potential production. Most of the stakeholders are in dilemma regarding individual benefits from such bioethanol production, as in some cases such production may turn out to be costlier compared to traditional fuel production. Also, in some cases such production indirectly may cause more GHG emissions, if the energy used for the conversion of bioethanol is from traditional sources. Karmee (2016) presented prospects and limitations of adoption of bioethanol generation and recommended detailed economic analysis of any industrial production considering all the factors including difference in prices of bioethanol and other fuel, as well as costs of establishing and maintaining such facility. For such analysis, costs of productions need to be optimised so that adoption of bioethanol yields a net benefit.

For an optimisation analysis, a mathematical model is a useful and efficient tool, which compares the current value of output energy to the costs of production process, incorporating major contributing factors as independent variables. Such modelling was never attempted for the case of bioethanol production from pineapple. Objective of this study was to develop a simple data-driven modelling framework, which can be applied to perform economic analysis of bioethanol production through the optimisation of magnitudes of input parameters. To the best of authors knowledge, this is a pioneer study on such data-driven modelling on bioethanol production from pineapple.

2. MATERIALS AND METHODS

2.1 Theoratical Background

Fermentation is the traditional process, which is used for the production of ethanol, and this is a common practice to use yeast as chemical precursors in the process of fermentation. The chemical equation of conversion of ethanol from sugar/glucose is as follows, details of which was provided by Maicas (2020):

$C_6H_{12}O_6$(glucose)/Fruits $\longrightarrow$ $2C_2H_5OH$(ethanol) / bioethanol fuel + CO_2 (carbon dioxide)

Hossain and Fazliny (2010) presented an in-depth experimental study on bioethanol generation from pineapple waste. They have experimented the influence of three salient factors such as pH, temperature and substrate concentrations on the generation of bioethanol from pineapple. This study develops a mathematical model for the quantification of bioethanol production based on the experimental results from Hossain and Fazliny (2010).

2.2 Methodology

Mathematical formulations were developed to expresses relationship between bioethanol general and each contributing factor studied in the study of Hossain and Fazliny (2010). The derived mathematical formulations were then integrated into a single equation as outlined shown Equation 1. Such type of mathematical function is commonly used for the predictions of algal/bacterial growth (Imteaz and Asaeda, 2000) and was recently successfully applied for the prediction of pollutants removal efficiency by Imteaz et al. (2021, 2020). Such formulation is based on the concept that there is a maximum level of achievable growth/removal/production for a certain process or system, which is affected and reduced by one or more limiting factor(s). Contributions of the factors to the maximum achievable magnitude can be amalgamated into the following single equation:

$$PEP=f(pH)*f(T)*f(SC)*MPP \qquad (1)$$

Where, PEP is the potential ethanol production as weight % of biomass used, f(pH) is the factor for the influence of pH, f(T) is the factor for the influence of temperature, f(FP) is the factor for the influence of fermentation period and MPC is the maximum potential production. From the experimental measured data of Hossain and Fazliny (2010), the relationships of f(pH), f(T), f(SC) were derived. Based on the study of Hossain and Fazliny (2010), the following expressions of f(pH), f(T), f(SC) are proposed:

$$f(pH) = \frac{(a_1 * pH^2 + b_1 * pH + C_1)}{Eth_{max}^{pH}} \tag{2}$$

$$f(T) = \frac{(a_2 * T^2 + b_2 * T + C_2)}{Eth_{max}^{T}} \tag{3}$$

$$f(SC) = \frac{(a_3 * SC + C_3)}{Eth_{max}^{SC}} \tag{4}$$

Where Eth_{max}^{pH}, Eth_{max}^{T} and Eth_{max}^{SC} are the maximum ethanol productions from individual experiments of varying pH, temperature and substrate concentration respectively. a_1, a_2, a_3 and b_1, b_2 are the coefficients. C_1, C_2, C_3 are the intercepts of the best-fit lines, when individual independent variable is zero. 'pH' is the pH of the solution, 'T' is the temperature in °C and 'SC' is the substrate concentration in 'gm/l'.

Potential ethanol production values for different combinations of independent parameters (pH, temperature and substrate concentration) were calculated using Equation 1. In the equation, the maximum potential production (MPP) was unknown. As such, MPP was calculated through trial assuming different values of MPP, until calculated PEP values closely matched with the corresponding measured values.

The following section describes final derived equation, its estimated values and comparison with the corresponding measured values. Performance of the developed model results were assessed with the common statistical measures such as Root Mean Squared Error (RMSE), Mean Absolute Error (MAE) and Relative Absolute Error (RAE), which are defined below. Also, a framework has been proposed for the proper analysis of benefit-cost ratio for such project considering time value of the money.

The RMSE of a predicted model with respect to the observed variable is defined with the equation.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(X_{obs,i} - X_{model,i})^2}{n}} \tag{5}$$

Where, X_{obs} is observed/measured values, X_{model} is modelled values at time i. 'n' is the number data.

The mean absolute error (MAE) is defined as the sum of the absolute value of the differences between all the measured values and modeled values, divided by the total number of predictions as outlined below:

$$MAE = \frac{\sum_{i=1}^{n}(X_{obs,i} - X_{model,i})}{n} \tag{6}$$

The Relative Absolute Error (RAE) is expressed as a ratio of cumulative errors to cumulative actual measured values, which is expressed as:

$$RAE = \frac{[\sum_{i=1}^{n}(X_{obs,i} - X_{model,i})^2]^{1/2}}{[\sum_{i=1}^{n}(X_{obs,i})^2]^{1/2}} \tag{7}$$

3. RESULTS

Experimental results of different bioethanol productions with varying pH, temperature and substrate concentration were extracted from Hossain and Fazliny (2010), which were the basis of current study on model development. In the study of Hossain and Fazliny (2010), there are nine sets of data with different combinations of input variables: pH, temperature and substrate concentration. As usual with other similar studies, for the assessment on the effect of a selected variable, the other variables were kept constant. Detailed derivations of f(pH), f(T) and f(SC) using the data from the experimental measurements of Hossain and Fazliny (2010) are described in the following section.

3.1 Derivation of Factors

While assessing the effect of varying pH, the temperature and substrate concentration were kept at 28°C and 1 gm/l respectively. Figure 1 shows the measured values of bioethanol production in % (v/v) for three different pH values. Figure 1 also shows the best-fit trendline with the pH values and corresponding bioethanol productions. From the trendline, the following best-fit equation of 2nd order polynomial is derived, which yields a coefficient of determination value of "1.0":

$$Eth_{pH} = -0.15*pH^2+1.7*pH+2.68 \tag{8}$$

Where, Eth_{Sh} is the ethanol production in % (v/v) for any pH value under a temperature of 28°C with a substrate concentration of 1 gm/l.

Figure 2 shows the measured values of bioethanol production in % (v/v) under varying temperature, when pH and substrate concentration were kept as 5.5 and 3 gm/l

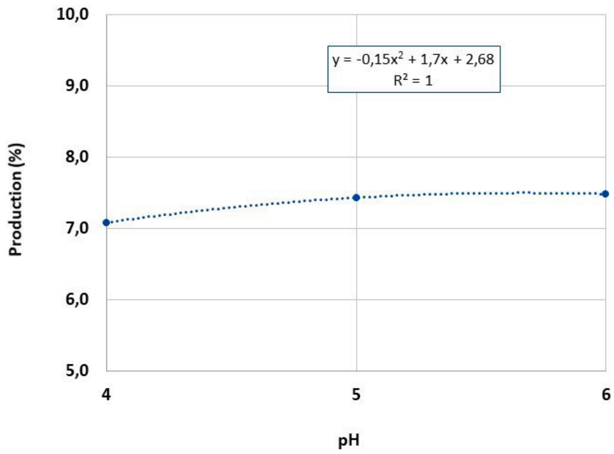

FIGURE 1: Effect of pH on bioethanol generation.

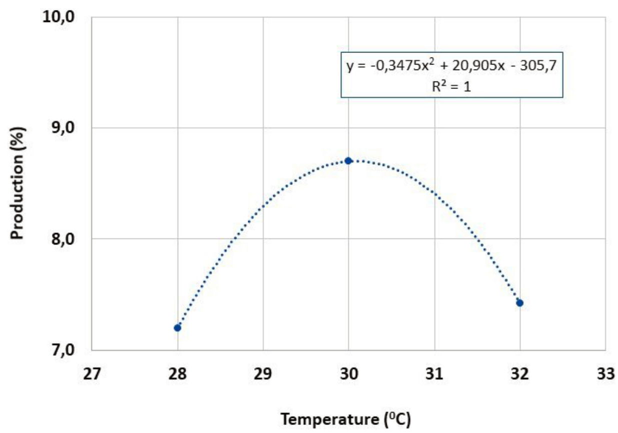

FIGURE 2: Effect of temperature on bioethanol generation.

respectively. Figure 2 also shows the best-fit trendline between the temperature and corresponding bioethanol production values. The best-fit trendline can be expressed with the following 2nd order polynomial, which yields a coefficient of determination value of "1.0":

$$Eth_T = -0.3475*T^2+20.905*T-305.7 \quad (9)$$

Where, Eth_T is the ethanol production in % (v/v) for any temperature (T) under a pH of 5.5 with a substrate concentration of 3 gm/l.

Figure 3 shows the measured values of bioethanol production in % (v/v) under varying substrate concentration, while pH and temperature were kept as 5.6 and 30°C respectively. Figure 3 also shows the best-fit trendline between the substrate concentrations and the corresponding bioethanol production values. The best-fit trendline can be expressed with the following liner equation, which yields a coefficient of determination value of "1.0":

$$Eth_{SC}=0.075*SC+7.735 \quad (10)$$

Where, Eth_{SC} is the ethanol production in % (v/v) for any substrate concentration (SC) under a temperature of 30°C with a pH of 5.6.

From the nine available measured values, replacing the derived functions for Eth_{pH}, Eth_T & Eth_{SC} into the Equations 2, 3 & 4 respectively, the corresponding values of f(pH), f(T) and f(SC) were evaluated. Eventually, replacing the calculated values of f(pH), f(T) and f(SC) into Equation 1, the potential bioethanol productions were calculated assuming the value of MPP (Maximum Production Production) through trials with the aim of achieving maximum correlation and least RMSE values between the measured and modelled values.

3.2 Developed Model

MPP value was determined through trial, assuming several reasonable values until a close fit between the measured ethanol productions and calculated productions was reached. Table 1 shows the calculated f(pH), f(T) and f(SC) values for different combinations of the selected independent variables; pH, temperature and substrate concentration. The table also shows the corresponding values of the model calculated potential productions, with the best 'MPP' value achieved of 9.0%.

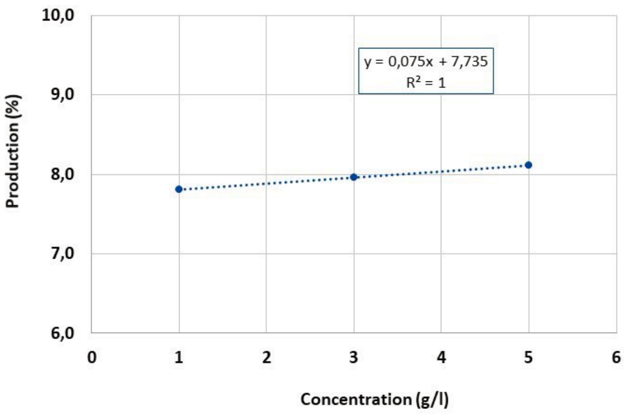

FIGURE 3: Effect of substrate concentration on bioethanol generation.

The usual practice of assessing such model results is to plot the model computed results with the experimental measured results on a single graph. Figure 4 shows the comparison between model calculated results and the experimental measured values. It is found that the model calculated values are having a correlation coefficient of 0.84 with the measured values. To evaluate the errors of the model calculated values the Root Mean Squared Error (RMSE), Mean Absolute Error (MAE) and Relative Absolute Error (RAE) values were calculated. The MAE, RMSE and RAE values evaluated for the model calculated values are "0.49", "0.39" and "0.06" respectively. All these values are quite low and can be considered as good achievement.

3.3 Framework for Economic Analysis

It is to be noted that in general the amount of yields from such bioethanol generation using fruit waste is not great and it is likely to take several years to achieve the payback of initial investment cost. Moreover, there will be ongoing operating and maintenance costs involved with such production. As the monetary benefit of the yields will be coming in future years, it is necessary to consider the present value of the future potential benefits which will be accumulated over the years using the Net Present Value (NPV) concept. Also, the future operation and maintenance costs need to be converted to net present values. Such eco-

TABLE 1: Calculated factors for different combinations of input variables.

Temperature (°C)	Substrate conc. (gm/l)	pH	f(T)	f(SC)	f(pH)	Estimated Production (%)
28	48	5.5	0.83	0.96	1.00	7.20
30	48	5.5	1.00	0.96	1.00	8.70
32	48	5.5	0.85	0.96	1.00	7.42
30	24	5.6	1.00	0.95	1.00	8.54
30	72	5.6	1.00	0.96	1.00	8.70
30	96	5.6	1.00	0.98	1.00	8.87
28	48	4.0	0.83	0.95	0.95	6.67
28	48	5.0	0.83	0.95	0.99	7.00
28	48	6.0	0.83	0.95	1.00	7.05

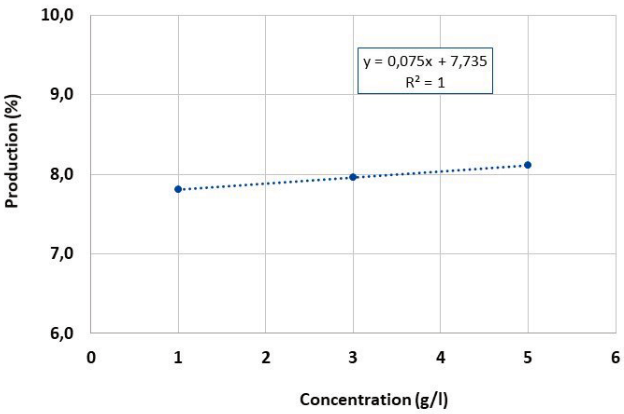

FIGURE 4: Comparison of model results with measured data.

nomic analysis is crucial for widescale implementations of bioethanol generation; without accurate estimations it may turn out to be not economically feasible. The total costs of the bioethanol generation can be calculated using following equation:

$$C = IC + \sum_{k=1}^{n} \frac{OM_k}{(1+r)^k} \tag{11}$$

Similarly, the accumulative benefits from the yields of the bioethanol production can be calculated considering variable price of bioethanol using the following equation:

$$B = \sum_{k=1}^{n} \frac{P_k}{(1+r)^k} \tag{12}$$

In the above equations, 'B' is the total accumulated benefit, 'C' is the total accumulated cost, r = internal rate of return (%/year), n = design life in years, 'P_k' is the variable future price of the bioethanol in in a year 'k', 'IC' is the initial investment cost of the system and 'OM_k' is the future annual operational and maintenance cost for a year 'k'. These equations should be considered simultaneously to evaluate total costs and return for a particular design life of the production system. Through comparing total costs and benefits the industries would be able to quantify actual benefits, which will encourage widespread implementations of such sustainable energy generations. For the current study, as no data was available on energy spent in the production process, as well as associated costs, the complete economic analysis was not performed.

4. CONCLUSIONS

With the aim of enhancing biofuel generation from different fruit/vegetable wastes, this paper presented development of a simple mathematical model for the estimation of potential bioethanol production from pineapple waste. The basic model was developed based on three contributing variables, which were extracted from an earlier experimental study on bioethanol productions from pineapple waste under different input conditions; pH, temperature and substrate concentration. For each of the studied variables, based on the earlier experimental measurement a contributing factor was derived. Then all the derived factors were multiplied with a maximum production capacity value to evaluate the potential bioethanol production. Model predicted values were compared with the experimental measurements and it is found that the model estimations are very close to the measured values having a good correlation coefficient of 0.84. Other standard statistical error parameters (RMSE, MAE and RAE) were also found to be low, revealing the fact on model's predictive capability. Such kind of model would be very useful for stakeholders of industrial-scale generation on their decision making while selecting appropriate magnitudes of the input variables related to the bioethanol production.

Such type of data-driven modelling approach was never explored for the generation of bioethanol from pineapple waste, although wider-scale implementations of such sustainable generation would help reducing carbon footprint through two ways; reducing waste and generating energy from sustainable source. From the experimental results it is clear that except substrate concentration, for other input variables there are certain optimum stages which yield maximum bioethanol productions. It is found that increasing temperature up to 30°C and a slightly acidic (pH<6) environment causes to maximise the production. Achieving such optimum conditions are associated with additional cost, which should be minimized to achieve a higher benefit-cost ratio. A framework for economic analysis incorporating net present values of the costs and yields is proposed. In the current study a complete economic analysis was not possible due to lack of data. It is recommended that future studies should incorporate a complete economic analysis with further data on cost and production amount.

It is to be mentioned that the proposed model was developed having three independent variables only, which was due to limited availability of the experimental data. One can explore to find additional factor(s) affecting the bioethanol production and if found the additional factor(s) can be easily incorporated in the existing model formulation. Nonetheless, the current model will be the foundation being a primitive effort in this data-driven model. More rigorous experimental measurements will be required to establish potential effect of any additional factor(s). Also, the proposed individual relationships of mentioned variables with the bioethanol generations are based on a single set of experiments with only 3 measurements for each variable. Validation of such relationships through more experiments warrants focus of any future study. Same methodology can be employed to develop similar data-driven models for other fruit/food waste.

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