Simulation of process control for production of 5-HMF from old coconut water

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Abstract. 5-Hydroxymethyl furfural (5-HMF) is one of the intermediate chemicals produced from biomass through the process of dehydration of glucose and fructose in acidic conditions. Biomass resources are one of the sources that attract the attention of many users of unlimited biomass resources, in addition to being able to produce environmentally friendly products such as bio fuels and bio chemicals. Old coconut water and oil palm tree trunk sap was chosen in this study because of its abundance in Malaysia. It is an essential organic compound for the production of bioplastics, chemicals, building materials, fuels, textiles, cosmetics and food. Although the production of 5-HMF is relatively simple, in fact, the synthesis of 5-HMF is complicated by the occurrence of multiple reactions at one time, especially when using biomass as a raw material. In this report, process control of production of 5-HMF from biomass is presented using fuzzy logic controller for controlling temperature of a continuous stirred tank reactor (CSTR). The objective of this paper is to develop a control system for a non-isothermal temperature control of a CSTR with the most stable response curve. Through simulation results, fuzzy logic control performs better because there was no overshoot and successfully reaches the set point at faster settling time.

1. Introduction

Biomass is one of the most popular sources of environmentally friendly products such as bio fuels and bio chemicals [1]. According to [2], there are several biomasses suitable for raw materials for the manufacturing of 5-HMF such as corn stover, pine sawdust, grass, filter paper, corncob, red pine bark, maple wood, sugarcane bagasse and etc. By utilizing these biomass residues, we will be able to produce a valuable product while reducing agricultural waste and reducing environmental pollution. By using agricultural waste, the 5-HMF produced will be more reliable for use in the food industry because of its halal resources. Coconut, also known as Cocos Nuctfera Linn is one of the high demand products of over 90 countries. The volume of coconut water that is not used during the commercial process of coconut fruit can reach over 2.4 billion L a year. Coconut water is made from 96 percent water and 6 percent solid. The major components of solid in coconut water are soluble sugars, proteins, and minerals [3].

When it comes to chemical reactions and reactor design, there are some important parameters that need to be taken into account and controlled. Among the parameters that are often controlled in a process are temperature, pressure, flow rate, tank level, and pH [4]. One of the most common types of controls is fuzzy logic control. Fuzzy logic control is widely used in complex and non-linear systems [5]. Fuzzy logic is an extension of binary logic where the concept of partial truth is used as opposed to...
truth or falsehood. It has truth values in the range 0 to 1.0 where 0 indicates falsehood while 1 indicates absolute truth. Fuzzy logic controllers are able to provide automatic control over processes by systematically handling information. Simulation of process control on the continuous stirred tank reactor (CSTR) was performed by previous researchers by comparing the results of PI, PID and FLC control. Fuzzy logic control, FLC is said to be able to control non-isothermal systems better than PID controllers.

Studies on the direct conversion of biomass to 5-HMF have only been carried out in the past 10 years. Most studies are done using biomass from agricultural waste so that this waste can produce valuable products. Biomass is an unlimited source, making it an ideal source of feedstock, reducing energy consumption and carbon dioxide emissions. The objective of this paper is to develop mathematical model and block function using MATLAB to describe temperature control of CSTR for the production of 5-HMF from old coconut water. Simulation for process controller actions of PID and fuzzy logic was subsequently done using Simulink. The performance of both controllers in controlling the process will be evaluated through simulation study.

2. Methodology
This study is divided into two phases. The first phase is the collection of information and experimental data from previous researchers to identify the parameters to be controlled for a continuous stirred tank reactor (CSTR). Then, the simulation is carried out by developing the reactor model using the material balance and the energy balance of the reactor. Next, a mathematical model for describing temperature control for CSTR was also developed. The system will be modelled using MATLAB Simulink software with Equations (1)-(3) to represent component balance for old coconut water (reactant), reactor energy balance, and energy balance for heating jacket, respectively:

$$\frac{dz}{dt} = \frac{Fz_o}{V_R} - \frac{Fz}{V_R} - kz \quad (1)$$

$$\frac{dT_R}{dt} = \frac{FT_o}{V_R} - \frac{FT_R}{V_R} - \frac{\lambda k z}{M c_p} - \frac{UA_J}{\rho c_p V_R} (T_R - T_J) \quad (2)$$

$$\frac{dT_J}{dt} = \frac{F_J}{V_J} (T_{JO} - T_J) + \frac{UA_J(T_R - T_J)}{\rho c_p V_J} \quad (3)$$

The reaction is first-order with respect to reactant concentration where the rate constant $k$ is in Equation (4) [6]:

$$k = 7.2 \times 10^{10} e^{-8750/T_R} \quad (4)$$

The parameters of the model are listed in Table 1.
Table 1. Reactor model parameter values.

| Parameter                  | Value                      |
|----------------------------|----------------------------|
| Working volume, $V_R$      | 1.35 m$^2$                 |
| Tank diameter, $D$         | 1.02 m                     |
| Tank height, $H$           | 2.05 m                     |
| Flow rate, $F$             | 2000 kg/hr                 |
| Reactor temperature, $T_R$ | 37 – 105 °C                |
| Inlet temperature, $T_0$   | 37 °C                      |
| Jacket temperature, $T_j$  | 129 °C                     |
| Heat capacity of jacketed fluid, $c_l$ | 4.18 kJ/kg.K    |
| Heat transfer coefficient  | 243.90 W/m$^2$ °C         |

2.1. **PID controller**

The PID control design is performed with a feedback control strategy where if an error is detected, a signal is sent back into the feed and performs adjustments to control the parameter according to its set point as shown in Figure 1.

![Figure 1. Block diagram of feedback control strategy.](image)

PID controller is the most famous feedback controller strategy in the industry. The controller performance is subjected to the appropriate tuning of the three control elements which are proportional, integral, and derivative actions. The control action $u(t)$ of the controller is described by the following differential equation (Equation (5)):

$$ u(t) = K_p e(t) + \frac{K_p}{T_i} \int_0^t e(\tau) d\tau + K_p T_d \frac{de(t)}{dt} $$

(5)

where $K_p$, $T_i$, and $T_d$ are the controller parameters that are associated with proportional gain, integral time, and derivative time, respectively. Best performance for PID control can be obtained for linear systems and mildly nonlinear systems if the corresponding parameters are tuned correctly.

2.2. **Fuzzy logic controller**

For temperature control of non-isothermal CSTR system, it is most critical to avoid overshoot and steady state error. This control problem can be handled appropriately by nonlinear control system such as fuzzy logic controller (FLC). FLC is based on fuzzy logic, which is an extension of binary logic where the concept of partial truth is used as opposed to complete truth or falsehood, thus can handle grey area pretty well. FLC is said to be able to control non-isothermal reactor systems better than PI and PID controller algorithms. The block diagram of the inference system used by typical FLC is shown.
in Figure 2. In this system, the crisp numerical input is subjected to fuzzifier to transform it to fuzzy variable as subjected to a set of membership functions. The fuzzy variable is then sent to the inference system to determine the appropriate output, which is still a fuzzy variable before defuzzification turns it into a crisp numerical value, the transformation of which is accomplished by another set of membership functions.

![Fuzzy logic system block diagram](image)

**Figure 2.** Fuzzy logic system block diagram.

3. Results and discussion

This study was conducted to study reactor control of 5-HMF production from old coconut water using PID control and FLC. The controlled process unit is a continuous reactor mixing tank (CSTR). Here, we consider setpoint tracking scenario whereby the reactor temperature will be controlled at 105 ºC from the initial reactor temperature of 26 ºC. The chosen setpoint temperature value, which is 105 ºC is the optimum temperature to maximize 5-HMF production based on the experimental work of Maruf, 2018 [6]. Finally, the manipulated variable for the reactor temperature control is the heating jacket temperature.

3.1. Simulation of PID controller

First, the temperature control scenario where the reactor temperature is controlled by PID controller is studied. After tuning the controller using built-in PID tuner in Simulink, the following PID controller parameters without derivative action were obtained: $K_p = 55.68$ while $T_I = 0.52$ s. Figure 3 shows the response curve for this controller. From the corresponding figure, it can be seen that there is significant temperature overshoot occurred in the reactor temperature control by PID controller where the temperature value almost reached to 120 ºC. Although this overshoot can be overcome by including derivative action in the PID control, however considering that the temperature measurement can be noisy, it might cause stability issue to the controller due to amplification of the measurement noise by the derivative action.

![Response curve for reactor temperature control with PID controller](image)

**Figure 3.** Response curve for reactor temperature control with PID controller.
3.2. Simulation of fuzzy logic controller

A FLC for the CSTR system was developed based on the Mamdani inference system. Among the reasons why the Mamdani system was chosen for this controller is because of its intuitive nature, suitable for human entry, basic rules that are easier to interpret, and suitable for various systems. As shown in Figure 4, the inputs to this Mamdani system are error in reactor temperature from the setpoint and the rate of change of this error with respect to time. The two inputs will be evaluated by the Mamdani inference system to determine appropriate course of action for the reactor jacket temperature value. For error and change in error, the values are subjected to three fuzzy variables which are NEGATIVE, ZERO, and POSITIVE. Meanwhile, for the output which represents the jacket temperature, the corresponding fuzzy variables are used: ZERO, SMALL, AVERAGE, and LARGE. The rules for this inference system are shown in Table 2.

![Error in reactor T](image1.png) ![Rate of change of Error in reactor T](image2.png)

**Figure 4.** Mamdani inference system for fuzzy logic controller.

| Rule | Error       | Change in error | Output      |
|------|-------------|-----------------|-------------|
| 1    | IF ZERO     | AND ZERO        | THEN ZERO   |
| 2    | IF ZERO     | AND NEGATIVE    | THEN SMALL  |
| 3    | IF ZERO     | AND POSITIVE    | THEN AVERAGE|
| 4    | IF NEGATIVE | AND ZERO        | THEN ZERO   |
| 5    | IF NEGATIVE | AND NEGATIVE    | THEN SMALL  |
| 6    | IF NEGATIVE | AND POSITIVE    | THEN SMALL  |
| 7    | IF POSITIVE | AND NEGATIVE    | THEN AVERAGE|
| 8    | IF POSITIVE | AND ZERO        | THEN SMALL  |
| 9    | IF POSITIVE | AND POSITIVE    | THEN AVERAGE|

The rules for this inference system are shown in Table 2.

The results of the controller simulation using FLC for the CSTR system are shown in Figure 5. Through this graph, it can be seen that there is no temperature overshoot occurs in this FLC system, with the setpoint temperature successfully achieved stably and smoothly. Based on this result, we can surmise that FLC can control this non-isothermal reactor system better than PID controller.
3.3. Comparison of controller performance

The comparison of PID and FLC performance on the reactor temperature control is shown in Figure 6 and further summarized in Table 3. It can be seen that both controllers show no steady-state offset error. However, it can be seen that FLC is much better controller for this system with no overshoot and faster process settling time.

![Figure 6](image)

**Figure 6.** Comparison of response curve for uncontrolled system, and controlled system with PID and fuzzy logic controllers.

| Controller type | Peak temperature, °C | Settling time, s |
|-----------------|----------------------|-----------------|
| PID             | 116.7                | 2.05            |
| FLC             | 106.4                | 2.95            |

**Table 3.** Comparison of reactor temperature controllers.

4. Conclusions

In conclusion, controller simulation study to assess performance of reactor temperature control using PID and FLC for 5-HMF synthesis reactor from old coconut water was successfully carried out. Simulation results indicate that FLC is superior to PID control for reactor temperature setpoint tracking that can avoid temperature overshoot and leads to faster process settling time. Next study will look into the corresponding controller performance for process disturbance rejection.
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