Application of thermodynamics and mathematical modeling on the optimization of the feeding flux rate on a fermentation process as a closed system

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Abstract. Fossil fuels are the main non-renewable energy source that supply communities and cities of electric and motor energy. The high demand for fossil fuels decreases reserves, making it a political, social, and environmental issue. Hence, bioethanol, considered a renewable source compared to other sources of energy, has become a viable alternative. Its manufacturing starts with the previous treatment of agroindustrial or food waste, followed by a fermentation process in a bioreactor and a distillation process for purification. However, the bioethanol production cost is higher than gasoline production because it requires identifying proper operating conditions of the process, traditionally done through trial and error. Therefore, this work describes the simulation of the fermentation of bioethanol, by considering the fermentation tank as a closed thermodynamical system and identifying the optimum biomass feeding flow rate by using the Cuckoo Search algorithm. The identification of the optimal biomass feeding flow rate reduces the substrate consumption time up to 30%, with respect to the process in a batch operation.

1. Introduction

Thermodynamics is one of the branches of physics that constantly interact with other natural sciences, like chemistry and biology, in the development of models for complex processes. Within chemistry, the manufacturing of bioethanol has become a very attractive activity since it represents a promising replacement for fossil fuels, aiding to reduce the environmental damage caused by the emission of greenhouse gasses [1]. Bioethanol manufacturing, typically relying on the understanding of chemical principles, can be studied from thermodynamics by developing models that can describe the mass-energy balance necessary for the transformation of primary matter into the final product [2]. The design, modeling, and optimization of fermentation systems for bioethanol bring numerous advantages by reducing the time required to complete the process [3]. Bioethanol fabrication starts with the pretreatment of the raw material where lignin and carbon sources are separated [4] acquiring must, a sugary solution, which is transferred to chemical reactor, considered as a closed system, since there is not a mass-energy exchange [5] where yeast (biomass) is added to start the fermentation process. The product of the fermentation will be biomass, bioethanol and subproducts (alcohols, aldehydes, organic
acids, etc.) and water. Finally, the bioethanol is purified with a concentration of 99.5% to 99.9% through a distillation process [6].

When the fermentation process comes to end, traditionally, the biomass is discarded or used as cattle feed [7]. On the contrary, Boinot in [8] demonstrated that the reincorporation of biomass into another fermentation process reduces the residence time inside the reactor, because the yeast does not require the stage of adaptation and growth in the medium [9].

The fermentation process can be described through mathematical models in which chemical and physical parameters determine the speed of the reaction [3]. Specifically, the rate at which the concentration of any reactant involved in the fermentation process, varies with time can be calculated by the Equation (1).

\[
\frac{dC_i * V}{dt} = V_{r_i} + (Q_e * C_{ie} - Q_s * C_{is}),
\]  

where the first term \( V_{r_i} \) represents the reaction velocity and the second term corresponds to the heat liberated by the reactant flux at the entry and exit points (respectively, \( C_{ie} \) and \( C_{is} \) represent the entry and exit reactant concentrations, while \( Q_e \) and \( Q_s \) represent the heat).

Typically the second term in Equation (1) is dismissed by assuming that the heath exchange produced during the reaction is negligible [10].

Traditionally, fermentation processes could be described using a mathematical model which representsthe reactants \( i \); known as states trajectory (substrate, biomass and bioethanol). Lee et al. in [11] reported a compendium of controlling and design equations to describe substrate rate consumption, biomass and bioethanol production in the three reactor operation modes which is defined from the magnitude of the biomass dosing flow [3]. The speed reaction equation (Equation (2)), substrate consumption rate in the Equation (3) and bioethanol and biomass production rate as show the Equation (4), and Equation (5).

\[
\mu(t) = \frac{\mu_{max} * S(t)}{K_S + S(t)} \left[ 1 - \frac{X(t)}{X_{max}} \right],
\]  

\[
\frac{dS(t)}{dt} = [-\frac{1}{Y_{PS}}] * \mu(t) * X(t) + \frac{F * V}{V} * X(t),
\]  

\[
\frac{dX}{dt} = \mu(t) * X(t) - \frac{F}{V} * X(t),
\]  

\[
\frac{dP(t)}{dt} = \frac{Q_{max} * S(t)}{S(t) + K_S} X - \frac{F}{V} * P(t).
\]

The parameters which describe the three differential equations and the reaction speed corresponds to: biomass dosing flow \( (F) \) in l/hr; volume of the reactor \( (V) \) in l, maximum biomass concentration in the medium \( X_{max} \) in gr bioethanol/gr of biomass \( * hr \) and kinetic constants of the substrate and product \( (K_S, Q_{max}) \) in g/l and \( \mu_{max} \) in 1/hr, respectively.

Equation (2), Equation (3), Equation (4), and Equation (5) were used to describe the biomass growth process of \textit{saccharomyces cerevisae} yeast [12] and \textit{streptomyces clavuligerus} [13] for the manufacture of bioethanol and clavunionic acid, respectively. In addition, this mathematical model has been incorporated into Fermenta and AnaBioPlus software, so that bioethanol manufacturers estimate the efficiency of the product from the variation of substrate and biomass before starting fermentation.

By having the experimental data and mathematical model that describes the fermentation process, the identification of the operation parameters of the model is performed. This stage can
be achieved analytically through the linearization of the system [3] or through software packages. In the reported proposals, the lsqcurvefit tool, available in the Matlab library, has been used in the identification of parameters of the clavuniolic acid [13] and protein model [14], beer [15], bioethanol [16], etc. These processes are developed in discontinuous operation mode.

The reactors that work in semi-batch or continuous operation modes are susceptible to receive a disturbance in the biomass feeding flow; reducing the yield of the desired products [3]. Therefore, the incorporation of a control system capable of returning the fermentation system to the nominal or desired values is of interest. The state feedback control systems were designed to track the predefined trajectory [17] as well as the return to the desired value in case of disturbances. The design and construction of the controller is based on the differential equations that describe the system of interest [18]. In addition to this, this scheme has a built-in PI controller that performs a correction action towards the desired value. This control scheme has shown high performance in polymerization processes [18], cooling tanks [19], exothermic reaction [20] and beer fermentation, [21], among others.

Since the biomass dosing flow is obtained through trial and error, it could be considered an optimization problem where the objective function is the substrate consumption in less time compared to the experimental process [19]. From the stochastic techniques reported in the open literature; bioinspired optimization methods have been able to improve the performance of a wide variety of industrial processes [22] and their efficiency is comparable with other strategies such as Genetic Algorithms [23] and Bee Swarm [24].

Unlike previous proposals where the identification of the biomass dosing is done through trial and error in the biomass growth, this work proposes via simulation, the identification of the optimum biomass feeding flow rate obtained through the Cuckoo Search stochastic algorithm in order to minimize the fermentation time in semibatch operation mode. Additionally, it is proposed to incorporate a feedback control system by states, which is capable of minimizing fluctuations in the biomass feeding flow, a disturbance that could compromise the performance of the fermentation process.

2. Methodology

Substrate, biomass and product experimental trajectories of biomass growth process were selected in order to establish the basis of this study. In these, Zapata and Peláez in [7] propose the use of Colombian bananas rejected for merchandising, Lin in [25] propose the use of analytical grade glucose as a carbon source and Rincón et al. in [26] propose the use of sugar cane molasses as substrate source. The initial concentration state and the quantification equipment for each yeast is shown in Table 1.

| Yeast                              | Substrate | Biomass | Product |
|-----------------------------------|-----------|---------|---------|
| Saccharomyces ceravisae            | 8         | 0.60    | 0       |
| Candida utilis                    | 80        | 0.31    | 0       |
| Gluconacetobacter diazotrophicus  | 130       | 0.50    | 0       |

Simulation and optimization of the experimental process was developed using Matlab 2017 Rb software and the control system was constructed using the Simulink model-based design environment. For this, the working environment was setup in a portable computer with an Intel Core i5 processor.

The mathematical model proposed by Lee et al. in [11] was selected to describe the experimental data of the yeast growth process as: speed reaction, $\mu$, substrate, biomass and
bioethanol. The lsqcurvefit tool of Matlab was used to identify the operation parameters. Moreover, the optimum speed biomass feeding flow identification was selected through an objective function in order to minimize the substrate concentration, because this is the only carbon source that biomass consumes [27]. For this, the Cuckoo Search algorithm was chosen as the optimization method under search criteria of 100 eggs with a 70% chance of survival and a reproduction rate of 100 generations. Selection of these criteria is based on results reported by Walton et al. in [28], in their study was identified the roots of nonlinear, trigonometric and nonlinear trigonometric functions.

3. Results

Experimental growth process of yeasts *saccharomyces cerevisae* (Sc) by Zapata and Peláez in [7], *candida utilis* (Cu) by Lin in [25] and *gluconacetobacter diazotrophicus* (Gd) by Rincón et al. in [26] through the mathematical model described in Equation (2), Equation (3), Equation (4), and Equation (5) of Lee et al. in [11] were described. Table 2 shows the mathematical model operation parameters identified using the numeric tool lsqcurvefit for each experiment.

| Operation parameter | Sc     | Cu       | Gd       |
|---------------------|--------|----------|----------|
| $Y_{PS}$            | 0.11   | 1.3015   | 0.1344   |
| $K_S$               | 34.00  | 5.85492  | 2099.7700|
| $\mu_{MAX}$         | 0.41   | 0.4912   | 0.1608   |
| $Q_{MAX}$           | 1.33   | 2.8000   | 2.5000   |

As Table 2 depicts, the magnitude of the $Q_{max}$ parameter in all cases is close to the maximum ethanol production capacity for each yeast as reported by Hui et al. in [29]. However, as can be observed, the $K_S$ operation parameter for *gluconacetobacter diazotrophicus* yeast is high because of the substrate, which means a low affinity; therefore, the conversion of substrate into bioethanol will require more time respect to the others fermentation processes.

A set of simulations were performed in order to obtain the mathematical model trajectories for each yeast’s fermentation process as show the Figure 1 using the operation parameters of Table 2 and the Equation (1), Equation (2), Equation (3), and Equation (4). The mathematical model was validated using experimental data reported by Zapata and Peláez in [7], Lin in [25] and Rincón et al. in [26] for determining the efficiency of the numeric tool lsqcurvefit.

Experimental data performance respect to mathematically modeled data is illustrated in Figure 1. As observed, modeled trajectories are spliced on the experimental data; hence, the experimental process is properly described by the magnitude of the operation parameters, identified by the numeric tool lsqcurvefit. Afterward, the Cuckoo Search algorithm was used for searching the biomass feeding flow into fermentation tank, throwing magnitudes of 0.015 L/hr, 0.35 L/hr, and 0.001 L/hr for the fermentation process with Sc, Cu, and Gd yeasts, respectively. These values were used into fermentation process simulation. Figure 2 shows the trajectories states with the optimized parameter in contrast with the experimental process by Zapata and Peláez in [7], Lin in [25] and Rincón et al. in [26].

In Figure 2 is shown that the three fermentation processes in batch and semi-batch modes match with the growth trajectories of the substrate, biomass and product, regardless of the biomass feeding flow rate. From the Figure 2(a) the optimized process requires 10.3 hours to reach the maximum biomass concentration inside the reactor respect to the 15.73 hours
consumed by the process using a biomass feeding flow in batch mode, as depicted in the Figure 3(a). Figure 2(b), the optimized biomass feeding flow consumes all the substrate in 12.2 hours respect to the 16 hours required by the batch mode. In the other hand, the fermentation process with Gd. Finally the Figure 2(c), shows that that the optimized process requires 440 hours to reach the maximum concentration of biomass respect to the 585 hours without feeding flow.

Figure 1. Mathematical model validation and operation parameters versus the experimental process for every yeast using (a) bananas rejected for merchandising, (b) analytical grade glucose, and (c) sugar cane molasses.

Figure 2. Biomass growth process performance versus the fermentation process using (a) bananas rejected for merchandising, (b) analytical grade glucose, and (c) sugar cane molasses.

Identifying that the fermentation process in semi-batch mode, under the optimized flow by the Cuckoo Search algorithm, reduces the time required to reach the maximum bioethanol concentration, it is necessary to incorporate a control system which guarantee the high performance of the system in case of disturbance. Therefore, for each fermentative system was incorporated a drop in the biomass feeding flow, evaluating the system using an open loop with respect to the feedback system. The magnitude of each disturbance and the states trajectories are shown in Figure 3.

Figure 3 depicts fermentation processes comparison for every yeast under a biomass feeding flow variation. As can be observed, in all cases, substrate consumption and biomass maximum concentration match with reported trajectories in open literature by Quintero in [30], Petre in [31] and Birol et al. in [32]. In the other hand, as is observed, the bioreactor coupled to the control system by states feedback does not show variations in time and in concentration of interest states, determining that , residence time into reactor or final concentration of the substrate, biomass and bioethanol with the incorporation of this scheme it is not affected.
Figure 3. Disturbance of the biomass feeding flow and its effect over biomass, substrate and bioethanol through an open loop system versus the control system fermentation process using (a) bananas rejected for merchandising, (b) analytical grade glucose, and (c) sugar cane molasses.

In relation with performance evaluation, in the Figure 3(a) which depicts *Saccharomyces cerevisiae* yeast fermentation process, it is observed that the time required by the open loop system is 15 hours in contrast with 10.03 hours required by the control system. It is expected that biomass growth process start when the disturbance comes to the end; however, in this study case the biomass reach its stationary state at 9.47 gr/l respect to the 10.47 gr/l quantified by the control system coupled to the bioreactor, this means, that the presence of unit disturbance in the feeding flow will generate an antagonistic effect on biomass growth. In same way, in the Figure 3(b) is observed *Candida utilis* yeast fermentation process, which requires 29.8 hours in the open loop system respect to 14 hours quantified by the control system, reaching 0.003 gr/l as minimum concentration; therefore, it requires more residence time for reach its biomass stationary state. Finally, the Figure 3(c) is observed *Gluconacetobacter diazotrophicus* yeast fermentation process with no significative differences in substrate consumption velocity or biomass or ethanol production due to the high fermentation time; hence, in this study case, controller incorporation will not affect process performance under a step disturbance.

4. Conclusions
This work reports the application of the Cuckoo Search algorithm to the thermodynamic and chemical equations describing bioethanol fermentation for calculating the optimal flux feeding rate, under the assumption that the fermentation tank can be represented as a closed system. To validate that the resulting mathematical model can describe this physicochemical process, three, previously reported, cases were considered. These fermentations processes with different yeasts was used to maximize ethanol concentration, these systems were evaluated in a batch mode (null flow) respect to a semibatch process using Cuckoo Search algorithm to identify the optimum biomass flow. In all cases was observed that the semibatch operation mode does not affect the final concentration of substrate, biomass and product. Additionally, the optimized magnitude was able of reduce residence time inside bioreactor. Considering the performance of the optimized trajectories of the three states with respect to experimental development, this stochastic process can be contemplated as a competitive tool for the reduction of biomass growth time.

In the other hand, to guarantee the high performance of the biomass growth process, a step disturbance was incorporated. Moreover, to minimize the antagonistic effects of the process, a state feedback control scheme was designed, constructed and implemented, being able to reach the biomass production trajectory in nominal operation without affecting the fermentation time or the trajectories of the three states of interest. Our work has led us to conclude that the control scheme proposed is a novel alternative to ensure an adequate performance in biomass...
growth process under conditions of optimized biomass feeding flow.

A future work, evaluating the accuracy of the Cuckoo Search algorithm into finding the optimal feeding/recirculating flux rates for a bioethanol fermentation reaction train (for both open and closed systems), is currently under development.

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