BRIGHAM YOUNG
UNIVERSITY

Department of Chemical Engineering
http://chemicalengineering.byu.edu//

April 13, 2016

Dr. John Hedengren
Brigham Young University
350 Clyde Building
Provo, UT 84602

Subject: Optimization of Ethanol Bioreactor System

Dear Dr. Hedengren,

We are pleased to submit our final report and findings regarding the optimization of an ethanol bioreactor system. Ethanol production is a major industry in the United States especially as it reduces global fossil-fuel consumption. The process of ethanol production involves simultaneous hydrolysis and fermentation reactions which respond oppositely to temperature conditions. For this reason, temperature optimization is extremely important to maximize production. A number of other studies have been completed to optimize ethanol production by adjusting the temperature of the reactor, but we were unable to find any studies that modeled and optimized the expensive refrigeration system for the ethanol plants. This is important for producers account for to maximize total profits.

We were able to include the refrigeration cycle by modeling an external heat exchanger and introducing a series of conditional equations to account for turning the refrigeration cycle on and off. The objective function accounted for the competing ethanol production and refrigeration cycle by assuming an increase in 1 g/mL was equivalent to a 1 hour decrease in time the chiller was operating. We found for 70°F (or colder) cooling water, the chiller should not be turned on; however, for 75°F cooling water the chiller should be started at 14.3 hours and stopped at 19.0 hours into the batch. Additional work should be done for other cooling water temperatures and a more accurate relationship between ethanol concentration and refrigeration operating time.

Sincerely,

Aaron Gillette

Trent Okeson

encl: Final Project Report

Please see the enclosed file.

Final Report:

Optimization of Ethanol Bioreactor System

Aaron Gillette and Trent Okeson

Brigham Young University, Provo, UT, 84604

April 13, 2016

Abstract

Ethanol production is a major industry in the United States and is favored as a method to reduce global fossil-fuel consumption. The process of ethanol production involves simultaneous hydrolysis and fermentation reactions which respond oppositely to temperature. For this reason, temperature optimization is extremely important to maximize production. A number of previous studies optimized ethanol production by adjusting the reactor temperatures; however, no studies existed that modeled and optimized the expensive refrigeration systems found in ethanol plants. Refrigeration cycles have a significant impact of the cost of running a plant and the overall profitability of a process. This study includes the refrigeration cycle by modeling an external heat exchanger and introducing a series of conditional equations to account for turning the refrigeration cycle on and off. The objective function accounted for the competing ethanol production and refrigeration cycle by assuming an increase in profits from increasing final ethanol concentrations by 1 g/L was equivalent to the cost of operating the refrigeration cycle for 1 hour. For 70°F (or colder) cooling water, using refrigeration cycles was not profitable; however, for 75°F cooling water the refrigeration cycle should be started at 14.3 hours and stopped at 19.0 hours into the batch. This use of the chiller results in a final ethanol concentration of 66.2 g/L.

1 Introduction

Corn biorefining to produce ethanol reduces global fossil-fuel consumption and is a major U.S. industry [1]. The United States produces the most biofuel in the world with projected production of 136 billion liters in 2022 [2]. This biofuel is typically produced by converting corn into ethanol through hydrolysis and fermentation. The simultaneous hydrolysis and fermentation reactions lead to complex reactor behavior. This complex behavior has been successfully modeled in several previous publications using a combination of experimentally collected data and first-principles models. These models have been used to optimize a variety of aspects of ethanol production.

Many of the ethanol optimization studies agree that the temperature profile for the batch reaction plays a major role in the overall reactor efficiency [3–6]. The efficiency is dependent on the rates of hydrolysis and fermentation. The hydrolysis reaction converts the feed dextrin to dextrose and is favored by higher temperatures. Fermentation, the conversion of dextrose to ethanol, happens faster at lower temperatures because the yeast, which makes the fermentation reaction possible, die faster at higher temperatures. These conflicting interests make an optimal temperature profile essential to maximize the conversion of biomass to ethanol.

Despite similar model equations, there is some discrepancy between optimal reactor temperatures. Janos Madar and his team reported the best temperature profile to be constant at about 50°F for the first 50% operation, then to dramatically decrease the temperature to for the next 40%, followed by a rapid ramp up to 68°F to finish the reaction [7]. James Bartee and his group ran a similar setup and found that a decrease in temperature starting about halfway through the reaction and periodic enzyme feed shots resulted in optimum ethanol production [6].

Another team, led by Wei Dai provided a more in depth analysis of the temperature profile. Wei Dai and his team found that decreasing the temperature much earlier than Madar resulted in a more optimal temperature profile [3]. They began cooling the reactor only 10% into the operation; however, the minimum reactor temperature was 86°F. This minimum temperature was used to incorporate realistic limitations on cooling systems for bioreactors. Wei Dai et al. used two minimum temperatures as conditions in separate runs (86°F and 88°F) and found the lower temperature resulted in a slightly higher ethanol production. Heating at the beginning of the process was also performed, but resulted in no further ethanol production. In addition to an optimal temperature profile, this group found that the enzyme should be injected into the reactor near the end of filling time instead of constantly during filling.

Although significant research has been done ethanol batch reactors, there is still significant room for further research. The models that have been used in past studies have included some significant simplifications. Heat transfer to and from the reactor is often been simplified, only specifying a fixed maximum heat transfer rate. Additionally, the reactors have been assumed to be well mixed. This assumption is a poor one because large reactors are often too big to have good mixing. In addition to the simplifications to the model, pH and Ammonia are known to effect ethanol production, but are poorly understood. Modeling these effects and including them in a reactor model would add significant depth to the optimization work already accomplished.

Of the various areas for improving past work on the optimization of ethanol production, this study modeled the cooling system of the reactor system to obtain a more realistic optimization profile. This allowed for a more accurate optimization of ethanol production while minimizing the need for running expensive

refrigeration cycles. To do this, a more extensive model of the cooling system was implemented. This study determined expensive refrigeration cycles should be used to cool the reactor. This will be important to companies invested in bioreactors to make sure they are optimizing profits instead of just optimizing ethanol production.

2 Model and Methods

The model used for this project was primarily based on work by Wei et al. [3]. For brevity the reactor model equations are not included in this paper but can be found elsewhere [3]. Wei et al. based their model on several previous papers; however, they re–regressed model parameters using data from industrial plants and expanded several of the models, introducing several new parameters. They also added an energy balance for the reactor. For this research, the model by Wei et al. was translated into the APMonitor modeling language. Heat exchanger modeling was then included. All of the optimization of the models in this paper were solved using the APOPT solver.

The temperature profile for the process was optimized and used to calculate cooling water flow rates to achieve the desired temperatures. Wei et al. put a limit on the minimum reactor temperature because the optimizer wanted to make the batch fermenter unrealistically cold to increase the ethanol production. Reactor temperatures below 85°F are unrealistic because cooling water is not always available below 65°F. This is especially problematic during summer months in plants located in the southern United States. The minimum reactor temperature constraint can ensure that the needed cooling will be achievable; however, these types of broad constraints have been shown to lead to conservative solutions in other applications [8].

While the model use by Wei et al. did calculate the heat transfer rates, a more detailed analysis involving specific parameters of the cooling water and reactor slurry such as temperature and flow rate were completed. The relationships of these parameters with the total heat transfer achieved are represented by Eqs. (1) to (3).

$$q = mC_p(T_{out} - T_{in}) \tag{1}$$

$$q = UAF\Delta T_{lm} \tag{2}$$

$$\Delta T_{lm} = \frac{(T_{hot,out} - T_{cold,in}) - (T_{hot,in} - T_{cold,out})}{ln\left(\frac{T_{hot,out} - T_{cold,in}}{T_{hot,in} - T_{cold,out}}\right)} \tag{3}$$

The discontinuities in Eq. (3) can cause significant problems for the solver. These discontinuities occur if natural log is negative or if the denominator is zero in the log-mean temperature calculation. To simplify the problem and remove the risk of infeasible solutions, the log-mean temperature equation was first rearranged

so the natural log was no longer in the denominator. To address the natural log, a model for the maximum possible heat transfer for a given cooling water temperature and reactor slurry temperature was created. This was done by assuming that the slurry and cooling water flow rates through the heat exchanger were at their maximum. The heat transfer was linearly dependent on the temperatures with no interactions between the two temperature variables. The resulted in a relatively simple model for the maximum heat transfer (Eq. (4)). This assumption significantly simplified the problem and ensured that the desired heating was achievable. The resulting heat transfer rates could then be used in a separate heat exchanger model to determine the for rates through the heat exchanger.

$$H_{cool} = 2424.8T - 2414.8T_{cool} \tag{4}$$

As previously mentioned, when the temperature gets higher during the summer months, the cooling water may not provide sufficient heat to keep the process running at optimal conditions. When this happens, a chiller (refrigeration unit) is used to cool the cooling water before going through the heat exchanger. To do this the model needed to turn the chiller on when more heat transfer was needed and to turn the chiller off when it wasn't needed. The function used to represent the heat transfer when the chiller was off was Eq. (4) and the function used for when the chiller was on was Eq. (5).

$$H_{cool,on} = 2424.8T - 2414.8(T_{cool} - 10) \tag{5}$$

To simplify the problem, the chiller was assumed to provide enough cooling to bring the cooling water temperature down by 10°F. This assumption resulted in a simple difference between Eq. (4) and Eq. (5). In reality the capability of the refrigeration system will be dependent on a variety of variables; however, modeling these dependencies was outside the scope of this work.

Next a series of conditional equations were needed to assign when Eq. (4) and Eq. (5) would be respectively used. To do this two new variables, t_{on} and t_{off}, were assigned. The variable t_{on} represented the time when the chiller turned on and t_{off} represented when the chiller turned back off. The following system of equations were developed to make this work:

$$0 \geq b \leq 1 \tag{6}$$

$$(1 - b)(tm - t_{on})(t_{off} - tm) \leq 0 \tag{7}$$

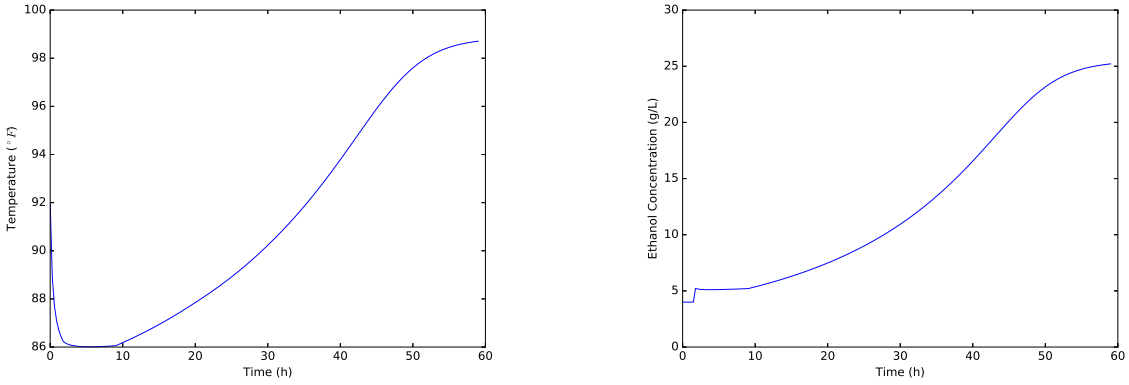
$$b(t_{on} - tm)(t_{off} - tm) \leq 0 \tag{8}$$

Eq. (6) introduces a continuous variable b between the values of 0 and 1. These equations make the only time the value of b is 1 is when t_{on} is less than tm and when t_{off} is greater than tm. For any other time interval b is 0. While 0 and 1 are the only two values that can be returned from the system of equations a continuous function is maintained using the inequalities and a mixed integer problem is avoided. This means a mixed integer solver is not needed. Using the conditional equations above and applying them to Eq. (4) and Eq. (5) results in Eq. (9) (with $S \geq 0$) which applies the appropriate function when the controller is on and off. This acts as an inequality constraint, ensuring that the cooling for the system will not exceed the maximum cooling that the heat exchangers can deliver.

$$S = (1-b)[2424.8T - 2414.8T_{cool} - H_{cool}] + b[2424.8T - 2414.8(T_{cool} - 10) - H_{cool}] \tag{9}$$

3 Simulation Results

The base model without an optimal solution resulted in the following profiles (Fig. 1 and Fig. 2). For these models it was assumed that the feed streams were 86°F and linearly increasing the cooling rate with respect to batch time. This was intended to offset the increased exothermic reaction rates as the batch progressed.



(a) Temperature profile with respect to time.

(b) Ethanol Concentration in g/L as the reaction progresses to completion.

Figure 1: Batch reactor profiles with no optimization of the cooling throughout the batch.

The temperature profile initially decreased because the feed to the reactor was cooler than the reactor temperature. At about 8 hours into the batch, the reactor was full so cooler feed was no longer added to the tank, resulting in a steady temperature. At that time, the reaction starts to proceed first converting the dextrin to dextrose and then subsequently dextrose to ethanol. Both of these reactions are exothermic, resulting in a steady increase in temperature throughout the remainder of the batch time.

The biomass feed containing yeast and the relatively low temperatures caused an initial spike in active yeast concentrations as shown in Fig. 2. This high concentration was not sustainable because the conversion rate of dextrin to dextrose was not high enough at these low temperatures. As time progressed the dextrose concentration increased with increasing temperature, allowing the yeast concentration to spike a second time. Eventually temperature and ethanol concentration became large enough, and the dextrose concentration became low enough, that the yeast was no longer able to thrive, driving the active yeast concentration back down.

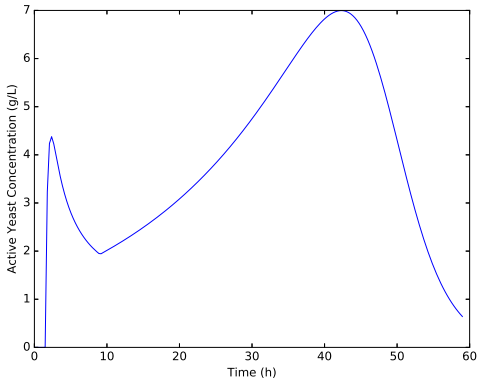


Figure 2: Active yeast concentrations in the reactor as the reaction progresses.

The sensitivity of ethanol concentration to temperature is displayed in Fig. 3 where the temperatures are held constant throughout the reaction. Even small changes in temperature can result in significant changes in final ethanol concentration.

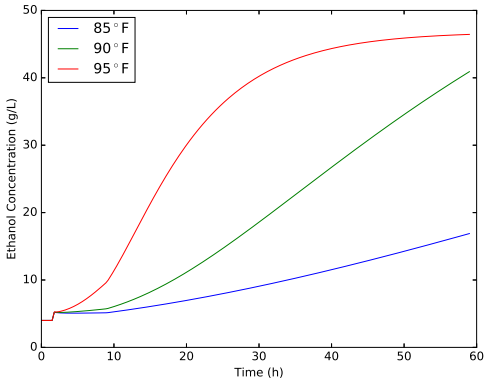
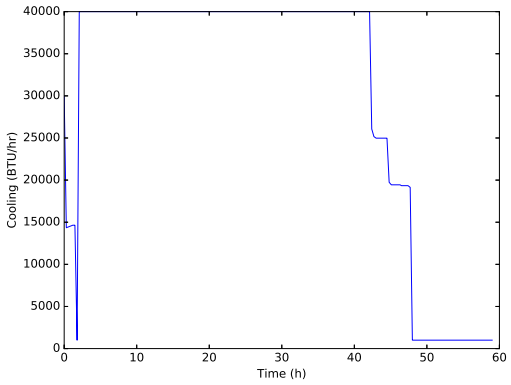


Figure 3: Ethanol concentration temperature sensitivity analysis

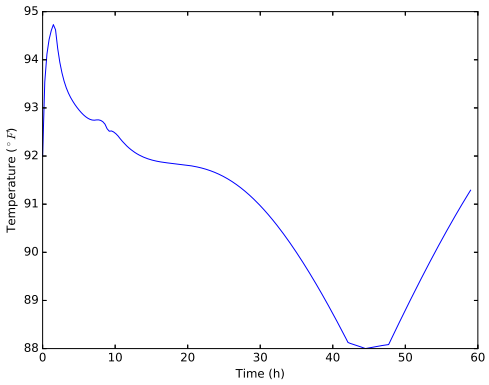
4 Dynamic Optimization Results

The final optimization of the cooling for the bioreactor was initialized though an iterative process of simpler optimization problems. Initially, the temperature profile of for the reactor was optimized. Using the results from this optimization, the cooling constraints were introduced to the problem and re–optimized. Finally, the chiller was introduced to the problem using Eqs. (6) to (9).

The first step in the optimization was optimizing temperature in the reactor. To get a successful solution, the time horizon was partitioned into 10 time periods, forcing the optimizer to choose one temperature for each time period. This significantly simplified the problem. This constraint was then relaxed and the solver was allowed to optimize the profile for all time steps. Using this solution, the heat transfer rate was optimized. For this optimization a maximum heat transfer of 40,000 BTU/min was placed on the cooling to realistically model heat exchanger limitations. The resulting profile is shown in Fig. 4 with a final ethanol concentration of 59.6 g/L. This solution is consistent with published results done previously. Initially, there is minimal cooling to help start the conversion of dextrin to dextrose. After the initial spike in temperature, the cooling was increased to favor the conversion of dextrose to ethanol. At the end of the batch, there was minimal effect of the rising temperature, so the cooling was reduced again to limit cooling water costs.



(a) Optimal cooling profile with respect to time.

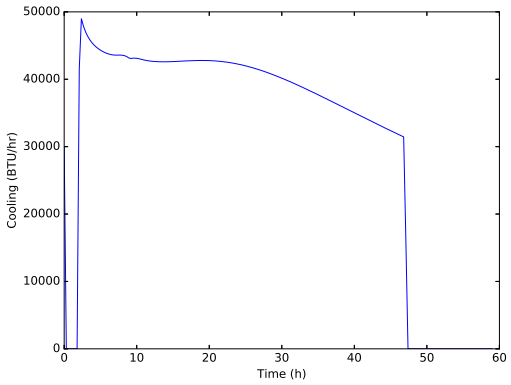


(b) Reactor temperature profile with respect to batch time.

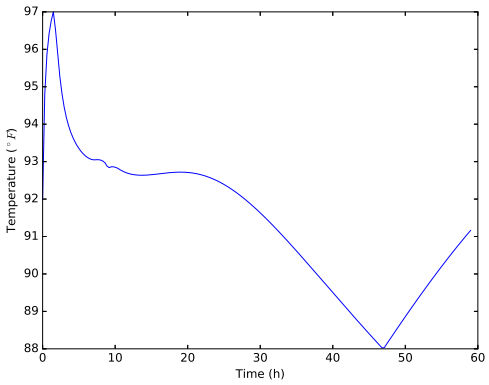
Figure 4: Batch reactor profiles with optimization of cooling throughout the batch and a maximum cooling set to 40,000 BTU/min for each of the heat exchangers.

The results in Fig. 4 are conservative because the maximum cooling was set to be relatively small to ensure that the cooling system will be able to successfully deliver the needed cooling. In order to push the cooling system to it's limits. The constraints for cooling were introduced to the model. This constraint is shown in Eq. (9) with $b = 0$. This allowed for more cooling at times when the reactor was warmer. The results from these optimizations with cooling water at 75°F and 70°F cooling water are shown in Figs. 5 and 6

respectively. With cooling water at 75°F, the final ethanol concentration was 60.8 g/L. For 70°F, the final ethanol concentration was 71.0g/L. This increase in final ethanol concentration from 59.6 g/L was due to the increased cooling capability throughout the batch. There was a minimal befit to using these constraints for cooling water at 75°F; however, when the cooling water was changed to be at 70°F the production of ethanol increased drastically.

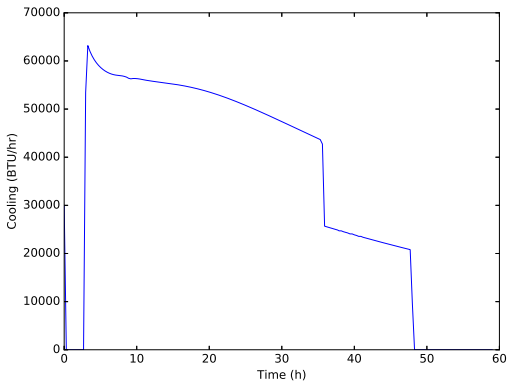


(a) Optimal cooling profile with respect to time.

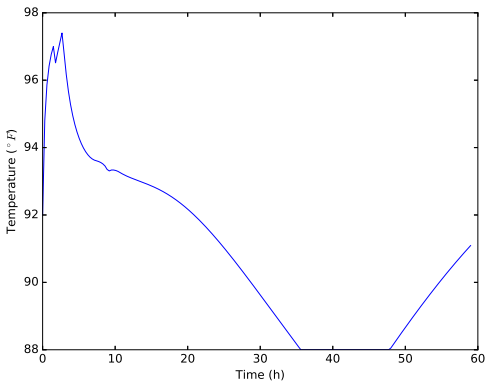


(b) The optimized temperature profile for the reactor.

Figure 5: Batch reactor profiles with optimization of cooling throughout the batch with cooling water at 70°F.



(a) Optimal cooling profile with respect to time.



(b) The optimized temperature profile for the reactor.

Figure 6: Batch reactor profiles with optimization of cooling throughout the batch with cooling water at 70°F.

The final optimization included the optimization of chiller on and off times. This problem was especially difficult because the solver would find local minima for a set of given start and stop times. This was due to the solver optimizing the cooling profile for a given start and stop time and then finding that adjusting the start and stop time did not directly improve the objective function. To overcome this challenge, a global

optimum was found by optimizing the cooling for given on and off times for the chiller. The on and off times were varied to create a surface plot of the objective function. To account for the cost of running a refrigeration cycle, 1 was subtracted from the final ethanol concentration for each hour of refrigeration. The calculations for each of the start and stop times were done in parallel. When the cooling water was available at 70°F or cooler, it was not advantageous to use the chiller; however, with higher cooling water temperatures, the chiller does produce enough extra ethanol to make chiller use advantageous. The chiller times were optimized for 75°F cooling water. The results from this study are shown in Fig. 7. The global optimal start and stop times were 14.3 hours and 19.0 hours.

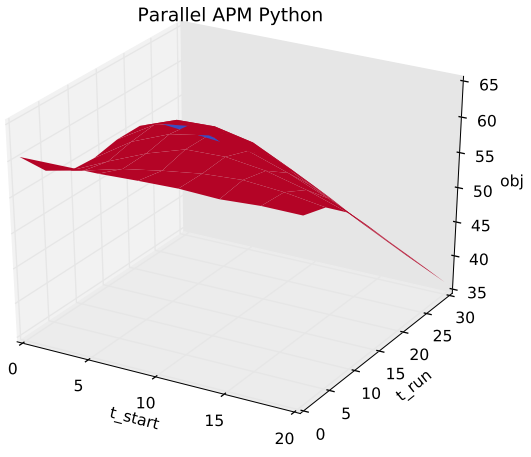
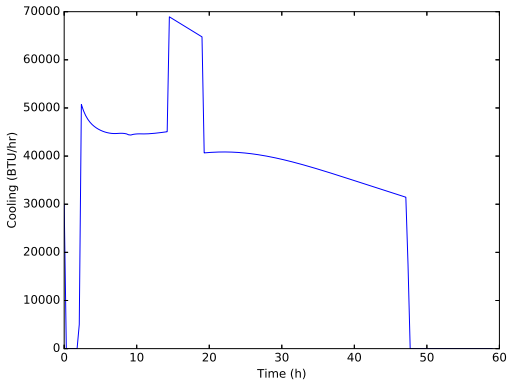


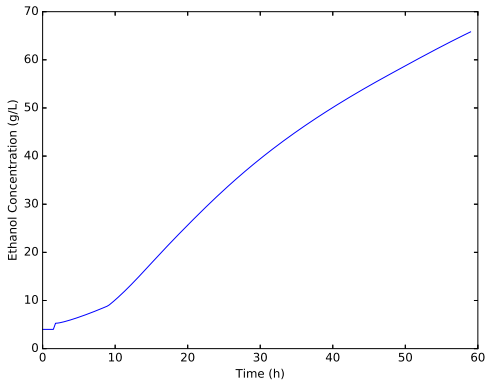
Figure 7: The objective function with respect to start and run times for the chiller. The cooling water for this study was available at 75°F.

Using these on and off times for the chiller, the new optimized profiles are shown in Figs. 8 and 9. As is seen the cooling remains relatively constant, at the maximum value, until the chiller turns on. Then once the chiller turns off, it stays at the maximum until near the end of the batch, when the end of the batch is reached the cooling turns off. This is because the change in temperature at the end has minimal effect on the final concentration and because there was a cost associated with the cooling. The final optimize concentration for the ethanol in the bio-reactor was 66.2 g/L.

The optimized profile with the chiller was very similar to the profiles without the chiller (5). The chiller allowed for more cooling creating a rapid decrease in temperature while it was running. This was advantageous for the yeast, making the conversion to ethanol greater. The time to run remained short due to the high cost that was placed on running the reactor.



(a) Optimal cooling profile with respect to time.



(b) Ethanol Concentration in g/L as the reaction progresses to completion.

Figure 8: Batch reactor profiles with optimization of cooling throughout the batch.

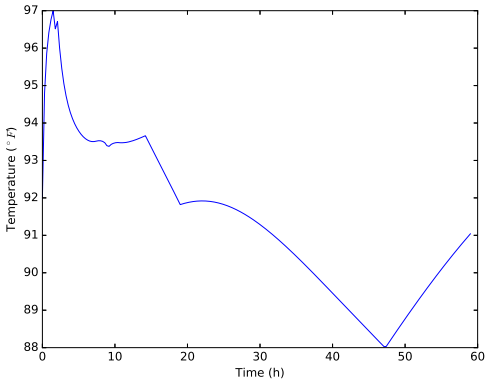


Figure 9: Temperature profile with respect to time for optimized cooling.

5 Conclusion

This work was successfully built on previous models for ethanol bioreactors. It included a model for the cooling systems associated with the reactor system. The system also included a model for a chiller. This changed the problem from a NLP problem to a MINLP. This was solved with a unique formulation removing the integer portion of the problem and allowing for the use of an active set method to optimize the problem. The optimization of the chiller operation was done using a sampling method due to the large number of local minima in the solution space. A global optimum was determined with associated chiller operation and cooling rates. Although the optimum found in this study resulted in less production of ethanol than the previous studies. The limitations on cooling were accurately modeled, making the solutions found more realistic. Some future work on the chiller would be valuable, since the chiller was assumed to cool the cooling water by 10°F.

References

[1] C A Cardona and O J Sanchez. Fuel ethanol production: process design trends and integration opportunities. *Bioresource technology*, 98(12):2415–2457, 2007.

[2] Graeme M. Walker. 125th anniversary review: Fuel alcohol: Current production and future challenges. *Journal of the Institute of Brewing*, 117(1):3–22, 2011.

[3] Wei Dai, Daniel P. Word, and Juergen Hahn. Modeling and dynamic optimization of fuel-grade ethanol fermentation using fed-batch process. *Control Engineering Practice*, 22(1):231–241, 2014.

[4] B. de Andrés-Toro, J.M. Girón-Sierra, J.a. López-Orozco, C. Fernández-Conde, J.M. Peinado, and F. Garca-Ochoa. A kinetic model for beer production under industrial operational conditions. *Mathematics and Computers in Simulation*, 48(1):65–74, 1998.

[5] Ye Sun and Jiayang Cheng. Hydrolysis of lignocellulosic materials for ethanol production: A review. *Bioresource Technology*, 83(1):1–11, 2002.

[6] James Bartee, Patrick Noll, Schweiger Axelrud, and Bijan Sayyar-Rodsari. Industrial Application of Nonlinear Model Predictive Control TEchnology for Fuel Ethanol Fermentation Process. *Journal of Chemical Information and Modeling*, 53:160, 1989.

[7] Janos Madar, Janos Abonyi, Balazs Balasko, and Ferenc Szeifert. Interactive Evolutionary Computation for Model based Optimization of Batch Fermentation. *System*.

[8] D. Mellinger, N. Michael, and V. Kumar. Trajectory generation and control for precise aggressive maneuvers with quadrotors. *The International Journal of Robotics Research*, 31(5):664–674, 2012.