

Optimal Feed Rate for Maximum Ethanol Production

Conor Keith

Loyola Marymount University

March 2, 2016

Outline

- **Chemostats and industrial ethanol manufacturing**
- *Saccharomyces cerevisiae* and the fermentation process
- The role of glucose feed concentration in the fermentation process
- A mathematical model of EtOH production in a chemostat environment
- Maximization of EtOH production using free final time optimal control problem
- Optimal feed flow rate

How Ethanol is produced on the industrial level

- Ethanol fermentation produces ethanol for use in food, beverages, and fuel.
- Yeast convert sugars, like glucose, into cellular energy .
- Ethanol and carbon dioxide are by products of this process.
- Fermentation occurs in large fermentation tanks.
- The enzyme alpha-amylase is added to tanks to break down corn starch into shorter carbohydrate chains called dextrins.
- During saccharification process the enzyme glucoamylase is added to mixture to break down dextrins into glucose.
- Starch is converted to simple sugars, yeast is added to convert glucose into ethanol and carbon dioxide.

https://www.osha.gov/dts/osta/otm/otm_iv/descriptions.pdf

Chemostats Can Be Used to Model Industrial Ethanol Production

- **Chemostat cultures have been used by researchers as a tool to simulate the different stages of industrial ethanol production.**
- **Chemostat cultures allows scientists to gather data regarding metabolic processes of yeast cells.**
- **Enable researchers to test the effects of specific nutrients on ethanol production.**

Outline

- Chemostats and industrial ethanol manufacturing
- ***Saccharomyces cerevisiae* and the fermentation process**
- The role of glucose feed concentration in the fermentation process
- A mathematical model of EtOH production in a chemostat environment
- Maximization of EtOH production using free final time optimal control problem
- Optimal feed flow rate

***Saccharomyces cerevisiae* is the Most Relevant Yeast Strain in Ethanol Production**

- ***Saccharomyces cerevisiae* is commonly used in winemaking, banking and brewing**
- ***S. cerevisiae* perform the most common type of fermentation**
- **Ethanol becomes toxic to yeast cells at high concentrations**
- ***S. cerevisiae* is a preferred yeast strain due to its high stress tolerance and its ability to efficiently use carbon and nitrogen resources**
- **Goal of industrial ethanol production is to produce maximum ethanol in shortest period of time**
- **Most ethanol is produced in later stages, i.e. at or near zero growth rates and stationary phase**

The Flexibility of *Saccharomyces cerevisiae*

- *S. cerevisiae* can rapidly switch between respiratory and fermentative sugar metabolism in response to changes in availability of oxygen and fermentable sugars
- *S. cerevisiae* can increase catabolic rates and start accumulating large amounts of ethanol upon this transfer
- Glucose starved yeast can adapt when introduced to high glucose concentrations within minutes
- Pathways responsible for fermentation process can suddenly catalyze sugar at very high rates, which is why *S. cerevisiae* is the most preferred yeast in industrial ethanol production (Van den Brink, et. al 2008).

Outline

- Chemostats and industrial ethanol manufacturing
- *Saccharomyces cerevisiae* and the fermentation process
- **The role of glucose feed concentration in the fermentation process**
- A mathematical model of EtOH production in a chemostat environment
- Maximization of EtOH production using free final time optimal control problem
- Optimal feed flow rate
- Conclusion

The Role of Glucose in Ethanol Fermentation

- **Yeast contain enzyme called zymase which catalyzes fermentation process**
- **Glucose zymase → Ethanol + Carbon Dioxide**
- **$\text{C}_6\text{H}_{12}\text{O}_6 (\text{aq}) \rightarrow 2\text{C}_2\text{H}_5\text{OH} (\text{aq}) + 2\text{CO}_2(\text{g})$**
- **Glycolysis breaks down glucose to form pyruvate.**
- **When oxygen is not present pyruvate undergoes fermentation.**

Outline

- Chemostats and industrial ethanol manufacturing
- *Saccharomyces cerevisiae* and the fermentation process
- The role of glucose feed concentration in the fermentation process
- **A mathematical model of EtOH production in a chemostat environment**
- Maximization of EtOH production using free final time optimal control problem
- Optimal feed flow rate

A mathematical model of Ethanol Production in a Continuous Culture

- $\frac{dX}{dt} = \mu X - \frac{F}{V} X$
- $\frac{dS}{dt} = -\frac{\mu}{Y} X + \frac{F}{V} (S_0 - S)$
- $\frac{dP}{dt} = \pi x - \frac{F}{V} P$
- $\frac{dV}{dt} = F$

Parameters and Constants in Model

- X = Cell mass concentration
- S = Glucose concentration
- P = Ethanol concentration
- μ = Specific growth rate
- π = Specific productivity
- F = Feed rate
- Notation used in Wang, et. al (1999)

Parameters and Constants Continued

- $\mu = \frac{\mu_0}{1 + \frac{P}{K_p}} * \frac{S}{K_s + S}$

- $\pi = \frac{\pi_0}{1 + \frac{P}{K_p}} * \frac{S}{K_s + S}$

- Growth equations from Wang, et. al (2008).

Outline

- Chemostats and industrial ethanol manufacturing
- *Saccharomyces cerevisiae* and the fermentation process
- The role of glucose feed concentration in the fermentation process
- A mathematical model of EtOH production in a chemostat environment
- Maximization of EtOH production using free final time optimal control problem
- Optimal feed flow rate

Brief Explanation of Dynamic Optimization

- $$\begin{cases} \dot{x} = f(x(t), u(t), t) \\ x(0) = x_0 \end{cases}$$
- **Goal: maximize objective function**
- $J(u) = \int_{t_0}^{t_f} F(x(t), u(t), t) dt + \lambda[x(t_1)]$
- **State variable depends on control variable.**
- **Decision maker chooses control variable at any given time**
- **Final time t_f in this case is free**
- **Dynamic optimization means we aren't looking for a single steady-state solution, but for an optimal path amongst all feasible paths for the system .**

Transversality Condition For Optimal Path

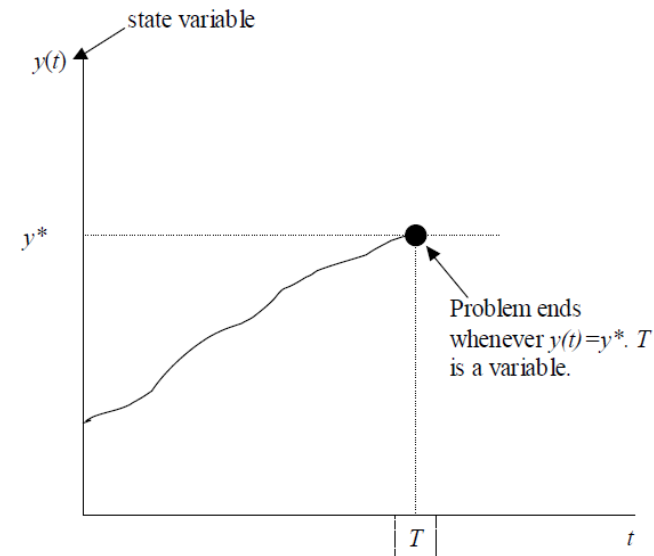
- $\dot{x} = f(X(t), S(t), P(t), V(t), u(t), t)$
- **The Hamiltonian:**
- $H(t) = f(X(t), S(t), P(t), V(t), u(t), t) + \lambda(t)g(X(t), S(t), P(t), V(t), u(t), t)$
- $H(t_f) = 0$, extending beyond t_f has no value because ethanol production has already been maximized
- $H(t_f)$ cannot be negative, in that case it would have been optimal to finish fermentation earlier
- State variables are the elevation of the road, control variable is the direction of the road at each point, and t_f is the length of the road.

A Mathematical Model of Ethanol Production in a Continuous Culture

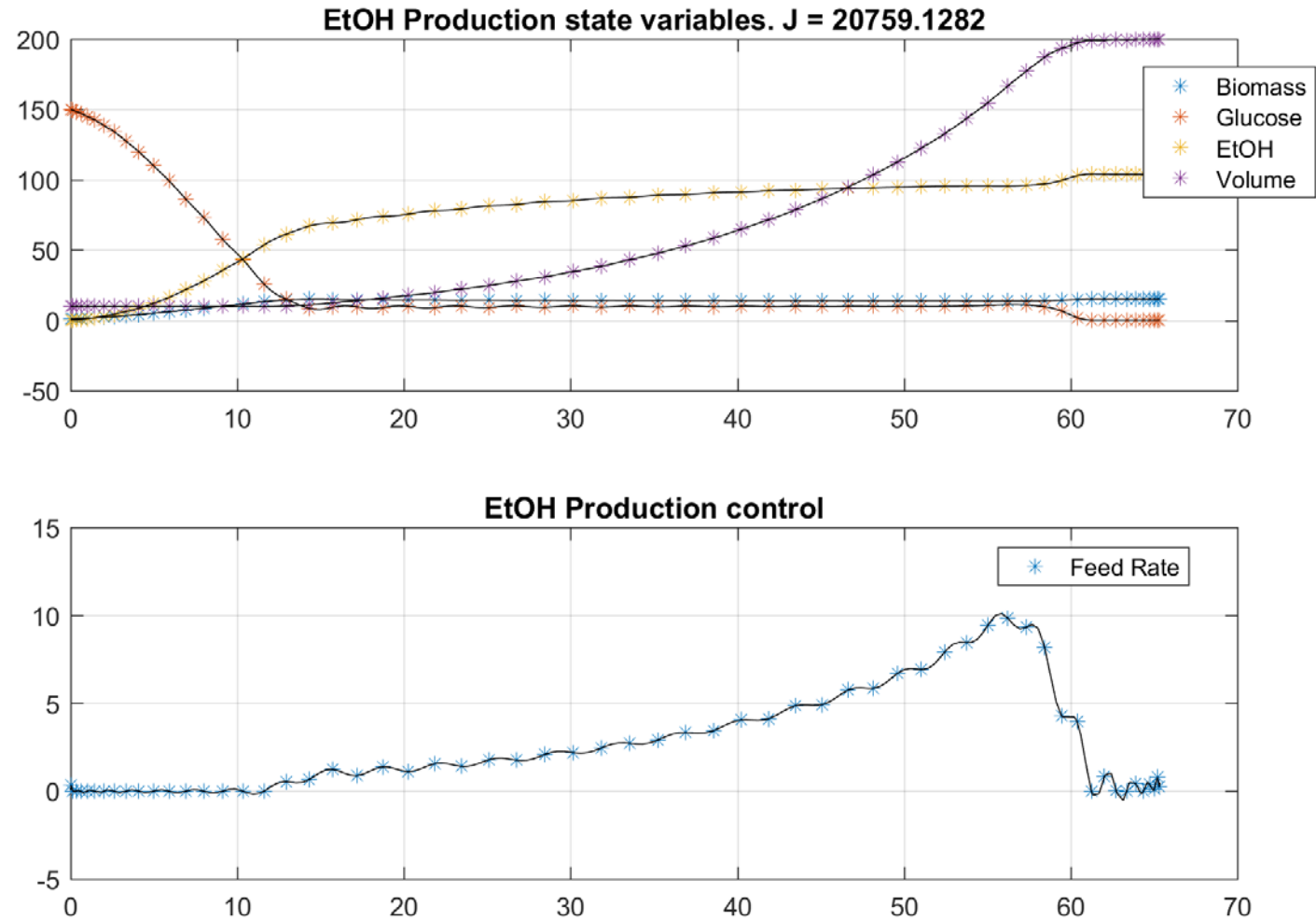
- $\frac{dX}{dt} = \mu X - \frac{F}{V} X$
- $\frac{dS}{dt} = -\frac{\mu}{Y} X + \frac{F}{V} (S_0 - S)$
- $\frac{dP}{dt} = \pi x - \frac{F}{V} P$
- $\frac{dV}{dt} = F$

Optimal control of Fermentation Process

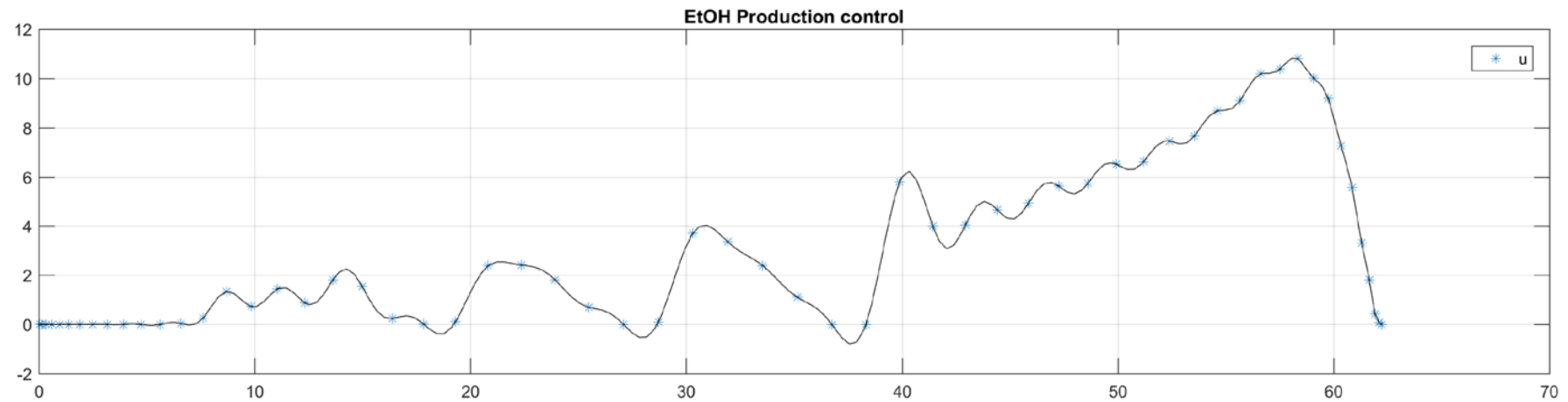
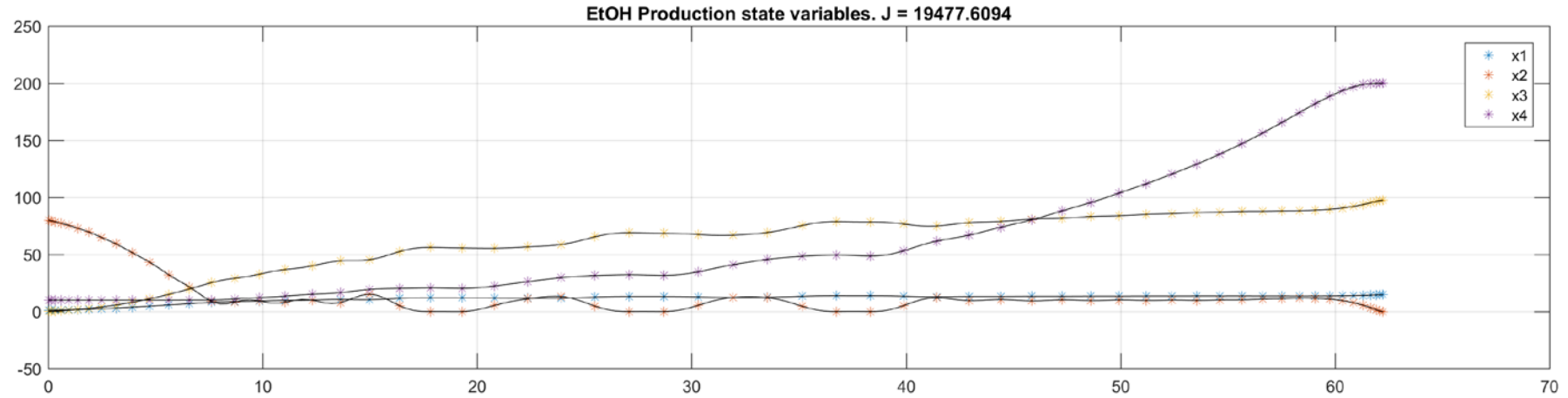
- Goal is to find optimal feeding rate, feed concentration, initial glucose concentration, and initial volume such that the ethanol production rate is maximized at the minimum fermentation time.
- The objective function is:
- $$\max_{F(t), S_o, S_f, V_0, t_f} J = P(t_f)V(t_f)$$
- My Matlab program used a direct collocation method to approximate numerical solutions for the optimal paths



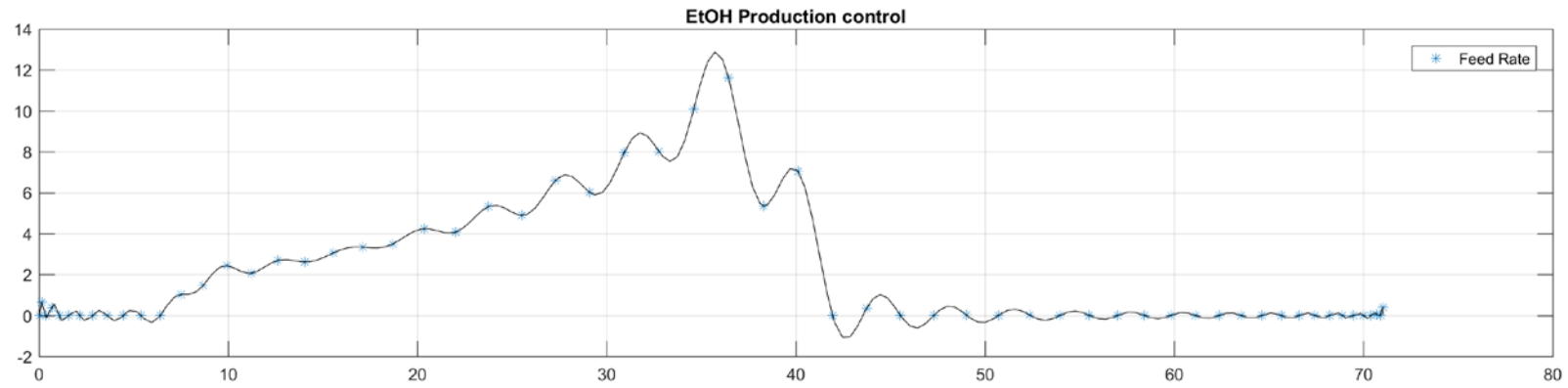
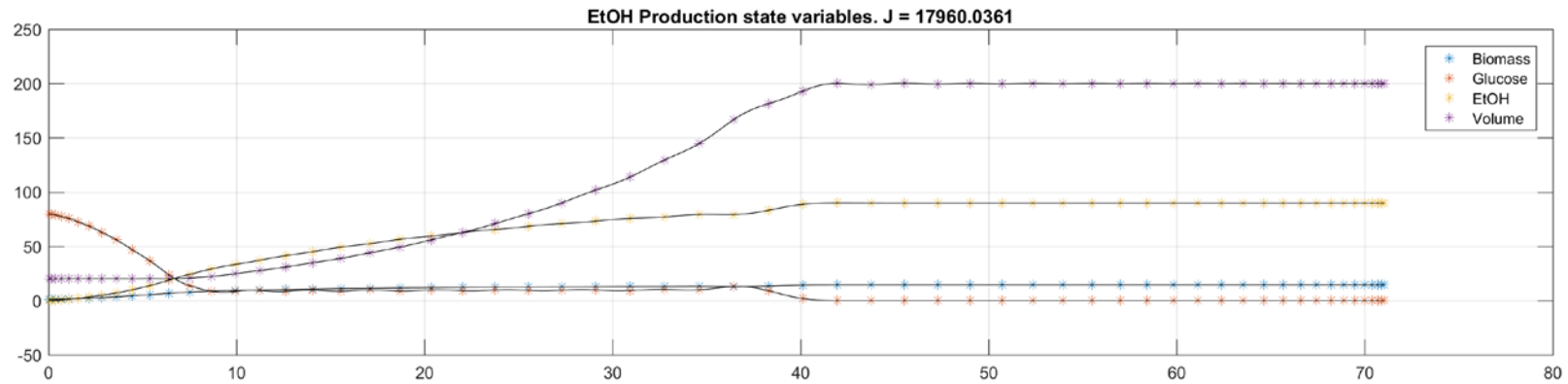
Optimal Paths For States and Control First Run



Optimal Paths With 70 g/L Reduction In Initial Glucose



Optimal Paths With 10 L Increase in Initial Volume



Results From Previous Research

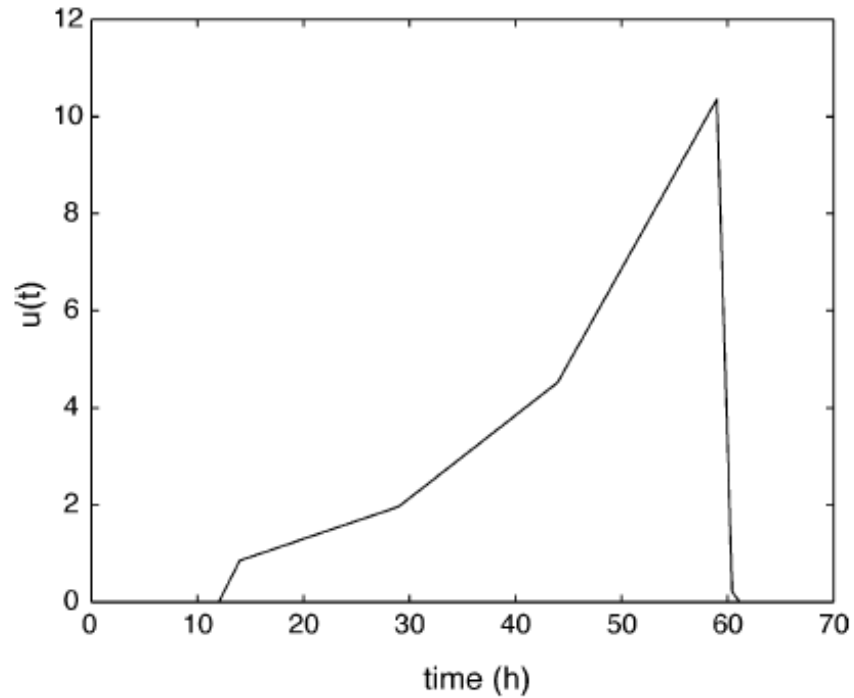


Fig. 7. Best optimal control ($J = 20839$, $t_f = 61.17$ h) for case study II.

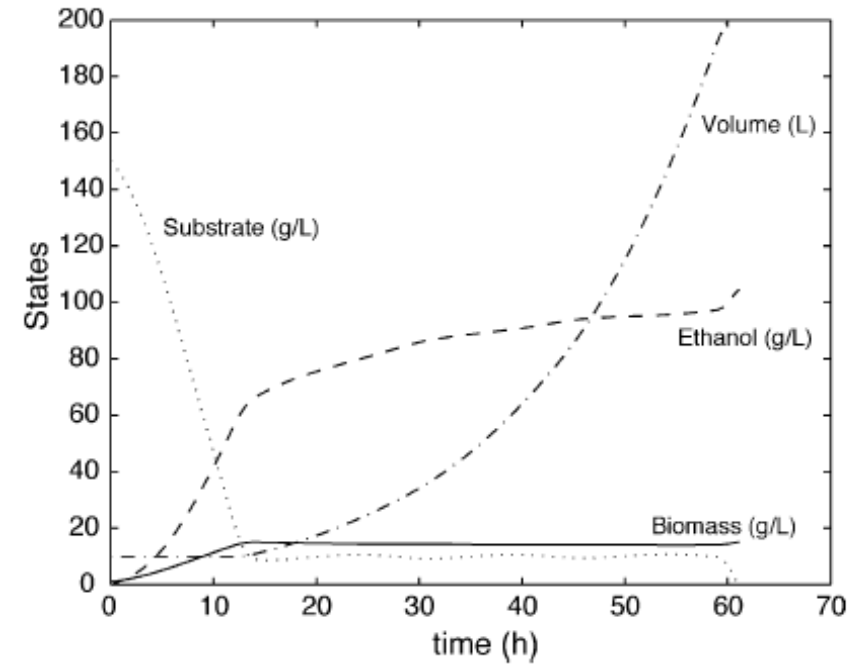


Fig. 8. State profiles for best optimal control, case study II.

Values For Optimal Production Rate and Final Time

- Optimal final time for my first simulation was about 65 hours and the maximum ethanol production rate was 4.22kg/hr.
- Optimal final time for my second simulation was about 61 hours and maximum ethanol production rate was 3.96 kg/hr
- Values are similar to values obtained by previous researchers using a similar model but with higher number of collocation points.
- The feed rate concentration had an optimal path similar to the paths found in other research.
- Once EtOH concentration hits a critical point, biomass decreases sharply towards initial point, but EtOH continues to increase.
- This is consistent with (paper), which states that most EtOH is produced in the later stages of fermentation.

Response to Varying Constraints

- Under the model I selected, maximum ethanol production is attained by adjusting feed rate concentration of glucose according to optimal path determined by solution to control problem.
- EtOH concentration increases despite decreases in biomass concentration of yeast.
- Feed rate and EtOH concentration are both constrained by total volume of chemostat/reactor.
- Reduction in initial glucose concentration by 70 g/l led to only a minor decrease in ethanol production rate.
- An increase in initial volume from 10 L to 20 L causes an increase in final time by > 10 hr

Conclusion

- It is possible to maximize EtOH production through optimal altering of feed rate over time.
- The optimal path of glucose feed rate is highly sensitive to changes in initial conditions.
- The maximum amount of ethanol production and maximum production rate are much less sensitive to changes in initial conditions.
- Maximum production is reached quickest when initial volume is low.

Acknowledgments

- I would like to thank Dr. Fitzpatrick, Dr. Dahlquist, and my fellow classmates.

References

- Brauer, M. J., Saldanha, A. J., Dolinski, K., & Botstein, D. (2005). Homeostatic adjustment and metabolic remodeling in glucose-limited yeast cultures. *Molecular biology of the cell*, 16(5), 2503-2517.
- Van den Brink, J., Canelas, A. B., Van Gulik, W. M., Pronk, J. T., Heijnen, J. J., De Winde, J. H., & Daran-Lapujade, P. (2008). Dynamics of glycolytic regulation during adaptation of *Saccharomyces cerevisiae* to fermentative metabolism. *Applied and environmental microbiology*, 74(18), 5710-5723.
- Wang, F. S., & Cheng, W. M. (1999). Simultaneous Optimization of Feeding Rate and Operation Parameters for Fed-Batch Fermentation Processes. *Biotechnology Progress*, 15(5), 949-952.
- Vázquez-Lima, F., Silva, P., Barreiro, A., Martínez-Moreno, R., Morales, P., Quirós, M., ... & Ferrer, P. (2014). Use of chemostat cultures mimicking different phases of wine fermentations as a tool for quantitative physiological analysis. *Microbial cell factories*, 13(1), 85.
- Gabriel, E., & Carrillo, U. (1999). *Optimal control of fermentation processes* (Doctoral dissertation, PhD Thesis, City University, London).
- Banga, J. R., Balsa-Canto, E., Moles, C. G., & Alonso, A. A. (2005). Dynamic optimization of bioprocesses: Efficient and robust numerical strategies. *Journal of Biotechnology*, 117(4), 407-419.