

Controller Design Project: Yeast Fermentation Bioreactor for Bioethanol Production

1. Introduction

Bioethanol is one of the most important products for the future of the chemical industry. Apart from its large-scale use as a biofuel, bioethanol has the potential to unlock a fully renewable chemical industry through the production of biobased ethylene, one of the two main feedstocks for current organic chemicals and materials. Bioethanol is typically produced by fermentation with the yeast *Saccharomyces Cerevisiae*, which has been used by humans for this purpose since the dawn of civilisation.

You have been put in charge of a project which will deliver a control strategy for a continuous bioreactor to produce ethanol from lignocellulosic glucose. The reactor has very complex kinetics and temperature is **controlled via a cooling jacket**, as the cells will die or underperform if the temperature is not maintained within the design range. Since production has already been delayed two years due to the COVID-19 pandemic, the bioreactor has already been installed, and you have only two weeks to design and test a control strategy before production commences. Simulink (MATLAB version **R2022b**) must be used to carry out calculations and simulations.

2. Project Information

The yeast fermenter has been developed as a bioreactor module (S-function) in Simulink. This mathematical model is **a first-principles model** of a continuous fermentation bioreactor for the production of ethanol from renewable feedstocks (e.g., lignocellulosic biomass). It accounts for various **non-linear characteristics of the process**, including **complex reaction kinetics with product inhibition**, a detailed **energy balance for the bioreactor and cooling jacket**, **the oxygen mass transfer within the fermentation broth**, **the effect of oxygen availability on by-product (i.e., glycerol) formation**, and **the effect of temperature dependence on the kinetic parameters, oxygen mass transfer, and by-product formation**.

The components tracked in this bioprocess include:

- Total cellular biomass (X_t)
- Viable cellular biomass (X_v)
- Glucose (S) as the carbon substrate
- Ethanol (P) as the product of interest
- Glycerol (G) as the by-product
- Oxygen (O)
- Feed Temperature
- Bioreactor Temperature
- Inlet coolant and jacket temperatures

Ethanol is produced during the exponential phase of the microbial culture (growth-associated production), but also a significant amount of ethanol is produced after the cells have reached their stationary phase (non-growth-associated production) (Aiba et al., 1968). Once ethanol production is decoupled from growth, lower temperatures favour product synthesis since the protein unfolding and enzyme deactivation effects are less profound (Aiba et al., 1968).

Like ethanol, glycerol is produced during the exponential phase of the microbial culture (growth-associated production), as well as after the stationary phase (non-growth-associated production). Glycerol is the main by-product of the process, which can account for up to 5% of the carbon source in industrial processes and is produced by the cell as a protective measure against the osmotic stress induced by the reduced water activity in the fermentation broth as a result of increased ethanol concentration in the broth (Alfenore et al., 2004; Hallsworth, 1998; Jones & Greenfield, 1986). Glycerol and polyols contribute to the thermal protection of proteins against denaturation and cell death (Amillastre et al., 2012; Back et al., 1979). Oxygen availability has been shown to affect glycerol formation, where improved aeration strategies lead to reduced glycerol production (Alfenore et al., 2004; Costenoble et al., 2000). Two dependencies are considered for the calculation of the equilibrium concentration of oxygen, namely its dependence on the temperature inside the bioreactor and on the oxygen that is supplied by an air inflow stream. Both dependencies are captured by Henry's law.

Glucose is assumed to be consumed for three distinct activities, namely (i) cellular biomass growth, (ii) ethanol production, and (iii) glycerol formation. Oxygen consumption takes place in the fermentation broth for cellular biomass growth and is assumed to follow saturation kinetics. Elevated temperatures have been shown to induce cell death in yeast cultures (Amillastre et al., 2012).

The reactor is equipped with thermocouples, flow metres, and an in-line HPLC to monitor the inlet and outlet conditions (temperature, flowrate and composition). It also has a mass spectrometer at the outlet to measure product composition. Process variables include:

- Dilution rate
- Feed glucose concentration
- Coolant flowrate
- Air flowrate
- Feed temperature
- Coolant inlet temperature

3. Control Objectives and Problem Statement

You are tasked with controlling the two key variables of the bioethanol production process: ethanol concentration (to keep distillation costs low) and bioreactor temperature (to ensure cell viability). You will do this by manipulating the coolant flowrate and glucose concentration in the feed (your two manipulated variables).

The first control objective is to maintain a steady ethanol production of 40 g/L. The second objective is to control the temperature of the bioreactor at 31.5°C.

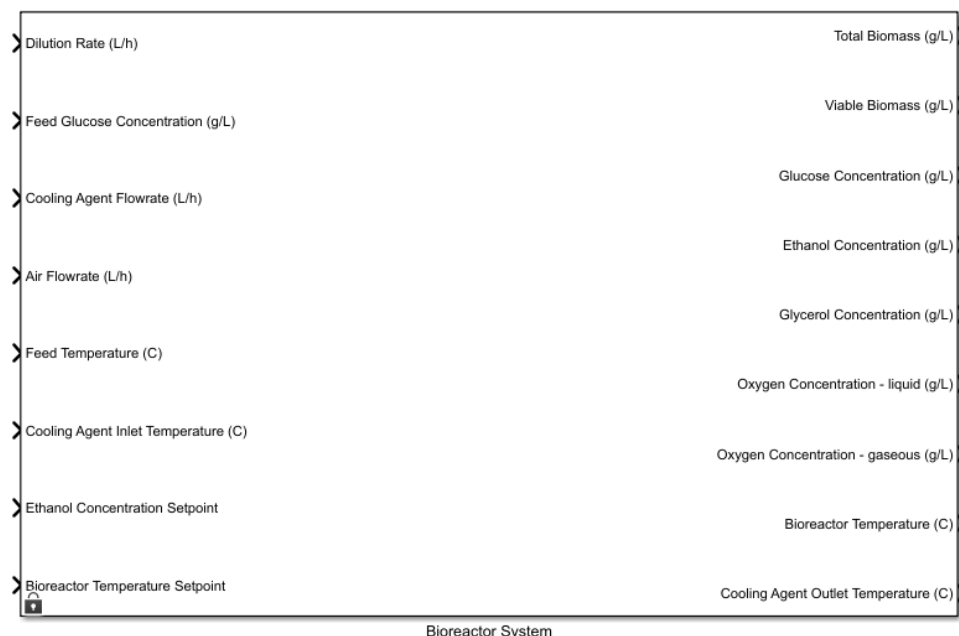
In order to achieve both objectives simultaneously, two potential manipulated variables are proposed: **the glucose concentration in the feed stream and the flowrate of the cooling agent.** The operating ranges of these variables are **20-1200 g/L** and **20-1000 L/h**, respectively. Your control scheme **must not exceed** the upper bounds of these ranges, as higher glucose concentrations would be difficult to solubilise in water and higher coolant flowrates would not be supported by the sizing of the existing piping of the plant.

Additionally, no control can be exerted on the other input variables as these are fixed by upstream processes and previous optimisation efforts. The input conditions for these input variables are as follows:

- Dilution Rate : **0.05** (fixed)
- Air Flowrate : **60,000 L/h** (fixed)
- Feed Temperature : **30°C** (fixed but subject to disturbances)
- Cooling Agent Inlet Temperature : **17.5°C** (fixed but subject to disturbances)

4. Development of a Distributed Control System in Simulink

The user interface of the bioethanol production process in Simulink is shown below **Error! Reference source not found.**(refer to the “Simulink FAQ” provided to you on Blackboard to familiarise yourself with Simulink). The Simulink block comprises **6 inputs** (corresponding to Dilution Rate, Feed Glucose Concentration, Cooling Agent Flowrate, Air Flowrate, Feed Temperature and Cooling Agent Inlet Temperature) and **9 outputs** (Total Biomass, Viable Biomass, Glucose Concentration, Ethanol Concentration, Glycerol Concentration, Oxygen Concentration-liquid, Oxygen Concentration-gaseous, Bioreactor Temperature, Cooling Jacket Temperature).



5. Step-by-Step Controller Design and Implementation

The following parts A-F describe a step-by-step procedure for the development of a controller for the bioethanol production process.

A. Monitor the output signal of key process variables

Make sure that you can monitor the 2 required variables: bioethanol concentration and bioreactor temperature. Choose a nominal state for your system (i.e., nominal values for your manipulated variables) that achieves steady-state bioethanol concentration and bioreactor temperature values close to the required set-points. Make sure that the values of your manipulated variables **never exceed** the physical limits of the system (see discussion in Section 3).

B. Process Identification (Transfer Function Model Identification)

It is useful to identify simple transfer function models to devise an efficient control scheme. Towards this goal, evaluate the **dynamic** response of your control variables with respect to the manipulated variables. In total, you are expected to derive 4 transfer function models by **considering all pairwise combinations of the manipulated variables and the control variables**. In doing so, pay special attention to the step changes imposed, and keep in mind that the process is non-linear (dependent of the value about which step changes are imposed) and valves can saturate. It is recommended to run multiple step tests around the nominal values of the manipulated variables (as chosen in A.) and average the responses.

C. Control Structure Selection (Loop Pairing)

Using Relative Gain Array analysis, compare the possible control structures. Select the best structure and explain your choice.

D. Bioreactor Temperature Control Loop

Design an appropriate feedback controller for the bioreactor temperature:

- Choose an appropriate feedback controller type (try P, PI, and PID).
- Try the Ziegler-Nichols tuning method and the Cohen-Coon tuning rules to select appropriate controller constants. Comment on the feasibility of both methods. The derived controller constants may serve as a first approximation, and then try to improve upon them directly in the plant.
- Observe how your controller affects the bioethanol concentration control loop.

E. Bioethanol Concentration Control Loop

Design an appropriate feedback controller for the bioethanol concentration:

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- Try the Ziegler-Nichols tuning method and the Cohen-Coon tuning rules to select appropriate controller constants. Comment on the feasibility of both methods. The derived controller constants may serve as a first approximation, and then try to improve upon them directly in the plant.
- Observe how your controller affects the bioreactor temperature control loop.

Requirements for sections D-E:

1. The controllers need not be active in the first 150h (allowing the system to stabilise).
You could use switches to make sure that this is the case.
2. The controllers should reach the required set points by 300h.

F. Controller test based on disturbance rejection

- On the morning of **Monday 13th February**, a list of disturbances on process inputs will become available on Blackboard for the groups to download.
- At that stage, you will be expected to have followed the methodology from sections A-E and have successfully designed suitable feedback control structures.
- You are tasked to review and comment on the ability of your existing control structures to reject the disturbances (i.e. does the system return to the set-points and, if so, how quickly?). Consider expanding your existing control structure by designing appropriate feed-forward controllers that minimising the impact of the disturbances on the controlled variables. Do **not** alter the tuning parameters for the feedback controllers.

6. Logistics

1. **Duration and assistance.** The project is available now. The project will run for two weeks (until February 17th). There will be GTA assistance available in person (room **RODH 203**) on Mondays, Tuesdays, Thursdays, and Fridays from 09:00-12:00. Your module coordinator will be available *via* Blackboard, or you can make an appointment *via* email to discuss any group issues.
2. **Groups.** You have been assigned to a group of (normally) 4 students for the duration of the project. Switching will not be permitted.
3. **Assessments.** The project will be assessed in the following ways:
 - a. Controller report (1 per group!) – 100%
4. **Notes**
 - a. You **MUST** use MATLAB version **R2022b** for your design and simulations.

7. Deliverables

1. You are to **email** (cleo.kontoravdi98@imperial.ac.uk) your best control system (Simulink.slx file) no later than **16:00 on Friday 17th February** (**ONE** email per group).
2. You are to **submit** your report no later than **16:00 on Friday 17th February on Blackboard** (**ONE** report per group).

Marking scheme for the report:

- Presentation: overall style, clarity, and organisation 30%
- Description of the theory 30%
- Discussion of the control strategy and simulations 40%

Report Guidelines

The following items are to be submitted:

(a) Report

The submission of one report by each group of students will be required. Please use the normal departmental template for report writing. A penalty will be imposed for reports that exceed the page limit. Arial 11-point font (minimum) and 2 cm margins (minimum).

Each report should not exceed 10 pages, including main body text, but excluding the title page, author names, abstract, and references.

Do not try to include all the results you generate, but include meaningful analyses to go with the figures or tables. Adopt compact and efficient ways to present the results. A compare-and-contrast approach may be helpful with overlaid plots from different simulations shown on the same graph with appropriate legends. For example, present results from single-loop controller performance, performance with both controllers, and performance with decoupled/detuned configurations on the same graph. You may also consider combining results from P, PI or PID controllers and present them on the same plots. This presentation will be efficient and easy to read.

The following is a **suggested** structure for the report and the topics for inclusion under the major headings. There is also a **suggestion** of an appropriate page limit for the different headings.

Table 1. Report structure.

Section	pages
Abstract	-
Introduction	2
Theory and Methodology	3
Results and discussion of system	1
Results and discussion of simulations	3
Conclusions	1

Overall page limit – 10

(i) Abstract and Keywords: The abstract must summarise the content of the report and the main conclusions. This is normally a short paragraph.

(ii) Introduction: The bioethanol process description; general aims and objectives of the reactor and controller design and specific aims for this bioethanol process.

(iii) Theory and Methodology: Only the theory and methods used in the work should be presented (the report is not a tutorial). It can cover the chosen reactor design elements and control strategy and any required details on mass balances, reactor modifications, model identification, feedback control, cascade control, and decouplers, etc., with salient equations and block diagrams as appropriate; methodology to implement these strategies or any experiments.

(iv) Results and analysis: Results and analysis (not all cases, but the ones that you judge as the most important); sample calculations; clear statements of parameters used and

simulations performed. The use of multiple plots on one set of axes is useful for showing comparisons.

(v) Discussion: The discussions must give insights. It is not enough to just describe the results. One way is to create tables or graphs showing trends and provide an explanation for the observed trends.

(vi) Conclusions and suggestions for future work to improve your design.

Report Marking

Reports are due to be submitted electronically (Blackboard) by **16:00 on Friday 17th February**. Late submissions will be penalised. It is wise to allow plenty of time when attempting submission at peak times in case the electronic submission system becomes overloaded.

Marks will be awarded for the quality of the results and presentation of the report. The assessors will look for: Good English and proper grammar including appropriate punctuation marks; organisation of the report in a coherent and logical manner with sections and sub-sections as necessary under the major headings; inclusion of proper citations and references; good formatting including figures with legible lines, appropriate background, legend positioned appropriately and figures of proper size (neither too big nor too small); titles for figures and tables placed appropriately (below the figures and above the tables) and labelled accordingly. Proofread carefully to identify typos.

Reports are checked against each other, as well as those from previous years, and against other electronic sources worldwide using the TurnItIn service.

Reports showing evidence of plagiarism are always penalised.

(b) Program listing

ONE copy of the controller should be sent by email to (cleo.kontoravdi98@imperial.ac.uk) indicating all group member names. Due by **16:00 on Friday 17th February**.

- Controller
 - Keep the name of your controller .slx files as the original one (i.e., 'CSTR_BioReactor_2023.slx'). Create a folder with all the associated controller files and ensure there is only one .slx file in that folder, corresponding to your best control scheme.
 - Compress this folder to a .zip and rename it to 'PC Group [Group number].zip'. So, for example, group 57 would submit 'PC Group 57.zip'
- Submission
 - Submit one .zip file to cleo.kontoravdi98@imperial.ac.uk with the subject line 'PC Group [Group Number] - files'. Send **ONE** email per group.

All additional calculations that were carried out in spreadsheets, etc. should be included in a data file and e-mailed along with the program files in the .zip folder.