

Date: December 11, 2020

To: Dr. Andrew Allman, Process Control Professor

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Subject: Analysis of Various Process Controller Design for a CSTR for Cyclopentadiene Synthesis

First-Principles Model

Our team was tasked with building and analyzing control systems for our CSTR reactor system by building a process model and using the process model to synthesize a controller architecture. The high-temperature CSTR is responsible for ensuring the spontaneous dimerization of cyclopentadiene (species A) to dicyclopentadiene (species B) shifts the equilibrium towards producing high concentrations of Cyclopentadiene needed for our production of a rubber copolymer product. In order to fulfill this process, we must manipulate the inlet flow rate as well as the heating rate in order to control the outlet temperature and concentration of A. This overall process can be modeled through two non-linear ODEs that describe the change in temperature and concentration of A over time as a function of the inlet flow-rate and heating rate.

Using energy and mass balances we derived the two nonlinear ODE's which resulted in the following:

$$\frac{dT}{dt} = \frac{q(T_i - T)}{V} - \frac{(A_{01} * \exp(\frac{-E_1}{RT}) * C_a^2 - A_{02} * \exp(\frac{-E_2}{RT}) * (C_{b,in} - \frac{C_a}{2})) * \Delta H_r}{C_p * \rho} + \frac{Q}{\rho * V * C_p}$$

$$\frac{dC_A}{dt} = \frac{-q * C_A}{V} + 2(A_{01} * \exp(\frac{-E_1}{RT}) * C_a^2 - A_{02} * \exp(\frac{-E_2}{RT}) * (C_{b,in} - \frac{C_a}{2}))$$

To derive these ODE's we assumed the rate law for the reversible reaction was in second order for CA in the forward reaction and first order in the reverse reaction. We also assumed the density, heat capacity, and volume in the CSTR tank are held constant. Instead of deriving an ODE for the concentration of species B, we related the concentration to the inlet B concentration and the outlet concentration of B through:

$$C_b = (C_{b,in} - \frac{C_a}{2})$$

Once we had our two ODEs we linearized the non-linear ODEs, the Temperature-dependent ODE took the form:

$$\frac{dT'}{dt} = a_1 q' + b_1 Q' + c_1 C_a' - d_1 T'$$

While the concentration ODE took the form:

$$\frac{dC_a'}{dt} = a q' + c C_a' - d T'$$

a_1, b_1, c_1, d_1 , and a, c, d were determined from our partial derivative fractions dependent upon the 2 manipulation variables and the 2 control variables and then plugging in our known numerical and nominal values into these equations. The following values for all constants are listed below:

$$a_1 = -2.52 \quad b_1 = .00676 \quad c_1 = .1189 \quad d_1 = -.09672$$

$$a = -.01396 \quad c = 6.3022 \times 10^{-5} \quad d = -.00146$$

Once we had our linearized ODEs, we took the Laplace transforms of each ODE. We should note that although the concentration ODE seemed to not be dependent upon the heating rate, it was dependent on temperature which was dependent upon the heating rate. Substituting $T(s)/Q(s)$, from our temperature Laplace transform equation, into the Concentration linearized ODE in place of T' allowed us to develop our 2 Concentration transfer functions. The following transform equations for both temperature and concentration are represented below:

$$\frac{T(s)}{Q(s)} = G_{21} = \frac{26.05}{-\frac{s}{.09672} + 1}$$

$$\frac{T(s)}{q(s)} = G_{22} = \frac{-.06911}{-\frac{s}{.09672} + 1}$$

$$\frac{C_a(s)}{Q(s)} = G_{11} = \frac{9.5}{-\frac{s}{.00146} + 1}$$

$$\frac{C_a(s)}{Q(s)} = G_{12} = \frac{.00302 \left(\frac{1}{.000146} s + 1 \right)}{\left(-\frac{s}{.09672} + 1 \right) \left(-\frac{s}{.00146} + 1 \right)}$$

As you can see in our transfer functions the τ_i is negative, in our transfer functions. A negative τ_i is not physically realizable, and believe the negative τ_i was the reason for the errors in our Ziegler-Nichols and ISE plots which are described later in the report. We believe we obtained negative τ_i values due to algebraic errors when deriving our non-linear ODEs and linearized equations. However, we believe it does make sense that the concentration transfer function dependent upon the heating rate is in second-order due to the concentration being dependent upon temperature which is dependent upon the heating rate Q even though the ODE for concentration did not contain Q .

Input/Output Pairing

After deriving the 4 transfer functions we plugged in all known variables as well as nominal values for our process allowing us to determine our gains k_{11} , k_{12} , k_{21} , and k_{22} to ultimately determine our lambda values which shaped our RGA matrix. k_{21} and k_{22} were dependent upon

the transfer functions $T(s)/q(s)$ and $T(s)/Q(s)$ respectively and equaled 26.05 and -.06911. k_{11} and k_{12} were dependent upon $Ca(s)/q(s)$ and $Ca(s)/Q(s)$ respectively, setting S to zero in these two transfer functions allowed us to simplify our transfer functions for an easier determination of our gains, especially in $Ca(s)/Q(s)$ which was a second-order transfer function. k_{11} and k_{12} equal to 9.5 and .00302. We used these relative gains to determine our λ_{11} which equals .893 and $1-\lambda_{11}$ equals .107. The resulting RGA matrix is:

$$\Lambda = \begin{bmatrix} .893 & .107 \\ .107 & .893 \end{bmatrix}$$

The RGA matrix corresponded to using G11 and G22 as our appropriate input/output pairing relating Ca to q (inlet flow rate) and T to Q (the heating input) due to the relative gain being closest to 1 compared to .107 for the non-recommended input/output pairing. Controlling the Concentration to the inlet flow rate makes the most physical sense because we want our controller to control the concentration by manipulating the inlet flow rate and minimizing the interactions between the input variables to have better control over the system. Allowing the controller to pair the temperature and heat rate minimize the interactions of the concentration allowing us to more accurately channel the closed loop function to achieve optimal concentration and outlet temperature for our CSTR process.

Ziegler-Nichols Controllers

Our team compared Ziegler-Nichols tuned P controllers in both the ideal and non-ideal pairing conditions. The ideal pairing of flow rate to cyclopentadiene (species A) concentration and the heat input to temperature was based on our assessment of ideal pairing from the previous RGA matrix. Our team decided that a P controller would be most appropriate for this scenario because the given set point tracking ranges (± 25 K and ± 0.1 M) allow for the justification of the expected offsets of a P controller. The following graphs show the Ziegler-Nichols tuned P controllers that are ideally paired at their stability limits when relating concentration and temperature to time using the provided Julia functions.

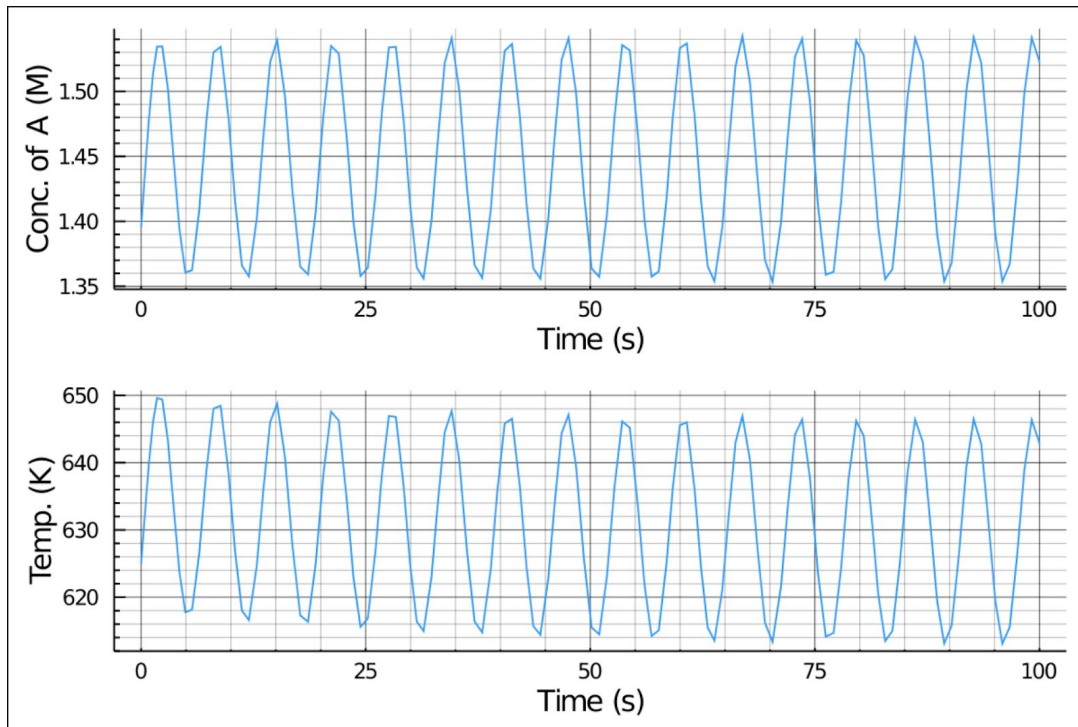


Figure 1: This is a representation of the stability limit of a P controller that pairs flow rate with concentration

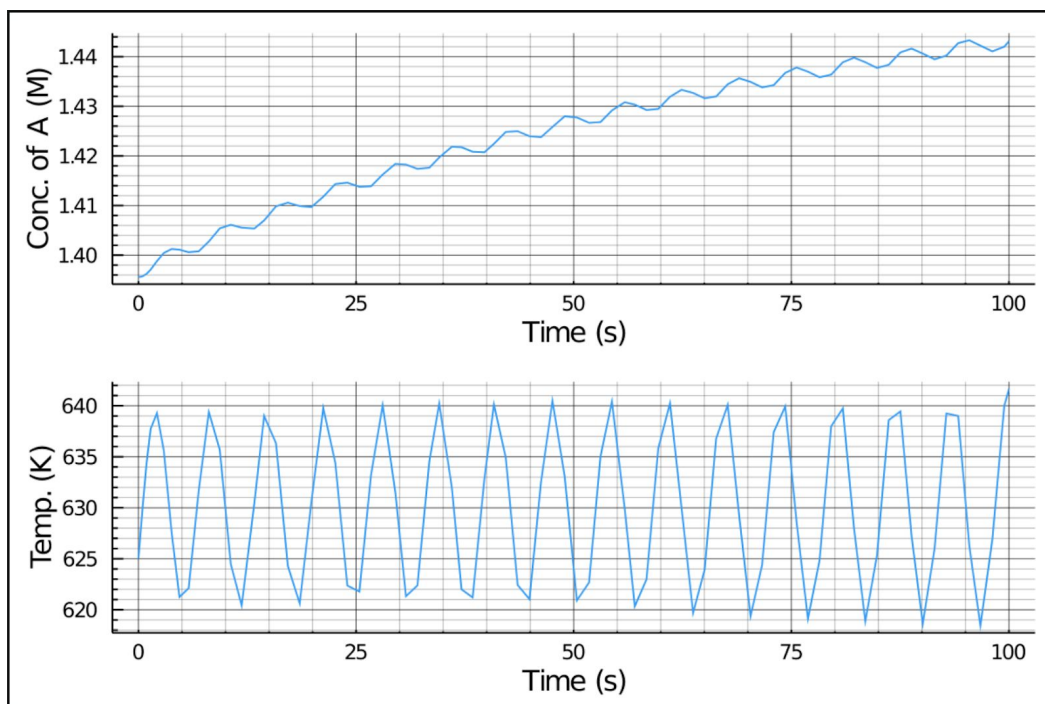


Figure 2: This is a representation of the stability limit of the P controller that pairs heat input with temperature.

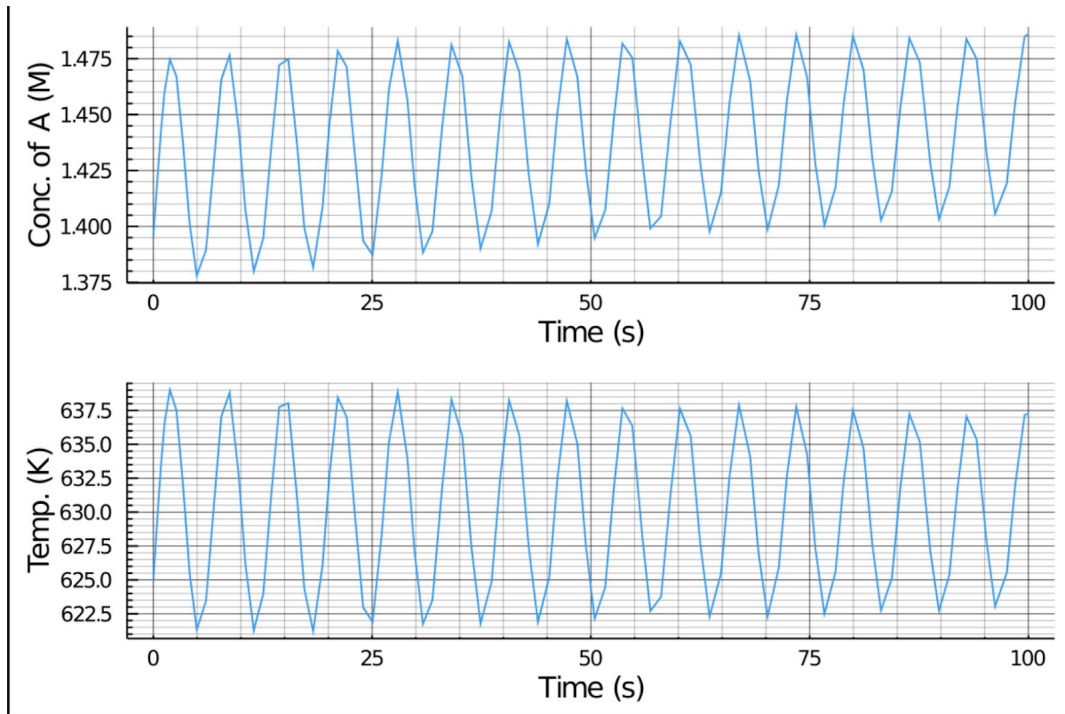


Figure 3: This is a representation of the stability limit of the P controller that pairs flow rate with temperature.

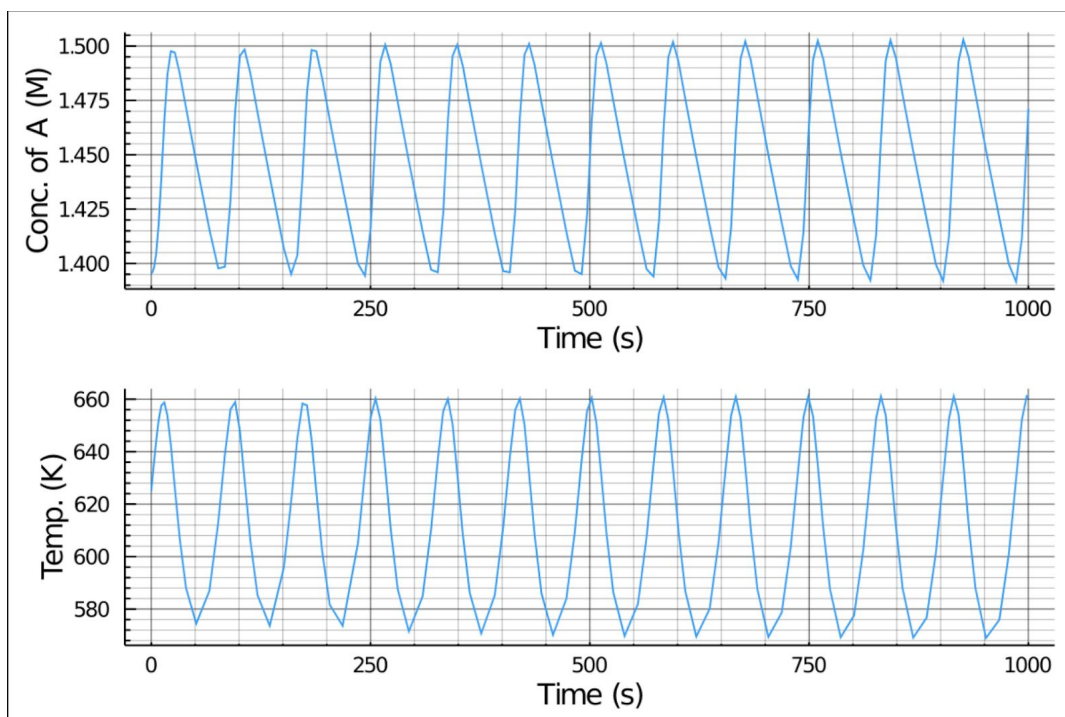


Figure 4: This is a representation of the stability limit of the P controller that pairs heat input with concentration.

From these graphs, we can tell that these controllers are at their stability limit because they output sustained oscillations. In Figures 1, 3, and 4 sustained oscillations are seen in all of the graphs when comparing concentration and temperature to time. In Figure 2 however, there are sustained oscillations in the graph comparing temperature and time which is expected for this controller but there is an increasing oscillation pattern seen in the graph comparing concentration and time that appears to plateau its sustained oscillations at around 1.45M. Since this is below the maximum concentration of 2.0M, this is a valid behavior for this controller. From these graphs, we can determine the ultimate period (P_u) of each P controller transfer function by measuring the distance between two sustained oscillation peaks. Using the ultimate period and K_c of both pairing conditioned controllers, we were able to tune the controllers and determined the following parameters.

	K_c	τ_i	τ_d
Flow and Concentration (Ideal)	-68.5	∞	0
Heat and Temperature (Ideal)	185,634	∞	0
Flow and Concentration (Non-Ideal)	-0.395	∞	0
Heat and Temperature (Non-Ideal)	5,250,000	∞	0

ISE Near-Optimal Controller

After calculations using the previous derived process transfer functions, we were able to develop ISE near-optimal controllers for the ideal pairing of inputs and outputs. The following equations were developed to model our PI controllers.

$$G_{C11} = \frac{1}{25.58s+1}$$

$$G_{C22} = \frac{1}{-9.67s+1}$$

A key simplification that was made for the derivation of these transfer functions is that the r value or “relative degree” was zero in both cases, resulting in the lack of a need for a filter. Another note that was taken about the derivation of G_{C22} is that the τ_i value in this transfer function was negative which is not seen in PI controllers in reality and can be assumed to be due to an arithmetic error in the first-principle model. Because of this, we must take into consideration of this error in further analysis of these controllers.

Comparison of Controllers

After tuning the Ziegler-Nichols P controllers and the development of the initial controller transfer functions, we were able to run a step point tracking test on all three controllers. Using the provided Julia functions, we were able to develop the following graphs.

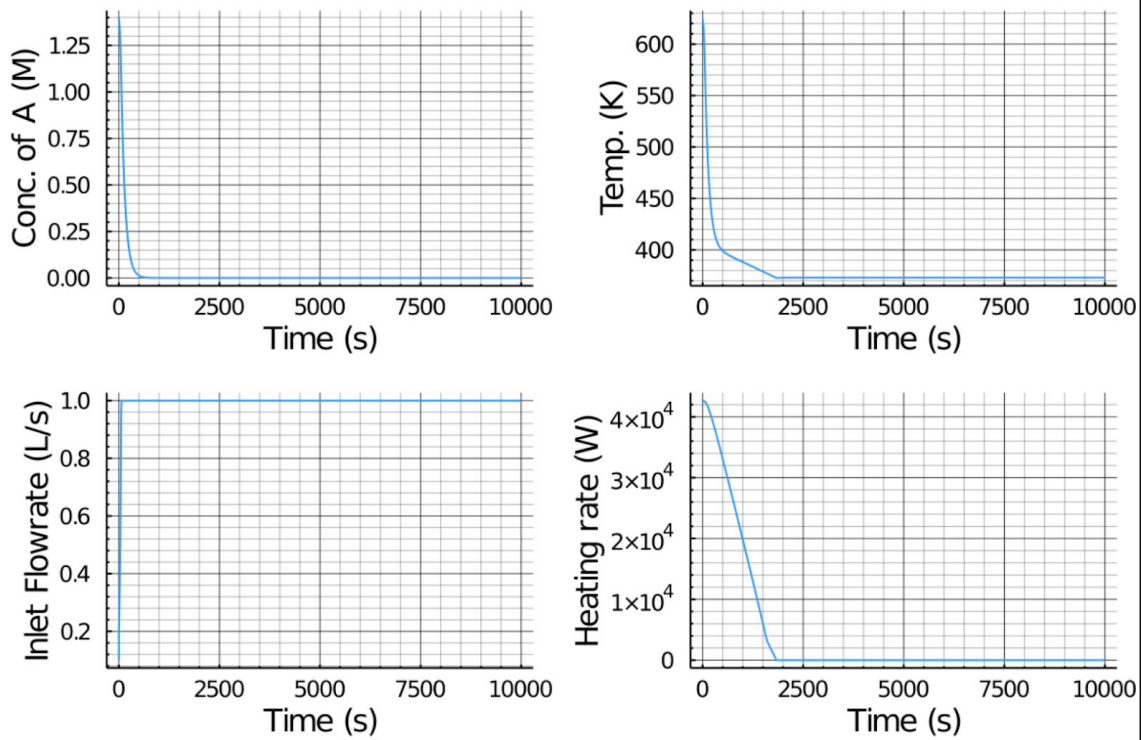


Figure 5: This is a representation of the set point tracking capabilities of the ideal pairing of the ISE near-optimal PI controllers

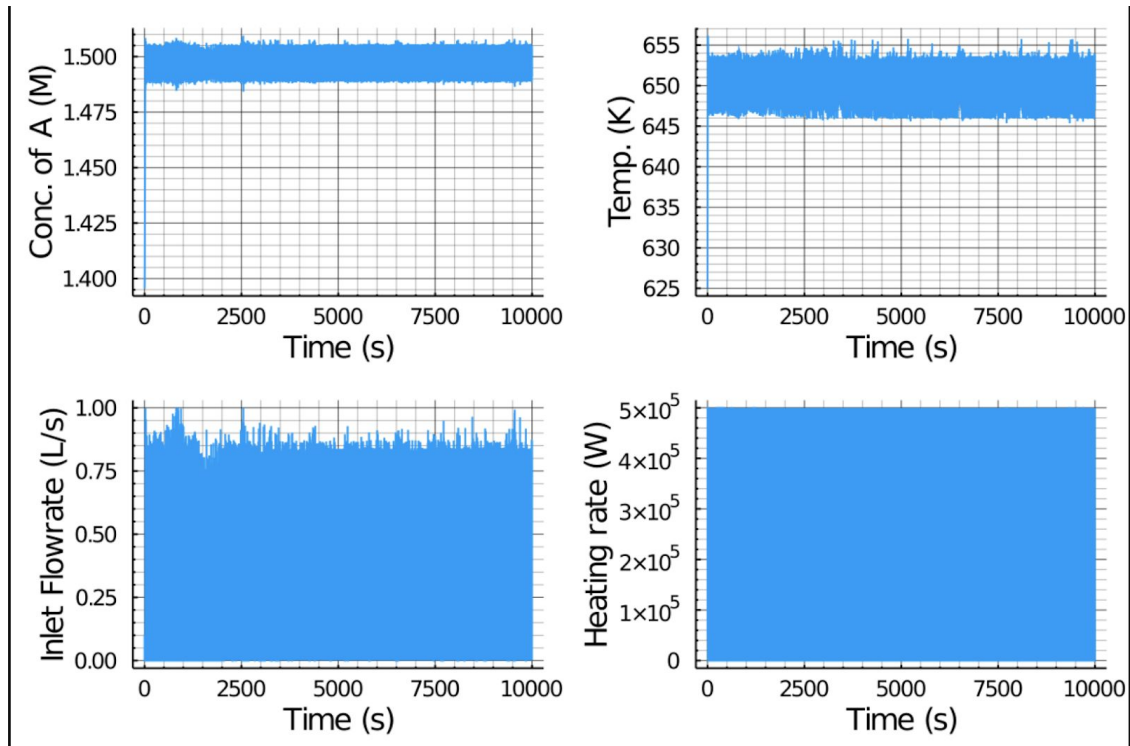


Figure 6: This is a representation of the set point tracking capabilities of the ideal pairing P controllers

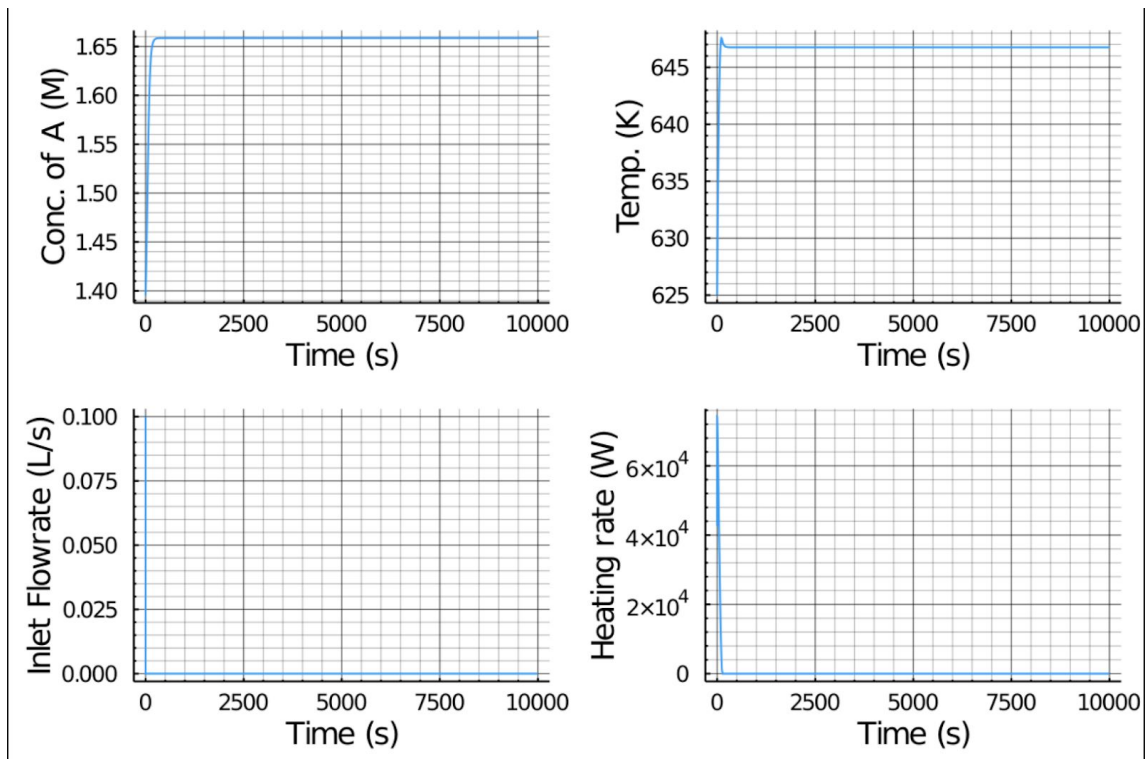


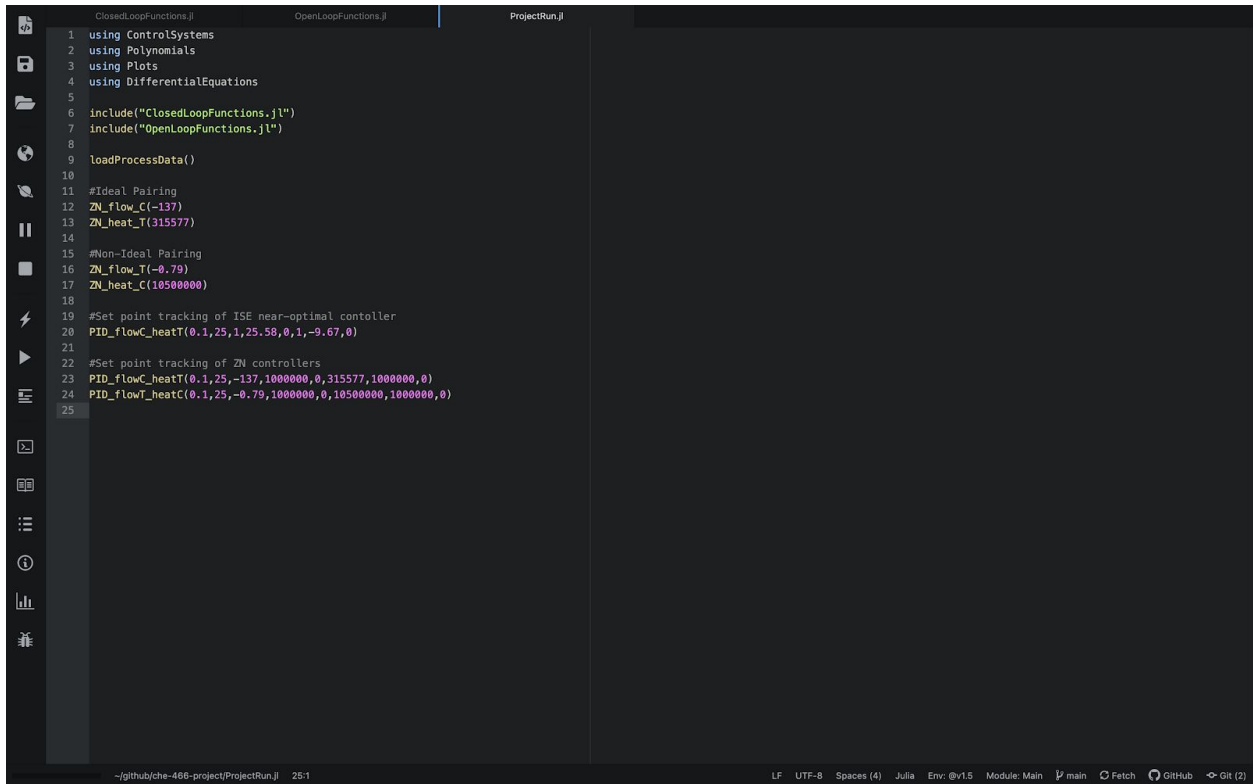
Figure 7: This is a representation of the set point tracking capabilities of the ideal pairing P controllers

From Figure 5, we can see that there is unrealistic behavior from both input and output parameters. After running the flow that keeps the CSTR concentration of species A at a constant 0 M and the temperature at a constant 370 K. This coupled with a constant flow rate of 1 L/s and a gradual decrease in heating rate to 0 W after about 1700 seconds makes this controller inappropriate for this scenario. However, this might not be the case if the arithmetic error present in the first-principles model were not present. From Figure 6, we can see that the ideal pairing keeps the CSTR concentration of species A at around 1.5 ± 0.015 M and keeps the temperature at around 650 ± 5 K. The inlet flow rate and heating rates fluctuate with changes in the outputs. The inlet flow rate is kept at around 0.80 ± 0.15 L/s and the heating rate is kept virtually constant at around 5×10^5 W. From Figure 7, there is completely unrealistic behavior that keeps the CSTR concentration of species A at a constant 1.66 M and the temperature at a constant 646.9 K. What makes these conditions unrealistic is that there is no fluctuation in the outlet parameters. On top of that, the input parameters have a single spike at 0 seconds with an inlet flow rate of 0.1 L/s and a heating rate at around 7.5×10^4 W. This would mean that the heat and flow of chemicals would only turn on once instantaneously at start and the conditions in the tank would remain constant for the next 10000 seconds. This is obviously an unrealistic assumption to make about the operating conditions of this CSTR and makes this pairing unideal for this scenario. Because the controllers for the ideal pairing conditions follow the desired boundary conditions for the outlet parameters, this would make for the highest recommended controller for this scenario compared to the other 2 developed controllers.

Discussion of Control Objectives

From an economic perspective, it can be beneficial to have a CSTR that maintains outputs at a relatively low fluctuation range as we saw from Figure 6 because it will be easy to compute the costs of operation without worrying about large fluctuations that may affect the expected cost of operation. This controller might not be the best from an environmental perspective when looking at the required heating rate for operation, but we can mitigate our environmental impact by using renewable sources of energy to provide this heat such as solar or wind power. Taking social factors into account of this controller design, we can take the financial advantage of using less of the inlet cyclopentadiene to decrease the price of our final copolymer rubber product such that it becomes more easily available to everyone that would want or need to purchase it. Finally from a safety perspective, this controller is ideal because it is not operating at the maximum boundary conditions for temperature or concentration which decreases the risk of runaway reactions from occurring in our CSTR, however, that should never decrease our attentiveness to any potential hazards in this process.

Julia Code



The screenshot shows a Julia IDE with three tabs: `ClosedLoopFunctions.jl`, `OpenLoopFunctions.jl`, and `ProjectRun.jl`. The `ProjectRun.jl` tab is active, displaying the following code:

```
1 using ControlSystems
2 using Polynomials
3 using Plots
4 using DifferentialEquations
5
6 include("ClosedLoopFunctions.jl")
7 include("OpenLoopFunctions.jl")
8
9 loadProcessData()
10
11 #Ideal Pairing
12 ZN_flow_C(-137)
13 ZN_heat_T(315577)
14
15 #Non-Ideal Pairing
16 ZN_flow_T(-0.79)
17 ZN_heat_C(10500000)
18
19 #Set point tracking of ISE near-optimal controller
20 PID_flow_heatT(0.1,25,1,25.58,0,1,-9.67,0)
21
22 #Set point tracking of ZN controllers
23 PID_flow_heatT(0.1,25,-137,1000000,0,315577,1000000,0)
24 PID_flow_heatC(0.1,25,-0.79,1000000,0,10500000,1000000,0)
25
```

The status bar at the bottom indicates the file path `~/github/che-486-project/ProjectRun.jl` at line 25, column 1. It also shows settings for LF line endings, UTF-8 encoding, 4 spaces for indentation, and the Julia environment. The module is set to `Main`, and the current branch is `main`. Git integration is shown with `Fetch` and `Git (2)` options.