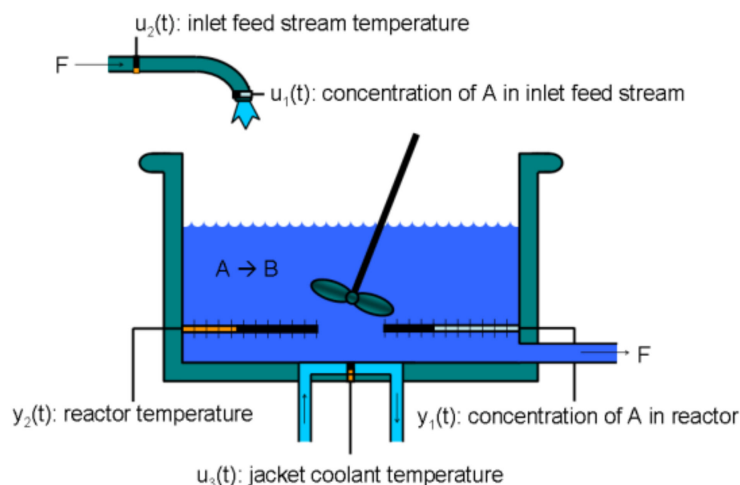


Chemical Process Optimization Overview

The process considered here is a Continuous Stirred Tank Reactor (CSTR) during transition from low to high conversion rate (high to low residual concentration). Because the chemical reaction is exothermic (produces heat), the reactor temperature must be controlled to prevent a thermal runaway. The control task is complicated by the fact that the process dynamics are nonlinear and transition from stable to unstable and back to stable as the conversion rate increases. The reactor dynamics are modeled in Simulink. The controlled variables (states) are the residual concentration C_r and the reactor temperature T_r , and the manipulated variable (action) is the temperature T_c of the coolant circulating in the reactor's cooling jacket.



This example shows how to use Project Bonsai's Machine Teaching strategies to learn a controller for a chemical reactor transitioning from low to high conversion rate. For background, see Seborg, D.E. et al., "Process Dynamics and Control", 2nd Ed., 2004, Wiley, pp. 34-36. This sample is largely adapted from the MathWorks' [Gain scheduled control of a chemical reactor](#).

Table of Contents

Model Overview.....	2
Objective and Constraints.....	3
Metrics.....	4
Experimental Setup.....	4
Benchmark Controller.....	5
Limitations of Benchmark Controller.....	6
Bonsai Brain.....	7
Machine Teaching Benefits.....	7
Brain Design.....	7
Run Gain-Scheduled Controller.....	8
Baseline - 2 Scenarios.....	8
Modifying Parameters.....	8
Important!.....	9
Train Bonsai Controller locally.....	10
Connect to Bonsai.....	10

The bonsaiConfig File.....	10
Run Bonsai Training with a Single\ Local Instance	11
Scale Bonsai training on the Cloud.....	11
Upload the Model.....	12
Train the Brain.....	13
Assessing Brain Performance	13
(2) Assess Brain locally in MATLAB while hosted in Bonai	14
(3) Assess exported Brain locally in Matlab.....	14

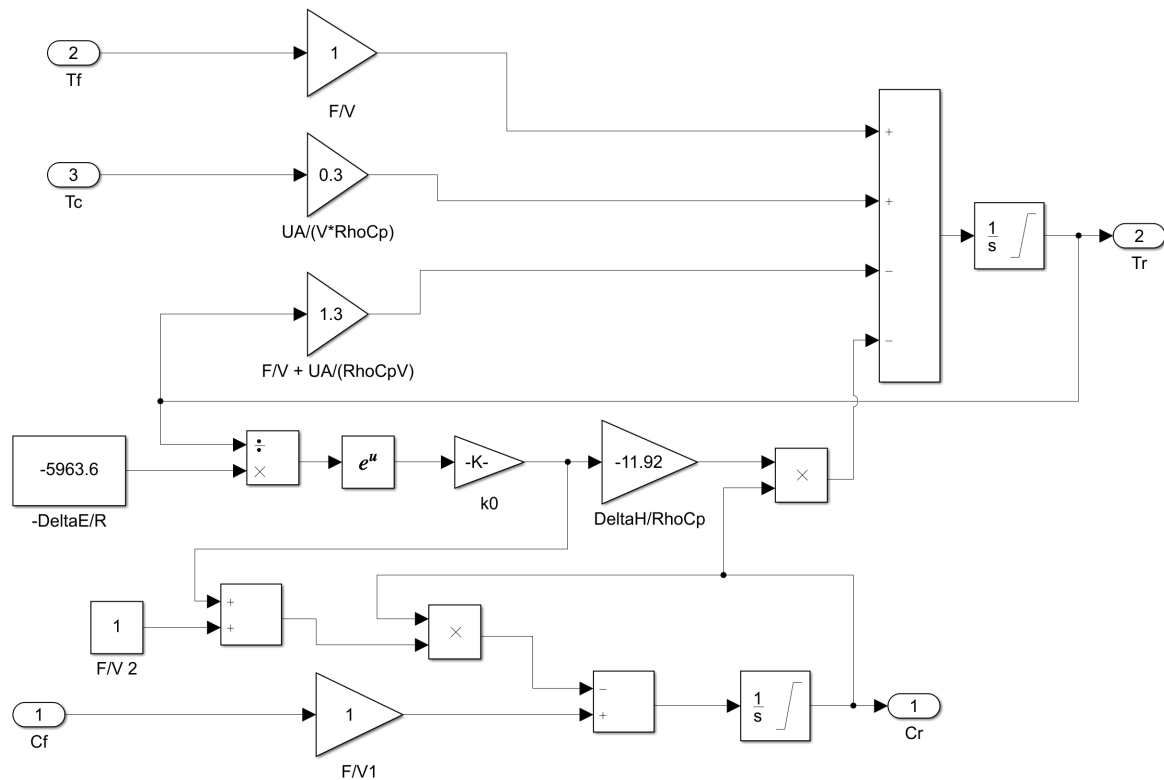
Model Overview

The Continuous Stirred Tank Reactor (CSTR) is modeled as dynamic simulation derived from Reynold's Transport Theorem with unsteady energy balance. The following assumptions are required to get the equations into a form that can be written and solved using Simulink.

1. The CSTR is perfectly mixed
2. The mass densities, ρ , of the feed and product streams are equal and constant
3. The liquid volume, V , in the reactor is kept constant constant by an overflow line
4. The thermal capacities of the coolant and the cooling oil are negligible compared to the thermal capacitance of the liquid in the tank
5. The heat of mixing is negligible compared to the heat of the reaction
6. Shaft work and heat losses to the ambient can be neglected

$$\frac{dT_r}{dt} = \frac{F}{V} T_f + \frac{UA}{V\rho C_p} T_c - \left(\frac{F}{V} + \frac{UA}{V\rho C_p} \right) T_r - \left(\frac{\Delta H}{\rho C_p} k_0 e^{\frac{-\Delta E}{RT_r}} \right) C_r$$

$$\frac{dC_r}{dt} = \frac{F}{V} C_f - \frac{F}{V} k_0 e^{\frac{-\Delta E}{RT_r}} C_r$$



The dynamic model of the CSTR is nonlinear as a result of the many product terms and exponential temperature dependencies. Simulink is used to solve these equations with a fixed timestep, T_s , of 0.5 minutes.

The residual concentration, Cr , has units of $\frac{kmol}{m^3}$. The temperatures T_f , T_c , and T_r are measured in Kelvin.

The following products are required to run the model:

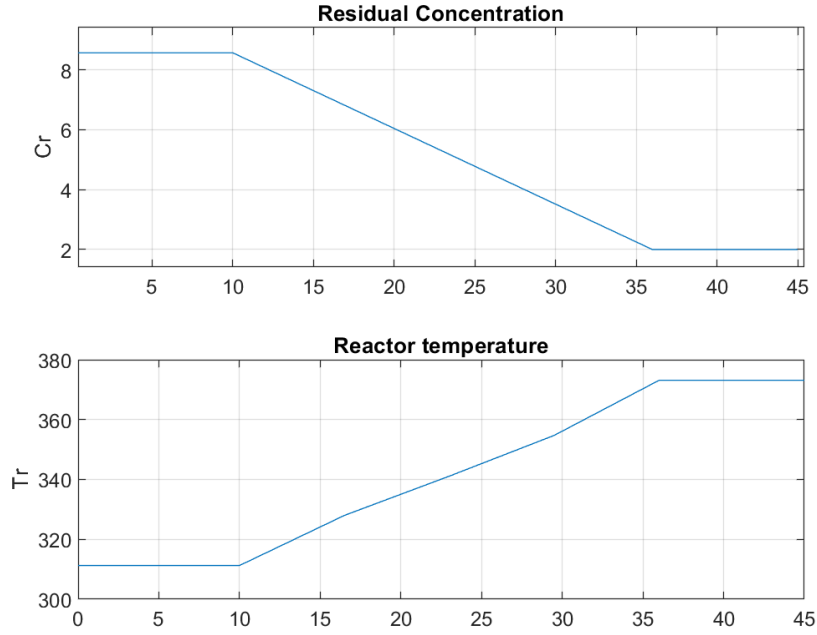
1. Simulink Version 10.0 (R2019b) or greater
2. Bonsai [Toolbox](#) 0.1.4
3. Bonsai [account](#)

Objective and Constraints

The chemical process requires transitioning a residual concentration of $8.57 \frac{kmol}{m^3}$ initially down to $2 \frac{kmol}{m^3}$.

This irreversible chemical reaction is unstable in the mid range and must be properly cooled to avoid thermal runaway. Thermal runaway is considered when the temperature of the reactor exceeds $400K$.

$$T_r < 400K$$



The target residual concentration and corresponding reactor temperatures at equilibrium are provided at each timestep for the ramp down. The transition lasts for 26 minutes long, however, the model is simulated for 45 minutes.

The coolant temperature, T_c , is manipulated as input to the simulation to satisfy the objectives and constraints. The coolant temperature adjustment, dT_c , is relative to the initial equilibrium $T_{cEQ}(1) = 297.88K$.

$$T_c = T_{cEQ}(1) + dT_c$$

The coolant temperature, T_c , is required to be rate limited to 10 degrees per minute (5 degrees per timestep). Inherently, the coolant temperature adjustment, dT_c , which is the variation from the initial equilibrium state, must be rate limited in the same manner. Thus, dT_c can be larger than 10, as long as the increment from previous timestep doesn't exceed 5 degrees Kelvin.

Metrics

In addition to the maximum reactor temperature, metrics like root mean squared (rms) error are useful in quantifying controller performance for a sequential decision making problem. This metric calculates the error from the reference at each timestep and basically aggregates the results throughout the chemical process.

$$C_r \text{ rms error} : 0.5641 \frac{kmol}{m^3}$$

$$T_r \text{ rms error} : 4.6046K$$

Experimental Setup

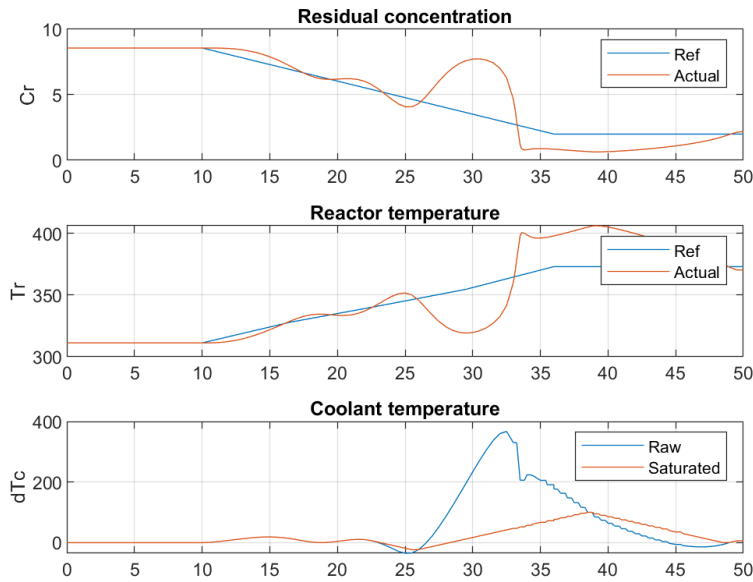
In this sample, we compare the performance of a benchmark Gain Scheduled Controller, to a Bonsai Brain, an Autonomous AI taught with the Microsoft Project Bonsai Platform.

Benchmark Controller

To achieve these requirements, a PI controller is used in an outer loop and a lead compensator is used in the inner loop. Due to the slow sampling rate, the lead compensator is needed to adequately stabilize the chemical reaction at the mid-range concentration $C_r = 5.28 \frac{\text{kmol}}{\text{m}^3}$. This means that there are essentially two controllers being utilized, where the output of the cascaded controllers is ultimately dT_c .

Typically, these controllers have fixed gains considering they are designed around equilibrium points. This problem has various equilibrium points as the residual concentration is transitioned from 8.57 to $2 \frac{\text{kmol}}{\text{m}^3}$. When using constant gains for both controllers, it is apparent that the performance requirements are not met due to the challenging nonlinear dynamics. In fact, the chemical reactor was induced into thermal runaway because T_r exceeds 400K .

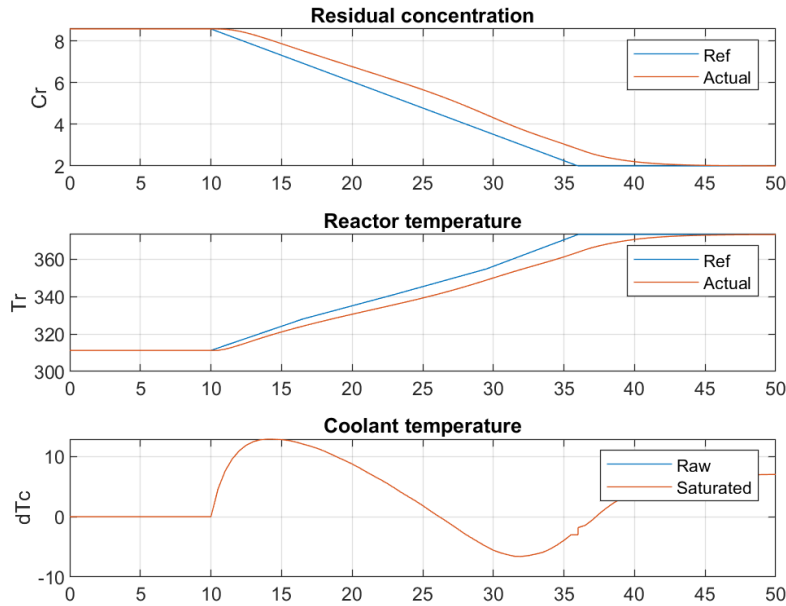
PI Controller Results



Because the reaction dynamics vary substantially with concentration, we further schedule the controller gains as a function of concentration. This is modeled in Simulink using Lookup Table blocks where this example simply provides the tuned gains for use. The design and tuning of these lookup tables involve using the Control System Design toolbox and more information can be found at [Gain scheduled control of a chemical reactor](#).

The benchmark controller successfully transitions the residual concentration from 8.57 to $2 \frac{\text{kmol}}{\text{m}^3}$ without inducing thermal runaway. The tuning of the individual gains also ensured T_c did not vary faster than 10 degrees per minute as shown by the raw and saturated dT_c plots being overlayed on top of one another.

Gain Scheduled PI Controller Results

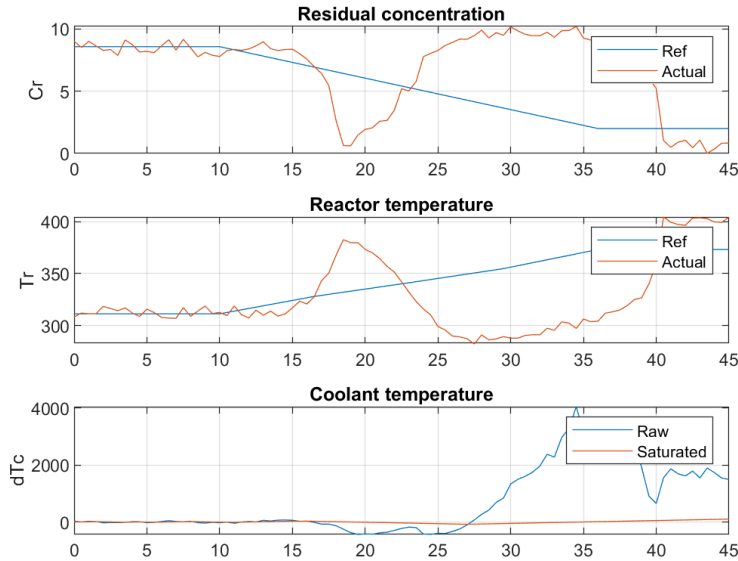


Limitations of Benchmark Controller

The gain scheduled controllers were specifically designed for this transition of 8.57 to $2 \frac{\text{kmol}}{\text{m}^3}$ for C_r . Choosing to specify a different starting and ending residual concentration would require calculating new initial equilibrium values for T_r , C_r , and T_c . Running the simulation with new target values without updating the initial conditions can lead to erroneous results. In order to re-design the gain scheduling for a new transition, we suggest obtaining the Control System Design toolbox and following the steps outlined in [Gain scheduled control of a chemical reactor](#).

When dealing with real-world problems, noisy sensor measurements of your states (control variables) may make controller performance struggle in selecting the ideal action (manipulated variable). Having the sensor provide a slightly wrong value as input to the controller will result in degraded controller performance, especially when ran sequentially. We take the benchmark controller with gain scheduling and introduce 5% Gaussian noise to C_r and T_r in simulation. The root mean squared (rms) error of C_r and T_r are reported and are worse than the benchmark with no noise. The system ran into thermal runaway because T_r exceeded 400K.

Gain Scheduled PI Controller with 5% noise Results



$$C_r \text{ rms error : } 3.8528 \frac{\text{kmol}}{\text{m}^3}$$

$$T_r \text{ rms error : } 39.212\text{K}$$

Bonsai Brain

A Bonsai Brain is an Autonomous AI controller. Microsoft Project Bonsai is a low-code platform that allows non-data science, and non-AI experts, to use Machine Teaching to build AI controllers.

Compared to PID control, AI can generalize across scenarios and handle uncertainty, like noise. Project Bonsai allows users to combine control and AI methods, specifically Reinforcement Learning (RL), to build autonomous systems. RL is not always a replacement of these technologies, rather it is a tool that can be used for targeted use cases and can enhance existing control methods.

Machine Teaching Benefits

Machine Teaching is the concept of injecting subject matter expertise into AI models. Project Bonsai's Machine Teaching can learn a controller to transition the residual concentration without thermal runaway just like the benchmark. Using Project Bonsai, a controller is learned through trial and error in simulation. The learned controller is an approximation that may be beneficial when noise is present in sensor readings.

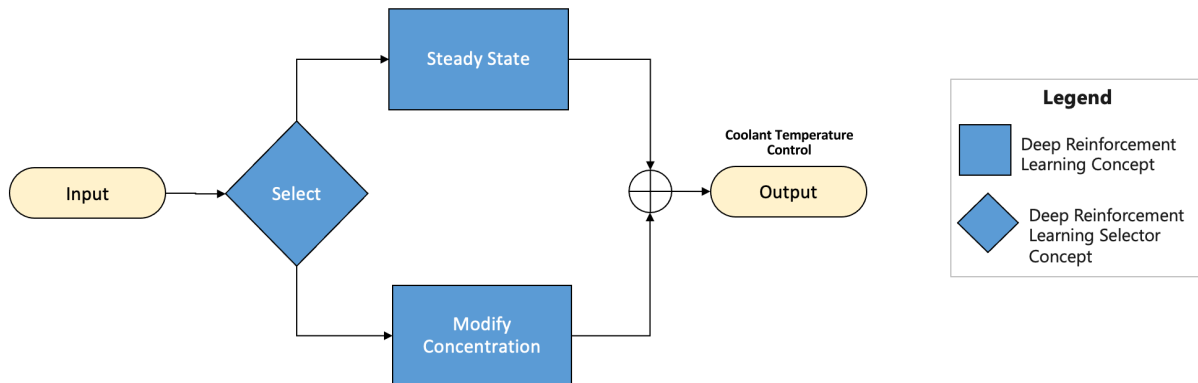
Brain Design

For this demo brain was design with multiple concepts that represent different operating conditions:

- The "steady state" concept controls the brain when the system is trying to produce the steady state residual concentration $8.57 \frac{\text{kmol}}{\text{m}^3}$.
- The "modify concentration" concept controls the brain when the sytem is trying to transition from producing 8.57 to $2 \frac{\text{kmol}}{\text{m}^3}$ over a period of 26 minutes.

- The "select" concept chooses either the "steady state" or "modify concentration" concept depending on the reactor conditions.

Brain Design Diagram



Run Gain-Scheduled Controller

To run the baseline controller (gain scheduled PI), first open the Simulink model:

```
CSTR_PI;
```

Now run the script:

```
run_PI;
```

After entering this command, the baseline will be run under 3 scenarios (see more below). Graphs will be shown for each of them independently.

Baseline - 2 Scenarios

These are the three scenarios that are run for using conventional controllers:

1. Gain Scheduling: This first scenario runs benchmark as engineered. It allows you to assess how well does the current system perform. New controllers (including Bonsai brains) will be compared against this scenario to assess over/under performance.
2. Benchmark with Noise: This second scenario assesses how well does benchmark perform under the influence of gaussian noise on the temperature/concentration read-outs. In a real application, read-outs might be subject to noise, as well as measurement error. This scenario tests robustness to noise.

Modifying Parameters

Each scenario is introduced in a separate section inside the `run_benchmark.m` script. There's 2 elements that you might be the most interested in changing:

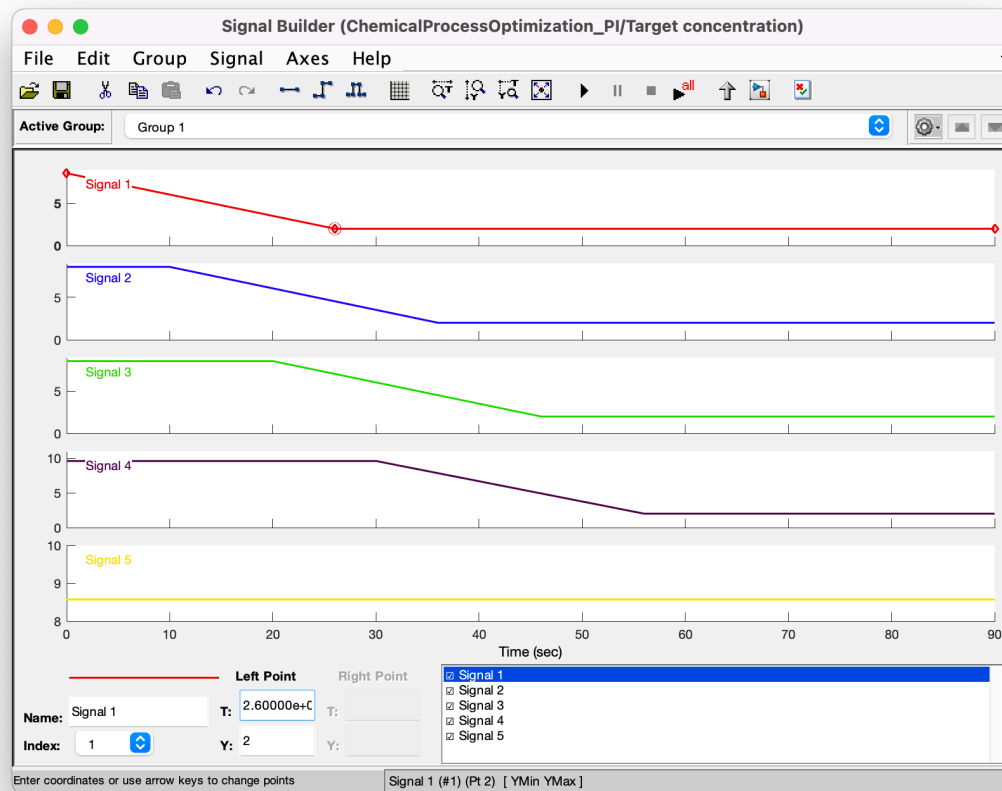
(1) Noise Magnitude: This is the amount of noise introduced to the states (controlled variables) in the model.

To modify the noise introduced during Benchmark Stretched, go and find the following line under "Benchmark (stretch - 5% noise)" section:

```
% Percentage of noise to include  
noise = 5;
```

Modify 5 to whichever value you desired within [0, 100] range.

(2) Signal Reference: This is the reference trajectory of Cref. There are 5 signals preconfigured in the signal builder. The default is signal 2.



Important!

To make sure that you don't run into issues when training with Bonsai, do not make changes to signals 1 - 5 of the signal builder. If you would like to experiment with different reference trajectories, create additional signals.

To modify the signal reference simulated, change the following line under "Initialization Workspace" section:

```
% Set Reference Signal  
Cref_signal = 2;
```

Train Bonsai Controller locally

After getting acclimated with the Chemical Process Optimization model and setting up a Bonsai account, you are now ready to train your first Bonsai brain for this simulation.

To train the Bonsai brain, first open the Simulink model:

```
CSTR_Bonsai;
```

In this model, the PI controller has been replaced with the Bonsai block.

Connect to Bonsai

Follow these steps to connect this model to Bonsai for the first time.

- (1) If you have not done so, you will need to create a Bonsai [account](#).
- (2) From the Bonsai UI, you will need to capture your Bonsai **Workspace ID** and **Access Key**. You can find this information by clicking on your username in the top right and selecting **Workspace Info**.
- (3) Save your workspace info in a hidden .env file. To do this, open **keys.env**, and enter your **Workspace ID** and **Access Key**, and save as **.env**.
- (4) Create a brain. In the Bonsai UI click **+Create Brain**. This will prompt for the type of brain to create. Select **Empty brain** and enter a name in the prompt. In this example, the brain is called **CSTR-demo**. Click the **Create brain** button.

This will create your brain and take you to the **Teach** tab. Note, the INK file will be empty. Now, open the **brain.ink** file. Copy the full content ("CTRL+a", then "CTRL+c") and paste it on the website.

You are now ready to train locally with the Bonsai Controller.

The bonsaiConfig File

The `bonsaiConfig` function is used to setup the connection between your model and the Bonsai platform. Here you describe several key factors:

- **name** - The name of your simulator (you will see this when you connect to Bonsai)
- **url** - Optional. The URL used to connect the Bonsai API service
- **timeout** -- Optional. The value in seconds for a timeout. A default value of 60 seconds is used if this is not explicitly set. **If you receive timeouts when running `bonsaiTrain`, increase this value up to 300*.*
- **workspace** - The workspace value obtained from the Bonsai platform. We recommend storing this value in a .env file.
- **accessKey** - the access key obtained from the Bonsai platform. We recommend storing this value in a .env file.
- **outputCSV** - Optional. When running locally, this can be helpful for debugging your model and the Bonsai connection.

- **stateSchema** - *Important.* This is the *order* of the values as they appear in the input parameter of the Bonsai block. Even if you use a Bus as your input the Bonsai block must understand the order of the values. These names must match what is in your inkling code in Bonsai.
- **actionSchema** - The actions the brain will perform. Input ports to the Moab subsystem. The names must match what is in your inkling code from Bonsai. Order is important.
- **configSchema** - The values that the Bonsai brain will send during a training episode. These are used as configuration parameters to initialize the model with different states, such as ball size, position, or velocity.

We recommend setting up environment variable for `SIM_WORKSPACE` and `SIM_ACCESS_KEY` in a **keys.env** file to prevent accidentally saving credentials into code revisions. See **template.env** for instructions. Another option is to save your Workspace ID and Access Key directly in `bonsaiConfig.m`. **Note: keys.env is an ignored file for git (.gitignore) but it will be uploaded into you workspace managed simulator.**

Run Bonsai Training with a Single\ Local Instance

Now that the connection to Bonsai has been configured, run the `bonsaiTrain` function. Once you see the Sim successfully registered message below or in the MATLAB Command Window, switch over to the [Bonsai UI](#), and click the **Train** button.

```
bonsaiTrain;
```

After clicking **Train**, select the Unmanaged simulator **Simulink-CSTR** (this assumes you left the `.name` value the same in `bonsaiConfig` and a simulator package named **CSTR** has not been uploaded to the platform).

After a short time (typically <2 minutes) the sim will connect. At this point the model is launched and parameters are set, so you may see a delay while this occurs and Mechanics Explorer launches.

After this process completes you will see the iterations per second displayed.

Check the MATLAB Command Window to see a series of outputs indicating communication with the Bonsai brain.

Connection speeds vary, but this model mostly operates at about 3-7 iterations per second.

To stop training, click **Stop Training** in the Bonsai UI.

Note: To terminate the simulation in MATLAB, use Ctrl+C in the Command Window. Be sure to disable Fast Restart from the Simulation tab in the Simulink model.

Scale Bonsai training on the Cloud

Scaling the model greatly improves training times. Once you have verified your model connects and runs locally, you can zip, upload, and scale your model on the cloud. Close Simulink and zip the entire contents of the folder that contains the model.

For example, if your folder structure is:

bonsai-cstr

```
└─ img
  └─ ... image files ...
├─ bonsaiAssess.m
├─ bonsaiConfig.m
├─ bonsaiTrain.m
├─ Chemical_Process_Optimization.mlx
├─ ChemicalProcessOptimization.slx
├─ cpo_tutorial_1.ink
├─ cpo_tutorial_2.ink
├─ CSTRData.mat
├─ init_vars.m
├─ LICENSE
├─ README.md
└─ run_benchmark.m
```

Then you only need to zip the parent **bonsai-cstr** folder. It is suggested you remove your `slprj` folder and `.slxc` files before zipping up the folder contents. You also do not need any `.csv` files, neither the `img/` folder. Call the file `bonsai-cstr.zip`.


Upload the Model


Back in the Bonsai UI, next to **Simulators**, click the **Add sim** button.

This will open a dialog. Select **MathWorks**. Then you can upload your zip file:

Add simulator — Upload model files

Make sure you have integrated the [Bonsai Simulink Toolbox](#) with your model before uploading. Additional terms apply to usage of this software.

 Simulator software
MathWorks Simulink ×


Select or drag and drop simulator model files
Expected file type: .zip, Max size: 150MB.

Simulator name

Create simulator

Cancel

Select or drag the `bonsai-cstr.zip` file created previously.

Give your simulator a name, then click **Create simulator**. In this demo, we use the name **CSTR**.

Note: It may take up to 20 minutes to create the simulator image. You will see the ACR path displayed after successful creation.

After the simulator is created you will see the new simulator appear under the **Simulators** section.

Note: Be sure your brain is not training prior to changing the package statement.

Train the Brain

The three concepts need to be trained separately. First, select the **SteadyState** concept and click the **Train** button. This will create several instances (from 1-50) using your uploaded model to train your brain. If you did not include the name of the simulator package in the inkling, you will be prompted to select the simulator package from the drop down window.

Each concept will need to be trained

Note: It may take up to 10 minutes for your simulators to connect.

Assessing Brain Performance

You can assess the trained brain in 2 ways:

(1) Assess Brain in Bonsai: This allows you to assess the trained brain using the Bonsai assessment feature while still hosting the brain in the Bonsai Platform. See [Assess trained brains in Bonsai - Bonsai | Microsoft Docs](#) for instructions.

(2) Assess Brain locally in MATLAB while hosted in Bonsai: see instructions below

(3) Assess exported Brain in locally in Matlab: see instructions below

(2) Assess Brain locally in MATLAB while hosted in Bonai

This allows you to test the performance of a trained brain in MATLAB while still hosting that brain in the Bonsai platform. The scenario simulated will be selected randomly from the lesson defined in Inking. Run:

```
bonsaiAssess;
```

This will begin assessment and connect to the Bonsai platform, similar to training. If your model is not open this will also open the model.

1. Click the **Run** button in Simulink.
2. In the Bonsai UI, click the **View Policy Performance** button in the Train Tab.
3. If the package statement is still in Inking, it will use a managed simulation for Assessment. To run an unmanaged simulator from your personal computer, uncomment the package statement in Inking (line 79). Then click the **Simulink - CSTR** simulator. Your local model will iterate using the brain in assessment mode. The scenario assessed (Cref_signal and noise) will be chosen from the lesson defined in the Inking.

If you receive the message "Last event was Unregister, done requesting events" then you may need to increase the timeout value in bonsaiConfig.

4. Once the assessment is complete, you can view the results by running the `plot_results` function:

```
plot_results(tout,simout,'Assessment')
```

(3) Assess exported Brain locally in Matlab

1. From you computer, login to docker (docker login) with credentials and make sure docker is running on your local system.
2. Export your brain from the Bonsai platfrom.
3. Pull the brain onto your local system using the "docker pull" command generated in the Deployment Instructions.
4. Start the brain using the "docker run" commands generated in the Deployment Instructions.
5. Configure the endpoint in bonsaiConfig.m or as an environment variable by the modifying **keys.env** files. (defaults to localhost:5000)
6. Run bonsaiExportConnect:

```
bonsaiExportConnect;
```

7. Run the following script to benchmark the exported Brain against the Gain Scheduled PI Controller.

This script will run 4 simulation scenarios and plot the results for comparison:

- 1st: Gain scheduled PI without noise
- 2nd: Gain scheduled PI with noise (as configured below)
- 3rd: Brain with no noise
- 4th: Brain with noise (as configured below)

```
run_benchmark;
```