Design & Simulation Lab
BTCH -18701

Semester: 7th

Department of Chemical Engineering

Sardar Beant Singh State University, Gurdaspur

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Course Objectives: To introduce students to use of software packages such as CHEMCAD, MATLAB, COMSOL for simulation, and also analyzing flow sheets.

Contents:

1. Introduction to Software Packages
2. Setting up models for simulation
3. Steady State simulation using CHEMCAD, Flow sheeting concepts (sequential modular, equation oriented)
4. Dynamic simulation using MATLAB
5. CFD simulations using COMSOL, geometry & meshing Practical Description

{Examples may be drawn from Fluid Flow, Heat Transfer, Reaction Engineering, Process Control}

Course Outcomes : Students will be able to:

1.Solve chemical engineering problems using advanced programming software

2.Use simulation software's like Chem-CAD & COMSOL

3.Analyse the techno-economic feasibility of chemical manufacturing facility

Part-1

(Simulation using Matlab or Python)

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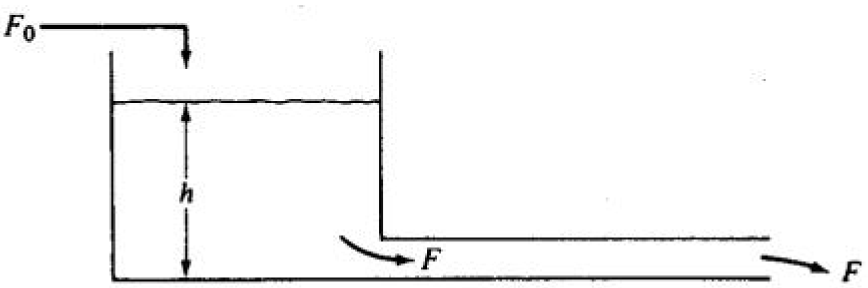
Experiment No.1 Mathematical Modeling & Programming of Gravity Flow Tank

[A tank having an incompressible liquid is pumped with a variable rate F. This inflow rate can vary with time because of changes in operations upstream.]

Assumptions:
Initial flow rate is 50% of design rate & Initial flow rate is 65% of design rate



Equation of Motion:
According to Newton second law of motion, force is equal to mass time acceleration for a system with constant mass.

$$F = \frac{M * a}{g_c}$$

Equation of Motion (Conservation of Momentum)

$$\frac{dv}{dt} = \frac{g}{L}h - \frac{K_f * g_c}{\rho * A_p}v^2$$

Simple ODE for assumption 1

$$\frac{dv}{dt} = 0.0107h - 0.00205v^2$$

Simple ODE for assumption 2

$$\frac{dh}{dt} = 0.311 - 0.0624v$$

Experiment No.2 Mathematical Modeling & Programming of Non Isothermal CSTR

Assumptions:

Irreversible and exothermic reaction.

Volume of the reactor (V) and inside the jacket (V_j) is constant.

nth order kinetics involved.

Heat of reaction is assumed to be λ.

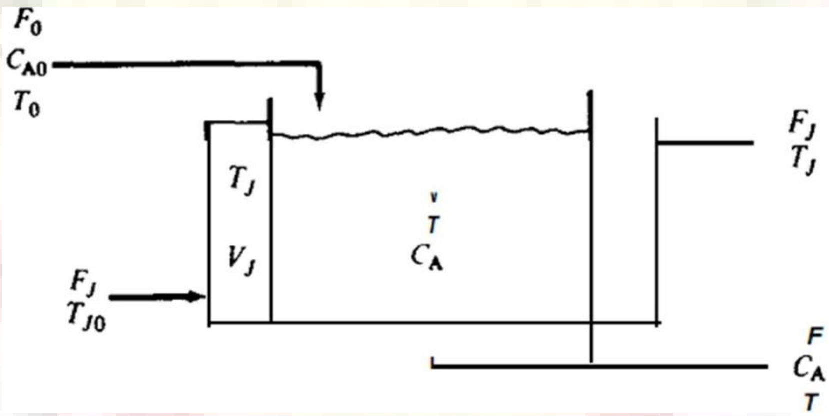
Density of a system is constant and negligible heat loss throughout.

Perfectly mixed CSTR.

Temperature everywhere in the jacket is Tj.

Energy Equation:

[Flow of internal, kinetic and potential energy into system by convection or diffusion] - [Flow of internal, kinetic and potential energy out of system by convection or diffusion] + [heat added to system by conduction, radiations and chemical reaction] - [work done by the system on surrounding (shaft work and PV work)]=[time rate of change of internal, kinetic and potential energy inside system]



- Energy equation for the Reactor:

$$\rho * Cp \frac{d(VT)}{dt} = \rho * Cp(F_0 T_0 - FT) - \lambda V (C_A)^n \alpha e^{-Ea/RT} - UA_H (T - T_j)$$

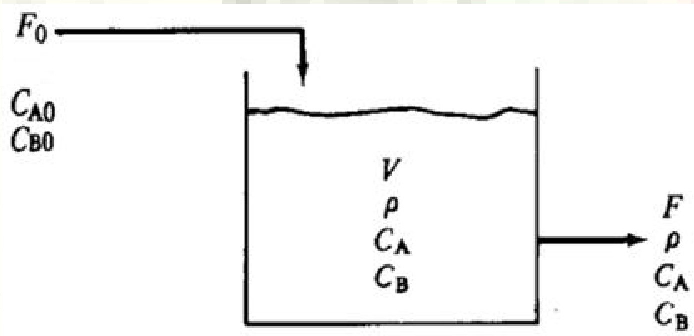
- Energy equation for the Reactor Jacket:

$$\rho_j * C_j \frac{d(T_j)}{dt} = \rho_j * C_j * F_j (T_{j0} - T_j) + UA_H (T - T_j)$$

Experiment No. 3 Mathematical Modeling and Programming of isothermal CSTR

Assumptions:
Reactor is perfectly mixed.
Volume of the reactor is constant.
First order kinetics involved.
Temperature is constant.
Density of a system is constant throughout.

Component Continuity Equation:
[Flow of moles of *jth* components into system] - [Flow of moles of *jth* components out of system] + [rate of formation of moles of *jth* components from chemical reaction]=[time rate of change of moles of *jth* components inside system]



Component continuity equation:

$$\frac{dC_A}{dt} = F_0 C_{A0} - FC_A - KC_A$$

Experiment No. 4 Mathematical Modeling and Programming of non-isothermal Batch Reactor

[Consider a batch reactor. Reactant is charged into the vessel. Steam is feed into the jacket to bring the reaction mass up to desired temperature. Cooling water must be added to the jacket to remove the exothermic heat of reaction and to make the reaction temperature follow the prescribed temperature-time curve.]

Assumptions:

Non isothermal conditions.

Exothermic, irreversible reaction.

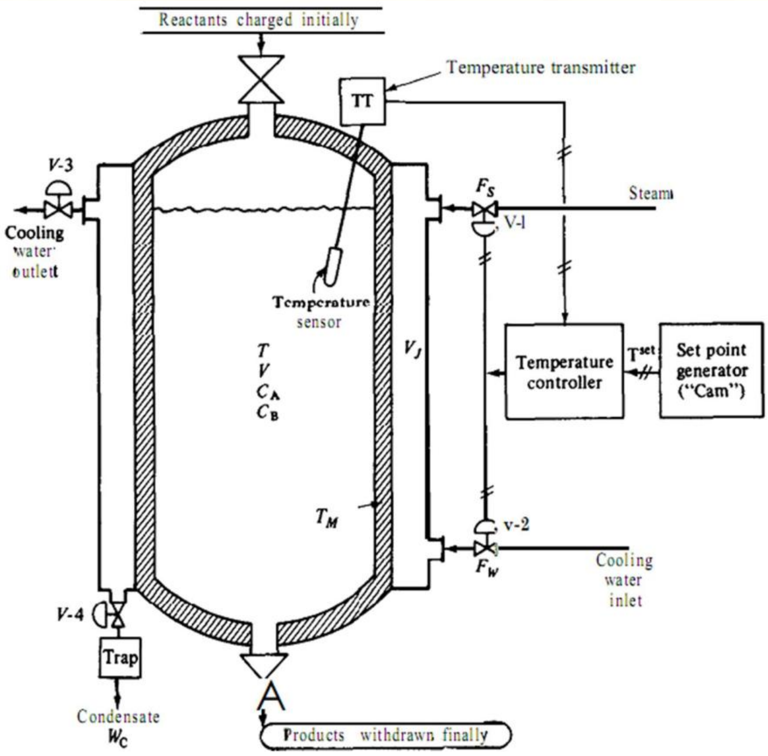
Kinetics of first order involved.

Assume optimum batch time, when reaction should stop.

Density of reacting liquid is constant.

Energy Equation:

[Flow of internal, kinetic and potential energy into system by convection or diffusion] - [Flow of internal, kinetic and potential energy out of system by convection or diffusion] + [heat added to system by conduction, radiations and chemical reaction] - [work done by the system on surrounding (shaft work and PV work)]=[time rate of change of internal, kinetic and potential energy inside system]



Energy Equation for process :

$$\rho V C p \frac{d(T)}{dt} = \lambda_1 V k_1 C_A - \lambda V k_2 C_B - h_i A_i (T - T_M)$$

Energy Equation for metal wall:

$$\rho_M V_M C_M \frac{d(T_M)}{dt} = h_0 A_0 (T_j - T_M) - h_i A_i (T_M - T)$$

Energy Equation for process:

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Experiment No.5 Mathematical Modeling and Programming of isothermal Distillation Column

[Distillation is used in many chemical processes for separating feed streams and for purification of final and intermediate product streams. Most column handle multi component feeds.]

Assumptions:

Binary system with constant relative volatility throughout the column.

A single feed stream is feed at saturated liquid onto the feed tray NF.

Neglect any dead time in vapor line from top of column to reflux drum & in the reflux line back to top tray.

Vapor density must smaller than liquid density.

Molar heat of vaporization of the two components is same.

Temperature changes from tray to tray are assumed to be negligible.

Negligible vapor hold ups. V1=V2=V3 V_N.

Component Continuity Equation:

[Flow of moles of *jth* components into system] - [Flow of moles of *jth* components out of system] + [rate of formation of moles of *jth* components from chemical reaction]=[time rate of change of moles of *jth* components inside system]

Total / Component Continuity Equation for Condenser & Reflux Drum:

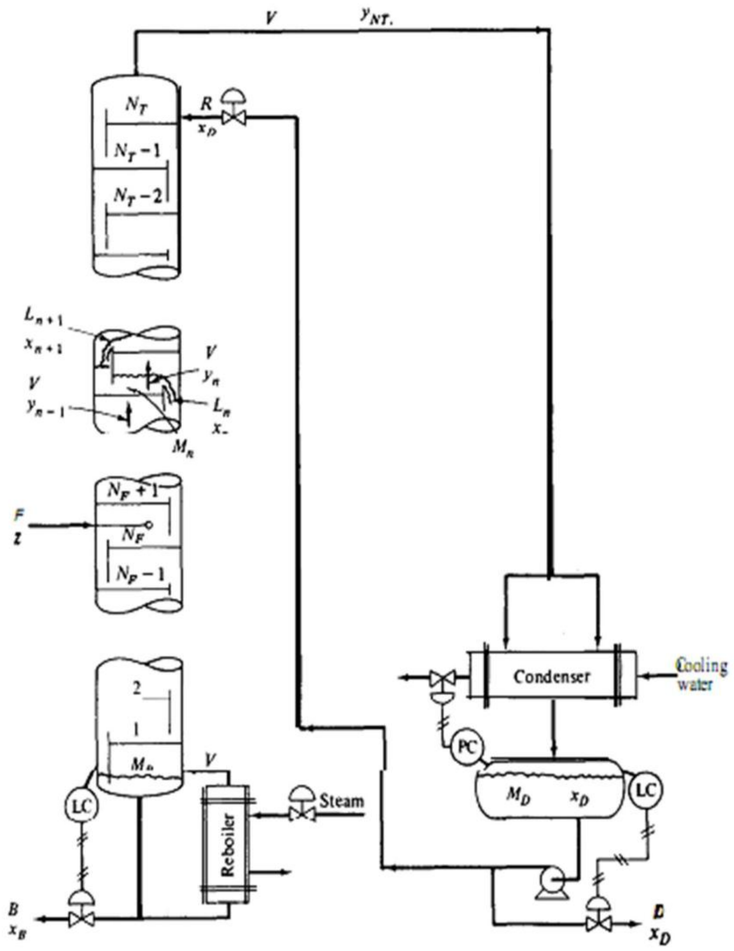
$$\frac{dM_D}{dt} = V - R - D$$

$$\frac{d(M_D x_D)}{dt} = Vy_{NT} - (R + D)x_D$$

Total / Component Continuity Equation For Top Tray ($n=N_T$)

$$\frac{dM_{NT}}{dt} = R - L_{NT}$$

$$\frac{d(M_{NT} x_{NT})}{dt} = Rx_D - L_{NT} x_{NT} + Vy_{NT-1} - Vy_{NT}$$



Total / Component Continuity Equation For nth Tray

$$\frac{dM_n}{dt} = L_{n+1} - L_n$$

$$\frac{d(M_n x_n)}{dt} = L_{n+1} x_{n+1} - L_n x_n + V y_{n-1} - V y_n$$

Total / Component Continuity Equation For feed Tray

$$\frac{dM_{NF}}{dt} = L_{NF+1} - L_{NF} + F$$

$$\frac{d(M_{NF} x_{NF})}{dt} = L_{NF+1} x_{NF+1} - L_{NF} x_{NF} + V y_{NF-1} - V y_{NF} + Fz$$

Total / Component Continuity Equation For first Tray

$$\frac{dM_1}{dt} = L_2 - L_1$$

$$\frac{dM_1 x_1}{dt} = L_2 x2 - L_1 x_1 + V y_B - V y_1$$

Total / Component Continuity Equation For Reboiler and Column Base

$$\frac{dM_B}{dt} = L_1 - V - B$$

$$\frac{dM_B x_B}{dt} = L_1 x_1 - V y_B - B x_B$$

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Experiment No 6

Objective: Estimate the stability of first order or higher order system (U tube manometer) with the help of computer and to study control problems by simulation

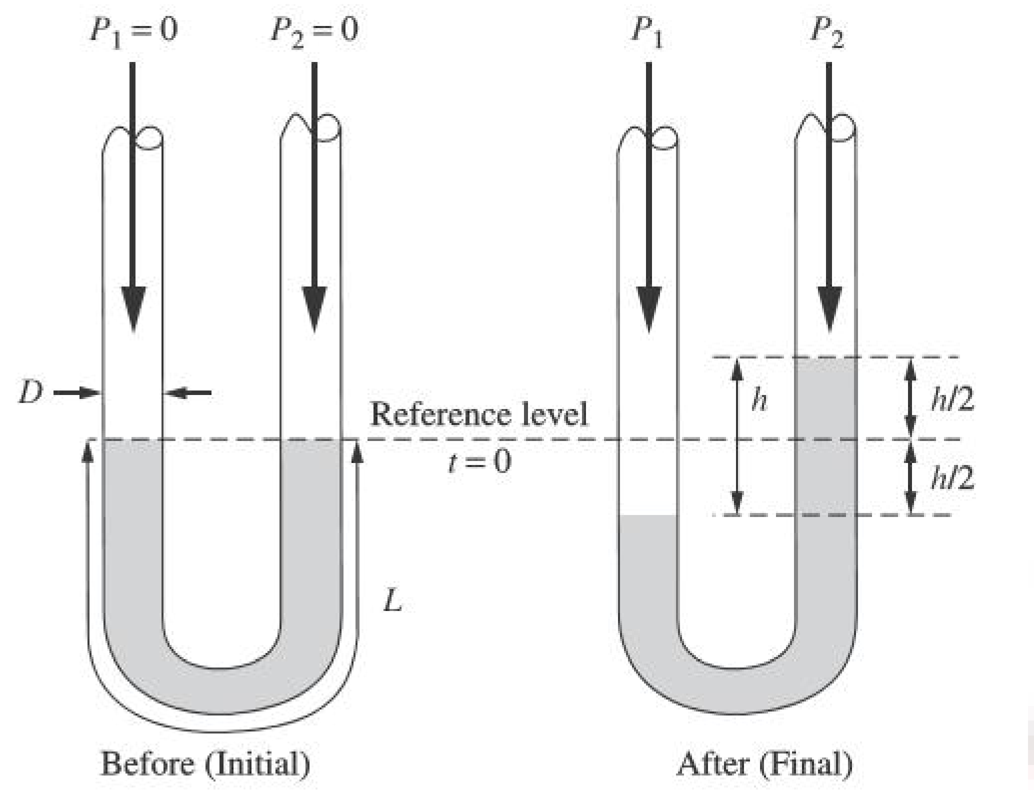
Investigation of the operation of controllers for proportional integral, proportional derivative and proportional integral derivative action using Simulink

Introduction:

Order of system is highest power of's^2' in the denominator of a closed loop transfer function. Second order systems are represented by a by a pair of poles. There may not be zeros in the transfer function, depending on whether there are derivative terms on the right-hand side of the differential equation. From the differential equation, the system function can be written directly. If we assume that the systems are causal, so that the step response is right-sided, then the ROC of the system function is implicitly specified to be to the right of the rightmost pole in the s-plane. The PID controller algorithm involves three separate constant parameters called three-term control like the proportional, the integral and derivative values, denoted P, I, and D. Simply, but these values can be interpreted in terms of time: P depends on the present error, I on the accumulation of past errors, and D is a prediction of future errors, based on current rate of change. The weighted sum of these three actions is used to adjust the process via a control element such as the position of a control valve, a damper, or the power supplied to a heating element.

Theory:

Consider a manometer as illustrated in figure. The manometer is being used to determine the pressure difference between two instrument taps on air line. The working fluid in the manometer is water. Determine the response of the manometer to a step change in pressure across the legs of the manometer.



Physical Data

L = 200cm

g = 980cm / s^2

μ = 1cP = 0.01g / (cm.s) } for the working fluid

ρ = 1.0g / cm^3

$$\frac{\Delta P}{\rho g} = \begin{cases} 0 & for\ t < 0 \\ 10\ cm & for\ t \geq 0 \end{cases}$$

D = 0.11 cm, 0.21 cm, 0.31 cm (Three cases)

Momentum balance on U tube manometer: It developed the differential equation for the manometer

$$\frac{2L}{3g}\frac{d^2\square}{dt^2} + \frac{16\mu L}{\rho D^2 g}\frac{d\square}{dt} + h = \frac{P_1 - P_2}{\rho g} = \frac{\Delta P}{\rho g}$$

The damping coefficient for the three different tube diameters

$$\zeta = \frac{8\mu}{\rho D^2}\sqrt{\frac{3L}{2g}} = \frac{8\,[\,0.01\frac{g}{cm.s}]}{\left(\frac{1.0g}{cm3}\right)(D^2)}\sqrt{\frac{3(200\ cm)}{2\left(980\frac{cm}{s^2}\right)}} = \frac{0.0443}{D^2}$$

Diameter (cm)	ζ
0.11	3.66
0.21	1.00
0.31	0.46

Clearly we have one under-damped system (ζ< 1), one critically damped system (ζ=1) and one over-damped d system (ζ >1).

Experiment Methodology:

(1) Develop the Simulink model for the following transfer function that developed from momentum transfer balance

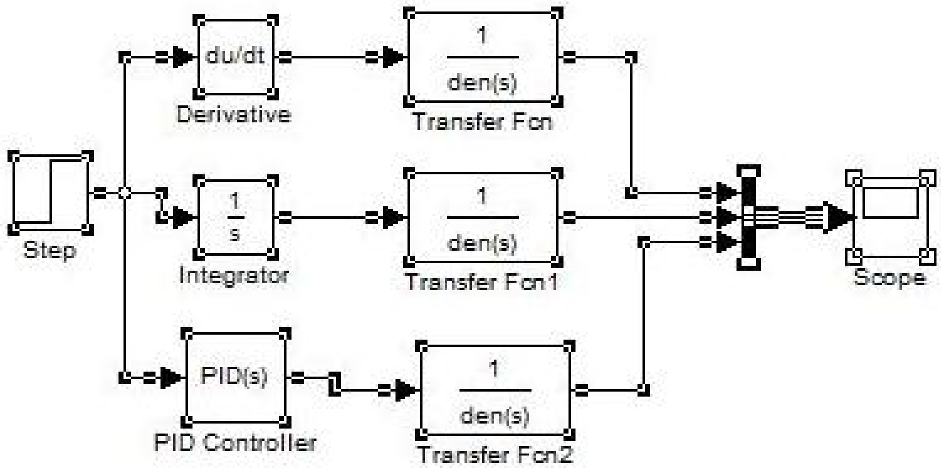
Diameter(cm)	τ	ζ	τ^2	$2\,\zeta\tau$	Transfer Function
0.11	0.369	3.66	0.136	2.70	$\frac{1}{0.136s^2 + 2.70s + 1}$
0.21	0.369	1.00	0.136	0.738	$\frac{1}{0.136s^2 + 0.738s + 1}$
0.31	0.369	0.46	0.136	0.340	$\frac{1}{0.136s^2 + 0.346s + 1}$

(2) The step input of magnitude of 10 units is for second order Laplace equation.

$\frac{Y(s)}{X(s)} = \frac{1}{\tau^2\, s^2 + 2\zeta\tau s + 1}$ and x= $\frac{10}{s}$

(3) Develop the Simulink model for three inputs without controller as shown in Figures.

(4) Develop the Simulink model for over damped system using proportional integral, proportional derivative and proportional integral derivative.



Results:

Discussion

Experiment No 7

Objective: To determine the best setting of controllers (bode plot) with controlling an actual process.

Theory: Bode diagram design is an interactive graphical method of modifying a compensator to achieve a specific open-loop response (loop shaping).The interactively shape the open-loop response using Control System Designer, the Bode Editor used. In the editor can adjust the open-loop bandwidth and design to gain and phase margin specifications. In addition to that adjust the loop shape, added poles and zeros to your compensator and adjust their values directly in the Bode Editor, or can use the Compensator Editor.

Plant Model and Requirements: The transfer function of the chemical process reactor, as described in SISO

$$G = \frac{\mathbf{1.5}}{s^2 + \mathbf{14}s + \mathbf{40.02}}$$

The design requirements are:

Rise time of less than 0.5 seconds, Steady-state error of less than 5%, Overshoot of less than 10%, Gain margin greater than 20 dB and Phase margin greater than 40 degrees

Modeling & Simulation in Open Control System Designer

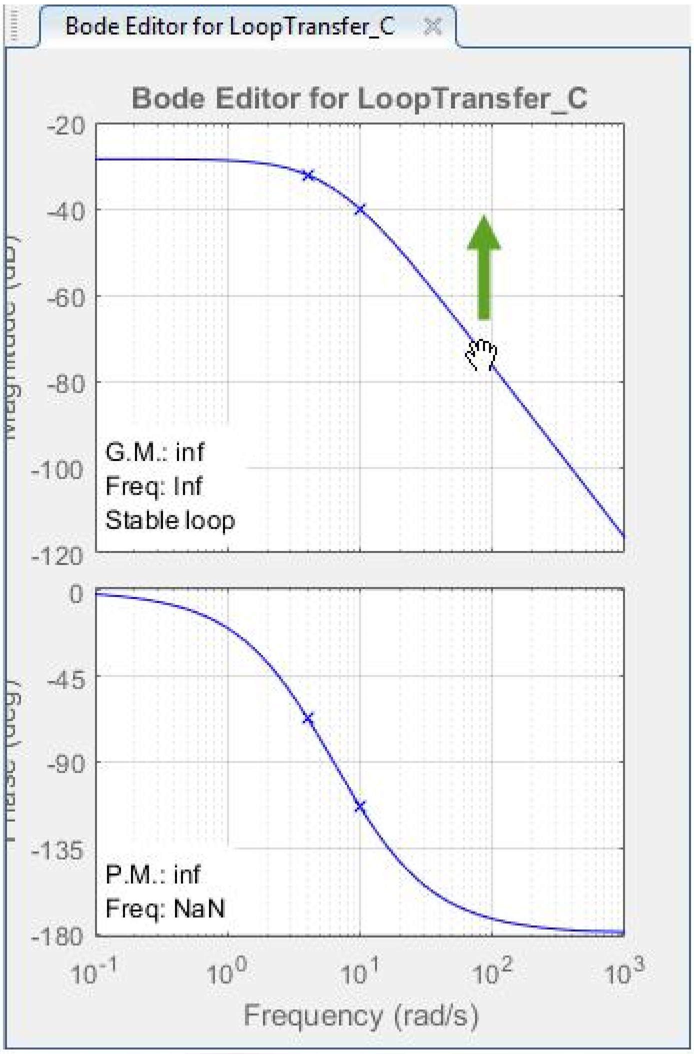
At the MATLAB command line creates a transfer function model of the plant, and open Control System Designer in the Bode Editor configuration.

```
G = tf (1.5, [1 14 40.02]);
ControlSystemDesigner ('bode', G);
```

Adjust Bandwidth

Since the design requires a rise time less than 0.5 seconds, set the open-loop crossover frequency to about 3 rad/s. To a first-order approximation, this crossover frequency corresponds to a time constant of 0.33 seconds.

To make the crossover easier to see, turn on the plot grid. Right-click the Bode Editor plot area and select Grid. The app adds a grid to the Bode response plots. To adjust the crossover frequency increases the compensator gain. In the Bode Editor plot, in the Magnitude response plot, drag the response upward. Doing so increases the gain of the compensator.

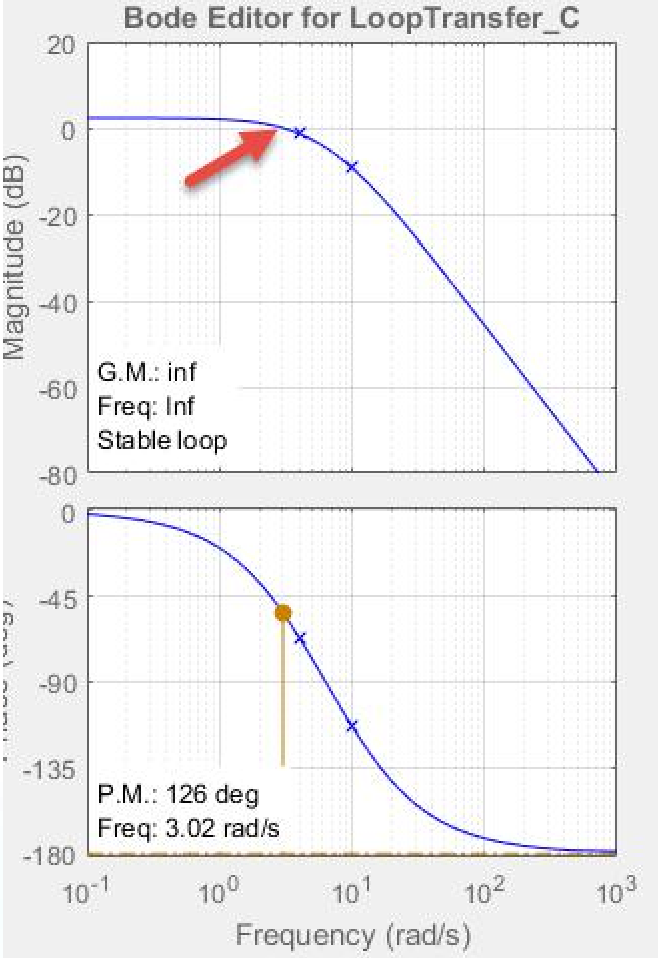


Drag the magnitude response upward until the crossover frequency is about 3 rad / s.

View Step Response Characteristics

To add the rise time to the Step Response plot, right-click the plot area, and select Characteristics > Rise Time

Similarly, to add the peak response to the Step Response plot, right-click the plot area, and select Characteristics > Peak Response.



Add Integrator to Compensator

To meet the 5% steady-state error requirement, eliminate steady-state error from the closed-loop step response by adding an integrator to your compensator. In the Bode Editor right-click in the plot area, and select Add Pole/Zero > Integrator

Adding an integrator produces zero steady-state error. However, changing the compensator dynamics also changes the crossover frequency, increasing the rise time. To reduce the rise time, increase the crossover frequency to around 3 rad/s.

Adjust Compensator Gain

To return the crossover frequency to around 3 rad/s, increase the compensator gain further. Right-click the Bode Editor plot area and select Edit Compensator. In the Compensator Editor dialog box, in the Compensator section, specify a gain of 99, and press Enter. The response plots update automatically.

The rise time is around 0.4 seconds, which satisfies the design requirements. However, the peak overshoot is around 32%. A compensator consisting of a gain and an integrator is not sufficient to meet the design requirements. Therefore, the compensator requires additional dynamics.

Add Lead Network to Compensator

In the Bode Editor, review the gain margin and phase margin for the current compensator design. The design requires a gain margin greater than 20 dB and phase margin greater than 40 degrees. The current design does not meet either of these requirements.

To increase the stability margins, add a lead network to the compensator.

In the Bode Editor, right-click and select Add Pole / Zero > Lead.

To specify the location of the lead network pole, click on the magnitude response. The app adds a real pole (red X) and real zero (red O) to the compensator and to the Bode Editor plot. In the Bode Editor, drag the pole and zero to change their locations. As you drag them, the app updates the pole / zero values and updates the response plots. To decrease the magnitude of a pole or zero, drag it towards the left. Since the pole and zero are on the negative real axis, dragging them to the left moves them closer to the origin in the complex plane.

The phase margin meets the design requirements; however, the gain margin is still too low.

Edit Lead Network Pole and Zero

To improve the controller performance, tune the lead network parameters. In the Compensator Editor Dialog box, in the Dynamics section, click the Lead row. In the Edit Selected Dynamics section, in the Real Zero text box, specify a location of -4.3, and press Enter.

Results:

Discussion

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Experiment No 8

Objective: Estimate the stability of first order or higher order system with the help of computer and to study control problems by simulation (step and impulse function).

Theory: Order of system is highest power of's' in the denominator of a closed loop transfer function. First-order systems are represented by a single pole in the s-plane, and second-order systems by a pair of poles. There may not be zeros in the transfer function, depending on whether there are derivative terms on the right-hand side of the differential equation. From the differential equation, the system function can be written directly. If we assume that the systems are causal, so that the impulse response is right-sided, then the ROC of the system function is implicitly specified to be to the right of the rightmost pole in the s-plane.

Command Matlab to Generate the step and Impulse Response to First Order System

```
>> num=[1];
>> den=[1,1];
>> sys=tf(num,den)
```

Transfer function:

$$\frac{1}{S+1}$$

```
>> [x,y]=impulse(sys)

>> num=[10];
>> den=[0.1 1];
>> step(num,den)
>> sys=tf(num,den)
```

Transfer function:

```
>> [temp,t]=step(sys);
```

Results:
Compare the output of both the input in term of response and draw the characteristics parameter for their evaluation in term of mathematical relation.

Part-B
(CHEMCAD Software)

Note: Student Can perform minimum four-five experiments using CHEMCAD tool