Process Simulation & Control using MATLAB and SIMULINK

Continuous Stirred Tank Reactor (Van-de-Vusse)

Dynamic model

- $\frac{dC_A}{dt} = \frac{F}{V}\left(C_{Af} - C_A\right) - k_1 C_A - k_3 C_A^2$
- $\frac{dC_B}{dt} = -\frac{F}{V} C_B + k_1 C_A - k_2 C_B$
- $\frac{dC_C}{dt} = -\frac{F}{V} C_C + k_2 C_B$
- $\frac{dC_D}{dt} = -\frac{F}{V} C_D + \frac{1}{2} k_3 C_A^2$

Reaction

$$A \overset{k_1}{\Rightarrow} B \overset{k_2}{\Rightarrow} C$$

$$A + A \overset{k_3}{\Rightarrow} 2D$$

Data for the CSTR

V = 5 l

F = 400 l/h

C_{Af} = 10 mol/l

k_l = 50 h^{-1}

k_2 = 100 h^{-1}

k_3 = 10 $l.mol^{-1}.h^{-1}$

Since our objective is to control C_B, the reduced order model should be

- $\frac{dC_A}{dt} = \frac{F}{V}\left(C_{Af} - C_A\right) - k_1 C_A - k_3 C_A^2 = f_1(C_A, C_B, F)$
- $\frac{dC_B}{dt} = -\frac{F}{V} C_B + k_1 C_A - k_2 C_B = f_2(C_A, C_B, F)$

Creating S function

1. In Matlab Command window type <edit sfuntmpl>

   >> edit sfuntmpl

2. It will open sfuntmpl.m file.
3. First line of the file is

function [sys,x0,str,ts,simStateCompliance] = sfuntmpl(t,x,u,flag)

4. Nice documentation is provided in this file describing the features.
5. Change the name of function ‘sfuntmpl’ to your function name. For eg., change to ‘vusse’
6. Save the file in your working folder as vusse.m

Creating S function (initialization)

6. Now edit the file as per your system of equations.
7. Do not change in the main function, i.e, vusse function.
8. Initialization should be done in the

function [sys,x0,str,ts,simStateCompliance]=mdlInitializeSizes

9. This system consist of 2 continuous state (C_A,C_B) 2 input (F and C_{Af})and 2 output variables (C_A,C_B).
10. Change statements in the function mdlInitializeSizes

```
sizes.NumContStates  = 2;
sizes.NumOutputs     = 2;
sizes.NumInputs      = 2;
x0=[0;0];  % initial condition
```

Creating S function (derivative)

6. Differential equations should be entered in
   function sys=mdlDerivatives(t,x,u)

```
function sys=mdlDerivatives(t,x,u)
% Inputs (2):
% Volumetric Flowrate (l/sec)
f = u(1);
% Feed Concentration (mol/l)
caf = u(2);
% States (2):
% Concentration of A in CSTR (mol/l)
ca = x(1);
% Concentration of B in CSTR (mol/l)
cb = x(2);
```

Creating S function (derivative)

```
% Parameters:
   k1 = 5/6; % rate constant for A --> B (min^-1)
   k2 = 5/3; % rate constant for B --> C (min^-1)
   k3 = 1/6; % rate constant for A + A --> D (mol/(liter min)
% Volume of CSTR (l)
V = 5;
fov=f/V;

% Compute xdot:
der1 = fov*(caf - ca) -k1*ca - k3*ca*ca;
der2 = -fov*cb + k1*ca - k2*cb;
sys=[der1;der2];
% end mdlDerivatives
```

Creating S function (output)

Output from the s-function block is defined in function

sys=mdlOutputs(t,x,u)

If all state variables are also output variables, i.e, C_A, C_B are also output then write the function as below:

```
function sys=mdlOutputs(t,x,u)
sys = x;
% end mdlOutputs
```

If output variable is different from state variable but a function of state and input variable, for e.g. conversion of C_A, C_B are the output then write function as below:

```
function sys=mdlOutputs(t,x,u)
sys = [(u(2)-x(1))/u(2); x(2)/u(2)];
% end mdlOutputs
```

Simulink model

1. Save the vusse.m after writing the functions as described in earlier slides.
2. Open Simulink model either

   typing <simulink> in the command window

   >> simulink

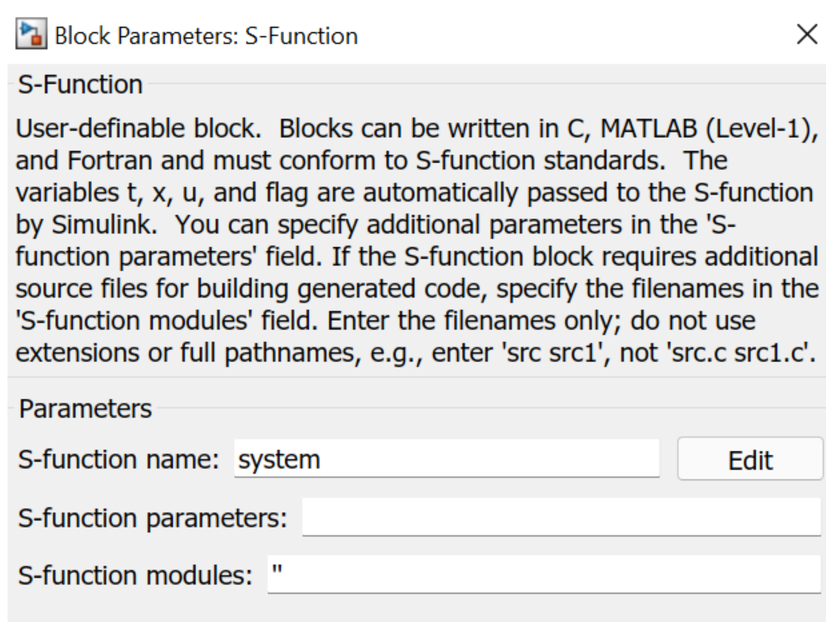
   or click <Home> -> <new> -> <simulink model>
3. Click on <blank model> to open blank model
4. Open library browser under tools menu. This will open built-in library function block available
5. Drag the s-function block from the library browser to the model window.

Simulink model

This will show in the model window as below

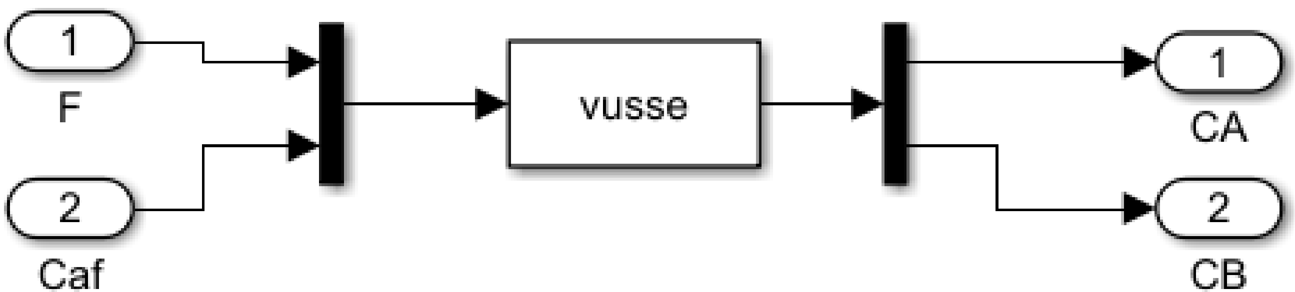
The system name should be changed by double clicking on the s-function block in the model window

Change the s-function Name from ‘system’ to ‘vusse’.



Simulink model

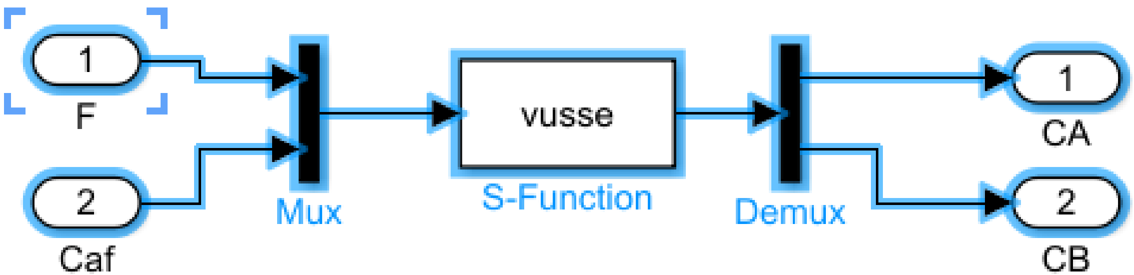
Now add input and output connection to the block. Since, 2 inputs (F and Caf) are required , we have to use ‘Mux’ block from library browser.



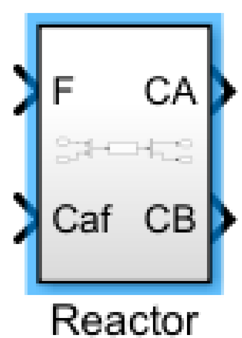
We also add two input ports block (‘In 1’) and rename them as ‘F’ And ‘Caf’.
Similarly for two output (CA and CB) from the block we use ‘Demux’ block from library browser.
Connect the Demux block with two output port block (‘out 1’) and Rename them CA and CB.

Simulink model (subsystem creation)

Select all the elements and block by pressing <ctrl> and A at the same time.



Create subsystem by clicking on ‘Create Subsystem’ under diagram menu and remove the ports and connecting lines.

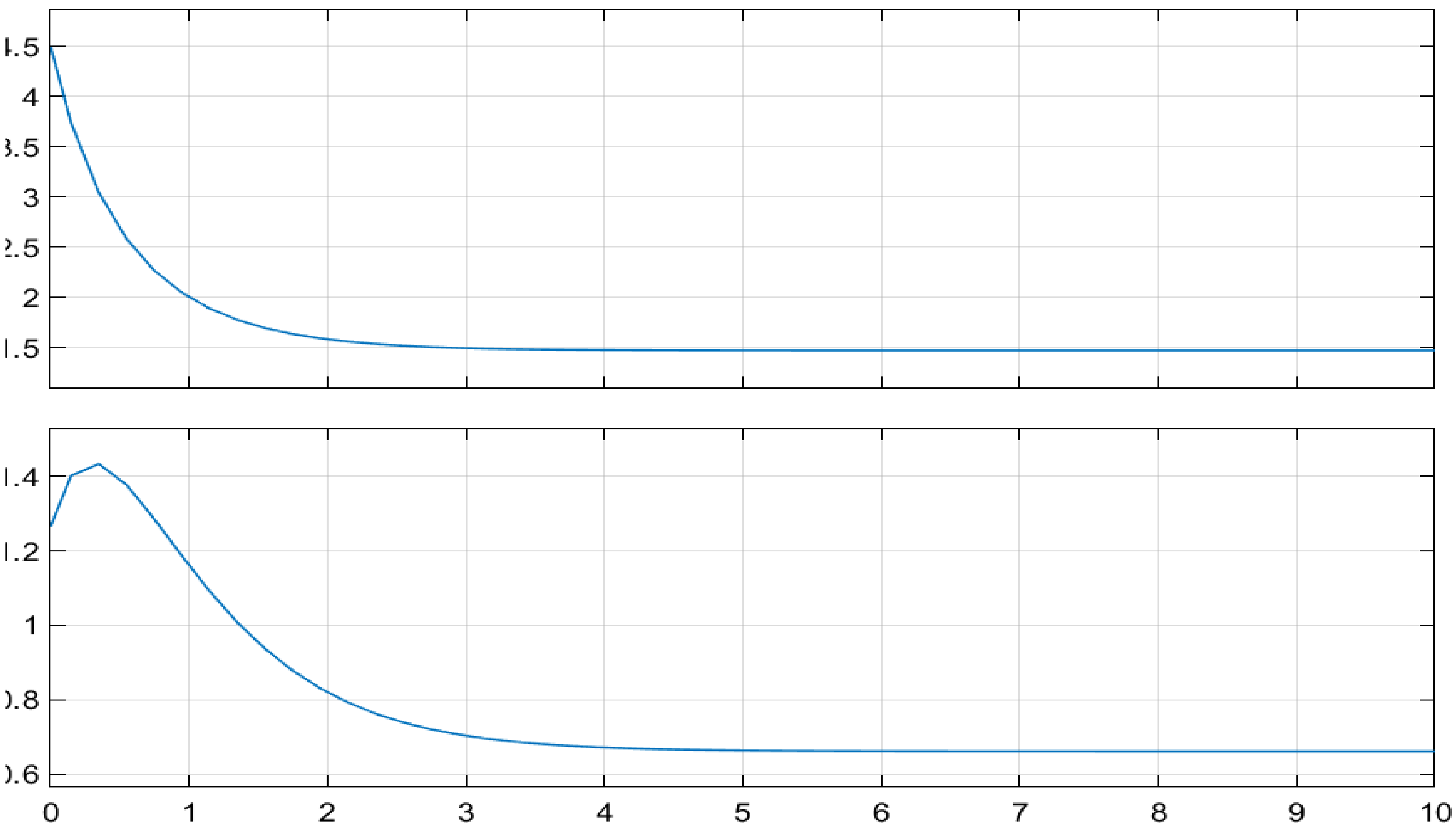


Simulink model (running vusse model)

Add input connection to the reactor for F and Caf using ‘const’ block and set values of F as 78/60 and Caf as 10.
Add ‘Scope’ block, modify scope block with 2 input port and connect outpout ports of reactor block

Simulink Model Vusse (Result)

Run the simulation for 10 mins



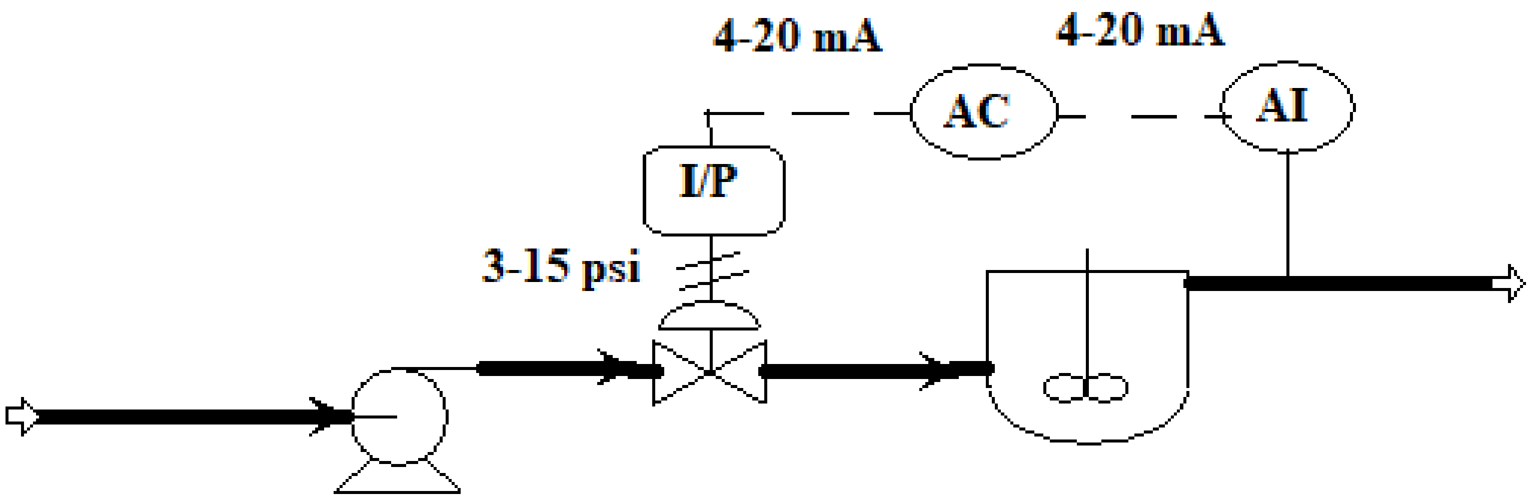
Process with instrumentation

The simulation of the Van-de-Vusse reactor is the basic process simulation where no instruments are attached to the process.

Most of the time we do control analysis based on this kind of process behavior/simulation because instrument gain and dynamics are neglected.

However, it is advised to include instrument dynamics in the overall process behavior so that any disturbances/noise due to instruments can be considered while designing/tuning the control system.

Process with instrumentation



Composition Analyzer

1. What should be the gain of the analyzer?
2. What is the measurement noise?
3. What is the measurement delay?

Steady State Behaviour

$$\frac{dC_A^S}{dt} = -k_3 {C_A^S}^2 - \left(k_1 + \frac{F^S}{V} C_{Af}^S\right) = 0$$

Solving the quadratic equation:

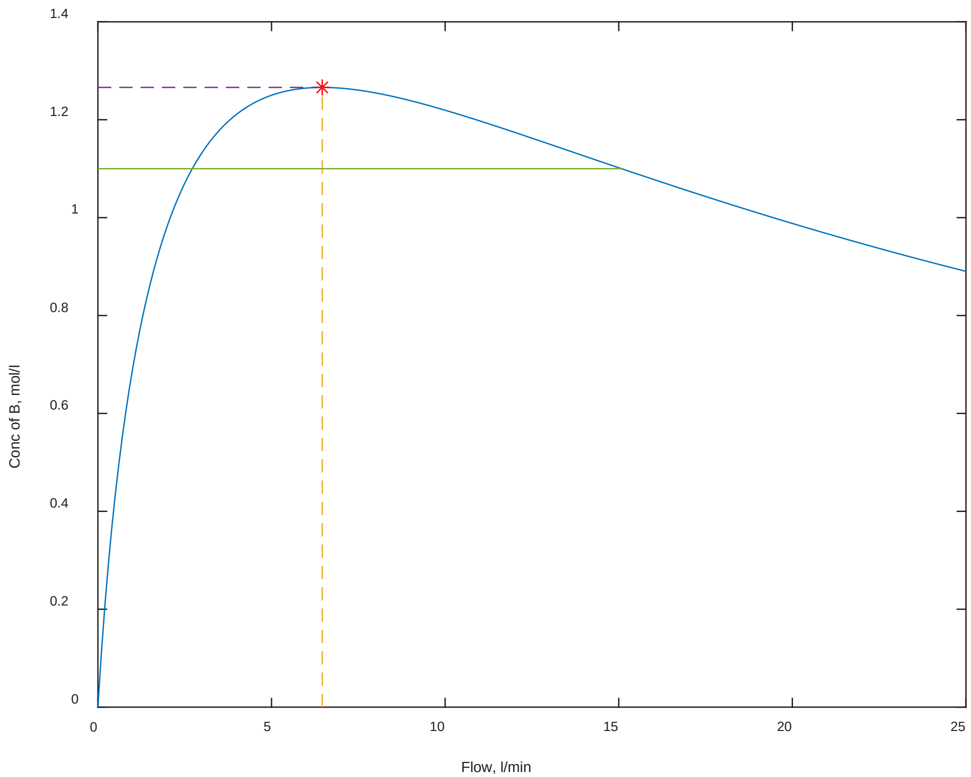
$$C_A^S = -\frac{\left(k_1 + \frac{F^S}{V}\right)}{2k_3} + \frac{\sqrt{\left(k_1 + \frac{F^S}{V}\right)^2 + \frac{4k_3 F^S}{V} C_{Af}^S}}{2k_3}$$

And

$$\frac{dC_B^S}{dt} = -\left(\frac{F^S}{V} + k_2\right) \mathrm{C_B^S} + \mathrm{k_1 C_A^S} = 0 \;\; \rightarrow \;\; C_B^S = \frac{\mathrm{k_1 C_A^S}}{\frac{F^S}{V} + k_2}$$

So, for known values of F^S, $C_A{}^S$ and $C_B{}^S$ can be calculated.

Steady State Behaviour



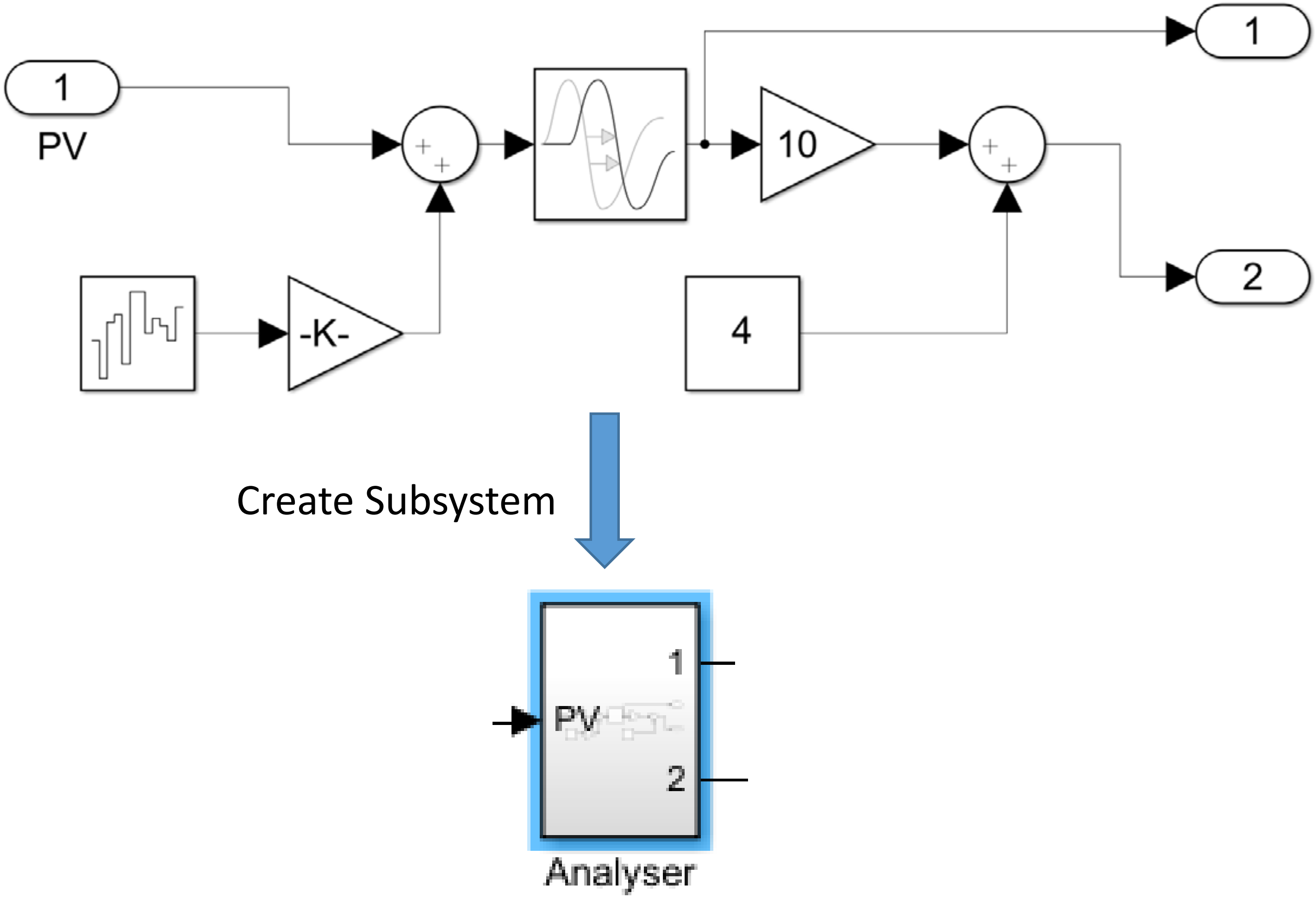
Maximum concentration of B = 1.266 mol/l at Flow 6.46 l/min

So, we take measuring instrument range 0-1.6 mol/l

$$Gain = \frac{20 - 4}{1.6 - 0} = 10$$

Normally, measurement delay and noise are specified by the manufacture.
Let us consider, the measurement delay is 3 min and noise is limited to ± 0.01

Sensor block : Simulink diagram



Control Valve

Valve Eqn. $Q = C_V\, f(x)\sqrt{\frac{\Delta p}{s.g}}$

For equal % valve: $f(x) = R^{x-1}$

We, choose C_V =10, R=40 and $\Delta p = 7 - 5^{x}$

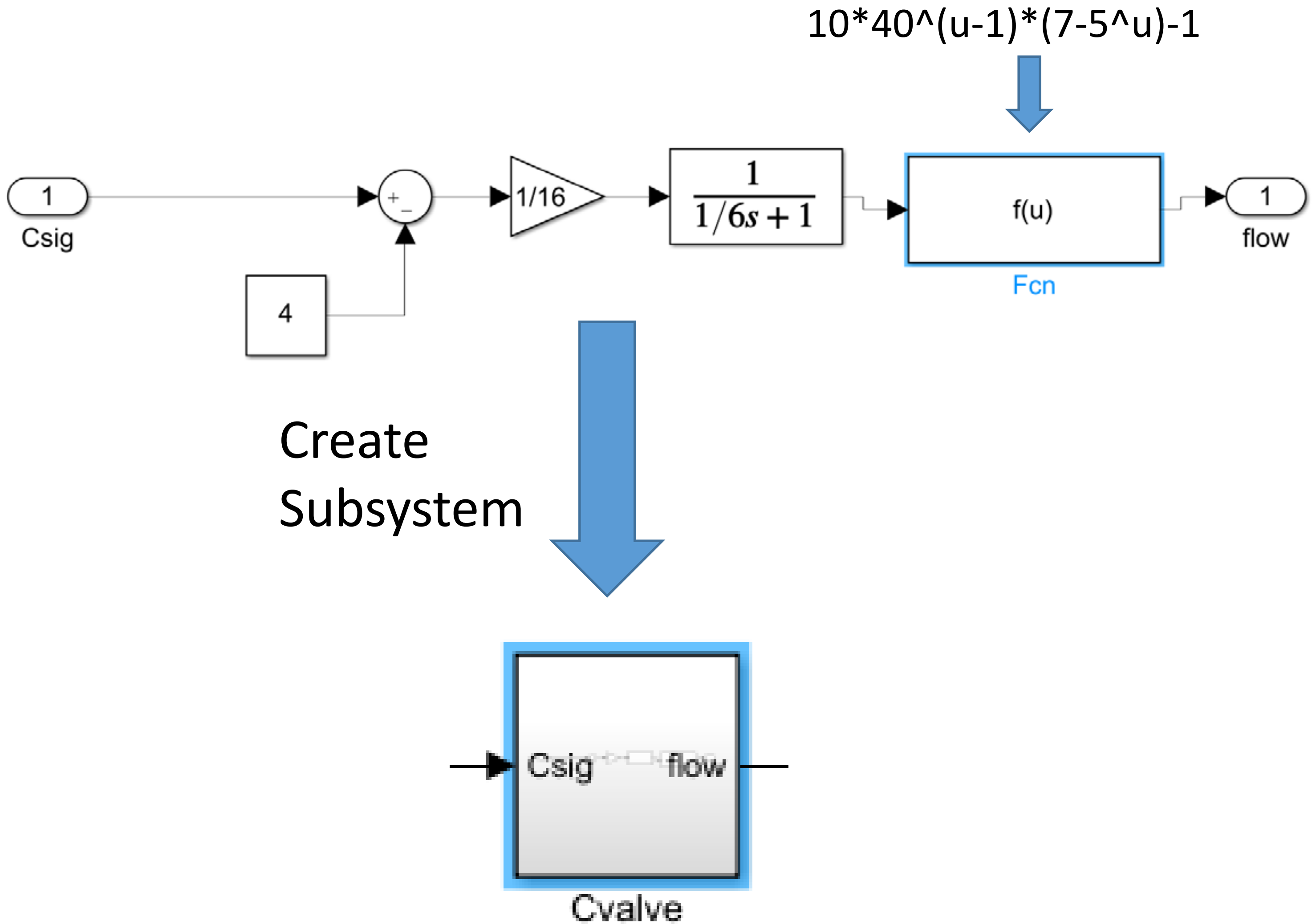
Q=10*40^(u-1)*(7-5^u)-1

At u=0.5, Q=6.53 liter/min, which is nearly the desired steady state flow.

I/P→fraction opening

$$\frac{15-3}{20-4}\,\frac{0-1}{15-3} = \frac{1}{16}$$

Control Valve: Simulink Diagram



PID Controller Block

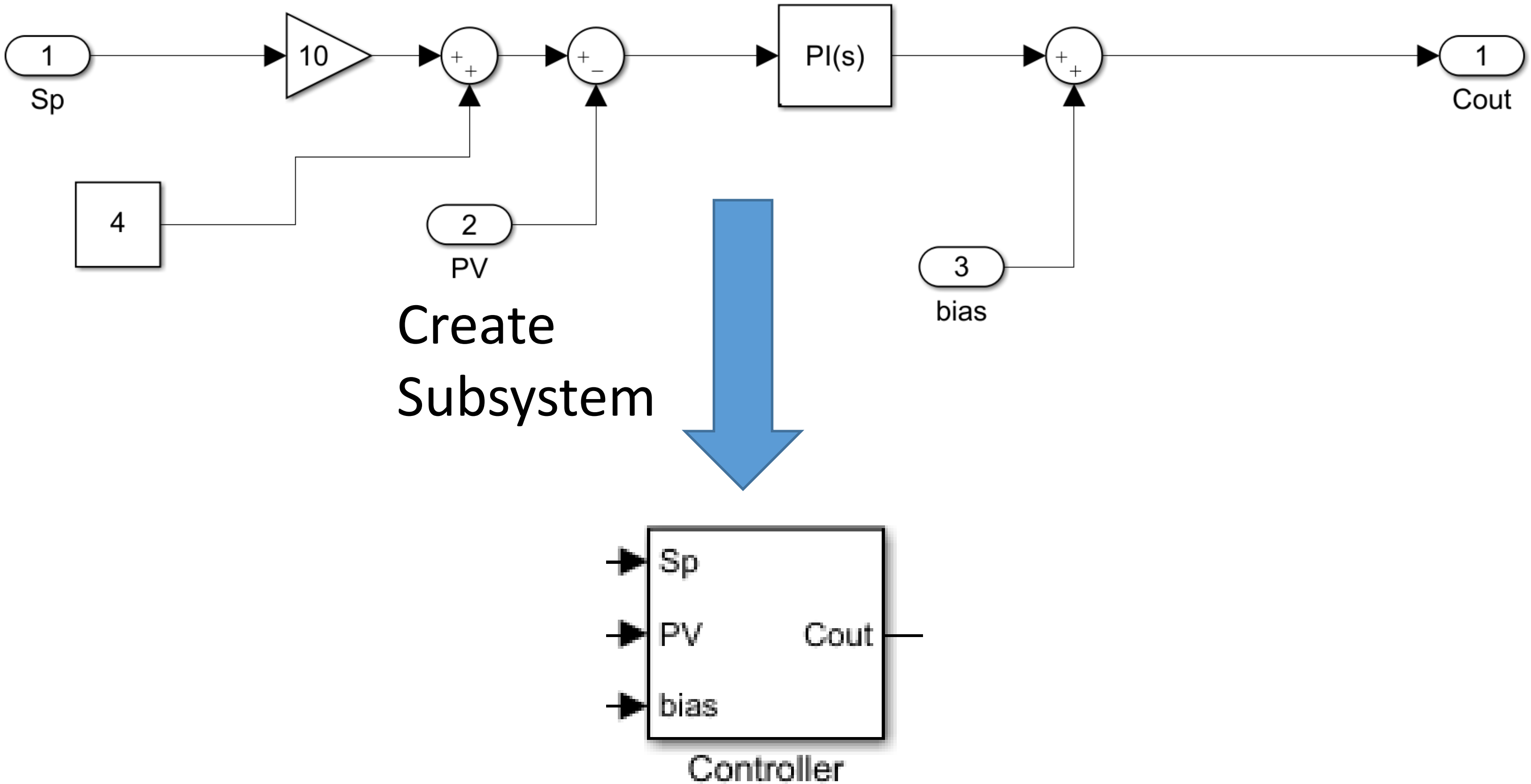
Simulink has a built-in PID controller block.

This block can be configured as P or PI or PD or PID controller

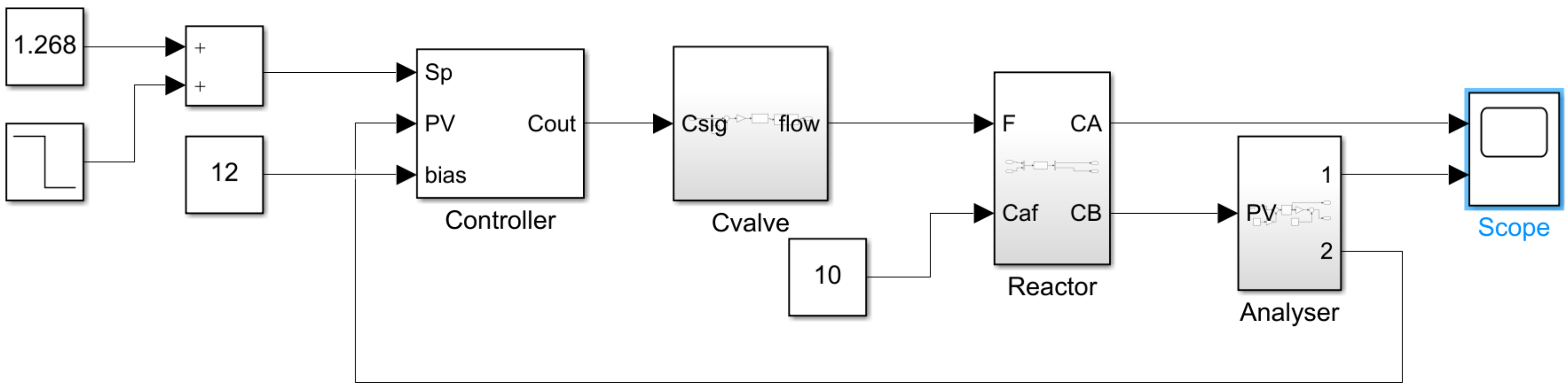
However, this block needs to be augmented with setpoint and bias.

Since, setpoint will be given in terms of process variable, measurement block gain needs to be included.

PID Controller: Simulink



Feedback Control Block diagram Simulink



Transfer Function Model

$x_1 = C_A - C_A^s$; $x_2 = C_B - C_B^s; u = F - F^s; \mathrm{d} = \mathrm{C_{Af}} - \mathrm{C_{Af}^s}$

Linearizing the equations, we get

$$\frac{dx_1}{dt} = a_{11}x_1 + a_{12}x_2 + b_{11}u + b_{12}d$$

$$\frac{dx_2}{dt} = a_{21}x_1 + a_{22}x_2 + b_{21}u + b_{22}d$$

Where,

$a_{11} = -\left(\frac{F^s}{V} + k_1 + 2k_3C_A^s\right)$; $a_{12} = 0$; $\mathrm{b}_{11} = \frac{\left(C_{Af}^s - C_A^s\right)}{V}$;

$b_{12} = \frac{F^s}{V}$; $a_{21} = k_1$; $a_{22} = -\left(\frac{F^s}{V} + k_2\right)$; $b_{21} = -\frac{C_b^s}{V}$;

$b_{22} = 0$;

Transfer Function Model

Taking Laplace Transform,

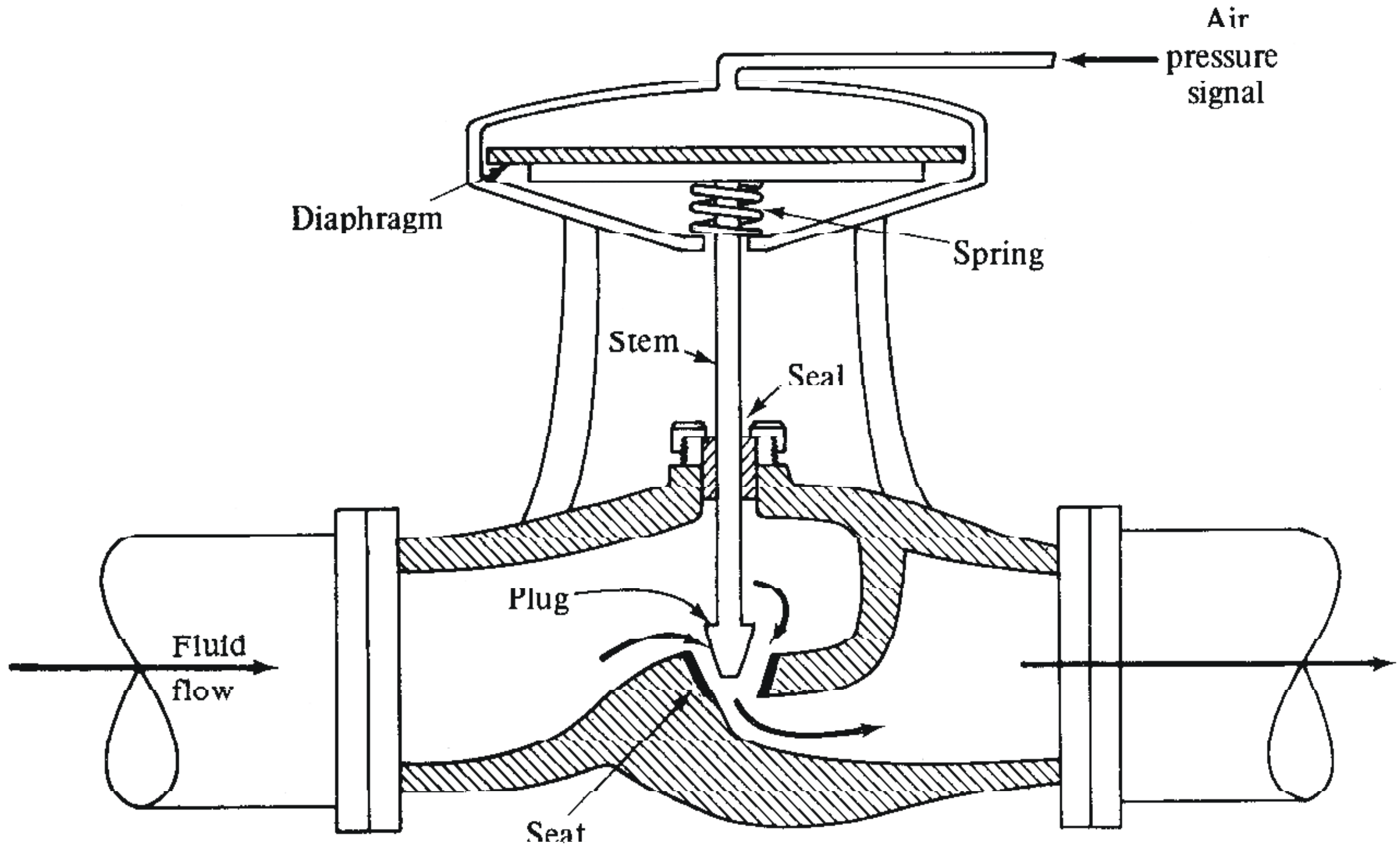
$$sx_1(s) = a_{11}x_1(s) + b_{11}u(s) + b_{12}d(s)$$

$$sx_2(s) = a_{21}x_1(s) + a_{22}x_2(s) + b_{21}u(s)$$

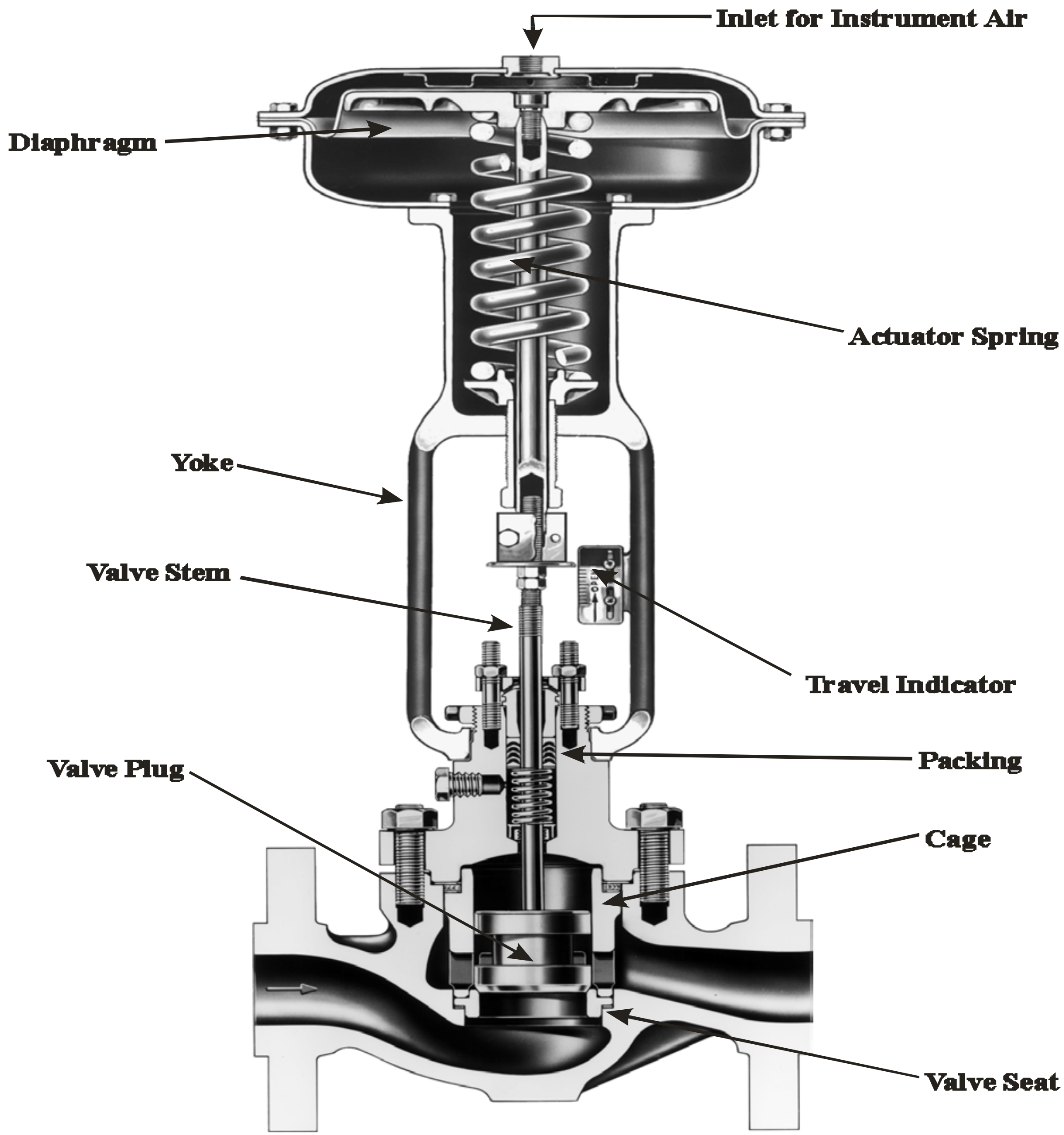
$$x_2(s) = \frac{[b_{21}s+(a_{21}b_{11}-a_{11}b_{21})]}{(s-a_{11})(s-a_{22})}u(s) + \frac{a_{21}b_{12}}{(s-a_{11})(s-a_{22})}d(s)$$

F	CA	CB
77.52552642454	4.4948977712609	1.265986323710897
60	4.0	1.25
100	5.0	1.25

Typical Globe Control Valve



Cross-section of a Globe Valve

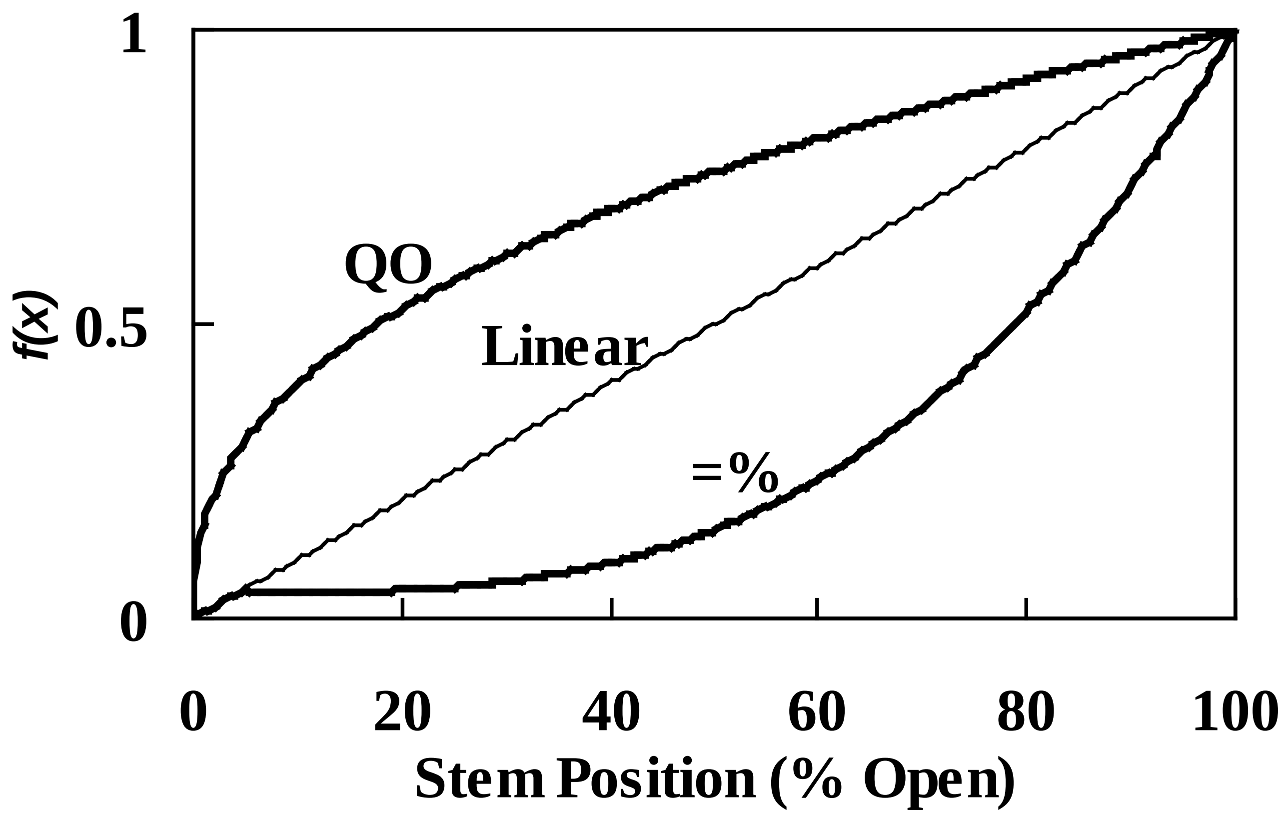


Types of Globe Valves

- Quick Opening- used for safety by-pass applications where quick opening is desired
- Equal Percentage- used for about 90% of control valve applications since it results in the most linear installed characteristics
- Linear- used when a relatively constant pressure drop is maintained across the valve

Inherent Valve Characteristics

Valve Eqn. $Q = C_V\, f(x)\sqrt{\frac{\Delta p}{s.g}}$



Linear:

$$f(x) = x$$

Quick opening

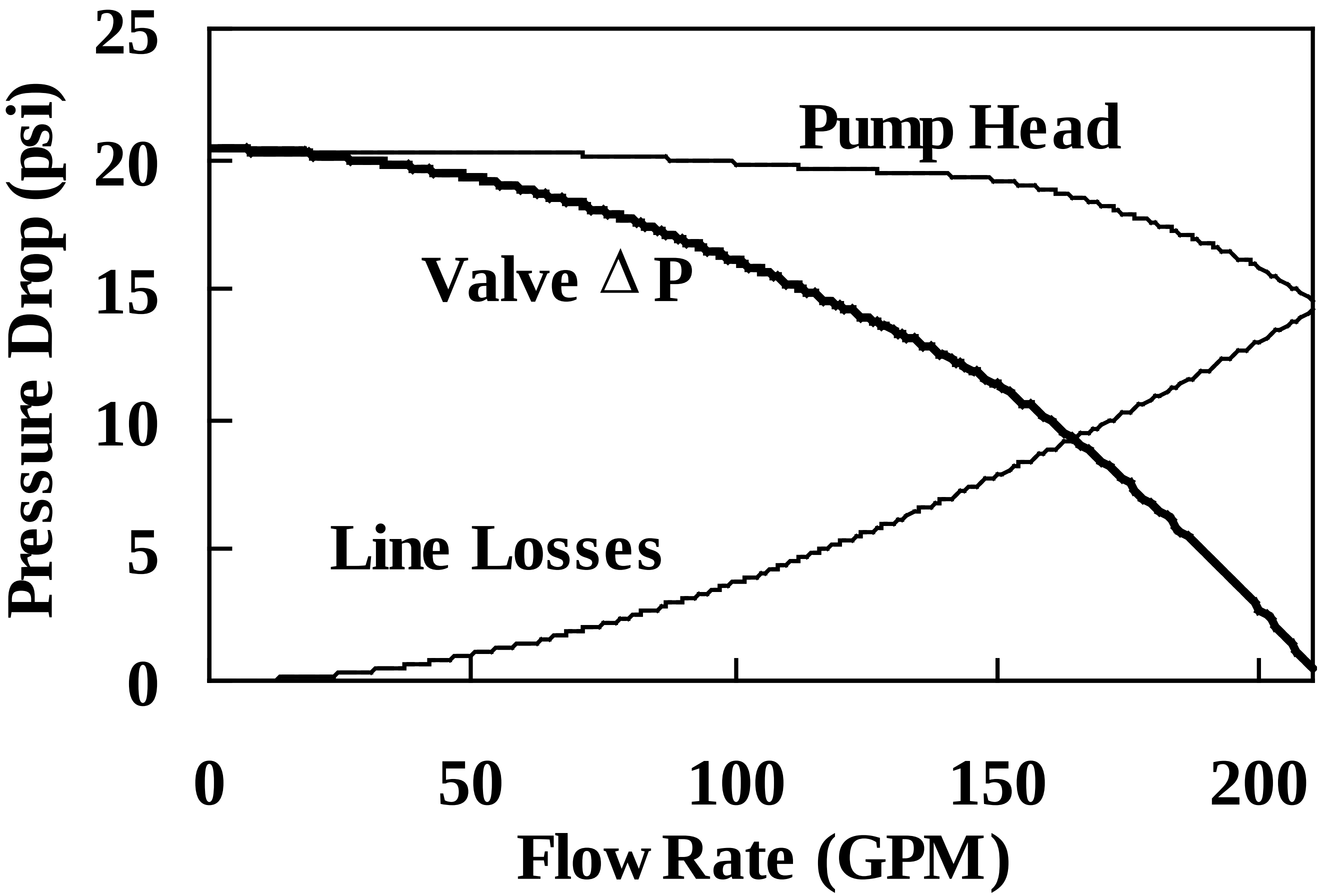
$$f(x) = \sqrt{x}$$

Equal %

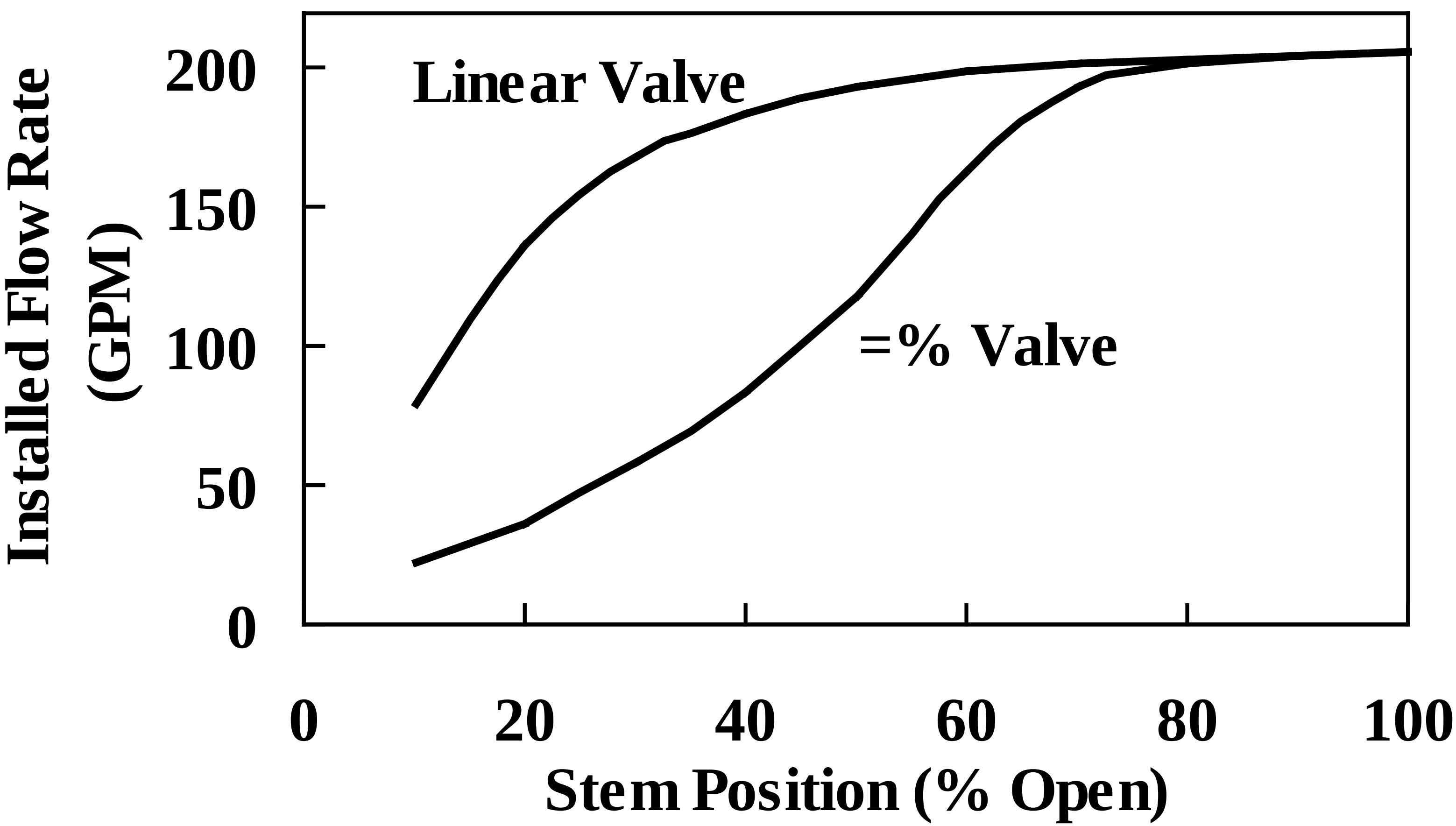
$$f(x) = R^{x-1}$$

R varies 20 to 50

Pressure Drop vs. Flow Rate



Installed Flow Characteristic



Control Valve Design Procedure

- Evaluate C_v at the maximum and minimum flow rate using the flow equation for a valve.
- Determine which valves can effectively provide the max and min flow rate remembering that, in general, the valve position should be greater than about 15% open for the minimum flow rate and less than 85% open for the maximum flow rate.
- Choose the smallest valve that meets the above criterion for the minimum capital investment or choose the largest valve to allow for future throughput expansion.

Additional Information Required to Size a Control Valve

- C_V versus % open for different valve sizes.
- Available pressure drop across the valve versus flow rate for each valve. Note that the effect of flow on the upstream and downstream pressure must be known.

Valve Deadband

- It is the maximum change in instrument air pressure to a valve that does not cause a change in the flow rate through the valve.
- Deadband determines the degree of precision that a control valve or flow controller can provide.
- Deadband is primarily affected by the friction between the valve stem and the packing.

Valve Actuator Selection

- Choose an air-to-open for applications for which it is desired to have the valve fail closed.
- Choose an air-to-close for applications for which it is desired to have the valve fail open.