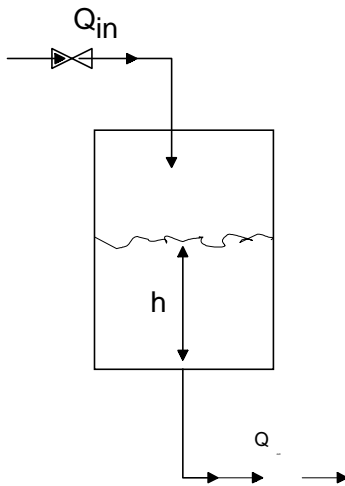


## EXAMPLES OF SOME SIMPLE MECHANISTIC MODELS



The diagram on the left shows a simple level system.  $Q_{in}$  [ $\text{m}^3 \text{min}^{-1}$ ] and  $Q_{out}$  [ $\text{m}^3 \text{min}^{-1}$ ] are the volumetric flows in and out of the tank. The level in the tank is given by  $h$  [m].

We wish to model the behaviour of the tank so that we can predict changes in level due to changes in flow conditions. Therefore, we need to develop the mass balance relationships. Since we are not considering temperature effects, there is no need to consider an energy balance.

However, the schematic does not provide sufficient information for a mass balance. The flows are volumetric flows. So, we need a density term ( $\rho$ ) to convert from volume units to mass units. We also need to know the cross-sectional area ( $A$ ) of the tank, so that we can determine the volume holdup in the tank, and hence the mass holdup.

Given these information, the mass balance of the tank can be written as:

$$\frac{d(\rho Ah)}{dt} = \rho Q_{in} - \rho Q_{out}$$

Since there is no heating effects, density can be assumed constant. Also, since the tank is cylindrical, it has constant cross-sectional area. Therefore, the ODE becomes:

$$\frac{\rho A dh}{dt} = \rho Q_{in} - \rho Q_{out} \quad \text{and hence} \quad \frac{A dh}{dt} = Q_{in} - Q_{out}$$

The above equation is correct as a mass balance, but is not really in the right form for solution. Note that the flow out,  $Q_{out}$ , is determined by the pressure exerted by the liquid, and is given by:

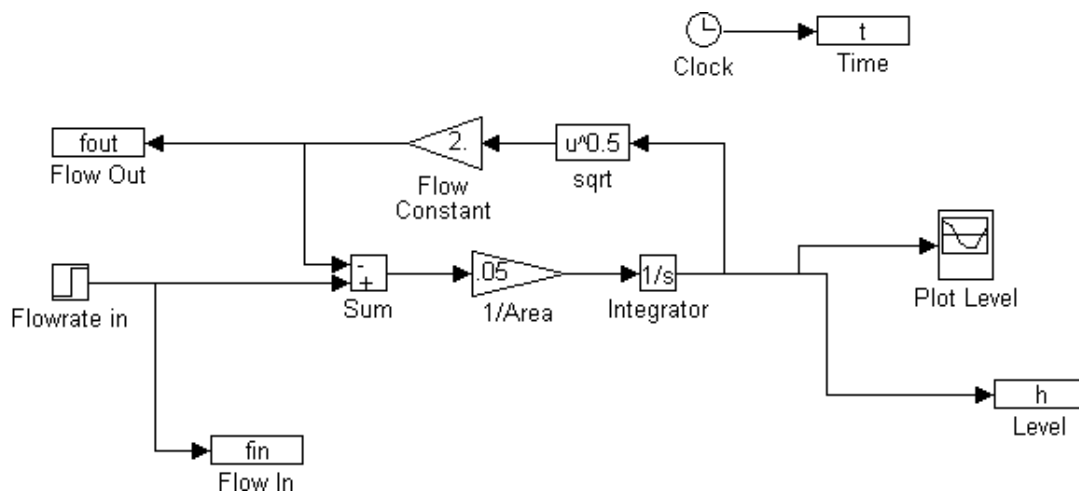
$$Q_{out} = k\sqrt{h}$$

Therefore, the mass balance should be written as:

$$\frac{A dh}{dt} = Q_{in} - k\sqrt{h} \quad \text{and finally as} \quad \frac{dh}{dt} = (Q_{in} - k\sqrt{h}) / A$$



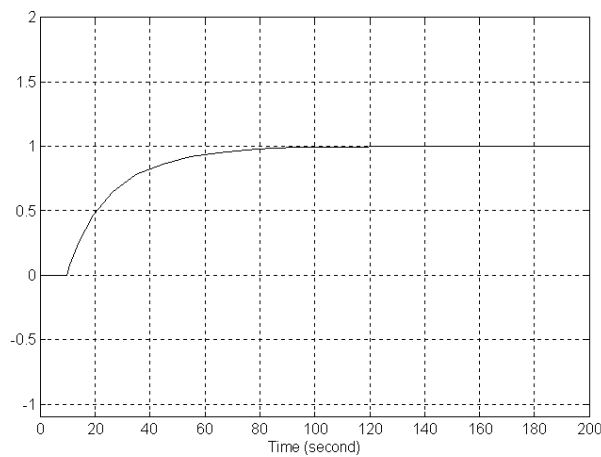
The solution can be performed in SIMULINK, and the corresponding simulation diagram is:



SIMULINK diagram to simulate a single tank system

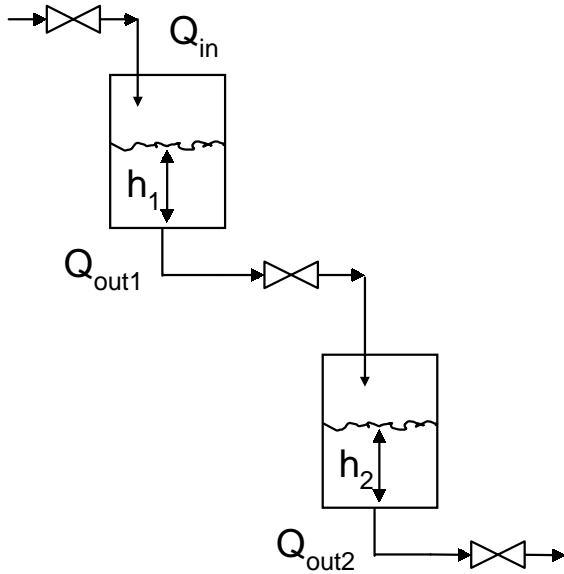
All the variables are named and sent to the MATLAB workspace. We also use a 'clock' to obtain the time instances at which the ODE is solved. Only the level is plotted.

Starting with zero initial conditions (set up through the 'integrator' block), the simulation gives the following response of level to a unit step change in the flowrate of liquid into the system.



Level response of single tank system





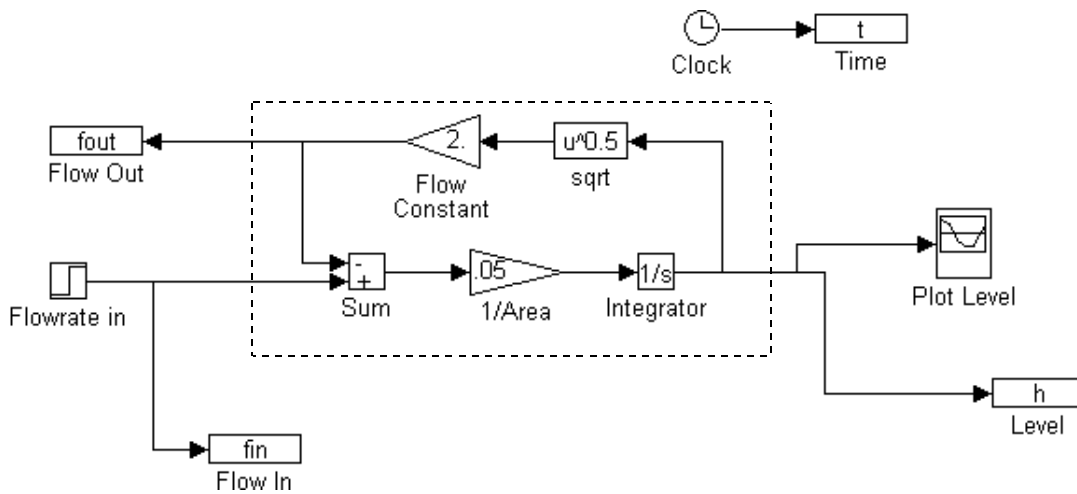
The figure on the left is a slight extension of the single tank system above. Here we have a 2 tank system, where the out flow from the first tank feeds the second tank. Following similar arguments as above, we can write the mass balance equations as:

$$\frac{dh_1}{dt} = (Q_{in} - k_1\sqrt{h_1}) / A_1$$

$$\frac{dh_2}{dt} = (k_1\sqrt{h_1} - k_2\sqrt{h_2}) / A_2$$

The subscripts '1' and '2' are used to distinguish between the properties and variables of the respective tanks.

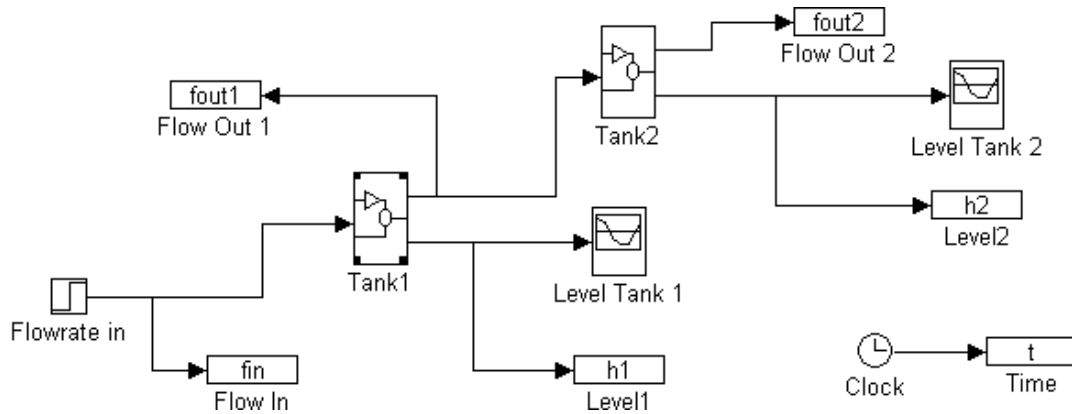
Again, we can develop the simulation diagram in SIMULINK to solve this set of ODE's. However, instead of developing the entire diagram from scratch, we can make use of the previous result to simplify the problem formulation.



Grouping of simulation blocks in SIMULINK

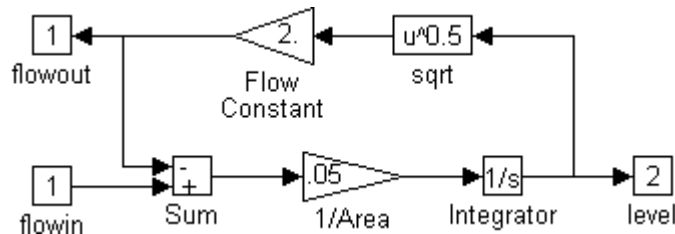
We can isolate the essential blocks on the simulation diagram for the single tank system, and 'group' it. This will give us a new block which represents a single tank, which can be re-used. Thus, the simulation diagram for the 2 tank system can be drawn as:





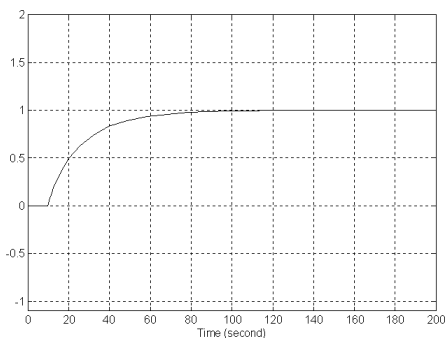
SIMULINK diagram to simulate a 2 tank system

Again, all the variables are sent to the workspace in case we want to save them to files, or subject them to further analysis. The blocks 'Tank1' and 'Tank2' are based on the following grouped module:

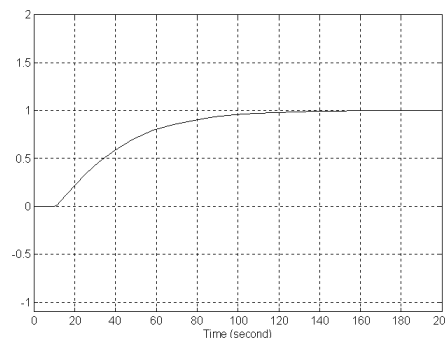


Module representing a single tank system

We can still set the parameters of each tank independently. A simulation run with 2 identical tanks gave the following results:



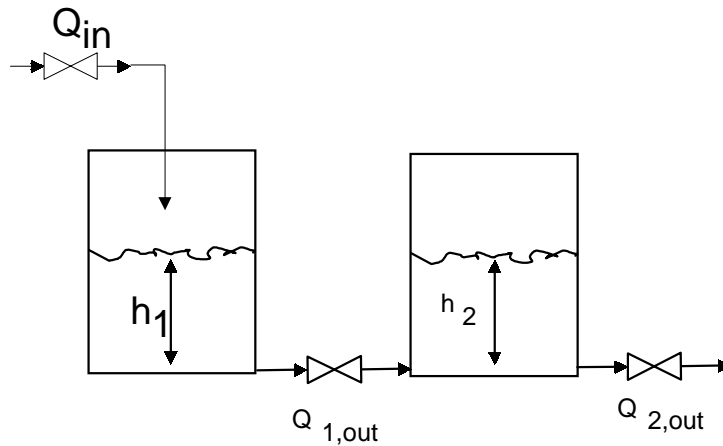
Level response of Tank 1



Level response of Tank 2

The ability to re-use simulation components is very useful, as it will allow the simulation of staged processes.





This 2 tank system shown schematic looks similar to the 2 tank system discussed previously. However the mass balance equations are very different. The mass balance for the first and second tank is respectively:

$$\frac{A_1 dh_1}{dt} = Q_{in} - Q_{1,out} \quad \text{and} \quad \frac{A_2 dh_2}{dt} = Q_{1,out} - Q_{2,out}$$

The flow out of the second tank is determined by the liquid head in that tank, i.e.

$$Q_{2,out} = k_2 \sqrt{h_2}$$

However, because of the coupling between the two tanks, the flow out of the first tank is determined by the difference in levels of the two tanks, i.e.

$$Q_{1,out} = k_1 \sqrt{h_1 - h_2}$$

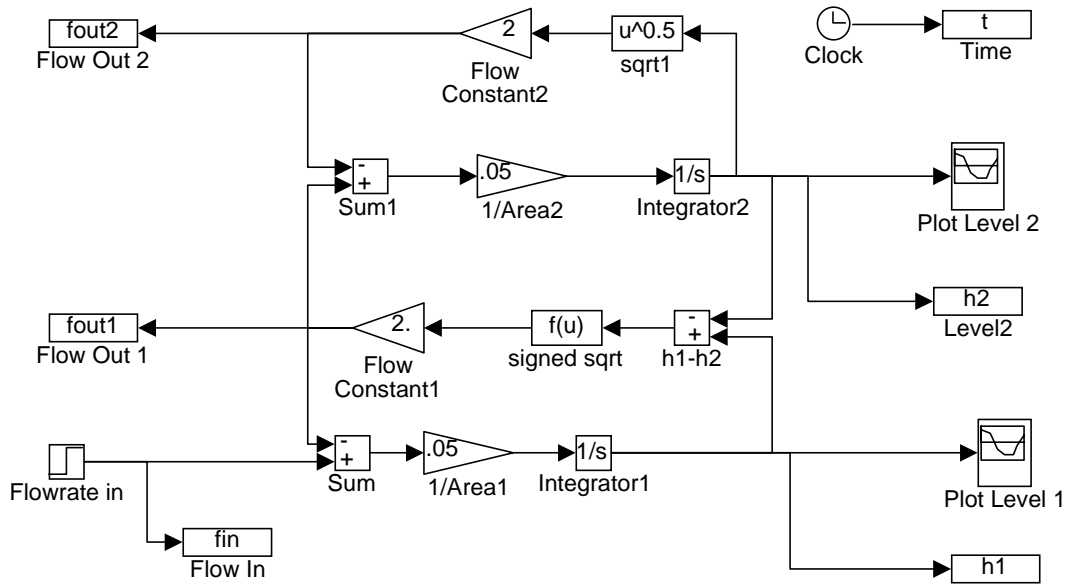
Thus the final set of ODE's that describe system behaviour is given by:

$$\frac{dh_1}{dt} = (Q_{in} - k_1 \sqrt{h_1 - h_2}) / A_1$$

$$\frac{dh_2}{dt} = (k_1 \sqrt{h_1 - h_2} - k_2 \sqrt{h_2}) / A_2$$

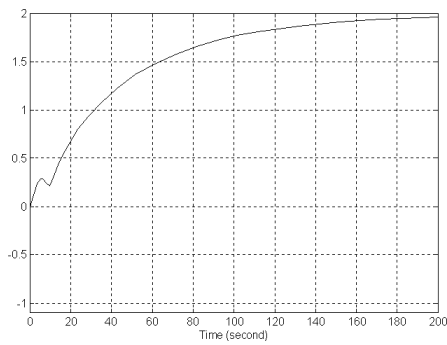
The corresponding SIMULINK diagram is:



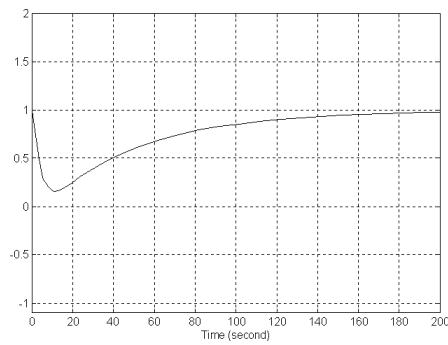


SIMULINK diagram for coupled tank system

Suppose the initial conditions are: Tank 1 is empty and Tank 2 has a level of 1 m. Then the results are as follows:



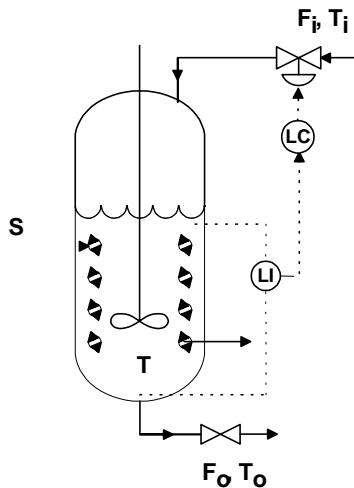
Level of Tank 1



Level of Tank 2

The responses are as expected.





The diagram on the left show a heated stirred tank. The heating medium's flow rate is  $S$  [ $\text{kgmin}^{-1}$ ]. The temperature of the bulk liquid is  $T$  [ $\text{degC}$ ]. Feed liquid enters the system at  $F_i$  [ $\text{kgmin}^{-1}$ ] and a temperature of  $T_i$  [ $\text{degC}$ ]. This flow is used to maintain the liquid level in the tank. The heated liquid leaves the tank with a flowrate of  $F_o$  [ $\text{kgmin}^{-1}$ ] and a temperature of  $T_o$  [ $\text{degC}$ ].

There are a number of ways to approach the modelling of this system..

Obviously, we need to write an energy balance to describe the heat effects. However, we can either consider a varying holding, which implies that the input and output liquid flows will be changing, or that the level controller will maintain a steady volume in the tank. This means that the liquid flows in and out of the tank will be constant in which case there is no need to develop a mass balance.

Let us, for the sake of simplicity, assume that liquid level is constant, in which case

$$F = F_i = F_o.$$

There are now several pieces of information to gather, namely:

$\lambda$  = latent heat of vaporisation of steam

$C_p$  = heat capacity of the liquid

To further simplify matters, we assume that heat is transferred to the system purely by condensing steam and that the heat capacity of the liquid is constant. Also, since the tank is being stirred, it is acceptable to assume that the temperature of the output stream is equal to the temperature of the liquid in the tank.

The general dynamic heat balance equation has the following form:

Rate of Energy Accumulation = Rate of Energy Input - Rate of Energy Consumption

Since the level is kept constant, then we do not have to consider the effects of changing mass in the tank on the rate of energy accumulation. Thus,

Rate of Energy Input =  $FC_p(T_i - T_a) + S\lambda$  where  $T_a$  is the ambient temperature.

Rate of Energy Consumption =  $FC_p(T_o - T_a)$



Rate of Energy Accumulation =  $MC_p \frac{dT_o}{dt}$  where  $M$  is the mass of liquid in the tank.

Thus the dynamic model of the stirred tank heating system is:

$$MC_p \frac{dT_o}{dt} = FC_p (T_i - T_a) + W_s \lambda - FC_p (T_o - T_a)$$

Simplification yields

$$MC_p \frac{dT_o}{dt} = FC_p (T_i - T_o) + W_s \lambda$$

or 
$$\frac{dT_o}{dt} = (FC_p (T_i - T_o) + W_s \lambda) / MC_p$$

which can then be set up in SIMULINK and simulated.

To develop a more representative description of the system, we can relax on some of the more contentious assumptions that we have made. If the controller does not provide perfect level control, then a mass balance will have to be written, but this will be as for the single tank example. That is,

$$\frac{dh}{dt} = (F_i - k\sqrt{h}) / A$$

where  $h$  is the level, and  $A$  is the cross sectional area of the tank. Since the flow in is being manipulated by the controller (proportional controller say), we will need to describe this as well.

$$F_i = k_c (h_s - h) + F_{i,0}$$

where  $F_{i,0}$  is the value of initial input flow rate;  $h_s$  is the desired level and  $k_c$  is the proportional gain. The energy balance will then have to be modified to:

$$MC_p \frac{dT_o}{dt} = F_i C_p (T_i - T_a) + W_s \lambda - F_o C_p (T_o - T_a)$$

Additionally, the heat capacity of some liquids change significantly with temperature, and this relationship is normally modelled as:

$$C_p = a + bT + cT^2$$

The more rigorous energy balance then becomes



$$MC_p \frac{dT_o}{dt} = F_i C_{p,i} (T_i - T_a) + W_s \lambda - F_o C_{p,o} (T_o - T_a)$$

We can even consider heat transfer into the system by the condensed steam, in which case we will need data about the heat transfer area and the heat transfer coefficients. By continuing to examine the system in further and further detail, the mass and energy balances become more complex. The most difficult scenario is to do away with the “well stirred” assumption. If we are to consider this scenario, then we will need to know the temperature distribution in the tank, and the problem becomes a two dimensional one; time and position. Nevertheless, the solution procedure is still the same. All that is required is to formulate the problem into a tractable form, and the choice of an appropriate solution strategy.

