

Process Dynamics and Control

Dynamic Modeling
The First Principles Approach

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1 Relationships Among Process Variables

1.1 Example set of variables

- Consider the reactor and separator system. There is a large set of variables related to the operation. For example, for the reactor the following sets of variables are identified.
 - Feed: temperature, composition, flow rate
 - Reactor: temperature, pressure, level of liquid, conversion
 - Outlet: composition, flow rate
 - Coolant: flow rate, temperature
- Some variables are measured while others are unmeasured.
- A process can be under a set of controllers or it may be operated without any control.

1.2 Using relations among variables for control

- Irrespective of whether a variable is measured or not, and whether a process is under control or without any control, variables experience cause and effect relations with other variables.
- For example, the temperature inside the reactor affects the rate and thus the conversion of reactants; the flow

rate of the coolant affects the reactor temperature and so on.

- The task of controllers is to exploit those relations to maintain certain variables at desired values.
- So, it is necessary that the relations among variables are well understood; this understanding, or in other words, some sort of model of relations among variables, is developed using a combination of process knowledge, scientific principles and process data.

1.3 Modelling steady state relations

1.3.1 Steady state relations: Example - distillation

- The relations between two variables can be expressed in different ways. For example, for a distillation column operation, there exists a relation between reflux ratio and product composition.
- These relations can be obtained by theoretical calculations considering material properties as well as column characteristics and operating conditions. Also the relations can be obtained by measuring the top composition at different reflux ratios. A hypothetical data set relating top composition of a distillation column and reflux ratio is presented in Figure 1.

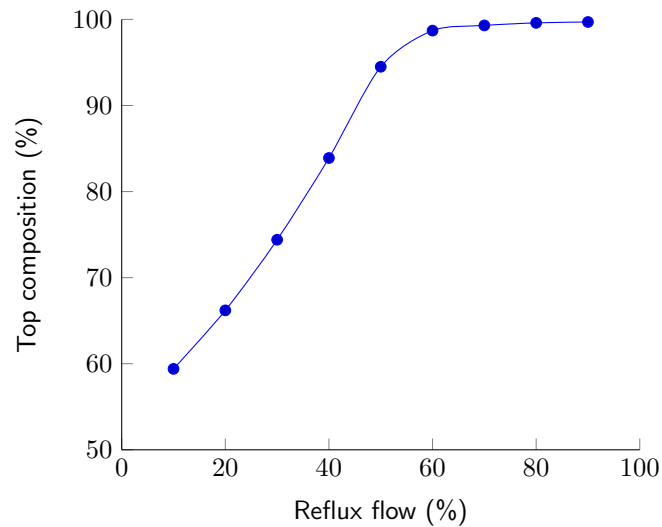


Figure 1: Typical relation between reflux flow and top product composition in a distillation column.

1.3.2 Steady state relations: Example - reactor

- Similar relations can be obtained for coolant flow rate and reactor temperature as shown in Figure 2, speed of car and fuel flow, level of liquid and inlet flow and so on.

1.3.3 Use of the steady state relations

- These relations are useful to determine what will be the value of one variable at a certain value of another.
- For example, if the coolant flow rate is maintained at a certain value, what will be the temperature in the reactor assuming that other variables remain the same.
- Such relations are known as steady state relations referring to the fact that transitional behavior are not captured therein.

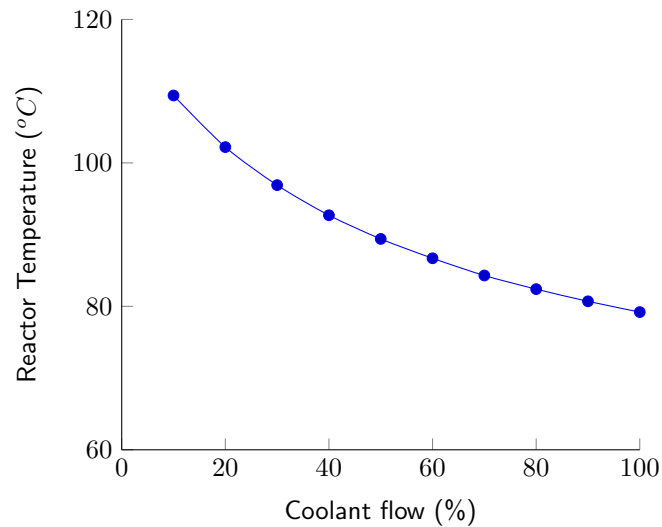


Figure 2: Typical relation between coolant flow and reactor temperature.

1.3.4 Limitations of the steady state relations

- However, it is not useful to determine how the temperature in the reactor will change if the coolant flow is changed from one value to another. Will the change be linear, monotonic or follow an oscillating path, is not determinable from these relations.
- Also how long will it take for the affected variable, e.g. the reactor temperature, to reach the next steady value, cannot be determined from these relations.
- To capture how an output changes with time when an input is changed, another type of models, namely, dynamic models are required.

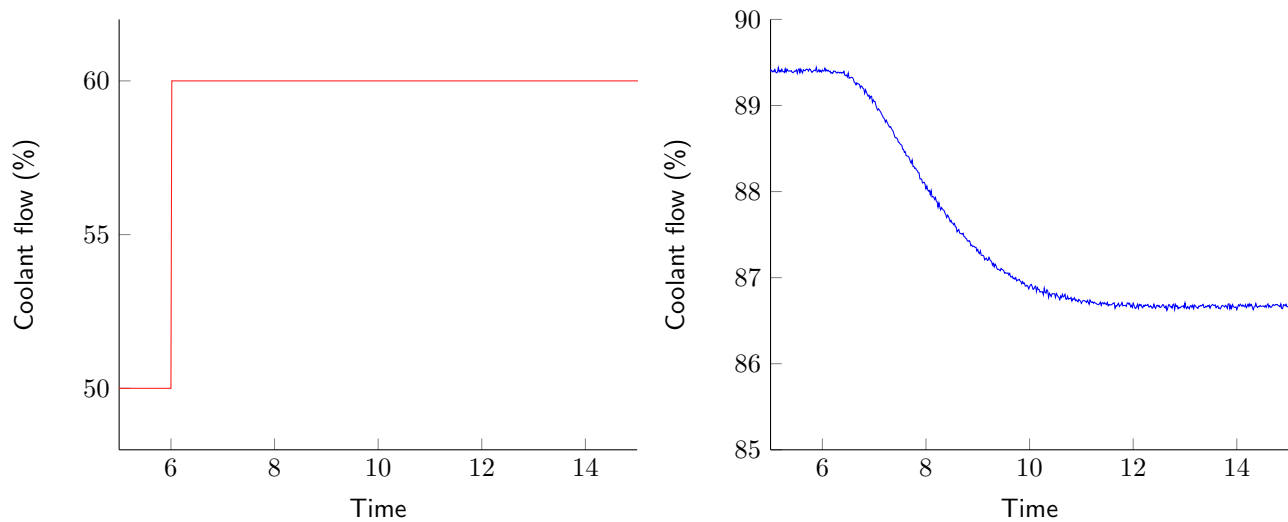


Figure 3: Typical transition in reactor temperature (right) with a change in coolant flow (left).

1.4 Dynamic Relations

1.4.1 Dynamic Relation example

- A dynamic relation expresses how one or a set of output changes with the change in one or a set of inputs as well as how the variables change with time.

1.4.2 Importance of dynamic relation for control

- The transitional behavior is important for control.
- The performance of control is, in fact, determined by how the transition from one steady state to another is attained or how a process is brought back to its steady state when any deviation is caused due to disturbances.
- For example, for the speed control of a car, if the driver wants to change the speed from one value, say 60 km/h to another, say, 80km/h, then how the fuel flow is ma-

nipulated to make this transition determines the driving control performance.

- For the pool level control problem, if it is desired to decrease the level of water in the pool by manipulating its inlet flow, one may choose to monotonically decrease the inlet flow. Alternatively, one can decrease the inlet flow by a large value and then increase it slowly. These two control actions will result in different patterns in how the level goes from its initial steady value to its final steady value. These pattern will depend on the dynamic relation between the level and inlet flow.

2 Workout: Modeling knowledge inventory

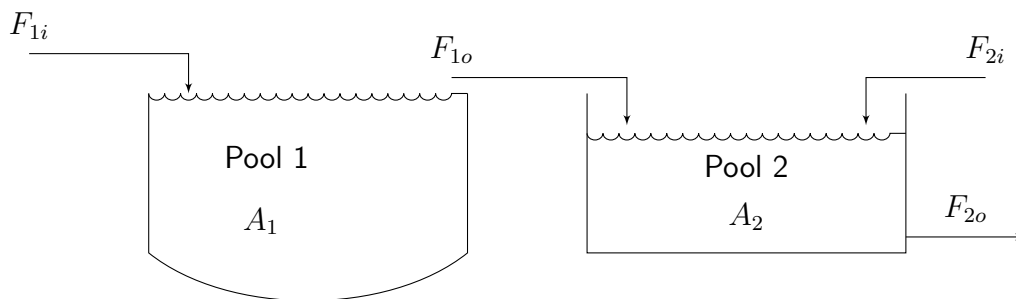


Figure 4: Schematic of the swimming pools. Standard notations for area (A) and flow rate (F) are used.

- Consider the pool example; we wanted to know whether Sam, the little boy in Pool 2 will drown when the inlet flow to pool 1 was increased suddenly. To know it we need a model for the process.

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- Using your knowledge on modeling, find a model for the swimming pools considering the above scenario.

3 Modeling Dynamic Relations

3.1 Governing laws

- Dynamic relations among process variables are governed by the laws of nature.
- For example, the downward flow of a liquid is governed by gravitational force and can be explained by laws of motion. The rate of a reaction and its dependence on reaction condition can be explained by the rate equations.
- Scientific principles those explain natural laws are the main tools for modelling dynamic relations. Principles of thermodynamics, mechanics, kinetics, heat transfer, mass transfer as well as the conservation principles form the bases for dynamic modelling.

3.2 Conservation principles

- Specifically which principles are required is determined by the specific problem in hand. However, often the three conservation principles are the starting point in dynamic modelling which are:

1. Conservation of mass
2. Conservation of energy
3. Conservation of momentum

For most process control problems, the momentum balance is not required. Also if the temperature is not within the input-output set, the energy balance equation becomes irrelevant.

3.2.1 Conservation of mass

The overall mass balance can be presented as

$$\left\{ \begin{array}{c} \textit{Rate of} \\ \textit{accumulation} \\ \textit{of mass} \end{array} \right\} = \left\{ \begin{array}{c} \textit{Rate of} \\ \textit{mass in} \end{array} \right\} - \left\{ \begin{array}{c} \textit{Rate of} \\ \textit{mass out} \end{array} \right\} \quad (1)$$

The component balance for any component i can be presented as

$$\begin{aligned}
 & \left\{ \begin{array}{c} \textit{Rate of} \\ \textit{accumulation} \\ \textit{of component } i \end{array} \right\} \\
 &= \left\{ \begin{array}{c} \textit{Rate of} \\ \textit{component} \\ \textit{ } i \textit{ in} \end{array} \right\} - \left\{ \begin{array}{c} \textit{Rate of} \\ \textit{component} \\ \textit{ } i \textit{ out} \end{array} \right\} \\
 &+ \left\{ \begin{array}{c} \textit{Rate of} \\ \textit{generation} \\ \textit{of } i \end{array} \right\} - \left\{ \begin{array}{c} \textit{Rate of} \\ \textit{consumption} \\ \textit{of } i \end{array} \right\} \quad (2)
 \end{aligned}$$

Here, the rate of generation and rate of consumption refer to generation and consumption due to chemical reactions. The overall material balance together with the component balance form the conservation of mass principles. It is worthwhile to note the basic principle behind the above equations; while a chemical species can be generated or consumed, the overall mass remains the same.

3.2.2 Conservation of energy

The conservation of energy equation can be written as:

$$\begin{aligned}
 & \left\{ \begin{array}{l} \textit{Rate of} \\ \textit{accumulation} \\ \textit{of energy} \end{array} \right\} \\
 = & \left\{ \begin{array}{l} \textit{Rate of} \\ \textit{energy in} \\ \textit{by convection} \end{array} \right\} - \left\{ \begin{array}{l} \textit{Rate of} \\ \textit{energy out} \\ \textit{by convection} \end{array} \right\} \\
 & + \left\{ \begin{array}{l} \textit{Rate of} \\ \textit{heat generation} \\ \textit{due to reaction} \end{array} \right\} + \left\{ \begin{array}{l} \textit{Rate of} \\ \textit{net heat addition} \end{array} \right\} \\
 & + \left\{ \begin{array}{l} \textit{Rate of} \\ \textit{net work done} \end{array} \right\} \qquad (3)
 \end{aligned}$$

4 An application example

4.1 Relevant principles

- Consider the pool control problem.
- If there is no concern about the temperature of water, the energy balance equation will be irrelevant.
- Also if the only component is water, there is no relevance of the component balance as well. This leaves the overall mass balance as the only conservation principle of interest.

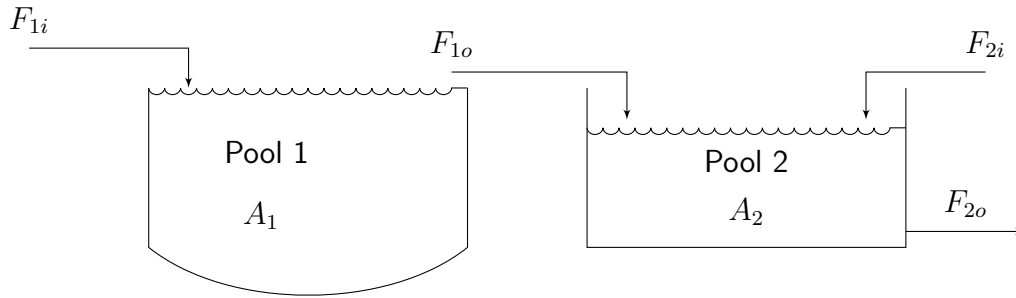


Figure 5: Schematic of the swimming pools.

4.2 Notations

- In general we will indicate level by h , volumetric flow rate by F , cross-sectional area of by A , and volume by V .
- Subscripts will be used for denoting pool numbers, 1 and 2 and a second subscript i and o will be used to denote inlet and outlet, respectively.
- t will be used to represent time. Regular notations for derivatives will also be used. Also we will assume a consistent set of units for all of the variables.

4.3 Pool 1 level model

The elements of the overall mass balance equation for pool 1 can be written as

$$\left\{ \begin{array}{l} \text{Rate of} \\ \text{Accumulation of mass} \end{array} \right\} = \frac{d(\rho V_1)}{dt} \quad (4)$$

$$\left\{ \begin{array}{l} \text{Rate of} \\ \text{mass in} \end{array} \right\} = \rho F_{1i} \quad (5)$$

$$\left\{ \begin{array}{l} \text{Rate of} \\ \text{mass out} \end{array} \right\} = \rho F_{1o} \quad (6)$$

The overall mass balance equation becomes

$$\frac{d(\rho V_1)}{dt} = \rho F_{1i} - \rho F_{1o} \quad (7)$$

Assuming the density of water to be constant, we have

$$\frac{dV_1}{dt} = F_{1i} - F_{1o} \quad (8)$$

For Pool 1, V_1 is constant and so $\frac{dV_1}{dt} = 0$. So we get

$$F_{1i} - F_{1o} = 0 \quad (9)$$

So we see that there is no dynamic relation associated with the level of water in the pool. It is also obvious from the structure that the level does not change with time.

4.3.1 Pool 2 level model

If the overall mass balance equation is written for Pool 2, we have

$$\frac{d(\rho V_2)}{dt} = \rho F_{1o} + \rho F_{2i} - \rho F_{2o} \quad (10)$$

Assuming constant density of water and using Eq.9, we have

$$\frac{dV_2}{dt} = F_{1i} + F_{2i} - F_{2o} \quad (11)$$

As we are modelling level, V_2 is expressed in terms of h_2 . From principles of fluid dynamics, F_{2o} can be expressed as $F_{2o} = c\sqrt{h_2}$, where c is a constant dependent on the resistance to flow in the pipeline. So we get

$$A_2 \frac{dh_2}{dt} + c\sqrt{h_2} = F_{1i} + F_{2i} \quad (12)$$

Eq. 12 is the dynamic model relating the level of water in pool 2 and the inlet flow rates into the pools. This example shows how using the conservation principle along with physical laws desired relations can be obtained.

5 First Principles Modeling

- The approach to find dynamic models utilizing the conservation principles along with principles of thermodynamics, mechanics, kinetics, is known as the first principles modelling.
- In this section a number of examples will be presented to illustrate the approach and develop dynamic model for simple systems.
- Before proceeding to the examples let us list the step by step procedure to systematize the first principles ap-

proach. The procedure can be divided into the following five steps.

5.1 Step 1 - Define modelling objective

- In the context of control, defining modelling objective refers to the selection of input-output pair which in turn defines the system boundary for the modelling exercise.
- In some cases, the output can be related to the input through other variables; the link between input and output is to be established first from process knowledge.

5.2 Step 2 - Gather process knowledge and information

- This step refers to identify knowledge regarding mechanics of fluid flow, kinetics of chemical reactions, mechanisms of heat and mass transfer and so on.
- Also information regarding equipment size and shape, valve characteristics, fluid properties and operational conditions are to be collected.

5.3 Step 3 - Develop model equations

- Model development refers to the use of conservation principles along with kinetic, mechanistic information, heat and mass transfer model to formulate the relations among the concerned variables.

- Note that to develop a model suitable for the purpose of control, assumptions are also required.

5.4 Step 4 - Simplify model equation and standardize

- This step refers to simplification of the developed equation to explicitly express the relations between an input and an output in a standard form.

5.5 Step 5 - Analyze and validate model

- The final step in the modelling exercise is to analyse the obtained model to validate it against process knowledge and data.
- A simplified model can be valid over a certain range; the user needs to know the range of the variables over which the model is valid.

6 Modeling example: Tanks in series

Consider the two tank system shown in Figure 6. To find a model of the system, let us follow the five step procedure described in Sec.5.

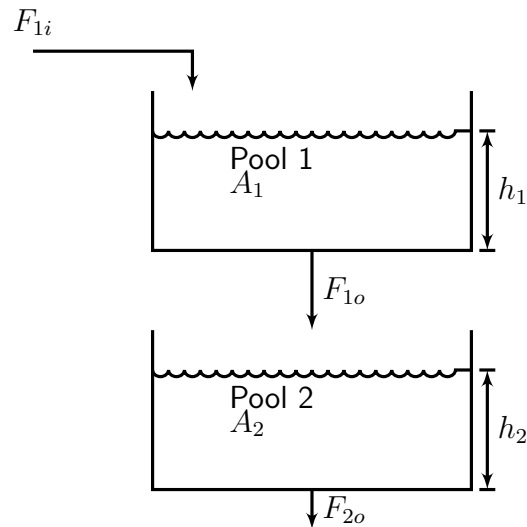


Figure 6: Schematic of two gravity drained tank in series.

6.1 Step 1 - Define modelling objective

- The objective this exercise is to find a model between the inlet flow to tank 1, F_{1i} , and the level of liquid in tank 2, h_2 .
- So the input is F_{1i} and the output is h_2 .
- Relating these two variables considering the two tanks as the system will result an accumulation term for both tanks.
- However, to express in terms of h_2 , the accumulation term of tank 2 should be considered separately.
- Now these variables are related through a couple of other variables. F_{1o} affects h_1 that affects F_{1o} . Finally F_{1o} affects h_2 .
- So the links of variables shown in Figure 7 are to be used to get the desired model. Equations are required to develop for each tank separately.

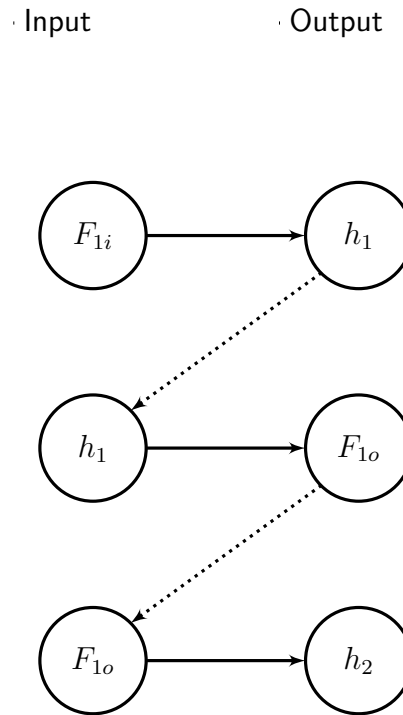


Figure 7: Links among variables for the two gravity drained tank in series.

6.2 Step 2 - Gather process knowledge and information

- To model the level, one needs to know how the outlet flow rate varies with the level of liquid in the tank.
- From the principles of fluid dynamics we know that outlet flow from a source due to gravity is proportional to the square root of pressure where pressure is directly proportional to level.

So we have

$$F_{1o} \propto \sqrt{h_1} \quad (13)$$

$$F_{1o} = c_1 \sqrt{h_1} \quad (14)$$

- Similar relations are valid for tank 2. The proportionality constant c_1 depends on the resistance to flow through the

outlet.

- There are no aspect of heat or mass transfer or reaction.
- In terms of process dimensions and operational conditions, we need to know the cross sectional areas of the two tanks, which are A_1 and A_2 .
- At this point, we also need to make assumptions about the system. We will assume that
 - the density of the liquid is constant

6.3 Step 3 - Develop model equations

The overall mass balance equation for tank 1 will lead to

$$\frac{d(\rho V_1)}{dt} = \rho F_{1i} - \rho F_{1o} \quad (15)$$

With the assumption of constant density, ρ , and applying Eq. 14, we get

$$A_1 \frac{dh_1}{dt} + c_1 \sqrt{h_1} = F_{1i} \quad (16)$$

- The relation between F_{1o} and h_1 is defined by Eq.14.
- To get the relation between F_{1o} and h_2 , the mass balance equation for tank 2 can be written which in combination with the tank 1 level equation and Eq. 14 form the relation between F_{1i} and h_2 .

$$A_1 \frac{dh_1}{dt} + c_1 \sqrt{h_1} = F_{1i} \quad (17)$$

$$F_{1o} = c_1 \sqrt{h_1} \quad (18)$$

$$A_2 \frac{dh_2}{dt} + c_2 \sqrt{h_2} = F_{1o} \quad (19)$$

Note how each of the equations corresponds to the links in Figure 7.

6.4 Step 4 - Simplify model equation and standardize

- The above model equations, although simple, require further simplifications to get those in the forms of ordinary differential equations (ODE).
- The nonlinear terms $\sqrt{h_i}$ are to be linearized. This will be discussed in the next chapter.
- Also we will use another tool, namely, the Laplace transformation to present the equations in the Laplace domain.
- As will be seen there, in the Laplace domain a single expression relating the liquid level in tank 2 and the inlet flow rate to tank 1 can be obtained in a standard form.

6.5 Step 5 - Analyze and validate model

- Model equations in the Laplace domain, when expressed in a standard form, allows to analyze the models in terms

of direction of change of the variables relative to one another.

- A qualitative analysis can be taken as an initial validation of a model.
- For further validation, input-output data from the process is required. A matching of the process data with the solution of the model ensures validity of the model within the range of process data.

7 Modeling example: Chlorination of pools

- So far for the pools we have consider pure water coming into the pool and the level of water in pool 2 was the only concern.
- However, if the pools are continuously chlorinated by adding chlorine in the pool 1 inlet flow and if the chlorine amount is suddenly increased, how that will affect the chlorine concentration in the pools. To find that out we will follow the same stepwise procedure.

7.1 Step 1 - Define modelling objective

- The modeling objective for this problem is to define the relation between inlet concentration of chlorine in stream F_{1i} , i.e. C_{1i} and the composition of chlorine in pool 1 and 2, i.e. C_1 and C_2 .

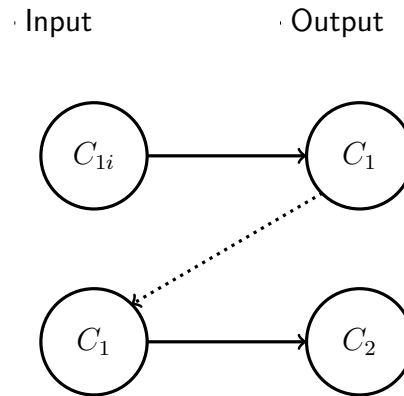


Figure 8: Links among variables for chlorination in swimming pools.

- Here, compositions are in terms of mass fraction of chlorine.
- Note that C_{1i} directly affects C_1 and C_2 is directly affected by C_1 . Thus the links are as shown in Figure.

7.2 Step 2 - Gather process knowledge and information

We will assume that the density of water does not change due to the variation in chlorine amount.

- the density of the liquid is constant

7.3 Step 3 - Develop model equations

To develop relation between inlet chlorine composition and that in the tanks we will assume that the flow rates remain constant. So the overall mass balance equation will result

in

$$F_{1i} = F_{1o} \quad (20)$$

$$F_{2o} = F_{1i} + F_{2i} \quad (21)$$

Component balance for pool 1 gives

$$\frac{d(\rho V_1 C_1)}{dt} = \rho F_{1i} C_{1i} - \rho F_{1o} C_1 \quad (22)$$

Component balance for pool 2 gives

$$\frac{d(\rho V_2 C_2)}{dt} = \rho F_{1o} C_1 + \rho F_{2i} C_{2i} - \rho F_{2o} C_2 \quad (23)$$

As $F_{1i} = F_{1o}$ and assuming that the inlet 2 is pure water Eq. 22 and Eq. 23 can be simplified to give

$$\frac{dC_1}{dt} + \frac{F_1}{V_1} C_1 = \frac{F_1}{V_1} C_{1i} \quad (24)$$

$$\frac{dC_2}{dt} + \frac{F_{2o}}{V_2} C_2 = \frac{F_1}{V_2} C_1 \quad (25)$$

Eqs.24 and 25 form the model equation to determine the effect of inlet chlorine concentration on that in pool 1 and pool 2.

7.4 Step 4 - Simplify model equation and standardize

This model equations do not contain any nonlinear term and as we will see in the next chapter, this is the standard form of ODE to translate the model into the Laplace domain.

7.5 Step 5 - Analyze and validate model

- Considering both flow rates and volume to be positive, the model equations show that the concentration in both pool 1 and pool 2 will increase due to the increase in inlet chlorine concentration.
- This is consistent with theoretical understanding of the phenomenon. The rate of change and pattern of the response curve can be verified from the solution of the equations.
- The solution can be compared with experimental data for further validation.

8 Modeling example: Reactor system

- Consider the reactor and separator system.
- There is a large number of variables associated with the system.
- To develop a dynamic model, we need to consider the input and output under consideration and define a sub-system boundary.
- An output can be affected by a set of variables.
- However, when modeling the relation between a pair of input and output, the other variables affecting the output can be assumed constant. This is valid due to the fact that how one variable affects another is determined by

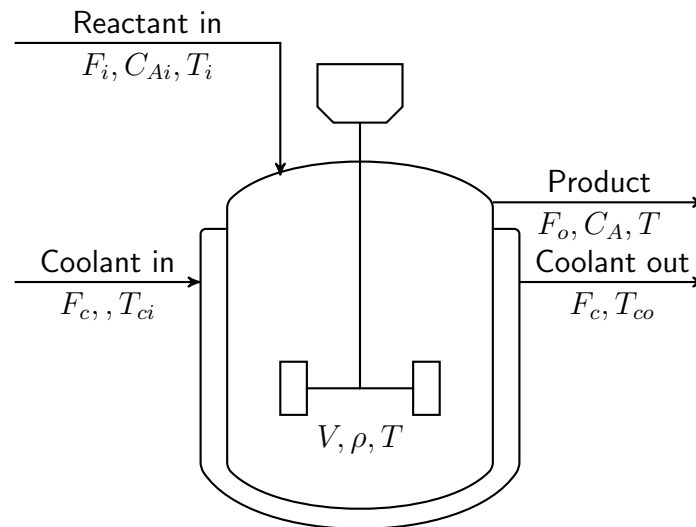


Figure 9: Schematic of CSTR with cooling jacket.

natural laws which remain unchanged.

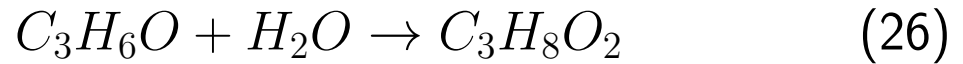
- Going back to the example, the modeling exercise will begin with the choice of input and output which is defined by the modeling objective.

8.1 Step 1 - Define modelling objective

- In this example the objective is to find a model between coolant flow rate, F_c and reactor temperature, T .
- From principles of chemical kinetics we know that temperature affects reaction rate which affects concentration of the chemical species and total heat generated by the reaction which, in turn, affects the temperature.
- So one needs to relate temperature, concentration of chemical species and reactant flow.

8.2 Step 2 - Gather process knowledge and information

The following reaction is considered in the CSTR.



The reaction takes place in excess of water and it is first order with respect to propylene oxide. For the sake of simplicity we will represent propylene oxide by A. So the rate of reaction is expressed as

$$r = kC_A \quad (27)$$

with

$$k = k_o e^{-E/RT} \quad (28)$$

The kinetic parameters can be found in the literature. Also fluid properties and reactor dimensions are to be used. Moreover, we need to make some assumptions as follows:

- densities and heat capacities of the reactants and product are same
- concentration and temperature are constants throughout the reactor
- reactor has a constant hold-up

8.3 Step 3 - Develop model equations

With all the information and process knowledge, we will move to write the balance equations. The overall mass

balance equation for the reactor will lead to

$$\frac{d(\rho V)}{dt} = \rho F_i - \rho F_o \quad (29)$$

With the assumption of constant hold-up Eq. 29 gives

$$F_i = F_o \quad (30)$$

Temperature is related to component A. So we will write the component balance for A only.

$$\frac{d(\rho V C_A)}{dt} = \rho F_i C_{Ai} - \rho F_o C_A - \rho V k C_A \quad (31)$$

Denoting $F_i = F_o = F$, the component balance can be expressed as

$$\frac{dC_A}{dt} = \frac{F}{V} (C_{Ai} - C_A) - k C_A \quad (32)$$

Note that the temperature term is implicit in k . Next we can write the energy balance equation.

$$\begin{aligned} \frac{d(\rho V C_p T)}{dt} = & \rho F_i C_p (T_i - T_{ref}) \\ & - \rho F_o C_p (T - T_{ref}) \\ & + (-\Delta H_R) V k C_A \\ & + \rho_c F_c C_{pc} (T_{ci} - T_{co}) \end{aligned} \quad (33)$$

Here, C_p and C_{pc} are the specific heat of the reactor materials and the coolant, respectively. Simplifying the above

equation we have

$$\begin{aligned} \rho V C_p \frac{dT}{dt} = & \rho F C_p (T_i - T) + (-\Delta H_R) V k C_A \\ & + \rho_c F_c C_{p_c} (T_{ci} - T_{co}) \end{aligned} \quad (34)$$

Eq. 30, Eq. 32 and Eq. 34 forms the model equation for the reactor temperature. Note that both T and C_A appears in both equations.

Depending on the system some further simplification is possible. For example, as this particular reaction takes place in the presence of excess water and we can assume the density of reactant and product same as that of water. Also typically the coolant is water. This assumption will lead to $\rho = \rho_c$ and $C_p = C_{p_c}$. So we get

$$\begin{aligned} \frac{dT}{dt} = & \frac{F}{V} (T_i - T) + \frac{(-\Delta H_R)}{\rho C_p} k C_A \\ & + \frac{F_c}{V} (T_{ci} - T_{co}) \end{aligned} \quad (35)$$

Also note that depending on the heating system the term net rate of heat addition by surrounding in the energy balance equation will be different. If there is a cooling system that absorbs the heat at a constant temperature T_c , the heat addition term will take the form

$$Q = U A_c (T_c - T) \quad (36)$$

where A_c is the heat transfer area of the cooling surface and U is the overall heat transfer coefficient.

8.4 Step 4 - Simplify model equation and standardize

Note the relation between k and T . This means that the third term in the model Eq. 32 and Eq. 34 has both C_A and T , representing a nonlinear term that needs to be linearized to express the equations in the form of ODE.

8.5 Step 5 - Analyze and validate model

Once linearized and standardized, the equations can be solved simultaneously and the model output can be compared with process data for validation.

9 Modeling example: Distillation column

- Consider the distillation column shown in Figure 10.
- Operation of a distillation column requires to consider aspects of both mass and heat transfer.
- Depending on the control problem, material and/or energy balance equation are needed to consider.
- Here we consider a tray column where compositions are changing from tray to tray. Consequently balance equations should be written around each tray.
- Let us see how to develop tray by tray balance equations for a specific control objective.

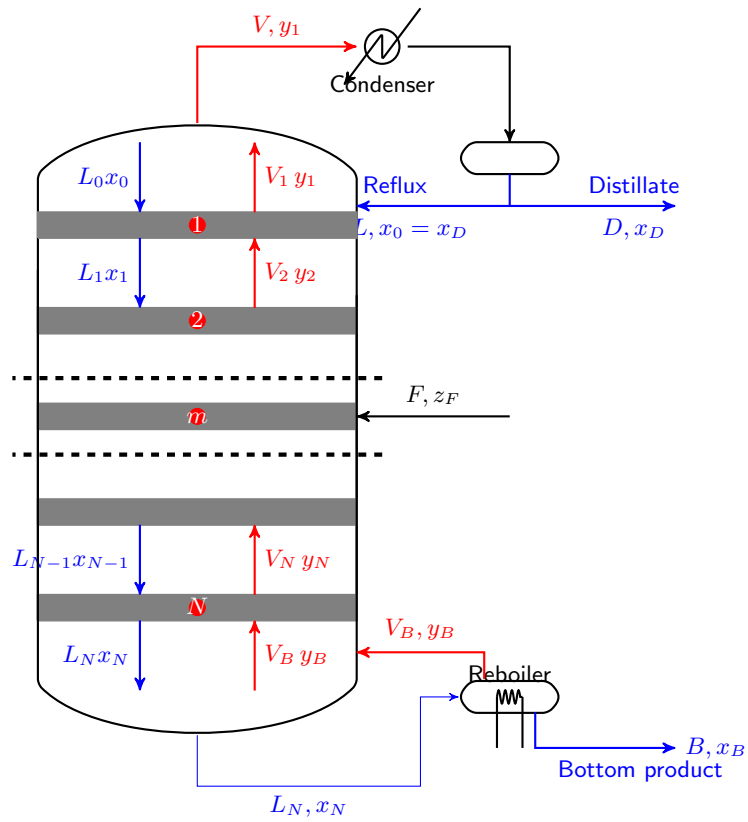


Figure 10: Tray by tray flow and nomenclature in a distillation column.

9.1 Step 1 - Define modelling objective

A common control configuration for distillation column is to manipulate the reflux flow (R) for top composition (x_D) control. For this purpose one needs to find the model between R and x_D .

9.2 Step 2 - Gather process knowledge and information

The process under consideration involves binary distillation. Equilibrium relations for the two components can be found in the literature. A number of assumptions are to be made to develop the required model equation.

1. Constant and equal liquid hold-up in each tray
2. Negligible vapor phase hold-up
3. Feed is saturated liquid
4. Constant molal overflow i.e equilibrium boiling with constant latent heat.

With the above assumptions, the required balance equations will be simpler. Also the constant molal overflow assumption will eliminate the need to write the energy balance equation.

9.3 Step 3 - Develop model equations

The component balance equation for the more volatile component for the condenser can be written as

$$H_c \frac{dx_D}{dt} = Vy_1 - (R + D)x_D \quad (37)$$

For a stage in the rectifying section, the component balance equation becomes

$$H_i \frac{dx_i}{dt} = V(y_{i+1} - y_i) + L_r(x_{i-1} - x_i) \quad (38)$$

for $i = 1, 2 \dots m$. For the feed tray considering the feed is saturated liquid

$$H_m \frac{dx_m}{dt} = V(y_{m+1} - y_m) + L_r x_{m-1} - L_s x_m + Fz_f \quad (39)$$

For any stage in the stripping section

$$H_j \frac{dx_j}{dt} = V(y_{j+1} - y_j) + L_s(x_{j-1} - x_j) \quad (40)$$

for $j = m + 1, m + 2 \dots N$. Finally for the reboiler

$$H_B \frac{dx_B}{dt} = -Vy_B + L_s x_N - Bx_B \quad (41)$$

Eq. 37 through Eq. 41 form a simpler representation of the distillation column composition model.

9.4 Step 4 - Simplify model equation and standardize

- Although a number of assumptions have been made to develop the above model, the equations are coupled; x_D appears in both condenser balance and balance around tray 1, x_1 appears both in the equations for tray 1 and tray 2 and so on.
- This will require a simultaneous solution. Also expressing the entire set into one high order equation becomes difficult.
- Moreover, such a complicated model, although useful for accurate prediction of composition, virtually useless for controller design. Model used for controller design needs to be much simpler.
- Later we will see that one needs to resort to data based modelling to develop simple model for such processes.

9.5 Step 5 - Analyze and validate model

The assumptions made to develop the model will limit its validity. If the reflux flow is varied over a wide range, the equations may become less accurate. Also for the data based model, the validation is within small range of input and output over which changes are made.

10 Use of Process Models

Models may have widely varying use. In the context of control, the main use of a model is to design controller. Following is a list of use of dynamic models.

Controller design :

Most controller design algorithms require either an explicit or an implicit model representing the dynamic behavior of the process.

Process simulation :

Models can be used to simulate process behavior over a range of operating conditions. This is helpful for predicting process behavior under conditions which may be costly to observe in real plants.

Operator training :

Model simulations can be used to train operators on how to control process and maintain safe operations during abnormal conditions.

Process optimization :

Using model predictions, data can be collected for large sets of operating conditions for the purpose of optimization.