Chemical Process Control
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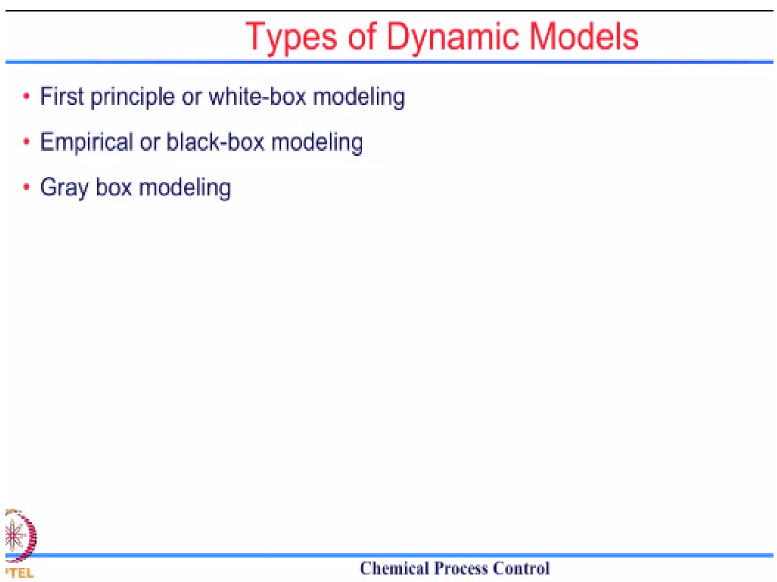
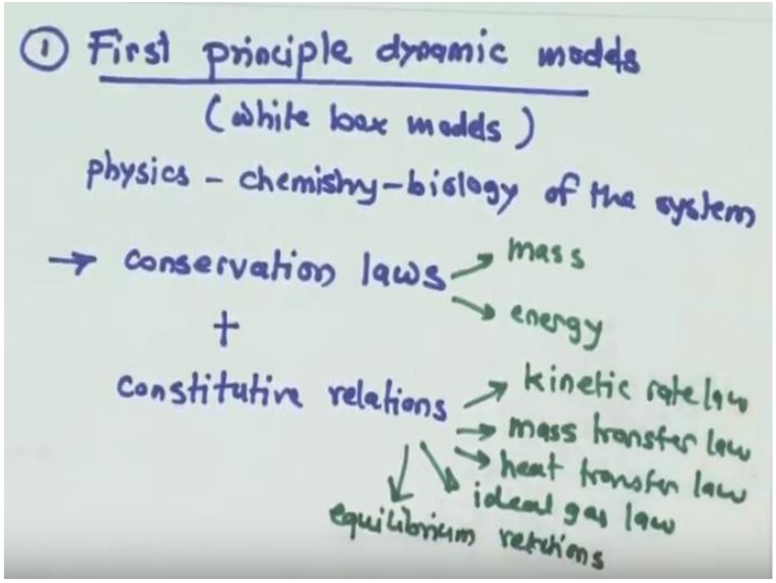
Lecture - 06
First Principle Dynamic Models

Now let us look at what are the different types of models which can be written for chemical processes and we are now actually interested in developing models which will be eventually used for process control. There are 3 types of dynamic models which can be written depending on how much information about the process is available and how much accuracy you require from each of those models.

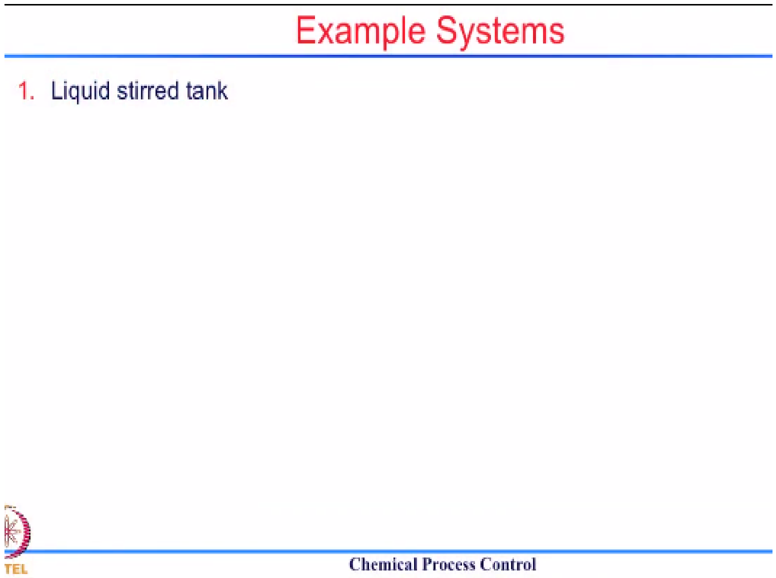




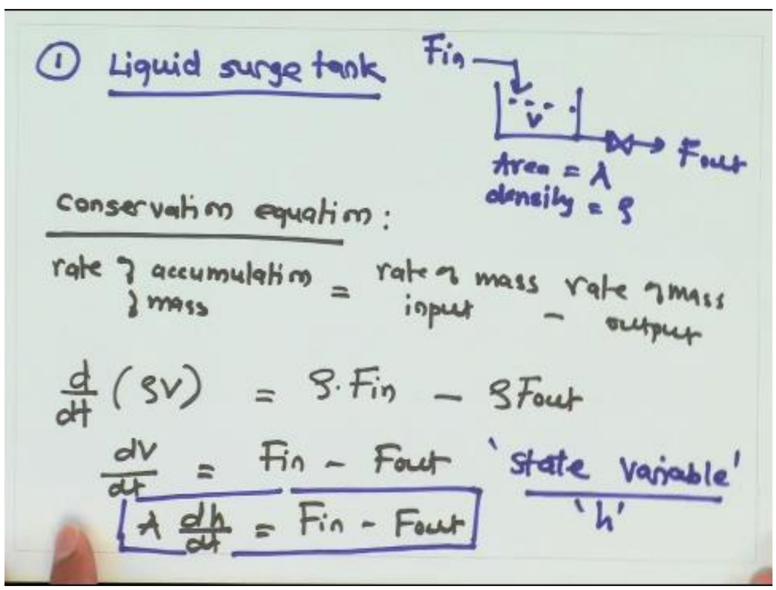
The first type of models is known as first principle models. We will also call them as white box models. As the name suggests, they are based on the first principles or principles of physics, chemistry, and biology. You can also call them as fundamental models based on the actual theory of the system and they will deal with conservation laws. So you know that in any process mass is conserved, energy is conserved.

When you write first principle dynamic models, you will try to ride on the fact that these conservation laws are valid on that particular system. And in addition to that, you also have constitutive relations. So you have conservation laws which will be conservation of mass, conservation of energy. You can also have constitutive relationships which are not captured directly by conservation laws but by some other either experimental equations or fundamental equations like kinetic rate laws or mass transfer relations, heat transfer law. It can be ideal gas law, can be an equilibrium relation. So when you combine all these theoretical aspects of that particular process and come up with a dynamic model of that particular system, it is known as the first principle dynamic model.

We will take a few examples and then try to write down first principle dynamic models for some of the simple systems.



The first example we are going to consider is the liquid surge tank.



If we have to write the first principle dynamic model, we will start with the conservation equation. For this system, there are no energetic effects. So all we need to write down an equation is for mass conservation. If I say the volume of the tank is ‘V’ and area of the tank is ‘A’, the density of the material is rho (‘ρ’). Then I can write down the equation,

$$Rate\ of\ accumulation\ of\ mass\ = Rate\ of\ mass\ input - Rate\ of\ mass\ output$$

As there are no reactions, there is no consumption of mass or there is no generation of mass. So the rate of accumulation of mass in the system will be,

$$\frac{d(\rho V)}{dt} = \rho F_{in} - \rho F_{out}$$

If we assume that density is constant, we can write down

$$\frac{dV}{dt} = F_{in} - F_{out}$$

And if we try to convert this volume into height, we can write down,

$$A\frac{dh}{dt} = F_{in} - F_{out}$$

This is our first principle dynamic model of the surge tank or the first pass at writing down the first principle dynamic model. Now here the time derivative comes for height. So 'h' is known as the state of the system because it tells me what is the status of this particular system. If the height is very close to the overflow condition then the status of the tank is it is going to overflow. Or if the height is very close to 0 the status is it is going to go dry.

So the variable which is typically written as a time derivative will give you the status of the system and therefore it is known as a state variable. For this particular example, 'h' is a state variable. It gives me the state of the system and extension of that is if this variable remains constant then we call it as a steady state and that is when you have a steady state, this dh/dt goes to 0.

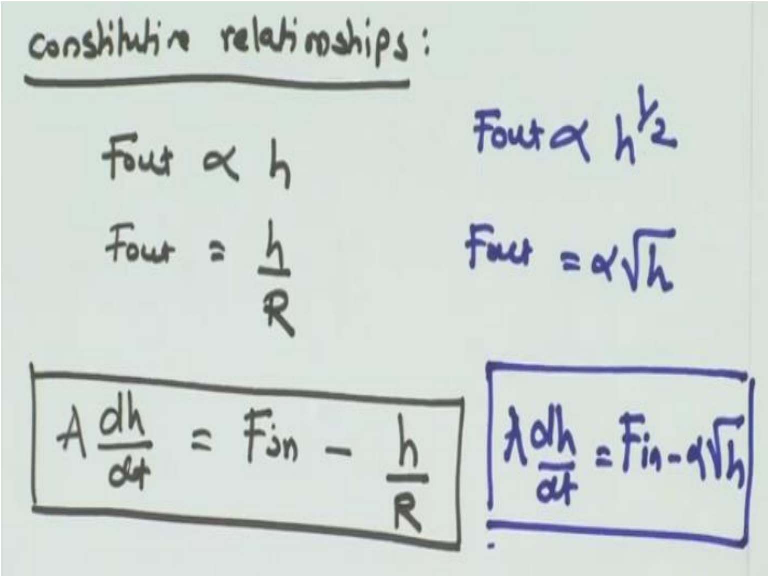
And therefore,

$$0 = F_{in} - F_{out}$$

Or

$$F_{in} = F_{out}$$

becomes your steady state condition. So steady state model can always be obtained from a first principle dynamic model by simply equating the time derivative of the state variable to 0. Now in this same example, we can also add constitutive relationships.



A very common assumption is that the outlet flow rate is proportional to the height inside the tank and which is very intuitive because if you look at this particular figure, if I have a lot of material inside the tank obviously the flow out of that tank will be very large as compared to if there is very little liquid in the tank, the outlet flow rate will be small. So it is quite common to assume that the outlet flow rate is proportional to height.

And we can write

$$F_{out} = \frac{h}{R}$$

Where R is known as the resistance of the valve. So if I use this constitutive relationship then my first principle dynamic model becomes,

$$A\frac{dh}{dt} = F_{in} - \frac{h}{R}$$

Now if I want to be more rigorous, then Fout is not proportional to h. It is actually proportional to the square root of the height and Fout can be written as,

$$F_{out} = \alpha \sqrt{h}$$

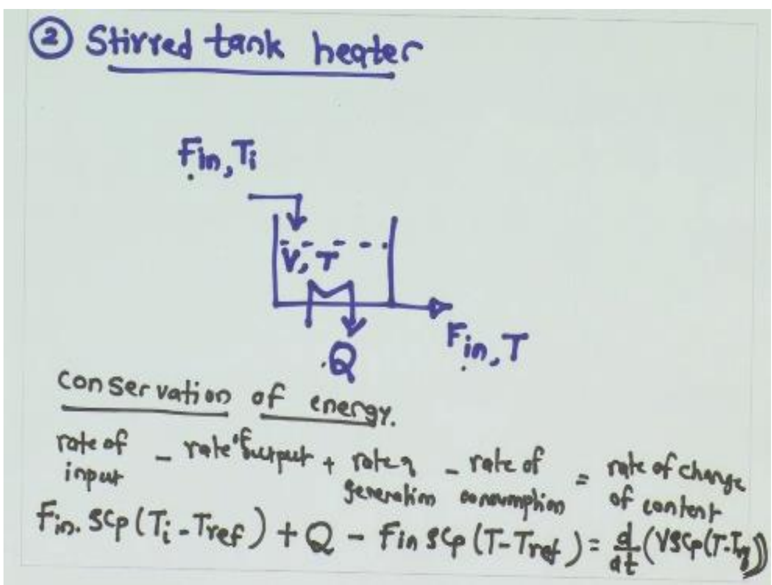
Where alpha is the valve constant.

In such a case the same dynamic model can be written more accurately as,

$$A\frac{dh}{dt} = F_{in} - \alpha\sqrt{h}$$

So depending on what constitutive relationship I am writing, the final form of the first principle dynamic model might change but a first principle dynamic model will always be written as a conservation equation followed by the constitutive relationships which may be some additional physical law or it may be some experimental correlation or relationship.

Let us now look at another example. This time the one which has significant energetic effects. We will consider an example of a stirred tank heater.



Similar to the previous example there is a tank, fluid comes in at an inlet flow rate and it leaves at a certain flow rate. For simplicity, let us assume that the inlet and outlet flow rate are equal so that the volume inside this tank remains constant. The inlet comes in at a temperature of 'Ti'. Heat is provided to this tank at the rate 'Q' and because of that the material inside the tank which is of amount 'V' gets heated to a temperature of 'T' and the stream leaving the tank also leaves at the temperature of 'T'.

For this example, as I said the material balance automatically gets satisfied because the amount of the material coming in is equal to the amount of material that is going out. We do not need to consider the conservation equation for mass. So we will start with conservation of energy. Now here let me point out that energy would consist of thermal energy, it may be potential energy or kinetic energy.

In chemical engineering systems, most of the times the potential and kinetic energy components are very insignificant compared to thermal energy or enthalpy. So most of the time even though we talk about the conservation of energy and writing energy balance, we are mostly inclined that we are trying to write an enthalpy balance. So let us try to write enthalpy balance for this particular system which will be,

$$Rate\ of\ input - Rate\ of\ output + Rate\ of\ generation - Rate\ of\ consumption = Rate\ of\ change\ of\ content$$

The rate of input of energy will be the enthalpy coming in through this input stream which will be,

$$Rate\ of\ input = F_{in}\ \rho\ C_p\ (T_i - T_{ref})$$

Where 'Tref' is the reference temperature for enthalpy calculation. There is one more input from this external source Q.

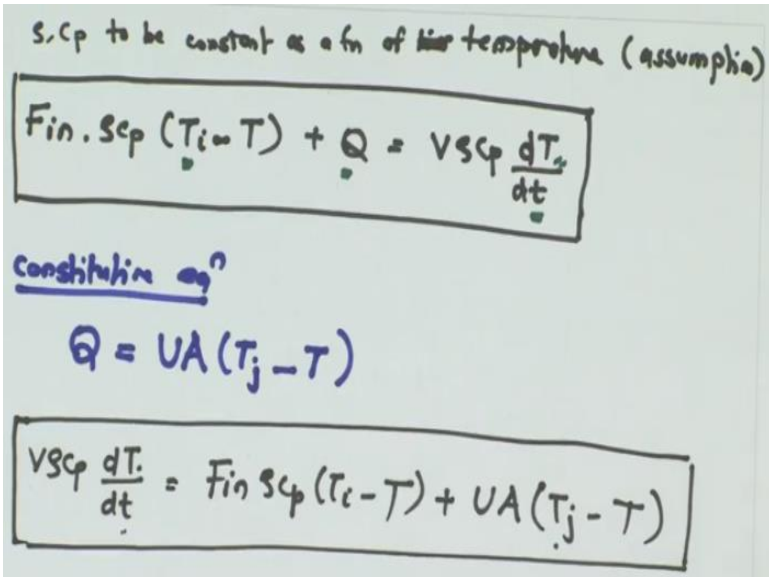
The rate of output will be written for this particular stream which will be,

$$Rate\ of\ output = F_{in}\rho C_p(T - T_{ref})$$

There is no generation or consumption of energy inside that system. So which will be equal to the rate of change of enthalpy content of this tank which will be,

$$Rate\ of\ change\ of\ content = \frac{d\left(V\rho C_p(T - T_{ref})\right)}{dt}$$

Let us now try to simplify this. We can assume that the density and heat capacity of this particular stream remains constant as a function of temperature.



So we can assume ρ, Cp to be constant as a function of temperature. We can simplify the previous equation as,

$$F_{in}\rho C_p(T_i - T) + Q = V\rho C_p\frac{dT}{dt}$$

This becomes a dynamic equation for the stirred tank heater. It gives the relationship between input which is Q to the output which is the temperature inside the tank or temperature leaving the tank.

It also gives the relationship between a potential disturbance which is ‘Ti’ and the output ‘T’ as a function of time. So it satisfies the definition of a dynamic model. Now at this point, we have not specified how that heat is entering into the system. It may be that there is a jacket around the stirred tank heater where steam is injected and then that hot steam will provide heat to the tank. So, in that case, we can write some constitutive equations.

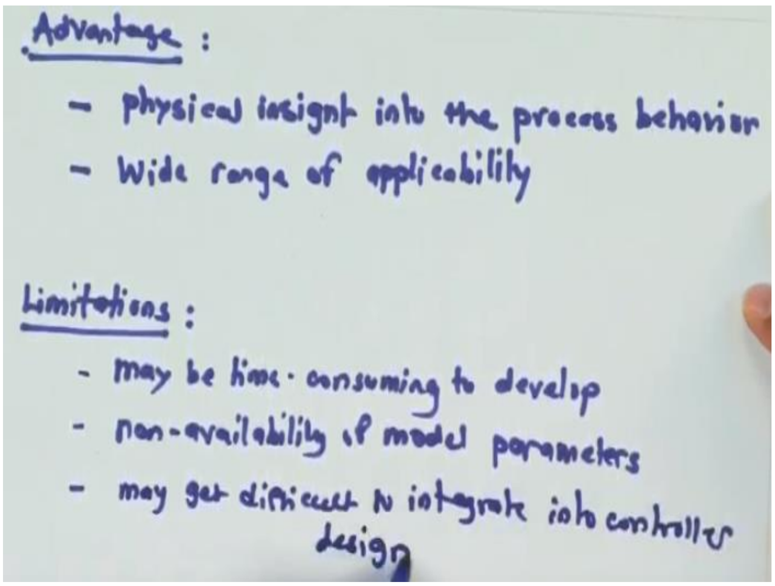
In this case, we can write the rate of heat transfer equation which will tell me that the rate of heat input will be UA times (T in the jacket – Tof the tank).

Using this equation we can refine our dynamic model as,

$$V\rho C_p \frac{dT}{dt} = F_{in}\rho C_p (T_i - T) + UA(T_j - T)$$

Even this can be used as a dynamic equation for this system which gives the relationship between jacket temperature and the output temperature as the function of time.

So we have seen 2 examples of first principle dynamic models. Now let us look at the advantages of first principle dynamic models.



The first advantage is that it gives a physical insight into the system. As it is built based on physical principles, it gives you how that system is going to behave under different sets of conditions. It also gives you what are the inherent parameters or which needs to be considered in order to understand the response of the process. The second advantage is it has a wide range of applicability.

As minimum assumptions are made and mostly physical laws are followed, these first principle dynamic models would be applicable over a wide range of operating conditions. Now having said that let us now look at what are the limitations of first principle models. The major limitation of a first principle model is that it may be time consuming to develop these equations.

We looked at very simple examples, so it was not evident that these can be difficult, but if you look at real chemical processes where multiple unit operations are interconnected and the number of variables may go into 100s, in that case writing dynamic equations for each and every process variable may be cumbersome.

It also gives us one additional limitation that many of the parameters which are part of the model may not be readily available. So non-availability of model parameters. These may be the mass transfer coefficient, reaction kinetics, or vapor-liquid equilibrium coefficient. So all the physical details or some of the parameters which are required in the model may not always be readily available and in that case applicability of first principle dynamic model gets restricted. Lastly, especially from the context of this course, we are interested in using these models for controller design.

In that case, if the model gets really complicated we will see later on that it will be very difficult to incorporate into the design of a control system. We typically tend to go for a simplistic model which can capture the response of a process. So, therefore, it may be difficult to integrate into controller design. Thank you.