MODULE TITLE : CONTROL SYSTEMS AND AUTOMATION

TOPIC TITLE : MODELLING OF PROCESSES

LESSON 1 : MATHEMATICAL MODELLING

CSA - 3 - 1

INTRODUCTION

Very often engineers use 'models' of a process to aid their understanding of how the process works and can be controlled. A model can be a description, a drawing, an actual physical model, or a mathematical/statistical construct that represents the approximate behaviour of the real, physical process, though often in a theoretical way.

In Lesson CSA - 1 - 1 (the first lesson of this module) we looked at a simple electrically heated, stirred tank with flow in and out. We developed a steady state model of the process using a mathematical equation which we called the control design equation. This was a very simple system as we set the conditions by making a series of assumptions (e.g. steady state, no change in density, etc.) to ensure we limited the complexity.

Thus the degree of complexity of a model is linked to decisions or assumptions made in the modelling process. Sometimes it is desirable to start with a *fundamental* or *first principles* model where modelling equations are developed starting from the material (mass) and energy balances, and chemical and physical laws.

In other cases, the fundamental behaviour of a process is poorly understood or prohibitively complex to model based on first principles. In these cases, models may be developed from experimental dynamic data. Developing a model from experimental data is often called *process identification*. Essentially, this approach 'curve fits' the data to produce what is sometimes called an 'Input/Output' or 'Black Box' model. This is shown diagrammatically overleaf.
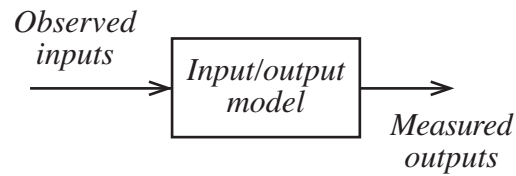
The choice of a model type depends on the scale of the problem.

We will concentrate mainly on fundamental modelling in more detail within this topic.

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YOUR AIMS
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At the end of this lesson you should be able to:

- give reasons for the modelling of processes

- produce simple mathematical models of processes, based on a series of assumptions, using
    – mass and energy balances
    – constitutive equations

- understand the use of the term 'degrees of freedom' in determining if a model is satisfactory

- list the stages in producing a model.

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FUNDAMENTAL OR FIRST PRINCIPLES MODELLING OF PROCESSES
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REASONS FOR CARRYING OUT MODELLING

A model can be a description, a drawing, an actual physical model, or a mathematical/statistical construct that represents the approximate behaviour of a real, physical process, though often in a very theoretical way. We will only be looking at mathematical modelling within this topic.

A mathematical model of a process is represented by a set of equations. It is only an approximation of the true process as it cannot incorporate all the features of the process. The more equations that are used, generally the better the approximation. However, the engineer must normally reach a compromise between the costs of producing and verifying the model (time and effort involved) and the level of approximation required.

Mathematical models can be helpful in process analysis and control in the following ways.

1. They help the engineer understand the process and can be used in computer simulations of possible behaviour within the process, without having the expense or hazards involved in using a real process.

2. Simulations, based on models, can be used to train operators.

3. Different control strategies can be developed, tested and evaluated.

4. Using computer simulations, it may be possible to devise controller settings to ensure that start up of the real process is more controlled and less hazardous.

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5. The optimal operating conditions for a new or existing process can be determined, especially when the nature of the feed or required products change. For example, operations at a refinery where the crude feedstock may vary with supplier and the requirement for certain products varies with time of year (e.g. a lower requirement for heating oil in summer compared to winter).

For many of the reasons above, particularly when new processes are being developed, the production of a viable model is critical to the success of the operation. Models can be classified into three categories depending upon how they are developed:

- theoretical or fundamental models developed from theoretical principles of chemistry and physics

- empirical or experimental (practice) models based on the mathematical analysis of experimental or process operating data

- semi-empirical models that are a compromise combination of theory and practice.

In the last category, data such as heat transfer coefficients, reaction rates, etc. are usually evaluated from data obtained in practice. This offers several advantages over the purely theoretical models as, being real values, they often take account of factors that might have been missed in the theoretical model.

PRODUCING A MODEL

The steps in developing a model are:

- Preparation.

    – Decide what kind of model is needed. What scale? How detailed? How accurate? What features cannot be neglected? What assumptions can we make?

    – Define and sketch the system.

    – Select variables.

- Model Development.

    – Write balance equations (mass, component, energy) to describe the system.

    – Write constitutive (descriptive) equations (e.g. equations for transport, equilibrium, reaction kinetics) needed to implement the balance equations.

    – Obtain and analyse practical data (if required).

    – Check for consistency of units and independence of equations.

- Solution (Simulation).

    – Solve the equations (analytically or numerically).

    – Check and verify the solution.

    – Run simulation.

Fundamental models will emerge as a system of differential balance equations (ordinary differential equations – ODEs – or partial differential equations – PDEs) accompanied by a set of algebraic constitutive equations. Depending on the intended use, this model can be adapted in several ways:

- made steady-state (the time derivatives approach a zero value)

- linearised

  - differential equation form
  - transformed to transfer function form (e.g. using Laplace Transform).

This process in summarized in FIGURE 1 below which will be explained in more detail throughout this lesson and topic.
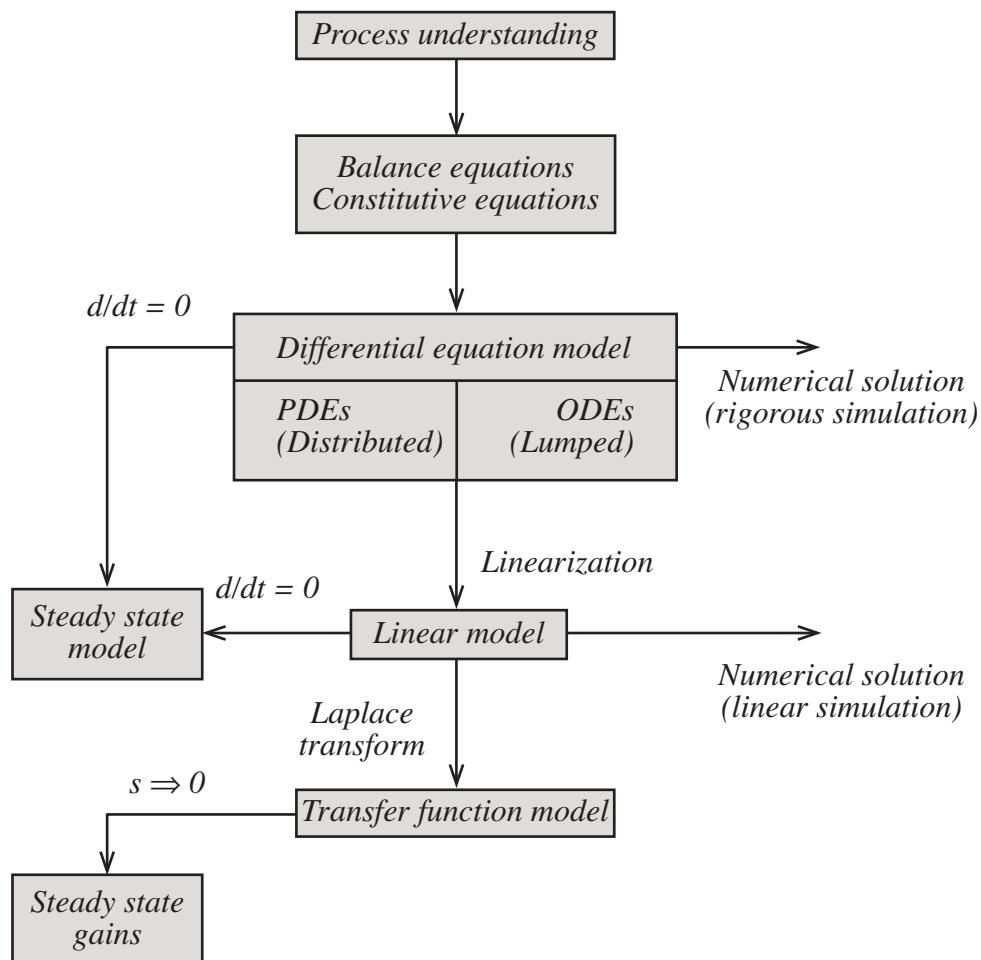

FIG. 1

When modelling, we often start by considering an unsteady state (or **dynamic**) model, as a steady state model can always be determined easily from the unsteady state model (though, as we have said previously, pure steady state processes do not actually exist but can be assumed with little inaccuracy in many cases).

BASIC MATHEMATICAL MODELLING EQUATIONS

Dynamic (non-steady state) models used for process modelling and control can be mathematically represented by a set of mass and energy balance equations (i.e. conservation of mass/energy equations).

Every dynamic model will include at least one balance equation. The balance equations will have a general form, which you may have met in other modules within the HNC course, i.e. for a given system

$$\text{mass in } = \text{ mass out } + \text{ accumulation}$$

$$\text{energy in } = \text{ energy out } + \text{ accumulation}$$

The accumulation term will be time dependent and thus involve a time derivative and thus produce a differential equation. The energy given to the surroundings is often ignored unless it is of significant value compared to the energy leaving the process in the flow out.

These balance equations may be supplemented by one or more constitutive equations that further define some of the terms in the balance equations.

CONSTITUTIVE EQUATIONS

All models will include one or more balance equations. Most will also use a set of *constitutive equations* to better define specific terms within the balance equations. Common constitutive relationships include:

- property relationships/equations of state

- transport flux relationships

- reaction rate expressions

- equilibrium expressions

- fluid flow relationships.

Property Relationships/Equations of State

Physical and thermodynamic properties (such as density, heat capacity, enthalpy, etc.) often vary with temperature, pressure, and composition. These relationships usually must be incorporated into dynamic models. For example, specific heat capacities may have values which change with temperature (T) according to equations of the form

$$C_{\mathrm{T}} \; = \; C_0 \; + \; aT \; + bT^2 \; + \; cT^3 \; + \; ....$$

where C_{T} is the specific heat capacity at temperature T

            C_0 is the specific heat capacity at temperature 0 (K or °C)

            T is temperature in K or °C

            a, b, c, etc. are constants for the given material.

Equations of state are typically used to express gas/vapour densities in terms of the system's temperature and pressure. Often, using the ideal gas equation is adequate, i.e.

$$\rho = \frac{pM_r}{RT}$$

where ρ = density (kg m^{-3})

p = absolute pressure (Pa)

M_r = relative molecular mass (kg kmol^{-1})

R is the ideal gas constant (J kmol^{-1} K^{-1})

and T is the absolute temperature (K).

Transport Flux Expressions

Transport flux expressions are usually used to quantify heat and mass transfer. When transport is purely molecular diffusion, these are nothing more than statements of Fick's law, Fourier's law, or Newton's law of viscosity. They then look like the one below for mass transfer by molecular diffusion:

$$N_A = -D_A \frac{dC_A}{dz}$$

where N_A = rate of molecular diffusion

D_A = diffusivity coefficient

C_A = concentration of A

z = distance.

When convective transport is significant, heat and mass transfer coefficients are typically used, leading to expressions like:

$$N_A \ = \ kA\mathrm{d}C_A$$

$$Q \ = \ hA\mathrm{d}T$$

where k and h are the mass transfer coefficient and heat transfer coefficient respectively.

Reaction Rate Expressions

The reaction rate expressions used in dynamic modelling are typically based on the principles of mass action. The **Arrhenius expression** must be incorporated directly when rate constants depend on temperature; otherwise, the energy balance won't adequately describe temperature changes. The Arrhenius expression for rate is:

$$r_A \ = \ k_0 e^{-\frac{E_A}{RT}} C_A$$

Equilibrium Expressions

Phase equilibrium expressions are often needed when modelling separation systems.

Chemical equilibrium expressions are needed less often. If they are needed, they are usually incorporated as part of the reaction rate expression.

Fluid Flow Relationships

Fluid flow relationships are typically used when it is necessary to relate pressure drop to flow rate. There are many equations for this and we will not cover these.

Let's look in more detail at how the basic and constitutive equations are obtained.

OVERALL MASS BALANCE

An overall mass balance is needed whenever you are interested in the 'hold-up' of a system. 'Hold-up' (accumulation/depletion) is typically measured in practice by using levels within vessels for liquid systems or pressures for gas/vapour systems.

A mass balance may be written over each system or subsystem that you can define within your process.

Constitutive equations may be needed to define system properties, such as density in terms of composition, temperature, pressure, etc.

As an example, let's consider a liquid storage tank as shown in FIGURE 2. We are going to do an overall mass balance over the tank.

Volumetric flow in,
$q_{vi}\ (m^3 s^{-1})$

V

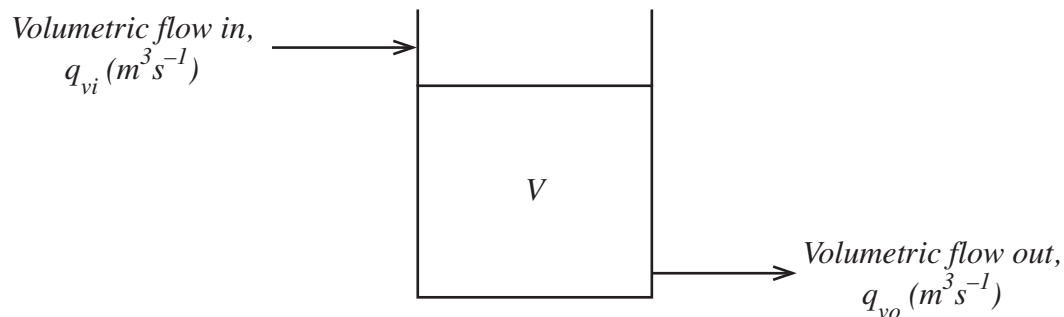*Volumetric flow out,*
$q_{vo}\ (m^3 s^{-1})$

FIG. 2

We cannot do a volume balance as the volume of a given mass of the material (density) may change. To do a mass balance we need to convert volume to mass.

$$\text{mass}\ (m)\ =\ \text{density}\ (\rho)\ \times\ \text{volume}\ (V)$$

and thus,   mass flow rate (q_m) = density (ρ) × volume flow rate (q_v)

If we let the subscripts $_i$ = input and $_o$ = output

Using the standard mass balance equation, over a given time period:

mass flow in = mass flow out + accumulation (the change in mass within the tank)

Note: accumulation can have a negative value (i.e. mass in tank can reduce).

For unit time,

$$\rho_i q_{vi} = \rho_o q_{vo} + \text{accumulation}$$

So the change in mass within the tank, with respect to time

$$= \frac{dm}{dt} = \frac{d\rho V}{dt} = \rho_i q_{vi} - \rho_o q_{vo}$$

where ρ is the average liquid density within the tank.

If the cross-sectional area of the tank is constant, the volume of liquid in the tank (V) can be determined as:

$$V = \text{cross-sectional area } (A) \text{ of the tank}$$
$$\times \text{ the height of liquid } (h) \text{ in the tank}$$

We can then determine just one process variable to represent this change in mass, i.e. the change in level of liquid in the tank.

Thus,
$$\frac{d\rho V}{dt} = \frac{Ad\rho h}{dt} = \rho_i q_{vi} - \rho_o q_{vo}$$

If the density of the liquid is constant i.e. $\rho_i = \rho_o = \rho$, then we can cancel by ρ and the final part of this equation can be simplified to:

$$\frac{A\,\mathrm{d}h}{\mathrm{d}t} = q_{vi} - q_{vo}$$

$$\text{or} \quad \frac{\mathrm{d}h}{\mathrm{d}t} = \frac{\left(q_{vi} - q_{vo}\right)}{A}$$

To obtain this equation, we have made the following assumptions, which are commonly made when compiling and simplifying mass balances.

1. Constant density of liquid (with respect to time) – true only if there is no change in temperature and no chemical reaction occurs.

2. Constant flow rates (with respect to time), i.e. the flow rates in and out do not fluctuate.

3. When dealing with mixtures of materials, there is perfect mixing so materials do not settle out due to density differences and thus we can use an average density to determine mass.

COMPONENT BALANCE (mass balance over individual components within a process)

Within most chemical processes it is usually the case that more than one chemical is present. A component balance must therefore be written whenever composition changes are to be examined. Thus almost all reactor or separator problems will involve a component balance. (Compositions are usually expressed in terms of mole fractions.)

If there is **no** reaction, then the balance equation for each component in the system is:

Rate of accumulation in mass of component in the system	=	Rate of mass flow of component into the system	–	Rate of mass flow of component out of the system

which has a form identical to the overall mass balance covered earlier.

With overall mass balance equations, however, it is immaterial whether reactions are occurring within the system; the total mass of all components will always remain the same. However, when components are present and reacting, the mass of individual components is not conserved. Components are both consumed and generated by chemical changes. Thus, to account for chemical reactions, the relevant expression to use when a component is reacting is:

Rate of accumulation in mass of component	=	Rate of mass flow of component into the system	–	Rate of mass flow of component out of the system	–	Rate of consumption of component by reaction

When a component is being formed, the last term becomes + rate of generation of component.

It should be borne in mind that a component balance can be written for each chemical species (component) in the system. Thus, if there are N components in a system, there could be N component balances. However, there is always only one overall mass balance equation for the system being considered. Since the sum of the individual masses of each component will give the total mass in the system, the component balances and the overall mass balance are related. Thus, it is sufficient to write $N - 1$ component balances and the overall mass balance, or N component balances and no overall balance to fully describe the mass flows within the system.

Initially, transport terms in a component balance will be expressed in terms of the component mass flow rates. Constitutive equations defining the component mass flow rates will thus be needed. When considering reactors (i.e. vessels where new components are formed as original components are used up), consumption and generation terms will be required and these will be written in terms of the constitutive equation for the reaction rate.

Let's look, as an example, at a constant stirred tank reactor (CSTR) with a simple irreversible reaction A $\rightarrow$ B occurring within it, as shown in FIGURE 3:
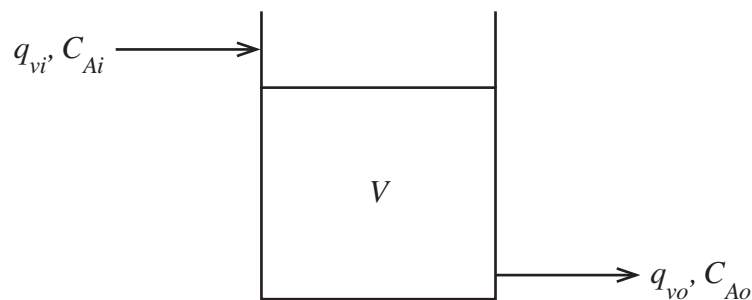
FIG. 3

NOTE: The 'constant' in constant stirred tank reactor is the liquid level (or volume) of the reactor.

The feed input consists of a mixture of components, with the concentration of component A being C_{Ai} moles m^{-3}. The overall flow rate entering is q_{vi} m^3 s^{-1}. The output rate is q_{vo} m^3 s^{-1} and the concentration of component A in the outlet is C_{Ao} moles m^{-3}. If we assume that the mixing is perfect within the tank then this outlet concentration will also be the concentration within the tank (C_A).

The rate of reaction per unit volume is given by

$$r = kC_A$$

where k is the reaction rate coefficient for component A with the units of s^{-1} and C_A = actual concentration of A in moles m^{-3} which will vary with time.

Typically, the rate coefficient k is strongly dependent upon temperature and can often be described by what is known as the **Arrhenius equation** as given by:

$$k = k_0 e^{\left(\frac{-E}{RT}\right)}$$

where k_0 is known as the frequency factor
            E is the activation energy for the reaction
            R is the gas constant
            T is the absolute temperature.

If we assume constant temperature then the reaction rate coefficient will be constant.

To convert moles to mass we need to multiply by the relative molecular mass of the component. Thus the mass of component A (in grams):

- entering, will be given by,

  $q_{vi}C_{Ai}M_{rA}$ (M_{rA} = relative molecular mass of component A in g mole^{-1})

- leaving, will be given by,

  $q_{vo}C_A M_{rA}$

- consumed by reaction, will be given by,

  $VkC_A M_{rA}$

- accumulating in the reactor, will be given by,

  $V\dfrac{dC_A}{dt}M_{rA}$

Since:

Rate of accumulation in mass of component A in		Rate of mass flow of component A into the system	−	Rate of mass flow of component A out of the system	−	Rate of consumption of component A by reaction
	=					

$$V\frac{dC_A}{dt}M_{rA} = q_{vi}C_{Ai}M_{rA} - q_{vo}C_A M_{rA} - VkC_A M_{rA}$$

$$\text{or} \quad V\frac{dC_A}{dt} = q_{vi}C_{Ai} - q_{vo}C_A - VkC_A$$

If the volumetric flow rates in and out are the same, $q_{vi} = q_{vo}$, (constant level in the tank) and there is constant temperature, there is no volumetric hold-up in the reactor (V is constant) and the equation simplifies to:

$$V\frac{dC_A}{dt} = q_v\left(C_{Ai} - C_A\right) - VkC_A$$

ENERGY BALANCE (enthalpy balance)

We will need to write an energy balance whenever the temperature within the system changes; temperature will almost always be inside the derivative term. The use of different reference temperatures for different types of enthalpy can complicate things, so we must be careful (e.g. reaction enthalpies are usually relative to 25°C whilst material enthalpies are referenced to 0°C).

An energy balance can be written for each separable system or subsystem.

In lesson PC - 1 - 1 we looked at the example of a heated, stirred tank, as shown in FIGURE 4 overleaf, to introduce the basics of process control and help define some of the terminology used in control theory.

In that case, the following process conditions were considered constant:

- input temperature (T_i)
- specific heat capacity of liquid (C)
- volume of liquid in tank (V)
- density of liquid (ρ)
- mass flow in = mass flow out (q_m)
- actual heat input (Q)

and we had perfect mixing and no heat lost to the surroundings. We had what is known as a steady-state process. We derived an expression for the amount of heat supplied in terms of the outlet temperature produced.
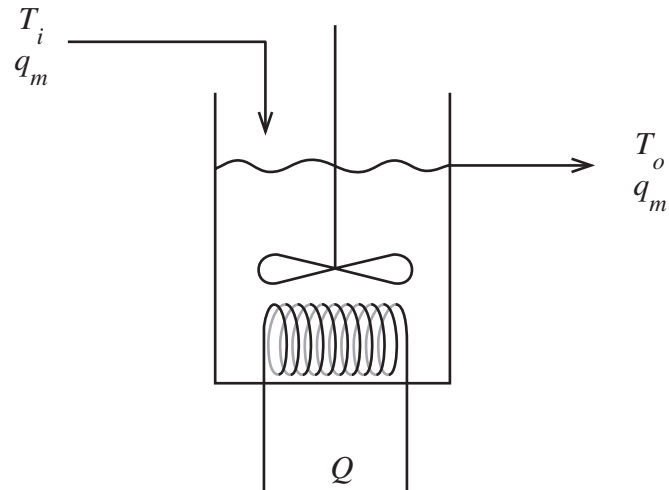
FIG. 4

Can you give the equation which links the heat input (Q) to the outlet temperature (T_o) under these 'steady state' conditions (we developed this in lesson PC - 1 - 1)?

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$$Q = q_m C(T_o - T_i)$$

A dynamic (unsteady state) energy balance of this process could differ from the steady state if q_{mi} and q_{mo} are made different values and hence a consumption/accumulation term is required (see FIGURE 5).
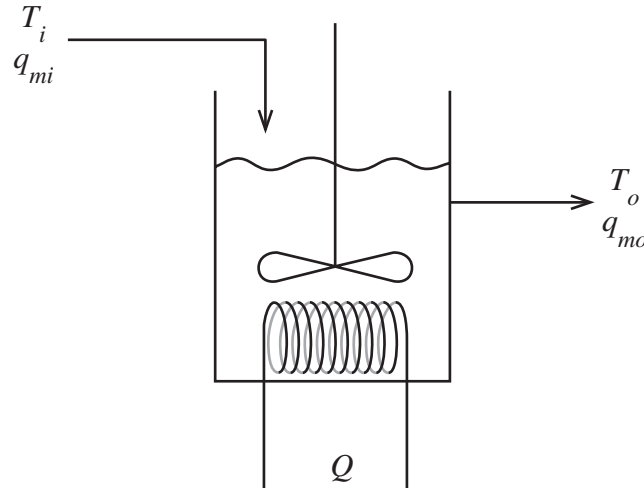
FIG. 5

The rate of energy accumulation

$$= q_{mi} C_i \left(T_i - T_{ref} \right) - q_{mo} C_o \left(T_o - T_{ref} \right) + Q$$

The rate of energy accumulation is also given by:

the rate of change of mass in vessel $\times$ the contents' specific heat capacity

$\times$ temperature change within the contents of the vessel

$$= \mathrm{d}m C \Delta T$$

or since mass (m) = volume(V) $\times$ density (ρ) of the contents

the rate of energy accumulation $= \dfrac{\mathrm{d}V \rho C \left(T - T_{ref} \right)}{\mathrm{d}t}$

Thus, equating the two equations

$$\frac{\mathrm{d}V\rho C\left(T - T_{\mathrm{ref}}\right)}{\mathrm{d}t} = q_{\mathrm{mi}}C_{\mathrm{i}}\left(T_{\mathrm{i}} - T_{\mathrm{ref}}\right) - q_{\mathrm{mo}}C_{\mathrm{o}}\left(T_{\mathrm{o}} - T_{\mathrm{ref}}\right) + Q$$

Energy transport fluxes and thermodynamic property relationships may require constitutive equations for fuller definition and more accurate modelling. For example, heat transfer rates may be given by $Q = UA\Delta T$ (U = overall heat transfer coefficient, A = area over which heat transfer occurs and ΔT is the temperature difference between the heater and the tank contents); density is a function of temperature ($\rho = f(T)$; specific heat capacities (C) may have values which change with temperature according to equations of the form $C_{\mathrm{T}} = C_0 + \mathrm{a}T + \mathrm{b}T^2 + \ldots$, etc.

Modelling assumptions which can be made to simplify this example include:

1.   perfect mixing (so $T = T_{\mathrm{o}}$)

2.   constant specific heat capacities ($C = C_{\mathrm{i}} = C_{\mathrm{o}}$)

3.   constant heat supply (Q)

4.   constant density

5.   constant volume in tank so that $\mathrm{d}V/\mathrm{d}t = 0$ and thus $q_{\mathrm{mi}} = q_{\mathrm{mo}} = q_{\mathrm{m}}$ which would then result in the equation becoming

$$0 = q_{\mathrm{m}}\left(T_{\mathrm{i}} - T_{\mathrm{o}}\right) + Q$$

or $Q = q_{\mathrm{m}}C\left(T_{\mathrm{o}} - T_{\mathrm{i}}\right)$ the steady state equation for the system.

Let's return to this example but this time create the unsteady state by varying the heat input via an electric heater whilst keeping the input and output mass flow rates equal, so there is no "hold-up" in the tank (see FIGURE 6) and therefore the mass of liquid in the tank is constant. If the density is constant then the volume within the tank is constant. Assuming that perfect mixing occurs within the tank then the outlet temperature T_o is equal to the temperature of the tank contents (T). Finally, for completeness we will also assume for simplicity that the heating of the tank itself and heat losses to atmosphere are minimal.

Let's suppose that the electrical heater has a significant thermal capacitance and that by varying the heat input the heating element's temperature (T_e) changes directly rather than the temperature of the tank contents.
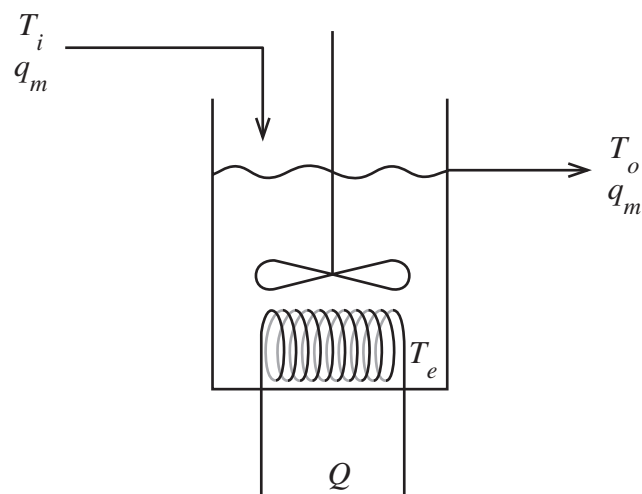

FIG. 6

From our knowledge of heat transfer, the heat actually transferred from the element to the contents $= hA(T_e - T)$, where h = film heat transfer coefficient for the element and A = area of element.

The heat content of the tank contents will change according to the equation $mC\dfrac{\mathrm{d}T}{\mathrm{d}t}$, where m = mass of tank contents, C = specific heat capacity of tank contents and $\dfrac{\mathrm{d}T}{\mathrm{d}t}$ is the rate of change of the tank contents' temperature with time. This will depend upon the heat content of the inlet flow relative to the tank temperature, $q_{\mathrm{m}}C(T_{\mathrm{i}} - T)$, and the heat transferred from the element, so that

$$mC\frac{\mathrm{d}T}{\mathrm{d}t} = q_{\mathrm{m}}C\big(T_{\mathrm{i}} - T\big) - hA\big(T_{\mathrm{e}} - T\big) \quad \text{............... (1)}$$

The change in heat content of the heating element with respect to time

$$= m_{\mathrm{e}}C_{\mathrm{e}}\frac{\mathrm{d}T_{\mathrm{e}}}{\mathrm{d}t}$$

where $\quad m_{\mathrm{e}}$ = mass of heating element
$\qquad\quad C_{\mathrm{e}}$ = specific heat capacity of heating element
$\qquad\quad \dfrac{\mathrm{d}T_{\mathrm{e}}}{\mathrm{d}t}$ = rate of change of heating element temperature with time.

If the heat actually supplied to the heating element is Q then the change in heat content of the element will be the difference between the heat added to the element and the heat lost by the element, i.e.

$$m_{\mathrm{e}}C_{\mathrm{e}}\frac{\mathrm{d}T_{\mathrm{e}}}{\mathrm{d}t} = Q - hA\big(T_{\mathrm{e}} - T\big) \quad \text{.................................. (2)}$$

Could we calculate the values of T_e and T from these two equations? How? The answer is in the text that follows.

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We want to calculate two unknowns (T_e and T) and we have two equations. In theory we should therefore be able to calculate the unknowns provided all the other terms in the equations are either constants or can be measured. For a specific set-up then m, m_e, C, C_e, h and A are known values related to the design of the tank and the heating element. The only other values required are for q_m, T_i and Q and these must be specified (or measured) as functions of time to enable the equations to be solved.

The model can then be solved for T and T_e as functions of time by integration between limits of the differential equations, provided the initial conditions of T and T_e are specified.

DEGREES OF FREEDOM IN MODELLING

To use a mathematical model for process simulation we must ensure that the model equations (differential and algebraic) provide a unique solution for different inputs and outputs. This is similar to the requirement that for a set of simultaneous equations to have a unique solution, the number of variables must equal the number of independent equations. It is not easy to make a similar evaluation for a large complicated steady state or dynamic model. However, for such a system of equations to have a unique solution, the number of unknown variables must equal the number of independent model equations. This is more conveniently stated as the degrees of freedom (N_f) of the system should be zero where:

$$N_f = N_v - N_E$$

where N_v = number of variables (unspecified inputs and outputs)
and N_E = number of independent equations (differential and algebraic).

If we carry out a degree of freedom analysis, three possible outcomes are possible.

1. $N_f = 0$: an exactly specified process as the number of equations = number of variables and thus a unique solution is possible. This is the only satisfactory case.

2. $N_f > 0$: an under specified process as the number of equations < number of variables and a unique solution is not possible. Additional independent equations are required to solve the problem or some of the variables must be re-specified as constants.

3. $N_f < 0$: an over specified process as the number of equations > number of variables and either additional variables may need to be identified or the independence of the equations should be checked.

To conclude this lesson we can summarise the steps required to obtain dynamic models as follows.

1. Draw a schematic diagram of the process and label all process variables.

2. List all assumptions to be used in developing the model. Try to make the model as simple as possible by using assumptions to minimise complexity (e.g. assume density is constant if the temperature change in a liquid is going to be small).

3. Write appropriate balance equations (overall mass, component, energy).

4. Introduce any constitutive equations (thermodynamic properties, reaction, etc.).

5. Identify the system parameters (constants).

6. Identify the model variables.

7. Determine the degrees of freedom.

8. If necessary, specify which inputs are to be fixed to reduce the number of degrees of freedom to 0.

9. If possible, solve the equations for the remaining variables. If this is not possible go back to Step 2 and try a simpler model.

You have now completed this lesson. Attempt the Self-Assessment Questions which follow to test your understanding of the content.

1. (a) What are the three main balance equations used in modelling simple chemical processes where no reaction occurs?

   (b) How would these be modified to produce model equations when a chemical reaction occurs?

2. Explain what is meant by constitutive equations, giving two examples.

3. In the diagram opposite, the contents of the tank are heated by dry saturated steam which is passed through a heating coil immersed in the liquid within the tank. The steam pressure is adjusted by a control valve. The pressure of steam controls the condensing temperature (T_s) within the coil, i.e. T_s is a function of pressure.

   The heat released by the steam at temperature T_s in the coil is transferred through the condensate film at the coil wall, which will then have a temperature T_w. The coil wall itself will present no resistance to heat transfer. The heat transferred through the coil wall will pass through the liquid film on the outside of the coil to the contents of the tank which heat up to a temperature T.

   (a) List other assumptions you are going to make when thinking about producing the model.

   (b) Produce the three equations which will model this process for the three variables T_s, T_w and T.

Steam in   Condensate out

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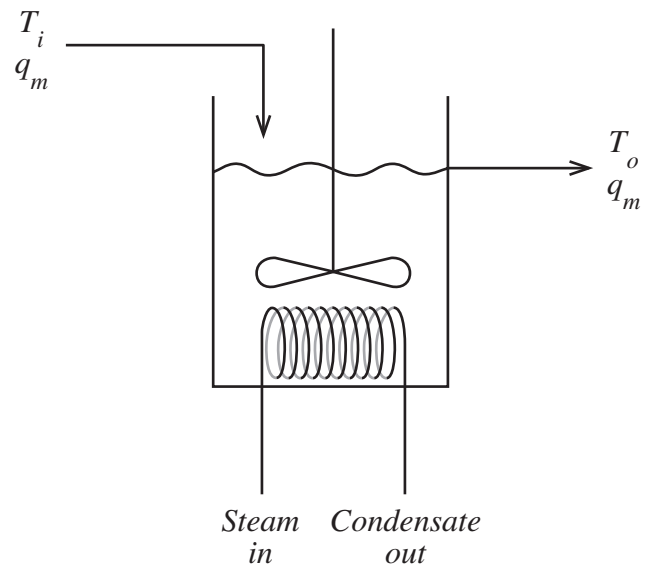
ANSWERS TO SELF-ASSESSMENT QUESTIONS

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1.   (a) Overall Mass balance

mass in = mass out + accumulation

Component Mass balance

mass of A in = mass of A out + accumulation

Energy balance

energy in = energy out + accumulation

– energy given to the surroundings

(b) The component mass balances would become

Rate of accumulation of mass of component A in the system		Rate of mass flow of component A into the system	Rate of mass flow of component A out of the system	Rate of consumption of component A by reaction
	=		–	–

Energy balance:

accumulation = energy in – energy out

– energy given to the surroundings

± energy of reaction

2. **Constitutive equations** better define specific terms within the balance equations.

For example:

Specific heat capacity C varies with temperature using relationships of the type

$$C_\mathrm{T} \;=\; C_0 \;+\; aT \;+\; bT^2 \;+\; cT^3 \;+\; \dots\dots\dots\dots$$

where C_T is the specific heat capacity at temperature T

$\quad\;\; C_0$ is the specific heat capacity at temperature 0 (K or °C)

$\quad\;\; T$ is temperature in K or °C

$\quad\;\; a, b, c \dots$ are constants for the given material.

Density of a gas can be determined using the ideal gas equation, i.e.

$$\rho \;=\; \frac{pM_\mathrm{r}}{RT}$$

Other examples mentioned in the lesson are:

- transport flux relationships

- reaction rate expressions

- equilibrium expressions

- fluid flow relationships.

3. (a) Assumptions to be made should include (depending on your knowledge of heat transfer you may not have got all of these).

- Flow in = flow out and constant density of liquid so that the mass within the tank is constant.

- T_i is constant.

- Perfect mixing so $T_o = T$.

- No heat loss to the surroundings.

- The thermal capacity of the condensate is 0 (this will be true if a steam trap is used to continuously remove the condensate).

- Specific heat capacities of the coil material and the liquid contents are constant.

(b) You are given that temperature T_s is a function of pressure. You are not given the actual relationship but can use the general expression

$$T_s = f(p_s)$$

where f = function of
and p_s = pressure of steam.

This is your first equation.

The temperature of the wall will vary with the amount of heat transferred to it from the steam through the condensate film on the inside of the coil and the amount of heat the wall transfers to the

contents through the liquid film on the outside of the coil. It will also depend on the mass of the coil and the specific heat capacity of the material it is constructed from. Thus an energy balance over the coil will give:

increase in heat content of coil wall $=$ heat supplied to the wall
$-$ heat lost by the wall

$$\therefore \quad m_c C_c \frac{dT_w}{dt} = h_s A_s \left(T_s - T_w \right) - h_L A_L \left(T_w - T \right)$$

where h_s $=$ film heat transfer coefficient on steam side
A_s $=$ area for heat transfer on steam side
h_L $=$ film heat transfer coefficient on liquid side
A_L $=$ area for heat transfer on liquid side.

This is the second equation.

The increase in temperature of the tank contents will be governed by the difference between the heat entering in the feed and heat leaving in the product and the heat supplied by the coil. It will also depend upon the mass of the tank contents and the specific heat capacity of the liquid contents.

Thus a heat balance over the tank contents will give

increase in heat content of contents $=$ heat difference between
inlet and outlet
$+$ heat supplied from the
coil wall

We assumed that perfect mixing gives $T_o = T$ and also that $q_{mi} = q_{mo} = q_m$

So
$$m_L C_L \frac{dT}{dt} = q_m C (T_i - T) + h_L A_L (T_w - T)$$

This is the third equation.

Three equations, 3 unknowns; we have no degrees of freedom and the model is therefore specified.

SUMMARY

Process modelling is important in determining correct operating procedures and in designing control systems for complex processes, though in this lesson we have dealt only with relatively simple processes.

The dynamic (non-steady state) models used for process modelling and control can be mathematically represented by a set of mass and energy balance equations (conservation of mass/energy equations) and constitutive equations, which better define specific terms within the balance equations.

Several examples of simple models for processes using either mass or energy balances or both were devised within the lesson.

The degrees of freedon (N_f) of the model is given by:

$$N_f \; = \; N_v \; - \; N_E$$

where N_v =   number of variables (unspecified inputs and outputs)
and N_E =   number of independent equations (differential and algebraic).

If we carry out a degree of freedom analysis, the only satisfactory state for solving the model is when $N_f = 0$, i.e. the number of equations = number of variables. This will enable a unique solution to the model.

The process for determining a dynamic models is as follows.

1. Draw a schematic diagram of the process and label all process variables.

2. List all assumptions to be used in developing the model. Try to make the model as simple as possible by using assumptions to minimise complexity (e.g. assume density is constant if the temperature change in a liquid is going to be small).

3. Write appropriate balance equations (overall mass, component, energy).

4. Introduce any constitutive equations (thermodynamic properties, reaction, etc.).

5. Identify the system parameters (constants).

6. Identify the model variables.

7. Determine the degrees of freedom.

8. If necessary, specify which inputs are to be fixed to reduce the number of degrees of freedom to 0.

9. If possible, solve the equations for the remaining variables. If this is not possible go back to Step 2 and try a simpler model.