Ordinary Differential Equations-Introduction

Differential equation

- An equation relating a dependent variable to one or more independent variables by means of its differential coefficients with respect to the independent variables is called a “differential equation”.

$$\frac{d^3y}{dx^3} - \left(\frac{dy}{dx}\right)^2 + 4y = 4e^x \cos x$$

$$\rho C_p \frac{\partial T}{\partial \theta} = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right)$$

Order and degree

- The order of a differential equation is equal to the order of the highest differential coefficient that it contains.
- The degree of a differential equation is the highest power of the highest order differential coefficient that the equation contains after it has been rationalized.

$$\frac{d^3y}{dx^3} - \left(\frac{dy}{dx}\right)^2 + 4y = 4e^x \cos x$$

3rd order O.D.E.

1st degree O.D.E.

Linear or non-linear

- Differential equations are said to be non-linear if any products exist between the dependent variable and its derivatives, or between the derivatives themselves.

$$\frac{d^3y}{dx^3} - \boxed{\left(\frac{dy}{dx}\right)^2} + 4y = 4e^x \cos x$$

Product between two derivatives ---- non-linear

$$\frac{dy}{dx} + 4\boxed{y^2} = \cos x$$

Product between the dependent variable themselves ---- non-linear

First order differential equations

- No general method of solutions of 1st ODEs because of their different degrees of complexity.
- Possible to classify them as:
  - exact equations
  - equations in which the variables can be separated
  - homogenous equations
  - equations solvable by an integrating factor
- First order linear differential equations occasionally arise in chemical engineering problems in the field of heat transfer, momentum transfer and mass transfer.

Separable-variables equations

- In the most simple first order differential equations, the independent variable and its differential can be separated from the dependent variable and its differential by the equality sign, using nothing more than the normal processes of elementary algebra.

$$y\frac{dy}{dx} = \sin x$$

Homogeneous equations

- Homogeneous/nearly homogeneous?
- A differential equation of the type, $\frac{dy}{dx} = f\left(\frac{y}{x}\right)$

  is termed a homogeneous differential equation of *the first order*.
- Such an equation can be solved by making the substitution $u = y/x$ and thereafter integrating the transformed equation.

Homogeneous equation example

- Liquid benzene is to be chlorinated batchwise by sparging chlorine gas into a reaction kettle containing the benzene. If the reactor contains such an efficient agitator that all the chlorine which enters the reactor undergoes chemical reaction, and only the hydrogen chloride gas liberated escapes from the vessel, estimate how much chlorine must be added to give the maximum yield of monochlorbenzene. The reaction is assumed to take place isothermally at 55 ºC when the ratios of the specific reaction rate constants are:

$$\begin{aligned}
&C_6H_6 + Cl_2 \rightarrow C_6H_5Cl + HCl\\
&C_6H_5Cl + Cl_2 \rightarrow C_6H_4Cl_2 + HCl\\
&C_6H_4Cl_2 + Cl_2 \rightarrow C_6H_3Cl_3 + HCl
\end{aligned}$$

Homogeneous equation example

Take a basis of 1 mole of benzene fed to the reactor and introduce the following variables to represent the stage of system at time θ,

p = moles of chlorine present
q = moles of benzene present
r = moles of monochlorbenzene present
s = moles of dichlorbenzene present
t = moles of trichlorbenzene present

Then q + r + s + t = 1
and the total amount of chlorine consumed is: y = r + 2s + 3t
From the material balances : *in - out = accumulation*

$$0 - k_1 pq = V\frac{dq}{d\theta}$$

$$k_1 pq - k_2 pr = V\frac{dr}{d\theta}$$

$$k_2 pr - k_3 ps = V\frac{ds}{d\theta}$$

$$k_3 ps = V\frac{dt}{d\theta}$$

$u = r/q$

$$\frac{dr}{dq} = \frac{k_2}{k_1}\left(\frac{r}{q}\right) - 1$$

Derivatives

Derivatives

Ordinary Derivatives

$$\frac{dv}{dt}$$

v is a function of one independent variable

Partial Derivatives

$$\frac{\partial u}{\partial y}$$

u is a function of more than one independent variable

Differential Equations

Differential Equations

Ordinary Differential Equations

$$\frac{d^2v}{dt^2} + 6tv = 1$$

involve one or more Ordinary derivatives of unknown functions

Partial Differential Equations

$$\frac{\partial^2 u}{\partial y^2} - \frac{\partial^2 u}{\partial x^2} = 0$$

involve one or more partial derivatives of unknown functions

Ordinary Differential Equations

Ordinary Differential Equations (ODE) involve one or more ordinary derivatives of unknown functions with respect to one independent variable

Examples:

$$\frac{dv(t)}{dt} - v(t) = e^t$$

$$\frac{d^2x(t)}{dt^2} - 5\frac{dx(t)}{dt} + 2x(t) = \cos(t)$$

x(t): unknown function

t: independent variable

Ordinary Differential Equations

Ordinary Differential Equations (ODE) involve one or more ordinary derivatives of unknown functions with respect to one independent variable

$$\frac{dv}{dt} = 9.8 - \frac{c}{M} v$$

(Dependent variable) unknown function to be determined

(independent variable) the variable with respect to which other variables are differentiated

Order of a Ordinary Differential Equation

The **order** of an ordinary differential equations is the order of the highest order derivative

Examples :

$$\frac{dx(t)}{dt} - x(t) = e^t$$ First order ODE

$$\frac{d^2x(t)}{dt^2} - 5\frac{dx(t)}{dt} + 2x(t) = \cos(t)$$ Second order ODE

$$\left(\frac{d^2x(t)}{dt^2}\right)^3 - \frac{dx(t)}{dt} + 2x^4(t) = 1$$ Second order ODE

Linear ODE

An ODE is linear if
The unknown function and its derivatives appear to power one
No product of the unknown function and/or its derivatives

Examples :

$$\frac{dx(t)}{dt} - x(t) = e^t$$ Linear ODE

$$\frac{d^2x(t)}{dt^2} - 5\frac{dx(t)}{dt} + 2t^2x(t) = \cos(t)$$ Linear ODE

$$\left(\frac{d^2x(t)}{dt^2}\right)^3 - \frac{dx(t)}{dt} + \sqrt{x(t)} = 1$$ Non-linear ODE

Non-Linear ODE

An ODE is linear if
The unknown function and its derivatives appear to power one
No product of the unknown function and/or its derivatives

Examples of nonlinear ODE :

$$\frac{dx(t)}{dt} - \cos(x(t)) = 1$$

$$\frac{d^2x(t)}{dt^2} - 5\frac{dx(t)}{dt}x(t) = 2$$

$$\frac{d^2x(t)}{dt^2} - \left|\frac{dx(t)}{dt}\right| + x(t) = 1$$

First ODE in heat transfer

An elevated horizontal cylindrical tank 1 m diameter and 2 m long is insulated with asbestos lagging of thickness l = 4 cm, and is employed as a maturing vessel for a batch chemical process. Liquid at 95 C is charged into the tank and allowed to mature over 5 days. If the data below applies, calculated the final temperature of the liquid and give a plot of the liquid temperature as a function of time.

Liquid film coefficient of heat transfer (h_1)	= 150 W/m²C
Thermal conductivity of asbestos (k)	= 0.2 W/m C
Surface coefficient of heat transfer by convection and radiation (h_2)	= 10 W/m²C
Density of liquid (ρ)	= 10^3 kg/m³
Heat capacity of liquid (s)	= 2500 J/kgC
Atmospheric temperature at time of charging	= 20 C
Atmospheric temperature (t)	t = 10 + 10 cos (πθ/12)
Time in hours (θ)	

Heat loss through supports is negligible. The thermal capacity of the lagging can be ignored.

First ODE in heat transfer

Area of tank (A) = (π x 1 x 2) + 2 (1 / 4 π x 1²) = 2.5π m²

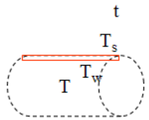
Rate of heat loss by liquid = h_1 A (T - T_w)
Rate of heat loss through lagging = kA/l (T_w - T_s)
Rate of heat loss from the exposed surface of the lagging = h_2 A (T_s - t)

At steady state, the three rates are equal:

$$h_1 A(T - T_w) = \frac{kA}{l}(T_w - T_s) = h_2 A(T_s - t) \implies T_s = 0.326\,T + 0.674\,t$$

Considering the thermal equilibrium of the liquid,

$$\textit{input rate - output rate = accumulation rate} \implies 0 - h_2 A(T_s - t) = V\rho s\,\frac{dT}{d\theta}$$



$$\boxed{\frac{dT}{d\theta} + 0.0235T = 0.235 + 0.235\cos(\pi\theta/12)}$$

B.C. θ = 0 , T = 95

Second ODE

- Likely to be reduced equations:
  - Non-linear
    - Equations where the dependent variable does not occur explicitly.
    - Equations where the independent variable does not occur explicitly.
    - Homogeneous equations.
  - Linear
    - The coefficients in the equation are constant
    - The coefficients are functions of the independent variable.

Second ODE

A graphite electrode 15 cm in diameter passes through a furnace wall into a water cooler which takes the form of a water sleeve. The length of the electrode between the outside of the furnace wall and its entry into the cooling jacket is 30 cm; and as a safety precaution the electrode in insulated thermally and electrically in this section, so that the outside furnace temperature of the insulation does not exceed 50 C.
If the lagging is of uniform thickness and the mean overall coefficient of heat transfer from the electrode to the surrounding atmosphere is taken to be 1.7 W/C m² of surface of electrode; and the temperature of the electrode just outside the furnace is 1500 C, estimate the duty of the water cooler if the temperature of the electrode at the entrance to the cooler is to be 150 C.
The following additional information is given.

Surrounding temperature	= 20 C
Thermal conductivity of graphite	$k_T = k_0 - \alpha T$ = 152.6 - 0.056 T W/m C

The temperature of the electrode may be assumed uniform at any cross-section.

Second ODE

The sectional area of the electrode A = 1/4 π x 0.15^2 = 0.0177 m^2

A heat balance over the length of electrode δx at distance x from the furnace is

input - output = accumulation

$$\left(-k_T A\frac{dT}{dx}\right)-\left(-k_T A\frac{dT}{dx}+\frac{d}{dx}(-k_T A\frac{dT}{dx})\delta x+\pi DU(T-T_0)\delta x\right)=0$$

where U = overall heat transfer coefficient from the electrode to the surroundings
D = electrode diameter

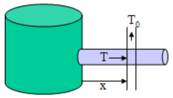
$$\frac{d}{dx}\left(\boxed{k_T}\frac{dT}{dx}\right)\delta x=\boxed{\frac{\pi DU}{A}}(T-T_0)\delta x \Rightarrow \frac{d}{dx}\left((k_0-\alpha T)\frac{dT}{dx}\right)-\beta(T-T_0)=0$$

$$\downarrow$$

$$(k_0-\alpha T)\frac{d^2T}{dx^2}-\alpha\left(\frac{dT}{dx}\right)^2-\beta(T-T_0)=0$$

$$p=\frac{dT}{dx} \quad \downarrow \quad p\frac{dp}{dT}=\frac{d^2T}{dx^2}$$

$$(k_0-\alpha T)p\frac{dp}{dT}-\alpha p^2-\beta(T-T_0)=0$$



Second ODE

$$(k_0-\alpha T)p\frac{dp}{dT}-\alpha p^2-\beta(T-T_0)=0$$

$$p^2=z \qquad y=(T-T_0)$$

$$[(k_0-\alpha T)-\alpha y]\frac{dz}{dy}-2\alpha z-2\beta y=0$$

Integrating factor $\exp\left(-\int\frac{2\alpha dy}{k_0-\alpha T_0-\alpha y}\right)=(k_0-\alpha T_0-\alpha y)^2$

$$\boxed{x=\int\frac{(k_0-\alpha T)dT}{\sqrt{[C+\beta(k_0-\alpha T)(T-T_0)^2-2/3\,\alpha\beta(T-T_0)^3]}}}$$

Linear differential equations

- They are frequently encountered in most chemical engineering fields of study, ranging from heat, mass, and momentum transfer to applied chemical reaction kinetics.
- The general linear differential equation of the nth order having constant coefficients may be written:

$$P_0\frac{d^n y}{dx^n}+P_1\frac{d^{n-1}y}{dx^{n-1}}+\ldots+P_{n-1}\frac{dy}{dx}+P_n y=\phi(x)$$

2^{nd} order linear differential equations

The general equation can be expressed in the form

$$P\frac{d^2y}{dx^2}+Q\frac{dy}{dx}+Ry=\phi(x)$$

where P,Q, and R are constant coefficients

Let the dependent variable y be replaced by the sum of the two new variables: $y=u+v$

Therefore

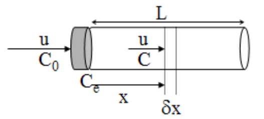
$$\left[P\frac{d^2u}{dx^2}+Q\frac{du}{dx}+Ru\right]+\boxed{\left[P\frac{d^2v}{dx^2}+Q\frac{dv}{dx}+Rv\right]=\phi(x)}$$

If v is a particular solution of the original differential equation

$$\left[P\frac{d^2u}{dx^2}+Q\frac{du}{dx}+Ru\right]=0$$

ODE in Chemical Engineering

- A tubular reactor of length L and 1 m^2 in cross section is employed to carry out a first order chemical reaction in which a material A is converted to a product B,
- The specific reaction rate constant is k s^{-1}. If the feed rate is u m^3/s, the feed concentration of A is C_o, and the diffusivity of A is assumed to be constant at D m^2/s. Determine the concentration of A as a function of length along the reactor. It is assumed that there is no volume change during the reaction, and that steady state conditions are established.



The concentration will vary in the entry section due to diffusion, but will not vary in the section following the reactor. (Wehner and Wilhelm, 1956)

→ section

	x	$x+\delta x$
Bulk flow of A	uC	$uC + u\dfrac{dC}{dx}\delta x$
Diffusion of A	$-D\dfrac{dC}{dx}$	$-D\dfrac{dC}{dx} + \dfrac{d}{dx}\left(-D\dfrac{dC}{dx}\right)\delta x$

A material balance can be taken over the element of length δx at a distance x form the inlet

Input - Output + Generation = ~~Accumulation~~

$$\left[(uC)+\left(-D\frac{dC}{dx}\right)\right]-\left[\left(uC+u\frac{dC}{dx}\delta x\right)+\left(-D\frac{dC}{dx}+\frac{d}{dx}\left(-D\frac{dC}{dx}\right)\delta x\right)\right]-kC\delta x=0$$

$$\left[(\cancel{uC})+\left(-D\cancel{\frac{dC}{dx}}\right)\right]-\left[\left(\cancel{uC}+u\frac{dC}{dx}\delta x\right)+\left(-D\cancel{\frac{dC}{dx}}+\frac{d}{dx}\left(-D\frac{dC}{dx}\right)\delta x\right)\right]-kC\delta x=0$$

$\downarrow$ dividing by δx

$$-\left[\left(u\frac{dC}{dx}\right)+\left(\frac{d}{dx}\left(-D\frac{dC}{dx}\right)\right)\right]-kC=0$$

$\downarrow$ rearranging

$$D\frac{d^2C}{dx^2}-u\frac{dC}{dx}-kC=0 \xrightarrow{\text{In the entry section}} D\frac{d^2\hat{C}}{dx^2}-u\frac{d\hat{C}}{dx}=0$$

$\downarrow$ auxillary function (both)

$$Dm^2-um-k=0 \qquad\qquad Dm^2-um=0$$

$$\downarrow \qquad\qquad \downarrow$$

$$C=A\exp\left[\frac{ux}{2D}(1+a)\right]+B\exp\left[\frac{ux}{2D}(1-a)\right] \qquad\qquad \hat{C}=\alpha+\beta\exp\left[\frac{ux}{D}\right]$$

$$a=\sqrt{\left(1+4kD/u^2\right)}$$

$$C=A\exp\left[\frac{ux}{2D}(1+a)\right]+B\exp\left[\frac{ux}{2D}(1-a)\right] \qquad\qquad \hat{C}=\alpha+\beta\exp\left[\frac{ux}{D}\right]$$

$\downarrow$ B. C. $\qquad\qquad$ $\downarrow$ B. C.

$$x=0 \quad \frac{dC}{dx}=\frac{d\hat{C}}{dx} \qquad\qquad x=-\infty \quad \hat{C}=C_0$$

$$x=L \quad \frac{dC}{dx}=0 \qquad\qquad x=0 \quad \hat{C}=C$$

$$\frac{C}{C_0}=\frac{2}{K}\exp\left(\frac{ux}{2D}\right)\left\{(a+1)\exp\left[\frac{ua}{2D}(L-x)\right]+(a-1)\exp\left[-\frac{ua}{2D}(L-x)\right]\right\}$$

$$K=(a+1)^2\exp(uLa/2D)-(a-1)^2\exp(-uLa/2D)$$

if diffusion is neglected (D→0) $\rightarrow$ $$\frac{C_0-C}{C_0}=1-\exp\left(\frac{-kx}{u}\right)$$

Simultaneous differential equations

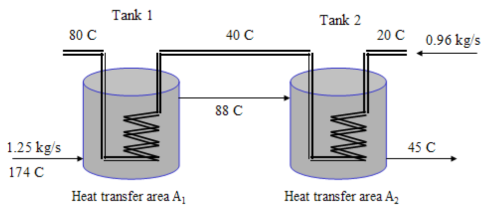
- These are groups of differential equations containing more than one dependent variable but only one independent variable.
- In these equations, all the derivatives of the different dependent variables are with respect to the one independent variable.

Use algebraic elimination of the variables until only one differential equation relating two of the variables remains.

Example of simultaneous differential equations

1.25 kg/s of sulphuric acid (heat capacity 1500 J/kg °C) is to be cooled in a two-stage counter-current cooler of the following type. Hot acid at 174 °C is fed to a tank where it is well stirred in contact with cooling coils. The continuous discharge from this tank at 88 °C flows to a second stirred tank and leaves at 45 °C. Cooling water at 20 °C flows into the coil of the second tank and thence to the coil of the first tank. The water is at 80 °C as it leaves the coil of the hot acid tank. To what temperatures would the contents of each tank rise if due to trouble in the supply, the cooling water suddenly stopped for 1h?

On restoration of the water supply, water is put on the system at the rate of 1.25 kg/s. Calculate the acid discharge temperature after 1 h. The capacity of each tank is 4500 kg of acid and the overall coefficient of heat transfer in the hot tank is 1150 W/m^2 °C and in the colder tank 750 W/m^2 °C. These constants may be assumed constant.



Steady state calculation:

Heat capacity of water 4200 J/kg C

$$1.25\times1500\times(174-45)=F_{water}\times4200\times(80-20) \longrightarrow F_{water}=0.96kg/s$$

$$1.25\times1500\times(88-45)=0.96\times4200\times(T_{middle}-20) \longrightarrow T_{middle}=40^{\circ}C$$

$$1.25\times1500\times(174-88)=1150\times A_1\times\Delta T$$

and

$$\Delta T=\frac{(88-80)-(88-40)}{\ln\left(\frac{(88-80)}{(88-40)}\right)}=22.32$$

Note:

$$\Delta T=\frac{(174-80)-(88-40)}{\ln\left(\frac{(174-80)}{(88-40)}\right)}=68.44$$

When water fails for 1 hour, heat balance for tank 1 and tank 2:

Tank 1 $\quad MCT_0-MCT_1=VC\frac{dT_1}{dt}$

Tank 2 $\quad MCT_1-MCT_2=VC\frac{dT_2}{dt}$

M: mass flow rate of acid
C: heat capacity of acid
V: mass capacity of tank
T_i: temperature of tank i

$$T_0-T_1=\frac{dT_1}{dt} \xrightarrow[\text{t = 0, } T_1 = 88]{\text{B.C.}} T_1=174-86e^{-t}$$

t = 1, T_1=142.4 C

$$T_1-T_2=\frac{dT_2}{dt}$$

$$174-86e^{-t}-T_2=\frac{dT_2}{dt} \xrightarrow{\text{integral factor, } e^t} T_2=174-(86t+129)e^{-t}$$

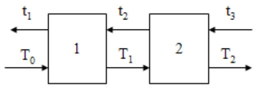
B.C.
t = 0, T_2 = 45

t = 1, T_2 = 94.9 C

When water supply restores after 1 hour, heat balance for tank 1 and tank 2:

Tank 1 $(WC_w t_2 + MCT_0) - (WC_w t_1 + MCT_1) = VC\dfrac{dT_1}{dt}$

Tank 2 $(WC_w t_3 + MCT_1) - (WC_w t_2 + MCT_2) = VC\dfrac{dT_2}{dt}$



W: mass flow rate of water
C_w: heat capacity of water
t_1: temperature of water leaving tank 1
t_2: temperature of water leaving tank 2
t_3: temperature of water entering tank 2

Heat transfer rate equations for the two tanks:

$$WC_w(t_1 - t_2) = U_1A_1\left[\frac{(T_1 - t_1) - (T_1 - t_2)}{\ln(T_1 - t_1) - \ln(T_1 - t_2)}\right]$$

$$WC_w(t_2 - t_3) = U_2A_2\left[\frac{(T_2 - t_2) - (T_2 - t_3)}{\ln(T_2 - t_2) - \ln(T_2 - t_3)}\right]$$

4 equations have to be solved simultaneously

$$(WC_w t_2 + MCT_0) - (WC_w t_1 + MCT_1) = VC\frac{dT_1}{dt}$$

$$(WC_w t_3 + MCT_1) - (WC_w t_2 + MCT_2) = VC\frac{dT_2}{dt}$$

$$\boxed{\begin{aligned} WC_w(t_1 - t_2) &= U_1A_1\left[\frac{(T_1 - t_1) - (T_1 - t_2)}{\ln(T_1 - t_1) - \ln(T_1 - t_2)}\right] \\ WC_w(t_2 - t_3) &= U_2A_2\left[\frac{(T_2 - t_2) - (T_2 - t_3)}{\ln(T_2 - t_2) - \ln(T_2 - t_3)}\right]\end{aligned}} \xrightarrow[\beta = e^{-\frac{U_2A_2}{WC_w}}]{\alpha = e^{-\frac{U_1A_1}{WC_w}}} \boxed{\begin{aligned} T_1(1-\alpha) &= t_1 - \alpha t_2 \\ T_2(1-\beta) &= t_2 - \beta t_3\end{aligned}}$$

$$\frac{d^2T_2}{dt^2} + 6.08\frac{dT_2}{dt} + 7.75T_2 = 309 \xrightarrow{\text{B.C. } t = 0,\ T_2 = 94.9\text{ C}} \text{Solve it}$$

Auxiliary conditions

auxiliary conditions

Initial Conditions

- all conditions are at one point of the independent variable

Boundary Conditions

- The conditions are not at one point of the independent variable

Initial value and Boundary-Value Problems

Initial-Value Problems

- The auxiliary conditions are at one point of the independent variable

$$\ddot{x} + 2\dot{x} + x = e^{-2t}$$

$$x(0) = 1, \quad \dot{x}(0) = 2.5$$

same

Boundary-Value Problems

- The auxiliary conditions are not at one point of the independent variable
- More difficult to solve than initial value problem

$$\ddot{x} + 2\dot{x} + x = e^{-2t}$$

$$x(0) = 1, \quad x(2) = 1.5$$

different

Classification of ODE

ODE can be classified in different ways

- Order
  - First order ODE
  - Second order ODE
  - N^{th} order ODE
- Linearity
  - Linear ODE
  - Nonlinear ODE
- Auxiliary conditions
  - Initial value problems
  - Boundary value problems

Analytical Solutions

- Analytical Solutions to ODE are available for linear ODE and special classes of nonlinear differential equations.

Numerical Solutions

- Numerical method are used to obtain a graph or a table of the unknown function
- Most of the Numerical methods used to solve ODE are based directly (or indirectly) on truncated Taylor series expansion

Classification of the Methods

Numerical Methods for solving ODE

Single-Step Methods

Estimates of the solution at a particular step are entirely based on information on the previous step

Multiple-Step Methods

Estimates of the solution at a particular step are based on information on more than one step