Ordinary Differential Equations

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".

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

Ordinary differential equation --------
only one independent variable involved: x

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

Partial differential equation ---------------
more than one independent variable involved: x, y, z, θ

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.

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

Product between two derivatives ---- non-linear

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

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

First order differential equations

- No general method of solutions of 1st O.D.E.s 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

Exact equations

- Exact? $$M(x,y)dx + N(x,y)dy = 0$$

$$\updownarrow \qquad \updownarrow$$

$$\frac{\partial F}{\partial x}dx + \frac{\partial F}{\partial y}dy = dF$$

General solution: F (x,y) = C

For example

$$x^3 - y\sin x + (\cos x + 2y)\frac{dy}{dx} = 0$$

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.

For example

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

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 C when the ratios of the specific reaction rate constants are:

$$k_1 = 8\ k_2\ ;\ k_2 = 30\ k_3$$

$$C_6H_6 + Cl_2 \rightarrow C_6H_5Cl + HCl$$
$$C_6H_5Cl + Cl_2 \rightarrow C_6H_4Cl_2 + HCl$$
$$C_6H_4Cl_2 + Cl_2 \rightarrow C_6H_3Cl_3 + HCl$$

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*

$$\left.\begin{aligned} 0 - k_1 pq &= V\frac{dq}{d\theta} \\ k_1 pq - k_2 pr &= V\frac{dr}{d\theta} \\ k_2 pr - k_3 ps &= V\frac{ds}{d\theta} \\ k_3 ps &= V\frac{dt}{d\theta} \end{aligned}\right\} \quad \frac{dr}{dq} = \frac{k_2}{k_1}\left(\frac{r}{q}\right) - 1$$

$u = r/q$

Equations solved by integrating factor

- There exists a factor by which the equation can be multiplied so that the one side becomes a complete differential equation. The factor is called "the integrating factor".

$$\frac{dy}{dx} + Py = Q$$ where P and Q are functions of x only

Assuming the integrating factor R is a function of x only, then

$$\left.\begin{aligned} R\frac{dy}{dx} + yRP &= RQ \\ R\frac{dy}{dx} + y\frac{dR}{dx} &= \frac{d}{dx}(Ry) \end{aligned}\right\} \quad R = \exp\left(\int P dx\right)$$ is the integrating factor

Example

Solve $xy - \frac{dy}{dx} = y^4 \exp\left(\frac{-3x^2}{2}\right)$

Let z = 1/y^3

$$\frac{dz}{dy} = -\frac{3}{y^4} \qquad \frac{dz}{dx} = -\frac{3}{y^4}\frac{dy}{dx}$$

$$3xz + \frac{dz}{dx} = 3\exp\left(\frac{-3x^2}{2}\right)$$

integral factor $\exp\left(\int 3x\,dx\right) = \exp\left(\frac{3x^2}{2}\right)$

$$3xz\exp\left(\frac{3x^2}{2}\right) + \frac{dz}{dx}\exp\left(\frac{3x^2}{2}\right) = 3$$

$$\frac{d}{dx}\left(z\exp\left(\frac{3x^2}{2}\right)\right) = 3$$

$$\left(z\exp\left(\frac{3x^2}{2}\right)\right) = 3x + C$$

$$\frac{1}{y^3}\exp\left(\frac{3x^2}{2}\right) = 3x + C$$

Summary of 1st O.D.E.

- First order linear differential equations occasionally arise in chemical engineering problems in the field of heat transfer, momentum transfer and mass transfer.

First O.D.E. 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/m^2C
Thermal conductivity of asbestos (k)	= 0.2 W/m C
Surface coefficient of heat transfer by convection and radiation (h_2)	= 10 W/m^2C
Density of liquid (ρ)	= 10^3 kg/m^3
Heat capacity of liquid (s)	= 2500 J/kgC
Atmospheric temperature at time of charging	= 20 C
Atmospheric temperature (t)	$t = 10 + 10 \cos(\pi\theta/12)$
Time in hours (θ)	

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

Area of tank (A) = (π x 1 x 2) + 2 (1 / 4 π x 1^2) = 2.5π m^2

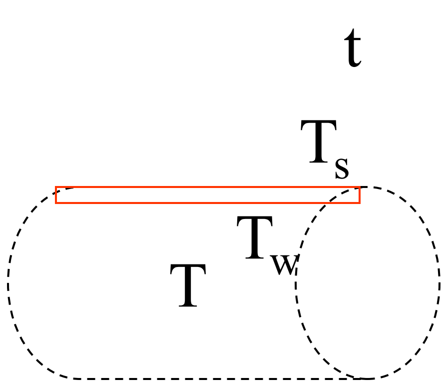
Rate of heat loss by liquid = h_1 A (T - T_w)
Rate of heat loss through lagging = kA/*l* (T_w - T_s)
Rate of heat loss from the exposed surface of the lagging = h_2 A (T_s - t)

At steady state, the three rates are equal:

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

Considering the thermal equilibrium of the liquid,

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



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

B.C. $\theta = 0$, T = 95

Second O.D.E.

- Purpose: reduce to 1st O.D.E.
- 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.

Non-linear 2nd O.D.E.

- Equations where the dependent variables does not occur explicitly

- They are solved by differentiation followed by the *p* substitution.
- When the *p* substitution is made in this case, the second derivative of *y* is replaced by the first derivative of *p* thus eliminating *y* completely and producing a first O.D.E. in *p* and *x*.

Solve $$\frac{d^2y}{dx^2} + x\frac{dy}{dx} = ax$$

Let $p = \frac{dy}{dx}$ and therefore $\frac{dp}{dx} = \frac{d^2y}{dx^2}$

$$\frac{dp}{dx} + xp = ax$$

integral factor $\exp\left(\frac{1}{2}x^2\right)$

$$\frac{dp}{dx}e^{\frac{1}{2}x^2} + xpe^{\frac{1}{2}x^2} = axe^{\frac{1}{2}x^2}$$

$$\frac{d}{dx}(pe^{\frac{1}{2}x^2}) = axe^{\frac{1}{2}x^2}$$

error function

Non-linear 2nd O.D.E.

- Equations where the independent variables does not occur explicitly

- They are solved by differentiation followed by the *p* substitution.
- When the *p* substitution is made in this case, the second derivative of *y* is replaced as

Let $p = \frac{dy}{dx}$

$$\therefore \frac{d^2y}{dx^2} = \frac{dp}{dx} = \frac{dp}{dy}\frac{dy}{dx} = p\frac{dp}{dy}$$

Solve $$y\frac{d^2y}{dx^2}+1=\left(\frac{dy}{dx}\right)^2$$

Let $p=\frac{dy}{dx}$ and therefore $\frac{d^2y}{dx^2}=p\frac{dp}{dy}$

$$yp\frac{dp}{dy}+1=p^2$$

Separating the variables

$$\frac{p}{p^2-1}dp=\frac{1}{y}dy$$

$$\ln y+\ln a=\frac{1}{2}\ln(p^2-1)$$

$$p=\frac{dy}{dx}=\sqrt{(a^2y^2+1)}$$

$$x=\int\frac{dy}{\sqrt{(a^2y^2+1)}}$$

$$x=\left(1/a\right)\sinh^{-1}(ay)+b$$

Non-linear 2nd O.D.E.- Homogeneous equations

- The homogeneous 1st O.D.E. was in the form: $\frac{dy}{dx}=f\left(\frac{y}{x}\right)$
- The corresponding dimensionless group containing the 2nd differential coefficient is $x\frac{d^2y}{dx^2}$
- In general, the dimensionless group containing the nth coefficient is $x^{n-1}\frac{d^ny}{dx^n}$
- The second order homogenous differential equation can be expressed in a form analogous to $\frac{dy}{dx}=f\left(\frac{y}{x}\right)$, viz.

$$x\frac{d^2y}{dx^2}=f\left(\frac{y}{x},\frac{dy}{dx}\right)$$

Assuming u = y/x →

$$x^2\frac{d^2u}{dx^2}=f\left(u,x\frac{du}{dx}\right)$$

Assuming x = e^t →

$$\frac{d^2u}{dt^2}-\frac{du}{dt}=f\left(u,\frac{du}{dt}\right)$$

If in this form, called homogeneous 2nd ODE

Solve $$2x^2 y \frac{d^2 y}{dx^2} + y^2 = x^2 \left(\frac{dy}{dx} \right)^2$$

Dividing by *2xy*

$$x \frac{d^2 y}{dx^2} + \frac{1}{2} \frac{y}{x} = \frac{1}{2} \frac{x}{y} \left(\frac{dy}{dx} \right)^2$$

homogeneous $x \frac{d^2 y}{dx^2} = f\left(\frac{y}{x}, \frac{dy}{dx} \right)$

Let $y = ux$

$$2ux^2 \frac{d^2 u}{dx^2} + 2ux \frac{du}{dx} = x^2 \left(\frac{du}{dx} \right)^2$$

Let $x = e^t$

$$2u \frac{d^2 u}{dt^2} = \left(\frac{du}{dt} \right)^2$$

$p = \frac{du}{dt}$

$$2up \frac{dp}{du} = p^2$$

General solution

$$y = x(B \ln x + C)^2$$

$y = Ax$ Singular solution

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.

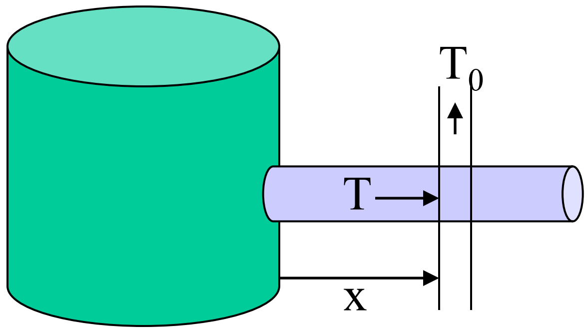
If the lagging is of uniform thickness and the mean overall coefficient of heat transfer from the electrode to the surrounding atmosphere is taken to be 1.7 W/C m^2 of surface of electrode; and the temperature of the electrode just outside the furnace is 1500 C, estimate the duty of the water cooler 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.



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

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

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

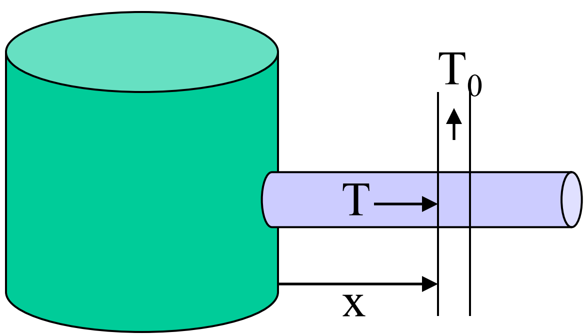
D = electrode diameter

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

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

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

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



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

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

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

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

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

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:

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

where $\varphi(x)$ is any function of x.

2nd 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

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

If v is a particular solution of the original differential equation

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

The general solution of the linear differential equation will be the sum of a "complementary function" and a "particular solution".

purpose

The complementary function

$$P\frac{d^2y}{dx^2} + Q\frac{dy}{dx} + Ry = 0$$

Let the solution assumed to be: $y = A_m e^{mx}$ $\quad \frac{dy}{dx} = A_m m e^{mx}$ $\quad \frac{d^2y}{dx^2} = A_m m^2 e^{mx}$

$$A_m e^{mx}(Pm^2 + Qm + R) = 0$$

auxiliary equation (characteristic equation)

→ Unequal roots / Equal roots

Real roots / Complex roots

Unequal roots to auxiliary equation

- Let the roots of the auxiliary equation be distinct and of values m_1 and m_2. Therefore, the solutions of the auxiliary equation are:

$$y = A_1 e^{m_1 x} \qquad\qquad y = A_2 e^{m_2 x}$$

- The most general solution will be

$$y = A_1 e^{m_1 x} + A_2 e^{m_2 x}$$

- If m_1 and m_2 are complex it is customary to replace the complex exponential functions with their equivalent trigonometric forms.

Solve $$\frac{d^2y}{dx^2} - 5\frac{dy}{dx} + 6y = 0$$

↓ auxiliary function

$$m^2 - 5m + 6 = 0$$

↓

$$m_1 = 2$$

$$m_2 = 3$$

↓

$$y = Ae^{2x} + Be^{3x}$$

Equal roots to auxiliary equation

- Let the roots of the auxiliary equation equal and of value $m_1 = m_2 = m$. Therefore, the solution of the auxiliary equation is: $y = Ae^{mx}$

Let $y = Ve^{mx}$ $\quad \frac{dy}{dx} = e^{mx}\frac{dV}{dx} + mVe^{mx}$ $\quad \frac{d^2y}{dx^2} = e^{mx}\frac{d^2V}{dx^2} + 2me^{mx}\frac{dV}{dx} + m^2Ve^{mx}$

where V is a function of x

$$P\frac{d^2y}{dx^2} + Q\frac{dy}{dx} + Ry = 0$$

$$\frac{d^2V}{dx^2} = 0 \rightarrow V = Cx + D$$

$$y = (Cx + d)e^{mx}$$

Solve $$\frac{d^2y}{dx^2}+6\frac{dy}{dx}+9y=0$$

$\downarrow$ auxiliary function

$$m^2+6m+9=0$$

$\downarrow$

$$m_1=m_2=-3$$

$\downarrow$

$$\boxed{y=(A+Bx)e^{-3x}}$$

Solve $\frac{d^2 y}{dx^2} - 4\frac{dy}{dx} + 5y = 0$

$\downarrow$ auxiliary function

$$m^2 - 4m + 5 = 0$$

$\downarrow$

$$m = 2 \pm i$$

$\downarrow$

$$y = Ae^{(2+i)x} + Be^{(2-i)x} \longrightarrow y = e^{2x}(E\cos x + F\sin x)$$

Particular integrals

- Two methods will be introduced to obtain the particular solution of a second linear O.D.E.
  - The method of undetermined coefficients
    - confined to linear equations with *constant coefficients* and *particular form of* $\varphi(x)$
  - The method of inverse operators
    - general applicability

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

Method of undetermined coefficients

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

- When *φ (x)* is constant, say C, a particular integral of equation is

$$y = C/R$$

- When *φ (x)* is a polynomial of the form $a_0+a_1x+a_2x^2+...+a_nx^n$ where all the coefficients are constants. The form of a particular integral is

$$y=\alpha_0+\alpha_1x+\alpha_2x^2+...+\alpha_nx^n$$

- When *φ (x)* is of the form Te^{rx}, where T and r are constants. The form of a particular integral is

$$y=\alpha e^{rx}$$

Method of undetermined coefficients

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

- When $\varphi(x)$ is of the form $G \sin nx + H \cos nx$, where G and H are constants, the form of a particular solution is

$$y = L\sin nx + M\cos nx$$

- Modified procedure when a term in the particular integral duplicates a term in the complementary function.

Solve $\frac{d^2y}{dx^2} - 4\frac{dy}{dx} + 4y = 4x + 8x^3$ → (auxiliary equation) $m^2 - 4m + 4m = 0$

$$y = p + qx + rx^2 + sx^3$$

$$\frac{dy}{dx} = q + 2rx + 3sx^2$$

$$\frac{d^2y}{dx^2} = 2r + 6sx$$

$$(2r + 6sx) - 4(q + 2rx + 3sx^2) + 4(p + qx + rx^2 + sx^3) = 4x + 8x^3$$

Equating coefficients of equal powers of x

$$\begin{cases} 2r - 4q + 4p = 0 \\ 6s - 8r + 4q = 4 \\ 4r - 12s = 0 \\ 4s = 8 \end{cases}$$

$$y_c = (A + Bx)e^{2x}$$

$$y_p = 7 + 10x + 6x^2 + 2x^3$$

$$y_{general} = y_c + y_p$$

Method of inverse operators

- Sometimes, it is convenient to refer to the symbol "D" as the differential operator:

$$Dy = \frac{dy}{dx}$$

$$D(Dy) = D^2 y = \frac{d^2 y}{dx^2}$$

$$\ldots$$

$$D^n y = \frac{d^n y}{dx^n}$$

But, $(Dy)^2 = \left(\frac{dy}{dx}\right)^2$

$$\frac{d^2 y}{dx^2} + 3\frac{dy}{dx} + 2y \longrightarrow D^2 y + 3Dy + 2y = (D^2 + 3D + 2)y = (D+1)(D+2)y$$

The differential operator D can be treated as an ordinary algebraic quantity with certain limitations.

(1) The distribution law:

$A(B+C) = AB + AC$

which applies to the differential operator D

(2) The commutative law:

$AB = BA$

which does not in general apply to the differential operator D

$Dxy \neq xDy$

$(D+1)(D+2)y = (D+2)(D+1)y$

(3) The associative law:

$(AB)C = A(BC)$

which does not in general apply to the differential operator D

$D(Dy) = (DD)y$

$D(xy) = (Dx)y + x(Dy)$

The basic laws of algebra thus apply to the pure operators, but the relative order of operators and variables must be maintained.

Differential operator to exponentials

$$De^{px} = pe^{px}$$

$$\cdots$$

$$D^n e^{px} = p^n e^{px}$$

$$f(D)e^{px} = f(p)e^{px}$$

$$(D^2 + 3D + 2)e^{px} = (p^2 + 3p + 2)e^{px}$$

$$D(ye^{px}) = e^{px}Dy + yDe^{px} = e^{px}(D + p)y$$

$$D^2(ye^{px}) = e^{px}(D + p)^2 y$$

$$\cdots$$

$$D^n(ye^{px}) = e^{px}(D + p)^n y$$

$$f(D)(ye^{px}) = e^{px} f(D + p)y$$

More convenient!

Differential operator to trigonometrical functions

$$D^n(\sin px) = D^n \operatorname{Im} e^{ipx} = \operatorname{Im} D^n e^{ipx} = \operatorname{Im}(ip)^n e^{ipx}$$

where "Im" represents the imaginary part of the function which follows it.

$$e^{ipx} = \cos px + i \sin px$$

$$D^{2n}(\sin px) = (-p^2)^n \sin px$$

$$D^{2n+1}(\sin px) = (-p^2)^n p \cos px$$

$$D^{2n}(\cos px) = (-p^2)^n \cos px$$

$$D^{2n+1}(\cos px) = -(-p^2)^n p \sin px$$

The inverse operator

The operator D signifies differentiation, i.e.

$$D\left[\int f(x)dx\right] = f(x) \longrightarrow \int f(x)dx = D^{-1} f(x)$$

- D^{-1} is the "inverse operator" and is an "intergrating" operator.
- It can be treated as an algebraic quantity in exactly the same manner as D

Solve $\frac{dy}{dx} - 4y = e^{2x}$

↓ differential operator

$$(D-4)y = e^{2x}$$

↓

$$y = \frac{1}{(D-4)} e^{2x} \xrightarrow[p=2]{f(D)e^{px} = f(p)e^{px}} y = \frac{1}{(2-4)} e^{2x}$$

↓

$$y = \frac{1}{4(1-\frac{1}{4}D)} e^{2x}$$

↓ binomial expansion

$$y = -\frac{1}{4} e^{2x} [1 + (\frac{1}{4}D) + (\frac{1}{4}D)^2 + (\frac{1}{4}D)^3 + \ldots]1$$

=2

↓

$$y = -\frac{1}{4} e^{2x} [1 + (\frac{1}{2}) + (\frac{1}{2})^2 + (\frac{1}{2})^3 + \ldots] \longrightarrow y = -\frac{1}{2} e^{2x}$$

$$y=\frac{1}{(D-4)}e^{2x}$$

$f(D)e^{px}=f(p)e^{px}$

$p=2$

$$y=\frac{1}{(2-4)}e^{2x}$$

$$\frac{1}{f(D)}e^{px}=\frac{1}{f(p)}e^{px}$$

如果 $f(p)=0$, 使用因次分析

$$\frac{1}{f(D)}e^{px}=\frac{1}{(D-p)^{n}\varphi(D)}e^{px}$$

非0的部分

$f(D)e^{px}=f(p)e^{px}$

$$\frac{1}{f(D)}e^{px}=\frac{e^{px}}{\varphi(p)}\frac{1}{(D-p)^{n}}$$

$f(D)ye^{px}=e^{px}f(D+p)y$

y = 1, p = 0, 即將 D-p換為 D

$$\frac{1}{f(D)}e^{px}=\frac{e^{px}}{\varphi(p)}\frac{1}{D^{n}}$$

$$\frac{1}{f(D)}e^{px}=\frac{e^{px}}{\varphi(p)}D^{-n}$$

integration

$$\frac{1}{f(D)}e^{px}=\frac{e^{px}}{\varphi(p)}\frac{x^{n}}{n!}$$

Solve

$$\frac{d^2y}{dx^2} - 8\frac{dy}{dx} + 16y = 6xe^{4x} \longrightarrow m^2 - 8m + 16 = 0$$

differential operator

$$(D^2 - 8D + 16)y = (D-4)^2 y = 6xe^{4x}$$

$$y_c = (A + Bx)e^{4x}$$

$$y_p = \frac{6}{(D-4)^2} xe^{4x}$$

$$y = y_c + y_p$$

f(p) = 0

$$f(D)e^{px} = e^{px} f(D+p)$$

$$y_p = 6xe^{4x} D^{-2}$$

integration

$$y_p = 6xe^{4x} \frac{x^2}{2!} \longrightarrow y_p = 3x^3 e^{4x}$$

Solve

$$\frac{d^2y}{dx^2} - \frac{dy}{dx} - 6y = 4x^3 + 3x^2 \longrightarrow m^2 - m - 6 = 0$$

differential operator

$$(D^2 - D - 6)y = (D-3)(D+2)y = 4x^3 + 3x^2$$

$$y_c = Ae^{3x} + Be^{-2x}$$

$$y_p = \frac{1}{(D-3)(D+2)}(4x^3 + 3x^2)$$

$$y = y_c + y_p$$

$$y_p = -\frac{1}{5}\left[\frac{1}{(3-D)} + \frac{1}{(2+D)}\right](4x^3 + 3x^2)$$

expanding each term by binomial theorem

$$y_p = -\frac{1}{5}\left[\left(\frac{1}{3} + \frac{D}{9} + \frac{D^2}{27} + \frac{D^3}{81} + \ldots\right) + \left(\frac{1}{2} - \frac{D}{4} + \frac{D^2}{8} - \frac{D^3}{16} + \ldots\right)\right](4x^3 + 3x^2)$$

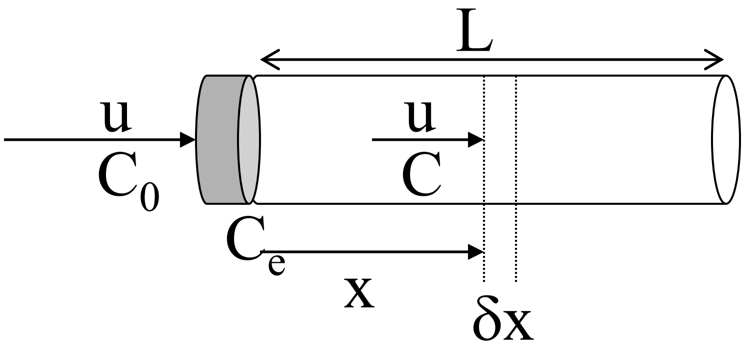
$$y_p = -\frac{4x^3 + 3x^2}{6} + \frac{12x^2 + 6x}{36} - \frac{7(24x + 6)}{216} + \frac{13 \times 24}{1296} - 0\ldots$$

O.D.E 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,

$$A \rightarrow B$$

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

→ 分開兩個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 fom the inlet

Input - Output + Generation = ~~Accumulation~~

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

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

↓ dividing by δx

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

↓ rearranging

$$D\frac{d^2C}{dx^2}-u\frac{dC}{dx}-kC=0$$

In the entry section →

$$D\frac{d^2\widehat{C}}{dx^2}-u\frac{d\widehat{C}}{dx}=0$$

↓ auxillary function (both)

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

↓

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

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

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

B. C.

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

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

$$\hat{C} = \alpha + \beta\exp\left[\frac{ux}{D}\right]$$

B. C.

$$x = -\infty \quad \hat{C} = C_0$$

$$x = 0 \quad \hat{C} = C$$

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

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

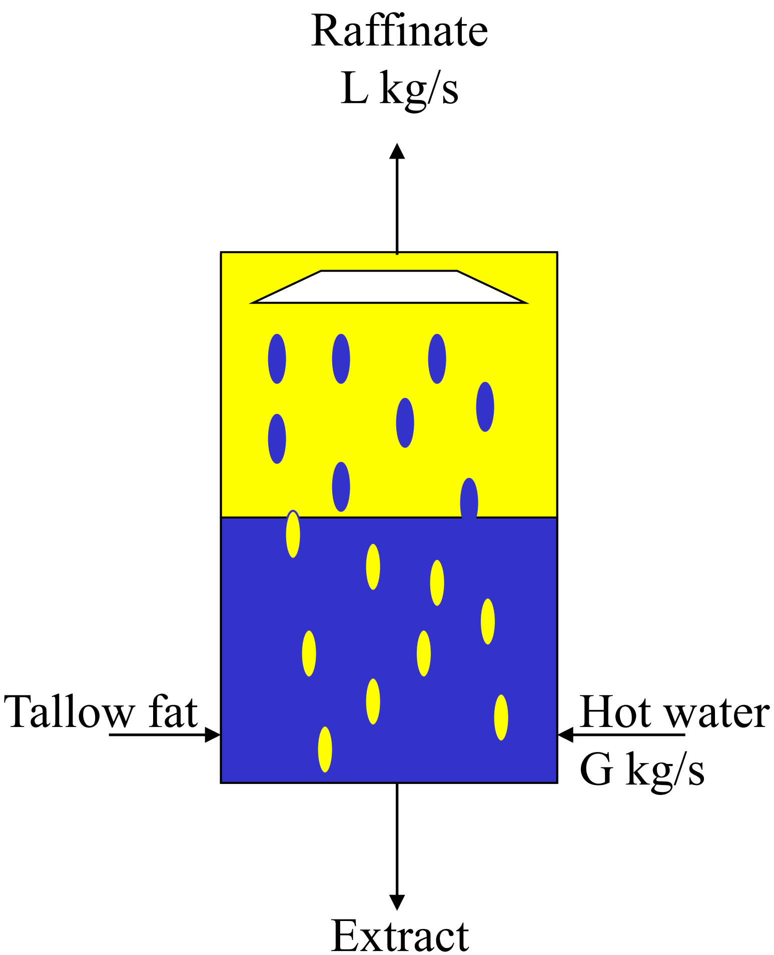
if diffusion is neglected (D→0)

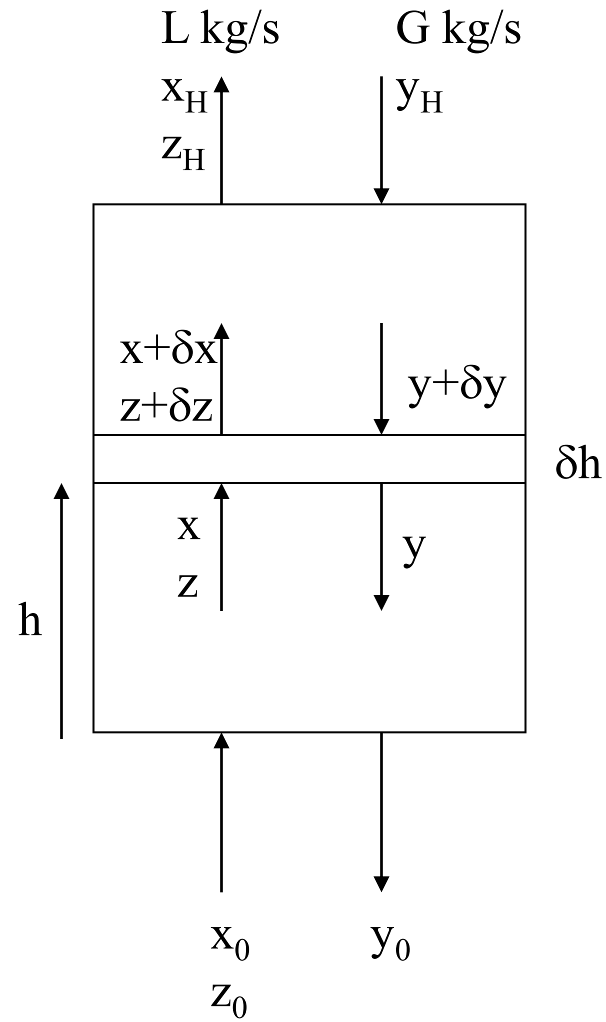
$$\frac{C_0 - C}{C_0} = 1 - \exp\left(\frac{-kx}{u}\right)$$

The continuous hydrolysis of tallow in a spray column 連續牛油水解

Glycerin, 甘油

1.017 kg/s of a tallow fat mixed with 0.286 kg/s of high pressure hot water is fed into the base of a spray column operated at a temperature 232 C and a pressure of 4.14 MN/m^2. 0.519kg/s of water at the same temperature and pressure is sprayed into the top of the column and descends in the form of droplets through the rising fat phase. Glycerine is generated in the fat phase by the hydrolysis reaction and is extracted by the descending water so that 0.701 kg/s of final extract containing 12.16% glycerine is withdrawn continuously from the column base. Simultaneously 1.121 kg/s of fatty acid raffinate containing 0.24% glycerine leaves the top of the column.
If the effective height of the column is 2.2 m and the diameter 0.66 m, the glycerine equivalent in the entering tallow 8.53% and the distribution ratio of glycerine between the water and the fat phase at the column temperature and pressure is 10.32, estimate the concentration of glycerine in each phase as a function of column height. Also find out what fraction of the tower height is required principally for the chemical reaction. The hydrolysis reaction is pseudo first order and the specific reaction rate constant is 0.0028 s^{-1}.





x = weight fraction of glycerine in raffinate

y = weight fraction of glycerine in extract

y^*= weight fraction of glycerine in extract in equilibrium with x

z = weight fraction of hydrolysable fat in raffinate

Consider the changes occurring in the element of column of height δh:

Glycerine transferred from fat to water phase, $KaS(y^* - y)\delta h$

Rate of destruction of fat by hydrolysis, $k\rho Sz\delta h$

Rate of production of glycerine by hydrolysis, $k\rho Sz\delta h / w$

S: sectional area of tower

a: interfacial area per volume of tower

K: overall mass transter coefficient

k: specific reaction rate constant

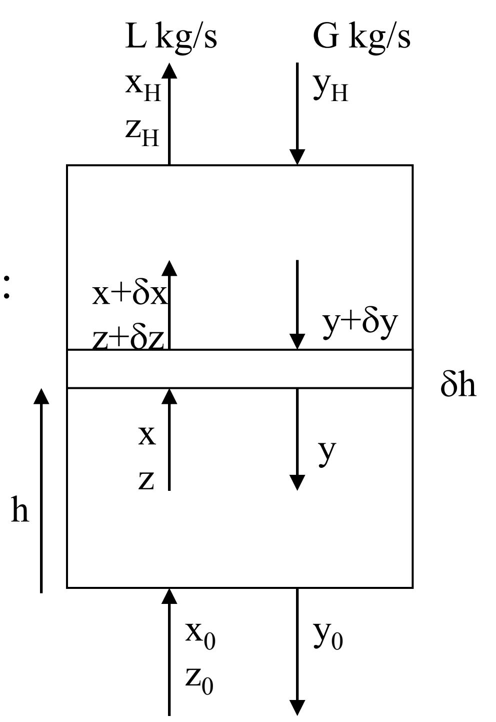
ρ: mass of fat per unit volume of column (730 kg/m^3)

w: kg fat per kg glycetine

A glycerine balance over the element δh is:

$$Lx - L\left(x + \frac{dx}{dh}\delta h\right) + \frac{(k\rho Sz\delta h)}{w} = KaS(y^* - y)\delta h$$ in the fat phase

$$G\left(y + \frac{dy}{dh}\delta h\right) - Gy = KaS(y - y^*)\delta h$$ in the extract phase



A glycerine balance between the element and the base of the tower is:

$$\left(Lx + \frac{Lz}{w} - \frac{Lz_0}{w}\right) = 0$$ in the fat phase

$$(Gy - Gy_0) = 0$$ in the extract phase

The glycerine equilibrium between the phases is:

$$y^* = mx$$

$$\frac{k\rho S^2 Ka}{LG}\left[\frac{mz_0}{w}+\frac{mG}{L}(y-y_0)\right]-\frac{k\rho S}{L}\left(\frac{KaS}{G}y-\frac{dy}{dh}\right)-\left(\frac{KaS}{G}\frac{dy}{dh}-\frac{d^2y}{dh^2}\right)+\frac{KaSm}{L}\frac{dy}{dh}=0$$

$$p=\frac{k\rho S}{L}$$

$$r=\frac{mG}{L}$$

$$q=\frac{KaS}{G}(r-1)$$

$$\frac{d^2y}{dh^2}+(p+q)\frac{dy}{dh}+pqy=\frac{pq}{r-1}\left(ry_0-\frac{mz_0}{w}\right)$$

2nd O.D.E. with constant coefficients

Complementary function

Particular solution

$$m^2+(p+q)m+pq=0$$

Constant at the right hand side, y_p = C/R

$$y_c = A\exp(-ph)+B\exp(-qh)$$

$$y_p=\frac{pq}{r-1}\left(ry_0-\frac{mz_0}{w}\right)/\,pq$$

$$y = A\exp(-ph) + B\exp(-qh) + \frac{1}{r-1}\left(ry_0 - \frac{mz_0}{w}\right)$$

↓ B.C.

We don't know y_0, either

$$\begin{cases} h = 0, x = 0 \\ h = H, y = 0 \end{cases}$$

We don't really want x here! → $$\begin{cases} h = 0, y = y_0 \\ h = H, y = 0 \end{cases}$$

↓ Apply the equations two slides earlier (replace y^* with mx)

$$mx = y - \frac{r-1}{q}\frac{dy}{dh}$$

↓

$$mx = y - \frac{r-1}{q}\left(-pA\exp(-ph) - qB\exp(-qh)\right)$$

↓

$$\begin{cases} y(ve^{-qH} - re^{-pH}) = \frac{1}{r-1}\left(ry_0 - \frac{mz_0}{w}\right)\left[(r - e^{-qH})e^{-pH} + (e^{-pH} - v)e^{-qh} + ve^{-qH} - re^{-pH}\right] \\ v = \frac{q + rp - p}{q} \end{cases}$$

Substitute y_0 in terms of other variables → ($h = 0, y = y_0$)

$$y = \frac{mz_0}{w(r-v)}\left[e^{-pH} + \left(\frac{e^{-pH}-v}{r-e^{-qH}}\right)e^{-qH} + \left(\frac{ve^{-qH}-re^{-pH}}{r-e^{-qH}}\right)\right]$$

$$L \sim \frac{1.017+1.121}{2} = 1.069$$

$$G \sim \frac{0.286+0.519}{2} = 0.403$$

$$y_0 \sim \frac{0.701\times 0.1216+0.276}{0.701+0.286} = 0.165$$

$$m = 10.32$$

$$k = 0.0028$$

$$S = \frac{\pi}{4}0.66^2$$

$$\rho = 730$$

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.

Our purpose: Use algebraic elemination of the variables until only one differential equation relating two of the variables remains.

Elimination of variable

Independent variable or dependent variables?

$$\frac{dx}{dt} = f_1(x, y)$$
$$\frac{dy}{dt} = f_2(x, y)$$

Elimination of independent variable →

$$\frac{dx}{dy} = \frac{f_1(x, y)}{f_2(x, y)}$$

較少用

Elimination of one or more dependent variables

It involves with equations of high order and
it would be better to make use of *matrices*

Solving differential equations simultaneously using matrices will be introduced later in the term

Elimination of dependent variables

Solve

$$(D^2+D-6)y+(D^2+6D+9)z=0$$
and
$$(D^2+3D-10)y+(D^2-3D+2)z=0$$

↓

$$(D+3)(D-2)y+(D+3)^2 z=0$$
and
$$(D-2)(D+5)y+(D-2)(D-1)z=0$$

$\times(D+5)$ → / $\times(D+3)$ →

$$(D+3)(D-2)(D+5)y+(D+5)(D+3)^2 z=0$$
and
$$(D+3)(D-2)(D+5)y+(D+3)(D-2)(D-1)z=0$$

↓

$$(D+5)(D+3)^2 z-(D+3)(D-2)(D-1)z=0$$
$$\therefore$$
$$(D+3)\left[(D^2+8D+15)-(D^2-3D+2)\right]z=0$$

←

$$(D+3)(11D+13)z=0$$

$$(D+3)(11D+13)z=0$$

$$z=Ae^{-\frac{13}{11}x}+Be^{-3x}$$

$(D^2+D-6)y+(D^2+6D+9)z=0$

$$(D^2+D-6)y=-\left[\left(\frac{13}{11}\right)^2-\left(\frac{6\times 13}{11}\right)+9\right]Ae^{-\frac{13}{11}x}$$

$= \mathrm{E}$

$$y_p=\frac{1}{(D^2+D-6)}Ee^{-\frac{13}{11}x}$$

$f(D)e^{px}=f(p)e^{px}$ $\quad p=-\frac{13}{11}$

$$y_p=\frac{1}{((-\frac{13}{11})^2+(-\frac{13}{11})-6)}Ee^{-\frac{13}{11}x}$$

$$y_p=-\frac{121}{700}Ee^{-\frac{13}{11}x}$$

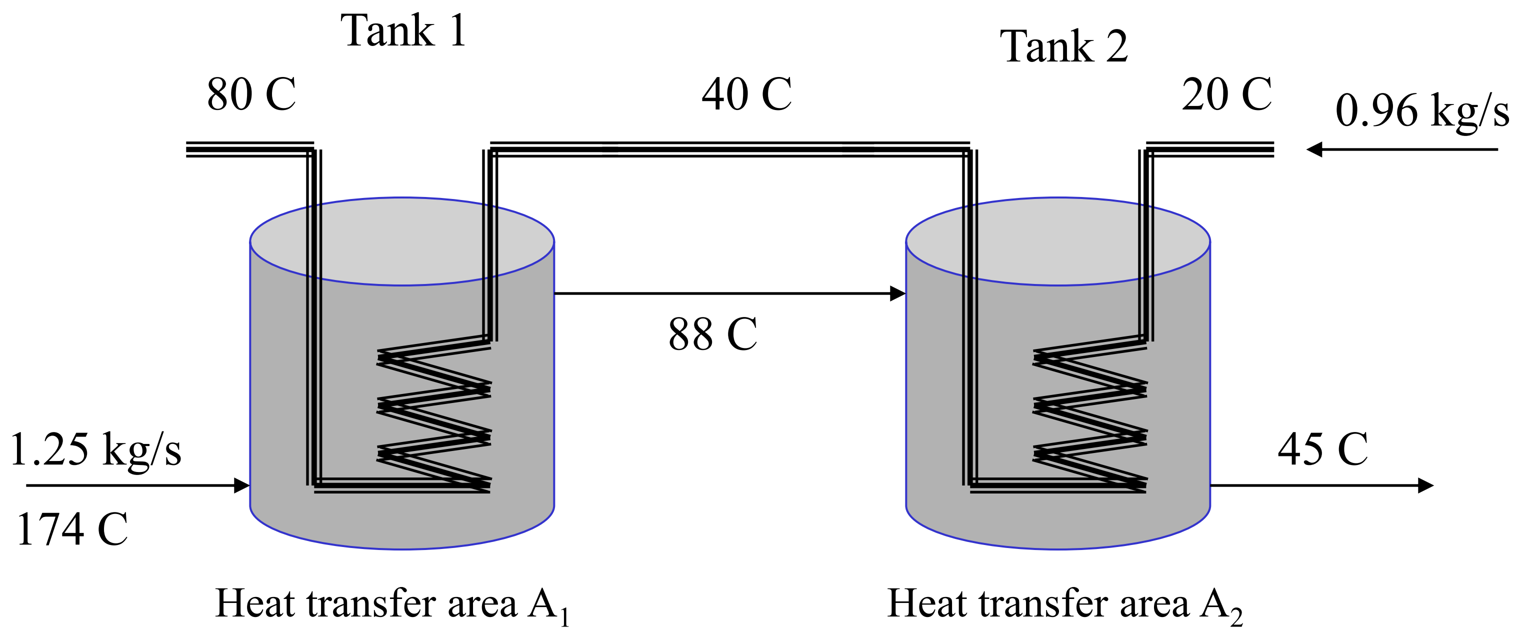
$$y_c=He^{2x}+Je^{-3x}$$

$$\mathrm{y}=\mathrm{y_c}+\mathrm{y_p}$$

Example of simultaneous O.D.E.s

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 45C. 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

$$1.25 \times 1500 \times (174 - 45) = F_{water} \times 4200 \times (80 - 20) \longrightarrow F_{water} = 0.96 kg/s$$

$$1.25 \times 1500 \times (88 - 45) = 0.96 \times 4200 \times (T_{middle} - 20) \longrightarrow T_{middle} = 40^{\circ} C$$

$$1.25 \times 1500 \times (174 - 88) = 1150 \times A_1 \times \Delta T$$

and

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

Note: 和單操課本不同

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

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

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

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

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

$$T_0 - T_1 = \frac{dT_1}{dt}$$

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

B.C.
t = 0, T_1 = 88 → $$T_1 = 174 - 86e^{-t}$$

t = 1, T_1=142.4 C

$$174 - 86e^{-t} - T_2 = \frac{dT_2}{dt}$$

integral factor, e^t → $$T_2 = 174 - (86t + 129)e^{-t}$$

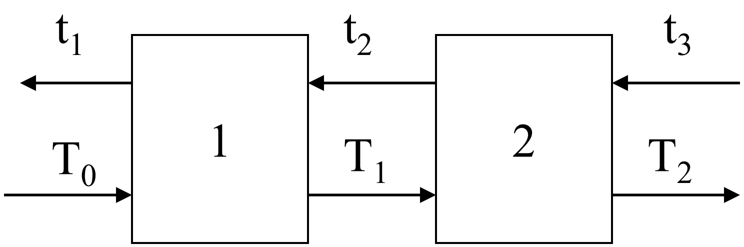
B.C.
t = 0, T_2 = 45

t = 1, T_2 = 94.9 C

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

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

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



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:

$$WC_w(t_1 - t_2) = U_1 A_1\left[\frac{(T_1 - t_1) - (T_1 - t_2)}{\ln(T_1 - t_1) - \ln(T_1 - t_2)}\right]$$

$$WC_w(t_2 - t_3) = U_2 A_2\left[\frac{(T_2 - t_2) - (T_2 - t_3)}{\ln(T_2 - t_2) - \ln(T_2 - t_3)}\right]$$

4 equations have to be solved simultaneously

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

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

$$WC_w(t_1 - t_2) = U_1 A_1 \left[\frac{(T_1 - t_1) - (T_1 - t_2)}{\ln(T_1 - t_1) - \ln(T_1 - t_2)} \right]$$

$$WC_w(t_2 - t_3) = U_2 A_2 \left[\frac{(T_2 - t_2) - (T_2 - t_3)}{\ln(T_2 - t_2) - \ln(T_2 - t_3)} \right]$$

$$\alpha = e^{-\frac{U_1 A_1}{WC_w}} \qquad \beta = e^{-\frac{U_2 A_2}{WC_w}} \longrightarrow$$

$$T_1(1-\alpha) = t_1 - \alpha t_2$$

$$T_2(1-\beta) = t_2 - \beta t_3$$

觀察各dependent variable 出現次數, 發現 t_1 出現次數最少，先消去！(i.e. t_1= ***代入)

再由出現次數次少的 t_2 消去

.....

代入各數值

.....

$$\frac{d^2T_2}{dt^2} + 6.08\frac{dT_2}{dt} + 7.75T_2 = 309 \xrightarrow{\text{B.C. } t = 0,\ T_2 = 94.9\text{ C}} \text{同時整理} T_1$$

基本上，1st order O.D.E. 應該都解的出來，方法不外乎：

- Check exact
- Separate variables
- homogenous equations, $u = y/x$
- equations solvable by an integrating factor

2nd order 以上的O.D.E → Non-linear O.D.E.

Non-linear O.D.E. ↓ 我們會解的部分

- 缺 x 的 O.D.E., reduced to 1st O.D.E.
- 缺 y 的 O.D.E., reduced to 1st O.D.E.
- homogeneous 的 O.D.E., $u = y/x$

2nd order 以上的O.D.E ↓ Linear O.D.E.

Linear O.D.E. ↓

General solution = complementary solution + particular solution

complementary solution ↓ 我們會解的部分 → constant coefficients

← variable coefficient? 用數列解，next course

particular solution ↓ 尋找特殊解的方法

- The method of undetermined coefficients
- The method of inverse operators