# References

- 1. J.ngham, I.J.Dunn, E.Heinzle, J. E. Prenosil, J.B.Snape, Chemical Engineering Dynamic, Wiley, 2007
- 2. V. G. Jenson and G. V. Jeffreys, Mathematical Methods in Chemical Engineering. McGraw-Hill, 1975
- 3. Zafer Ahsen, Differential Equations and Their Applications. Prentice Hall of India, 2007
- R. G. Rice, D. D. Do, Applied Mathematics And Modeling For Chemical Engineers, John Wiley and Sons, 995
- 5. İ.Tosun, Modeling in Transport Phenomena, Elsevier, 2007

### INTRODUCTION

Nearly, All applied science and engineering deal with performing experiments and interpreting the results. This may be done quantitatively by taking accurate measurements of the system variables or qualitatively by investigating the general behavior of the system in terms of one variable influencing another. This is done alternatively by looking for an mathematical model of the system. There are three step for an mathematical model of the system

- 1. Drawing a picture of the system to be modeled.
- 2. Collection of all relevant physical information in the form of conservation laws and rate equations.

3. Writing the conservation of chemical species, conservation of momentum , and conservation of energy . Express the relationship between flow rate and driving force in the fields of fluid flow, Heat transfer, and diffusion of matter. These are then applied to the model, and the results should be a mathematical equation which describes the system.

The type of equations (algebraic, differential, finite difference, etc.) will depend upon both the system under investigation, and the detail of its model.

## Dependent, Independent Variables, and Parameters

Any solution of a differential equation is an algebraic equation involving symbols. These symbols fall into three classes.

- Independent variables,
- Dependent variables
- Parameters

Independent Variables: Examples of independent variables are time and coordinate variables (t, x, y, z)

Dependent Variables: These are properties of the system which change when the independent variables are altered in value. The relationship between independent and dependent variables is one of cause and effect; the independent variable measures the cause and the dependent variable measures the effect of a particular action. Examples of dependent variables are temperature, concentration, etc.

- Parameters: This is by far the largest group, consisting mainly of the characteristic properties of the apparatus and the physical properties of the materials. Examples are overall dimensions of the apparatus, flow rates, heat transfer coefficients, thermal conductivity, specific heat, density, initial or boundary values of the dependent variables.
- ----- Single independent variable give rise to ordinary differential equations.

---- when more than one independent variable is needed to describe a system, the usual result is a partial differential equations.

#### Ordinary Differential Equations

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 equations. If there is only one independent variables the equation is said to be an ordinary differential equation

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

If there are two or more independent variables and the equation contains differential coefficient with respect to each of these, the equation is said to be a partial differential equation.

$$D_{AB} \frac{\partial^2 C_A}{\partial x^2} = \frac{\partial C_A}{\partial t}$$
 CA, y :Depandent variable  
x, t : Indepandent variable

#### Order and Degree

The order of a differential equation is equal to the order of the highest differential coefficient that it contains. Thus in equation 1 the order of highest differential coefficient is three and therefore equation 1 is third order differential equation. 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. Eq 1 is of the first degree, even though it contains the first order differential coefficient raised to the second power and the cube of the independent variable.

Eq 1 a third order first degree non linear ordinary differential equation.

$$\frac{d^3y}{dx^3} - x\frac{d^2y}{dx^2} + 6(\frac{dy}{dx})^2 + 5x^3\frac{dy}{dx} + 8y = 8e^x\cos x \tag{1}$$

# **Boundary Conditions**

An ordinary differential equation usually arises in any problem which involves a single independent variable. The general solution of this differential equation will contain arbitrary constants of integration, the number of constants being equal to the order of the differential equation. To complete the solution of a particular problem, these arbitrary constants have to be evaluated.

# EXAMPLES

1-)  $k \cdot (1-x) = \frac{dx}{dt}$ 

 $\frac{d^2C}{dx^2}$ 

$$kdt = \frac{dx}{(1-x)} \implies kt = -\ln(1-x) +$$

The order of the differential equation is one

The number of constants is one 2-)

$$-6x = 0 \qquad \frac{dC}{dx} = P \qquad \frac{d}{dx} \left(\frac{dC}{dx}\right) - 6x = 0 \quad \Rightarrow \frac{dP}{dx} = 6x \Rightarrow P = 3x^2 + c$$

The order of the differential equation is two The number of constants are two

$$P = 3x^{2} + c_{1} \Longrightarrow \frac{dC}{dx} = 3x^{2} + c_{1} \qquad C = x^{3} + c_{1}x + c_{2}$$

3-) 
$$\frac{d^2 V}{dy^2} - 5V = 0 \quad D = \frac{d}{dy} \quad D^2 V - 5V = 0 \rightarrow D^2 - 5 = 0 \rightarrow D_{1,2} = \pm \sqrt{5}$$
$$V = c_1 e^{\sqrt{5}y} + c_2 e^{-\sqrt{5}y}$$

The order of the differential equation is two

The number of constants are two

# LINEAR DIFFERENTIAL EQUATIONS:

A differential equation is said to be linear if the dependent variable y and its differential coefficients occur only in the first degree and are not multiplied together. The linear differential equation of the first order is of the form

$$\frac{dy}{dx} + P(x)y = Q(x)...(2)$$

Where P and Q are constants or functions of x alone. To solve such an equation, multiply both sides of Eq(2) by 1

$$\lambda y = \int \lambda Q(x) dx + c$$

$$\frac{dz}{dx} - \frac{2}{x}z = \frac{2}{3}x^{4} \qquad x^{-2}z = \int x^{-2}\frac{2}{3}x^{4}dx \qquad \lambda = e^{\int P(x)dx} = e^{-\int \frac{2}{x}dx} = e^{-2\ln|x|} = e^{\ln x^{-2}} = x^{-2}$$

$$x^{-2}z = \int \frac{2}{3}x^{2}dx \qquad \longrightarrow \qquad x^{-2}z = \frac{2}{3}\frac{x^{3}}{3} + c \qquad \longrightarrow \qquad z(x) = \frac{2}{9}x^{5} + cx^{2}$$

#### Step by Step Procedure for an Mathematical Model of The System

- Draw a sketch of the system to be modeled and label/define the various geometric, physical and chemical quantities
- Select the important dependent (response) variables
- Select the possible independent variable, changes in which must necessarily affect the dependent variables
- List the parameters (physical size and shape ) that are expected to be important : also note the possibility of no constant parameters (e.g., termal conductivity changing with temperature, m(T))
- Draw a sketch of the expected behavior of the dependent variable (s)
- Establish a control volume for a differential or finite element of the system to be modeled; sketch the element and indicate all inflowoutflow paths.
- Write the conservation law for the volume element: Express flux and reaction rate terms using general symbols, which are then as positive quantities, so that signs are introduced only as terms are inserted according to the roles of the conservation law,
- Write out all possibilities for boundary values of the dependent variables
- Search out solution methods

#### From mathematical viewpoint, these models can be classified into two broad classes

- Distributed parameter model: Relationship between the variables involved as functions of time and space.
- Lumped parameter models: These models lump all the variables involved are treated as functions time alone.

("We can study model at macroscopic level where the transport equations (**Momentum, Energy, Mass**) are developed by balancing of physical quantities as input and output streams in a control volume in which quantities such as temperature and concentration varied only whit respect to time. It cannot provide information at local level. Whereas, the transport phenomena at microscopic level, where the transport equations are developed by balancing physical quantities for a small control volume and then allowing the control volume to approach zero results in transport equations which are valid at each point in the fluid. Theses equations may be solved by using appropriate assumptions and boundary conditions. Microscopic level of study of system gives the chance to study the systems in much more details and provides more accurate description of the transport phenomena occurring in the system. If required, these equations may be integrated for the whole system for better understanding of the overall performance of the system")

- **Momentum transport** deals with the transport of momentum in fluids and is also known as fluid dynamics. Solution of equation of motion provides information about the velocity distribution in the system.
- **Energy transport** deals with the transport of different forms of energy in a system and is also commonly known as heat transfer. Solution of basic equation of thermal energy provides the information about the temperature distribution in the system.
- **Mass transport** deals with the transport of various chemical species in a system. The solution of convective diffusion equation provides the information about the concentration distribution in the system.

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