Fundamentals of Vector Spaces

Equation Forms in Process Modeling

Distributed Parameter Models and Abstract Equation Forms

Differential Algebraic Equations

Most of the systems encountered in chemical engineering are distributed parameter systems. Even though behavior of some of these systems can be adequately represented by lumped parameter models, such simplifying assumptions may fail to provide accurate picture of system behavior in many situations and variations of variables along time and space have to be considered while modeling. This typically results in a set of partial di¤erential equations (PDEs) or ordinary di¤erential equations with boundary conditions speci…ed (ODE-Boundary value Problems or ODE-BVP). This is illustrated through examples in this sub-section.

Example 10

Consider the double pipe heat exchanger in which a liquid flowing in the inner tube is heated by steam flowing countercurrently around the tube (Figure 10). The temperature in the pipe changes not only with time but also along the axial direction z. While developing the model, it is assumed that the temperature does not change along the radius of the pipe. Consequently , we have only two independent variables, i.e. z and t. To perform the energy balance,we consider an element of length Δz as shown in the figure. For this element, over a period of time Δt

$$\rho C_p A \Delta z[(T)_{t+\Delta t} - (T)_t] = \rho C_p VA(T)_z \Delta t - \rho C_p VA(T)_{z+\Delta z}\Delta t + Q\Delta t(\pi D \Delta z) \quad \text{----(75)}$$

This equation can be explained as

[accumulation of the enthalpy during the time period Δt]

= [flow in of the enthalpy during Δt] - [flow out of the enthalpy during Δt]

[enthalpy transferred from steam to the liquid through wall during Δt]

where

Q : amount of heat transferred from the steam to the liquid per unit time and per unit heat transfer area.

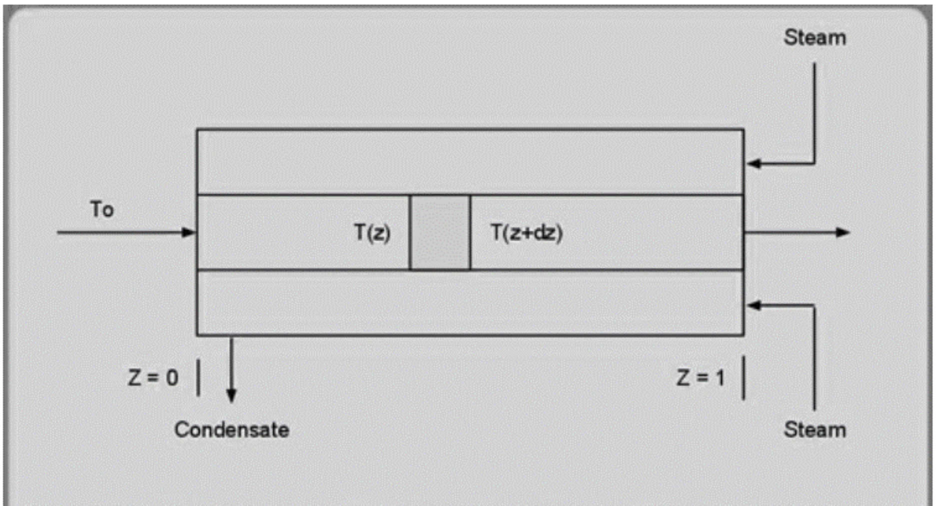

Figure 10: Double Pipe Heat Exchanger (Steam on Shell Side)

A : cross section area of the inner tube.

V : average velocity of the liquid(assumed constant).

D : external diameter of the inner tube.

Dividing both the sides by ($\Delta z \Delta t$) and taking limit as $\Delta t \to 0$ and $\Delta z \to 0$, we have

$$\rho C_p A \frac{\partial T(z,t)}{\partial t} = -\rho C_p VA \frac{\partial T(z,t)}{\partial z} + \pi DQ \quad \text{----(76)}$$

$$Q = U[T_{st} - T] \quad \text{----(77)}$$

Boundary conditions:

$$T(t, z = 0) = T_1 \, for \, t \geq 0$$

Initial condition

$$T(t = 0, z) = T_0(0, z) \quad \text{----(78)}$$

Steady State Simulation: Find $T(z)$ given $T(z = 0) = T_1$ when $\partial T / \partial t = 0$, i.e. solve for

$$\rho C_p VA \frac{\partial T}{\partial z} = \pi DQ = \pi DQU(T_{st} - T) \quad \text{----(79)}$$

$$T(0) = T_1 \quad \text{----(80)}$$

This results in a ODE-IVP, which can be solved to obtain steady state profiles $T(z)$ for specified heat load and liquid velocity.

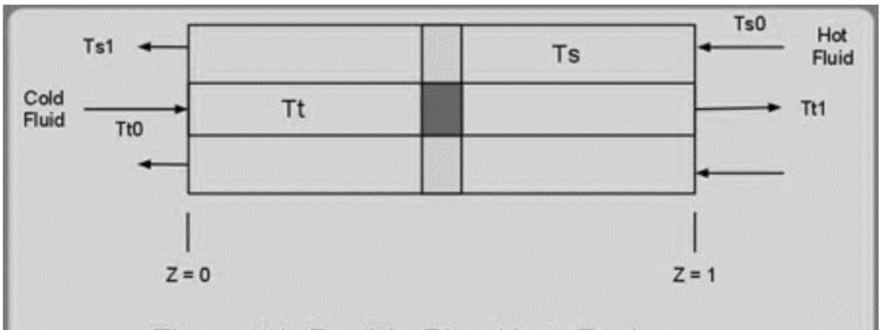

Figure 11: Double Pipe Heat Exchanger

This results in a ODE-IVP, which can be solved to obtain steady state profiles $T(z)$ for specified heat load and liquid velocity.

DynamicSimulation

$$\rho C_p A \frac{\partial T}{\partial t} = -\rho C_p VA \frac{\partial T}{\partial z} + \pi DQ \quad \text{----(81)}$$

with

$$T(t, 0) = T_1 \, at \, z = 0 \, and \, t \geq 0 \quad : \quad \textit{Boundary condition} \quad \text{----(82)}$$

$$T(0, z) = T_0(z) \quad : \quad \textit{Initial temperature profile} \quad \text{----(83)}$$

This results in a Partial Differential Equation (PDE) model for the distributed parameter system.

Example 11

Now, let us consider the situation where the some hot liquid is used on the shell side to heat the tube side fluid (see Figure 11). The model equations for this case can be stated as

$$\rho_t C_{pt} A_t \frac{\partial T_t(z,t)}{\partial t} = -\rho_t C_{pt} V_t A_t \frac{\partial T_t(z,t)}{\partial z} + \pi D Q(z,t) \quad \text{----(84)}$$

$$\rho_s C_{pt} A_s \frac{\partial T_s(z,t)}{\partial t} = \rho_s C_{ps} V_s A_s \frac{\partial T_s(z,t)}{\partial z} - \pi D Q(z,t) \quad \text{----(85)}$$

$$Q(z,t) = U[T_s(z,t) - T_t(z,t)] \quad \text{----(86)}$$

where subscript t denotes tube side and subscript s denotes shell side. The initial and boundary conditions become

$$T_t(t,0) = T_{t0} \text{ at } z = 0 \text{ and } t \geq 0 \quad : \text{ Boundary condition} \quad \text{----(87)}$$

$$T(0,z) = T_{t0}(z) \quad : \text{ Initial temperature profile} \quad \text{----(88)}$$

$$T_s(t,1) = T_{s1} \text{ at } z = 1 \text{ and } t \geq 0 \quad : \text{ Boundary condition} \quad \text{----(89)}$$

$$T(0,z) = T_{s0}(z) \quad : \text{ Initial temperature profile} \quad \text{----(90)}$$

These are coupled PDEs and have to be solved simultaneously to understand the transient behavior. The steady state problem can be stated as

$$\rho_t C_{pt} V_t A_t \frac{dT_t(z,t)}{dz} = \pi D U[T_s(z) - T_t(z)] \quad \text{----(91)}$$

$$\rho_s C_{ps} V_s A_s \frac{dT_s(z,t)}{dz} = \pi D U[T_s(z) - T_t(z)] \quad \text{----(92)}$$

$$T_t(0) = T_{t0} \quad \text{at } z = 0 \quad \text{----(93)}$$

$$T_s(1) = T_{s1} \quad \text{at } z = 1 \quad \text{----(94)}$$

Equations (91-92) represent coupled ordinary differential equations. The need to compute steady state profiles for the counter-current double pipe heat exchanger results in a boundary value problem (ODE-BVP) as one variable is specified at $z = 0$ while the other is specified at at $z = 1$.

Before we conclude this section, we briefly review some terminology associated with PDEs, which will be used in the later modules.

Definition 12

Order of PDE: Order of a PDE is highest order of derivative occurring in PDE.

Definition 13

Degree of PDE: Power to which highest order derivative is raised.

Example 14

Consider PDE

$$\partial u/\partial t + (d^2u/dz^2)^n = u^3 \quad \text{----(95)}$$

Here, the $Oredr = 2$ and $Degree = n$. Solutions of PDEs are sought such that it is satisfied in the domain and on the boundaries . A problem is said to be well posed when the solution is uniquely determined and it is sufficiently smooth and differentiable function of the independent variables. The boundary conditions have to be consistent with one another in order for a problem to be well posed. This implies that at the points common to boundaries, the conditions should not violet each other.

A linear PDE can be classified as:

- Homogeneous equations:Differential equation that does not contain any terms other than dependent variables and their derivatives.

$$\partial^2 u/\partial x^2 + \partial^2 u/\partial y^2 = 0$$
$$\partial u/\partial t = \partial u^2/\partial x^2 \quad \text{----(96)}$$

- Non homogeneous equations: Contain terms other than dependent variables

$$\partial u/\partial t = \partial^2 u/\partial x^2 + \sin x \quad \text{----(97)}$$

$$\partial^2 u/\partial x^2 + \partial^2 u/\partial y^2 = \sin x \ \sin y \quad \text{----(98)}$$

Similarly,the boundary conditions can be homogeneous or non homogeneous depending on whether they contain terms independent of dependent variables.

The PDEs typically encountered in engineering applications are 2^{nd} order PDEs (reaction-diffusion systems, heat transfer, fluid-flow etc.)

Classification of 2^{nd} order PDEs:

Consider a 2^{nd} order PDE in n independent variables $(x_1, x_2, x_3, x_4) = (x, y, z, t)$. This can be written as

$$\sum_{i=1}^{4}\sum_{j=1}^{4} a_{ij}\frac{\partial^2 u}{\partial x_i \partial x_j} = f[\partial u/\partial x_1, \ldots, \partial u/\partial x_4, , u, x_1, \ldots, x_4] \quad \text{----(99)}$$

a_{ij} are assumed to be independent of $'u'$ and its derivative. They can be functions of (x_i). a_{ij} can always be written as $a_{ij} = a_{ji}$ for i $\neq$ j as

$$\frac{\partial^2 u}{\partial x_i \partial x_j} = \frac{\partial^2 u}{\partial x_j \partial x_i} \quad \text{----(100)}$$

Thus, a_{ij} are elements of a real symmetric matrix A. Obviously A has real eigen values. The PDE is called

- **Elliptic:** if all eigenvalues are +ve or-ve.
- **Hyperbolic:** if some eigenvalues are +ve and rest are -ve.
- **Parabolic:** if at-least one eigen value is zero.

The classification is global if a_{ij} are independent of x_i, else it is local. Typical partial differential equations we come across in engineering applications are of the form

$$\nabla^2 u = a\frac{\partial u}{\partial t} + b\frac{\partial^2 u}{\partial t^2} + cu + f(x_1, x_2, x_3, t) \quad \text{----(101)}$$

subject to appropriate boundary conditions and initial conditions. This PDE is solved in a three dimensional region V, which can be bounded or unbounded. The boundary of V is denoted by S. On the spatial surface S, we have boundary conditions of the form

$$(\alpha(s,t)\hat{n}).\nabla u + \beta(s,t)u = h(s,t) \quad \text{----(102)}$$

where $\hat{n}$ is the outward normal direction to S and s represents spatial coordinate along S. We can classify the PDEs as follows

- Elliptic: $a = b = 0$
- Parabolic: $a \neq 0, b = 0$
- Hyperbolic: $b > 0$

Elliptic Problems typically arise while studying steady-state behavior of diffusive systems. Parabolic or hyperbolic problems typically arise when studying transient behavior of diffusive systems.

Elliptic boundary value problem

An **elliptic boundary value problem** is a special kind of boundary value problem which can be thought of as the stable state of an evolution problem. For example, the Dirichlet problem for the Laplacian gives the eventual distribution of heat in a room several hours after the heating is turned on.

Differential equations describe a large class of natural phenomena, from the heat equation describing the evolution of heat in (for instance) a metal plate, to the Navier-Stokes equation describing the movement of fluids, including Einstein's equations describing the physical universe in a relativistic way. Although all these equations are boundary value problems, they are further subdivided into categories. This is necessary because each category must be analysed using different techniques. The present article deals with the category of boundary value problems known as linear elliptic problems.

Boundary value problems and partial differential equations specify relations between two or more quantities. For instance, in the heat equation, the rate of change of temperature at a point is related to the difference of temperature between that point and the nearby points so that, over time, the heat flows from hotter points to cooler points. Boundary value problems can involve space, time and other quantities such as temperature, velocity, pressure, magnetic field, etc...

Some problems do not involve time. For instance, if one hangs a clothesline between the house and a tree, then in the absence of wind, the clothesline will not move and will adopt a gentle hanging curved shape known as the catenary. This curved shape can be computed as the solution of a differential equation relating position, tension, angle and gravity, but since the shape does not change over time, there is no time variable.

Elliptic boundary value problems are a class of problems which do not involve the time variable, and instead only depend on space variables.

The main example

In two dimensions, let x, y be the coordinates. We will use the notation u_x, u_{xx} for the first and second partial derivatives of u with respect to x, and a similar notation for y. We will use the symbols D_x and D_y for the partial differential operators in x and y. The second partial derivatives will be denoted D_x^2 and D_y^2. We also define the gradient $\nabla u = (u_x, u_y)$, the Laplace operator

$\Delta u = u_{xx} + u_{yy}$ and the divergence $\nabla \cdot (u, v) = u_x + v_y$. Note from the definitions that $\Delta u = \nabla \cdot (\nabla u)$.

The main example for boundary value problems is the Laplace operator,

$$\Delta u = f \text{ in } \Omega,$$
$$u = 0 \text{ on } \partial\Omega;$$

where Ω is a region in the plane and $\partial\Omega$ is the boundary of that region. The function f is known data and the solution u is what must be computed. This example has the same essential properties as all other elliptic boundary value problems.

The solution u can be interpreted as the stationary or limit distribution of heat in a metal plate shaped like Ω, if this metal plate has its boundary adjacent to ice (which is kept at zero degrees, thus the Dirichlet boundary condition.) The function f represents the intensity of heat generation at each point in the plate (perhaps there is an electric heater resting on the metal plate, pumping heat into the plate at rate $f(x)$, which does not vary over time, but may be nonuniform in space on the metal plate.) After waiting for a long time, the temperature distribution in the metal plate will approach u.

Nomenclature

Let $Lu = au_{xx} + bu_{yy}$ where a and b are constants. $L = aD_x^2 + bD_y^2$ is called a second order differential operator. If we formally replace the derivatives D_x by x and D_y by y, we obtain the expression

$$ax^2 + by^2.$$

If we set this expression equal to some constant k, then we obtain either an ellipse (if a, b, k are all the same sign) or a hyperbola (if a and b are of opposite signs.) For that reason, L is said to be elliptic when $ab > 0$ and hyperbolic if $ab < 0$. Similarly, the operator $L = D_x + D_y^2$ leads to a parabola, and so this L is said to be parabolic.

We now generalize the notion of ellipticity. While it may not be obvious that our generalization is the right one, it turns out that it does preserve most of the necessary properties for the purpose of analysis.

General linear elliptic boundary value problems of the second degree

Let $x_1, \ldots, x_n$ be the space variables. Let $a_{ij}(x), b_i(x), c(x)$ be real valued functions of $x = (x_1, \ldots, x_n)$. Let L be a second degree linear operator. That is,

$$Lu(x) = \sum_{i,j=1}^{n} (a_{ij}(x)u_{x_i})_{x_j} + \sum_{i=1}^{n} b_i(x)u_{x_i}(x) + c(x)u(x) \text{ (divergence form).}$$

$$Lu(x) = \sum_{i,j=1}^{n} a_{ij}(x)u_{x_i x_j} + \sum_{i=1}^{n} \tilde{b}_i(x)u_{x_i}(x) + c(x)u(x) \text{ (nondivergence form)}$$

We have used the subscript $\cdot_{x_i}$ to denote the partial derivative with respect to the space variable x_i. The two formulae are equivalent, provided that

$$\tilde{b}_i(x) = b_i(x) + \sum_j a_{ij,x_j}(x).$$

In matrix notation, we can let $a(x)$ be an $n \times n$ matrix valued function of x and $b(x)$ be a n -dimensional column vector-valued function of x, and then we may write

$$Lu = \nabla \cdot (a \nabla u) + b^T \nabla u + cu \text{ (divergence form).}$$

One may assume, without loss of generality, that the matrix a is symmetric (that is, for all i, j, x, $a_{ij}(x) = a_{ji}(x)$. We make that assumption in the rest of this article.

We say that the operator L is *elliptic* if, for some constant $\alpha > 0$, any of the following equivalent conditions hold:

1. $\lambda_{\min}(a(x)) > \alpha \quad \forall x$ (see eigenvalue).
2. $u^T a(x) u > \alpha u^T u \quad \forall u \in \mathbb{R}^n$.
3. $\sum_{i,j=1}^{n} a_{ij} u_i u_j > \alpha \sum_{i=1}^{n} u_i^2 \quad \forall u \in \mathbb{R}^n$.

An elliptic boundary value problem is then a system of equations like

$Lu = f \text{ in } \Omega$ (the PDE) and
$u = 0 \text{ on } \partial\Omega$ (the boundary value).

This particular example is the Dirichlet problem. The Neumann problem is

$Lu = f \text{ in } \Omega$ and
$u_\nu = g \text{ on } \partial\Omega$

where u_ν is the derivative of u in the direction of the outwards pointing normal of $\partial\Omega$. In general, if B is any trace operator, one can construct the boundary value problem

$Lu = f \text{ in } \Omega$ and
$Bu = g \text{ on } \partial\Omega$.

In the rest of this article, we assume that L is elliptic and that the boundary condition is the Dirichlet condition $u = 0 \text{ on } \partial\Omega$.

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