CHAPTER 1
INTRODUCTION

The chapter briefs introductory concept of mathematical modeling and its role in formulating complex real-world problems into a simplified mathematical formulation to address various industrial problems. Besides, it also throws light on the concept of boundary value problems, the pulp washing process, and its types.

1.1 MATHEMATICAL MODELING

To understand real-world problems, researchers frequently develop various models that are considered as a simplified abstract view of complex reality. Mathematical modeling is a procedure to develop a suitable mathematical framework for any problem. In this process, the real-world situation is transferred into an abstract world comprising mathematical concepts (Dundar et al., 2012). In other words, it is the art of converting the problems or phenomena occurring in the real world into a mathematical form (Sari et al., 2010). According to Berry and Houstan (1995), it aids in simulating the effects of different important factors on the physical process. Therefore, it can be concluded that it is a skill of transforming problems from an industry into a suitable mathematical formulation whose theoretical and numerical analysis provides insight, answers, and guidance useful for the originating application.

In recent times, mathematical modeling has emerged as one of the most effective tools for solving practical problems in engineering, sciences, medical, banking, and other domains. According to Jiwari et al. (2018), various processes in engineering and biosciences such as reaction-diffusion and heat conduction are described by mathematical modeling. Besides, some authors such as Liu et al. (2011) highlighted that it is not only beneficial in physical systems but also in other fields such as psychology, economics, sociology, music, philosophy, political science, linguistics, etc. In addition, the main advantage of a mathematical model is that one can study the behavior of the system and the effect of different components, which are helpful in future prediction (Szukiewicz, 2001). These models play an important role not only in understanding the intricate processes but also help in increasing the profits of the industry (Szukiewicz, 2001; Ewing and Wangh, 2001).

Consequently, some advantages of mathematical modeling can be listed as under:

- It is very useful in many application areas.
- It provides exactness and direction in solving the problem of industries.
- It enables a comprehensive understanding of the modeled system.
- It helps in preparing the way for a better understanding to design the system and control the system.
- Modern computing capabilities are efficiently used in this process.

According to (Ganaie et al., 2014), mathematical model problems are generally categorized as black-box or white-box models based on the priori availability of information. The models for which priori information is not available are black-box type model systems. The models for which all necessary information is available are white box-type model systems. In practical situations, all systems lie within the white-box and black-box models. However, it is preferred if the priori information is available to a sufficient extent, then the developed models can provide accurate results. Besides this, the mathematical models can be categorized according to the structure, nature, and basic initial assumptions of the system such as linear, nonlinear, static, dynamic, explicit, implicit, discrete, continuous, deterministic, probabilistic (stochastic), deductive, inductive, strategic, non-strategic (Mittal, 2015). Further, mathematical models generally comprise of relationships between variables that are described by functions and differential operators. The system was usually described with a set of equations and a set of variables that establish the relationships between the variables (Szukiewicz, 2000).
Moreover, the environmental issues related to industries such as emission pollution, deforestation, global warming, the greenhouse effect, and climate change can also be reduced through effective mathematical modeling. According to Kadalbajoo and Awasthi (2008), the solution of mathematical models helps in the simulation of the behavior of a physical process and systems. The process of simulation involves the representation of specific key behaviors or physical characteristics of an abstract or physical system (Berry and Houstan, 1995). Besides, simulation and modeling is a practice to develop a level of understanding of the relations between the parts of a system or whole system. Further, in terms of system engineering, the word simulation is used for the task of forming the mathematical model of a system and using that model for a systematic investigation of the actual system (Guillaume, 2018).

According to some other researchers, an important part of the modeling process is the assessment of whether or not a given model accurately fits the system (Sari et al., 2010). Initially, the model is solved and manipulated with the appropriate mathematical and computational techniques. Thereafter, it is evaluated based on its fitness for experimental or empirical data. The common approach to check the fitness of the model is based on splitting data into two disjoint parts training and verification of data. The parameters of the model are estimated with training data. In many cases, the accuracy of the model is judged by its closeness with the verification data (Arora et al., 2005). However, lack of agreement relating theoretical framework and experimental measurements often directs toward important advancements in the development of other suitable theories (Sari et al., 2010).

It can be concluded from the above discussion that a thorough study and physical framework are essential for the development of the model and thereafter, its fitness to determine the physical properties of real-world problems. The steps in the mathematical modeling process include:

- Identification of Real-world problem
- Detailed understanding of the physical process
- Mathematical model formulation
- Analytic/Numerical solution of the mathematical model
- Validation with the experimental data
- Interpretation of the results.

This modeling process is diagrammatically shown in Figure 1.1.

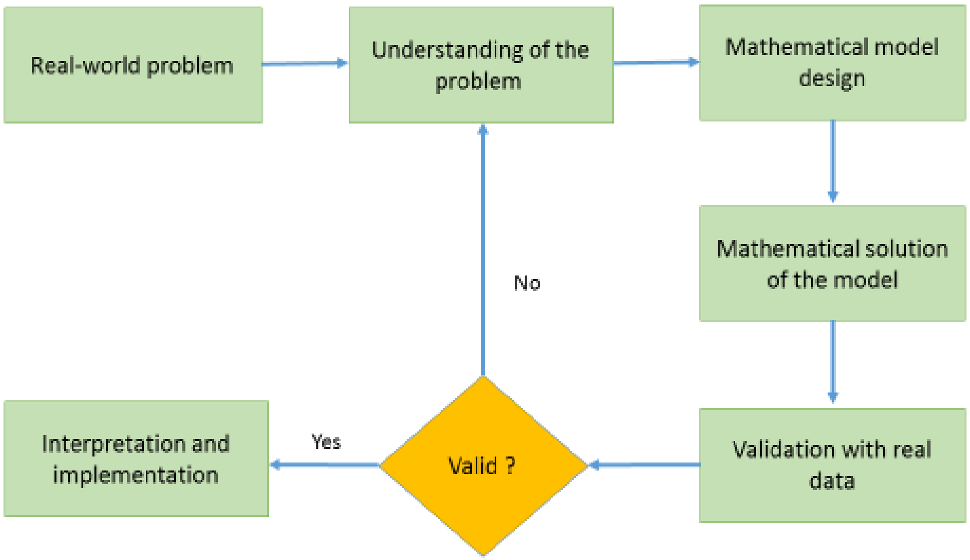

Figure 1.1 A schematic modeling process

1.2 BOUNDARY VALUE PROBLEMS

Many mathematical models applicable in engineering involves the rate of change of physical quantities therefore, quantitative treatment of these models usually emerges in the form of differential equations (Dumont, 1986; Liu et al., 2011). Besides according to Coimbra et al. (2004), many engineering problems are based on mathematical modeling which is developed in the form of partial differential equations (PDEs). Further, the differential equations along with some specified conditions at different points are known as boundary value problems (BVPs) (Rapp, 2017). Mathematically, the BVP is a differential equation along with an additional set of constraints known as boundary conditions. BVPs have applications in the areas of physics, chemistry, and various engineering streams. In most common situations, the values of solution and derivatives are specified at two boundary points and are defined as two-point BVPs (Boyce and Diprima, 2021). The boundary condition that specifies the value of the function itself is the first-type boundary condition and is known as the Dirichlet boundary condition. On the other hand, the boundary condition that specifies the value of the normal derivate of the function is the second-type boundary condition and known as the Neumann boundary condition. Besides, the boundary condition that specifies the value of the variable itself and the normal derivative is known as the Cauchy boundary condition (Rapp, 2017).

In recent years, researchers are concerned with the solution of models using BVPs and are focusing on the steady-state condition or the kind of material of experiment performed (Mittal et al., 2013). The steady-state procedure involved is the solution of second-order ordinary differential equations (ODEs) along with conditions at two boundary ends expressed in the form of two-point BVPs. One such two-point BVP associated with the pulp-washing process involved in industrial practice is related to the displacement of an initially homogeneous solute from a medium of finite length by the introduction of a solvent (Mittal and Kukreja, 2015). Because of the involvement of various parameters, these are usually exhibited as PDEs. Obtaining the optimum solution to these model equations is of paramount importance. Previous studies suggest that linear BVPs are having analytical solutions and nonlinear BVPs are approximated with numerical solutions (Lang and Sloan, 2002). In pursuit of the accuracy of results, various advancements in numerical methods are usually seen for solving BVPs.

1.3 PULP WASHING

Pulp and paper industries are interactive chemical processing plants with a wider scope of recycling. Pulp washing is a common process used by paper industry in the recovery of solid and liquid products as well as chemicals. According to Dumont (1986), the pulping processes can be chemical, mechanical, or a mixture of both. Pulping is attained when the wood chips are cooked using a chemical solution known as liquor in a digester. Solute removal from packed beds of porous particles with the introduction of wash liquor is a conventional washing operation in many industries (Tervola, 2006). The pulp washing is concerned with detaching cellulose fibres from black liquor with the use of a minimal amount of wash liquor (Gupta and Kukreja, 2012). Further, to get the fine-quality paper, it is essential to remove the coloring compounds and residual lignin through a process known as bleaching (Gupta and Kukreja, 2012). In case of mechanical pulp washing process, Dumont (1986) explained that pulp quality is mainly affected by the parameters such as area, fiber length, and distribution. In this regard, Potůček and Hájková (2016) reported that the morphological properties, chemical composition, and strength properties of non-woody pulp fibres together with pulping procedures of non-woody plants also influence pulp washing.

Also, this is an area of interest for various chemical and process industries such as polymer separation by assorted polymerization, fiber purification before drying, pulp fiber purification during the paper making, etc. (Roininen and Alopaeus, 2011). The main motive of the process industry is not only to maintain the quality of the product but also to maximize production and minimize the use of washing liquid with less environmental load (Singh et al., 2008). The whole washing process is described by the material balance equation (Tervola, 2006). It is expressed as:

$$\left\{\begin{matrix} Rate\ of\ \ mass \\ entering \\ due\ to\ bulk\ fluid \end{matrix}\right\} + \left\{\begin{matrix} Rate\ of\ \ mass \\ entering \\ due\ to\ dispersion \end{matrix}\right\} = \left\{\begin{matrix} Rate\ of\ \ mass \\ leaving \\ due\ to\ bulk\ fluid \end{matrix}\right\} + \left\{\begin{matrix} Rate\ of\ \ mass \\ due\ to \\ accumulation \end{matrix}\right\} + \left\{\begin{matrix} Rate\ of\ \ mass \\ accumulated \\ in\ solid\ phase \end{matrix}\right\}$$

1.3.1 Types of Pulp Washing

The dilution-thickening and displacement washing are the two pulp-washing operations that are abundantly used in the paper industry. In the first type of washing, the slurry of the pulp is weakened and completely mixed with the wash liquor. Thereafter, it is condensed by pressing or filtering. Whereas displacement washing deals with replacing the liquor residing in the pulp bed with washed liquor instead of mixing the two liquors (Seupel and Peuker, 2021). To achieve better washing efficiency Arora and Potuček (2012), suitable displacement washing is of utmost importance. At the initial stage of displacement, the discharged portion from the pulp bed is mainly concentrated with the mother liquor. The concentration of lignin starts decreasing rapidly when the first portion of the wash liquor passes through the bed. Thereafter, a major part of the mother liquor present in the inter-particle voids is removed and replaced by wash liquid. Finally, the remains of black liquor are removed from the narrow pores of fiber in the last period. A better pulp-washing process is achieved with a decrease in the concentration of mother liquor present at the initial stage of washing.

While studying the washing process in the paper industry, Tervola (2006) found that multistage countercurrent washing is a common technique applied in the washing process in which the solid flow and wash liquid are in opposite directions. In the final stage, the uncontaminated wash liquid is used to wash the cleanest pulp. The wash discharge obtained from each stage is recycled as wash fluid in its previous stage. Thus, separate recoveries are attained at different stages. Thereafter, the wash discharge from the first segment of the second stage is drained into the first segment of the first stage and the wash waste from the second segment of the second stage is drained to the second segment of the first stage, and so on. The maximum polluted wash waste portion obtained from the stage is utilized to wash the most polluted cake in the preceding stage. Besides, the slightest polluted wash waste part from the stage is used to wash the slightest polluted cake in the preceding stage. A usual washing system in the industry consists of three to four washers in the pulp washing process. These washers are in a series of counter flow with set up such as the final wash is performed with clean water (Kumar et al., 2010).

According to Kumar et al. (2010), the segregated wash effluent circulation is an attractive option to recover the solute in the process of cake washing and is frequently applied in the pulping industry. The target of clean cake can be achieved by making the amount of the leaving wash effluent small which is possible with a low wash ratio. Generally, these processes consist of porous material and hence solute is completely removed with multistage operations because the solute is slowly displaced with the introduction of wash liquor. According to Mittal (2014), the remains of dissolved solids (expressed as BOD, COD, or in the form of Na_2SO_4) attached to the washed pulp increase the cost of the chemical treatment, effluent makeup, pulping, bleaching, and fuel consumption. Also, with the excess use of wash water, the cost of evaporation in the dilution of the recovered liquor is increased, and to heat the excess wash water, the environmental load is also increased. Therefore, the optimum washing focuses on two aspects i.e., soluble solids do not overflow along with pulp (causing the least soda loss) and restriction of pulp overflow with the effluents.

1.3.2 Approaches to Pulp Washing Models

Various investigators have summarized three approaches of modeling which are mainly used in pulp washing viz.

- Process modeling
- Statistical modeling
- Physical modeling.

Pekkanen and Norden (1985) presented a complete review of different process models beneficial in describing the pulp washing process. These models are beneficial for the process of design calculations and provide less information about how to design or operate the washer so that efficiency can be improved. Statistical modeling is based on statistical assumptions and makes estimates regarding the real-world problems for the sample data. Physical models explain the washing process in terms of mass transfer and fundamental fluid flow principles which occur at the microscopic level during displacement washing of pulp fibre bed. These models include mass transfer and longitudinal dispersion coefficient parameters which are classified based mass transfer principles such as microscopic (dispersion models), macroscopic (differential contact model), and semi-quantitative models. The macroscopic models provide only an outside description of the process considering material balance. The microscopic models are about the basic mechanism of fluid dynamics. Semi-quantitative models are in-between among these two models.

In a study, Ganaie et al. (2014) described the three physical rates associated with a microscopic model for pulp-packed beds such as:

- Axial dispersion that occurs in the flowing liquor (bulk fluid)
- Fick's second law of diffusion
- Mass transfer of the liquid phase accounts for the solute transport from the surface of fiber to the flowing liquid.

1.3.3 Diffusion-dispersion and Adsorption-desorption Phenomenon

In the industry, it is not an easy task to meet the above-mentioned ideal stipulations. Therefore, the industry needs optimum consumption of water, power, chemicals, and the number of stages. The pulp washing process involves adsorption-desorption, diffusion-dispersion phenomenon (Kukreja, 1996; Gupta et al., 2015). Ganaie et al. (2013) revealed that solute removal is a process that relates to diffusion-like dispersion towards the direction of flow known as longitudinal dispersion. In this process, dispersion takes place due to back mixing, diffusion happens due to concentration gradient and adsorption-desorption occur due to relative affinity of various solute towards the fibre surface. Further, the study described that most of the researchers used a one-dimensional axial dispersion model to describe the washing operation of the pulp fibre bed. The study also illustrated that the axial dispersion coefficient is a robust parameter that serves the role of diffusion coefficient as well as dispersion. Likewise, Roininen and Alopaeus (2011) supported that the models of axial dispersion involve the diffusion term of second order that describes the rate of change of concentration in spatial and temporal directions. However, Karahan (2006) explained that the problems associated with environmental pollution for groundwater, rivers, and coasts can be handled with the mathematical model of diffusion–dispersion that describes the diffusion and transport process. Likewise, Jiwari et al. (2018) also revealed that advection-diffusion-reaction has great application in the study of patterns for physical, chemical, and biological systems in nature.

1.4 SUMMARY

The chapter presents a brief background of the various concepts involved in the present study. It points out the role of mathematical modeling in transforming problems experienced by industry into a suitable mathematical formulation whose theoretical and numerical analysis provides insight, answers, and guidance useful for the originating application. Further, it emphasizes on the pulp washing process, which is a major industrial problem that needs to be addressed efficiently. The continuous efforts made in this direction can benefit a lot in increasing the efficiency of the industry and decreasing the environmental load.